Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 02:11 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

1   Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.228
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.0%
RSRZ outliers		0.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
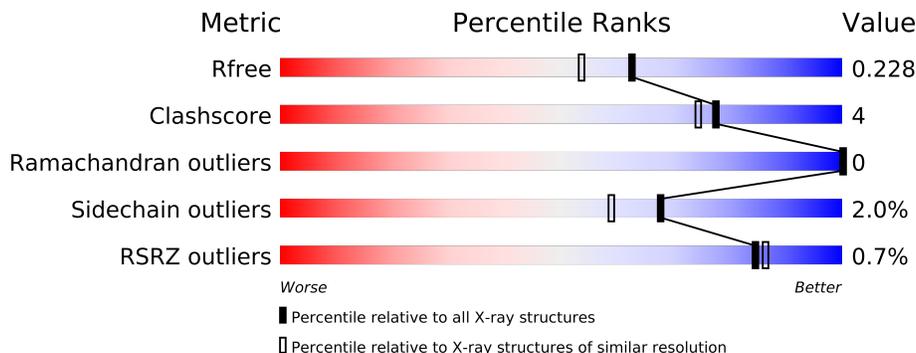
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (1.90-1.86)

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 >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	207	
1	B	207	
1	C	207	
1	D	207	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6881 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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:
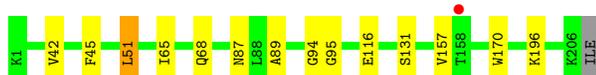
- Molecule 1: Superoxide dismutase [Mn], mitochondrial

Chain B:

- Molecule 1: Superoxide dismutase [Mn], mitochondrial

Chain C:

- Molecule 1: Superoxide dismutase [Mn], mitochondrial

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.21 (at 1.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.190 , 0.231 0.187 , 0.228	Depositor DCC
R_{free} test set	3039 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 34.7	EDS
Estimated twinning fraction	0.012 for -h,-l,-k	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 59870 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6881	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	57	0	0	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (49) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:D:131:SER:HB3	1:D:170:TRP:CE2	2.45	0.52
1:B:3:THR:HG23	3:B:411:HOH:O	2.09	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:D:182:MLY:HH22	1:D:182:MLY:HD3	1.56	0.45
1:B:119:MLY:O	1:B:123:THR:HG23	2.16	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:D:99:PRO:HB3	1:D:195:TRP:HB3	1.99	0.43
1:C:172:HIS:HE1	3:C:457:HOH:O	1.99	0.43
1:B:181:MLY:HH12	1:B:181:MLY:HD2	1.82	0.43
1:D:187:MLY:HH23	1:D:187:MLY:HD2	1.80	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:68[A]:GLN:OE1	1:D:71:ILE:HB	2.20	0.41
1:B:46:GLN:HE22	1:C:46:GLN:NE2	2.18	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:D:2:VAL:HG23	1:D:35:VAL:HG13	2.03	0.41
1:B:4:LEU:HD13	1:B:27:TYR:CZ	2.56	0.41
1:A:89:ALA:O	1:A:95:GLY:HA3	2.21	0.41
1:A:51:LEU:HA	1:A:51:LEU:HD12	1.91	0.41
1:B:2:VAL:HG23	1:B:35:VAL:HG13	2.03	0.40
1:C:131:SER:HB3	1:C:170:TRP:CE2	2.55	0.40
1:C:124:MLY:HH22	1:C:124:MLY:HD2	1.73	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

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	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%)	69	61
1	B	154/154 (100%)	150 (97%)	4 (3%)	59	46
1	C	155/154 (101%)	152 (98%)	3 (2%)	69	61
1	D	156/154 (101%)	153 (98%)	3 (2%)	69	61
All	All	619/616 (100%)	606 (98%)	13 (2%)	68	56

