



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 07:42 am BST

PDB ID : 2F4I
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

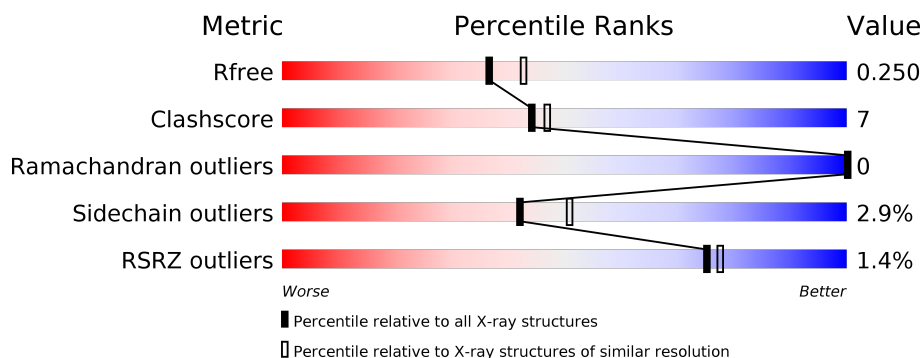
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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 on 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	<div> <div style="width: 79%;"></div> <div style="width: 10%;"></div> <div style="width: 11%;"></div> </div> <div>79% 10% 11%</div>
1	B	197	<div> <div style="width: 80%;"></div> <div style="width: 9%;"></div> <div style="width: 10%;"></div> </div> <div>80% 9% 10%</div>
1	C	197	<div> <div style="width: 76%;"></div> <div style="width: 14%;"></div> <div style="width: 10%;"></div> </div> <div>76% 14% 10%</div>
1	D	197	<div> <div style="width: 5%;"></div> <div style="width: 72%;"></div> <div style="width: 17%;"></div> <div style="width: 11%;"></div> </div> <div>5% 72% 17% 11%</div>

2 Entry composition

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

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	LEADER SEQUENCE	UNP Q9X052
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9X052
A	-9	SER	-	LEADER SEQUENCE	UNP Q9X052
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9X052
A	-7	MLY	-	LEADER SEQUENCE	UNP Q9X052
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9X052
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9X052
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9X052
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9X052
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9X052
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9X052
A	0	HIS	-	LEADER SEQUENCE	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

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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	-	LEADER SEQUENCE	UNP Q9X052
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9X052
B	-9	SER	-	LEADER SEQUENCE	UNP Q9X052
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9X052
B	-7	MLY	-	LEADER SEQUENCE	UNP Q9X052
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9X052
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9X052
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9X052
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9X052
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9X052
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9X052
B	0	HIS	-	LEADER SEQUENCE	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
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B	142	MLY	LYS	MODIFIED RESIDUE	UNP Q9X052
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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	-	LEADER SEQUENCE	UNP Q9X052

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9X052
C	-9	SER	-	LEADER SEQUENCE	UNP Q9X052
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9X052
C	-7	MLY	-	LEADER SEQUENCE	UNP Q9X052
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9X052
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9X052
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9X052
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9X052
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9X052
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9X052
C	0	HIS	-	LEADER SEQUENCE	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	-	LEADER SEQUENCE	UNP Q9X052
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9X052
D	-9	SER	-	LEADER SEQUENCE	UNP Q9X052
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9X052
D	-7	MLY	-	LEADER SEQUENCE	UNP Q9X052
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9X052
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9X052
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9X052
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9X052
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9X052
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9X052
D	0	HIS	-	LEADER SEQUENCE	UNP Q9X052

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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 (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: 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

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

- Molecule 1: hypothetical protein TM0957



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 29.85 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.83-2.25) 99.8 (29.85-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.24Å)	Xtriage
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	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6251	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage'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: MG, MLY, CL

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	0.87	0/1342	0.76	0/1825
1	B	0.78	0/1372	0.76	0/1863
1	C	0.78	0/1384	0.76	0/1876
1	D	0.70	0/1329	0.77	0/1805
All	All	0.79	0/5427	0.76	0/7369

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 [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	1397	23	0
1	B	1453	0	1423	9	0
1	C	1466	0	1455	16	0
1	D	1416	0	1380	28	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	143	0	0	1	0
4	D	89	0	0	0	0
All	All	6251	0	5655	76	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 76 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 ⓘ

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

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%)	139 (99%)	2 (1%)	67	76
1	B	145/150 (97%)	138 (95%)	7 (5%)	25	28
1	C	147/150 (98%)	144 (98%)	3 (2%)	55	64
1	D	139/150 (93%)	132 (95%)	7 (5%)	24	26
All	All	572/600 (95%)	553 (97%)	19 (3%)	42	46

