



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:28 PM UTC

PDB ID : 2ZZE / pdb_00002zze
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 : 2009-02-10
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

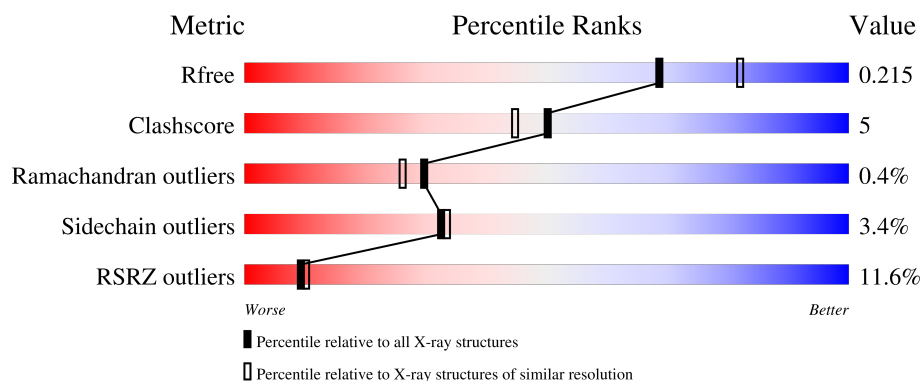
1 Overall quality at a glance

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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	752	

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 (CCD ID: ZN) (formula: Zn).

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

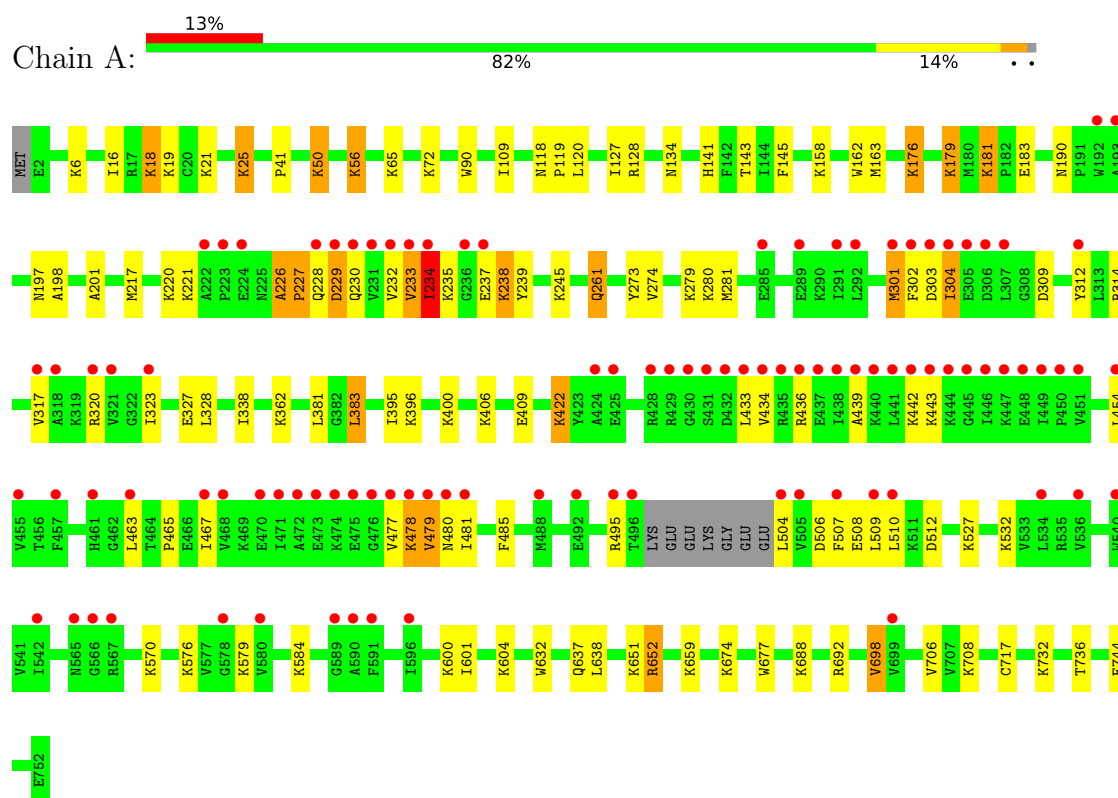
- Molecule 3 is water.

