



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 02:36 am BST

PDB ID : 3LOY  
Title : Crystal structure of a Copper-containing benzylamine oxidase from Hansenula Polymorpha  
Authors : Klema, V.J.; Johnson, B.J.; Wilmot, C.M.  
Deposited on : 2010-02-04  
Resolution : 2.00 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

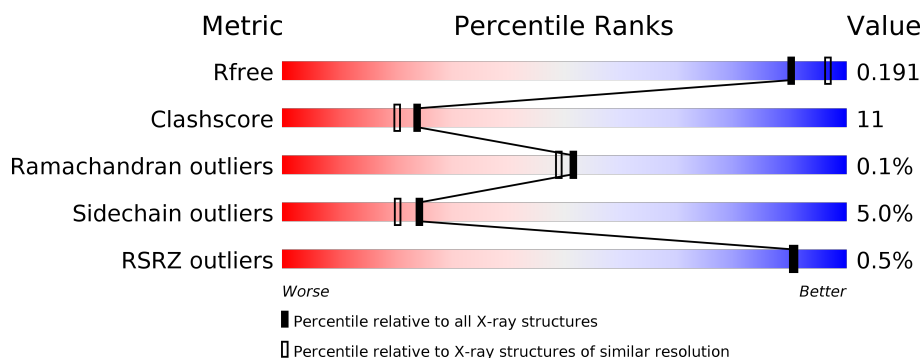
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	633	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>83%</span> <span>14%</span> <span>..</span> </div> </div>
1	B	633	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>77%</span> <span>19%</span> <span>..</span> </div> </div>
1	C	633	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>15%</span> <span>..</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	637	-	X	-	-
3	GOL	B	639	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18610 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 copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	6	0
			5115	3275	870	944	26			
1	B	633	Total	C	N	O	S	0	6	0
			5120	3276	874	943	27			
1	C	633	Total	C	N	O	S	0	1	0
			5086	3255	867	939	25			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

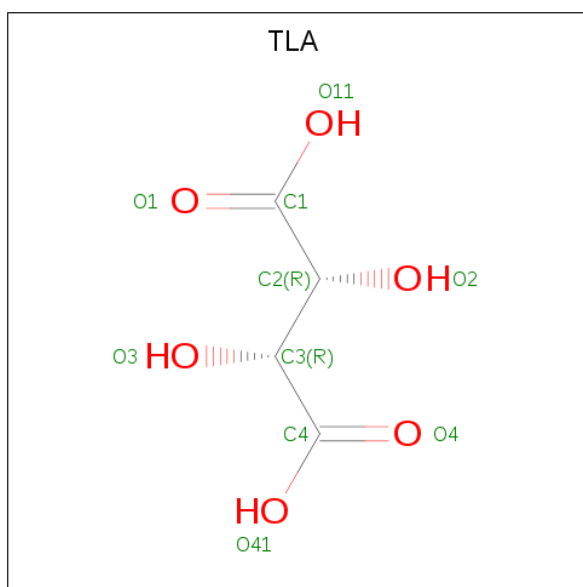
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

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



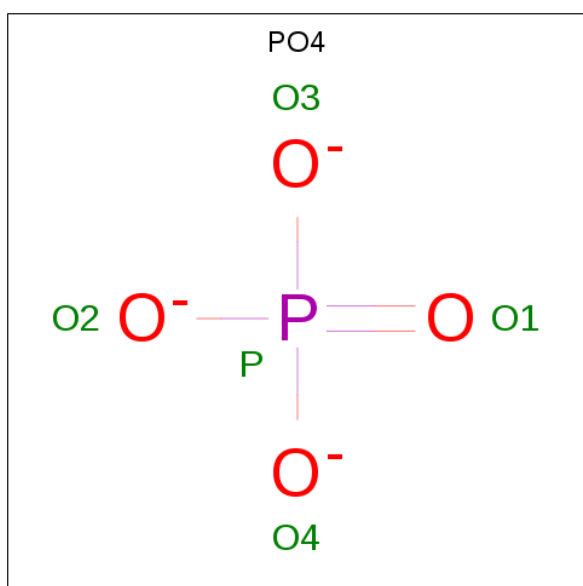
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total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

