



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:49 AM UTC

PDB ID : 2F4I / pdb_00002f4i
Title : Crystal structure of an ob-fold protein (tm0957) from thermotoga maritima msb8 at 1.90 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-11-23
Resolution : 2.25 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

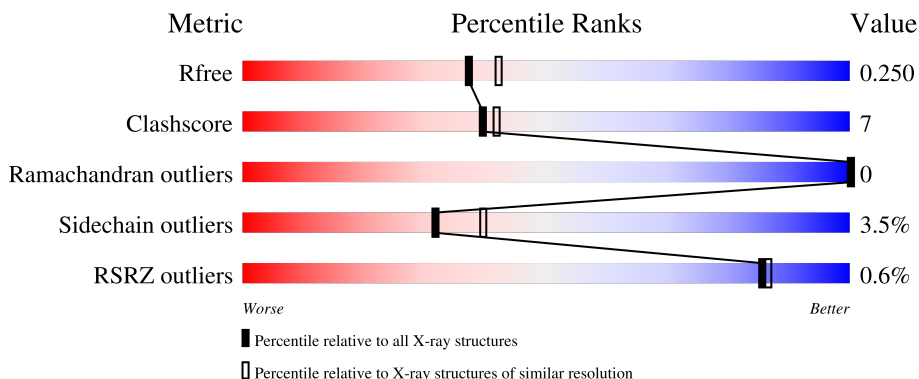
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	197	 77% 11% • 11%
1	B	197	 80% 9% • 10%
1	C	197	 76% 13% • 10%
1	D	197	 69% 20% • 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6251 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 hypothetical protein TM0957.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	176	1428	933	227	265	3	0	6	0
1	B	178	1453	946	234	270	3	0	7	0
1	C	177	1466	954	242	266	4	0	9	0
1	D	176	1416	922	229	262	3	0	4	0

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP Q9X052
A	-10	GLY	-	expression tag	UNP Q9X052
A	-9	SER	-	expression tag	UNP Q9X052
A	-8	ASP	-	expression tag	UNP Q9X052
A	-7	MLY	-	expression tag	UNP Q9X052
A	-6	ILE	-	expression tag	UNP Q9X052
A	-5	HIS	-	expression tag	UNP Q9X052
A	-4	HIS	-	expression tag	UNP Q9X052
A	-3	HIS	-	expression tag	UNP Q9X052
A	-2	HIS	-	expression tag	UNP Q9X052
A	-1	HIS	-	expression tag	UNP Q9X052
A	0	HIS	-	expression tag	UNP Q9X052
A	35	MSE	MET	modified residue	UNP Q9X052
A	37	MLY	LYS	modified residue	UNP Q9X052
A	42	MLY	LYS	modified residue	UNP Q9X052
A	51	MLY	LYS	modified residue	UNP Q9X052
A	55	MSE	MET	modified residue	UNP Q9X052
A	56	MSE	MET	modified residue	UNP Q9X052
A	81	MLY	LYS	modified residue	UNP Q9X052
A	84	MLY	LYS	modified residue	UNP Q9X052
A	106	MLY	LYS	modified residue	UNP Q9X052