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

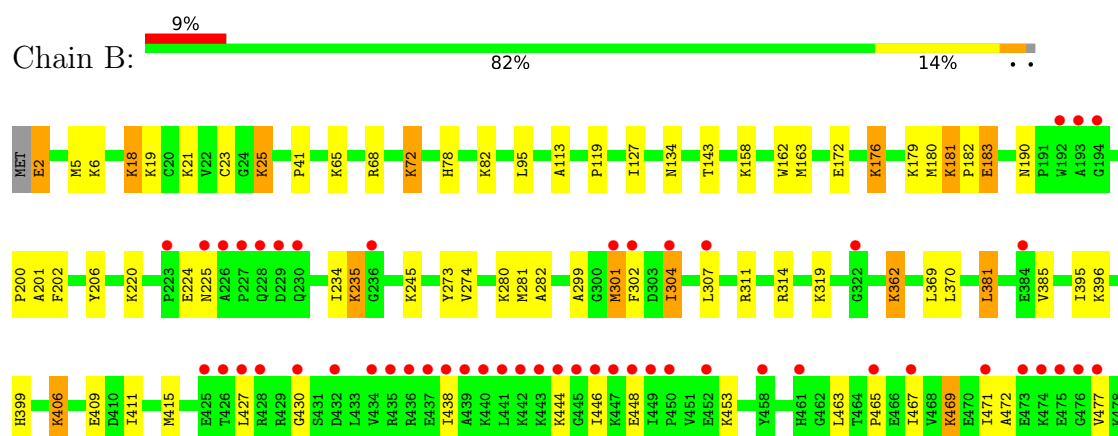
3 Residue-property plots [i](#)

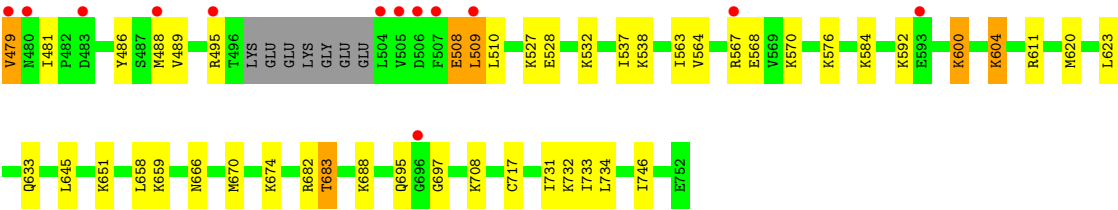
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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, α , β , γ	89.06Å 130.15Å 94.86Å 90.00° 117.46° 90.00°	Depositor
Resolution (Å)	38.58 – 2.16 38.58 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.58-2.16) 98.1 (38.58-2.16)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.227 0.217 , 0.215	Depositor DCC
R_{free} test set	5053 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, ZN, 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	0.52	0/5843	0.77	4/7933 (0.1%)
1	B	0.52	0/5843	0.75	2/7933 (0.0%)
All	All	0.52	0/11686	0.76	6/15866 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LYS	N-CA-C	6.25	119.54	110.42
1	B	224	GLU	CB-CA-C	-6.03	109.03	117.23
1	B	509	LEU	N-CA-C	-5.56	105.16	112.72
1	A	302	PHE	N-CA-C	5.54	117.13	108.20
1	A	226	ALA	CA-C-N	5.42	126.61	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	B	508	GLU	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	6139	0	6195	75	0
1	B	6141	0	6200	55	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	12395	130	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 130 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:411:ILE:HG22	1:B:415:MET:HE2	1.58	0.85
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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	21	15
1	B	702/752 (93%)	686 (98%)	14 (2%)	2 (0%)	36	34
All	All	1404/1504 (93%)	1365 (97%)	33 (2%)	6 (0%)	30	26

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%)	31	31
1	B	610/614 (99%)	588 (96%)	22 (4%)	31	31
All	All	1220/1228 (99%)	1176 (96%)	44 (4%)	32	31