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

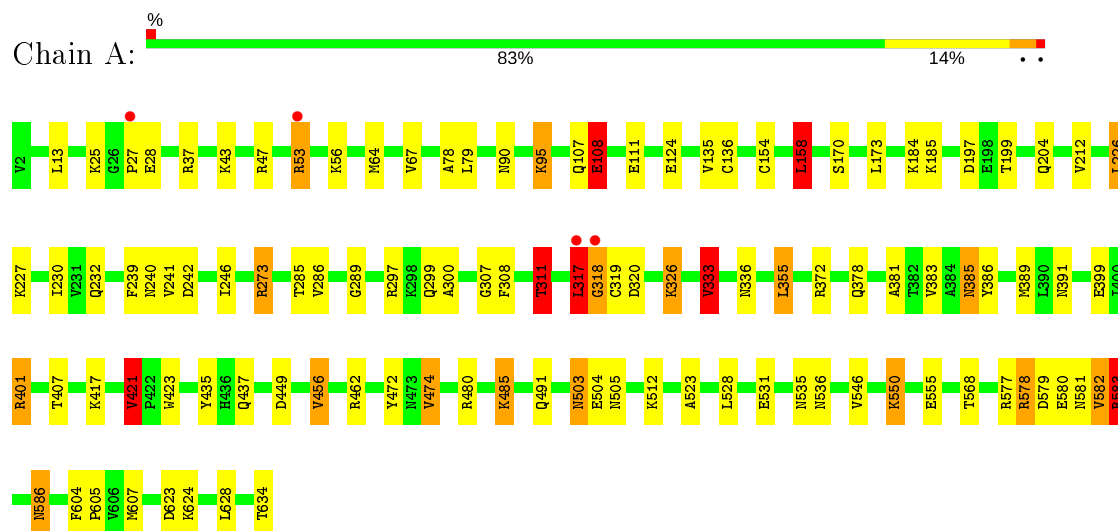
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1028	Total 1028	O 1028	0	0
6	B	1051	Total 1051	O 1051	0	0
6	C	1116	Total 1116	O 1116	0	0

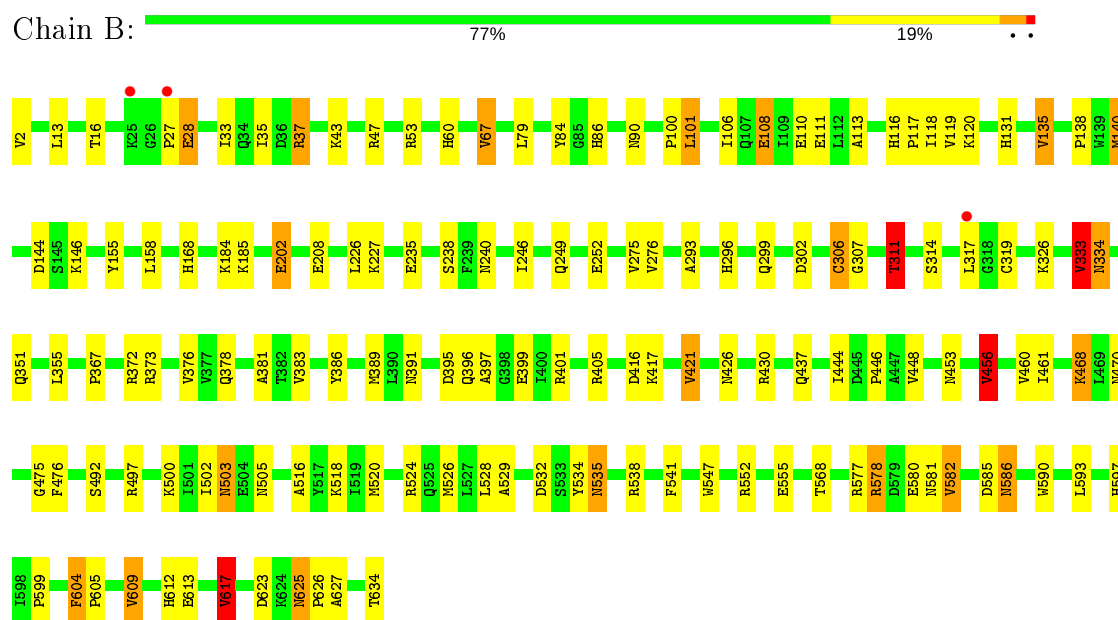
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: copper amine oxidase



