



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2017 – 08:12 AM EDT

PDB ID : 2ZZE  
Title : Crystal structure of alanyl-tRNA synthetase without oligomerization domain in lysine-methylated form  
Authors : Sokabe, M.; Ose, T.; Tokunaga, K.; Nakamura, A.; Nureki, O.; Yao, M.; Tanaka, I.  
Deposited on : unknown  
Resolution : 2.16 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 : rb-20030345  
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) : rb-20030345

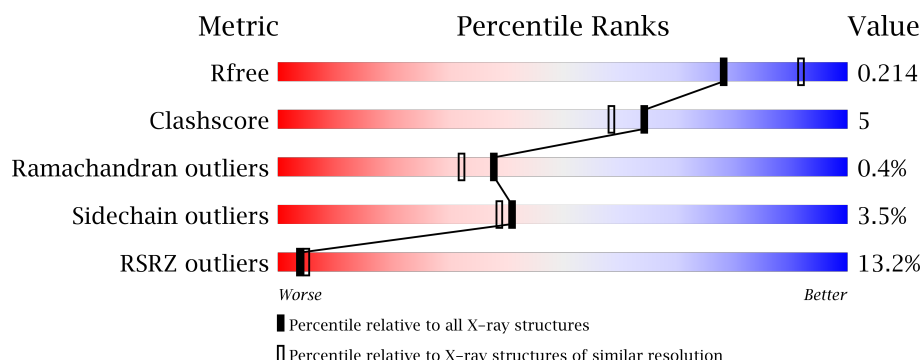
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (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. 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	752	<div> <div>15%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	752	<div> <div>10%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13125 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 Alanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	744	Total	C	N	O	S	0	3	0
			6139	3977	1034	1096	32			
1	B	744	Total	C	N	O	S	0	3	0
			6141	3979	1034	1096	32			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

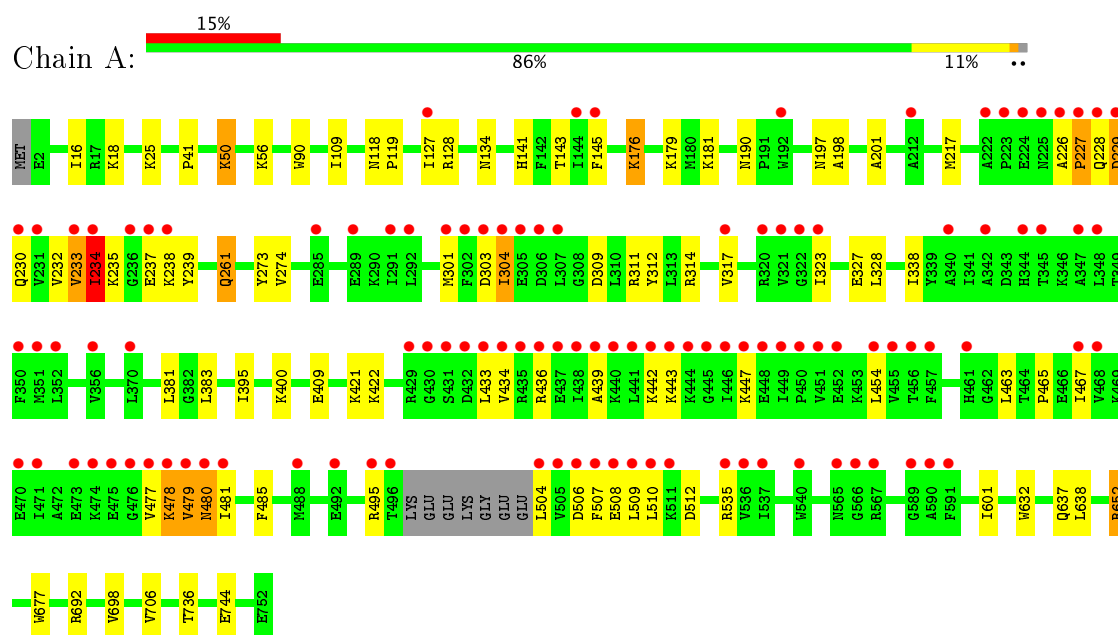
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	414	Total	O	0	0
			414	414		
3	B	429	Total	O	0	0
			429	429		

