



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:44 am BST

PDB ID : 5THM  
Title : Esterase-6 from *Drosophila melanogaster*  
Authors : Fraser, N.J.; Jackson, C.J.  
Deposited on : 2016-09-29  
Resolution : 2.15 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](mailto: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 ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

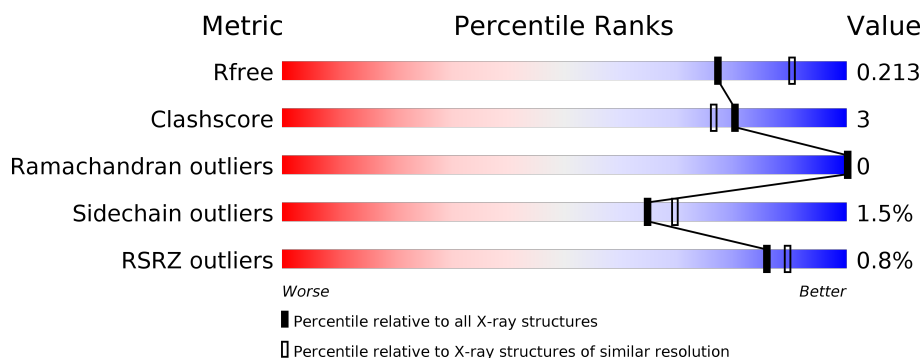
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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  $\leq 5\%$ . 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	533	<div> <div></div> <div>91%</div> <div>6%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4586 atoms, of which 8 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.

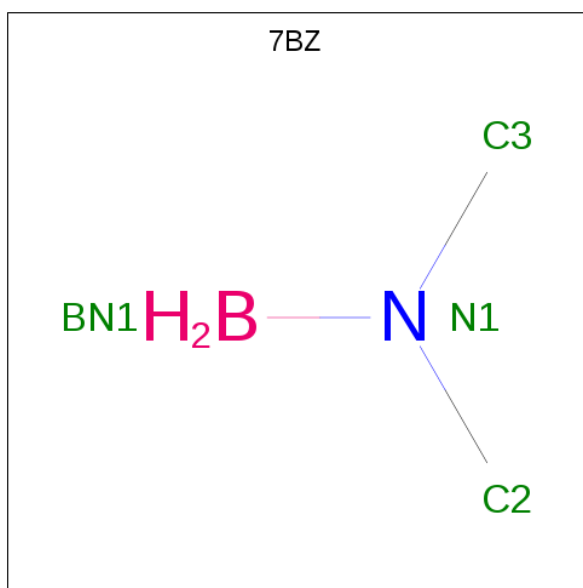
- Molecule 1 is a protein called Esterase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	8	0
			4252	2728	713	797	14			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP P08171
A	-8	HIS	-	expression tag	UNP P08171
A	-7	HIS	-	expression tag	UNP P08171
A	-6	HIS	-	expression tag	UNP P08171
A	-5	HIS	-	expression tag	UNP P08171
A	-4	HIS	-	expression tag	UNP P08171
A	-3	HIS	-	expression tag	UNP P08171
A	-2	ASP	-	expression tag	UNP P08171
A	-1	HIS	-	expression tag	UNP P08171
A	0	MET	-	expression tag	UNP P08171
A	15	VAL	LYS	engineered mutation	UNP P08171
A	145	LEU	VAL	engineered mutation	UNP P08171
A	208	MLY	ARG	engineered mutation	UNP P08171
A	229	GLU	GLY	engineered mutation	UNP P08171
A	237	SER	ASN	engineered mutation	UNP P08171
A	247	ALA	THR	engineered mutation	UNP P08171
A	290	GLY	ASP	engineered mutation	UNP P08171
A	292	PHE	ILE	engineered mutation	UNP P08171
A	335	VAL	ILE	engineered mutation	UNP P08171
A	383	GLY	GLU	engineered mutation	UNP P08171
A	400	GLY	SER	engineered mutation	UNP P08171
A	416	VAL	ALA	engineered mutation	UNP P08171
A	450	SER	PHE	engineered mutation	UNP P08171
A	456	SER	PHE	engineered mutation	UNP P08171
A	485	ASP	ASN	engineered mutation	UNP P08171
A	511	THR	ILE	engineered mutation	UNP P08171

