wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:48 PM GMT

PDB ID	:	1H5Q
Title	:	MANNITOL DEHYDROGENASE FROM AGARICUS BISPORUS
Authors	:	Horer, S.; Stoop, J.; Mooibroek, H.; Baumann, U.; Sassoon, J.
Deposited on	:	2001-05-24
Resolution	:	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
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 (1)) were used in the production of this report:

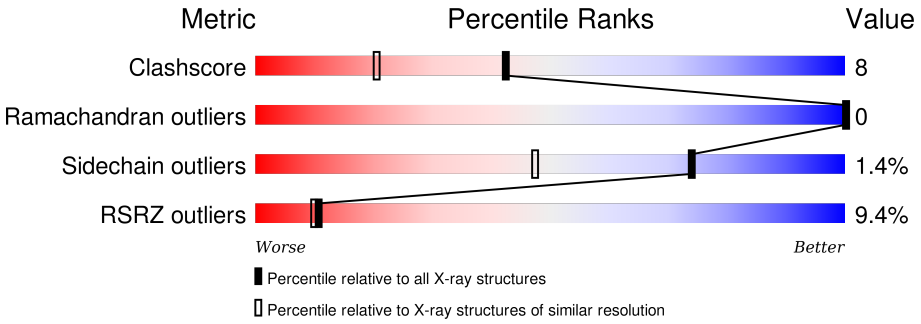
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (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 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.

Mol	Chain	Length	Quality of chain
1	A	265	36% 65% 31%
1	B	265	11% 79% 17%
1	C	265	8% 82% 15%
1	D	265	13% 85% 13%
1	E	265	5% 86% 12%
1	F	265	5% 86% 11%
1	G	265	9% 84% 13%

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Mol	Chain	Length	Quality of chain
1	H	265	3% 83% 14%
1	I	265	5% 86% 11%
1	J	265	7% 87% 11%
1	K	265	4% 85% 12%
1	L	265	3% 86% 11%

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
3	NI	B	2263	-	-	-	X
3	NI	J	3263	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27197 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 NADP-DEPENDENT MANNITOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	B	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	C	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	D	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	E	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	F	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	G	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	H	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	I	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	J	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	K	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	L	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PRO	ALA	CONFLICT	UNP O93868
B	89	PRO	ALA	CONFLICT	UNP O93868
C	89	PRO	ALA	CONFLICT	UNP O93868
D	89	PRO	ALA	CONFLICT	UNP O93868
E	89	PRO	ALA	CONFLICT	UNP O93868

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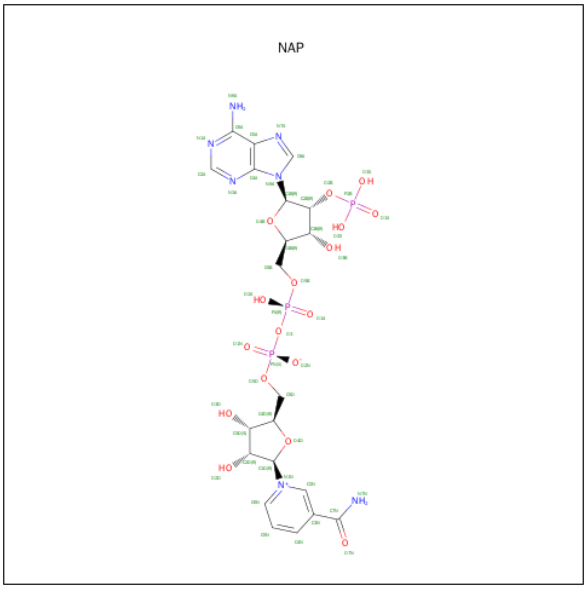
Chain	Residue	Modelled	Actual	Comment	Reference
F	89	PRO	ALA	CONFLICT	UNP O93868
G	89	PRO	ALA	CONFLICT	UNP O93868
H	89	PRO	ALA	CONFLICT	UNP O93868
I	89	PRO	ALA	CONFLICT	UNP O93868
J	89	PRO	ALA	CONFLICT	UNP O93868
K	89	PRO	ALA	CONFLICT	UNP O93868
L	89	PRO	ALA	CONFLICT	UNP O93868

