



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 02:44 am BST

PDB ID : 3LSU  
Title : Crystal Structure of SOD2 from *Saccharomyces cerevisiae*  
Authors : Sheng, Y.; Cascio, D.; Valentine, J.S.  
Deposited on : 2010-02-12  
Resolution : 1.90 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](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	:	2.11
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

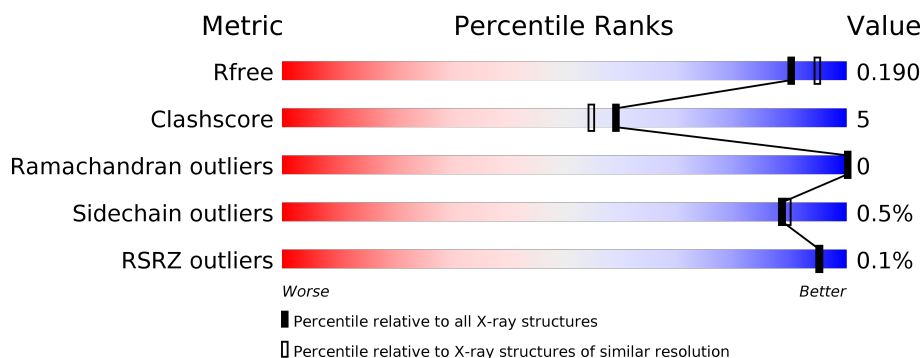
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	<div> <div></div> <div>92%7%</div> </div>
1	B	207	<div> <div></div> <div>92%8%</div> </div>
1	C	207	<div> <div></div> <div>91%9%</div> </div>
1	D	207	<div> <div></div> <div>91%9%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7111 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	276	304	3			
1	B	207	Total	C	N	O	S	0	0	0
			1668	1084	277	305	2			
1	C	206	Total	C	N	O	S	0	0	0
			1660	1078	276	304	2			
1	D	207	Total	C	N	O	S	0	0	0
			1668	1084	277	305	2			

- 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 GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	104	Total	O	0	0
			104	104		
5	C	107	Total	O	0	0
			107	107		
5	D	102	Total	O	0	0
			102	102		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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:  92% 8%



- Molecule 1: Superoxide dismutase [Mn], mitochondrial

Chain C:  91% 9%



- Molecule 1: Superoxide dismutase [Mn], mitochondrial

Chain D:  91% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.66Å 64.93Å 66.55Å 109.36° 106.35° 109.68°	Depositor
Resolution (Å)	32.38 – 1.90 37.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.2 (32.38-1.90) 89.2 (37.01-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.162 , 0.195 0.158 , 0.190	Depositor DCC
$R_{free}$ test set	3034 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for k,h,-h-k-l 0.005 for -k,-h,l 0.010 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: GOL, MN, MLY, NA

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	0.36	0/1537	0.49	0/2109
1	B	0.37	0/1537	0.50	0/2110
1	C	0.36	0/1529	0.50	0/2099
1	D	0.36	0/1537	0.50	0/2110
All	All	0.36	0/6140	0.50	0/8428

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	1632	22	0
1	B	1668	0	1634	12	0
1	C	1660	0	1624	13	0
1	D	1668	0	1636	27	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	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	8	0	0
3	D	12	0	16	1	0
4	C	1	0	0	0	0
5	A	108	0	0	1	0
5	B	104	0	0	0	0
5	C	107	0	0	2	0
5	D	102	0	0	1	0
All	All	7111	0	6558	62	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 5.