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	304	ILE
1	B	444	LYS
1	B	307	LEU
1	B	370	LEU
1	B	488[A]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	ASN
1	B	637	GLN
1	B	695	GLN
1	B	666	ASN
1	A	316	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	179	1	9,10,11	0.40	0	6,11,13	2.56	4 (66%)
1	MLY	B	396	1	9,10,11	0.44	0	6,11,13	2.26	4 (66%)
1	MLY	B	422	1	7,8,11	0.53	0	3,8,13	0.22	0
1	MLY	A	527	1	9,10,11	0.41	0	6,11,13	2.27	4 (66%)
1	MLY	A	732	1	9,10,11	0.50	0	6,11,13	2.18	3 (50%)
1	MLY	A	406	1	9,10,11	0.44	0	6,11,13	2.32	4 (66%)
1	MLY	A	220	1	9,10,11	0.47	0	6,11,13	2.27	3 (50%)
1	MLY	A	221	1	9,10,11	0.40	0	6,11,13	2.23	3 (50%)
1	MLY	B	179	1	9,10,11	0.33	0	6,11,13	2.51	4 (66%)
1	MLY	B	532	1	9,10,11	0.47	0	6,11,13	2.13	3 (50%)
1	MLY	B	732	1	9,10,11	0.47	0	6,11,13	2.10	2 (33%)
1	MLY	A	584	1	9,10,11	0.40	0	6,11,13	2.32	4 (66%)
1	MLY	A	604	1	9,10,11	0.41	0	6,11,13	2.24	4 (66%)
1	MLY	B	406	1	9,10,11	0.51	0	6,11,13	2.39	4 (66%)
1	MLY	B	453	1	9,10,11	0.42	0	6,11,13	2.29	4 (66%)
1	MLY	B	6	1	9,10,11	0.55	0	6,11,13	2.30	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	B	576	1	9,10,11	0.50	0	6,11,13	2.36	4 (66%)
1	MLY	A	592	1	7,8,11	0.49	0	3,8,13	0.27	0
1	MLY	B	592	1	9,10,11	0.38	0	6,11,13	2.18	3 (50%)
1	MLY	B	56	1	7,8,11	0.48	0	3,8,13	0.30	0
1	MLY	B	674	1	9,10,11	0.43	0	6,11,13	2.26	4 (66%)
1	MLY	A	6	1	9,10,11	0.51	0	6,11,13	2.21	3 (50%)
1	MLY	B	604	1	9,10,11	0.50	0	6,11,13	2.07	2 (33%)
1	MLY	B	245	1	9,10,11	0.43	0	6,11,13	2.41	4 (66%)
1	MLY	B	362	1	9,10,11	0.31	0	6,11,13	2.34	4 (66%)
1	MLY	A	25	1	9,10,11	0.46	0	6,11,13	2.21	4 (66%)
1	MLY	B	280	1	9,10,11	0.41	0	6,11,13	2.45	4 (66%)
1	MLY	B	469	1	9,10,11	0.40	0	6,11,13	2.35	4 (66%)
1	MLY	A	21	1	9,10,11	0.44	0	6,11,13	2.31	4 (66%)
1	MLY	A	65	1	9,10,11	0.38	0	6,11,13	2.27	4 (66%)
1	MLY	A	532	1	9,10,11	0.45	0	6,11,13	2.35	4 (66%)
1	MLY	A	181	1	9,10,11	0.37	0	6,11,13	2.09	2 (33%)
1	MLY	B	279	1	7,8,11	0.52	0	3,8,13	0.20	0
1	MLY	A	600	1	9,10,11	0.42	0	6,11,13	2.26	4 (66%)
1	MLY	B	651	1	9,10,11	0.43	0	6,11,13	2.13	2 (33%)
1	MLY	A	235	1	7,8,11	0.59	0	3,8,13	0.45	0
1	MLY	B	600	1	9,10,11	0.39	0	6,11,13	2.25	3 (50%)
1	MLY	B	158	1	9,10,11	0.37	0	6,11,13	2.49	4 (66%)