- Molecule 2 is N,N-dimethylboranamine (three-letter code: 7BZ) (formula:  $C_2H_8BN$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	H	N	0	0
			12	1	2	8	1		

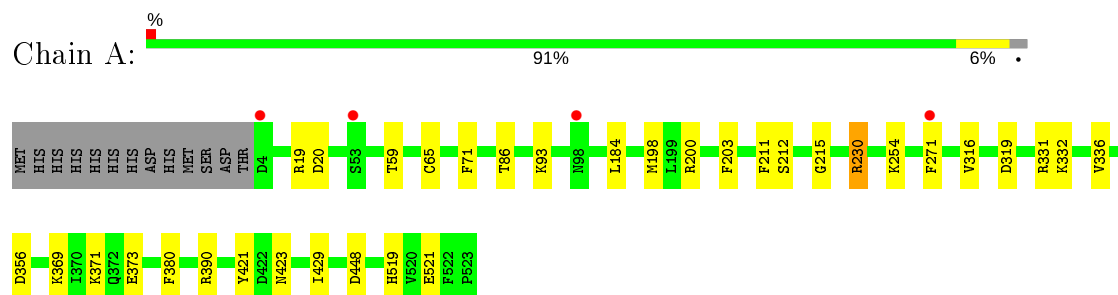
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	322	Total	O	0	0
			322	322		

### 3 Residue-property plots [i](#)

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: Esterase-6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.71Å 80.64Å 107.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.32 – 2.15 41.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.4 (40.32-2.15) 96.4 (41.99-2.15)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.65 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.155 , 0.210 0.158 , 0.213	Depositor DCC
$R_{free}$ test set	1589 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MLY, 7BZ

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	0.44	1/4006 (0.0%)	0.62	3/5454 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	ARG	CZ-NH2	-5.67	1.25	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	NE-CZ-NH2	-15.01	112.80	120.30
1	A	230	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	A	230	ARG	CD-NE-CZ	5.93	131.91	123.60

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	4252	0	4135	23	0
2	A	4	8	0	0	0
3	A	322	0	0	1	0
All	All	4578	8	4135	23	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 3.

All (23) 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:65[A]:CYS:SG	3:A:960:HOH:O	2.10	1.06
1:A:331:ARG:HB3	1:A:332:MLY:HE3	1.55	0.87
1:A:271:PHE:HZ	1:A:336:VAL:CG1	2.13	0.61
1:A:271:PHE:CZ	1:A:336:VAL:CG1	2.84	0.60
1:A:271:PHE:HZ	1:A:336:VAL:HG13	1.75	0.52
1:A:316:VAL:HG12	1:A:421:TYR:HB3	1.91	0.51
1:A:371:MLY:HE2	1:A:380:PHE:CE2	2.45	0.51
1:A:19:ARG:NH1	1:A:59:THR:O	2.44	0.49
1:A:369:MLY:HE3	1:A:373:GLU:OE1	2.12	0.48
1:A:271:PHE:CZ	1:A:336:VAL:HG13	2.50	0.47
1:A:71:PHE:CZ	1:A:429:ILE:HD11	2.50	0.46
1:A:198[B]:MET:HA	1:A:203:PHE:CG	2.51	0.46
1:A:369:MLY:HH12	1:A:373:GLU:OE2	2.17	0.44
1:A:20:ASP:OD2	1:A:93:MLY:HH23	2.17	0.44
1:A:212:SER:HB3	1:A:215:GLY:O	2.17	0.44
1:A:254:MLY:HH22	1:A:254:MLY:HD3	1.77	0.43
1:A:230:ARG:NH2	1:A:356:ASP:OD2	2.51	0.43
1:A:421:TYR:CZ	1:A:423:ASN:HB3	2.53	0.43
1:A:198[A]:MET:HE2	1:A:198[A]:MET:HB3	1.83	0.43
1:A:421:TYR:CD2	1:A:448:ASP:HB3	2.54	0.43
1:A:519:HIS:HB3	1:A:521:GLU:O	2.19	0.42
1:A:198[A]:MET:HA	1:A:203:PHE:CG	2.54	0.41
1:A:332:MLY:HG2	1:A:332:MLY:H	1.63	0.41