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 chains 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	A	1	1	10,10,11	6.18	4 (40%)	9,11,13	2.66	1 (11%)
1	MLY	A	105	1	10,10,11	6.59	2 (20%)	9,11,13	0.97	1 (11%)
1	MLY	A	119	1	10,10,11	6.22	2 (20%)	9,11,13	0.94	1 (11%)
1	MLY	A	124	1	10,10,11	5.55	2 (20%)	9,11,13	1.20	1 (11%)
1	MLY	A	138	1	10,10,11	6.21	2 (20%)	9,11,13	2.41	1 (11%)
1	MLY	A	145	1	10,10,11	5.64	2 (20%)	9,11,13	0.70	0
1	MLY	A	181	1	10,10,11	5.73	2 (20%)	9,11,13	1.26	1 (11%)
1	MLY	A	182	1	10,10,11	5.77	2 (20%)	9,11,13	1.19	1 (11%)
1	MLY	A	187	1	10,10,11	5.77	2 (20%)	9,11,13	0.75	0
1	MLY	A	196	1	10,10,11	6.16	2 (20%)	9,11,13	1.93	1 (11%)
1	MLY	A	206	1	10,10,11	5.75	2 (20%)	9,11,13	1.57	1 (11%)
1	MLY	A	29	1	10,10,11	5.57	2 (20%)	9,11,13	0.77	0
1	MLY	A	54	1	10,10,11	5.41	2 (20%)	9,11,13	0.71	0
1	MLY	A	63	1	10,10,11	7.35	2 (20%)	9,11,13	0.71	0
1	MLY	A	72	1	10,10,11	5.77	2 (20%)	9,11,13	1.15	1 (11%)
1	MLY	A	8	1	10,10,11	5.66	2 (20%)	9,11,13	1.28	1 (11%)
1	MLY	B	1	1	10,10,11	6.06	2 (20%)	9,11,13	1.57	2 (22%)
1	MLY	B	105	1	10,10,11	5.82	2 (20%)	9,11,13	1.11	1 (11%)
1	MLY	B	119	1	10,10,11	6.18	2 (20%)	9,11,13	0.92	1 (11%)
1	MLY	B	124	1	10,10,11	5.88	2 (20%)	9,11,13	0.87	0
1	MLY	B	138	1	10,10,11	6.01	2 (20%)	9,11,13	2.68	1 (11%)
1	MLY	B	145	1	10,10,11	5.50	2 (20%)	9,11,13	0.80	0
1	MLY	B	181	1	10,10,11	5.81	2 (20%)	9,11,13	0.73	0
1	MLY	B	182	1	10,10,11	5.93	2 (20%)	9,11,13	0.93	0
1	MLY	B	187	1	10,10,11	5.81	2 (20%)	9,11,13	0.88	0
1	MLY	B	196	1	10,10,11	6.07	2 (20%)	9,11,13	1.63	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MLY	B	206	1	10,10,11	5.85	2 (20%)	9,11,13	1.04	1 (11%)
1	MLY	B	29	1	10,10,11	5.75	2 (20%)	9,11,13	0.74	0
1	MLY	B	54	1	10,10,11	5.89	2 (20%)	9,11,13	0.71	0
1	MLY	B	63	1	10,10,11	7.09	2 (20%)	9,11,13	0.61	0