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Ni	0	0
			1	1		
3	E	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		
3	I	1	Total	Ni	0	0
			1	1		
3	A	1	Total	Ni	0	0
			1	1		
3	F	1	Total	Ni	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	202	Total	O	0	0
			202	202		
4	C	251	Total	O	0	0
			251	251		
4	D	190	Total	O	0	0
			190	190		
4	E	342	Total	O	0	0
			342	342		
4	F	313	Total	O	0	0
			313	313		

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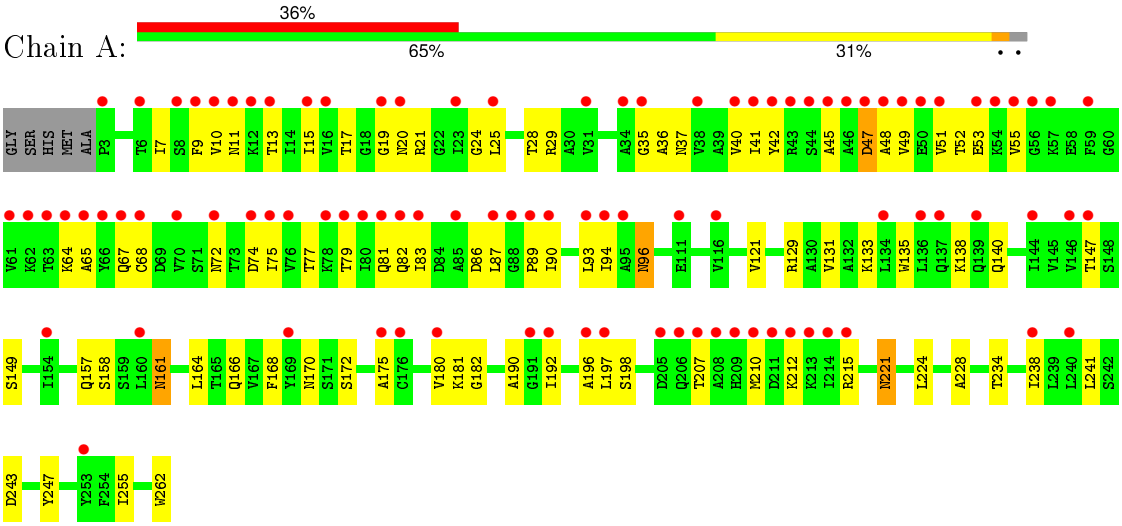
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	291	Total O 291 291	0	0
4	H	302	Total O 302 302	0	0
4	I	311	Total O 311 311	0	0
4	J	268	Total O 268 268	0	0
4	K	284	Total O 284 284	0	0
4	L	307	Total O 307 307	0	0

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.

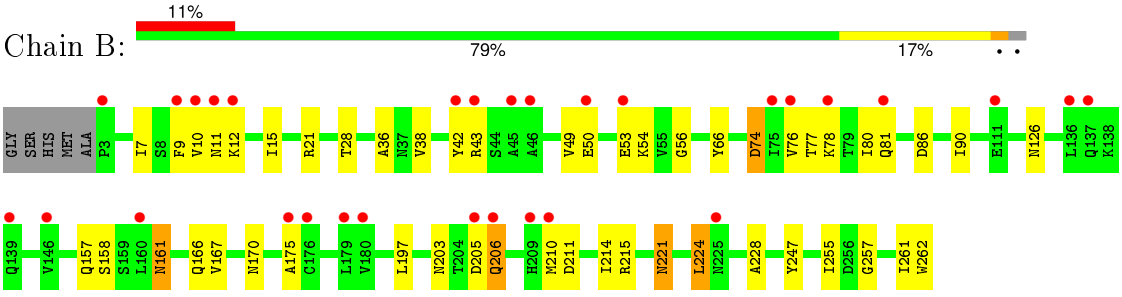
- Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain A:



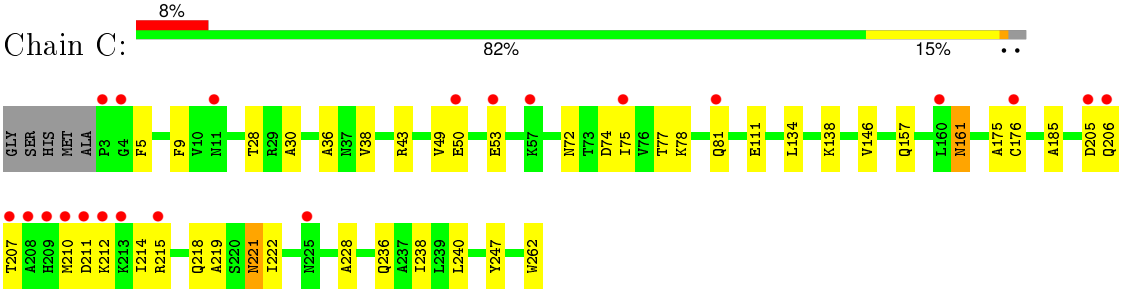
- Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain B:



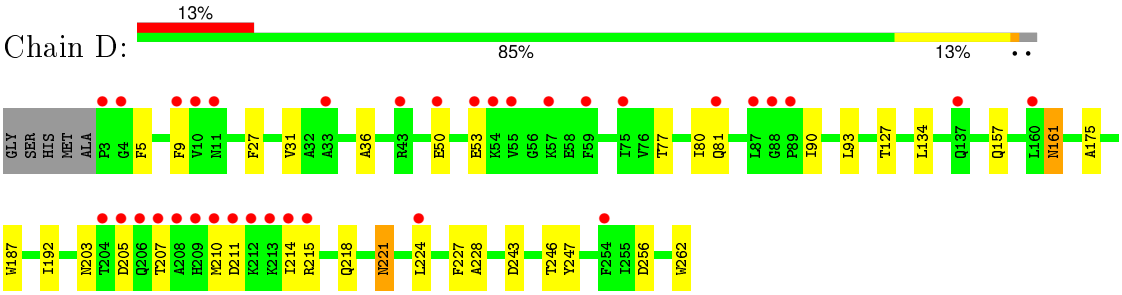
- Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain C:



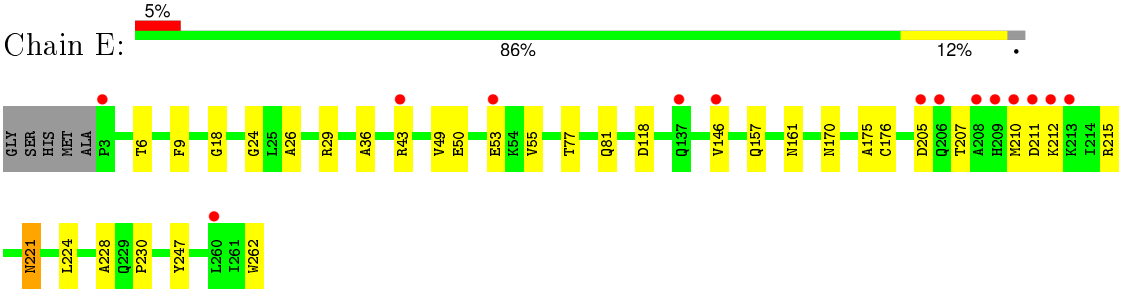
- Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain D:



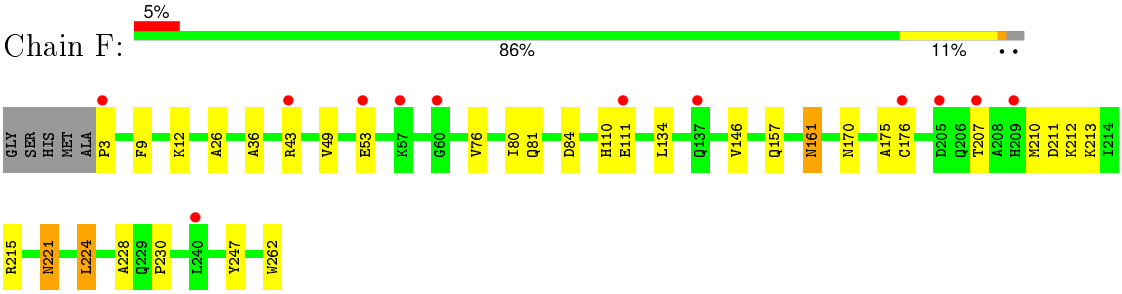
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain E:



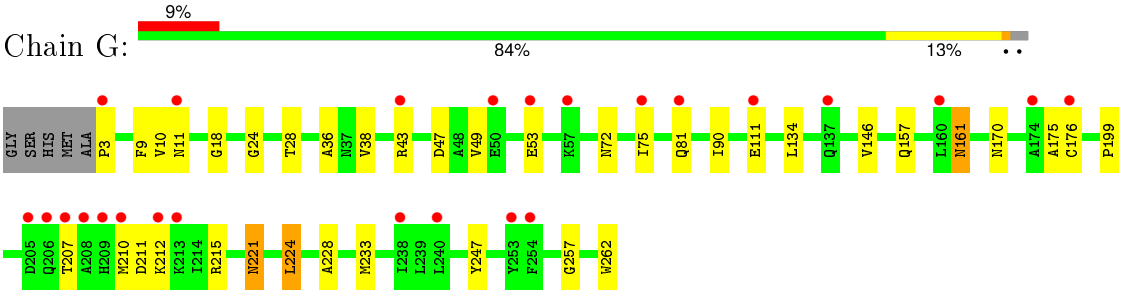
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain F:



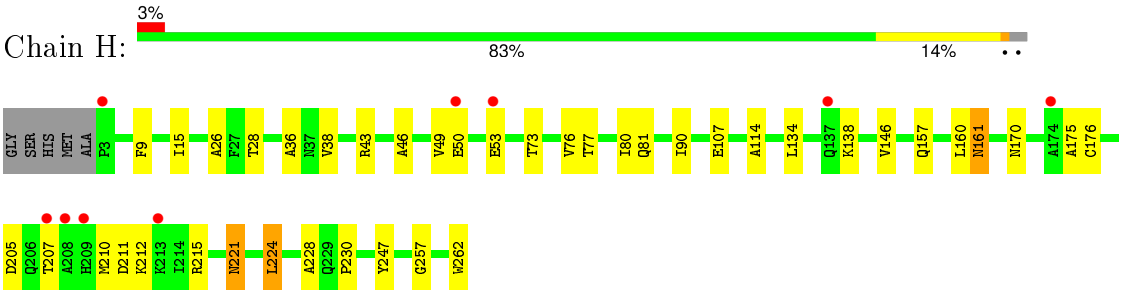
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain G:



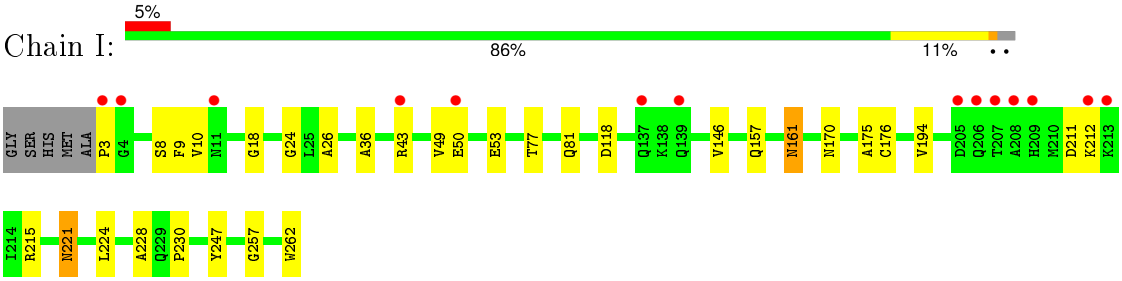
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain H:



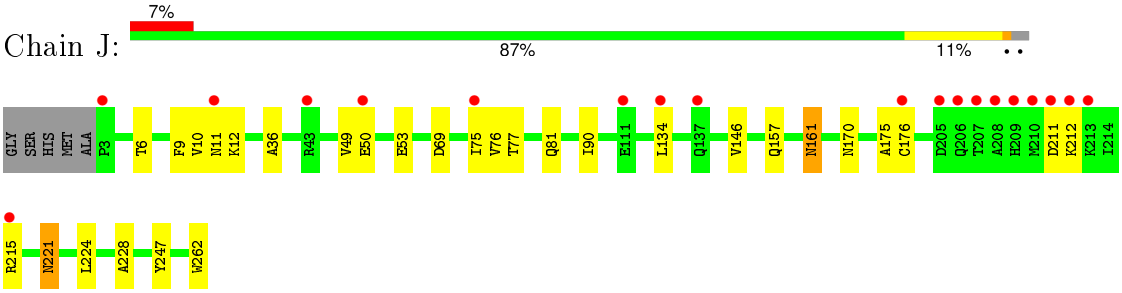
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain I:



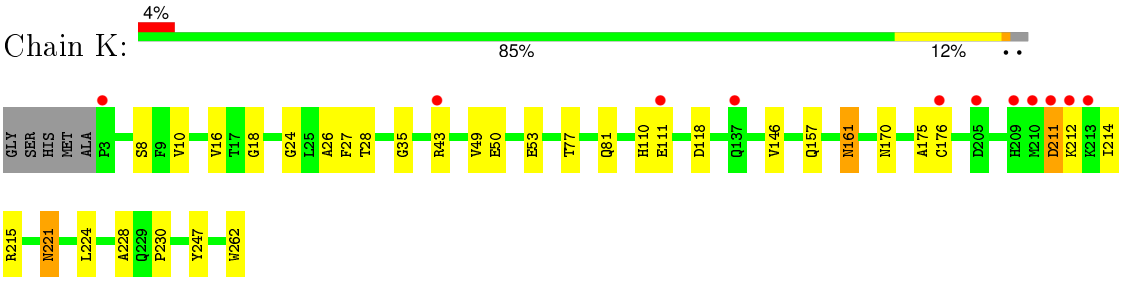
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain J:



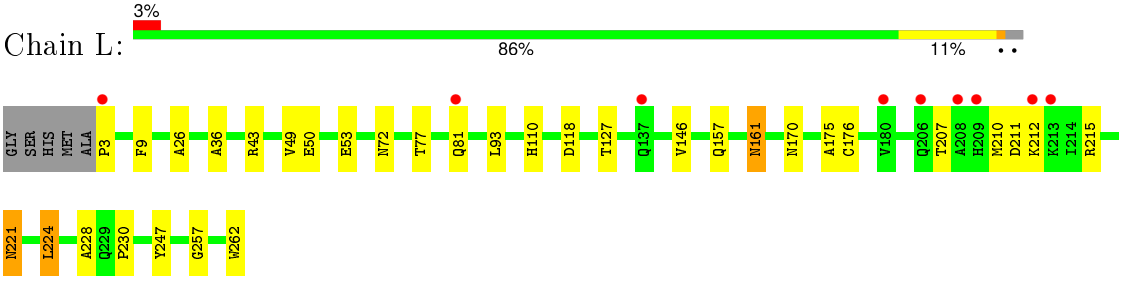
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain K:



• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.25Å 124.85Å 132.69Å 90.00° 118.54° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 39.89 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.50) 98.3 (39.89-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.209 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 508942 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27197	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.30	0/1985	0.70	3/2693 (0.1%)
1	B	0.30	0/1985	0.68	2/2693 (0.1%)
1	C	0.32	0/1985	0.68	2/2693 (0.1%)
1	D	0.31	0/1985	0.67	3/2693 (0.1%)
1	E	0.36	0/1985	0.68	2/2693 (0.1%)
1	F	0.36	0/1985	0.68	1/2693 (0.0%)
1	G	0.34	0/1985	0.67	2/2693 (0.1%)
1	H	0.35	0/1985	0.69	2/2693 (0.1%)
1	I	0.35	0/1985	0.68	2/2693 (0.1%)
1	J	0.35	0/1985	0.67	1/2693 (0.0%)
1	K	0.35	0/1985	0.68	1/2693 (0.0%)
1	L	0.35	0/1985	0.69	1/2693 (0.0%)
All	All	0.34	0/23820	0.68	22/32316 (0.1%)

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	211	ASP	CB-CG-OD2	6.40	124.06	118.30
1	H	211	ASP	CB-CG-OD2	6.28	123.96	118.30
1	K	211	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	211	ASP	CB-CG-OD2	6.06	123.75	118.30
1	E	211	ASP	CB-CG-OD2	6.04	123.74	118.30

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	1952	0	1949	88	0
1	B	1952	0	1949	52	1
1	C	1952	0	1949	35	0
1	D	1952	0	1949	28	0
1	E	1952	0	1949	34	0
1	F	1952	0	1949	36	0
1	G	1952	0	1949	40	0
1	H	1952	0	1949	36	0
1	I	1952	0	1949	32	0
1	J	1952	0	1949	31	1
1	K	1952	0	1949	39	0
1	L	1952	0	1949	31	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	24	0	0
2	F	48	0	25	0	0
2	G	48	0	24	0	0
2	H	48	0	25	0	0
2	I	48	0	25	0	0
2	J	48	0	25	0	0
2	K	48	0	24	0	0
2	L	48	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	130	0	0	14	0
4	B	202	0	0	17	0
4	C	251	0	0	5	0
4	D	190	0	0	3	0
4	E	342	0	0	9	1
4	F	313	0	0	9	1
4	G	291	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	302	0	0	7	0
4	I	311	0	0	6	0
4	J	268	0	0	7	0
4	K	284	0	0	11	0
4	L	307	0	0	4	0
All	All	27197	0	23685	397	2

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 397 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:K:16:VAL:HG11	4:K:2029:HOH:O	1.60	1.01
1:C:50:GLU:HG3	4:C:2061:HOH:O	1.66	0.95
1:F:157:GLN:HE22	1:H:221:ASN:HD21	1.11	0.95
1:L:50:GLU:HG3	4:L:2074:HOH:O	1.64	0.94
1:A:212:LYS:HD2	1:F:3:PRO:HD2	1.46	0.93

All (2) 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:B:86:ASP:O	1:J:11:ASN:OD1[3_546]	1.88	0.32
4:E:2145:HOH:O	4:F:2169:HOH:O[2_656]	2.17	0.03