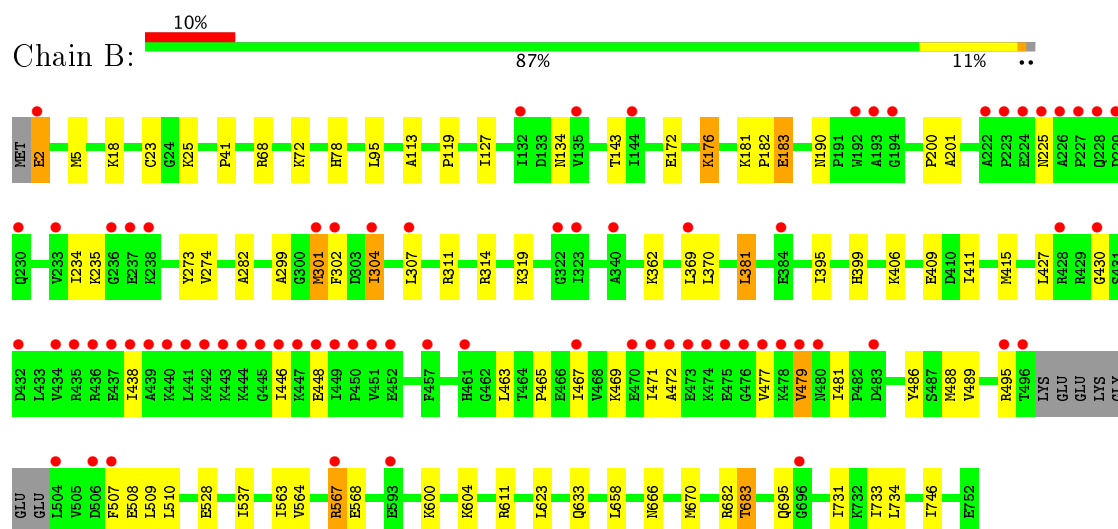
### 3 Residue-property plots

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: Alanyl-tRNA synthetase



#### • Molecule 1: Alanyl-tRNA synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.06Å 130.15Å 94.86Å 90.00° 117.46° 90.00°	Depositor
Resolution (Å)	38.58 – 2.16 38.56 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.58-2.16) 98.0 (38.56-2.16)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.189 , 0.227 0.216 , 0.214	Depositor DCC
$R_{free}$ test set	5035 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: ZN, MLY, OCS

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	0.41	0/5843	0.55	0/7933
1	B	0.41	0/5843	0.53	0/7933
All	All	0.41	0/11686	0.54	0/15866

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	VAL	Peptide
1	B	508	GLU	Peptide

### 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	6139	0	6192	70	0
1	B	6141	0	6200	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	414	0	0	6	0
3	B	429	0	0	2	0
All	All	13125	0	12392	118	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 5.

The worst 5 of 118 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:477:VAL:HG22	1:A:478:LYS:H	1.39	0.88
1:B:134:ASN:HD21	1:B:304:ILE:H	1.25	0.84
1:A:507:PHE:CD2	1:A:508:GLU:N	2.46	0.83
1:B:666:ASN:HD21	1:B:731:ILE:H	1.22	0.82
1:A:234:ILE:O	1:A:235:MLY:HB3	1.83	0.77

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	702/752 (93%)	679 (97%)	19 (3%)	4 (1%)	28	20
1	B	702/752 (93%)	686 (98%)	14 (2%)	2 (0%)	44	41
All	All	1404/1504 (93%)	1365 (97%)	33 (2%)	6 (0%)	38	32

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	PRO
1	A	234	ILE
1	A	478	LYS
1	B	448	GLU
1	B	446	ILE

