



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1LA2  
Title : Structural analysis of *Saccharomyces cerevisiae* myo-inositol phosphate synthase  
Authors : Kniewel, R.; Buglino, J.A.; Shen, V.; Chadna, T.; Beckwith, A.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYS-GXRC)  
Deposited on : 2002-03-27  
Resolution : 2.65 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.

---

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

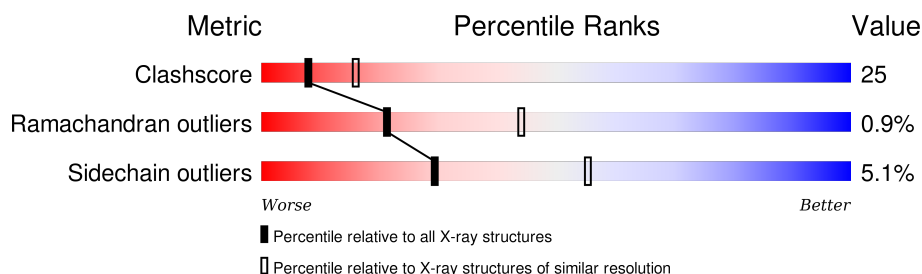
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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	 55% 39% . .
1	B	533	 53% 41% . .
1	C	533	 53% 40% . .
1	D	533	 53% 40% . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17040 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	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			
1	B	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			
1	C	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			
1	D	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP P11986
A	14	VAL	LEU	SEE REMARK 999	UNP P11986
A	?	-	PHE	SEE REMARK 999	UNP P11986
A	60	LEU	GLU	SEE REMARK 999	UNP P11986
A	69	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	?	-	ALA	SEE REMARK 999	UNP P11986
A	98	GLU	LYS	SEE REMARK 999	UNP P11986
A	109	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	136	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	140	ASN	LYS	SEE REMARK 999	UNP P11986
A	141	ASP	HIS	SEE REMARK 999	UNP P11986
A	158	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	176	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	201	ASN	GLN	SEE REMARK 999	UNP P11986
A	261	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	405	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	415	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	423	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	444	PRO	ALA	SEE REMARK 999	UNP P11986
A	452	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	?	-	ARG	SEE REMARK 999	UNP P11986

*Continued on next page...*

*Continued from previous page...*

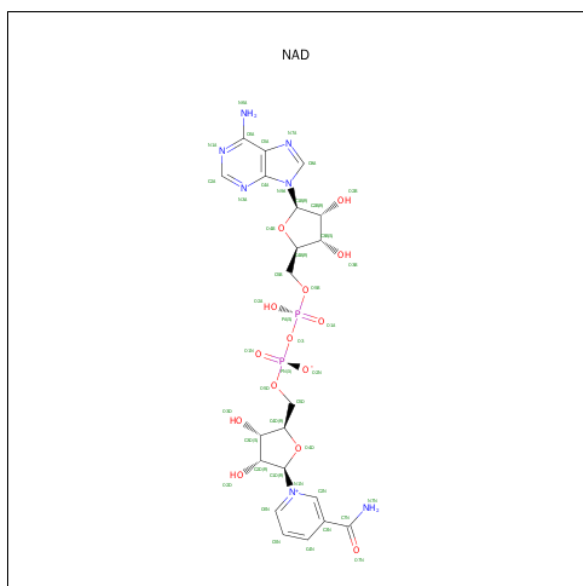
Chain	Residue	Modelled	Actual	Comment	Reference
B	14	VAL	LEU	SEE REMARK 999	UNP P11986
B	?	-	PHE	SEE REMARK 999	UNP P11986
B	60	LEU	GLU	SEE REMARK 999	UNP P11986
B	69	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	?	-	ALA	SEE REMARK 999	UNP P11986
B	98	GLU	LYS	SEE REMARK 999	UNP P11986
B	109	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	136	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	140	ASN	LYS	SEE REMARK 999	UNP P11986
B	141	ASP	HIS	SEE REMARK 999	UNP P11986
B	158	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	176	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	201	ASN	GLN	SEE REMARK 999	UNP P11986
B	261	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	405	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	415	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	423	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	444	PRO	ALA	SEE REMARK 999	UNP P11986
B	452	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	?	-	ARG	SEE REMARK 999	UNP P11986
C	14	VAL	LEU	SEE REMARK 999	UNP P11986
C	?	-	PHE	SEE REMARK 999	UNP P11986
C	60	LEU	GLU	SEE REMARK 999	UNP P11986
C	69	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	?	-	ALA	SEE REMARK 999	UNP P11986
C	98	GLU	LYS	SEE REMARK 999	UNP P11986
C	109	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	136	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	140	ASN	LYS	SEE REMARK 999	UNP P11986
C	141	ASP	HIS	SEE REMARK 999	UNP P11986
C	158	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	176	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	201	ASN	GLN	SEE REMARK 999	UNP P11986
C	261	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	405	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	415	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	423	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	444	PRO	ALA	SEE REMARK 999	UNP P11986
C	452	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	?	-	ARG	SEE REMARK 999	UNP P11986
D	14	VAL	LEU	SEE REMARK 999	UNP P11986
D	?	-	PHE	SEE REMARK 999	UNP P11986

