



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:33 PM BST

PDB ID : 4E4E  
Title : Crystal Structure of the Y34F mutant of *Saccharomyces cerevisiae* Manganese Superoxide Dismutase  
Authors : Sheng, Y.; Cascio, D.; Valentine, J.S.  
Deposited on : 2012-03-12  
Resolution : 1.88 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

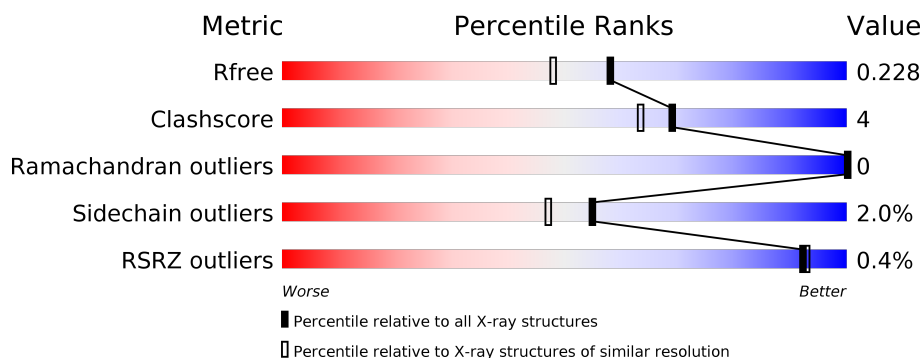
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	207	 92% 7%
1	B	207	 86% 14%
1	C	207	 87% 12%
1	D	207	 86% 12%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6881 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 Superoxide dismutase [Mn], mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	1	0
			1665	1082	277	304	2			
1	B	207	Total	C	N	O	S	0	0	0
			1667	1084	277	304	2			
1	C	205	Total	C	N	O	S	0	2	0
			1655	1075	274	304	2			
1	D	203	Total	C	N	O	S	0	3	0
			1659	1081	274	302	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	PHE	TYR	ENGINEERED MUTATION	UNP P00447
B	34	PHE	TYR	ENGINEERED MUTATION	UNP P00447
C	34	PHE	TYR	ENGINEERED MUTATION	UNP P00447
D	34	PHE	TYR	ENGINEERED MUTATION	UNP P00447

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	61	Total 61	O 61	0	0
3	C	57	Total 57	O 57	0	0
3	D	56	Total 56	O 56	0	0

### 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: Superoxide dismutase [Mn], mitochondrial

Chain A:  92% 7%




- Molecule 1: Superoxide dismutase [Mn], mitochondrial

Chain B:  86% 14%




- Molecule 1: Superoxide dismutase [Mn], mitochondrial

Chain C:  87% 12%



- Molecule 1: Superoxide dismutase [Mn], mitochondrial

Chain D:  86% 12%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.14Å 63.02Å 63.94Å 112.19° 106.78° 103.88°	Depositor
Resolution (Å)	32.18 – 1.88 52.66 – 1.88	Depositor EDS
% Data completeness (in resolution range)	94.5 (32.18-1.88) 94.6 (52.66-1.88)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, $R_{free}$	0.190 , 0.231 0.187 , 0.228	Depositor DCC
$R_{free}$ test set	3042 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6881	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.45	0/1537	0.56	0/2109
1	B	0.43	0/1536	0.56	0/2108
1	C	0.45	0/1541	0.57	0/2115
1	D	0.44	0/1549	0.55	0/2125
All	All	0.44	0/6163	0.56	0/8457

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	1665	0	1630	13	0
1	B	1667	0	1635	16	0
1	C	1655	0	1622	15	0
1	D	1659	0	1627	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	61	0	0	1	0
3	C	57	0	0	1	0
3	D	56	0	0	0	0
All	All	6881	0	6514	49	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 4.