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	494/533 (93%)	478 (97%)	16 (3%)	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	416/421 (99%)	409 (98%)	7 (2%)	60	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	THR
1	A	184	LEU
1	A	200[A]	ARG
1	A	200[B]	ARG
1	A	211	PHE
1	A	319	ASP
1	A	390	ARG

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 molecules in this entry.

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

32 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	302	1	9,10,11	0.65	0	6,11,13	0.71	0
1	MLY	A	91	1	9,10,11	0.62	0	6,11,13	1.13	0
1	MLY	A	208	1	9,10,11	0.70	0	6,11,13	0.65	0
1	MLY	A	251	1	9,10,11	0.47	0	6,11,13	0.78	0
1	MLY	A	254	1	9,10,11	0.54	0	6,11,13	1.17	1 (16%)
1	MLY	A	369	1	9,10,11	0.58	0	6,11,13	0.69	0
1	MLY	A	256	1	9,10,11	0.66	0	6,11,13	1.03	0
1	MLY	A	489	1	9,10,11	0.76	0	6,11,13	0.85	0
1	MLY	A	332	1	9,10,11	0.69	0	6,11,13	0.86	0
1	MLY	A	225	1	9,10,11	0.51	0	6,11,13	1.02	0
1	MLY	A	169	1	9,10,11	0.56	0	6,11,13	0.73	0
1	MLY	A	371	1	9,10,11	0.50	0	6,11,13	0.95	0
1	MLY	A	329	1	9,10,11	0.62	0	6,11,13	0.85	0
1	MLY	A	305	1	9,10,11	0.79	0	6,11,13	0.48	0
1	MLY	A	361	1	9,10,11	0.65	0	6,11,13	0.52	0
1	MLY	A	77	1	9,10,11	0.55	0	6,11,13	1.07	0
1	MLY	A	93	1	9,10,11	0.52	0	6,11,13	0.70	0
1	MLY	A	360	1	9,10,11	0.68	0	6,11,13	0.61	0
1	MLY	A	129	1	9,10,11	0.52	0	6,11,13	0.81	0
1	MLY	A	503	1	9,10,11	0.82	0	6,11,13	0.83	0
1	MLY	A	267	1	9,10,11	0.67	0	6,11,13	0.75	0
1	MLY	A	166	1	9,10,11	0.59	0	6,11,13	0.74	0
1	MLY	A	51	1	9,10,11	0.65	0	6,11,13	0.75	0
1	MLY	A	96	1	9,10,11	0.56	0	6,11,13	0.55	0
1	MLY	A	250	1	9,10,11	0.50	0	6,11,13	0.65	0
1	MLY	A	413	1	9,10,11	0.65	0	6,11,13	0.65	0
1	MLY	A	427	1	9,10,11	0.57	0	6,11,13	0.94	0
1	MLY	A	410	1	9,10,11	0.92	0	6,11,13	0.40	0
1	MLY	A	49	1	9,10,11	0.75	0	6,11,13	0.64	0
1	MLY	A	358	1	9,10,11	0.65	0	6,11,13	0.85	0
1	MLY	A	60	1	9,10,11	0.55	0	6,11,13	0.90	0
1	MLY	A	496	1	9,10,11	0.68	0	6,11,13	0.65	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	302	1	-	2/8/9/11	-
1	MLY	A	91	1	-	1/8/9/11	-
1	MLY	A	208	1	-	4/8/9/11	-
1	MLY	A	251	1	-	1/8/9/11	-
1	MLY	A	254	1	-	0/8/9/11	-
1	MLY	A	369	1	-	1/8/9/11	-
1	MLY	A	256	1	-	0/8/9/11	-
1	MLY	A	489	1	-	2/8/9/11	-
1	MLY	A	332	1	-	6/8/9/11	-
1	MLY	A	225	1	-	0/8/9/11	-
1	MLY	A	169	1	-	1/8/9/11	-
1	MLY	A	371	1	-	2/8/9/11	-
1	MLY	A	329	1	-	1/8/9/11	-
1	MLY	A	305	1	-	0/8/9/11	-
1	MLY	A	361	1	-	0/8/9/11	-
1	MLY	A	77	1	-	2/8/9/11	-
1	MLY	A	93	1	-	2/8/9/11	-
1	MLY	A	360	1	-	2/8/9/11	-
1	MLY	A	129	1	-	1/8/9/11	-
1	MLY	A	503	1	-	0/8/9/11	-
1	MLY	A	267	1	-	2/8/9/11	-
1	MLY	A	166	1	-	5/8/9/11	-
1	MLY	A	51	1	-	1/8/9/11	-
1	MLY	A	96	1	-	3/8/9/11	-
1	MLY	A	250	1	-	3/8/9/11	-
1	MLY	A	413	1	-	2/8/9/11	-
1	MLY	A	427	1	-	0/8/9/11	-
1	MLY	A	410	1	-	0/8/9/11	-
1	MLY	A	49	1	-	1/8/9/11	-
1	MLY	A	358	1	-	3/8/9/11	-
1	MLY	A	60	1	-	0/8/9/11	-
1	MLY	A	496	1	-	1/8/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	MLY	CD-CE-NZ	-2.37	107.38	113.79

