wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:02 PM GMT

PDB ID	:	1DO8
Title	:	CRYSTAL STRUCTURE OF A CLOSED FORM OF HUMAN MITOCHONDRIAL NAD(P)+-DEPENDENT MALIC ENZYME
Authors	:	Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.
Deposited on	:	1999-12-19
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

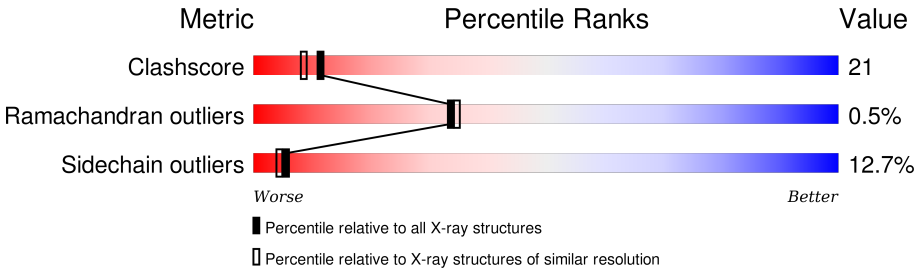
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 >=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 <=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	564	59% 31% 8% •
1	B	564	57% 35% 5% •
1	C	564	63% 30% 5% •
1	D	564	63% 28% 7% •

2 Entry composition (i)

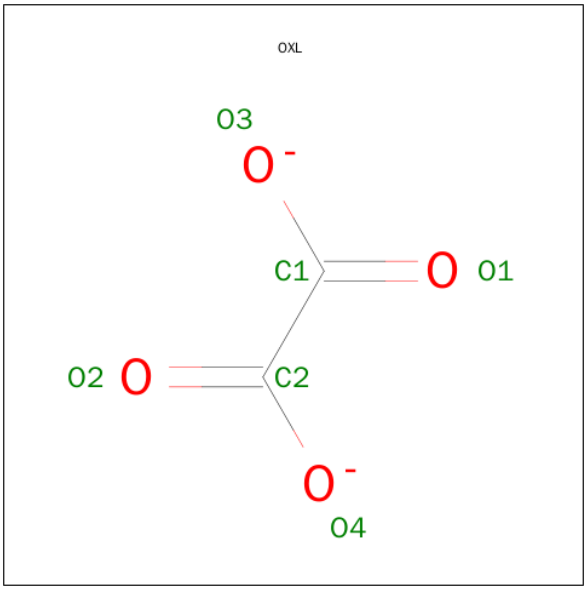
There are 5 unique types of molecules in this entry. The entry contains 18807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	C	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	D	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	2	4		
2	B	1	Total	C	O	0	0
			6	2	4		

Continued on next page...

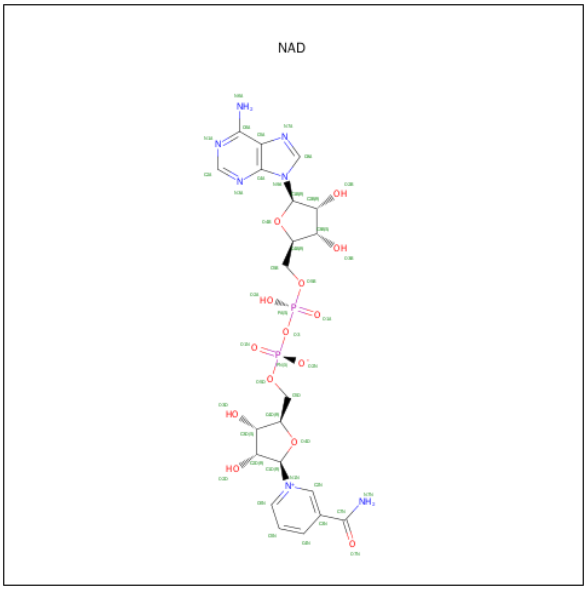
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 2 4	0	0
2	D	1	Total C O 6 2 4	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 44 21 7 14 2	0	0
4	A	1	Total C N O P 44 21 7 14 2	9	0
4	B	1	Total C N O P 44 21 7 14 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	9	0
			44	21	7	14	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	0
			239	239		
5	B	199	Total	O	0	0
			199	199		
5	C	275	Total	O	0	0
			275	275		
5	D	246	Total	O	0	0
			246	246		