### 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	610/614 (99%)	588 (96%)	22 (4%)	40	38
1	B	610/614 (99%)	587 (96%)	23 (4%)	38	35
All	All	1220/1228 (99%)	1175 (96%)	45 (4%)	41	36

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	638	LEU
1	B	225	ASN
1	B	567	ARG
1	B	2	GLU
1	B	301[A]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	633	GLN
1	A	740	GLN
1	B	666	ASN
1	A	608	GLN
1	B	608	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

82 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	158	1	10,10,11	0.55	0	8,11,13	1.88	3 (37%)
1	MLY	A	179	1	10,10,11	0.45	0	8,11,13	2.21	4 (50%)
1	MLY	A	18	1	10,10,11	0.48	0	8,11,13	2.09	2 (25%)
1	MLY	A	181	1	10,10,11	0.44	0	8,11,13	1.91	2 (25%)
1	MLY	A	19	1	10,10,11	0.44	0	8,11,13	2.01	3 (37%)
1	MLY	A	21	1	10,10,11	0.46	0	8,11,13	2.05	4 (50%)
1	MLY	A	220	1	10,10,11	0.48	0	8,11,13	2.01	3 (37%)
1	MLY	A	221	1	10,10,11	0.36	0	8,11,13	1.97	3 (37%)
1	MLY	A	235	1	8,8,11	0.80	0	5,8,13	0.72	0
1	MLY	A	245	1	10,10,11	0.39	0	8,11,13	2.02	3 (37%)
1	MLY	A	25	1	10,10,11	0.54	0	8,11,13	2.05	4 (50%)
1	MLY	A	279	1	10,10,11	0.43	0	8,11,13	2.19	4 (50%)
1	MLY	A	280	1	10,10,11	0.44	0	8,11,13	2.12	4 (50%)
1	MLY	A	362	1	10,10,11	0.42	0	8,11,13	2.09	3 (37%)
1	MLY	A	396	1	10,10,11	0.50	0	8,11,13	1.96	3 (37%)
1	MLY	A	406	1	10,10,11	0.44	0	8,11,13	2.05	4 (50%)
1	MLY	A	422	1	10,10,11	0.43	0	8,11,13	2.15	4 (50%)
1	MLY	A	453	1	8,8,11	0.99	1 (12%)	5,8,13	0.77	0
1	MLY	A	469	1	8,8,11	0.99	1 (12%)	5,8,13	0.93	0
1	MLY	A	527	1	10,10,11	0.36	0	8,11,13	2.01	4 (50%)
1	MLY	A	532	1	10,10,11	0.41	0	8,11,13	2.07	4 (50%)
1	MLY	A	538	1	8,8,11	1.02	1 (12%)	5,8,13	0.96	0
1	MLY	A	56	1	10,10,11	0.39	0	8,11,13	2.14	4 (50%)
1	MLY	A	570	1	10,10,11	0.43	0	8,11,13	2.11	4 (50%)
1	MLY	A	576	1	10,10,11	0.42	0	8,11,13	2.03	4 (50%)
1	MLY	A	579	1	10,10,11	0.45	0	8,11,13	2.13	4 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	584	1	10,10,11	0.36	0	8,11,13	2.09	4 (50%)
1	MLY	A	592	1	8,8,11	0.90	1 (12%)	5,8,13	0.82	0
1	MLY	A	6	1	10,10,11	0.44	0	8,11,13	2.20	4 (50%)
1	MLY	A	600	1	10,10,11	0.38	0	8,11,13	2.07	4 (50%)
1	MLY	A	604	1	10,10,11	0.47	0	8,11,13	2.00	4 (50%)
1	MLY	A	65	1	10,10,11	0.51	0	8,11,13	2.01	4 (50%)
1	MLY	A	651	1	10,10,11	0.45	0	8,11,13	1.86	2 (25%)
1	MLY	A	659	1	10,10,11	0.63	0	8,11,13	2.06	4 (50%)
1	MLY	A	674	1	10,10,11	0.36	0	8,11,13	2.22	5 (62%)
1	MLY	A	688	1	10,10,11	0.54	0	8,11,13	1.97	3 (37%)