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	MLY	LYS	modified residue	UNP Q9X052
A	119	MLY	LYS	modified residue	UNP Q9X052
A	142	MLY	LYS	modified residue	UNP Q9X052
A	143	MSE	MET	modified residue	UNP Q9X052
A	161	MLY	LYS	modified residue	UNP Q9X052
A	164	MLY	LYS	modified residue	UNP Q9X052
A	173	MLY	LYS	modified residue	UNP Q9X052
A	177	MLY	LYS	modified residue	UNP Q9X052
A	196	MLY	LYS	modified residue	UNP Q9X052
A	201	MLY	LYS	modified residue	UNP Q9X052
B	-11	MSE	-	expression tag	UNP Q9X052
B	-10	GLY	-	expression tag	UNP Q9X052
B	-9	SER	-	expression tag	UNP Q9X052
B	-8	ASP	-	expression tag	UNP Q9X052
B	-7	MLY	-	expression tag	UNP Q9X052
B	-6	ILE	-	expression tag	UNP Q9X052
B	-5	HIS	-	expression tag	UNP Q9X052
B	-4	HIS	-	expression tag	UNP Q9X052
B	-3	HIS	-	expression tag	UNP Q9X052
B	-2	HIS	-	expression tag	UNP Q9X052
B	-1	HIS	-	expression tag	UNP Q9X052
B	0	HIS	-	expression tag	UNP Q9X052
B	35	MSE	MET	modified residue	UNP Q9X052
B	37	MLY	LYS	modified residue	UNP Q9X052
B	42	MLY	LYS	modified residue	UNP Q9X052
B	51	MLY	LYS	modified residue	UNP Q9X052
B	55	MSE	MET	modified residue	UNP Q9X052
B	56	MSE	MET	modified residue	UNP Q9X052
B	81	MLY	LYS	modified residue	UNP Q9X052
B	84	MLY	LYS	modified residue	UNP Q9X052
B	106	MLY	LYS	modified residue	UNP Q9X052
B	113	MLY	LYS	modified residue	UNP Q9X052
B	119	MLY	LYS	modified residue	UNP Q9X052
B	142	MLY	LYS	modified residue	UNP Q9X052
B	143	MSE	MET	modified residue	UNP Q9X052
B	161	MLY	LYS	modified residue	UNP Q9X052
B	164	MLY	LYS	modified residue	UNP Q9X052
B	173	MLY	LYS	modified residue	UNP Q9X052
B	177	MLY	LYS	modified residue	UNP Q9X052
B	196	MLY	LYS	modified residue	UNP Q9X052
B	201	MLY	LYS	modified residue	UNP Q9X052
C	-11	MSE	-	expression tag	UNP Q9X052

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	expression tag	UNP Q9X052
C	-9	SER	-	expression tag	UNP Q9X052
C	-8	ASP	-	expression tag	UNP Q9X052
C	-7	MLY	-	expression tag	UNP Q9X052
C	-6	ILE	-	expression tag	UNP Q9X052
C	-5	HIS	-	expression tag	UNP Q9X052
C	-4	HIS	-	expression tag	UNP Q9X052
C	-3	HIS	-	expression tag	UNP Q9X052
C	-2	HIS	-	expression tag	UNP Q9X052
C	-1	HIS	-	expression tag	UNP Q9X052
C	0	HIS	-	expression tag	UNP Q9X052
C	35	MSE	MET	modified residue	UNP Q9X052
C	37	MLY	LYS	modified residue	UNP Q9X052
C	42	MLY	LYS	modified residue	UNP Q9X052
C	51	MLY	LYS	modified residue	UNP Q9X052
C	55	MSE	MET	modified residue	UNP Q9X052
C	56	MSE	MET	modified residue	UNP Q9X052
C	81	MLY	LYS	modified residue	UNP Q9X052
C	84	MLY	LYS	modified residue	UNP Q9X052
C	106	MLY	LYS	modified residue	UNP Q9X052
C	113	MLY	LYS	modified residue	UNP Q9X052
C	119	MLY	LYS	modified residue	UNP Q9X052
C	142	MLY	LYS	modified residue	UNP Q9X052
C	143	MSE	MET	modified residue	UNP Q9X052
C	161	MLY	LYS	modified residue	UNP Q9X052
C	164	MLY	LYS	modified residue	UNP Q9X052
C	173	MLY	LYS	modified residue	UNP Q9X052
C	177	MLY	LYS	modified residue	UNP Q9X052
C	196	MLY	LYS	modified residue	UNP Q9X052
C	201	MLY	LYS	modified residue	UNP Q9X052
D	-11	MSE	-	expression tag	UNP Q9X052
D	-10	GLY	-	expression tag	UNP Q9X052
D	-9	SER	-	expression tag	UNP Q9X052
D	-8	ASP	-	expression tag	UNP Q9X052
D	-7	MLY	-	expression tag	UNP Q9X052
D	-6	ILE	-	expression tag	UNP Q9X052
D	-5	HIS	-	expression tag	UNP Q9X052
D	-4	HIS	-	expression tag	UNP Q9X052
D	-3	HIS	-	expression tag	UNP Q9X052
D	-2	HIS	-	expression tag	UNP Q9X052
D	-1	HIS	-	expression tag	UNP Q9X052
D	0	HIS	-	expression tag	UNP Q9X052