The worst 5 of 62 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:72:MLY:HH23	1:D:68:GLN:HE22	1.28	0.95
1:D:87:ASN:HD22	1:D:201:ARG:HH12	1.17	0.91
1:A:87:ASN:HD22	1:A:201:ARG:HH12	1.21	0.88
1:B:87:ASN:HD22	1:B:201:ARG:HH12	1.24	0.85
1:C:87:ASN:HD22	1:C:201:ARG:HH12	1.27	0.82

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%)	187 (98%)	4 (2%)	0	100	100
1	B	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
1	C	190/207 (92%)	188 (99%)	2 (1%)	0	100	100
1	D	190/207 (92%)	186 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	761/828 (92%)	747 (98%)	14 (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%)	153 (99%)	1 (1%)	86	87
1	B	154/154 (100%)	153 (99%)	1 (1%)	86	87
1	C	153/154 (99%)	152 (99%)	1 (1%)	84	84
1	D	154/154 (100%)	154 (100%)	0	100	100
All	All	615/616 (100%)	612 (100%)	3 (0%)	88	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	B	160	PRO
1	C	150	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	87	ASN
1	C	153	ASN
1	D	68	GLN
1	B	153	ASN
1	D	46	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

64 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	196	1	9,10,11	1.12	1 (11%)	6,11,13	0.96	0
1	MLY	A	206	1	9,10,11	1.17	1 (11%)	6,11,13	1.00	0
1	MLY	C	124	1	9,10,11	0.82	0	6,11,13	0.70	0
1	MLY	A	124	1	9,10,11	0.91	0	6,11,13	0.61	0
1	MLY	C	54	1	9,10,11	0.91	0	6,11,13	0.96	1 (16%)
1	MLY	C	72	1	9,10,11	0.99	0	6,11,13	0.74	0
1	MLY	C	119	1	9,10,11	1.13	1 (11%)	6,11,13	0.89	0
1	MLY	B	54	1	9,10,11	0.99	0	6,11,13	0.88	0
1	MLY	C	196	1	9,10,11	1.05	0	6,11,13	0.99	0
1	MLY	D	182	1	9,10,11	1.07	1 (11%)	6,11,13	0.83	0
1	MLY	A	196	1	9,10,11	0.98	0	6,11,13	0.62	0
1	MLY	C	63	1	9,10,11	0.91	0	6,11,13	0.88	0
1	MLY	D	8	1	9,10,11	1.02	0	6,11,13	0.79	0
1	MLY	D	181	1	9,10,11	0.80	0	6,11,13	0.56	0
1	MLY	A	8	1	9,10,11	1.09	1 (11%)	6,11,13	0.88	0
1	MLY	A	54	1	9,10,11	0.95	0	6,11,13	0.75	0
1	MLY	C	187	1	9,10,11	1.13	1 (11%)	6,11,13	0.86	0
1	MLY	D	206	1	9,10,11	1.07	1 (11%)	6,11,13	1.16	1 (16%)
1	MLY	C	145	1	9,10,11	1.04	0	6,11,13	1.06	1 (16%)
1	MLY	B	145	1	9,10,11	0.82	0	6,11,13	0.72	0
1	MLY	D	119	1	9,10,11	0.98	0	6,11,13	0.69	0
1	MLY	B	206	1	9,10,11	0.97	0	6,11,13	1.00	0