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	213	ILE
1	C	149	ILE
1	D	144	GLU
1	B	198[B]	GLU
1	D	147	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	C	196	1	7,8,11	0.71	0	3,8,13	0.63	0
1	MLY	B	106	1	7,8,11	0.57	0	3,8,13	1.19	0
1	MLY	A	161	1	7,8,11	0.71	0	3,8,13	0.52	0
1	MLY	B	142	1	7,8,11	0.77	0	3,8,13	0.50	0
1	MLY	C	84	1	7,8,11	0.60	0	3,8,13	0.42	0
1	MLY	B	201	1	5,6,11	0.49	0	2,6,13	0.16	0
1	MLY	D	42	1	9,10,11	1.11	1 (11%)	6,11,13	1.06	1 (16%)
1	MLY	B	42	1	9,10,11	1.11	1 (11%)	6,11,13	0.66	0
1	MLY	B	164	1	6,7,11	0.62	0	2,7,13	0.17	0
1	MLY	C	81	1	7,8,11	0.63	0	3,8,13	0.65	0
1	MLY	D	177	1	4,5,11	0.67	0	1,5,13	0.25	0
1	MLY	A	106	1	7,8,11	0.59	0	3,8,13	1.09	0
1	MLY	A	196	1	7,8,11	0.97	0	3,8,13	0.37	0
1	MLY	C	177	1	7,8,11	0.86	0	3,8,13	0.14	0
1	MLY	D	173	1	7,8,11	0.44	0	3,8,13	0.26	0
1	MLY	A	177	1	6,7,11	0.78	0	2,7,13	0.24	0
1	MLY	B	113	1	9,10,11	0.60	0	6,11,13	0.72	0
1	MLY	C	51	1	7,8,11	0.72	0	3,8,13	0.46	0
1	MLY	A	42	1	7,8,11	0.87	0	3,8,13	0.31	0
1	MLY	A	81[B]	-	9,10,11	1.02	0	6,11,13	0.97	0
1	MLY	A	113	1	7,8,11	1.48	1 (14%)	3,8,13	0.52	0
1	MLY	A	81[A]	-	9,10,11	1.00	0	6,11,13	1.00	0
1	MLY	B	119	1	5,6,11	0.71	0	2,6,13	0.34	0
1	MLY	A	201	1	6,7,11	0.61	0	2,7,13	0.19	0
1	MLY	C	106	1	9,10,11	0.83	0	6,11,13	0.76	0
1	MLY	A	119	1	5,6,11	0.88	0	2,6,13	0.44	0
1	MLY	B	173	1	7,8,11	1.04	0	3,8,13	0.27	0
1	MLY	D	201	1	6,7,11	0.55	0	2,7,13	0.21	0
1	MLY	D	84	1	9,10,11	0.93	0	6,11,13	1.19	0
1	MLY	B	81	1	7,8,11	0.63	0	3,8,13	0.32	0
1	MLY	A	84	1	9,10,11	0.89	0	6,11,13	1.23	1 (16%)
1	MLY	C	161	1	7,8,11	0.61	0	3,8,13	0.23	0
1	MLY	C	113	1	7,8,11	0.69	0	3,8,13	0.52	0
1	MLY	D	119	1	5,6,11	0.62	0	2,6,13	0.10	0
1	MLY	B	51	1	5,6,11	0.84	0	2,6,13	0.82	0
1	MLY	B	177	1	9,10,11	0.54	0	6,11,13	0.60	0
1	MLY	D	196	1	7,8,11	0.87	0	3,8,13	0.26	0
1	MLY	C	164[B]	-	9,10,11	1.23	1 (11%)	6,11,13	1.24	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	164	1	7,8,11	0.61	0	3,8,13	0.54	0