- Molecule 1: copper amine oxidase



- Molecule 1: copper amine oxidase

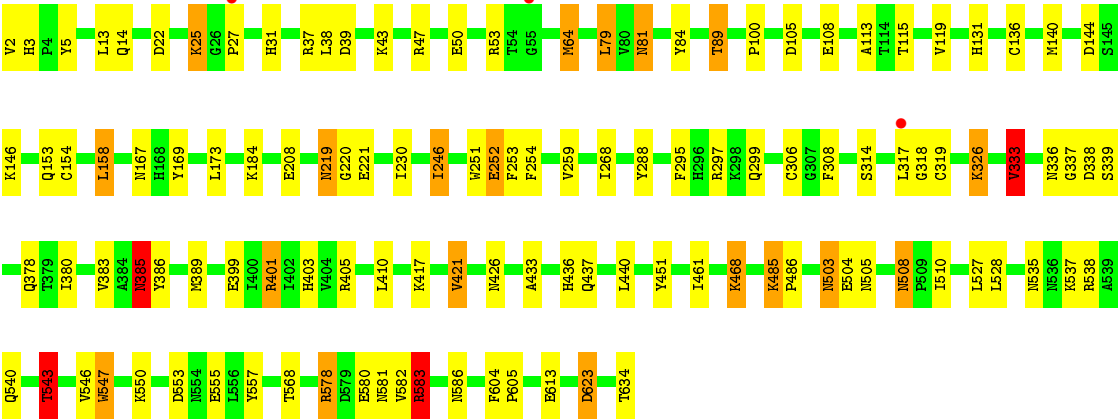


Chain C: 

81%

15%

••



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	288.51Å 91.06Å 151.10Å 90.00° 117.23° 90.00°	Depositor
Resolution (Å)	37.42 – 2.00 37.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.4 (37.42-2.00) 90.4 (37.42-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.145 , 0.191 0.146 , 0.191	Depositor DCC
$R_{free}$ test set	10514 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	18610	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 3.51% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, CU, TLA, TPQ

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	1.17	3/5253 (0.1%)	1.08	22/7149 (0.3%)
1	B	1.22	13/5255 (0.2%)	1.05	16/7151 (0.2%)
1	C	1.25	7/5212 (0.1%)	1.06	21/7096 (0.3%)
All	All	1.21	23/15720 (0.1%)	1.06	59/21396 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLU	CB-CG	-8.01	1.36	1.52
1	C	295	PHE	CE1-CZ	7.79	1.52	1.37
1	B	202	GLU	CG-CD	7.31	1.62	1.51
1	C	546	VAL	CB-CG2	-7.24	1.37	1.52
1	C	254	PHE	CE1-CZ	6.72	1.50	1.37

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	583	ARG	NE-CZ-NH1	15.74	128.17	120.30
1	A	578	ARG	NE-CZ-NH2	-14.90	112.85	120.30
1	B	578	ARG	NE-CZ-NH2	-13.37	113.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	583	ARG	NE-CZ-NH1	12.97	126.78	120.30
1	A	583	ARG	NE-CZ-NH2	-12.44	114.08	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	LEU	Peptide
1	A	318	GLY	Peptide
1	C	385	ASN	Mainchain

## 5.2 Too-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 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	5115	0	5032	87	0
1	B	5120	0	5034	145	1
1	C	5086	0	4991	111	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	24	0	32	2	0
3	B	24	0	31	9	0
3	C	18	0	24	3	0
4	A	10	0	4	0	0
4	C	10	0	4	1	0
5	B	5	0	0	0	0
6	A	1028	0	0	36	0
6	B	1051	0	0	44	1
6	C	1116	0	0	46	0
All	All	18610	0	15152	340	2

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 11.