All (49) 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:68[B]:GLN:OE1	1:D:68[B]:GLN:NE2	2.04	0.90
1:B:62:ARG:HG3	1:C:79[A]:THR:HG21	1.78	0.66
1:D:94:GLY:HA3	1:D:196:MLY:HH13	1.82	0.62
1:A:157:VAL:O	1:D:62:ARG:NH2	2.35	0.58
1:A:68[B]:GLN:HB2	1:D:68[B]:GLN:HE21	1.71	0.56
1:B:75:GLY:O	1:B:79:THR:HG23	2.06	0.54
1:A:65:ILE:O	1:A:68[B]:GLN:HG3	2.08	0.53
1:B:3:THR:HG23	3:B:411:HOH:O	2.09	0.52
1:D:131:SER:HB3	1:D:170:TRP:CE2	2.45	0.52
1:D:75:GLY:O	1:D:79:THR:HG23	2.09	0.52
1:A:45:PHE:HD2	1:D:45[B]:PHE:CE2	2.29	0.51
1:B:163:PRO:HG2	1:B:207:ILE:HG21	1.94	0.49
1:A:45:PHE:CE1	1:A:68[A]:GLN:NE2	2.81	0.49
1:B:65:ILE:O	1:B:68:GLN:HG3	2.12	0.49
1:A:131:SER:HB3	1:A:170:TRP:CE2	2.48	0.48
1:A:42:VAL:HG22	1:D:64:MET:HE1	1.96	0.47
1:C:64:MET:HA	1:C:64:MET:HE3	1.96	0.47
1:C:2:VAL:HG23	1:C:35:VAL:HG13	1.98	0.46
1:D:15:GLU:HG2	1:D:19:SER:HA	1.98	0.46
1:B:119:MLY:O	1:B:123:THR:HG23	2.16	0.45
1:D:182:MLY:HH22	1:D:182:MLY:HD3	1.56	0.45
1:C:54:MLY:HD3	1:C:54:MLY:HH22	1.76	0.45
1:A:94:GLY:HA3	1:A:196:MLY:HH23	1.99	0.45
1:B:72:MLY:HD2	1:B:72:MLY:HH23	1.78	0.44
1:B:131:SER:HB3	1:B:170:TRP:CE2	2.53	0.44
1:A:170:TRP:CH2	1:B:130:GLY:HA2	2.53	0.44
1:B:149:VAL:HG21	1:B:157:VAL:HG11	1.99	0.43
1:C:172:HIS:HE1	3:C:457:HOH:O	1.99	0.43
1:D:99:PRO:HB3	1:D:195:TRP:HB3	1.99	0.43
1:B:181:MLY:HH12	1:B:181:MLY:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:MLY:HH23	1:D:187:MLY:HD2	1.80	0.43
1:B:196:MLY:HD3	1:B:196:MLY:HH13	1.64	0.43
1:C:97:GLU:HA	1:C:98:PRO:HD3	1.80	0.42
1:B:161:LEU:O	1:C:62:ARG:NH2	2.50	0.42
1:C:52:LEU:HD12	1:C:56:PRO:HA	2.01	0.42
1:C:72:MLY:HD2	1:C:72:MLY:HH23	1.68	0.42
1:C:72:MLY:HE3	1:C:155:ASP:OD1	2.18	0.42
1:B:46:GLN:HE22	1:C:46:GLN:NE2	2.18	0.41
1:A:68[A]:GLN:OE1	1:D:71:ILE:HB	2.20	0.41
1:C:176:LEU:HD23	1:D:176:LEU:HD23	2.02	0.41
1:C:8:MLY:HH22	1:C:86:GLU:OE1	2.21	0.41
1:B:4:LEU:HD13	1:B:27:TYR:CZ	2.56	0.41
1:D:2:VAL:HG23	1:D:35:VAL:HG13	2.03	0.41
1:A:51:LEU:HA	1:A:51:LEU:HD12	1.91	0.41
1:A:89:ALA:O	1:A:95:GLY:HA3	2.21	0.41
1:B:2:VAL:HG23	1:B:35:VAL:HG13	2.03	0.40
1:C:124:MLY:HH22	1:C:124:MLY:HD2	1.73	0.40
1:C:131:SER:HB3	1:C:170:TRP:CE2	2.55	0.40
1:D:72:MLY:HD2	1:D:72:MLY:HH23	1.79	0.40

