



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 01:00 AM EDT

PDB ID : 1Z1Y
Title : Crystal structure of Methylated Pvs25, an ookinete protein from Plasmodium vivax
Authors : Saxena, A.K.; Singh, K.; Su, H.P.; Klein, M.M.; Stowers, A.W.; Saul, A.J.; Long, C.A.; Garboczi, D.N.
Deposited on : 2005-03-07
Resolution : 2.00 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

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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

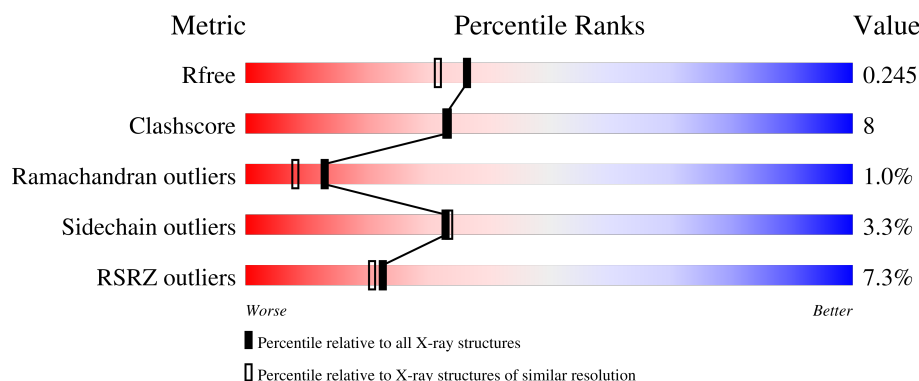
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	186	 4% 77% 16% • 5%
1	B	186	 9% 78% 15% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2829 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 ookinete surface protein Pvs25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1376	850	224	276	26			
1	B	175	Total	C	N	O	S	0	0	0
			1356	838	218	274	26			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLU	-	cloning artifact	UNP O96555
A	-3	ALA	-	cloning artifact	UNP O96555
A	-2	GLU	-	cloning artifact	UNP O96555
A	-1	ALA	-	cloning artifact	UNP O96555
A	0	SER	-	cloning artifact	UNP O96555
A	9	MLY	LYS	modified residue	UNP O96555
A	21	MLY	LYS	modified residue	UNP O96555
A	39	MLY	LYS	modified residue	UNP O96555
A	43	MLY	LYS	modified residue	UNP O96555
A	44	MLY	LYS	modified residue	UNP O96555
A	49	MLY	LYS	modified residue	UNP O96555
A	70	MLY	LYS	modified residue	UNP O96555
A	80	MLY	LYS	modified residue	UNP O96555
A	92	MLY	LYS	modified residue	UNP O96555
A	119	MLY	LYS	modified residue	UNP O96555
A	127	MLY	LYS	modified residue	UNP O96555
A	128	MLY	LYS	modified residue	UNP O96555
A	131	MLY	LYS	modified residue	UNP O96555
A	140	MLY	LYS	modified residue	UNP O96555
A	149	MLY	LYS	modified residue	UNP O96555
A	156	MLY	LYS	modified residue	UNP O96555
A	167	MLY	LYS	modified residue	UNP O96555
A	169	MLY	LYS	modified residue	UNP O96555
A	174	GLY	-	expression tag	UNP O96555
A	175	PRO	-	expression tag	UNP O96555