1	MLY	A	173	1	7,8,11	0.72	0	3,8,13	0.38	0
1	MLY	D	113	1	9,10,11	0.78	0	6,11,13	0.63	0
1	MLY	D	106	1	7,8,11	0.52	0	3,8,13	1.12	0
1	MLY	A	164	1	9,10,11	1.36	2 (22%)	6,11,13	1.33	1 (16%)
1	MLY	D	81	1	6,7,11	0.67	0	2,7,13	0.41	0
1	MLY	C	164[A]	-	9,10,11	0.64	0	6,11,13	0.57	0
1	MLY	B	196	1	7,8,11	0.75	0	3,8,13	0.49	0
1	MLY	D	142	1	4,5,11	0.84	0	1,5,13	0.74	0
1	MLY	C	42	1	9,10,11	0.78	0	6,11,13	0.81	0
1	MLY	B	84	1	9,10,11	1.34	1 (11%)	6,11,13	0.39	0
1	MLY	A	51	1	7,8,11	0.85	0	3,8,13	0.69	0
1	MLY	B	161	1	7,8,11	0.66	0	3,8,13	0.73	0
1	MLY	D	51	1	6,7,11	0.82	0	2,7,13	0.22	0
1	MLY	C	119	1	5,6,11	0.85	0	2,6,13	0.09	0
1	MLY	C	142	1	9,10,11	0.81	0	6,11,13	1.02	0
1	MLY	A	142	1	4,5,11	0.60	0	1,5,13	0.49	0
1	MLY	C	201	1	5,6,11	0.71	0	2,6,13	0.29	0
1	MLY	D	161	1	7,8,11	0.65	0	3,8,13	0.35	0
1	MLY	C	173	1	9,10,11	1.23	1 (11%)	6,11,13	0.60	0
1	MLY	B	37	1	3,4,11	0.93	0	2,4,13	1.01	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	C	196	1	-	0/6/7/11	-
1	MLY	B	106	1	-	0/6/7/11	-
1	MLY	A	161	1	-	1/6/7/11	-
1	MLY	B	142	1	-	0/6/7/11	-
1	MLY	C	84	1	-	0/6/7/11	-
1	MLY	B	201	1	-	3/4/5/11	-
1	MLY	D	42	1	-	3/8/9/11	-
1	MLY	B	42	1	-	1/8/9/11	-
1	MLY	B	164	1	-	1/5/6/11	-
1	MLY	C	81	1	-	3/6/7/11	-
1	MLY	D	177	1	-	0/3/4/11	-
1	MLY	A	106	1	-	0/6/7/11	-
1	MLY	A	196	1	-	1/6/7/11	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	51	1	-	0/5/6/11	-
1	MLY	C	119	1	-	1/4/5/11	-
1	MLY	C	142	1	-	0/8/9/11	-
1	MLY	A	142	1	-	1/3/4/11	-
1	MLY	C	201	1	-	3/4/5/11	-
1	MLY	D	161	1	-	2/6/7/11	-
1	MLY	C	173	1	-	1/8/9/11	-
1	MLY	B	37	1	-	0/0/2/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	MLY	CB-CA	3.00	1.57	1.53
1	A	164	MLY	CE-NZ	2.81	1.56	1.46
1	C	164[B]	MLY	CE-NZ	2.79	1.56	1.46
1	C	173	MLY	CE-NZ	2.66	1.56	1.46
1	D	42	MLY	CE-NZ	2.42	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	2.85	121.51	113.79
1	C	164[B]	MLY	CD-CE-NZ	2.70	121.11	113.79
1	A	84	MLY	CD-CE-NZ	2.51	120.59	113.79
1	D	42	MLY	CD-CE-NZ	2.13	119.54	113.79