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	191/207 (92%)	188 (98%)	3 (2%)	0	100	100
1	B	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
1	C	191/207 (92%)	187 (98%)	4 (2%)	0	100	100
1	D	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
All	All	762/828 (92%)	747 (98%)	15 (2%)	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	154/154 (100%)	151 (98%)	3 (2%)	57	49
1	B	154/154 (100%)	150 (97%)	4 (3%)	46	36
1	C	155/154 (101%)	152 (98%)	3 (2%)	57	49
1	D	156/154 (101%)	153 (98%)	3 (2%)	57	49
All	All	619/616 (100%)	606 (98%)	13 (2%)	55	45

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	87	ASN
1	A	116	GLU
1	B	3	THR
1	B	64	MET
1	B	87	ASN
1	B	115	ASP
1	C	9	TRP
1	C	47	GLU
1	C	87	ASN
1	D	21[A]	GLN
1	D	21[B]	GLN
1	D	87	ASN

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

Mol	Chain	Res	Type
1	B	46	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

62 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	B	1	1	9,10,11	0.69	0	6,11,13	1.34	1 (16%)
1	MLY	B	145	1	9,10,11	0.60	0	6,11,13	0.95	0
1	MLY	A	8	1	9,10,11	0.60	0	6,11,13	0.83	0
1	MLY	C	187	1	9,10,11	0.70	0	6,11,13	0.61	0
1	MLY	A	119	1	9,10,11	0.70	0	6,11,13	0.73	0
1	MLY	B	182	1	9,10,11	0.64	0	6,11,13	1.00	0
1	MLY	D	145	1	9,10,11	0.60	0	6,11,13	0.99	0
1	MLY	C	105	1	9,10,11	0.69	0	6,11,13	0.88	0
1	MLY	C	54	1	9,10,11	0.52	0	6,11,13	0.77	0
1	MLY	A	1	1	9,10,11	3.60	2 (22%)	6,11,13	0.85	0
1	MLY	D	196	1	9,10,11	0.54	0	6,11,13	0.89	0
1	MLY	D	124	1	9,10,11	0.55	0	6,11,13	0.84	0
1	MLY	A	181	1	9,10,11	0.58	0	6,11,13	0.65	0
1	MLY	A	124	1	9,10,11	0.55	0	6,11,13	0.88	0
1	MLY	A	182	1	9,10,11	0.60	0	6,11,13	0.82	0
1	MLY	D	54	1	9,10,11	0.53	0	6,11,13	1.10	1 (16%)
1	MLY	B	138	1	9,10,11	0.66	0	6,11,13	0.65	0
1	MLY	B	29	1	9,10,11	0.66	0	6,11,13	0.71	0
1	MLY	A	206	1	9,10,11	0.61	0	6,11,13	0.66	0
1	MLY	A	187	1	9,10,11	0.59	0	6,11,13	0.73	0
1	MLY	B	187	1	9,10,11	0.57	0	6,11,13	0.64	0
1	MLY	C	29	1	9,10,11	0.72	0	6,11,13	0.65	0