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Chain	Residue	Modelled	Actual	Comment	Reference
A	176	HIS	-	expression tag	UNP O96555
A	177	HIS	-	expression tag	UNP O96555
A	178	HIS	-	expression tag	UNP O96555
A	179	HIS	-	expression tag	UNP O96555
A	180	HIS	-	expression tag	UNP O96555
A	181	HIS	-	expression tag	UNP O96555
B	-4	GLU	-	cloning artifact	UNP O96555
B	-3	ALA	-	cloning artifact	UNP O96555
B	-2	GLU	-	cloning artifact	UNP O96555
B	-1	ALA	-	cloning artifact	UNP O96555
B	0	SER	-	cloning artifact	UNP O96555
B	9	MLY	LYS	modified residue	UNP O96555
B	21	MLY	LYS	modified residue	UNP O96555
B	39	MLY	LYS	modified residue	UNP O96555
B	43	MLY	LYS	modified residue	UNP O96555
B	44	MLY	LYS	modified residue	UNP O96555
B	49	MLY	LYS	modified residue	UNP O96555
B	70	MLY	LYS	modified residue	UNP O96555
B	80	MLY	LYS	modified residue	UNP O96555
B	92	MLY	LYS	modified residue	UNP O96555
B	119	MLY	LYS	modified residue	UNP O96555
B	127	MLY	LYS	modified residue	UNP O96555
B	128	MLY	LYS	modified residue	UNP O96555
B	131	MLY	LYS	modified residue	UNP O96555
B	140	MLY	LYS	modified residue	UNP O96555
B	149	MLY	LYS	modified residue	UNP O96555
B	156	MLY	LYS	modified residue	UNP O96555
B	167	MLY	LYS	modified residue	UNP O96555
B	169	MLY	LYS	modified residue	UNP O96555
B	174	GLY	-	expression tag	UNP O96555
B	175	PRO	-	expression tag	UNP O96555
B	176	HIS	-	expression tag	UNP O96555
B	177	HIS	-	expression tag	UNP O96555
B	178	HIS	-	expression tag	UNP O96555
B	179	HIS	-	expression tag	UNP O96555
B	180	HIS	-	expression tag	UNP O96555
B	181	HIS	-	expression tag	UNP O96555

- Molecule 2 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total Yb 7 7	0	0
2	B	2	Total Yb 2 2	0	0

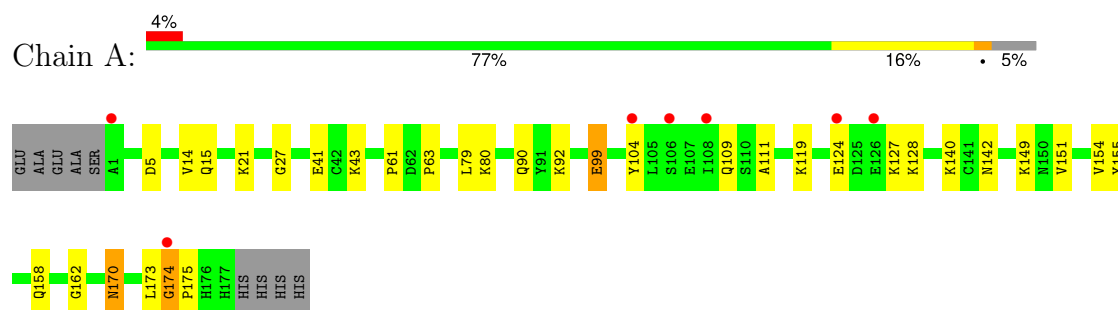
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	54	Total O 54 54	0	0
3	B	34	Total O 34 34	0	0

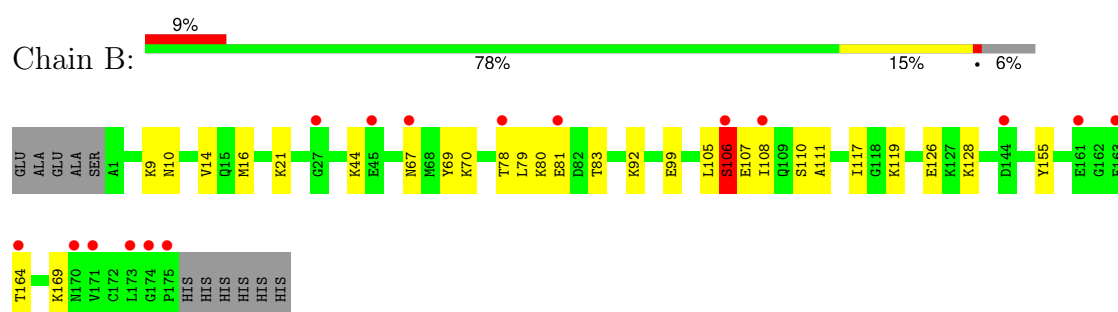
3 Residue-property plots

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: ookinete surface protein Pvs25



- Molecule 1: ookinete surface protein Pvs25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.16Å 43.70Å 65.65Å 90.00° 103.15° 90.00°	Depositor
Resolution (Å)	28.60 – 2.00 28.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.60-2.00) 98.7 (28.60-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.244 , 0.276 0.239 , 0.245	Depositor DCC
R_{free} test set	1095 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2829	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.53% 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, YB