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	302	MLY	O-C-CA-CB
1	A	208	MLY	O-C-CA-CB
1	A	332	MLY	N-CA-CB-CG
1	A	332	MLY	C-CA-CB-CG
1	A	77	MLY	O-C-CA-CB
1	A	96	MLY	N-CA-CB-CG
1	A	96	MLY	C-CA-CB-CG
1	A	332	MLY	CD-CE-NZ-CH1
1	A	208	MLY	CD-CE-NZ-CH2
1	A	166	MLY	CD-CE-NZ-CH2
1	A	250	MLY	CD-CE-NZ-CH1
1	A	250	MLY	CD-CE-NZ-CH2
1	A	413	MLY	CD-CE-NZ-CH1
1	A	413	MLY	CD-CE-NZ-CH2
1	A	369	MLY	CG-CD-CE-NZ
1	A	51	MLY	CG-CD-CE-NZ
1	A	358	MLY	CG-CD-CE-NZ
1	A	169	MLY	CG-CD-CE-NZ
1	A	371	MLY	CG-CD-CE-NZ
1	A	208	MLY	CD-CE-NZ-CH1
1	A	166	MLY	CD-CE-NZ-CH1
1	A	96	MLY	CD-CE-NZ-CH2
1	A	358	MLY	CD-CE-NZ-CH2
1	A	166	MLY	CG-CD-CE-NZ
1	A	129	MLY	CG-CD-CE-NZ
1	A	250	MLY	CG-CD-CE-NZ
1	A	489	MLY	CD-CE-NZ-CH1
1	A	371	MLY	CD-CE-NZ-CH2
1	A	49	MLY	CD-CE-NZ-CH2
1	A	358	MLY	CD-CE-NZ-CH1
1	A	332	MLY	CD-CE-NZ-CH2
1	A	329	MLY	CG-CD-CE-NZ
1	A	166	MLY	CE-CD-CG-CB
1	A	332	MLY	CE-CD-CG-CB
1	A	496	MLY	CA-CB-CG-CD
1	A	208	MLY	CE-CD-CG-CB
1	A	77	MLY	CE-CD-CG-CB
1	A	360	MLY	CG-CD-CE-NZ
1	A	267	MLY	CG-CD-CE-NZ
1	A	93	MLY	CG-CD-CE-NZ
1	A	166	MLY	CA-CB-CG-CD
1	A	332	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	A	267	MLY	CD-CE-NZ-CH1
1	A	302	MLY	CD-CE-NZ-CH2
1	A	251	MLY	CE-CD-CG-CB
1	A	93	MLY	CE-CD-CG-CB
1	A	91	MLY	CE-CD-CG-CB
1	A	489	MLY	CD-CE-NZ-CH2
1	A	360	MLY	CA-CB-CG-CD