1	MLY	A	138	1	9,10,11	0.72	0	6,11,13	0.87	0
1	MLY	A	54	1	9,10,11	0.49	0	6,11,13	0.86	0
1	MLY	D	105	1	9,10,11	0.70	0	6,11,13	0.83	0
1	MLY	C	63	1	9,10,11	0.83	0	6,11,13	0.74	0
1	MLY	D	1	1	9,10,11	0.59	0	6,11,13	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	B	206	1	9,10,11	0.77	0	6,11,13	0.63	0
1	MLY	A	72	1	9,10,11	0.70	0	6,11,13	1.05	0
1	MLY	D	72	1	9,10,11	0.56	0	6,11,13	0.99	0
1	MLY	C	145	1	9,10,11	0.53	0	6,11,13	0.87	0
1	MLY	B	72	1	9,10,11	0.62	0	6,11,13	0.82	0
1	MLY	A	105	1	9,10,11	0.76	0	6,11,13	0.69	0
1	MLY	C	119	1	9,10,11	0.59	0	6,11,13	0.77	0
1	MLY	C	138	1	9,10,11	0.70	0	6,11,13	1.14	1 (16%)
1	MLY	C	72	1	9,10,11	0.57	0	6,11,13	1.30	0
1	MLY	B	63	1	9,10,11	0.78	0	6,11,13	0.67	0
1	MLY	C	181	1	9,10,11	0.55	0	6,11,13	0.99	0
1	MLY	D	181	1	9,10,11	0.55	0	6,11,13	0.61	0
1	MLY	B	105	1	9,10,11	0.77	0	6,11,13	0.88	0
1	MLY	D	182	1	9,10,11	0.56	0	6,11,13	0.86	0
1	MLY	A	196	1	9,10,11	0.86	0	6,11,13	0.74	0
1	MLY	D	29	1	9,10,11	0.65	0	6,11,13	0.78	0
1	MLY	C	196	1	9,10,11	0.60	0	6,11,13	0.76	0
1	MLY	D	138	1	9,10,11	0.66	0	6,11,13	1.08	0
1	MLY	B	119	1	9,10,11	0.71	0	6,11,13	0.73	0
1	MLY	C	182	1	9,10,11	0.57	0	6,11,13	0.97	0
1	MLY	C	1	1	9,10,11	0.60	0	6,11,13	0.89	0
1	MLY	A	145	1	9,10,11	0.64	0	6,11,13	0.80	0
1	MLY	D	187	1	9,10,11	0.60	0	6,11,13	0.86	0
1	MLY	D	119	1	9,10,11	0.63	0	6,11,13	0.83	0
1	MLY	D	8	1	9,10,11	0.51	0	6,11,13	0.70	0
1	MLY	A	29	1	9,10,11	0.59	0	6,11,13	0.94	0
1	MLY	B	196	1	9,10,11	0.66	0	6,11,13	0.87	0
1	MLY	C	8	1	9,10,11	0.54	0	6,11,13	0.83	0
1	MLY	C	124	1	9,10,11	0.79	0	6,11,13	0.71	0
1	MLY	B	8	1	9,10,11	0.69	0	6,11,13	1.13	1 (16%)
1	MLY	B	54	1	9,10,11	0.60	0	6,11,13	0.78	0
1	MLY	A	63	1	9,10,11	0.74	0	6,11,13	0.88	0
1	MLY	B	181	1	9,10,11	0.74	0	6,11,13	0.45	0
1	MLY	D	63	1	9,10,11	0.54	0	6,11,13	0.88	0
1	MLY	B	124	1	9,10,11	0.48	0	6,11,13	0.84	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	B	1	1	-	0/8/9/11	-
1	MLY	B	145	1	-	1/8/9/11	-
1	MLY	A	8	1	-	1/8/9/11	-