1	MLY	A	145	1	9,10,11	1.00	1 (11%)	6,11,13	0.70	0
1	MLY	B	138	1	9,10,11	0.92	0	6,11,13	1.23	1 (16%)
1	MLY	D	138	1	9,10,11	0.91	0	6,11,13	0.54	0
1	MLY	B	8	1	9,10,11	1.04	1 (11%)	6,11,13	0.98	0
1	MLY	D	54	1	9,10,11	1.04	0	6,11,13	1.01	0
1	MLY	B	181	1	9,10,11	0.89	0	6,11,13	0.85	0
1	MLY	A	105	1	9,10,11	1.09	1 (11%)	6,11,13	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	1	1	9,10,11	0.94	0	6,11,13	0.91	0
1	MLY	B	1	1	9,10,11	1.11	1 (11%)	6,11,13	1.09	0
1	MLY	B	119	1	9,10,11	1.02	0	6,11,13	1.01	0
1	MLY	C	105	1	9,10,11	1.10	1 (11%)	6,11,13	0.87	0
1	MLY	D	72	1	9,10,11	0.95	0	6,11,13	0.96	0
1	MLY	B	72	1	9,10,11	1.10	1 (11%)	6,11,13	1.04	0
1	MLY	C	206	1	9,10,11	1.04	1 (11%)	6,11,13	0.96	0
1	MLY	D	105	1	9,10,11	1.07	1 (11%)	6,11,13	0.95	0
1	MLY	C	182	1	9,10,11	1.14	1 (11%)	6,11,13	1.10	0
1	MLY	B	63	1	9,10,11	0.93	0	6,11,13	0.82	0
1	MLY	C	29	1	9,10,11	1.00	1 (11%)	6,11,13	0.74	0
1	MLY	A	63	1	9,10,11	0.99	0	6,11,13	0.83	0
1	MLY	A	72	1	9,10,11	0.95	0	6,11,13	0.99	0
1	MLY	A	181	1	9,10,11	0.90	0	6,11,13	0.75	0
1	MLY	A	182	1	9,10,11	1.04	0	6,11,13	0.86	0
1	MLY	D	196	1	9,10,11	1.01	0	6,11,13	0.96	1 (16%)
1	MLY	A	29	1	9,10,11	0.96	0	6,11,13	0.65	0
1	MLY	A	138	1	9,10,11	0.85	0	6,11,13	0.63	0
1	MLY	B	124	1	9,10,11	0.90	0	6,11,13	0.96	0
1	MLY	B	187	1	9,10,11	1.06	1 (11%)	6,11,13	1.10	1 (16%)
1	MLY	A	187	1	9,10,11	1.04	1 (11%)	6,11,13	0.88	0
1	MLY	A	119	1	9,10,11	1.02	1 (11%)	6,11,13	0.81	0
1	MLY	D	124	1	9,10,11	0.91	0	6,11,13	0.61	0
1	MLY	D	29	1	9,10,11	1.10	1 (11%)	6,11,13	0.66	0
1	MLY	D	187	1	9,10,11	0.97	0	6,11,13	0.86	0
1	MLY	B	29	1	9,10,11	0.92	0	6,11,13	0.67	0
1	MLY	D	1	1	9,10,11	1.00	1 (11%)	6,11,13	1.05	0
1	MLY	B	105	1	9,10,11	1.06	1 (11%)	6,11,13	0.96	0
1	MLY	C	8	1	9,10,11	0.96	1 (11%)	6,11,13	0.77	0
1	MLY	C	181	1	9,10,11	0.78	0	6,11,13	0.68	0
1	MLY	D	63	1	9,10,11	0.97	0	6,11,13	0.92	0
1	MLY	B	182	1	9,10,11	0.94	0	6,11,13	1.06	1 (16%)
1	MLY	D	145	1	9,10,11	0.94	0	6,11,13	0.90	0
1	MLY	C	1	1	9,10,11	1.03	1 (11%)	6,11,13	1.12	1 (16%)
1	MLY	C	138	1	9,10,11	0.91	0	6,11,13	0.61	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	196	1	-	2/8/9/11	-
1	MLY	A	206	1	-	7/8/9/11	-