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	254	MLY	1	0
1	A	369	MLY	2	0
1	A	332	MLY	2	0
1	A	371	MLY	1	0
1	A	93	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
2	7BZ	A	601	-	2,3,3	0.26	0	1,3,3	5.35	1 (100%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	601	7BZ	C2-N1-C3	5.35	120.00	111.36

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

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, 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	488/533 (91%)	-0.44	4 (0%) 86 89	8, 16, 33, 64	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ASP	7.6
1	A	271	PHE	3.8
1	A	98	ASN	2.3
1	A	53	SER	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains

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<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	B-factors(Å <sup>2</sup> )	Q<0.9
1	MLY	A	332	11/12	0.80	0.33	58,66,77,79	0
1	MLY	A	49	11/12	0.90	0.22	30,37,58,72	0
1	MLY	A	208	11/12	0.91	0.16	12,16,58,63	0
1	MLY	A	305	11/12	0.91	0.14	18,23,56,60	0
1	MLY	A	96	11/12	0.91	0.20	32,45,68,81	0
1	MLY	A	254	11/12	0.91	0.12	12,19,32,48	0
1	MLY	A	329	11/12	0.92	0.15	15,24,52,57	0
1	MLY	A	93	11/12	0.93	0.13	23,29,46,49	0
1	MLY	A	358	11/12	0.93	0.10	13,14,23,33	0
1	MLY	A	51	11/12	0.94	0.20	31,40,48,51	0
1	MLY	A	361	11/12	0.94	0.20	13,19,51,67	0
1	MLY	A	413	11/12	0.94	0.22	18,26,46,47	0
1	MLY	A	410	11/12	0.94	0.15	12,21,46,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	267	11/12	0.94	0.11	11,19,45,46	0
1	MLY	A	91	11/12	0.94	0.10	14,20,28,30	0
1	MLY	A	250	11/12	0.95	0.14	12,18,37,48	0
1	MLY	A	371	11/12	0.95	0.11	11,16,24,27	0
1	MLY	A	166	11/12	0.95	0.15	15,19,59,70	0
1	MLY	A	77	11/12	0.95	0.12	14,18,42,50	0
1	MLY	A	129	11/12	0.95	0.12	15,21,50,51	0
1	MLY	A	60	11/12	0.95	0.19	16,27,56,58	0
1	MLY	A	496	11/12	0.95	0.17	14,22,52,55	0
1	MLY	A	169	11/12	0.96	0.09	17,22,40,48	0
1	MLY	A	225	11/12	0.96	0.12	11,15,39,50	0
1	MLY	A	360	11/12	0.96	0.09	15,18,23,28	0
1	MLY	A	427	11/12	0.96	0.11	13,18,32,41	0
1	MLY	A	251	11/12	0.96	0.17	17,19,49,53	0
1	MLY	A	503	11/12	0.96	0.10	11,16,27,29	0
1	MLY	A	369	11/12	0.96	0.12	10,15,33,41	0
1	MLY	A	489	11/12	0.96	0.09	11,22,35,38	0
1	MLY	A	302	11/12	0.96	0.10	13,20,38,42	0
1	MLY	A	256	11/12	0.97	0.08	12,15,24,28	0

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	7BZ	A	601	4/4	0.76	0.28	20,20,20,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.