

wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2023 – 02:55 AM EDT

:	1DO1
:	CARBONMONOXY-MYOGLOBIN MUTANT L29W AT 105K
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:	1999-12-18
:	1.50 Å(reported)
	:

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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
Clashscore		IL	1
Ramachandran outliers			0
Sidechain outliers			0
	Worse	Bette	r
	Percentile relative to all X-ray structures		
	Percentile relative to X-ray structures of similar	resolution	

Metric	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	А	154	97%
2	В	2	100%



1DO1

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 1492 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 MYOGLOBIN.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	153	Total 1223	C 788	N 218	0 215	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	FME	MET	modified residue	UNP P02185
А	29	TRP	LEU	engineered mutation	UNP P02185
А	122	ASN	ASP	engineered mutation	UNP P02185

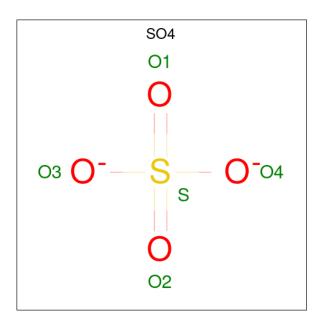
• Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	At	\mathbf{oms}		ZeroOcc	AltConf	Trace
2	В	2	Total 23	C 12	0 11	0	0	0

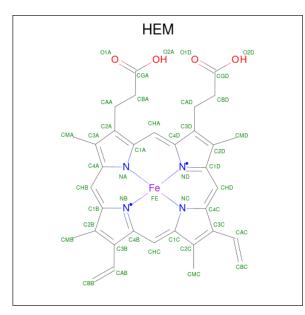
• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

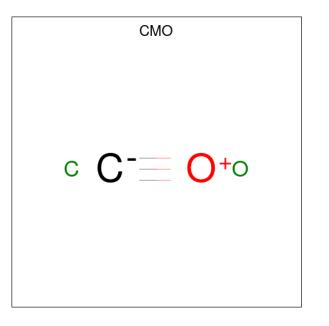
• Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
4	Δ	1	Total	С	Fe	Ν	0	0	0
4	4 A	1	43	34	1	4	4	0	0



• Molecule 5 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 2 1 1 \end{array}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	191	Total O 191 191	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. 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. 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.

Note EDS was not executed.

• Molecule 1: MYOGLOBIN

Chain B:

GLC1 GLC2 100%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 6	Depositor	
Cell constants	90.46Å 90.46Å 45.26Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	7.00 - 1.50	Depositor	
% Data completeness	94.5 (7.00-1.50)	Depositor	
(in resolution range)	54.0 (1.00-1.00)	Depositor	
R_{merge}	0.04	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	X-PLOR 3.1	Depositor	
R, R_{free}	0.189 , 0.215	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1492	wwPDB-VP	
Average B, all atoms $(Å^2)$	11.0	wwPDB-VP	



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: HEM, SO4, GLC, CMO

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.33	0/1253	0.50	0/1683	

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	А	1223	0	1243	3	0
2	В	23	0	21	0	0
3	А	10	0	0	0	0
4	А	43	0	30	0	0
5	А	2	0	0	0	0
6	А	191	0	0	1	0
All	All	1492	0	1294	3	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 1.

All (3) 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:83:GLU:H	1:A:83:GLU:CD	2.16	0.49	
1:A:151:TYR:CE2	1:A:153:GLY:HA2	2.55	0.42	
1:A:118:ARG:NH2	6:A:212:HOH:O	2.53	0.41	

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 Allowe		Outliers	Percentiles		
1	А	151/154~(98%)	148 (98%)	3~(2%)	0	100	100	

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	А	125/125~(100%)	125~(100%)	0	100 100	

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

2 monosaccharides 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).

Mal	Mol Type Chain	Chain	Chain Res	Res Link	Bo	Bond lengths			Bond angles		
		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
2	GLC	В	1	2	11,11,12	1.30	1 (9%)	$15,\!15,\!17$	2.66	4 (26%)	
2	GLC	В	2	2	12,12,12	1.17	1 (8%)	$17,\!17,\!17$	1.78	3 (17%)	

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
2	GLC	В	1	2	-	0/2/19/22	0/1/1/1
2	GLC	В	2	2	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

M	ol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2		В	1	GLC	O5-C5	2.70	1.48	1.43
2		В	2	GLC	O5-C5	2.12	1.49	1.44