1	MLY	C	187	1	-	1/8/9/11	-
1	MLY	A	119	1	-	1/8/9/11	-
1	MLY	B	182	1	-	4/8/9/11	-
1	MLY	D	145	1	-	4/8/9/11	-
1	MLY	C	105	1	-	5/8/9/11	-
1	MLY	C	54	1	-	1/8/9/11	-
1	MLY	A	1	1	-	2/8/9/11	-
1	MLY	D	196	1	-	2/8/9/11	-
1	MLY	D	124	1	-	1/8/9/11	-
1	MLY	A	181	1	-	2/8/9/11	-
1	MLY	A	124	1	-	1/8/9/11	-
1	MLY	A	182	1	-	0/8/9/11	-
1	MLY	D	54	1	-	3/8/9/11	-
1	MLY	B	138	1	-	1/8/9/11	-
1	MLY	B	29	1	-	1/8/9/11	-
1	MLY	A	206	1	-	3/8/9/11	-
1	MLY	A	187	1	-	4/8/9/11	-
1	MLY	B	187	1	-	0/8/9/11	-
1	MLY	C	29	1	-	0/8/9/11	-
1	MLY	A	138	1	-	2/8/9/11	-
1	MLY	A	54	1	-	2/8/9/11	-
1	MLY	D	105	1	-	2/8/9/11	-
1	MLY	C	63	1	-	2/8/9/11	-
1	MLY	D	1	1	-	2/8/9/11	-
1	MLY	B	206	1	-	6/8/9/11	-
1	MLY	A	72	1	-	3/8/9/11	-
1	MLY	D	72	1	-	0/8/9/11	-
1	MLY	C	145	1	-	0/8/9/11	-
1	MLY	B	72	1	-	2/8/9/11	-
1	MLY	A	105	1	-	1/8/9/11	-
1	MLY	C	119	1	-	2/8/9/11	-
1	MLY	C	138	1	-	0/8/9/11	-
1	MLY	C	72	1	-	0/8/9/11	-
1	MLY	B	63	1	-	2/8/9/11	-
1	MLY	C	181	1	-	1/8/9/11	-
1	MLY	D	181	1	-	0/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	105	1	-	4/8/9/11	-
1	MLY	D	182	1	-	4/8/9/11	-
1	MLY	A	196	1	-	2/8/9/11	-
1	MLY	D	29	1	-	0/8/9/11	-
1	MLY	C	196	1	-	0/8/9/11	-
1	MLY	D	138	1	-	1/8/9/11	-
1	MLY	B	119	1	-	1/8/9/11	-
1	MLY	C	182	1	-	2/8/9/11	-
1	MLY	C	1	1	-	0/8/9/11	-
1	MLY	A	145	1	-	3/8/9/11	-
1	MLY	D	187	1	-	0/8/9/11	-
1	MLY	D	119	1	-	0/8/9/11	-
1	MLY	D	8	1	-	1/8/9/11	-
1	MLY	A	29	1	-	0/8/9/11	-
1	MLY	B	196	1	-	2/8/9/11	-
1	MLY	C	8	1	-	3/8/9/11	-
1	MLY	C	124	1	-	4/8/9/11	-
1	MLY	B	8	1	-	3/8/9/11	-
1	MLY	B	54	1	-	2/8/9/11	-
1	MLY	A	63	1	-	2/8/9/11	-
1	MLY	B	181	1	-	2/8/9/11	-
1	MLY	D	63	1	-	3/8/9/11	-
1	MLY	B	124	1	-	0/8/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MLY	CA-N	-10.05	1.17	1.48
1	A	1	MLY	CB-CA	3.69	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MLY	CD-CE-NZ	-2.66	106.60	113.79
1	C	138	MLY	CH2-NZ-CH1	-2.25	103.92	109.73
1	B	8	MLY	CH2-NZ-CH1	-2.12	104.24	109.73
1	D	54	MLY	CD-CE-NZ	-2.03	108.30	113.79