1	MLY	C	124	1	-	2/8/9/11	-
1	MLY	A	124	1	-	2/8/9/11	-
1	MLY	C	54	1	-	2/8/9/11	-
1	MLY	C	72	1	-	1/8/9/11	-
1	MLY	C	119	1	-	2/8/9/11	-
1	MLY	B	54	1	-	5/8/9/11	-
1	MLY	C	196	1	-	3/8/9/11	-
1	MLY	D	182	1	-	0/8/9/11	-
1	MLY	A	196	1	-	0/8/9/11	-
1	MLY	C	63	1	-	4/8/9/11	-
1	MLY	D	8	1	-	0/8/9/11	-
1	MLY	D	181	1	-	0/8/9/11	-
1	MLY	A	8	1	-	2/8/9/11	-
1	MLY	A	54	1	-	1/8/9/11	-
1	MLY	C	187	1	-	1/8/9/11	-
1	MLY	D	206	1	-	5/8/9/11	-
1	MLY	C	145	1	-	4/8/9/11	-
1	MLY	B	145	1	-	1/8/9/11	-
1	MLY	D	119	1	-	2/8/9/11	-
1	MLY	B	206	1	-	2/8/9/11	-
1	MLY	A	145	1	-	0/8/9/11	-
1	MLY	B	138	1	-	1/8/9/11	-
1	MLY	D	138	1	-	2/8/9/11	-
1	MLY	B	8	1	-	4/8/9/11	-
1	MLY	D	54	1	-	3/8/9/11	-
1	MLY	B	181	1	-	3/8/9/11	-
1	MLY	A	105	1	-	2/8/9/11	-
1	MLY	A	1	1	-	4/8/9/11	-
1	MLY	B	1	1	-	1/8/9/11	-
1	MLY	B	119	1	-	2/8/9/11	-
1	MLY	C	105	1	-	2/8/9/11	-
1	MLY	D	72	1	-	2/8/9/11	-
1	MLY	B	72	1	-	2/8/9/11	-
1	MLY	C	206	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	105	1	-	2/8/9/11	-
1	MLY	C	182	1	-	3/8/9/11	-
1	MLY	B	63	1	-	2/8/9/11	-
1	MLY	C	29	1	-	0/8/9/11	-
1	MLY	A	63	1	-	0/8/9/11	-
1	MLY	A	72	1	-	2/8/9/11	-
1	MLY	A	181	1	-	0/8/9/11	-
1	MLY	A	182	1	-	4/8/9/11	-
1	MLY	D	196	1	-	3/8/9/11	-
1	MLY	A	29	1	-	0/8/9/11	-
1	MLY	A	138	1	-	2/8/9/11	-
1	MLY	B	124	1	-	3/8/9/11	-
1	MLY	B	187	1	-	3/8/9/11	-
1	MLY	A	187	1	-	2/8/9/11	-
1	MLY	A	119	1	-	2/8/9/11	-
1	MLY	D	124	1	-	2/8/9/11	-
1	MLY	D	29	1	-	1/8/9/11	-
1	MLY	D	187	1	-	2/8/9/11	-
1	MLY	B	29	1	-	0/8/9/11	-
1	MLY	D	1	1	-	3/8/9/11	-
1	MLY	B	105	1	-	2/8/9/11	-
1	MLY	C	8	1	-	2/8/9/11	-
1	MLY	C	181	1	-	2/8/9/11	-
1	MLY	D	63	1	-	2/8/9/11	-
1	MLY	B	182	1	-	0/8/9/11	-
1	MLY	D	145	1	-	4/8/9/11	-
1	MLY	C	1	1	-	5/8/9/11	-
1	MLY	C	138	1	-	2/8/9/11	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	29	MLY	CB-CA	2.60	1.57	1.53
1	C	187	MLY	CB-CA	2.55	1.57	1.53
1	A	206	MLY	CB-CA	2.46	1.56	1.53
1	B	1	MLY	CB-CA	2.44	1.56	1.53
1	C	119	MLY	CB-CA	2.39	1.56	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	206	MLY	CD-CE-NZ	2.61	120.84	113.79
1	B	138	MLY	CD-CE-NZ	2.53	120.65	113.79
1	C	1	MLY	CD-CE-NZ	2.18	119.68	113.79
1	B	182	MLY	CD-CE-NZ	2.12	119.53	113.79
1	B	187	MLY	CD-CE-NZ	2.10	119.48	113.79