1	MLY	A	708	1	9,10,11	0.52	0	6,11,13	2.05	2 (33%)
1	MLY	B	181	1	9,10,11	0.44	0	6,11,13	2.10	2 (33%)
1	MLY	B	72	1	9,10,11	0.39	0	6,11,13	2.30	4 (66%)
1	MLY	B	235	1	9,10,11	0.42	0	6,11,13	2.28	4 (66%)
1	MLY	A	570	1	9,10,11	0.47	0	6,11,13	2.34	4 (66%)
1	MLY	A	688	1	9,10,11	0.48	0	6,11,13	2.16	3 (50%)
1	MLY	B	19	1	9,10,11	0.52	0	6,11,13	2.35	4 (66%)
1	MLY	A	579	1	9,10,11	0.44	0	6,11,13	2.44	4 (66%)
1	MLY	B	688	1	9,10,11	0.43	0	6,11,13	2.39	4 (66%)
1	MLY	A	19	1	9,10,11	0.50	0	6,11,13	2.23	3 (50%)
1	MLY	A	651	1	9,10,11	0.47	0	6,11,13	2.07	2 (33%)
1	MLY	A	659	1	9,10,11	0.42	0	6,11,13	2.33	4 (66%)
1	MLY	B	538	1	9,10,11	0.35	0	6,11,13	2.24	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	396	1	9,10,11	0.42	0	6,11,13	2.21	3 (50%)
1	MLY	B	708	1	9,10,11	0.45	0	6,11,13	2.15	2 (33%)
1	MLY	B	21	1	9,10,11	0.41	0	6,11,13	2.16	2 (33%)
1	MLY	B	65	1	9,10,11	0.41	0	6,11,13	2.27	4 (66%)
1	MLY	A	158	1	9,10,11	0.40	0	6,11,13	2.08	3 (50%)
1	MLY	A	538	1	7,8,11	0.63	0	3,8,13	0.26	0
1	MLY	A	674	1	9,10,11	0.40	0	6,11,13	2.35	4 (66%)
1	MLY	B	221	1	7,8,11	0.47	0	3,8,13	0.49	0
1	MLY	A	576	1	9,10,11	0.46	0	6,11,13	2.31	4 (66%)
1	MLY	A	453	1	7,8,11	0.52	0	3,8,13	0.15	0
1	MLY	B	82	1	9,10,11	0.43	0	6,11,13	2.27	4 (66%)
1	MLY	A	56	1	9,10,11	0.44	0	6,11,13	2.41	4 (66%)
1	MLY	A	469	1	7,8,11	0.50	0	3,8,13	0.36	0
1	MLY	B	579	1	7,8,11	0.57	0	3,8,13	0.27	0
1	MLY	A	280	1	9,10,11	0.41	0	6,11,13	2.39	4 (66%)
1	MLY	B	584	1	9,10,11	0.45	0	6,11,13	2.30	4 (66%)
1	MLY	B	220	1	9,10,11	0.42	0	6,11,13	2.16	2 (33%)
1	OCS	B	717	1	6,8,9	1.17	0	7,11,13	1.44	2 (28%)
1	MLY	A	362	1	9,10,11	0.38	0	6,11,13	2.23	3 (50%)
1	MLY	B	570	1	9,10,11	0.48	0	6,11,13	2.12	3 (50%)
1	MLY	A	245	1	9,10,11	0.45	0	6,11,13	2.30	3 (50%)
1	MLY	A	279	1	9,10,11	0.42	0	6,11,13	2.29	4 (66%)
1	MLY	A	18	1	9,10,11	0.52	0	6,11,13	2.30	2 (33%)
1	OCS	A	717	1	6,8,9	1.17	0	7,11,13	1.76	1 (14%)
1	MLY	B	659	1	9,10,11	0.34	0	6,11,13	2.27	3 (50%)
1	MLY	B	25	1	9,10,11	0.57	0	6,11,13	2.50	4 (66%)
1	MLY	A	82	1	7,8,11	0.62	0	3,8,13	0.06	0
1	MLY	B	527	1	9,10,11	0.36	0	6,11,13	2.29	4 (66%)
1	MLY	A	72	1	9,10,11	0.40	0	6,11,13	2.32	3 (50%)
1	MLY	A	422	1	9,10,11	0.41	0	6,11,13	2.44	4 (66%)
1	MLY	B	18	1	9,10,11	0.48	0	6,11,13	2.24	2 (33%)