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	145	MLY	O-C-CA-CB
1	A	1	MLY	O-C-CA-CB
1	A	206	MLY	N-CA-CB-CG
1	A	206	MLY	C-CA-CB-CG
1	B	206	MLY	C-CA-CB-CG
1	D	182	MLY	O-C-CA-CB
1	B	8	MLY	O-C-CA-CB
1	B	182	MLY	CD-CE-NZ-CH1
1	B	182	MLY	CD-CE-NZ-CH2
1	D	145	MLY	CD-CE-NZ-CH1
1	D	145	MLY	CD-CE-NZ-CH2
1	D	54	MLY	CD-CE-NZ-CH1
1	D	54	MLY	CD-CE-NZ-CH2
1	A	187	MLY	CD-CE-NZ-CH1
1	A	138	MLY	CD-CE-NZ-CH1
1	A	138	MLY	CD-CE-NZ-CH2
1	A	54	MLY	CD-CE-NZ-CH2
1	D	1	MLY	CD-CE-NZ-CH1
1	B	206	MLY	CD-CE-NZ-CH2
1	A	72	MLY	CD-CE-NZ-CH1
1	A	72	MLY	CD-CE-NZ-CH2
1	B	63	MLY	CD-CE-NZ-CH1
1	B	105	MLY	CD-CE-NZ-CH1
1	A	196	MLY	CD-CE-NZ-CH2
1	C	124	MLY	CD-CE-NZ-CH1
1	B	8	MLY	CD-CE-NZ-CH1
1	D	63	MLY	CD-CE-NZ-CH1
1	C	124	MLY	CG-CD-CE-NZ
1	D	182	MLY	CG-CD-CE-NZ
1	A	124	MLY	CG-CD-CE-NZ
1	A	1	MLY	CG-CD-CE-NZ
1	B	196	MLY	CG-CD-CE-NZ
1	D	54	MLY	CG-CD-CE-NZ
1	A	206	MLY	CG-CD-CE-NZ
1	A	187	MLY	CG-CD-CE-NZ
1	D	63	MLY	CG-CD-CE-NZ
1	C	105	MLY	CD-CE-NZ-CH1
1	A	187	MLY	CD-CE-NZ-CH2
1	A	54	MLY	CD-CE-NZ-CH1
1	B	63	MLY	CD-CE-NZ-CH2
1	D	182	MLY	CD-CE-NZ-CH2
1	A	145	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	B	181	MLY	CD-CE-NZ-CH1
1	D	63	MLY	CD-CE-NZ-CH2
1	A	181	MLY	CG-CD-CE-NZ
1	C	182	MLY	CG-CD-CE-NZ
1	D	196	MLY	CG-CD-CE-NZ
1	B	105	MLY	CG-CD-CE-NZ
1	C	187	MLY	CD-CE-NZ-CH1
1	D	105	MLY	CD-CE-NZ-CH1
1	B	119	MLY	CD-CE-NZ-CH2
1	B	196	MLY	CD-CE-NZ-CH1
1	A	63	MLY	CD-CE-NZ-CH1
1	B	206	MLY	CG-CD-CE-NZ
1	A	72	MLY	CG-CD-CE-NZ
1	D	105	MLY	CD-CE-NZ-CH2
1	B	206	MLY	CD-CE-NZ-CH1
1	B	105	MLY	CD-CE-NZ-CH2
1	C	124	MLY	CD-CE-NZ-CH2
1	C	8	MLY	CG-CD-CE-NZ
1	A	119	MLY	CD-CE-NZ-CH1
1	A	105	MLY	CE-CD-CG-CB
1	C	105	MLY	CA-CB-CG-CD
1	A	187	MLY	CA-CB-CG-CD
1	C	124	MLY	CA-CB-CG-CD
1	D	1	MLY	CD-CE-NZ-CH2
1	A	196	MLY	CD-CE-NZ-CH1
1	A	145	MLY	CD-CE-NZ-CH1
1	B	181	MLY	CG-CD-CE-NZ
1	B	182	MLY	CE-CD-CG-CB
1	A	181	MLY	CD-CE-NZ-CH2
1	C	54	MLY	CE-CD-CG-CB
1	C	63	MLY	CD-CE-NZ-CH2
1	C	63	MLY	CE-CD-CG-CB
1	C	119	MLY	CE-CD-CG-CB
1	D	182	MLY	CE-CD-CG-CB
1	B	105	MLY	CE-CD-CG-CB
1	D	196	MLY	CE-CD-CG-CB
1	A	145	MLY	CA-CB-CG-CD
1	B	72	MLY	CE-CD-CG-CB
1	D	145	MLY	CE-CD-CG-CB
1	C	105	MLY	CD-CE-NZ-CH2
1	A	8	MLY	CA-CB-CG-CD
1	C	105	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	A	63	MLY	CG-CD-CE-NZ
1	C	181	MLY	CD-CE-NZ-CH1
1	B	54	MLY	CD-CE-NZ-CH1
1	C	105	MLY	N-CA-CB-CG
1	C	8	MLY	N-CA-CB-CG
1	C	119	MLY	C-CA-CB-CG
1	C	182	MLY	CE-CD-CG-CB
1	B	145	MLY	CA-CB-CG-CD
1	B	206	MLY	CE-CD-CG-CB
1	D	138	MLY	CD-CE-NZ-CH2
1	B	29	MLY	CD-CE-NZ-CH1
1	C	8	MLY	C-CA-CB-CG
1	B	72	MLY	CA-CB-CG-CD
1	B	54	MLY	CE-CD-CG-CB
1	D	124	MLY	CA-CB-CG-CD
1	B	138	MLY	CD-CE-NZ-CH2
1	D	8	MLY	CA-CB-CG-CD
1	B	182	MLY	CG-CD-CE-NZ
1	B	206	MLY	N-CA-CB-CG
1	B	8	MLY	CD-CE-NZ-CH2