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	35	MSE	MET	modified residue	UNP Q9X052
D	37	MLY	LYS	modified residue	UNP Q9X052
D	42	MLY	LYS	modified residue	UNP Q9X052
D	51	MLY	LYS	modified residue	UNP Q9X052
D	55	MSE	MET	modified residue	UNP Q9X052
D	56	MSE	MET	modified residue	UNP Q9X052
D	81	MLY	LYS	modified residue	UNP Q9X052
D	84	MLY	LYS	modified residue	UNP Q9X052
D	106	MLY	LYS	modified residue	UNP Q9X052
D	113	MLY	LYS	modified residue	UNP Q9X052
D	119	MLY	LYS	modified residue	UNP Q9X052
D	142	MLY	LYS	modified residue	UNP Q9X052
D	143	MSE	MET	modified residue	UNP Q9X052
D	161	MLY	LYS	modified residue	UNP Q9X052
D	164	MLY	LYS	modified residue	UNP Q9X052
D	173	MLY	LYS	modified residue	UNP Q9X052
D	177	MLY	LYS	modified residue	UNP Q9X052
D	196	MLY	LYS	modified residue	UNP Q9X052
D	201	MLY	LYS	modified residue	UNP Q9X052

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	118	Total O 118 118	0	0
4	B	134	Total O 134 134	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	143	Total 143	O 143	0	0
4	D	89	Total 89	O 89	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.68Å 78.08Å 82.49Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	29.83 – 2.25 29.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.83-2.25) 99.8 (29.83-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.248 0.195 , 0.250	Depositor DCC
R_{free} test set	1989 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtrriage
Anisotropy	0.425	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6251	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, MLY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	0/1342	0.91	1/1825 (0.1%)
1	B	0.89	1/1372 (0.1%)	0.87	0/1863
1	C	0.94	0/1384	0.87	0/1876
1	D	0.85	2/1329 (0.2%)	0.87	0/1805
All	All	0.92	3/5427 (0.1%)	0.88	1/7369 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	129	ILE	CA-CB	6.45	1.61	1.53
1	B	207	ILE	CA-CB	5.38	1.59	1.53
1	D	207	ILE	CA-CB	5.02	1.59	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	SER	N-CA-C	5.11	116.69	110.41

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	1428	0	1398	23	0
1	B	1453	0	1423	9	0
1	C	1466	0	1456	16	0
1	D	1416	0	1381	29	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	118	0	0	1	0
4	B	134	0	0	0	0
4	C	143	0	0	1	0
4	D	89	0	0	0	0
All	All	6251	0	5658	77	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 7.

The worst 5 of 77 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:164:MLY:HH23	1:A:169:ASN:HD21	1.08	1.16
1:A:56:MSE:HE1	1:A:209:LEU:CB	1.80	1.09
1:A:56:MSE:HE1	1:A:209:LEU:HB2	1.40	1.01
1:A:164:MLY:HH23	1:A:169:ASN:ND2	1.86	0.90
1:D:110:ILE:HD13	1:D:112:VAL:CG2	2.06	0.85

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	165/197 (84%)	163 (99%)	2 (1%)	0	100	100
1	B	169/197 (86%)	167 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	168/197 (85%)	167 (99%)	1 (1%)	0	100	100
1	D	164/197 (83%)	161 (98%)	3 (2%)	0	100	100
All	All	666/788 (84%)	658 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	141/150 (94%)	137 (97%)	4 (3%)	38	48
1	B	145/150 (97%)	138 (95%)	7 (5%)	23	25
1	C	147/150 (98%)	143 (97%)	4 (3%)	39	49
1	D	139/150 (93%)	131 (94%)	8 (6%)	18	19
All	All	572/600 (95%)	549 (96%)	23 (4%)	32	34

