



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:33 PM GMT

PDB ID : 1PL7  
Title : Human Sorbitol Dehydrogenase (apo)  
Authors : Pauly, T.A.; Ekstrom, J.L.; Beebe, D.A.; Chrnyk, B.; Cunningham, D.; Griffor, M.; Kamath, A.; Lee, S.E.; Madura, R.; McGuire, D.; Subashi, T.; Wasilko, D.; Watts, P.; Mylari, B.L.; Oates, P.J.; Adams, P.D.; Rath, V.L.  
Deposited on : 2003-06-07  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

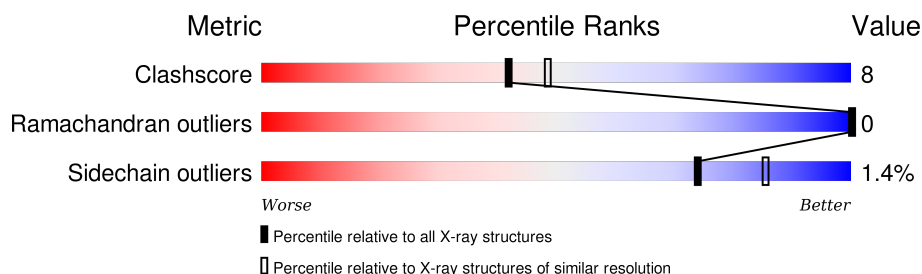
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	356	 84% 15% •
1	B	356	 87% 13%
1	C	356	 83% 17%
1	D	356	 85% 15%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12009 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 Sorbitol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	4	0
			2712	1721	472	498	21			
1	B	356	Total	C	N	O	S	0	4	0
			2712	1721	472	498	21			
1	C	356	Total	C	N	O	S	0	4	0
			2712	1721	472	498	21			
1	D	356	Total	C	N	O	S	0	4	0
			2712	1721	472	498	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLN	LEU	SEE REMARK 999	UNP Q00796
B	238	GLN	LEU	SEE REMARK 999	UNP Q00796
C	238	GLN	LEU	SEE REMARK 999	UNP Q00796
D	238	GLN	LEU	SEE REMARK 999	UNP Q00796

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

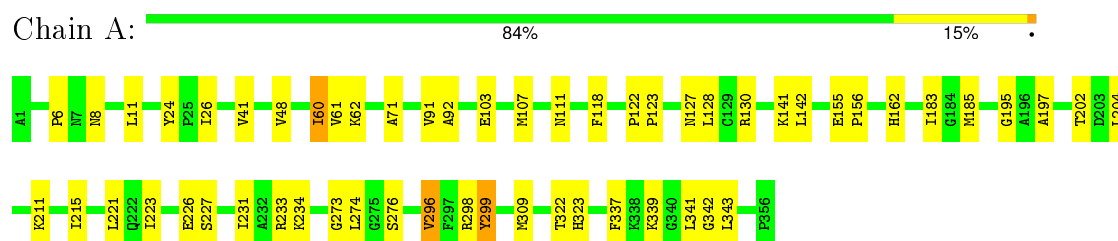
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	297	Total 297	O 297	0	0
3	B	269	Total 269	O 269	0	0
3	C	282	Total 282	O 282	0	0
3	D	309	Total 309	O 309	0	0

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

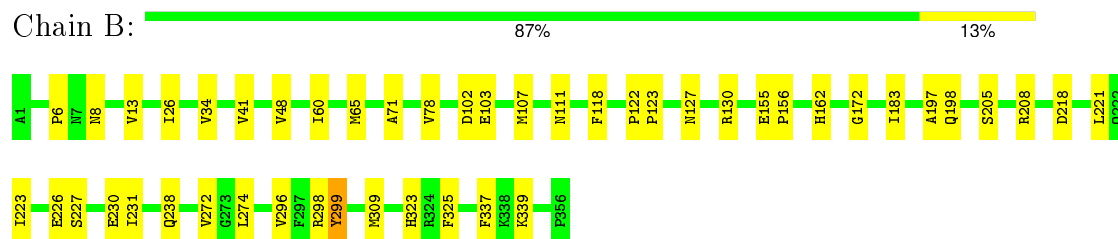
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