1	MLY	A	708	1	10,10,11	0.45	0	8,11,13	1.86	3 (37%)
1	OCS	A	717	1	8,8,9	1.11	0	7,11,13	2.90	1 (14%)
1	MLY	A	72	1	10,10,11	0.36	0	8,11,13	2.17	4 (50%)
1	MLY	A	732	1	10,10,11	0.45	0	8,11,13	1.94	3 (37%)
1	MLY	A	82	1	8,8,11	0.89	0	5,8,13	0.87	0
1	MLY	B	158	1	10,10,11	0.42	0	8,11,13	2.22	4 (50%)
1	MLY	B	179	1	10,10,11	0.31	0	8,11,13	2.22	4 (50%)
1	MLY	B	18	1	10,10,11	0.42	0	8,11,13	2.09	3 (37%)
1	MLY	B	181	1	10,10,11	0.47	0	8,11,13	1.93	2 (25%)
1	MLY	B	19	1	10,10,11	0.46	0	8,11,13	2.10	4 (50%)
1	MLY	B	21	1	10,10,11	0.45	0	8,11,13	1.94	2 (25%)
1	MLY	B	220	1	10,10,11	0.44	0	8,11,13	1.93	2 (25%)
1	MLY	B	221	1	8,8,11	0.80	0	5,8,13	0.90	0
1	MLY	B	235	1	10,10,11	0.49	0	8,11,13	2.02	3 (37%)
1	MLY	B	245	1	10,10,11	0.40	0	8,11,13	2.11	4 (50%)
1	MLY	B	25	1	10,10,11	0.54	0	8,11,13	2.34	5 (62%)
1	MLY	B	279	1	8,8,11	0.91	1 (12%)	5,8,13	0.91	0
1	MLY	B	280	1	10,10,11	0.40	0	8,11,13	2.18	4 (50%)
1	MLY	B	362	1	10,10,11	0.41	0	8,11,13	2.09	4 (50%)
1	MLY	B	396	1	10,10,11	0.53	0	8,11,13	2.02	4 (50%)
1	MLY	B	406	1	10,10,11	0.53	0	8,11,13	2.12	4 (50%)
1	MLY	B	422	1	8,8,11	0.81	0	5,8,13	0.76	0
1	MLY	B	453	1	10,10,11	0.46	0	8,11,13	2.02	4 (50%)
1	MLY	B	469	1	10,10,11	0.40	0	8,11,13	2.20	5 (62%)
1	MLY	B	527	1	10,10,11	0.32	0	8,11,13	2.06	4 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	B	532	1	10,10,11	0.42	0	8,11,13	1.90	3 (37%)
1	MLY	B	538	1	10,10,11	0.41	0	8,11,13	2.14	4 (50%)
1	MLY	B	56	1	8,8,11	0.79	0	5,8,13	0.75	0
1	MLY	B	570	1	10,10,11	0.43	0	8,11,13	2.01	3 (37%)
1	MLY	B	576	1	10,10,11	0.44	0	8,11,13	2.11	4 (50%)
1	MLY	B	579	1	8,8,11	1.18	1 (12%)	5,8,13	0.69	0
1	MLY	B	584	1	10,10,11	0.40	0	8,11,13	2.05	3 (37%)
1	MLY	B	592	1	10,10,11	0.36	0	8,11,13	2.00	3 (37%)
1	MLY	B	6	1	10,10,11	0.47	0	8,11,13	2.28	5 (62%)
1	MLY	B	600	1	10,10,11	0.37	0	8,11,13	2.48	4 (50%)
1	MLY	B	604	1	10,10,11	0.51	0	8,11,13	1.89	2 (25%)
1	MLY	B	65	1	10,10,11	0.40	0	8,11,13	2.00	3 (37%)
1	MLY	B	651	1	10,10,11	0.39	0	8,11,13	1.89	2 (25%)
1	MLY	B	659	1	10,10,11	0.38	0	8,11,13	2.03	3 (37%)
1	MLY	B	674	1	10,10,11	0.38	0	8,11,13	2.02	3 (37%)
1	MLY	B	688	1	10,10,11	0.39	0	8,11,13	2.28	5 (62%)
1	MLY	B	708	1	10,10,11	0.40	0	8,11,13	1.94	2 (25%)
1	OCS	B	717	1	8,8,9	1.20	0	7,11,13	2.31	2 (28%)
1	MLY	B	72	1	10,10,11	0.34	0	8,11,13	2.13	4 (50%)
1	MLY	B	732	1	10,10,11	0.41	0	8,11,13	1.89	2 (25%)
1	MLY	B	82	1	10,10,11	0.41	0	8,11,13	2.08	4 (50%)