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	214[B]	GLN
1	D	143	MSE
1	D	117[B]	ASN
1	D	144	GLU
1	B	112	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	53	GLN
1	D	53	GLN
1	D	97	GLN
1	B	97	GLN
1	A	53	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

59 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	D	142	1	4,5,11	0.86	0	1,5,13	0.03	0
1	MLY	A	81[B]	-	9,10,11	1.03	0	6,11,13	0.96	0
1	MLY	B	177	1	9,10,11	0.53	0	6,11,13	0.62	0
1	MLY	B	119	1	5,6,11	0.68	0	2,6,13	0.42	0
1	MLY	B	113	1	9,10,11	0.60	0	6,11,13	0.71	0
1	MLY	B	173	1	7,8,11	1.05	0	3,8,13	0.26	0
1	MLY	A	51	1	7,8,11	0.88	0	3,8,13	0.66	0
1	MLY	D	42	1	9,10,11	1.13	1 (11%)	6,11,13	1.10	1 (16%)
1	MLY	C	106	1	9,10,11	0.82	0	6,11,13	0.76	0
1	MLY	B	161	1	7,8,11	0.68	0	3,8,13	0.73	0
1	MLY	D	84	1	9,10,11	0.91	0	6,11,13	1.20	0
1	MLY	A	113	1	7,8,11	1.41	1 (14%)	3,8,13	0.54	0
1	MLY	A	177	1	6,7,11	0.81	0	2,7,13	0.26	0
1	MLY	A	106	1	7,8,11	0.61	0	3,8,13	1.04	0
1	MLY	D	161	1	7,8,11	0.66	0	3,8,13	0.34	0
1	MLY	C	173	1	9,10,11	1.25	1 (11%)	6,11,13	0.59	0
1	MLY	D	81	1	6,7,11	0.69	0	2,7,13	0.40	0
1	MLY	B	81	1	7,8,11	0.64	0	3,8,13	0.31	0
1	MLY	A	119	1	5,6,11	0.83	0	2,6,13	0.43	0
1	MLY	A	164	1	9,10,11	1.38	2 (22%)	6,11,13	1.39	1 (16%)
1	MLY	B	201	1	5,6,11	0.51	0	2,6,13	0.16	0
1	MLY	D	119	1	5,6,11	0.61	0	2,6,13	0.12	0
1	MLY	D	196	1	7,8,11	0.85	0	3,8,13	0.26	0
1	MLY	B	142	1	7,8,11	0.76	0	3,8,13	0.48	0
1	MLY	C	164[A]	-	9,10,11	0.64	0	6,11,13	0.58	0
1	MLY	A	84	1	9,10,11	0.88	0	6,11,13	1.28	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	C	161	1	7,8,11	0.62	0	3,8,13	0.23	0
1	MLY	C	196	1	7,8,11	0.73	0	3,8,13	0.65	0
1	MLY	A	161	1	7,8,11	0.73	0	3,8,13	0.54	0
1	MLY	A	201	1	6,7,11	0.64	0	2,7,13	0.21	0
1	MLY	C	142	1	9,10,11	0.81	0	6,11,13	1.01	0
1	MLY	B	42	1	9,10,11	1.12	1 (11%)	6,11,13	0.63	0
1	MLY	A	173	1	7,8,11	0.72	0	3,8,13	0.39	0
1	MLY	A	81[A]	-	9,10,11	1.01	0	6,11,13	1.02	0
1	MLY	B	37	1	3,4,11	0.99	0	2,4,13	0.99	0
1	MLY	A	196	1	7,8,11	0.96	0	3,8,13	0.37	0
1	MLY	C	42	1	9,10,11	0.77	0	6,11,13	0.79	0
1	MLY	D	113	1	9,10,11	0.80	0	6,11,13	0.62	0
1	MLY	D	106	1	7,8,11	0.52	0	3,8,13	1.08	0
1	MLY	D	177	1	4,5,11	0.68	0	1,5,13	0.32	0
1	MLY	B	106	1	7,8,11	0.58	0	3,8,13	1.13	0
1	MLY	A	142	1	4,5,11	0.62	0	1,5,13	0.09	0
1	MLY	A	42	1	7,8,11	0.85	0	3,8,13	0.30	0
1	MLY	D	164	1	7,8,11	0.60	0	3,8,13	0.51	0
1	MLY	B	84	1	9,10,11	1.33	1 (11%)	6,11,13	0.39	0
1	MLY	C	81	1	7,8,11	0.63	0	3,8,13	0.61	0
1	MLY	C	113	1	7,8,11	0.72	0	3,8,13	0.49	0
1	MLY	C	177	1	7,8,11	0.88	0	3,8,13	0.12	0
1	MLY	C	119	1	5,6,11	0.81	0	2,6,13	0.13	0
1	MLY	C	201	1	5,6,11	0.75	0	2,6,13	0.31	0