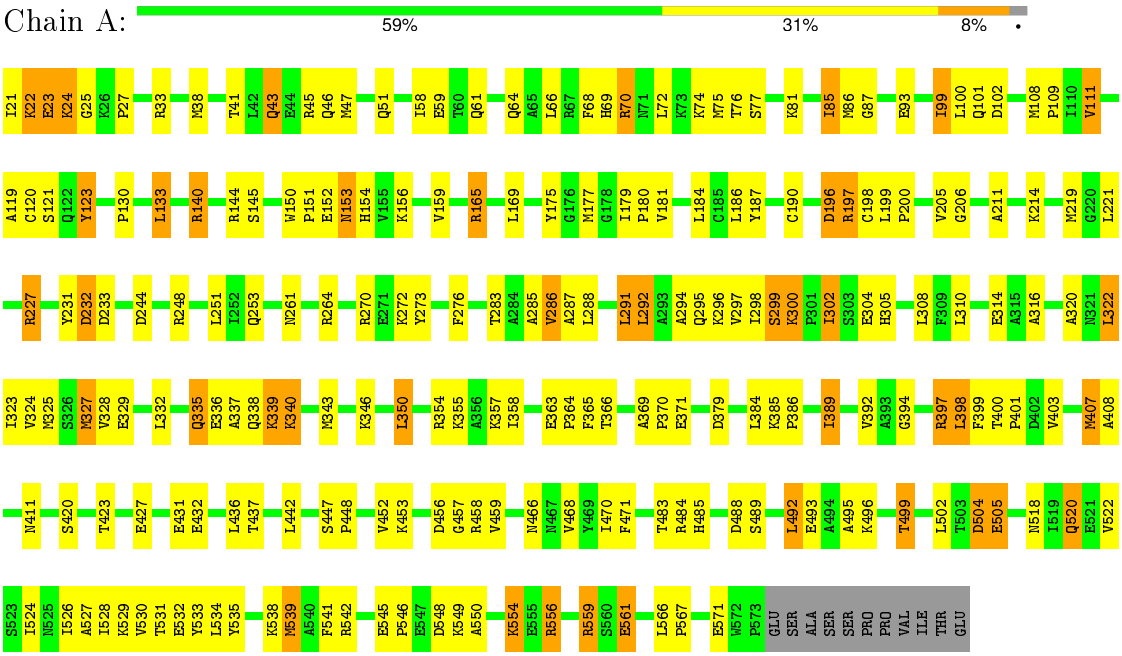
3 Residue-property plots (i)

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.