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	158	1	-	0/7/9/11	0/0/0/0
1	MLY	A	179	1	-	0/7/9/11	0/0/0/0
1	MLY	A	18	1	-	0/7/9/11	0/0/0/0
1	MLY	A	181	1	-	0/7/9/11	0/0/0/0
1	MLY	A	19	1	-	0/7/9/11	0/0/0/0
1	MLY	A	21	1	-	0/7/9/11	0/0/0/0
1	MLY	A	220	1	-	0/7/9/11	0/0/0/0
1	MLY	A	221	1	-	0/7/9/11	0/0/0/0
1	MLY	A	235	1	-	0/5/7/11	0/0/0/0
1	MLY	A	245	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	25	1	-	0/7/9/11	0/0/0/0
1	MLY	A	279	1	-	0/7/9/11	0/0/0/0
1	MLY	A	280	1	-	0/7/9/11	0/0/0/0
1	MLY	A	362	1	-	0/7/9/11	0/0/0/0
1	MLY	A	396	1	-	0/7/9/11	0/0/0/0
1	MLY	A	406	1	-	0/7/9/11	0/0/0/0
1	MLY	A	422	1	-	0/7/9/11	0/0/0/0
1	MLY	A	453	1	-	0/5/7/11	0/0/0/0
1	MLY	A	469	1	-	0/5/7/11	0/0/0/0
1	MLY	A	527	1	-	0/7/9/11	0/0/0/0
1	MLY	A	532	1	-	0/7/9/11	0/0/0/0
1	MLY	A	538	1	-	0/5/7/11	0/0/0/0
1	MLY	A	56	1	-	0/7/9/11	0/0/0/0
1	MLY	A	570	1	-	0/7/9/11	0/0/0/0
1	MLY	A	576	1	-	0/7/9/11	0/0/0/0
1	MLY	A	579	1	-	0/7/9/11	0/0/0/0
1	MLY	A	584	1	-	0/7/9/11	0/0/0/0
1	MLY	A	592	1	-	0/5/7/11	0/0/0/0
1	MLY	A	6	1	-	0/7/9/11	0/0/0/0
1	MLY	A	600	1	-	0/7/9/11	0/0/0/0
1	MLY	A	604	1	-	0/7/9/11	0/0/0/0
1	MLY	A	65	1	-	0/7/9/11	0/0/0/0
1	MLY	A	651	1	-	0/7/9/11	0/0/0/0
1	MLY	A	659	1	-	0/7/9/11	0/0/0/0
1	MLY	A	674	1	-	0/7/9/11	0/0/0/0
1	MLY	A	688	1	-	0/7/9/11	0/0/0/0
1	MLY	A	708	1	-	0/7/9/11	0/0/0/0
1	OCS	A	717	1	-	1/4/7/9	0/0/0/0
1	MLY	A	72	1	-	0/7/9/11	0/0/0/0
1	MLY	A	732	1	-	0/7/9/11	0/0/0/0
1	MLY	A	82	1	-	0/5/7/11	0/0/0/0
1	MLY	B	158	1	-	0/7/9/11	0/0/0/0
1	MLY	B	179	1	-	0/7/9/11	0/0/0/0
1	MLY	B	18	1	-	0/7/9/11	0/0/0/0
1	MLY	B	181	1	-	0/7/9/11	0/0/0/0
1	MLY	B	19	1	-	0/7/9/11	0/0/0/0
1	MLY	B	21	1	-	0/7/9/11	0/0/0/0
1	MLY	B	220	1	-	0/7/9/11	0/0/0/0
1	MLY	B	221	1	-	0/5/7/11	0/0/0/0
1	MLY	B	235	1	-	0/7/9/11	0/0/0/0
1	MLY	B	245	1	-	0/7/9/11	0/0/0/0
1	MLY	B	25	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	279	1	-	0/5/7/11	0/0/0/0
1	MLY	B	280	1	-	0/7/9/11	0/0/0/0
1	MLY	B	362	1	-	0/7/9/11	0/0/0/0
1	MLY	B	396	1	-	0/7/9/11	0/0/0/0
1	MLY	B	406	1	-	0/7/9/11	0/0/0/0
1	MLY	B	422	1	-	0/5/7/11	0/0/0/0
1	MLY	B	453	1	-	0/7/9/11	0/0/0/0
1	MLY	B	469	1	-	0/7/9/11	0/0/0/0
1	MLY	B	527	1	-	0/7/9/11	0/0/0/0
1	MLY	B	532	1	-	0/7/9/11	0/0/0/0
1	MLY	B	538	1	-	0/7/9/11	0/0/0/0
1	MLY	B	56	1	-	0/5/7/11	0/0/0/0
1	MLY	B	570	1	-	0/7/9/11	0/0/0/0
1	MLY	B	576	1	-	0/7/9/11	0/0/0/0
1	MLY	B	579	1	-	0/5/7/11	0/0/0/0
1	MLY	B	584	1	-	0/7/9/11	0/0/0/0
1	MLY	B	592	1	-	0/7/9/11	0/0/0/0
1	MLY	B	6	1	-	0/7/9/11	0/0/0/0
1	MLY	B	600	1	-	0/7/9/11	0/0/0/0
1	MLY	B	604	1	-	0/7/9/11	0/0/0/0
1	MLY	B	65	1	-	0/7/9/11	0/0/0/0
1	MLY	B	651	1	-	0/7/9/11	0/0/0/0
1	MLY	B	659	1	-	0/7/9/11	0/0/0/0
1	MLY	B	674	1	-	0/7/9/11	0/0/0/0
1	MLY	B	688	1	-	0/7/9/11	0/0/0/0
1	MLY	B	708	1	-	0/7/9/11	0/0/0/0
1	OCS	B	717	1	-	1/4/7/9	0/0/0/0
1	MLY	B	72	1	-	0/7/9/11	0/0/0/0
1	MLY	B	732	1	-	0/7/9/11	0/0/0/0
1	MLY	B	82	1	-	0/7/9/11	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	592	MLY	CA-C	2.23	1.53	1.50
1	B	279	MLY	CA-C	2.24	1.53	1.50
1	A	538	MLY	CA-C	2.39	1.53	1.50
1	A	453	MLY	CA-C	2.50	1.53	1.50
1	A	469	MLY	CA-C	2.51	1.53	1.50