1	MLY	D	201	1	6,7,11	0.53	0	2,7,13	0.21	0
1	MLY	B	164	1	6,7,11	0.62	0	2,7,13	0.15	0
1	MLY	C	84	1	7,8,11	0.62	0	3,8,13	0.40	0
1	MLY	B	51	1	5,6,11	0.88	0	2,6,13	0.84	0
1	MLY	D	173	1	7,8,11	0.44	0	3,8,13	0.24	0
1	MLY	B	196	1	7,8,11	0.74	0	3,8,13	0.50	0
1	MLY	C	164[B]	-	9,10,11	1.23	1 (11%)	6,11,13	1.30	1 (16%)
1	MLY	C	51	1	7,8,11	0.70	0	3,8,13	0.48	0
1	MLY	D	51	1	6,7,11	0.80	0	2,7,13	0.23	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	D	142	1	-	2/3/4/11	-
1	MLY	A	81[B]	-	-	4/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	177	1	-	1/8/9/11	-
1	MLY	B	119	1	-	0/4/5/11	-
1	MLY	B	113	1	-	1/8/9/11	-
1	MLY	B	173	1	-	0/6/7/11	-
1	MLY	A	51	1	-	0/6/7/11	-
1	MLY	D	42	1	-	3/8/9/11	-
1	MLY	C	106	1	-	1/8/9/11	-
1	MLY	B	161	1	-	0/6/7/11	-
1	MLY	D	84	1	-	0/8/9/11	-
1	MLY	A	113	1	-	4/6/7/11	-
1	MLY	A	177	1	-	2/5/6/11	-
1	MLY	A	106	1	-	0/6/7/11	-
1	MLY	D	161	1	-	2/6/7/11	-
1	MLY	C	173	1	-	1/8/9/11	-
1	MLY	D	81	1	-	3/5/6/11	-
1	MLY	B	81	1	-	2/6/7/11	-
1	MLY	A	119	1	-	0/4/5/11	-
1	MLY	A	164	1	-	3/8/9/11	-
1	MLY	B	201	1	-	3/4/5/11	-
1	MLY	D	119	1	-	1/4/5/11	-
1	MLY	D	196	1	-	2/6/7/11	-
1	MLY	B	142	1	-	0/6/7/11	-
1	MLY	C	164[A]	-	-	1/8/9/11	-
1	MLY	A	84	1	-	3/8/9/11	-
1	MLY	C	161	1	-	1/6/7/11	-
1	MLY	C	196	1	-	0/6/7/11	-
1	MLY	A	161	1	-	1/6/7/11	-
1	MLY	A	201	1	-	1/5/6/11	-
1	MLY	C	142	1	-	0/8/9/11	-
1	MLY	B	42	1	-	0/8/9/11	-
1	MLY	A	173	1	-	0/6/7/11	-
1	MLY	A	81[A]	-	-	4/8/9/11	-
1	MLY	B	37	1	-	0/1/2/11	-
1	MLY	A	196	1	-	1/6/7/11	-
1	MLY	C	42	1	-	2/8/9/11	-
1	MLY	D	113	1	-	3/8/9/11	-
1	MLY	D	106	1	-	0/6/7/11	-
1	MLY	D	177	1	-	0/3/4/11	-
1	MLY	B	106	1	-	0/6/7/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	142	1	-	1/3/4/11	-
1	MLY	A	42	1	-	0/6/7/11	-
1	MLY	D	164	1	-	2/6/7/11	-
1	MLY	B	84	1	-	4/8/9/11	-
1	MLY	C	81	1	-	3/6/7/11	-
1	MLY	C	113	1	-	2/6/7/11	-
1	MLY	C	177	1	-	1/6/7/11	-
1	MLY	C	119	1	-	1/4/5/11	-
1	MLY	C	201	1	-	3/4/5/11	-
1	MLY	D	201	1	-	3/5/6/11	-
1	MLY	B	164	1	-	1/5/6/11	-
1	MLY	C	84	1	-	0/6/7/11	-
1	MLY	B	51	1	-	3/4/5/11	-
1	MLY	D	173	1	-	0/6/7/11	-
1	MLY	B	196	1	-	2/6/7/11	-
1	MLY	C	164[B]	-	-	3/8/9/11	-
1	MLY	C	51	1	-	2/6/7/11	-
1	MLY	D	51	1	-	0/5/6/11	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	MLY	CE-NZ	2.84	1.56	1.46
1	C	164[B]	MLY	CE-NZ	2.82	1.56	1.46
1	C	173	MLY	CE-NZ	2.68	1.56	1.46
1	A	113	MLY	CB-CA	2.63	1.57	1.53
1	D	42	MLY	CE-NZ	2.44	1.55	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	MLY	CD-CE-NZ	3.02	121.51	113.71
1	C	164[B]	MLY	CD-CE-NZ	2.86	121.11	113.71
1	A	84	MLY	CD-CE-NZ	2.66	120.59	113.71
1	D	42	MLY	CD-CE-NZ	2.26	119.54	113.71