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	179	1	-	1/8/9/11	-
1	MLY	B	396	1	-	3/8/9/11	-
1	MLY	B	422	1	-	3/6/7/11	-
1	MLY	A	527	1	-	5/8/9/11	-
1	MLY	A	732	1	-	1/8/9/11	-
1	MLY	A	406	1	-	3/8/9/11	-
1	MLY	A	220	1	-	2/8/9/11	-
1	MLY	A	221	1	-	2/8/9/11	-
1	MLY	B	179	1	-	1/8/9/11	-
1	MLY	B	532	1	-	2/8/9/11	-
1	MLY	B	732	1	-	3/8/9/11	-
1	MLY	A	584	1	-	3/8/9/11	-
1	MLY	A	604	1	-	2/8/9/11	-
1	MLY	B	406	1	-	5/8/9/11	-
1	MLY	B	453	1	-	3/8/9/11	-
1	MLY	B	6	1	-	3/8/9/11	-
1	MLY	B	576	1	-	4/8/9/11	-
1	MLY	A	592	1	-	0/6/7/11	-
1	MLY	B	592	1	-	5/8/9/11	-
1	MLY	B	56	1	-	1/6/7/11	-
1	MLY	B	674	1	-	4/8/9/11	-
1	MLY	A	6	1	-	2/8/9/11	-
1	MLY	B	604	1	-	5/8/9/11	-
1	MLY	B	245	1	-	1/8/9/11	-
1	MLY	B	362	1	-	5/8/9/11	-
1	MLY	A	25	1	-	3/8/9/11	-
1	MLY	B	280	1	-	2/8/9/11	-
1	MLY	B	469	1	-	4/8/9/11	-
1	MLY	A	21	1	-	4/8/9/11	-
1	MLY	A	65	1	-	2/8/9/11	-
1	MLY	A	532	1	-	2/8/9/11	-
1	MLY	A	181	1	-	2/8/9/11	-
1	MLY	B	279	1	-	2/6/7/11	-
1	MLY	A	600	1	-	5/8/9/11	-
1	MLY	B	651	1	-	1/8/9/11	-
1	MLY	A	235	1	-	2/6/7/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	600	1	-	1/8/9/11	-
1	MLY	B	158	1	-	3/8/9/11	-
1	MLY	A	708	1	-	1/8/9/11	-
1	MLY	B	181	1	-	1/8/9/11	-
1	MLY	B	72	1	-	3/8/9/11	-
1	MLY	B	235	1	-	5/8/9/11	-
1	MLY	A	570	1	-	4/8/9/11	-
1	MLY	A	688	1	-	6/8/9/11	-
1	MLY	B	19	1	-	1/8/9/11	-
1	MLY	A	579	1	-	2/8/9/11	-
1	MLY	B	688	1	-	4/8/9/11	-
1	MLY	A	19	1	-	2/8/9/11	-
1	MLY	A	651	1	-	1/8/9/11	-
1	MLY	A	659	1	-	1/8/9/11	-
1	MLY	B	538	1	-	3/8/9/11	-
1	MLY	A	396	1	-	1/8/9/11	-
1	MLY	B	708	1	-	1/8/9/11	-
1	MLY	B	21	1	-	1/8/9/11	-
1	MLY	B	65	1	-	1/8/9/11	-
1	MLY	A	158	1	-	1/8/9/11	-
1	MLY	A	538	1	-	2/6/7/11	-
1	MLY	A	674	1	-	2/8/9/11	-
1	MLY	B	221	1	-	0/6/7/11	-
1	MLY	A	576	1	-	2/8/9/11	-
1	MLY	A	453	1	-	0/6/7/11	-
1	MLY	B	82	1	-	6/8/9/11	-
1	MLY	A	56	1	-	3/8/9/11	-
1	MLY	A	469	1	-	1/6/7/11	-
1	MLY	B	579	1	-	2/6/7/11	-
1	MLY	A	280	1	-	2/8/9/11	-
1	MLY	B	584	1	-	3/8/9/11	-
1	MLY	B	220	1	-	1/8/9/11	-
1	OCS	B	717	1	-	3/4/7/9	-
1	MLY	A	362	1	-	3/8/9/11	-
1	MLY	B	570	1	-	2/8/9/11	-
1	MLY	A	245	1	-	2/8/9/11	-
1	MLY	A	279	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	18	1	-	3/8/9/11	-
1	OCS	A	717	1	-	4/4/7/9	-
1	MLY	B	659	1	-	2/8/9/11	-
1	MLY	B	25	1	-	3/8/9/11	-
1	MLY	A	82	1	-	2/6/7/11	-
1	MLY	B	527	1	-	3/8/9/11	-
1	MLY	A	72	1	-	3/8/9/11	-
1	MLY	A	422	1	-	5/8/9/11	-
1	MLY	B	18	1	-	3/8/9/11	-