1	MLY	B	72	1	10,10,11	5.88	2 (20%)	9,11,13	0.66	0
1	MLY	B	8	1	10,10,11	5.89	2 (20%)	9,11,13	1.23	2 (22%)
1	MLY	C	1	1	10,10,11	5.93	2 (20%)	9,11,13	1.11	1 (11%)
1	MLY	C	105	1	10,10,11	5.65	2 (20%)	9,11,13	0.93	0
1	MLY	C	119	1	10,10,11	5.98	2 (20%)	9,11,13	0.63	0
1	MLY	C	124	1	10,10,11	6.05	2 (20%)	9,11,13	0.60	0
1	MLY	C	138	1	10,10,11	5.97	2 (20%)	9,11,13	1.66	2 (22%)
1	MLY	C	145	1	10,10,11	5.92	2 (20%)	9,11,13	0.74	0
1	MLY	C	181	1	10,10,11	6.02	2 (20%)	9,11,13	1.07	1 (11%)
1	MLY	C	182	1	10,10,11	5.90	2 (20%)	9,11,13	1.13	1 (11%)
1	MLY	C	187	1	10,10,11	5.91	2 (20%)	9,11,13	0.53	0
1	MLY	C	196	1	10,10,11	5.62	2 (20%)	9,11,13	0.81	0
1	MLY	C	29	1	10,10,11	5.80	2 (20%)	9,11,13	1.01	1 (11%)
1	MLY	C	54	1	10,10,11	5.73	2 (20%)	9,11,13	0.61	0
1	MLY	C	63	1	10,10,11	7.26	2 (20%)	9,11,13	0.64	0
1	MLY	C	72	1	10,10,11	5.69	2 (20%)	9,11,13	1.17	0
1	MLY	C	8	1	10,10,11	5.63	2 (20%)	9,11,13	1.16	1 (11%)
1	MLY	D	1	1	10,10,11	5.87	2 (20%)	9,11,13	0.59	0
1	MLY	D	105	1	10,10,11	5.74	2 (20%)	9,11,13	1.07	1 (11%)
1	MLY	D	119	1	10,10,11	5.94	2 (20%)	9,11,13	1.19	1 (11%)
1	MLY	D	124	1	10,10,11	5.87	2 (20%)	9,11,13	1.01	1 (11%)
1	MLY	D	138	1	10,10,11	5.85	2 (20%)	9,11,13	2.36	1 (11%)
1	MLY	D	145	1	10,10,11	5.63	2 (20%)	9,11,13	1.06	0
1	MLY	D	181	1	10,10,11	5.81	2 (20%)	9,11,13	0.85	1 (11%)
1	MLY	D	182	1	10,10,11	5.60	2 (20%)	9,11,13	1.30	1 (11%)
1	MLY	D	187	1	10,10,11	5.99	2 (20%)	9,11,13	0.78	0
1	MLY	D	196	1	10,10,11	6.32	2 (20%)	9,11,13	1.12	1 (11%)
1	MLY	D	29	1	10,10,11	6.03	2 (20%)	9,11,13	0.66	0
1	MLY	D	54	1	10,10,11	5.79	2 (20%)	9,11,13	1.24	2 (22%)
1	MLY	D	63	1	10,10,11	5.70	2 (20%)	9,11,13	0.90	0
1	MLY	D	72	1	10,10,11	5.62	2 (20%)	9,11,13	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MLY	D	8	1	10,10,11	5.99	2 (20%)	9,11,13	0.88	1 (11%)