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	0.63	0/1195	0.69	0/1625
1	B	0.61	0/1173	0.69	0/1595
All	All	0.62	0/2368	0.69	0/3220

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	1376	0	1306	24	0
1	B	1356	0	1293	19	1
2	A	7	0	0	0	0
2	B	2	0	0	0	1
3	A	54	0	0	2	0
3	B	34	0	0	1	0
All	All	2829	0	2599	41	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (41) 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:B:126:GLU:OE2	1:B:128:MLY:HE2	1.69	0.92
1:B:78:THR:HB	3:B:210:HOH:O	1.72	0.87
1:A:128:MLY:HH13	3:A:199:HOH:O	1.79	0.82
1:B:80:MLY:HE3	1:B:81:GLU:OE2	1.78	0.82
1:A:80:MLY:HE3	1:A:90:GLN:O	1.94	0.68
1:A:104:TYR:CE1	1:A:109:GLN:HG2	2.34	0.62
1:B:105:LEU:O	1:B:106:SER:C	2.39	0.60
1:A:5:ASP:OD1	1:A:140:MLY:HH13	2.02	0.59
1:B:105:LEU:O	1:B:106:SER:O	2.20	0.59
1:B:21:MLY:HH22	1:B:99:GLU:OE2	2.03	0.57
1:A:173:LEU:O	1:A:174:GLY:O	2.24	0.56
1:B:92:MLY:HG2	1:B:111:ALA:HB1	1.91	0.53
1:A:92:MLY:HG2	1:A:111:ALA:HB1	1.90	0.52
1:A:14:VAL:HB	1:A:154:VAL:HG22	1.93	0.51
1:B:117:ILE:HG12	1:B:155:TYR:CE2	2.48	0.48
1:A:27:GLY:O	3:A:198:HOH:O	2.20	0.47
1:B:78:THR:HG22	1:B:79:LEU:N	2.29	0.47
1:B:16:MET:SD	1:B:21:MLY:HE3	2.55	0.47
1:B:169:MLY:HH13	1:B:169:MLY:HD2	1.70	0.47
1:A:61:PRO:O	1:A:63:PRO:HD3	2.15	0.46
1:A:15:GLN:HB3	1:A:155:TYR:HB2	1.98	0.46
1:A:21:MLY:HH13	1:A:99:GLU:OE2	2.16	0.46
1:B:9:MLY:HD2	1:B:10:ASN:OD1	2.16	0.46
1:B:80:MLY:HH22	1:B:81:GLU:OE2	2.15	0.45
1:A:41:GLU:HB2	1:A:43:MLY:HH12	1.97	0.45
1:A:149:MLY:HH12	1:B:108:ILE:HD11	1.99	0.45
1:A:14:VAL:CG2	1:A:154:VAL:HG21	2.46	0.44
1:A:162:GLY:O	1:A:175:PRO:HA	2.17	0.44
1:A:151:VAL:O	1:A:154:VAL:HG12	2.18	0.44
1:B:67:ASN:ND2	1:B:69:TYR:O	2.50	0.44
1:A:149:MLY:HH22	1:A:158:GLN:OE1	2.17	0.43
1:A:92:MLY:HG2	1:A:111:ALA:CB	2.49	0.43
1:A:170:ASN:HD22	1:A:170:ASN:C	2.21	0.43
1:A:124:GLU:O	1:A:124:GLU:HG2	2.19	0.43
1:A:149:MLY:HE3	1:B:108:ILE:HG12	2.00	0.43
1:A:92:MLY:HH11	1:A:127:MLY:HB3	2.01	0.42
1:B:21:MLY:HH23	1:B:21:MLY:HD3	1.83	0.42
1:A:14:VAL:HG21	1:A:154:VAL:HG21	2.02	0.42
1:B:119:MLY:HH22	1:B:119:MLY:HD2	1.81	0.41
1:B:70:MLY:HD3	1:B:70:MLY:HH22	1.67	0.40
1:A:149:MLY:HH22	1:A:149:MLY:HD3	1.70	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLU:OE1	2:B:182:YB:YB[2_645]	1.96	0.24