The worst 5 of 340 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:623:ASP:HB3	6:A:3187:HOH:O	1.15	1.32
1:C:623:ASP:HB3	6:C:2705:HOH:O	1.20	1.30
1:B:623:ASP:HB3	6:B:1917:HOH:O	1.28	1.28
1:B:43:LYS:HB2	6:B:1590:HOH:O	1.27	1.27
1:C:634:THR:HA	6:C:2441:HOH:O	1.49	1.11

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:TYR:OH	1:B:86:HIS:NE2[2_556]	2.02	0.18
6:B:1986:HOH:O	6:B:2006:HOH:O[2_556]	2.17	0.03

## 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	636/633 (100%)	618 (97%)	17 (3%)	1 (0%)	47	44
1	B	636/633 (100%)	619 (97%)	17 (3%)	0	100	100
1	C	631/633 (100%)	613 (97%)	18 (3%)	0	100	100
All	All	1903/1899 (100%)	1850 (97%)	52 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	LEU

### 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	563/558 (101%)	534 (95%)	29 (5%)	23	19
1	B	563/558 (101%)	534 (95%)	29 (5%)	23	19
1	C	558/558 (100%)	533 (96%)	25 (4%)	27	24
All	All	1684/1674 (101%)	1601 (95%)	83 (5%)	24	21

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	140	MET
1	B	333	VAL
1	C	468	LYS
1	B	146	LYS
1	B	246	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	391	ASN
1	B	503	ASN
1	C	437	GLN
1	B	426	ASN
1	B	453	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	TPQ	C	386	1	13,14,15	1.54	4 (30%)	15,19,21	1.61	3 (20%)
1	TPQ	B	386	1	13,14,15	1.89	6 (46%)	15,19,21	1.63	4 (26%)
1	TPQ	A	386	1	13,14,15	2.44	6 (46%)	15,19,21	1.98	2 (13%)

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	TPQ	C	386	1	-	0/5/22/24	0/1/1/1
1	TPQ	B	386	1	-	0/5/22/24	0/1/1/1
1	TPQ	A	386	1	-	0/5/22/24	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	TPQ	O2-C2	4.18	1.35	1.24
1	A	386	TPQ	O5-C5	4.04	1.35	1.24
1	A	386	TPQ	C3-C4	3.97	1.41	1.35
1	B	386	TPQ	O5-C5	3.08	1.32	1.24
1	C	386	TPQ	O5-C5	2.90	1.32	1.24

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	TPQ	CB-CA-C	-5.86	100.48	111.47
1	B	386	TPQ	CB-CA-C	-3.87	104.21	111.47
1	C	386	TPQ	CB-CA-C	-3.44	105.01	111.47
1	A	386	TPQ	C6-C1-C2	3.29	121.16	118.64
1	C	386	TPQ	C6-C5-C4	2.69	121.59	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	386	TPQ	1	0
1	B	386	TPQ	1	0
1	A	386	TPQ	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	A	638	-	5,5,5	1.04	0	5,5,5	1.05	1 (20%)
3	GOL	C	638	-	5,5,5	0.57	0	5,5,5	1.03	0
3	GOL	B	640	-	5,5,5	0.34	0	5,5,5	0.99	0
3	GOL	B	637	-	5,5,5	0.42	0	5,5,5	0.73	0
5	PO4	B	638	-	4,4,4	0.90	0	6,6,6	0.61	0
4	TLA	C	637	-	3,9,9	0.50	0	6,12,12	1.97	2 (33%)
4	TLA	A	640	-	3,9,9	1.76	1 (33%)	6,12,12	1.32	1 (16%)
3	GOL	B	639	-	5,5,5	0.66	0	5,5,5	1.11	0
3	GOL	A	639	-	5,5,5	0.48	0	5,5,5	0.96	1 (20%)
3	GOL	C	636	-	5,5,5	0.97	0	5,5,5	0.93	0
3	GOL	C	639	-	5,5,5	0.39	0	5,5,5	0.79	0
3	GOL	A	636	-	5,5,5	0.46	0	5,5,5	1.30	1 (20%)
3	GOL	B	636	-	5,5,5	1.05	0	5,5,5	0.85	0
3	GOL	A	637	-	5,5,5	0.36	0	5,5,5	1.95	2 (40%)