There are no ring outliers.

13 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	54	MLY	1	0
1	D	196	MLY	1	0
1	D	72	MLY	1	0
1	B	72	MLY	1	0
1	C	72	MLY	2	0
1	D	182	MLY	1	0
1	A	196	MLY	1	0
1	B	119	MLY	1	0
1	D	187	MLY	1	0
1	B	196	MLY	1	0
1	C	8	MLY	1	0
1	C	124	MLY	1	0
1	B	181	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	190/207 (91%)	-0.21	1 (0%) 91 91	18, 27, 39, 45	0
1	B	191/207 (92%)	-0.17	2 (1%) 82 83	18, 26, 39, 46	0
1	C	190/207 (91%)	-0.27	0 100 100	19, 26, 38, 44	0
1	D	188/207 (90%)	-0.20	0 100 100	19, 27, 42, 48	0
All	All	759/828 (91%)	-0.21	3 (0%) 92 93	18, 26, 40, 48	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158	THR	3.1
1	B	207	ILE	2.5
1	B	115	ASP	2.2

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	MLY	B	206	11/12	0.80	0.33	33,48,63,65	0
1	MLY	A	206	11/12	0.81	0.22	41,45,56,59	0
1	MLY	B	54	11/12	0.84	0.21	36,40,58,60	0
1	MLY	A	196	11/12	0.85	0.22	26,35,52,52	0
1	MLY	D	54	11/12	0.85	0.19	42,50,61,62	0
1	MLY	A	1	11/12	0.86	0.21	36,46,70,71	0
1	MLY	A	105	11/12	0.88	0.19	26,36,56,58	0
1	MLY	C	1	11/12	0.88	0.16	35,39,60,65	0
1	MLY	C	105	11/12	0.88	0.24	31,36,67,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	C	196	11/12	0.89	0.20	28,32,63,69	0
1	MLY	C	8	11/12	0.89	0.16	34,39,52,53	0
1	MLY	A	187	11/12	0.89	0.19	22,28,60,60	0
1	MLY	D	196	11/12	0.90	0.25	26,32,58,62	0
1	MLY	C	119	11/12	0.90	0.21	27,32,57,57	0
1	MLY	A	63	11/12	0.90	0.12	28,30,44,48	0
1	MLY	D	105	11/12	0.91	0.19	29,36,71,71	0
1	MLY	C	124	11/12	0.91	0.15	25,28,51,53	0
1	MLY	C	145	11/12	0.91	0.13	21,24,42,48	0
1	MLY	A	145	11/12	0.91	0.13	23,26,42,46	0
1	MLY	D	63	11/12	0.91	0.14	27,32,54,56	0
1	MLY	C	54	11/12	0.92	0.15	24,28,49,49	0
1	MLY	D	8	11/12	0.92	0.12	27,33,43,46	0
1	MLY	A	72	11/12	0.92	0.14	24,29,48,50	0
1	MLY	B	63	11/12	0.92	0.13	25,32,46,51	0
1	MLY	B	1	11/12	0.92	0.15	22,29,47,47	0