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	157/186 (84%)	150 (96%)	5 (3%)	2 (1%)	10	5
1	B	155/186 (83%)	148 (96%)	6 (4%)	1 (1%)	22	17
All	All	312/372 (84%)	298 (96%)	11 (4%)	3 (1%)	13	8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	GLY
1	B	106	SER
1	A	142	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	138/145 (95%)	135 (98%)	3 (2%)	47	51
1	B	136/145 (94%)	130 (96%)	6 (4%)	24	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	274/290 (94%)	265 (97%)	9 (3%)	33	33

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	99	GLU
1	A	170	ASN
1	B	14	VAL
1	B	83	THR
1	B	106	SER
1	B	107	GLU
1	B	110	SER
1	B	164	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	B	18	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

36 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	49	1	9,10,11	0.60	0	6,11,13	0.61	0
1	MLY	B	9	1	9,10,11	0.58	0	6,11,13	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	B	44	1	9,10,11	0.52	0	6,11,13	1.11	1 (16%)
1	MLY	B	92	1	9,10,11	0.53	0	6,11,13	0.83	0
1	MLY	B	43	1	9,10,11	0.67	0	6,11,13	0.85	0
1	MLY	A	119	1	9,10,11	0.66	0	6,11,13	1.22	1 (16%)
1	MLY	B	70	1	9,10,11	0.61	0	6,11,13	0.52	0
1	MLY	B	128	1	9,10,11	0.50	0	6,11,13	0.59	0
1	MLY	B	167	1	9,10,11	0.53	0	6,11,13	0.77	0
1	MLY	B	80	1	9,10,11	0.65	0	6,11,13	0.63	0
1	MLY	A	127	1	9,10,11	0.53	0	6,11,13	0.81	0
1	MLY	B	119	1	9,10,11	0.63	0	6,11,13	0.51	0
1	MLY	B	127	1	9,10,11	0.62	0	6,11,13	0.73	0
1	MLY	A	156	1	9,10,11	0.62	0	6,11,13	0.85	0
1	MLY	A	21	1	9,10,11	0.74	0	6,11,13	0.58	0
1	MLY	A	167	1	9,10,11	0.69	0	6,11,13	0.93	0
1	MLY	A	131	1	9,10,11	0.50	0	6,11,13	0.90	0
1	MLY	B	131	1	9,10,11	0.59	0	6,11,13	0.88	0
1	MLY	A	44	1	9,10,11	0.52	0	6,11,13	0.91	0
1	MLY	B	149	1	9,10,11	0.57	0	6,11,13	0.82	0
1	MLY	A	39	1	9,10,11	0.57	0	6,11,13	0.78	0