There are no bond length outliers.

The worst 5 of 237 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	MLY	CH2-NZ-CH1	4.37	120.91	109.72
1	B	245	MLY	CH2-NZ-CH1	4.10	120.23	109.72
1	B	600	MLY	CH2-NZ-CH1	4.07	120.15	109.72
1	B	659	MLY	CH2-NZ-CH1	4.02	120.03	109.72
1	A	18	MLY	CH2-NZ-CH1	3.99	119.95	109.72

There are no chirality outliers.

5 of 205 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	56	MLY	O-C-CA-CB
1	A	72	MLY	O-C-CA-CB
1	A	235	MLY	N-CA-CB-CG
1	A	235	MLY	C-CA-CB-CG
1	A	362	MLY	O-C-CA-CB

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	B	406	MLY	1	0
1	B	604	MLY	1	0
1	B	362	MLY	2	0
1	A	25	MLY	1	0

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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, 95th 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 ²)	Q<0.9
1	A	703/752 (93%)	0.73	99 (14%) 6 7	10, 22, 40, 72	3 (0%)
1	B	703/752 (93%)	0.42	64 (9%) 15 16	9, 20, 44, 65	3 (0%)
All	All	1406/1504 (93%)	0.58	163 (11%) 9 10	9, 21, 44, 72	6 (0%)

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	GLY	7.8
1	A	234	ILE	7.0
1	A	438	ILE	6.9
1	A	446	ILE	6.8
1	A	477	VAL	6.3