The worst 5 of 7 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	1	GLC	O5-C5-C6	-8.63	93.67	107.20
2	В	2	GLC	O5-C5-C6	-5.02	93.95	106.44
2	В	1	GLC	O3-C3-C4	-2.70	104.12	110.35
2	В	2	GLC	O3-C3-C4	-2.64	104.25	110.35
2	В	1	GLC	C2-C3-C4	-2.19	107.11	110.89

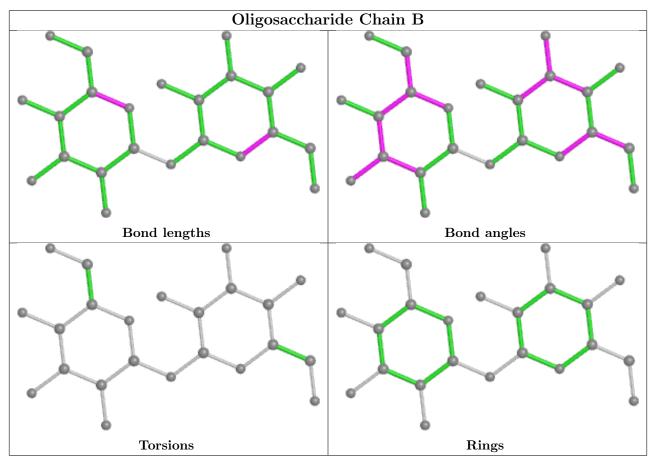
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

4 ligands 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).

Mal	Mol Type Chain H		Dec	Res Link	Bo	ond leng	ths	Bond angles		
	Type Chain N	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
3	SO4	А	348	-	4,4,4	0.52	0	6,6,6	0.20	0
4	HEM	А	154	1,5	41,50,50	1.31	4 (9%)	45,82,82	1.06	4 (8%)
3	SO4	А	347	-	4,4,4	0.47	0	6,6,6	0.34	0
5	CMO	А	155	4	0,1,1	-	-	-		

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
4	HEM	А	154	1,5	-	5/12/54/54	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	А	154	HEM	C3C-CAC	-3.15	1.41	1.47
4	А	154	HEM	CBB-CAB	2.94	1.44	1.30
4	А	154	HEM	CAB-C3B	-2.45	1.40	1.47
4	А	154	HEM	CBC-CAC	2.40	1.45	1.29

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	А	154	HEM	C2B-C1B-NB	2.46	112.76	109.84
4	А	154	HEM	C4C-CHD-C1D	2.38	125.70	122.56
4	А	154	HEM	CMC-C2C-C3C	2.37	129.12	124.68
4	А	154	HEM	C4B-CHC-C1C	2.14	125.38	122.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
4	А	154	HEM	CAD-CBD-CGD-O2D
4	А	154	HEM	CAA-CBA-CGA-O2A

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	Chain	1	1 0	Atoms
4	А	154	HEM	CAA-CBA-CGA-O1A
4	А	154	HEM	CAD-CBD-CGD-O1D
4	А	154	HEM	C2A-CAA-CBA-CGA

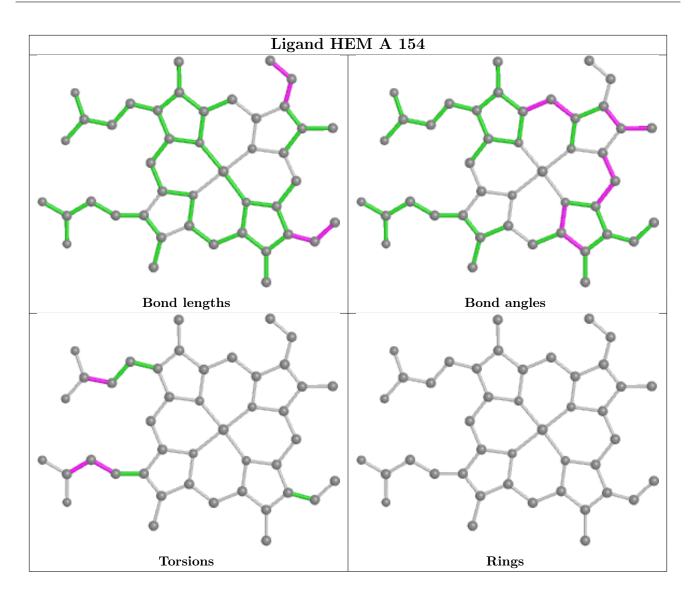
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There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