1	MLY	A	43	1	9,10,11	0.59	0	6,11,13	0.45	0
1	MLY	B	140	1	9,10,11	0.51	0	6,11,13	0.83	0
1	MLY	A	149	1	9,10,11	0.59	0	6,11,13	1.02	0
1	MLY	A	9	1	9,10,11	0.45	0	6,11,13	0.65	0
1	MLY	A	70	1	9,10,11	0.90	0	6,11,13	1.05	0
1	MLY	B	39	1	9,10,11	0.57	0	6,11,13	0.94	0
1	MLY	A	92	1	9,10,11	0.74	0	6,11,13	0.72	0
1	MLY	A	169	1	9,10,11	0.57	0	6,11,13	1.02	0
1	MLY	B	169	1	9,10,11	0.62	0	6,11,13	0.33	0
1	MLY	B	21	1	9,10,11	0.78	0	6,11,13	0.54	0
1	MLY	A	80	1	9,10,11	0.73	0	6,11,13	0.57	0
1	MLY	A	140	1	9,10,11	0.62	0	6,11,13	0.54	0
1	MLY	A	128	1	9,10,11	0.60	0	6,11,13	0.74	0
1	MLY	B	156	1	9,10,11	0.52	0	6,11,13	0.70	0
1	MLY	B	49	1	9,10,11	0.49	0	6,11,13	0.96	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	49	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	9	1	-	3/8/9/11	-
1	MLY	B	44	1	-	2/8/9/11	-
1	MLY	B	92	1	-	5/8/9/11	-
1	MLY	B	43	1	-	4/8/9/11	-
1	MLY	A	119	1	-	3/8/9/11	-
1	MLY	B	70	1	-	2/8/9/11	-
1	MLY	B	128	1	-	1/8/9/11	-
1	MLY	B	167	1	-	6/8/9/11	-
1	MLY	B	80	1	-	1/8/9/11	-
1	MLY	A	127	1	-	1/8/9/11	-
1	MLY	B	119	1	-	7/8/9/11	-
1	MLY	B	127	1	-	5/8/9/11	-
1	MLY	A	156	1	-	3/8/9/11	-
1	MLY	A	21	1	-	3/8/9/11	-
1	MLY	A	167	1	-	3/8/9/11	-
1	MLY	A	131	1	-	2/8/9/11	-
1	MLY	B	131	1	-	2/8/9/11	-
1	MLY	A	44	1	-	0/8/9/11	-
1	MLY	B	149	1	-	4/8/9/11	-
1	MLY	A	39	1	-	3/8/9/11	-
1	MLY	A	43	1	-	2/8/9/11	-
1	MLY	B	140	1	-	3/8/9/11	-
1	MLY	A	149	1	-	1/8/9/11	-
1	MLY	A	9	1	-	5/8/9/11	-
1	MLY	A	70	1	-	3/8/9/11	-
1	MLY	B	39	1	-	4/8/9/11	-
1	MLY	A	92	1	-	6/8/9/11	-
1	MLY	A	169	1	-	1/8/9/11	-
1	MLY	B	169	1	-	4/8/9/11	-
1	MLY	B	21	1	-	2/8/9/11	-
1	MLY	A	80	1	-	2/8/9/11	-
1	MLY	A	140	1	-	2/8/9/11	-
1	MLY	A	128	1	-	2/8/9/11	-
1	MLY	B	156	1	-	4/8/9/11	-
1	MLY	B	49	1	-	3/8/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	MLY	CD-CE-NZ	-2.49	107.27	113.71
1	A	119	MLY	CD-CE-NZ	-2.43	107.44	113.71