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	60	LEU	GLU	SEE REMARK 999	UNP P11986
D	69	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	?	-	ALA	SEE REMARK 999	UNP P11986
D	98	GLU	LYS	SEE REMARK 999	UNP P11986
D	109	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	136	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	140	ASN	LYS	SEE REMARK 999	UNP P11986
D	141	ASP	HIS	SEE REMARK 999	UNP P11986
D	158	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	176	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	201	ASN	GLN	SEE REMARK 999	UNP P11986
D	261	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	405	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	415	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	423	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	444	PRO	ALA	SEE REMARK 999	UNP P11986
D	452	MSE	MET	MODIFIED RESIDUE	UNP P11986

- 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		

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 3 is water.

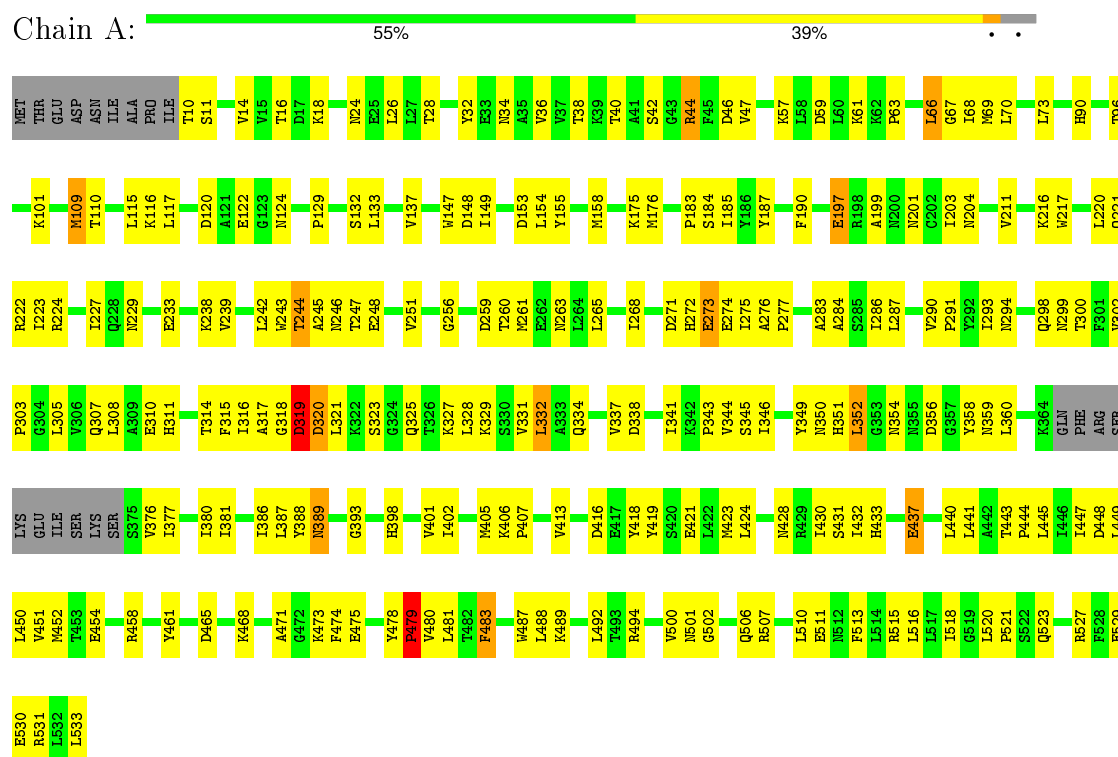
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	188	Total	O	0	0
			188	188		
3	C	194	Total	O	0	0
			194	194		
3	D	165	Total	O	0	0
			165	165		

### 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 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: Myo-inositol-1-phosphate synthase



