



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2018 – 09:49 pm GMT

PDB ID : 1JKF  
Title : Holo 1L-myo-inositol-1-phosphate Synthase  
Authors : Stein, A.J.; Geiger, J.H.  
Deposited on : 2001-07-12  
Resolution : 2.40 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

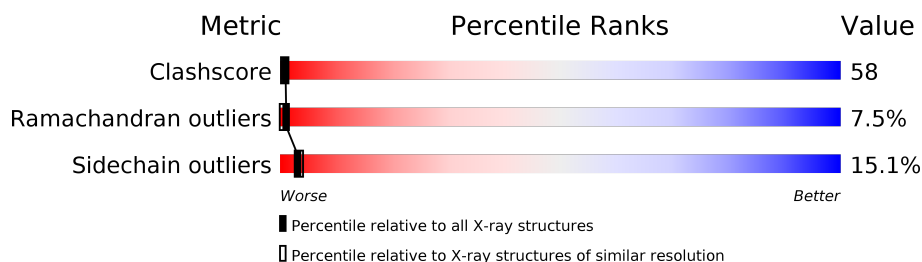
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	122078	3953 (2.40-2.40)
Ramachandran outliers	120005	3894 (2.40-2.40)
Sidechain outliers	119972	3895 (2.40-2.40)

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	533	
1	B	533	

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
2	NAD	B	610	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7971 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 myo-inositol-1-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3675	2338	617	706	14			
1	B	465	Total	C	N	O	S	0	0	0
			3670	2336	616	704	14			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

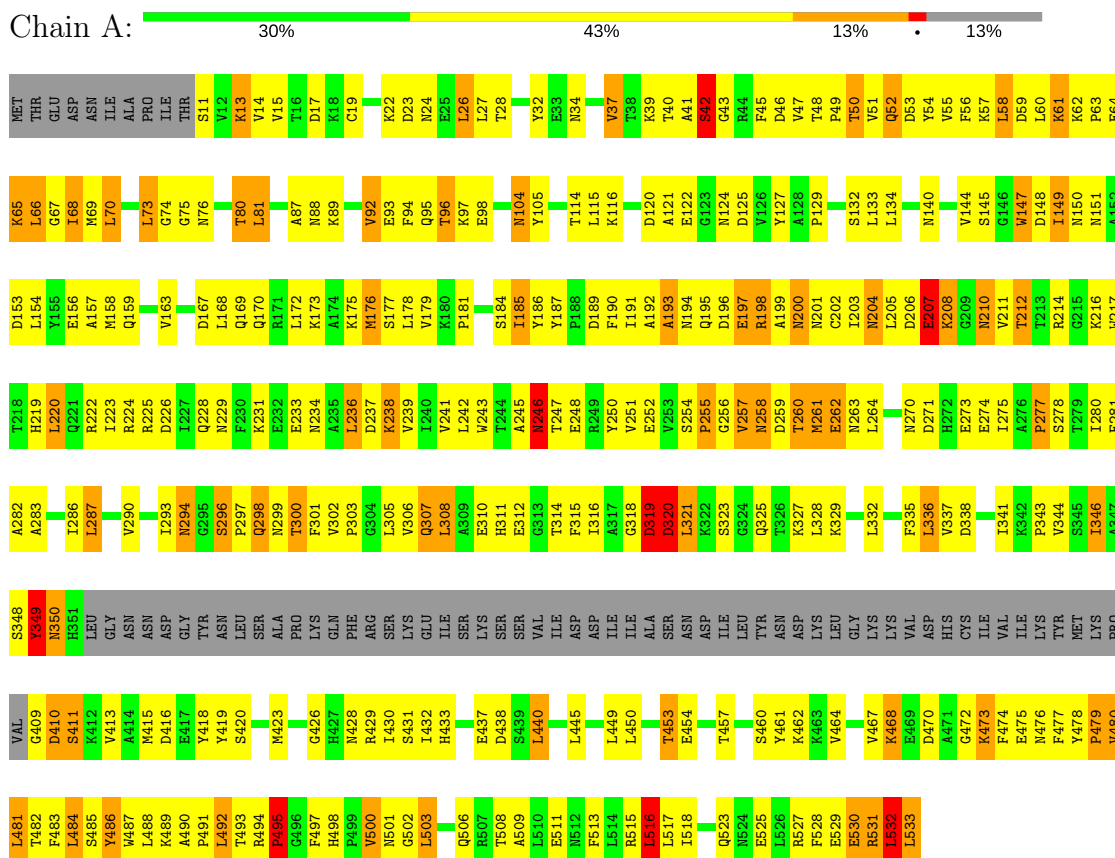
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	256	Total 256	O 256	0	0
3	B	282	Total 282	O 282	0	0