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	258/265 (97%)	239 (93%)	19 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	258/265 (97%)	245 (95%)	13 (5%)	0	100	100
1	C	258/265 (97%)	251 (97%)	7 (3%)	0	100	100
1	D	258/265 (97%)	250 (97%)	8 (3%)	0	100	100
1	E	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	F	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	G	258/265 (97%)	252 (98%)	6 (2%)	0	100	100
1	H	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	I	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	J	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	K	258/265 (97%)	252 (98%)	6 (2%)	0	100	100
1	L	258/265 (97%)	252 (98%)	6 (2%)	0	100	100
All	All	3096/3180 (97%)	3006 (97%)	90 (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	208/211 (99%)	204 (98%)	4 (2%)	65	31
1	B	208/211 (99%)	204 (98%)	4 (2%)	65	31
1	C	208/211 (99%)	206 (99%)	2 (1%)	82	62
1	D	208/211 (99%)	205 (99%)	3 (1%)	74	47
1	E	208/211 (99%)	206 (99%)	2 (1%)	82	62
1	F	208/211 (99%)	205 (99%)	3 (1%)	74	47
1	G	208/211 (99%)	205 (99%)	3 (1%)	74	47
1	H	208/211 (99%)	205 (99%)	3 (1%)	74	47
1	I	208/211 (99%)	206 (99%)	2 (1%)	82	62
1	J	208/211 (99%)	205 (99%)	3 (1%)	74	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	208/211 (99%)	205 (99%)	3 (1%)	74 47
1	L	208/211 (99%)	205 (99%)	3 (1%)	74 47
All	All	2496/2532 (99%)	2461 (99%)	35 (1%)	74 47

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	161	ASN
1	G	221	ASN
1	L	161	ASN
1	F	221	ASN
1	F	224	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	110	HIS
1	G	161	ASN
1	L	110	HIS
1	F	161	ASN
1	F	221	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)

Of 18 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
2	NAP	A	263	-	42,52,52	1.60	3 (7%)	54,80,80	2.20	11 (20%)
2	NAP	B	263	-	42,52,52	1.49	3 (7%)	54,80,80	2.12	9 (16%)
2	NAP	C	263	-	42,52,52	1.53	4 (9%)	54,80,80	2.19	8 (14%)
2	NAP	D	263	-	42,52,52	1.53	4 (9%)	54,80,80	2.31	9 (16%)
2	NAP	E	263	-	42,52,52	1.56	4 (9%)	54,80,80	2.27	10 (18%)
2	NAP	F	263	-	42,52,52	1.53	4 (9%)	54,80,80	2.21	12 (22%)
2	NAP	G	263	-	42,52,52	1.52	4 (9%)	54,80,80	2.35	11 (20%)
2	NAP	H	263	-	42,52,52	1.53	4 (9%)	54,80,80	2.28	11 (20%)
2	NAP	I	263	-	42,52,52	1.57	4 (9%)	54,80,80	2.02	8 (14%)
2	NAP	J	263	-	42,52,52	1.47	5 (11%)	54,80,80	2.23	11 (20%)
2	NAP	K	263	-	42,52,52	1.53	4 (9%)	54,80,80	2.19	9 (16%)
2	NAP	L	263	-	42,52,52	1.52	4 (9%)	54,80,80	2.35	8 (14%)

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	NAP	A	263	-	-	0/27/67/67	0/5/5/5
2	NAP	B	263	-	-	0/27/67/67	0/5/5/5
2	NAP	C	263	-	-	0/27/67/67	0/5/5/5
2	NAP	D	263	-	-	0/27/67/67	0/5/5/5
2	NAP	E	263	-	-	0/27/67/67	0/5/5/5
2	NAP	F	263	-	-	0/27/67/67	0/5/5/5
2	NAP	G	263	-	-	0/27/67/67	0/5/5/5
2	NAP	H	263	-	-	0/27/67/67	0/5/5/5
2	NAP	I	263	-	-	0/27/67/67	0/5/5/5
2	NAP	J	263	-	-	0/27/67/67	0/5/5/5
2	NAP	K	263	-	-	0/27/67/67	0/5/5/5
2	NAP	L	263	-	-	0/27/67/67	0/5/5/5