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	81[A]	MLY	C-CA-CB-CG
1	A	81[B]	MLY	C-CA-CB-CG
1	A	113	MLY	C-CA-CB-CG
1	A	177	MLY	C-CA-CB-CG
1	A	201	MLY	O-C-CA-CB

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	84	MLY	1	0
1	C	173	MLY	1	0
1	A	164	MLY	3	0
1	D	196	MLY	1	0
1	C	164[A]	MLY	1	0
1	C	142	MLY	1	0
1	D	113	MLY	1	0
1	C	177	MLY	1	0
1	B	196	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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

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	159/197 (80%)	-0.17	0 100 100	11, 18, 26, 32	5 (3%)
1	B	160/197 (81%)	-0.11	1 (0%) 85 86	11, 18, 26, 35	7 (4%)
1	C	160/197 (81%)	-0.08	1 (0%) 85 86	9, 18, 28, 43	7 (4%)
1	D	159/197 (80%)	0.19	2 (1%) 75 76	9, 18, 25, 31	4 (2%)
All	All	638/788 (80%)	-0.04	4 (0%) 85 86	9, 18, 27, 43	23 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	59	GLY	2.8
1	C	130	PHE	2.5
1	D	58[A]	GLU	2.2
1	B	212	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	37	5/12	0.67	0.15	32,36,38,38	0
1	MLY	D	196	9/12	0.70	0.14	18,21,21,21	0
1	MLY	D	106	9/12	0.81	0.12	19,21,25,25	0
1	MLY	D	84	11/12	0.81	0.12	17,23,28,29	0
1	MLY	C	173	11/12	0.82	0.15	19,25,32,32	0
1	MLY	D	177	6/12	0.82	0.11	19,19,21,21	0
1	MLY	B	196	9/12	0.82	0.10	18,21,22,22	0
1	MLY	C	142	11/12	0.83	0.15	16,20,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MLY	A	177	8/12	0.84	0.12	19,21,24,24	0
1	MLY	C	81	9/12	0.84	0.11	19,20,25,25	0
1	MLY	B	84	11/12	0.85	0.12	18,24,29,31	0
1	MLY	C	106	11/12	0.85	0.11	19,22,28,28	0
1	MLY	D	173	9/12	0.86	0.11	19,21,26,27	0
1	MLY	A	164	11/12	0.86	0.14	18,26,31,31	0
1	MLY	D	51	8/12	0.86	0.13	16,21,26,26	0
1	MLY	D	201	8/12	0.86	0.10	19,23,27,27	0
1	MLY	C	119	7/12	0.87	0.12	16,17,19,19	0
1	MLY	C	196	9/12	0.87	0.09	18,20,21,21	0
1	MLY	B	201	7/12	0.87	0.10	19,22,26,27	0
1	MLY	C	84	9/12	0.88	0.12	17,20,26,27	0
1	MLY	B	177	11/12	0.88	0.10	19,21,24,24	0