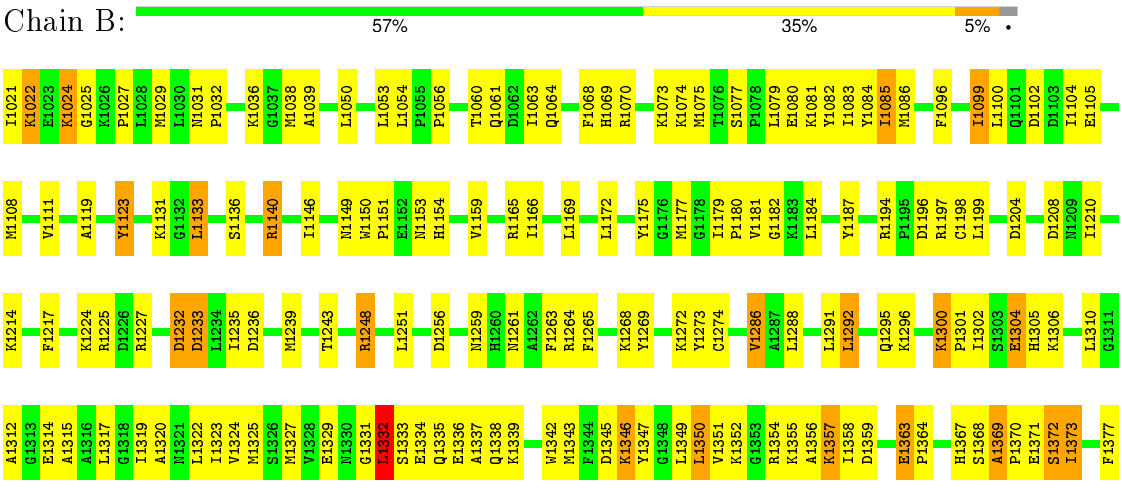
- Molecule 1: MALIC ENZYME

Chain A:



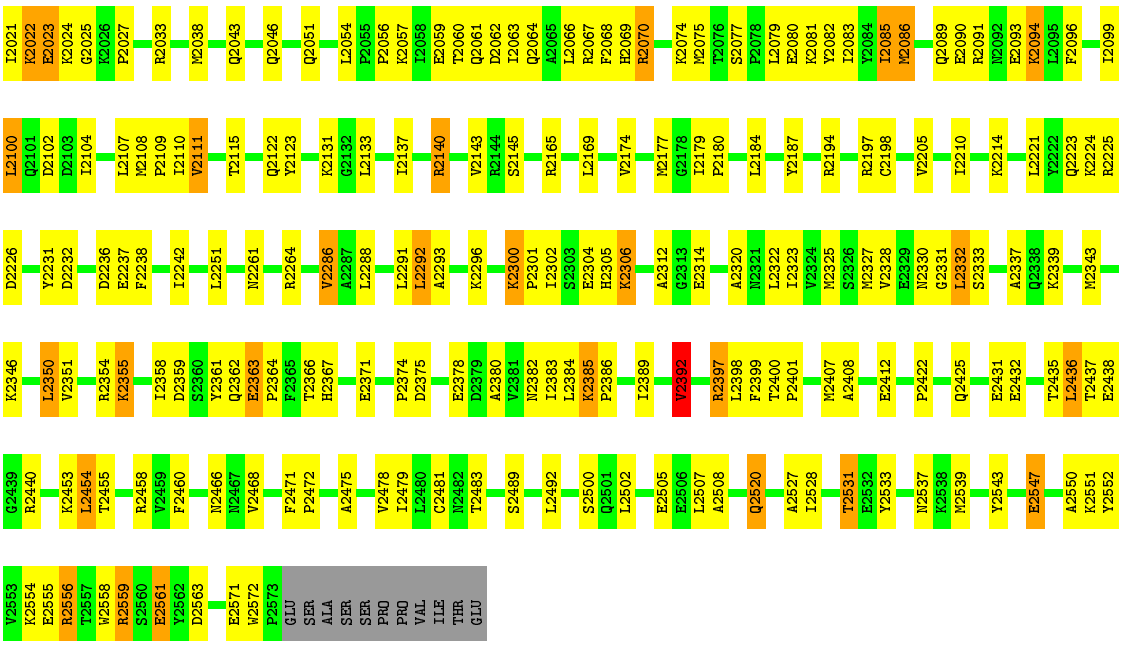
- Molecule 1: MALIC ENZYME

Chain B:



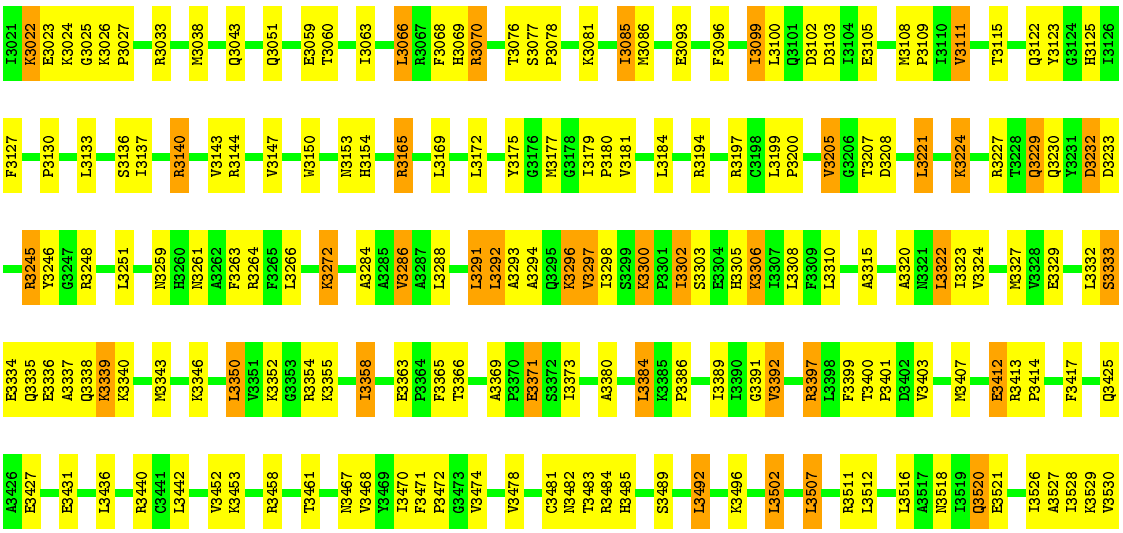
• Molecule 1: MALIC ENZYME

Chain C:



• Molecule 1: MALIC ENZYME

Chain D:




T3531
E3532
N3537
K3538
M3539
A3540
E3545
P3546
E3547
D3548
K3549
A3550
K3551
E3555
R3556
T3557
W3558
R3559
E3571
W3572
P3573
GLU
SER
ALA
SER
SER
PRO
PRO
VAL
ILE
THR
GLU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	229.00Å 118.70Å 113.00Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18807	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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: OXL, MN, 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	0.37	0/4447	0.61	0/5998
1	B	0.37	0/4447	0.61	0/5998
1	C	0.38	0/4447	0.61	0/5998
1	D	0.38	0/4447	0.60	0/5998
All	All	0.37	0/17788	0.61	0/23992

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

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	4367	0	4407	203	0
1	B	4367	0	4407	229	0
1	C	4367	0	4407	141	0
1	D	4367	0	4407	179	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	1	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	88	0	52	2	0
4	B	88	0	52	3	0
4	C	88	0	52	2	0
4	D	88	0	52	1	0
5	A	239	0	0	14	0
5	B	199	0	0	30	0
5	C	275	0	0	18	0
5	D	246	0	0	12	0
All	All	18807	0	17836	731	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 21.

The worst 5 of 731 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:177:MSE:HE2	1:A:181:VAL:HG23	1.29	1.14
1:D:3177:MSE:HE2	1:D:3181:VAL:HG23	1.35	1.08
1:A:123:TYR:HD2	1:A:219:MSE:HE1	1.18	1.06
1:B:1358:ILE:HG22	5:B:4650:HOH:O	1.54	1.06
1:A:140:ARG:HH22	1:A:233:ASP:HB3	1.14	1.05

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	551/564 (98%)	530 (96%)	19 (3%)	2 (0%)	39 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	551/564 (98%)	522 (95%)	26 (5%)	3 (0%)	34 35
1	C	551/564 (98%)	530 (96%)	17 (3%)	4 (1%)	26 25
1	D	551/564 (98%)	528 (96%)	20 (4%)	3 (0%)	34 35
All	All	2204/2256 (98%)	2110 (96%)	82 (4%)	12 (0%)	34 35

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1332	LEU
1	C	2332	LEU
1	A	397	ARG
1	C	2392	VAL
1	D	3302	ILE