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	201	MLY	N-CA-CB-CG
1	B	201	MLY	C-CA-CB-CG
1	C	81	MLY	N-CA-CB-CG
1	C	81	MLY	C-CA-CB-CG
1	A	177	MLY	C-CA-CB-CG

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	177	MLY	1	0

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [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	159/197 (80%)	-0.21	0	100 100	15, 18, 26, 32	0
1	B	160/197 (81%)	-0.13	0	100 100	13, 18, 26, 35	0
1	C	160/197 (81%)	-0.13	0	100 100	12, 18, 28, 43	0
1	D	159/197 (80%)	0.23	9 (5%)	23 25	13, 18, 25, 31	0
All	All	638/788 (80%)	-0.06	9 (1%)	75 77	12, 18, 27, 43	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	39	PHE	3.6
1	D	150	ILE	3.1
1	D	79	HIS	2.9
1	D	148	ARG	2.8
1	D	59	GLY	2.6

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	D	196	9/12	0.77	0.26	18,21,21,21	0
1	MLY	B	37	5/12	0.77	0.23	32,36,38,38	0
1	MLY	D	84	11/12	0.83	0.18	17,23,28,29	0
1	MLY	B	196	9/12	0.85	0.16	18,21,22,22	0
1	MLY	C	173	11/12	0.86	0.20	19,25,32,32	0
1	MLY	A	164	11/12	0.86	0.20	18,26,31,31	0
1	MLY	A	173	9/12	0.88	0.24	19,21,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	C	142	11/12	0.88	0.18	16,20,26,26	0
1	MLY	C	196	9/12	0.89	0.14	18,20,21,21	0
1	MLY	B	84	11/12	0.90	0.17	18,24,29,31	0
1	MLY	A	177	8/12	0.90	0.26	19,21,24,24	0
1	MLY	D	113	11/12	0.91	0.19	17,21,24,24	0
1	MLY	D	173	9/12	0.91	0.20	19,21,26,27	0
1	MLY	D	51	8/12	0.91	0.18	16,21,26,26	0
1	MLY	D	142	6/12	0.92	0.18	16,18,20,21	0
1	MLY	B	201	7/12	0.92	0.14	19,22,26,27	0
1	MLY	B	164	8/12	0.92	0.15	18,20,26,27	0
1	MLY	C	51	9/12	0.92	0.17	16,21,29,29	0
1	MLY	D	201	8/12	0.92	0.13	19,23,27,27	0
1	MLY	A	106	9/12	0.92	0.12	19,20,26,26	0
1	MLY	D	106	9/12	0.93	0.11	19,21,25,25	0
1	MLY	A	201	8/12	0.93	0.14	19,23,26,27	0
1	MLY	C	164[A]	11/12	0.93	0.21	18,20,20,21	7
1	MLY	A	161	9/12	0.93	0.12	17,19,21,22	0
1	MLY	C	81	9/12	0.93	0.11	19,20,25,25	0
1	MLY	C	42	11/12	0.93	0.13	18,22,25,25	0
1	MLY	B	177	11/12	0.93	0.14	19,21,24,24	0
1	MLY	B	42	11/12	0.93	0.14	16,22,26,26	0
1	MLY	C	164[B]	11/12	0.93	0.21	18,21,23,23	7
1	MLY	A	42	9/12	0.93	0.13	17,20,24,25	0
1	MLY	A	113	9/12	0.93	0.12	17,19,23,24	0
1	MLY	D	177	6/12	0.94	0.18	19,19,21,21	0
1	MLY	C	106	11/12	0.94	0.14	19,22,28,28	0
1	MLY	D	42	11/12	0.94	0.13	17,22,25,26	0
1	MLY	A	196	9/12	0.94	0.12	17,20,23,23	0
1	MLY	A	51	9/12	0.94	0.15	17,21,29,29	0
1	MLY	B	81	9/12	0.94	0.14	18,20,24,24	0
1	MLY	B	51	7/12	0.94	0.11	16,19,27,28	0
1	MLY	D	161	9/12	0.94	0.11	17,18,21,22	0
1	MLY	D	81	8/12	0.94	0.13	19,20,23,24	0
1	MLY	C	84	9/12	0.94	0.13	17,20,26,27	0
1	MLY	B	142	9/12	0.95	0.13	15,19,23,24	0
1	MLY	C	177	9/12	0.95	0.14	19,21,26,26	0
1	MLY	A	81[B]	11/12	0.95	0.13	15,19,20,20	4
1	MLY	D	164	9/12	0.95	0.12	18,20,26,26	0
1	MLY	B	113	11/12	0.95	0.15	17,21,25,25	0
1	MLY	B	161	9/12	0.95	0.12	17,19,22,25	0
1	MLY	A	81[A]	11/12	0.95	0.13	17,19,20,20	4
1	MLY	C	119	7/12	0.95	0.15	16,17,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	A	84	11/12	0.95	0.13	17,22,25,26	0
1	MLY	C	201	7/12	0.95	0.15	19,22,26,27	0
1	MLY	C	161	9/12	0.95	0.11	17,19,21,23	0
1	MLY	C	113	9/12	0.95	0.13	17,19,24,25	0
1	MLY	B	119	7/12	0.95	0.12	15,17,19,20	0
1	MLY	B	106	9/12	0.96	0.09	19,21,25,26	0
1	MLY	A	119	7/12	0.96	0.11	15,16,19,21	0
1	MLY	B	173	9/12	0.96	0.11	19,21,26,26	0
1	MLY	D	119	7/12	0.96	0.12	15,16,19,20	0
1	MLY	A	142	6/12	0.97	0.08	15,18,20,22	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.92	0.07	44,44,44,44	0
3	MG	C	4	1/1	0.92	0.15	32,32,32,32	0
2	CL	A	3	1/1	0.94	0.20	43,43,43,43	0
2	CL	B	2	1/1	0.98	0.06	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.