### 3 Residue-property plots

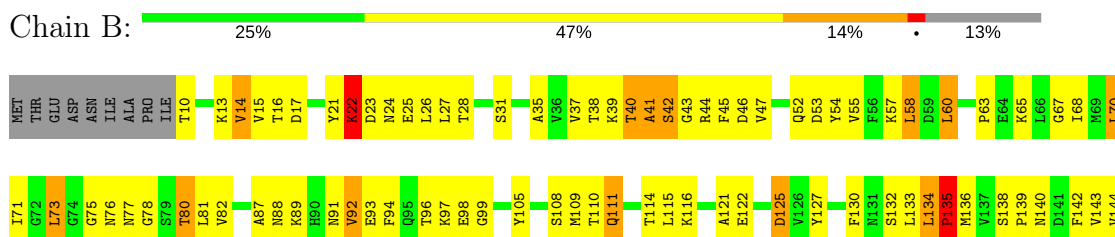
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

- Molecule 1: myo-inositol-1-phosphate synthase



- Molecule 1: myo-inositol-1-phosphate synthase





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.04Å 95.96Å 121.29Å 90.00° 126.04° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	57.3 (10.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.205 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7971	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

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	0.52	1/3748 (0.0%)	0.78	2/5083 (0.0%)
1	B	0.53	0/3743	0.81	3/5077 (0.1%)
All	All	0.52	1/7491 (0.0%)	0.79	5/10160 (0.0%)

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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	MET	CG-SD	-5.11	1.67	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	GLY	N-CA-C	6.76	130.00	113.10
1	A	516	LEU	CA-CB-CG	6.10	129.34	115.30
1	A	73	LEU	CA-CB-CG	5.91	128.90	115.30
1	B	524	ASN	N-CA-C	-5.29	96.71	111.00
1	B	526	LEU	N-CA-C	-5.14	97.13	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	349	TYR	Sidechain
1	B	349	TYR	Sidechain

## 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	3675	0	3666	417	2
1	B	3670	0	3666	493	1
2	A	44	0	26	8	0
2	B	44	0	26	29	0
3	A	256	0	0	35	1
3	B	282	0	0	52	0
All	All	7971	0	7384	864	3

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 58.

The worst 5 of 864 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:B:149:ILE:HD11	1:B:195:GLN:HE21	1.04	1.13
1:B:315:PHE:HB3	1:B:481:LEU:HD11	1.30	1.12
1:B:293:ILE:HD11	1:B:453:THR:HG21	1.28	1.12
1:B:70:LEU:HD21	1:B:81:LEU:HD23	1.33	1.08
1:A:533:LEU:HG	1:B:494:ARG:HH22	0.92	1.08

All (3) 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:A:229:ASN:OD1	1:B:178:LEU:O[3_455]	1.70	0.50
3:A:696:HOH:O	3:A:696:HOH:O[2_555]	2.08	0.12
1:A:23:ASP:OD2	1:A:23:ASP:OD2[2_556]	2.10	0.10

## 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	462/533 (87%)	389 (84%)	46 (10%)	27 (6%)	2	0
1	B	461/533 (86%)	360 (78%)	59 (13%)	42 (9%)	1	0
All	All	923/1066 (87%)	749 (81%)	105 (11%)	69 (8%)	1	0

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	207	GLU
1	A	298	GLN
1	A	319	ASP
1	B	22	LYS

### 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	410/471 (87%)	348 (85%)	62 (15%)	3	3
1	B	410/471 (87%)	348 (85%)	62 (15%)	3	3
All	All	820/942 (87%)	696 (85%)	124 (15%)	3	3

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	HIS

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Mol	Chain	Res	Type
1	B	80	THR
1	B	473	LYS
1	A	500	VAL
1	B	14	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	ASN
1	B	24	ASN
1	B	307	GLN
1	A	501	ASN
1	A	504	ASN

### 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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	A	600	1	40,48,48	2.62	11 (27%)	44,73,73	1.48	5 (11%)
2	NAD	B	610	-	40,48,48	2.81	15 (37%)	44,73,73	1.46	4 (9%)

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	NAD	A	600	1	-	0/22/62/62	0/5/5/5
2	NAD	B	610	-	-	0/22/62/62	0/5/5/5

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	610	NAD	C3N-C7N	-4.77	1.43	1.50
2	A	600	NAD	O4B-C1B	-3.99	1.35	1.41
2	A	600	NAD	C3N-C7N	-3.47	1.45	1.50
2	B	610	NAD	C2D-C3D	-2.32	1.47	1.53
2	B	610	NAD	O5B-C5B	2.07	1.52	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	NAD	N3A-C2A-N1A	-5.60	124.07	128.86
2	B	610	NAD	N3A-C2A-N1A	-4.85	124.71	128.86
2	B	610	NAD	C5N-C4N-C3N	-2.65	117.23	120.35
2	A	600	NAD	C5N-C4N-C3N	-2.42	117.50	120.35
2	B	610	NAD	O7N-C7N-N7N	-2.29	119.27	122.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	NAD	8	0
2	B	610	NAD	29	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.