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	1	1	-	0/7/9/11	0/0/0/0
1	MLY	A	105	1	-	0/7/9/11	0/0/0/0
1	MLY	A	119	1	-	0/7/9/11	0/0/0/0
1	MLY	A	124	1	-	0/7/9/11	0/0/0/0
1	MLY	A	138	1	-	0/7/9/11	0/0/0/0
1	MLY	A	145	1	-	0/7/9/11	0/0/0/0
1	MLY	A	181	1	-	0/7/9/11	0/0/0/0
1	MLY	A	182	1	-	0/7/9/11	0/0/0/0
1	MLY	A	187	1	-	0/7/9/11	0/0/0/0
1	MLY	A	196	1	-	0/7/9/11	0/0/0/0
1	MLY	A	206	1	-	0/7/9/11	0/0/0/0
1	MLY	A	29	1	-	0/7/9/11	0/0/0/0
1	MLY	A	54	1	-	0/7/9/11	0/0/0/0
1	MLY	A	63	1	-	0/7/9/11	0/0/0/0
1	MLY	A	72	1	-	0/7/9/11	0/0/0/0
1	MLY	A	8	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1	1	-	0/7/9/11	0/0/0/0
1	MLY	B	105	1	-	0/7/9/11	0/0/0/0
1	MLY	B	119	1	-	0/7/9/11	0/0/0/0
1	MLY	B	124	1	-	0/7/9/11	0/0/0/0
1	MLY	B	138	1	-	0/7/9/11	0/0/0/0
1	MLY	B	145	1	-	0/7/9/11	0/0/0/0
1	MLY	B	181	1	-	0/7/9/11	0/0/0/0
1	MLY	B	182	1	-	0/7/9/11	0/0/0/0
1	MLY	B	187	1	-	0/7/9/11	0/0/0/0
1	MLY	B	196	1	-	0/7/9/11	0/0/0/0
1	MLY	B	206	1	-	0/7/9/11	0/0/0/0
1	MLY	B	29	1	-	0/7/9/11	0/0/0/0
1	MLY	B	54	1	-	0/7/9/11	0/0/0/0
1	MLY	B	63	1	-	0/7/9/11	0/0/0/0
1	MLY	B	72	1	-	0/7/9/11	0/0/0/0
1	MLY	B	8	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1	1	-	0/7/9/11	0/0/0/0
1	MLY	C	105	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	C	119	1	-	0/7/9/11	0/0/0/0
1	MLY	C	124	1	-	0/7/9/11	0/0/0/0
1	MLY	C	138	1	-	0/7/9/11	0/0/0/0
1	MLY	C	145	1	-	0/7/9/11	0/0/0/0
1	MLY	C	181	1	-	0/7/9/11	0/0/0/0
1	MLY	C	182	1	-	0/7/9/11	0/0/0/0
1	MLY	C	187	1	-	0/7/9/11	0/0/0/0
1	MLY	C	196	1	-	0/7/9/11	0/0/0/0
1	MLY	C	29	1	-	0/7/9/11	0/0/0/0
1	MLY	C	54	1	-	0/7/9/11	0/0/0/0
1	MLY	C	63	1	-	0/7/9/11	0/0/0/0
1	MLY	C	72	1	-	0/7/9/11	0/0/0/0
1	MLY	C	8	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1	1	-	0/7/9/11	0/0/0/0
1	MLY	D	105	1	-	0/7/9/11	0/0/0/0
1	MLY	D	119	1	-	0/7/9/11	0/0/0/0
1	MLY	D	124	1	-	0/7/9/11	0/0/0/0
1	MLY	D	138	1	-	0/7/9/11	0/0/0/0
1	MLY	D	145	1	-	0/7/9/11	0/0/0/0
1	MLY	D	181	1	-	0/7/9/11	0/0/0/0
1	MLY	D	182	1	-	0/7/9/11	0/0/0/0
1	MLY	D	187	1	-	0/7/9/11	0/0/0/0
1	MLY	D	196	1	-	0/7/9/11	0/0/0/0
1	MLY	D	29	1	-	0/7/9/11	0/0/0/0
1	MLY	D	54	1	-	0/7/9/11	0/0/0/0
1	MLY	D	63	1	-	0/7/9/11	0/0/0/0
1	MLY	D	72	1	-	0/7/9/11	0/0/0/0
1	MLY	D	8	1	-	0/7/9/11	0/0/0/0