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	A	638	-	-	0/4/4/4	-
3	GOL	C	638	-	-	4/4/4/4	-
3	GOL	B	640	-	-	3/4/4/4	-
3	GOL	B	637	-	-	0/4/4/4	-
4	TLA	C	637	-	-	0/4/12/12	-
4	TLA	A	640	-	-	0/4/12/12	-
3	GOL	B	639	-	-	2/4/4/4	-
3	GOL	A	639	-	-	0/4/4/4	-
3	GOL	C	636	-	-	2/4/4/4	-
3	GOL	C	639	-	-	0/4/4/4	-
3	GOL	A	636	-	-	2/4/4/4	-
3	GOL	B	636	-	-	2/4/4/4	-
3	GOL	A	637	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	640	TLA	O2-C2	2.23	1.47	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	637	TLA	C1-C2-C3	-3.30	106.01	113.11
4	C	637	TLA	O3-C3-C4	-2.98	103.92	111.10
3	A	637	GOL	O3-C3-C2	-2.93	96.17	110.20
3	A	637	GOL	O2-C2-C1	2.82	121.55	109.12
4	A	640	TLA	C4-C3-C2	-2.45	107.83	113.11

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	640	GOL	C1-C2-C3-O3
3	C	638	GOL	O1-C1-C2-C3
3	C	638	GOL	C1-C2-C3-O3
3	C	636	GOL	O1-C1-C2-C3
3	A	636	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	638	GOL	1	0
3	B	640	GOL	3	0
4	C	637	TLA	1	0
3	B	639	GOL	6	0
3	A	639	GOL	2	0
3	C	639	GOL	2	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 [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, 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	632/633 (99%)	-0.78	4 (0%) 89 88	17, 24, 39, 59	0
1	B	632/633 (99%)	-0.79	3 (0%) 91 90	16, 25, 40, 62	0
1	C	632/633 (99%)	-0.86	3 (0%) 91 90	15, 22, 36, 57	0
All	All	1896/1899 (99%)	-0.81	10 (0%) 91 90	15, 24, 39, 62	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	LEU	7.0
1	A	317	LEU	3.9
1	C	317	LEU	3.4
1	A	53	ARG	2.6
1	A	27	PRO	2.4

### 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, 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	TPQ	B	386	14/15	0.96	0.10	18,24,27,28	1
1	TPQ	C	386	14/15	0.97	0.13	16,22,29,29	1
1	TPQ	A	386	14/15	0.98	0.14	18,26,29,29	1

### 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(Å <sup>2</sup> )	Q<0.9
5	PO4	B	638	5/5	0.82	0.34	125,125,126,126	0
3	GOL	B	640	6/6	0.87	0.14	40,52,54,60	0
3	GOL	B	639	6/6	0.91	0.13	48,56,57,57	0
3	GOL	C	639	6/6	0.91	0.13	53,54,57,58	0
3	GOL	A	637	6/6	0.92	0.13	35,41,44,45	0
3	GOL	A	639	6/6	0.93	0.11	39,43,46,51	0
3	GOL	B	636	6/6	0.95	0.09	20,26,31,31	0
3	GOL	B	637	6/6	0.95	0.13	41,42,45,47	0
3	GOL	A	638	6/6	0.96	0.08	21,27,29,30	0
3	GOL	A	636	6/6	0.96	0.18	49,53,56,56	0
3	GOL	C	638	6/6	0.96	0.12	41,51,57,58	0
3	GOL	C	636	6/6	0.96	0.08	21,30,31,31	0
4	TLA	A	640	10/10	0.98	0.06	21,25,28,28	0
4	TLA	C	637	10/10	0.99	0.05	24,27,30,30	0
2	CU	B	635	1/1	1.00	0.07	24,24,24,24	0
2	CU	C	635	1/1	1.00	0.07	21,21,21,21	0
2	CU	A	635	1/1	1.00	0.07	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.