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	469/465 (101%)	406 (87%)	63 (13%)	5 4
1	B	469/465 (101%)	412 (88%)	57 (12%)	6 5
1	C	469/465 (101%)	409 (87%)	60 (13%)	5 4
1	D	469/465 (101%)	410 (87%)	59 (13%)	5 4
All	All	1876/1860 (101%)	1637 (87%)	239 (13%)	5 4

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1502	LEU
1	C	2122	GLN
1	D	3358	ILE
1	B	1507	LEU
1	C	2022	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1425	GLN
1	C	2064	GLN
1	D	3482	ASN
1	B	1520	GLN
1	C	2069	HIS

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)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
4	NAD	A	601	-	38,48,48	1.77	9 (23%)	47,73,73	1.96	5 (10%)
4	NAD	A	602	-	38,48,48	1.89	11 (28%)	47,73,73	1.92	4 (8%)
2	OXL	A	603	3	0,5,5	0.00	-	0,6,6	0.00	-
4	NAD	B	1601	-	38,48,48	1.70	10 (26%)	47,73,73	2.00	6 (12%)
4	NAD	B	1602	-	38,48,48	2.02	10 (26%)	47,73,73	1.98	5 (10%)
2	OXL	B	1603	3	0,5,5	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAD	C	2601	-	38,48,48	1.56	6 (15%)	47,73,73	1.97	6 (12%)
4	NAD	C	2602	-	38,48,48	2.26	10 (26%)	47,73,73	2.04	6 (12%)
2	OXL	C	2603	3	0,5,5	0.00	-	0,6,6	0.00	-
4	NAD	D	3601	-	38,48,48	1.83	9 (23%)	47,73,73	1.99	6 (12%)
4	NAD	D	3602	-	38,48,48	1.92	8 (21%)	47,73,73	1.97	5 (10%)
2	OXL	D	3603	3	0,5,5	0.00	-	0,6,6	0.00	-

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	NAD	A	601	-	-	0/22/62/62	0/5/5/5
4	NAD	A	602	-	-	0/22/62/62	0/5/5/5
2	OXL	A	603	3	-	0/0/4/4	0/0/0/0
4	NAD	B	1601	-	-	0/22/62/62	0/5/5/5
4	NAD	B	1602	-	-	0/22/62/62	0/5/5/5
2	OXL	B	1603	3	-	0/0/4/4	0/0/0/0
4	NAD	C	2601	-	-	0/22/62/62	0/5/5/5
4	NAD	C	2602	-	-	0/22/62/62	0/5/5/5
2	OXL	C	2603	3	-	0/0/4/4	0/0/0/0
4	NAD	D	3601	-	-	0/22/62/62	0/5/5/5
4	NAD	D	3602	-	-	0/22/62/62	0/5/5/5
2	OXL	D	3603	3	-	0/0/4/4	0/0/0/0

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2601	NAD	C5A-C4A	-3.30	1.33	1.40
4	D	3601	NAD	C5A-C4A	-3.17	1.33	1.40
4	A	601	NAD	C5A-C4A	-3.16	1.33	1.40
4	D	3602	NAD	C5A-C4A	-2.97	1.33	1.40
4	B	1601	NAD	C5A-C4A	-2.90	1.33	1.40

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3602	NAD	N3A-C2A-N1A	-10.70	120.70	128.89
4	A	601	NAD	N3A-C2A-N1A	-10.62	120.76	128.89
4	B	1601	NAD	N3A-C2A-N1A	-10.61	120.77	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2601	NAD	N3A-C2A-N1A	-10.59	120.79	128.89
4	B	1602	NAD	N3A-C2A-N1A	-10.53	120.83	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAD	2	0
4	B	1601	NAD	3	0
4	C	2601	NAD	1	0
4	C	2602	NAD	1	0
4	D	3602	NAD	1	0
2	D	3603	OXL	1	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.