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	MLY	O-C	22.94	1.27	1.11
1	C	63	MLY	O-C	22.46	1.26	1.11
1	B	63	MLY	O-C	22.12	1.26	1.11
1	A	105	MLY	O-C	20.51	1.25	1.11
1	D	196	MLY	O-C	19.80	1.25	1.11
1	A	138	MLY	O-C	19.42	1.24	1.11
1	A	119	MLY	O-C	19.39	1.24	1.11
1	B	119	MLY	O-C	19.25	1.24	1.11
1	A	196	MLY	O-C	19.10	1.24	1.11
1	B	1	MLY	O-C	18.92	1.24	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	MLY	O-C	18.90	1.24	1.11
1	C	181	MLY	O-C	18.82	1.24	1.11
1	C	124	MLY	O-C	18.79	1.24	1.11
1	B	138	MLY	O-C	18.79	1.24	1.11
1	D	8	MLY	O-C	18.77	1.24	1.11
1	D	29	MLY	O-C	18.74	1.24	1.11
1	C	119	MLY	O-C	18.66	1.24	1.11
1	D	187	MLY	O-C	18.64	1.24	1.11
1	C	138	MLY	O-C	18.49	1.24	1.11
1	D	119	MLY	O-C	18.49	1.24	1.11
1	B	182	MLY	O-C	18.47	1.24	1.11
1	C	1	MLY	O-C	18.46	1.24	1.11
1	C	145	MLY	O-C	18.42	1.24	1.11
1	B	124	MLY	O-C	18.41	1.24	1.11
1	B	8	MLY	O-C	18.39	1.24	1.11
1	C	187	MLY	O-C	18.35	1.24	1.11
1	D	124	MLY	O-C	18.35	1.24	1.11
1	B	54	MLY	O-C	18.33	1.24	1.11
1	B	72	MLY	O-C	18.33	1.24	1.11
1	D	1	MLY	O-C	18.33	1.24	1.11
1	C	182	MLY	O-C	18.33	1.24	1.11
1	B	206	MLY	O-C	18.25	1.24	1.11
1	B	187	MLY	O-C	18.19	1.23	1.11
1	D	138	MLY	O-C	18.16	1.23	1.11
1	D	181	MLY	O-C	18.13	1.23	1.11
1	B	105	MLY	O-C	18.04	1.23	1.11
1	C	29	MLY	O-C	18.01	1.23	1.11
1	B	181	MLY	O-C	18.00	1.23	1.11
1	D	54	MLY	O-C	18.00	1.23	1.11
1	A	187	MLY	O-C	18.00	1.23	1.11
1	A	182	MLY	O-C	17.97	1.23	1.11
1	A	72	MLY	O-C	17.94	1.23	1.11
1	C	54	MLY	O-C	17.94	1.23	1.11
1	A	206	MLY	O-C	17.92	1.23	1.11
1	A	181	MLY	O-C	17.88	1.23	1.11
1	D	105	MLY	O-C	17.78	1.23	1.11
1	D	63	MLY	O-C	17.77	1.23	1.11
1	B	29	MLY	O-C	17.73	1.23	1.11
1	C	72	MLY	O-C	17.72	1.23	1.11
1	A	1	MLY	O-C	17.66	1.23	1.11
1	A	8	MLY	O-C	17.62	1.23	1.11
1	C	8	MLY	O-C	17.58	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	105	MLY	O-C	17.56	1.23	1.11
1	C	196	MLY	O-C	17.53	1.23	1.11
1	A	145	MLY	O-C	17.52	1.23	1.11
1	D	145	MLY	O-C	17.51	1.23	1.11
1	D	72	MLY	O-C	17.50	1.23	1.11
1	D	182	MLY	O-C	17.48	1.23	1.11
1	A	124	MLY	O-C	17.37	1.23	1.11
1	A	29	MLY	O-C	17.28	1.23	1.11
1	B	145	MLY	O-C	17.02	1.23	1.11
1	A	54	MLY	O-C	16.84	1.23	1.11