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	206	MLY	N-CA-CB-CG
1	A	206	MLY	C-CA-CB-CG
1	C	54	MLY	O-C-CA-CB
1	D	206	MLY	N-CA-CB-CG
1	D	206	MLY	C-CA-CB-CG

There are no ring outliers.

16 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	124	MLY	1	0
1	C	72	MLY	1	0
1	C	119	MLY	1	0
1	C	145	MLY	1	0
1	D	119	MLY	1	0
1	B	181	MLY	1	0
1	A	1	MLY	1	0
1	C	105	MLY	1	0
1	C	182	MLY	1	0
1	C	29	MLY	1	0
1	A	72	MLY	2	0
1	B	124	MLY	1	0
1	B	29	MLY	1	0
1	C	8	MLY	1	0
1	C	181	MLY	1	0
1	D	145	MLY	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
3	GOL	C	210	4	5,5,5	0.37	0	5,5,5	0.38	0
3	GOL	B	209	-	5,5,5	0.40	0	5,5,5	0.23	0
3	GOL	D	209	-	5,5,5	0.43	0	5,5,5	0.60	0
3	GOL	D	210	-	5,5,5	0.44	0	5,5,5	0.38	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
3	GOL	C	210	4	-	0/4/4/4	-
3	GOL	B	209	-	-	4/4/4/4	-
3	GOL	D	209	-	-	2/4/4/4	-
3	GOL	D	210	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	209	GOL	O1-C1-C2-C3
3	B	209	GOL	C1-C2-C3-O3
3	B	209	GOL	O2-C2-C3-O3
3	D	209	GOL	O1-C1-C2-C3
3	D	210	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	210	GOL	1	0

## 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%)	-0.33	0	100 100	18, 23, 32, 43	0
1	B	191/207 (92%)	-0.49	0	100 100	17, 22, 34, 42	0
1	C	190/207 (91%)	-0.51	0	100 100	17, 22, 32, 41	0
1	D	191/207 (92%)	-0.33	1 (0%)	91 92	17, 22, 35, 44	0
All	All	762/828 (92%)	-0.41	1 (0%)	95 95	17, 22, 33, 44	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	45	PHE	3.1