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. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
1	MLY	A	235	9/12	0.48	0.25	48,48,50,50	0
1	MLY	A	469	9/12	0.68	0.20	38,38,39,39	0
1	MLY	B	235	11/12	0.70	0.17	41,42,47,47	0
1	MLY	A	576	11/12	0.72	0.17	29,31,39,39	0
1	MLY	A	453	9/12	0.72	0.14	34,34,34,35	0
1	MLY	B	469	11/12	0.74	0.17	43,43,43,43	0
1	MLY	A	538	9/12	0.76	0.14	29,29,30,31	0
1	MLY	B	453	11/12	0.76	0.18	40,41,43,43	0
1	MLY	A	579	11/12	0.76	0.16	30,30,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	B	221	9/12	0.77	0.14	32,34,35,35	0
1	MLY	A	422	11/12	0.78	0.19	28,29,39,39	0
1	MLY	A	592	9/12	0.79	0.14	28,29,29,30	0
1	MLY	B	406	11/12	0.79	0.13	25,27,32,32	0
1	MLY	B	604	11/12	0.80	0.16	18,19,34,34	0
1	MLY	B	538	11/12	0.81	0.14	24,24,29,30	0
1	MLY	A	280	11/12	0.81	0.14	26,28,34,34	0
1	MLY	A	279	11/12	0.82	0.13	24,25,31,31	0
1	MLY	A	221	11/12	0.83	0.18	28,30,37,37	0
1	MLY	B	422	9/12	0.84	0.13	31,32,34,34	0
1	MLY	A	584	11/12	0.84	0.12	28,28,30,30	0
1	MLY	A	532	11/12	0.84	0.14	25,26,27,27	0
1	MLY	B	280	11/12	0.84	0.13	20,22,26,26	0
1	MLY	A	604	11/12	0.84	0.15	21,22,33,33	0
1	MLY	A	220	11/12	0.85	0.12	24,26,31,31	0
1	MLY	B	576	11/12	0.85	0.13	24,25,35,35	0
1	MLY	B	579	9/12	0.85	0.12	23,24,29,29	0
1	MLY	B	532	11/12	0.85	0.13	21,22,30,30	0
1	MLY	A	570	11/12	0.86	0.13	27,27,33,33	0
1	MLY	A	600	11/12	0.86	0.13	24,24,30,30	0
1	MLY	A	72	11/12	0.86	0.12	17,18,27,28	0
1	MLY	B	82	11/12	0.86	0.15	18,19,32,33	0
1	MLY	B	6	11/12	0.87	0.12	20,22,30,31	0
1	MLY	B	600	11/12	0.87	0.13	19,20,32,34	0
1	MLY	A	362	11/12	0.87	0.14	21,22,34,35	0
1	MLY	A	65	11/12	0.88	0.09	15,15,21,22	0
1	MLY	B	25	11/12	0.88	0.12	14,14,30,30	0
1	MLY	B	584	11/12	0.88	0.11	21,21,30,30	0
1	MLY	A	179	11/12	0.88	0.12	16,16,28,28	0
1	MLY	A	688	11/12	0.88	0.12	22,23,35,36	0
1	MLY	B	362	11/12	0.89	0.12	15,16,27,27	0
1	MLY	A	245	11/12	0.89	0.12	15,18,32,32	0
1	MLY	A	406	11/12	0.89	0.11	25,26,32,33	0
1	MLY	A	6	11/12	0.89	0.12	14,15,29,30	0
1	MLY	A	82	9/12	0.89	0.12	16,17,22,23	0
1	MLY	B	19	11/12	0.89	0.12	12,13,25,25	0
1	MLY	B	279	9/12	0.90	0.10	18,20,22,24	0
1	MLY	B	72	11/12	0.90	0.10	16,17,22,22	0
1	MLY	A	396	11/12	0.90	0.09	22,23,31,32	0
1	MLY	B	179	11/12	0.90	0.10	16,17,27,28	0
1	MLY	B	220	11/12	0.90	0.11	27,29,30,30	0
1	MLY	A	527	11/12	0.90	0.11	25,26,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	A	732	11/12	0.90	0.12	17,18,28,28	0
1	MLY	B	245	11/12	0.91	0.10	14,15,26,26	0
1	MLY	B	396	11/12	0.91	0.11	20,20,29,29	0
1	MLY	A	56	11/12	0.91	0.10	18,19,30,31	0
1	MLY	B	592	11/12	0.91	0.09	20,21,30,30	0
1	MLY	A	19	11/12	0.91	0.12	11,13,24,25	0
1	MLY	B	570	11/12	0.91	0.10	19,21,28,29	0
1	MLY	B	674	11/12	0.91	0.11	17,19,32,32	0
1	MLY	B	65	11/12	0.92	0.08	14,15,21,22	0
1	MLY	A	181	11/12	0.92	0.10	16,16,23,24	0
1	MLY	A	158	11/12	0.92	0.10	12,13,25,25	0
1	MLY	B	56	9/12	0.92	0.08	19,20,24,26	0
1	MLY	B	651	11/12	0.92	0.08	17,17,19,20	0
1	MLY	B	527	11/12	0.92	0.11	22,23,31,31	0
1	MLY	B	688	11/12	0.92	0.09	19,20,30,30	0
1	MLY	B	18	11/12	0.93	0.09	13,13,16,17	0
1	MLY	A	21	11/12	0.93	0.09	12,12,21,22	0
1	MLY	A	659	11/12	0.93	0.09	16,17,24,25	0
1	MLY	B	158	11/12	0.93	0.12	14,15,27,28	0
1	MLY	A	674	11/12	0.93	0.10	20,20,33,34	0
1	MLY	A	651	11/12	0.94	0.08	15,16,20,22	0
1	MLY	A	25	11/12	0.94	0.09	11,13,26,27	0
1	MLY	B	659	11/12	0.94	0.10	15,16,22,23	0
1	MLY	B	181	11/12	0.94	0.07	16,16,20,20	0
1	OCS	A	717	9/10	0.94	0.09	24,25,27,29	0
1	MLY	B	708	11/12	0.94	0.09	17,18,25,25	0
1	MLY	B	21	11/12	0.95	0.07	11,12,16,17	0
1	MLY	A	708	11/12	0.95	0.08	18,19,27,27	0
1	MLY	A	18	11/12	0.95	0.07	12,13,14,15	0
1	MLY	B	732	11/12	0.95	0.08	16,17,24,25	0
1	OCS	B	717	9/10	0.97	0.07	21,21,23,23	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	ZN	A	753	1/1	0.99	0.05	16,16,16,16	0
2	ZN	B	753	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.