1	A	1	MLY	CB-CA	6.39	1.58	1.53
1	A	1	MLY	CA-N	-4.42	1.17	1.49
1	C	63	MLY	CA-C	4.27	1.56	1.48
1	A	63	MLY	CA-C	3.63	1.55	1.48
1	B	29	MLY	CA-C	3.55	1.55	1.48
1	C	138	MLY	CA-C	3.38	1.54	1.48
1	B	63	MLY	CA-C	3.33	1.54	1.48
1	D	105	MLY	CA-C	3.22	1.54	1.48
1	A	105	MLY	CA-C	3.20	1.54	1.48
1	C	145	MLY	CA-C	3.20	1.54	1.48
1	B	145	MLY	CA-C	3.18	1.54	1.48
1	D	54	MLY	CA-C	3.12	1.54	1.48
1	D	138	MLY	CA-C	3.08	1.54	1.48
1	A	1	MLY	CA-C	3.06	1.54	1.48
1	C	124	MLY	CA-C	3.05	1.54	1.48
1	D	29	MLY	CA-C	3.05	1.54	1.48
1	C	182	MLY	CA-C	3.05	1.54	1.48
1	A	29	MLY	CA-C	3.05	1.54	1.48
1	C	187	MLY	CA-C	3.04	1.54	1.48
1	A	145	MLY	CA-C	3.02	1.54	1.48
1	B	119	MLY	CA-C	3.01	1.54	1.48
1	B	54	MLY	CA-C	3.01	1.54	1.48
1	B	196	MLY	CA-C	2.98	1.53	1.48
1	D	187	MLY	CA-C	2.97	1.53	1.48
1	A	72	MLY	CA-C	2.95	1.53	1.48
1	D	119	MLY	CA-C	2.92	1.53	1.48
1	C	29	MLY	CA-C	2.92	1.53	1.48
1	C	1	MLY	CA-C	2.91	1.53	1.48
1	B	181	MLY	CA-C	2.90	1.53	1.48
1	A	196	MLY	CA-C	2.86	1.53	1.48
1	C	119	MLY	CA-C	2.85	1.53	1.48
1	C	105	MLY	CA-C	2.84	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	MLY	CA-C	2.84	1.53	1.48
1	D	63	MLY	CA-C	2.83	1.53	1.48
1	A	8	MLY	CA-C	2.80	1.53	1.48
1	D	72	MLY	CA-C	2.77	1.53	1.48
1	C	72	MLY	CA-C	2.77	1.53	1.48
1	B	105	MLY	CA-C	2.75	1.53	1.48
1	A	182	MLY	CA-C	2.74	1.53	1.48
1	A	119	MLY	CA-C	2.72	1.53	1.48
1	D	145	MLY	CA-C	2.71	1.53	1.48
1	B	72	MLY	CA-C	2.70	1.53	1.48
1	D	1	MLY	CA-C	2.65	1.53	1.48
1	D	181	MLY	CA-C	2.62	1.53	1.48
1	B	182	MLY	CA-C	2.60	1.53	1.48
1	A	187	MLY	CA-C	2.58	1.53	1.48
1	C	181	MLY	CA-C	2.56	1.53	1.48
1	A	206	MLY	CA-C	2.56	1.53	1.48
1	C	8	MLY	CA-C	2.55	1.53	1.48
1	A	138	MLY	CA-C	2.55	1.53	1.48
1	B	138	MLY	CA-C	2.50	1.53	1.48
1	C	196	MLY	CA-C	2.50	1.52	1.48
1	D	182	MLY	CA-C	2.49	1.52	1.48
1	D	124	MLY	CA-C	2.49	1.52	1.48
1	D	196	MLY	CA-C	2.48	1.52	1.48
1	B	8	MLY	CA-C	2.41	1.52	1.48
1	A	181	MLY	CA-C	2.41	1.52	1.48
1	B	124	MLY	CA-C	2.40	1.52	1.48
1	D	8	MLY	CA-C	2.33	1.52	1.48
1	B	1	MLY	CA-C	2.31	1.52	1.48
1	B	187	MLY	CA-C	2.31	1.52	1.48
1	B	206	MLY	CA-C	2.26	1.52	1.48
1	C	54	MLY	CA-C	2.22	1.52	1.48
1	A	124	MLY	CA-C	2.12	1.52	1.48