### 6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	A	206	11/12	0.82	0.32	34,45,60,64	0
1	MLY	C	1	11/12	0.85	0.20	32,42,59,63	0
1	MLY	C	206	11/12	0.86	0.21	31,41,69,71	0
1	MLY	B	54	11/12	0.89	0.24	43,47,63,65	0
1	MLY	A	1	11/12	0.89	0.25	31,37,57,58	0
1	MLY	A	8	11/12	0.91	0.13	24,27,39,40	0
1	MLY	D	1	11/12	0.91	0.13	25,30,47,53	0
1	MLY	C	105	11/12	0.91	0.25	26,31,59,59	0
1	MLY	A	72	11/12	0.92	0.14	20,24,50,52	0
1	MLY	D	196	11/12	0.92	0.23	21,32,58,60	0
1	MLY	A	119	11/12	0.92	0.19	22,26,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	105	11/12	0.92	0.28	21,28,55,57	0
1	MLY	B	187	11/12	0.92	0.19	18,24,66,67	0
1	MLY	D	8	11/12	0.92	0.13	28,30,39,39	0
1	MLY	C	119	11/12	0.93	0.13	22,25,40,42	0
1	MLY	A	187	11/12	0.93	0.17	21,24,68,69	0
1	MLY	C	72	11/12	0.93	0.13	20,23,40,40	0
1	MLY	C	187	11/12	0.93	0.15	19,22,47,52	0
1	MLY	C	181	11/12	0.93	0.14	19,21,40,46	0
1	MLY	D	54	11/12	0.93	0.35	38,44,69,72	0
1	MLY	B	181	11/12	0.93	0.12	19,23,35,38	0
1	MLY	C	196	11/12	0.94	0.13	21,30,49,52	0
1	MLY	C	63	11/12	0.94	0.12	22,25,44,47	0
1	MLY	D	206	11/12	0.94	0.10	27,30,43,49	0
1	MLY	B	206	11/12	0.94	0.13	22,27,39,46	0
1	MLY	B	182	11/12	0.94	0.13	19,20,43,46	0
1	MLY	A	145	11/12	0.94	0.11	19,22,34,39	0
1	MLY	B	196	11/12	0.94	0.19	21,26,55,58	0
1	MLY	A	182	11/12	0.94	0.13	16,22,46,46	0
1	MLY	A	124	11/12	0.95	0.10	19,20,39,44	0
1	MLY	C	8	11/12	0.95	0.12	24,26,41,48	0
1	MLY	B	124	11/12	0.95	0.11	19,22,40,44	0
1	MLY	B	119	11/12	0.95	0.19	20,26,55,56	0
1	MLY	C	145	11/12	0.95	0.12	19,21,31,39	0
1	MLY	B	29	11/12	0.95	0.09	18,21,38,40	0
1	MLY	D	72	11/12	0.95	0.12	20,23,40,40	0
1	MLY	B	72	11/12	0.95	0.11	17,20,40,41	0
1	MLY	D	119	11/12	0.95	0.12	20,24,44,44	0
1	MLY	D	63	11/12	0.95	0.13	29,33,51,55	0
1	MLY	D	105	11/12	0.95	0.16	21,29,66,67	0
1	MLY	D	182	11/12	0.95	0.10	18,21,33,37	0
1	MLY	B	1	11/12	0.96	0.09	20,26,39,45	0
1	MLY	C	182	11/12	0.96	0.09	17,20,41,47	0
1	MLY	D	124	11/12	0.96	0.09	18,21,35,38	0
1	MLY	D	187	11/12	0.96	0.12	17,21,57,57	0
1	MLY	A	196	11/12	0.96	0.10	20,22,32,33	0
1	MLY	C	29	11/12	0.96	0.09	17,20,33,33	0
1	MLY	B	105	11/12	0.96	0.13	22,28,58,60	0
1	MLY	A	63	11/12	0.96	0.09	23,26,47,49	0
1	MLY	A	181	11/12	0.96	0.10	19,24,41,45	0
1	MLY	C	124	11/12	0.96	0.09	19,23,41,44	0
1	MLY	A	54	11/12	0.96	0.10	21,25,42,47	0
1	MLY	B	138	11/12	0.96	0.10	16,18,25,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	D	138	11/12	0.97	0.09	17,20,25,25	0
1	MLY	B	8	11/12	0.97	0.12	22,31,37,42	0
1	MLY	A	138	11/12	0.97	0.08	16,18,28,29	0
1	MLY	C	54	11/12	0.97	0.08	17,24,37,38	0
1	MLY	D	145	11/12	0.97	0.09	19,22,42,42	0
1	MLY	B	63	11/12	0.97	0.11	23,28,47,50	0
1	MLY	B	145	11/12	0.97	0.09	16,19,31,33	0
1	MLY	D	181	11/12	0.97	0.08	17,20,23,26	0
1	MLY	D	29	11/12	0.97	0.08	19,22,37,38	0
1	MLY	C	138	11/12	0.97	0.07	19,22,30,30	0
1	MLY	A	29	11/12	0.98	0.08	17,20,36,38	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, 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
3	GOL	D	210	6/6	0.88	0.13	24,35,37,42	0
3	GOL	C	210	6/6	0.90	0.15	29,32,35,43	0
3	GOL	B	209	6/6	0.91	0.13	33,37,38,43	0
3	GOL	D	209	6/6	0.93	0.13	23,24,28,30	0
4	NA	C	209	1/1	0.94	0.08	32,32,32,32	0
2	MN	A	208	1/1	1.00	0.08	19,19,19,19	0
2	MN	C	208	1/1	1.00	0.09	19,19,19,19	0
2	MN	D	208	1/1	1.00	0.07	18,18,18,18	0
2	MN	B	208	1/1	1.00	0.08	18,18,18,18	0

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

There are no such residues in this entry.