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	MLY	CB-CA-C	-4.18	104.77	111.65
1	A	179	MLY	CD-CE-NZ	-3.26	104.92	113.77
1	B	158	MLY	CD-CE-NZ	-3.08	105.39	113.77
1	B	179	MLY	CD-CE-NZ	-2.99	105.64	113.77
1	A	422	MLY	CD-CE-NZ	-2.95	105.74	113.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	717	OCS	SG-CB-CA-N
1	A	717	OCS	SG-CB-CA-N

There are no ring outliers.

17 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	179	MLY	1	0
1	A	18	MLY	1	0
1	A	181	MLY	1	0
1	A	235	MLY	2	0
1	A	25	MLY	1	0
1	A	422	MLY	1	0
1	A	56	MLY	1	0
1	B	18	MLY	1	0
1	B	181	MLY	1	0
1	B	235	MLY	1	0
1	B	25	MLY	1	0
1	B	362	MLY	2	0
1	B	406	MLY	1	0
1	B	469	MLY	1	0
1	B	600	MLY	1	0
1	B	604	MLY	1	0
1	B	72	MLY	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are 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

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	703/752 (93%)	0.84	111 (15%) 2 3	10, 22, 40, 72	0
1	B	703/752 (93%)	0.49	74 (10%) 7 10	11, 20, 44, 65	0
All	All	1406/1504 (93%)	0.67	185 (13%) 4 5	10, 21, 44, 72	0

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	VAL	10.5
1	A	438	ILE	10.4
1	A	236	GLY	10.0
1	A	446	ILE	9.3
1	A	441	LEU	8.5