#### • Molecule 1: Myo-inositol-1-phosphate synthase







I286	SER	P444	N524
LYS	LYS	L445	E525
GLU	GLU	I446	L526
ILE	ILE	I447	R527
I293	SER	D448	E530
I298	LYS	L449	R531
	SER	L450	L532
V302	S376	V451	L533
P303	I377	M452	
G304		T453	
L305	I380	E454	
V306	I381	T457	
Q307		R458	
E310	I386	V459	
	L387	S460	
T314	Y388	Y461	
F315	N389	D465	
I316	D390	P466	
A317		V467	
G318	G393	K468	
D319	K394	E469	
D320	D397	Y478	
L321	H398	P479	
K322	C399		
S323	I400	T482	
	V401	F483	
K327	I402	L484	
L328	K403		
K329	Y404	M487	
	M405	L489	
L332	K406	T493	
	P407	R494	
V337	V408		
D338		F497	
	S411	R498	
K342	K412	P499	
F343	V413	V500	
V344	A414	N501	
S345	M415	G502	
	D416	K505	
Y349	E417	Q506	
I350	Y418	R507	
H351	Y419		
L352	S420	L510	
G353		E511	
N354	N423	H512	
		F513	
G357	S431	L514	
Y358	I432	R515	
N359	H433	L516	
L360	N434	L517	
S361			
A362	E437	L520	
P363		Q523	
K364	L440		
GLN	L441		
PHE	A442		
ARG	T443		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.69Å 187.35Å 98.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.65	Depositor
% Data completeness (in resolution range)	99.4 (19.96-2.65)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.224 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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: 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	0.26	0/4112	0.47	0/5561
1	B	0.26	0/4112	0.48	0/5561
1	C	0.26	0/4112	0.48	0/5561
1	D	0.25	0/4112	0.47	0/5561
All	All	0.26	0/16448	0.47	0/22244

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	4043	0	4038	216	0
1	B	4043	0	4038	212	0
1	C	4043	0	4038	216	0
1	D	4043	0	4038	226	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	2	0
3	A	145	0	0	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	188	0	0	5	0
3	C	194	0	0	11	0
3	D	165	0	0	10	0
All	All	17040	0	16256	809	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 25.

The worst 5 of 809 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:423:MSE:HE3	1:D:444:PRO:HG3	1.27	1.11
1:A:437:GLU:HG3	1:A:440:LEU:HD12	1.29	1.09
1:D:437:GLU:HG3	1:D:440:LEU:HD12	1.35	1.08
1:A:129:PRO:HG2	1:A:132:SER:HB3	1.45	0.96
1:D:96:THR:HG23	1:D:98:GLU:H	1.34	0.93

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	510/533 (96%)	471 (92%)	36 (7%)	3 (1%)	30	54
1	B	510/533 (96%)	462 (91%)	41 (8%)	7 (1%)	14	31
1	C	510/533 (96%)	468 (92%)	37 (7%)	5 (1%)	19	41
1	D	510/533 (96%)	456 (89%)	50 (10%)	4 (1%)	24	47
All	All	2040/2132 (96%)	1857 (91%)	164 (8%)	19 (1%)	21	44

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	ALA
1	B	319	ASP
1	D	320	ASP
1	D	469	GLU
1	C	319	ASP

### 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	452/461 (98%)	431 (95%)	21 (5%)	33	61
1	B	452/461 (98%)	427 (94%)	25 (6%)	27	51
1	C	452/461 (98%)	430 (95%)	22 (5%)	31	58
1	D	452/461 (98%)	428 (95%)	24 (5%)	28	54
All	All	1808/1844 (98%)	1716 (95%)	92 (5%)	29	55

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	465	ASP
1	C	109	MSE
1	D	359	ASN
1	B	475	GLU
1	C	22	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	433	HIS
1	C	194	ASN
1	D	350	ASN
1	B	523	GLN
1	C	95	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAD	A	900	-	38,48,48	2.35	8 (21%)	47,73,73	1.94	11 (23%)
2	NAD	B	901	-	38,48,48	2.39	8 (21%)	47,73,73	1.90	12 (25%)
2	NAD	C	902	-	38,48,48	2.35	8 (21%)	47,73,73	1.99	13 (27%)
2	NAD	D	903	-	38,48,48	2.37	8 (21%)	47,73,73	1.92	12 (25%)

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	900	-	-	0/22/62/62	0/5/5/5
2	NAD	B	901	-	-	0/22/62/62	0/5/5/5
2	NAD	C	902	-	-	0/22/62/62	0/5/5/5
2	NAD	D	903	-	-	0/22/62/62	0/5/5/5

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	NAD	O4B-C1B	-3.40	1.36	1.41
2	D	903	NAD	O4B-C1B	-3.18	1.37	1.41
2	C	902	NAD	O4B-C1B	-2.88	1.37	1.41
2	A	900	NAD	O4B-C1B	-2.50	1.38	1.41
2	A	900	NAD	C7N-N7N	2.03	1.37	1.33

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	NAD	O7N-C7N-C3N	-5.90	113.14	119.59
2	D	903	NAD	O7N-C7N-C3N	-5.86	113.19	119.59
2	A	900	NAD	O7N-C7N-C3N	-5.83	113.23	119.59
2	B	901	NAD	O7N-C7N-C3N	-5.80	113.25	119.59
2	A	900	NAD	PN-O3-PA	-4.31	120.62	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	NAD	2	0
2	B	901	NAD	1	0
2	C	902	NAD	2	0
2	D	903	NAD	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 ⓘ

### 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.