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	MLY	C-CA-N	-7.86	105.97	113.83
1	A	1	MLY	C-CA-N	-7.47	106.37	113.83
1	A	138	MLY	C-CA-N	-6.90	106.94	113.83
1	D	138	MLY	C-CA-N	-6.58	107.25	113.83
1	A	196	MLY	C-CA-N	-5.30	108.54	113.83
1	B	196	MLY	C-CA-N	-4.34	109.50	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	MLY	C-CA-N	-4.31	109.52	113.83
1	C	138	MLY	C-CA-N	-4.18	109.66	113.83
1	A	181	MLY	C-CA-N	-3.46	110.37	113.83
1	B	1	MLY	C-CA-N	-3.37	110.47	113.83
1	D	182	MLY	C-CA-N	-3.33	110.51	113.83
1	A	8	MLY	C-CA-N	-3.27	110.56	113.83
1	D	119	MLY	C-CA-N	-2.95	110.88	113.83
1	A	182	MLY	C-CA-N	-2.95	110.89	113.83
1	A	124	MLY	C-CA-N	-2.94	110.89	113.83
1	C	8	MLY	C-CA-N	-2.78	111.06	113.83
1	B	1	MLY	CD-CE-NZ	-2.67	106.60	113.59
1	B	206	MLY	C-CA-N	-2.65	111.18	113.83
1	D	196	MLY	C-CA-N	-2.59	111.24	113.83
1	C	29	MLY	C-CA-N	-2.55	111.28	113.83
1	D	54	MLY	C-CA-N	2.55	116.37	113.83
1	C	1	MLY	C-CA-N	-2.52	111.31	113.83
1	C	182	MLY	C-CA-N	-2.48	111.35	113.83
1	B	8	MLY	C-CA-N	-2.48	111.36	113.83
1	D	105	MLY	C-CA-N	-2.47	111.36	113.83
1	B	105	MLY	C-CA-N	-2.37	111.46	113.83
1	D	124	MLY	C-CA-N	-2.31	111.53	113.83
1	A	105	MLY	C-CA-N	-2.30	111.53	113.83
1	A	72	MLY	C-CA-N	-2.21	111.62	113.83
1	A	119	MLY	C-CA-N	-2.19	111.64	113.83
1	C	138	MLY	CH2-NZ-CH1	-2.14	103.92	109.75
1	C	181	MLY	C-CA-N	-2.11	111.72	113.83
1	B	119	MLY	C-CA-N	-2.06	111.77	113.83
1	D	181	MLY	C-CA-N	-2.06	111.77	113.83
1	D	8	MLY	C-CA-N	-2.03	111.80	113.83
1	B	8	MLY	CH2-NZ-CH1	-2.03	104.24	109.75
1	D	54	MLY	CD-CE-NZ	-2.02	108.30	113.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