### 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. 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	221	11/12	0.86	0.41	-	28,30,37,37	0
1	MLY	A	158	11/12	0.91	0.13	-	12,13,25,25	0
1	MLY	B	19	11/12	0.91	0.16	-	12,13,25,25	0
1	MLY	B	406	11/12	0.82	0.23	-	25,27,32,32	0
1	MLY	A	708	11/12	0.95	0.12	-	18,19,27,27	0
1	MLY	A	659	11/12	0.94	0.15	-	16,17,24,25	0
1	MLY	B	56	9/12	0.94	0.11	-	19,20,24,26	0
1	MLY	B	279	9/12	0.91	0.13	-	18,20,22,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	362	11/12	0.87	0.21	-	21,22,34,35	0
1	MLY	B	6	11/12	0.91	0.17	-	20,22,30,31	0
1	MLY	B	659	11/12	0.96	0.14	-	15,16,22,23	0
1	MLY	B	181	11/12	0.95	0.15	-	16,16,20,20	0
1	MLY	A	406	11/12	0.87	0.22	-	25,26,32,33	0
1	MLY	B	422	9/12	0.87	0.17	-	31,32,34,34	0
1	MLY	A	56	11/12	0.92	0.13	-	18,19,30,31	0
1	MLY	A	584	11/12	0.83	0.23	-	28,28,30,30	0
1	MLY	B	179	11/12	0.92	0.18	-	16,17,27,28	0
1	MLY	B	221	9/12	0.85	0.28	-	32,34,35,35	0
1	MLY	B	65	11/12	0.95	0.08	-	14,15,21,22	0
1	MLY	A	18	11/12	0.96	0.09	-	12,13,14,15	0
1	MLY	A	19	11/12	0.92	0.15	-	11,13,24,25	0
1	MLY	A	65	11/12	0.93	0.11	-	15,15,21,22	0
1	MLY	B	532	11/12	0.90	0.15	-	21,22,30,30	0
1	MLY	A	179	11/12	0.88	0.18	-	16,16,28,28	0
1	MLY	B	18	11/12	0.94	0.13	-	13,13,16,17	0
1	MLY	B	453	11/12	0.80	0.33	-	40,41,43,43	0
1	MLY	A	422	11/12	0.84	0.20	-	28,29,39,39	0
1	MLY	B	280	11/12	0.83	0.24	-	20,22,26,26	0
1	MLY	A	576	11/12	0.86	0.19	-	29,31,39,39	0
1	MLY	B	651	11/12	0.94	0.10	-	17,17,19,20	0
1	MLY	A	6	11/12	0.91	0.16	-	14,15,29,30	0
1	MLY	A	280	11/12	0.86	0.22	-	26,28,34,34	0
1	MLY	A	527	11/12	0.92	0.17	-	25,26,34,34	0
1	MLY	A	21	11/12	0.95	0.11	-	12,12,21,22	0
1	MLY	B	220	11/12	0.93	0.16	-	27,29,30,30	0
1	MLY	A	25	11/12	0.94	0.10	-	11,13,26,27	0
1	OCS	A	717	9/10	0.96	0.12	-	24,25,27,29	0
1	MLY	B	25	11/12	0.90	0.16	-	14,14,30,30	0
1	OCS	B	717	9/10	0.98	0.13	-	21,21,23,23	0
1	MLY	B	158	11/12	0.93	0.17	-	14,15,27,28	0
1	MLY	A	651	11/12	0.92	0.12	-	15,16,20,22	0
1	MLY	B	396	11/12	0.91	0.24	-	20,20,29,29	0
1	MLY	A	674	11/12	0.94	0.20	-	20,20,33,34	0