1	MLY	B	72	11/12	0.92	0.16	19,26,46,50	0
1	MLY	B	119	11/12	0.92	0.16	24,29,52,57	0
1	MLY	A	124	11/12	0.93	0.13	24,25,42,48	0
1	MLY	C	182	11/12	0.93	0.13	23,24,44,48	0
1	MLY	A	182	11/12	0.93	0.14	18,22,47,48	0
1	MLY	D	187	11/12	0.93	0.23	22,27,65,67	0
1	MLY	D	1	11/12	0.93	0.11	29,32,56,59	0
1	MLY	C	187	11/12	0.93	0.16	22,24,59,62	0
1	MLY	B	105	11/12	0.93	0.14	26,36,61,65	0
1	MLY	B	8	11/12	0.93	0.15	28,36,51,53	0
1	MLY	D	182	11/12	0.93	0.17	21,23,42,47	0
1	MLY	B	182	11/12	0.93	0.14	21,23,40,42	0
1	MLY	A	8	11/12	0.93	0.10	24,29,40,43	0
1	MLY	B	124	11/12	0.93	0.13	22,26,42,44	0
1	MLY	B	196	11/12	0.94	0.17	24,29,68,70	0
1	MLY	A	119	11/12	0.94	0.21	21,25,50,52	0
1	MLY	D	72	11/12	0.94	0.17	22,29,49,55	0
1	MLY	C	63	11/12	0.94	0.16	25,31,61,63	0
1	MLY	D	145	11/12	0.94	0.11	25,28,42,44	0
1	MLY	D	124	11/12	0.94	0.12	26,28,44,45	0
1	MLY	D	119	11/12	0.94	0.20	24,34,59,61	0
1	MLY	D	29	11/12	0.94	0.11	20,25,45,47	0
1	MLY	A	54	11/12	0.95	0.11	28,29,40,40	0
1	MLY	C	181	11/12	0.95	0.12	21,28,45,47	0
1	MLY	D	181	11/12	0.95	0.12	20,24,35,36	0
1	MLY	A	181	11/12	0.95	0.15	21,27,49,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	B	187	11/12	0.95	0.14	20,26,47,54	0
1	MLY	A	138	11/12	0.95	0.10	22,26,35,35	0
1	MLY	B	181	11/12	0.95	0.14	22,28,45,46	0
1	MLY	C	72	11/12	0.95	0.12	22,30,58,58	0
1	MLY	A	29	11/12	0.95	0.11	19,22,38,42	0
1	MLY	B	138	11/12	0.96	0.13	20,23,32,35	0
1	MLY	B	29	11/12	0.96	0.09	20,22,37,40	0
1	MLY	C	29	11/12	0.96	0.10	20,21,38,38	0
1	MLY	B	145	11/12	0.96	0.10	18,25,33,34	0
1	MLY	C	138	11/12	0.96	0.09	21,23,32,34	0
1	MLY	D	138	11/12	0.97	0.09	20,24,34,35	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	B	301	1/1	1.00	0.09	18,18,18,18	0
2	MN	C	301	1/1	1.00	0.08	18,18,18,18	0
2	MN	A	301	1/1	1.00	0.08	17,17,17,17	0
2	MN	D	301	1/1	1.00	0.08	19,19,19,19	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.