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	70	MLY	N-CA-CB-CG
1	A	70	MLY	C-CA-CB-CG
1	A	92	MLY	N-CA-CB-CG
1	A	92	MLY	C-CA-CB-CG
1	A	127	MLY	O-C-CA-CB
1	A	140	MLY	O-C-CA-CB
1	B	39	MLY	O-C-CA-CB
1	B	92	MLY	C-CA-CB-CG
1	B	119	MLY	N-CA-CB-CG
1	B	119	MLY	C-CA-CB-CG
1	B	127	MLY	O-C-CA-CB
1	B	140	MLY	O-C-CA-CB
1	B	149	MLY	O-C-CA-CB
1	B	156	MLY	N-CA-CB-CG
1	B	156	MLY	C-CA-CB-CG
1	B	167	MLY	N-CA-CB-CG
1	B	167	MLY	C-CA-CB-CG
1	A	9	MLY	CD-CE-NZ-CH2
1	A	92	MLY	CD-CE-NZ-CH1
1	A	92	MLY	CD-CE-NZ-CH2
1	A	119	MLY	CD-CE-NZ-CH1
1	A	119	MLY	CD-CE-NZ-CH2
1	A	156	MLY	CD-CE-NZ-CH1
1	B	39	MLY	CD-CE-NZ-CH1
1	B	43	MLY	CD-CE-NZ-CH1
1	B	43	MLY	CD-CE-NZ-CH2
1	B	49	MLY	CD-CE-NZ-CH2
1	B	92	MLY	CD-CE-NZ-CH1
1	B	127	MLY	CD-CE-NZ-CH2
1	B	167	MLY	CD-CE-NZ-CH1
1	B	167	MLY	CD-CE-NZ-CH2
1	B	39	MLY	CG-CD-CE-NZ
1	A	9	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	A	49	MLY	CD-CE-NZ-CH2
1	A	156	MLY	CD-CE-NZ-CH2
1	A	167	MLY	CD-CE-NZ-CH1
1	B	39	MLY	CD-CE-NZ-CH2
1	B	49	MLY	CD-CE-NZ-CH1
1	B	92	MLY	CD-CE-NZ-CH2
1	B	119	MLY	CD-CE-NZ-CH1
1	B	127	MLY	CD-CE-NZ-CH1
1	B	131	MLY	CD-CE-NZ-CH1
1	B	131	MLY	CD-CE-NZ-CH2
1	B	119	MLY	CG-CD-CE-NZ
1	B	169	MLY	CG-CD-CE-NZ
1	A	128	MLY	CD-CE-NZ-CH1
1	B	21	MLY	CD-CE-NZ-CH2
1	B	119	MLY	CD-CE-NZ-CH2
1	B	169	MLY	CD-CE-NZ-CH1
1	B	21	MLY	CG-CD-CE-NZ
1	A	167	MLY	CG-CD-CE-NZ
1	A	92	MLY	CG-CD-CE-NZ
1	B	70	MLY	CG-CD-CE-NZ
1	A	39	MLY	CD-CE-NZ-CH1
1	A	39	MLY	CD-CE-NZ-CH2
1	A	49	MLY	CD-CE-NZ-CH1
1	A	128	MLY	CD-CE-NZ-CH2
1	B	70	MLY	CD-CE-NZ-CH2
1	B	128	MLY	CD-CE-NZ-CH1
1	B	149	MLY	CD-CE-NZ-CH2
1	B	156	MLY	CG-CD-CE-NZ
1	B	119	MLY	CA-CB-CG-CD
1	B	167	MLY	CG-CD-CE-NZ
1	A	149	MLY	CD-CE-NZ-CH2
1	A	43	MLY	CE-CD-CG-CB
1	B	140	MLY	CG-CD-CE-NZ
1	B	149	MLY	CD-CE-NZ-CH1
1	A	21	MLY	CE-CD-CG-CB
1	B	43	MLY	CE-CD-CG-CB
1	B	127	MLY	CG-CD-CE-NZ
1	A	131	MLY	CE-CD-CG-CB
1	B	9	MLY	CA-CB-CG-CD
1	B	156	MLY	CE-CD-CG-CB
1	A	70	MLY	CE-CD-CG-CB
1	B	140	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	B	149	MLY	CE-CD-CG-CB
1	B	167	MLY	CE-CD-CG-CB
1	A	9	MLY	CE-CD-CG-CB
1	B	92	MLY	CA-CB-CG-CD
1	B	169	MLY	CE-CD-CG-CB
1	A	92	MLY	CA-CB-CG-CD
1	A	39	MLY	CG-CD-CE-NZ
1	A	156	MLY	CE-CD-CG-CB
1	B	44	MLY	CE-CD-CG-CB
1	B	9	MLY	CG-CD-CE-NZ
1	B	119	MLY	CE-CD-CG-CB
1	A	119	MLY	CA-CB-CG-CD
1	A	167	MLY	CE-CD-CG-CB
1	B	169	MLY	C-CA-CB-CG
1	A	80	MLY	CE-CD-CG-CB
1	B	92	MLY	N-CA-CB-CG
1	B	80	MLY	CA-CB-CG-CD
1	A	43	MLY	CD-CE-NZ-CH2
1	B	49	MLY	CE-CD-CG-CB
1	B	44	MLY	CA-CB-CG-CD
1	B	9	MLY	CE-CD-CG-CB
1	B	43	MLY	CG-CD-CE-NZ
1	A	140	MLY	CE-CD-CG-CB
1	A	21	MLY	CG-CD-CE-NZ
1	B	127	MLY	CA-CB-CG-CD
1	A	131	MLY	CD-CE-NZ-CH2
1	A	169	MLY	C-CA-CB-CG
1	A	9	MLY	CA-CB-CG-CD
1	A	21	MLY	CA-CB-CG-CD
1	A	9	MLY	CG-CD-CE-NZ
1	A	80	MLY	CA-CB-CG-CD