1	MLY	A	592	9/12	0.85	0.34	-	28,29,29,30	0
1	MLY	A	688	11/12	0.88	0.15	-	22,23,35,36	0
1	MLY	A	469	9/12	0.78	0.35	-	38,38,39,39	0
1	MLY	B	584	11/12	0.89	0.18	-	21,21,30,30	0
1	MLY	A	453	9/12	0.82	0.24	-	34,34,34,35	0
1	MLY	B	235	11/12	0.84	0.27	-	41,42,47,47	0
1	MLY	B	688	11/12	0.94	0.10	-	19,20,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	B	708	11/12	0.93	0.13	-	17,18,25,25	0
1	MLY	B	362	11/12	0.88	0.17	-	15,16,27,27	0
1	MLY	B	600	11/12	0.89	0.19	-	19,20,32,34	0
1	MLY	A	279	11/12	0.88	0.18	-	24,25,31,31	0
1	MLY	B	527	11/12	0.92	0.19	-	22,23,31,31	0
1	MLY	A	532	11/12	0.89	0.21	-	25,26,27,27	0
1	MLY	A	600	11/12	0.88	0.18	-	24,24,30,30	0
1	MLY	B	538	11/12	0.77	0.29	-	24,24,29,30	0
1	MLY	B	732	11/12	0.96	0.15	-	16,17,24,25	0
1	MLY	A	245	11/12	0.92	0.13	-	15,18,32,32	0
1	MLY	A	579	11/12	0.81	0.18	-	30,30,34,34	0
1	MLY	A	396	11/12	0.89	0.18	-	22,23,31,32	0
1	MLY	B	72	11/12	0.93	0.14	-	16,17,22,22	0
1	MLY	B	579	9/12	0.91	0.16	-	23,24,29,29	0
1	MLY	B	592	11/12	0.91	0.15	-	20,21,30,30	0
1	MLY	B	674	11/12	0.90	0.20	-	17,19,32,32	0
1	MLY	A	72	11/12	0.89	0.17	-	17,18,27,28	0
1	MLY	A	220	11/12	0.89	0.14	-	24,26,31,31	0
1	MLY	A	604	11/12	0.85	0.24	-	21,22,33,33	0
1	MLY	A	235	9/12	0.39	0.54	-	48,48,50,50	0
1	MLY	B	245	11/12	0.95	0.10	-	14,15,26,26	0
1	MLY	A	82	9/12	0.89	0.19	-	16,17,22,23	0
1	MLY	A	732	11/12	0.92	0.15	-	17,18,28,28	0
1	MLY	B	21	11/12	0.96	0.11	-	11,12,16,17	0
1	MLY	B	82	11/12	0.84	0.26	-	18,19,32,33	0
1	MLY	A	181	11/12	0.89	0.15	-	16,16,23,24	0
1	MLY	B	469	11/12	0.86	0.31	-	43,43,43,43	0
1	MLY	B	576	11/12	0.90	0.15	-	24,25,35,35	0
1	MLY	B	604	11/12	0.84	0.19	-	18,19,34,34	0
1	MLY	A	570	11/12	0.90	0.26	-	27,27,33,33	0
1	MLY	B	570	11/12	0.90	0.17	-	19,21,28,29	0
1	MLY	A	538	9/12	0.82	0.34	-	29,29,30,31	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. 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
2	ZN	A	753	1/1	0.99	0.12	1.50	16,16,16,16	0
2	ZN	B	753	1/1	1.00	0.13	1.18	17,17,17,17	0

## 6.5 Other polymers

There are no such residues in this entry.