1	MLY	A	201	8/12	0.88	0.11	19,23,26,27	0
1	MLY	D	113	11/12	0.88	0.11	17,21,24,24	0
1	MLY	D	42	11/12	0.89	0.10	17,22,25,26	0
1	MLY	D	142	6/12	0.89	0.09	16,18,20,21	0
1	MLY	B	81	9/12	0.89	0.11	18,20,24,24	0
1	MLY	D	81	8/12	0.89	0.08	19,20,23,24	0
1	MLY	A	51	9/12	0.89	0.12	17,21,29,29	0
1	MLY	B	42	11/12	0.89	0.12	16,22,26,26	0
1	MLY	B	106	9/12	0.90	0.09	19,21,25,26	0
1	MLY	D	119	7/12	0.90	0.09	15,16,19,20	0
1	MLY	B	142	9/12	0.90	0.09	15,19,23,24	0
1	MLY	D	161	9/12	0.90	0.10	17,18,21,22	0
1	MLY	D	164	9/12	0.90	0.09	18,20,26,26	0
1	MLY	A	161	9/12	0.90	0.09	17,19,21,22	0
1	MLY	A	106	9/12	0.90	0.10	19,20,26,26	0
1	MLY	A	173	9/12	0.90	0.10	19,21,27,27	0
1	MLY	C	51	9/12	0.90	0.11	16,21,29,29	0
1	MLY	C	177	9/12	0.91	0.09	19,21,26,26	0
1	MLY	A	196	9/12	0.91	0.09	17,20,23,23	0
1	MLY	C	42	11/12	0.91	0.09	18,22,25,25	0
1	MLY	C	113	9/12	0.91	0.09	17,19,24,25	0
1	MLY	C	161	9/12	0.92	0.07	17,19,21,23	0
1	MLY	C	164[A]	11/12	0.92	0.12	18,20,20,21	7
1	MLY	C	164[B]	11/12	0.92	0.12	18,21,23,23	7
1	MLY	B	164	8/12	0.92	0.10	18,20,26,27	0
1	MLY	A	119	7/12	0.92	0.08	15,16,19,21	0
1	MLY	B	173	9/12	0.93	0.07	19,21,26,26	0
1	MLY	B	113	11/12	0.93	0.09	17,21,25,25	0
1	MLY	B	119	7/12	0.93	0.09	15,17,19,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	C	201	7/12	0.93	0.09	19,22,26,27	0
1	MLY	A	84	11/12	0.93	0.08	17,22,25,26	0
1	MLY	A	113	9/12	0.93	0.07	17,19,23,24	0
1	MLY	A	42	9/12	0.94	0.07	17,20,24,25	0
1	MLY	B	51	7/12	0.95	0.08	16,19,27,28	0
1	MLY	B	161	9/12	0.95	0.08	17,19,22,25	0
1	MLY	A	81[A]	11/12	0.95	0.11	17,19,20,20	4
1	MLY	A	81[B]	11/12	0.95	0.11	15,19,20,20	4
1	MLY	A	142	6/12	0.96	0.06	15,18,20,22	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(\AA^2)	Q<0.9
2	CL	A	1	1/1	0.88	0.11	44,44,44,44	0
2	CL	A	3	1/1	0.93	0.13	43,43,43,43	0
3	MG	C	4	1/1	0.93	0.09	32,32,32,32	0
2	CL	B	2	1/1	0.97	0.09	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.