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	263	NAP	O3B-C3B	-2.91	1.36	1.43
2	E	263	NAP	O3B-C3B	-2.78	1.36	1.43
2	G	263	NAP	O3B-C3B	-2.60	1.36	1.43
2	F	263	NAP	O3B-C3B	-2.53	1.36	1.43
2	C	263	NAP	O3B-C3B	-2.47	1.37	1.43

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	263	NAP	N3A-C2A-N1A	-12.57	119.27	128.89
2	L	263	NAP	N3A-C2A-N1A	-12.36	119.43	128.89
2	A	263	NAP	N3A-C2A-N1A	-12.15	119.59	128.89
2	G	263	NAP	N3A-C2A-N1A	-11.76	119.89	128.89
2	B	263	NAP	N3A-C2A-N1A	-11.67	119.96	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	263	NAP	1	0
2	B	263	NAP	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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	260/265 (98%)	1.89	96 (36%) 0 1	26, 49, 74, 82	0
1	B	260/265 (98%)	0.86	30 (11%) 6 6	21, 29, 38, 45	0
1	C	260/265 (98%)	0.38	21 (8%) 15 14	17, 23, 33, 41	0
1	D	260/265 (98%)	0.80	34 (13%) 5 4	18, 29, 41, 55	0
1	E	260/265 (98%)	0.16	14 (5%) 29 30	14, 18, 25, 30	0
1	F	260/265 (98%)	0.29	12 (4%) 36 37	14, 19, 28, 34	0
1	G	260/265 (98%)	0.38	25 (9%) 10 10	14, 21, 31, 36	0
1	H	260/265 (98%)	0.27	9 (3%) 48 50	14, 18, 27, 30	0
1	I	260/265 (98%)	0.23	14 (5%) 29 30	14, 19, 27, 32	0
1	J	260/265 (98%)	0.36	19 (7%) 18 18	15, 21, 31, 36	0
1	K	260/265 (98%)	0.29	11 (4%) 40 42	14, 20, 29, 37	0
1	L	260/265 (98%)	0.23	9 (3%) 48 50	14, 19, 27, 31	0
All	All	3120/3180 (98%)	0.51	294 (9%) 11 10	14, 21, 45, 82	0

The worst 5 of 294 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	PRO	11.6
1	D	208	ALA	9.4
1	A	208	ALA	8.3
1	B	11	ASN	8.3
1	I	3	PRO	8.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NI	B	2263	1/1	0.88	0.41	11.81	78,78,78,78	0
3	NI	J	3263	1/1	0.98	0.17	2.98	16,16,16,16	0
2	NAP	J	263	48/48	0.95	0.09	-0.09	18,20,24,28	0
2	NAP	A	263	48/48	0.86	0.17	-0.09	40,54,62,68	0
2	NAP	K	263	48/48	0.95	0.08	-0.20	16,18,22,27	0
3	NI	A	2263	1/1	0.96	0.11	-0.22	32,32,32,32	0
2	NAP	H	263	48/48	0.95	0.09	-0.22	15,18,21,28	0
2	NAP	D	263	48/48	0.94	0.09	-0.26	22,25,30,32	0
2	NAP	C	263	48/48	0.95	0.09	-0.27	17,21,25,30	0
2	NAP	I	263	48/48	0.96	0.08	-0.30	16,18,22,28	0
2	NAP	B	263	48/48	0.91	0.10	-0.37	22,28,31,34	0
2	NAP	G	263	48/48	0.95	0.09	-0.39	16,20,23,26	0
2	NAP	E	263	48/48	0.96	0.08	-0.40	15,17,20,25	0
3	NI	I	3263	1/1	1.00	0.10	-0.41	21,21,21,21	0
2	NAP	L	263	48/48	0.96	0.08	-0.45	15,18,22,27	0
3	NI	F	3263	1/1	0.99	0.10	-0.52	20,20,20,20	0
2	NAP	F	263	48/48	0.96	0.08	-0.52	15,17,21,27	0
3	NI	E	3263	1/1	1.00	0.09	-1.07	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.