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.

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 ⓘ

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(Å²)	Q<0.9
1	A	206/207 (99%)	-0.15	1 (0%)	88	90	18, 27, 40, 53	0
1	B	207/207 (100%)	-0.10	2 (0%)	79	81	18, 26, 41, 51	0
1	C	205/207 (99%)	-0.18	1 (0%)	88	90	19, 27, 41, 49	0
1	D	203/207 (98%)	-0.12	2 (0%)	79	81	19, 27, 42, 52	0
All	All	821/828 (99%)	-0.14	6 (0%)	84	86	18, 27, 41, 53	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	MLY	3.9
1	B	207	ILE	3.0
1	A	158	THR	2.7
1	C	105	MLY	2.1
1	D	196	MLY	2.0
1	D	187	MLY	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å²)	Q<0.9
1	MLY	A	187	11/12	0.20	14.98	22,28,60,60	0
1	MLY	C	187	11/12	0.17	13.03	22,24,59,62	0
1	MLY	D	187	11/12	0.26	10.48	22,27,65,67	0
1	MLY	D	182	11/12	0.18	9.55	21,23,42,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MLY	A	1	11/12	0.24	7.27	36,46,70,71	0
1	MLY	C	182	11/12	0.13	6.12	23,24,44,48	0
1	MLY	D	196	11/12	0.26	5.79	26,32,58,62	0
1	MLY	A	206	11/12	0.19	5.56	41,45,56,59	0
1	MLY	B	187	11/12	0.16	5.49	20,26,47,54	0
1	MLY	B	206	11/12	0.37	5.13	33,48,63,65	0
1	MLY	C	181	11/12	0.13	4.43	21,28,45,47	0
1	MLY	C	124	11/12	0.16	4.36	25,28,51,53	0
1	MLY	C	1	11/12	0.17	4.34	35,39,60,65	0
1	MLY	A	182	11/12	0.13	3.74	18,22,47,48	0
1	MLY	B	196	11/12	0.20	3.63	24,29,68,70	0
1	MLY	B	182	11/12	0.14	3.61	21,23,40,42	0
1	MLY	C	105	11/12	0.27	3.56	31,36,67,71	0
1	MLY	A	124	11/12	0.14	3.51	24,25,42,48	0
1	MLY	A	181	11/12	0.15	3.15	21,27,49,53	0
1	MLY	D	105	11/12	0.20	3.13	29,36,71,71	0
1	MLY	D	119	11/12	0.20	2.84	24,34,59,61	0
1	MLY	B	181	11/12	0.14	2.64	22,28,45,46	0
1	MLY	B	72	11/12	0.17	2.53	19,26,46,50	0
1	MLY	A	119	11/12	0.21	2.29	21,25,50,52	0
1	MLY	D	181	11/12	0.12	2.27	20,24,35,36	0
1	MLY	C	119	11/12	0.20	2.18	27,32,57,57	0
1	MLY	C	63	11/12	0.17	2.14	25,31,61,63	0
1	MLY	A	196	11/12	0.22	2.07	26,35,52,52	0
1	MLY	C	196	11/12	0.21	2.03	28,32,63,69	0
1	MLY	B	54	11/12	0.19	1.90	36,40,58,60	0
1	MLY	D	124	11/12	0.12	1.90	26,28,44,45	0
1	MLY	B	138	11/12	0.13	1.86	20,23,32,35	0
1	MLY	B	124	11/12	0.12	1.59	22,26,42,44	0
1	MLY	A	105	11/12	0.18	1.47	26,36,56,58	0
1	MLY	D	72	11/12	0.17	1.43	22,29,49,55	0
1	MLY	B	1	11/12	0.15	1.28	22,29,47,47	0
1	MLY	B	119	11/12	0.17	1.24	24,29,52,57	0
1	MLY	C	29	11/12	0.11	1.22	20,21,38,38	0
1	MLY	C	145	11/12	0.13	1.03	21,24,42,48	0
1	MLY	C	72	11/12	0.13	0.94	22,30,58,58	0
1	MLY	A	29	11/12	0.10	0.89	19,22,38,42	0
1	MLY	B	8	11/12	0.15	0.85	28,36,51,53	0
1	MLY	A	145	11/12	0.13	0.79	23,26,42,46	0
1	MLY	B	105	11/12	0.15	0.75	26,36,61,65	0
1	MLY	B	29	11/12	0.09	0.74	20,22,37,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
1	MLY	A	72	11/12	0.14	0.70	24,29,48,50	0
1	MLY	D	54	11/12	0.18	0.65	42,50,61,62	0
1	MLY	C	54	11/12	0.14	0.63	24,28,49,49	0
1	MLY	D	1	11/12	0.12	0.59	29,32,56,59	0
1	MLY	D	29	11/12	0.11	0.48	20,25,45,47	0
1	MLY	C	8	11/12	0.16	0.44	34,39,52,53	0
1	MLY	D	63	11/12	0.14	0.30	27,32,54,56	0
1	MLY	D	8	11/12	0.13	0.30	27,33,43,46	0
1	MLY	B	63	11/12	0.13	0.24	25,32,46,51	0
1	MLY	D	145	11/12	0.12	0.14	25,28,42,44	0
1	MLY	C	138	11/12	0.09	-0.16	21,23,32,34	0
1	MLY	A	63	11/12	0.12	-0.25	28,30,44,48	0
1	MLY	A	54	11/12	0.10	-0.44	28,29,40,40	0
1	MLY	A	138	11/12	0.09	-0.44	22,26,35,35	0
1	MLY	D	138	11/12	0.09	-0.50	20,24,34,35	0
1	MLY	B	145	11/12	0.10	-0.60	18,25,33,34	0
1	MLY	A	8	11/12	0.10	-0.61	24,29,40,43	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å²)	Q<0.9
2	MN	A	301	1/1	0.09	1.55	17,17,17,17	0
2	MN	B	301	1/1	0.09	1.07	18,18,18,18	0
2	MN	C	301	1/1	0.08	0.81	18,18,18,18	0
2	MN	D	301	1/1	0.08	0.48	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.