There are no ring outliers.

16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	9	MLY	1	0
1	B	92	MLY	1	0
1	B	70	MLY	1	0
1	B	128	MLY	1	0
1	B	80	MLY	2	0
1	A	127	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	119	MLY	1	0
1	A	21	MLY	1	0
1	A	43	MLY	1	0
1	A	149	MLY	4	0
1	A	92	MLY	3	0
1	B	169	MLY	1	0
1	B	21	MLY	3	0
1	A	80	MLY	1	0
1	A	140	MLY	1	0
1	A	128	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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

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, 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	159/186 (85%)	0.45	7 (4%) 39 38	17, 29, 41, 52	0
1	B	157/186 (84%)	0.80	16 (10%) 13 12	21, 34, 61, 65	0
All	All	316/372 (84%)	0.62	23 (7%) 22 21	17, 30, 52, 65	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	SER	7.9
1	A	124	GLU	6.0
1	A	174	GLY	3.9
1	B	164	THR	3.8
1	A	1	ALA	3.6
1	B	161	GLU	3.0
1	A	126	GLU	2.7
1	B	170	ASN	2.7
1	B	173	LEU	2.6
1	B	78	THR	2.5
1	B	27	GLY	2.4
1	B	108	ILE	2.4
1	A	106	SER	2.3
1	B	45	GLU	2.3
1	B	175	PRO	2.2
1	B	171	VAL	2.2
1	A	108	ILE	2.2
1	B	81	GLU	2.2
1	A	104	TYR	2.2
1	B	67	ASN	2.2
1	B	163	PHE	2.1
1	B	174	GLY	2.1
1	B	144	ASP	2.1

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, 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	B	167	11/12	0.71	0.17	64,64,66,66	0
1	MLY	B	169	11/12	0.71	0.14	64,64,64,64	0
1	MLY	A	80	11/12	0.77	0.17	34,35,43,43	0
1	MLY	A	149	11/12	0.77	0.14	28,30,40,41	0
1	MLY	A	167	11/12	0.78	0.14	29,31,42,42	0
1	MLY	B	127	11/12	0.78	0.15	37,38,51,51	0
1	MLY	B	131	11/12	0.81	0.18	39,40,46,47	0
1	MLY	A	140	11/12	0.83	0.12	27,30,36,36	0
1	MLY	B	80	11/12	0.83	0.14	34,36,39,40	0
1	MLY	B	156	11/12	0.84	0.10	35,37,41,41	0
1	MLY	A	49	11/12	0.84	0.15	26,28,38,38	0
1	MLY	B	92	11/12	0.84	0.13	38,38,41,42	0
1	MLY	A	43	11/12	0.85	0.12	29,31,40,40	0
1	MLY	A	119	11/12	0.85	0.14	19,22,40,41	0
1	MLY	B	119	11/12	0.86	0.10	33,34,40,41	0
1	MLY	B	70	11/12	0.86	0.13	26,29,40,41	0
1	MLY	B	149	11/12	0.87	0.14	41,42,46,46	0
1	MLY	A	39	11/12	0.87	0.11	24,27,36,36	0
1	MLY	A	92	11/12	0.87	0.12	29,31,38,39	0
1	MLY	A	70	11/12	0.87	0.13	30,31,41,41	0
1	MLY	A	169	11/12	0.88	0.09	27,28,31,33	0
1	MLY	B	39	11/12	0.88	0.10	27,28,42,43	0
1	MLY	A	156	11/12	0.88	0.10	23,25,39,39	0
1	MLY	B	21	11/12	0.89	0.09	23,25,32,33	0
1	MLY	A	9	11/12	0.89	0.15	23,25,39,40	0
1	MLY	B	128	11/12	0.89	0.12	33,35,36,36	0
1	MLY	B	43	11/12	0.89	0.10	33,35,41,41	0
1	MLY	B	140	11/12	0.89	0.09	36,37,38,38	0
1	MLY	B	44	11/12	0.89	0.12	34,34,37,38	0
1	MLY	A	21	11/12	0.89	0.13	20,23,34,36	0
1	MLY	A	127	11/12	0.89	0.14	21,24,39,39	0
1	MLY	A	44	11/12	0.89	0.10	27,29,30,30	0
1	MLY	A	131	11/12	0.91	0.09	23,24,27,28	0
1	MLY	B	49	11/12	0.91	0.13	24,25,34,36	0
1	MLY	B	9	11/12	0.93	0.08	26,26,38,38	0
1	MLY	A	128	11/12	0.93	0.08	20,22,26,27	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	YB	A	185	1/1	0.95	0.06	61,61,61,61	0
2	YB	A	186	1/1	0.96	0.06	65,65,65,65	0
2	YB	A	188	1/1	0.96	0.04	50,50,50,50	0
2	YB	A	187	1/1	0.97	0.05	62,62,62,62	0
2	YB	A	184	1/1	0.97	0.05	53,53,53,53	0
2	YB	A	182	1/1	0.98	0.03	21,21,21,21	0
2	YB	B	182	1/1	0.98	0.03	30,30,30,30	0
2	YB	B	183	1/1	0.98	0.14	75,75,75,75	0
2	YB	A	183	1/1	0.99	0.03	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.