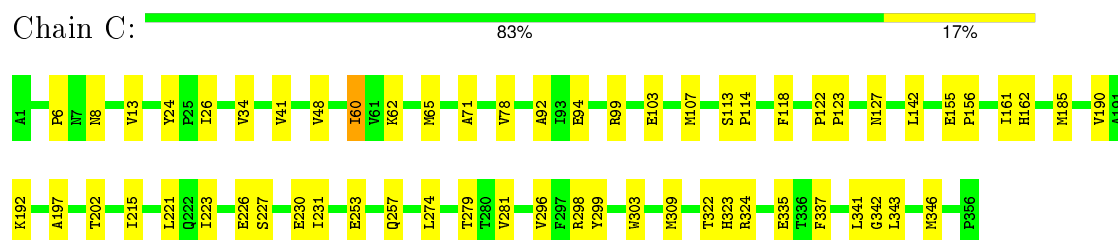
- Molecule 1: Sorbitol dehydrogenase



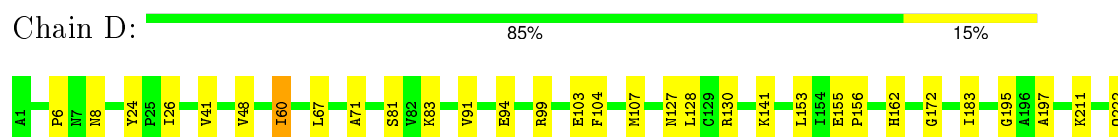
- Molecule 1: Sorbitol dehydrogenase



- Molecule 1: Sorbitol dehydrogenase



- Molecule 1: Sorbitol dehydrogenase



I223	E226	S227	E230	I231	R232	R233	Q238	E253	Q257	L274	V296	Y299	W303	R309	T322	R323	R324	E335	T336	F337	R338	R339	G340	L341	G342	L343	R344	I345	W346	P356
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.95Å 134.95Å 224.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.17 – 2.20	Depositor
% Data completeness (in resolution range)	88.4 (43.17-2.20)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.200 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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: ZN

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	0.31	0/2769	0.61	0/3750
1	B	0.31	0/2769	0.60	0/3750
1	C	0.31	0/2769	0.60	0/3750
1	D	0.31	0/2769	0.60	0/3750
All	All	0.31	0/11076	0.60	0/15000

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	2712	0	2761	53	0
1	B	2712	0	2761	51	0
1	C	2712	0	2761	55	0
1	D	2712	0	2761	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	297	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	269	0	0	9	0
3	C	282	0	0	4	0
3	D	309	0	0	6	0
All	All	12009	0	11044	185	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 8.

The worst 5 of 185 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:C:223:ILE:HD12	1:C:231:ILE:HD12	1.47	0.97
1:A:223:ILE:HD12	1:A:231:ILE:HD12	1.48	0.95
1:B:223:ILE:HD12	1:B:231:ILE:HD12	1.51	0.92
1:D:223:ILE:HD12	1:D:231:ILE:HD12	1.55	0.87
1:B:162:HIS:HD2	1:B:296:VAL:HG23	1.40	0.85

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	358/356 (101%)	346 (97%)	12 (3%)	0	100	100
1	B	358/356 (101%)	349 (98%)	9 (2%)	0	100	100
1	C	358/356 (101%)	348 (97%)	10 (3%)	0	100	100
1	D	358/356 (101%)	345 (96%)	13 (4%)	0	100	100
All	All	1432/1424 (101%)	1388 (97%)	44 (3%)	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	A	294/290 (101%)	288 (98%)	6 (2%)	63	76
1	B	294/290 (101%)	291 (99%)	3 (1%)	82	91
1	C	294/290 (101%)	291 (99%)	3 (1%)	82	91
1	D	294/290 (101%)	290 (99%)	4 (1%)	74	85
All	All	1176/1160 (101%)	1160 (99%)	16 (1%)	74	85

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	ASN
1	B	299	TYR
1	D	60	ILE
1	B	60	ILE
1	D	127	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	355	ASN
1	C	127	ASN
1	C	355	ASN
1	B	257	GLN
1	C	257	GLN

### 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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.