



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:06 PM GMT

PDB ID : 1S20
Title : A novel NAD binding protein revealed by the crystal structure of E. Coli 2,3-diketogulonate reductase (YiaK) NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET ER82
Authors : Forouhar, F.; Lee, I.; Benach, J.; Kulkarni, K.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2004-01-07
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
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

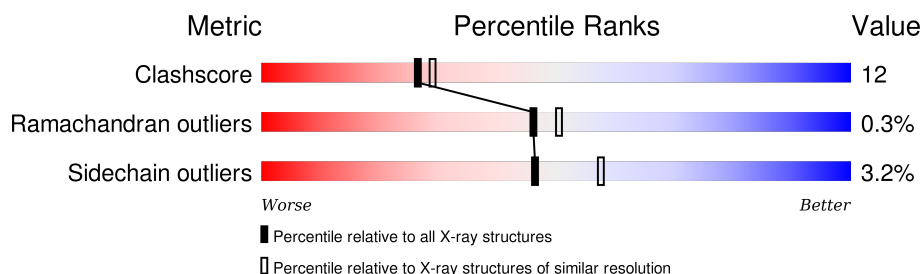
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 $\leq 5\%$. 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	340	
1	B	340	
1	C	340	
1	D	340	
1	E	340	
1	F	340	
1	G	340	

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Mol	Chain	Length	Quality of chain
1	H	340	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 74%, a yellow segment representing 22%, and a small grey segment at the end. Below the green segment is the label '74%' and below the yellow segment is the label '22%'. To the right of the grey segment are two small black dots.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22358 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 Hypothetical oxidoreductase yiaK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	Se	0	0	0
			2579	1615	453	493	3	15			
1	B	334	Total	C	N	O	S	Se	0	0	0
			2579	1615	453	493	3	15			
1	C	334	Total	C	N	O	S	Se	0	0	0
			2579	1615	453	493	3	15			
1	D	334	Total	C	N	O	S	Se	0	0	0
			2579	1615	453	493	3	15			
1	E	334	Total	C	N	O	S	Se	0	0	0
			2579	1615	453	493	3	15			
1	F	333	Total	C	N	O	S	Se	0	0	0
			2570	1610	452	490	3	15			
1	G	335	Total	C	N	O	S	Se	0	0	0
			2589	1621	456	494	3	15			
1	H	334	Total	C	N	O	S	Se	0	0	0
			2579	1615	453	493	3	15			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	32	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	93	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	94	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	118	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	144	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	170	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	173	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	175	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	177	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	182	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	221	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	229	MSE	MET	MODIFIED RESIDUE	UNP P37672

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Chain	Residue	Modelled	Actual	Comment	Reference
A	235	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	285	MSE	MET	MODIFIED RESIDUE	UNP P37672
A	333	LEU	-	CLONING ARTIFACT	UNP P37672
A	334	GLU	-	CLONING ARTIFACT	UNP P37672
A	335	HIS	-	EXPRESSION TAG	UNP P37672
A	336	HIS	-	EXPRESSION TAG	UNP P37672
A	337	HIS	-	EXPRESSION TAG	UNP P37672
A	338	HIS	-	EXPRESSION TAG	UNP P37672
A	339	HIS	-	EXPRESSION TAG	UNP P37672
A	340	HIS	-	EXPRESSION TAG	UNP P37672
B	1	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	32	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	93	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	94	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	118	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	144	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	170	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	173	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	175	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	177	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	182	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	221	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	229	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	235	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	285	MSE	MET	MODIFIED RESIDUE	UNP P37672
B	333	LEU	-	CLONING ARTIFACT	UNP P37672
B	334	GLU	-	CLONING ARTIFACT	UNP P37672
B	335	HIS	-	EXPRESSION TAG	UNP P37672
B	336	HIS	-	EXPRESSION TAG	UNP P37672
B	337	HIS	-	EXPRESSION TAG	UNP P37672
B	338	HIS	-	EXPRESSION TAG	UNP P37672
B	339	HIS	-	EXPRESSION TAG	UNP P37672
B	340	HIS	-	EXPRESSION TAG	UNP P37672
C	1	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	32	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	93	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	94	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	118	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	144	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	170	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	173	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	175	MSE	MET	MODIFIED RESIDUE	UNP P37672

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Chain	Residue	Modelled	Actual	Comment	Reference
C	177	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	182	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	221	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	229	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	235	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	285	MSE	MET	MODIFIED RESIDUE	UNP P37672
C	333	LEU	-	CLONING ARTIFACT	UNP P37672
C	334	GLU	-	CLONING ARTIFACT	UNP P37672
C	335	HIS	-	EXPRESSION TAG	UNP P37672
C	336	HIS	-	EXPRESSION TAG	UNP P37672
C	337	HIS	-	EXPRESSION TAG	UNP P37672
C	338	HIS	-	EXPRESSION TAG	UNP P37672
C	339	HIS	-	EXPRESSION TAG	UNP P37672
C	340	HIS	-	EXPRESSION TAG	UNP P37672
D	1	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	32	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	93	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	94	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	118	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	144	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	170	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	173	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	175	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	177	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	182	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	221	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	229	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	235	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	285	MSE	MET	MODIFIED RESIDUE	UNP P37672
D	333	LEU	-	CLONING ARTIFACT	UNP P37672
D	334	GLU	-	CLONING ARTIFACT	UNP P37672
D	335	HIS	-	EXPRESSION TAG	UNP P37672
D	336	HIS	-	EXPRESSION TAG	UNP P37672
D	337	HIS	-	EXPRESSION TAG	UNP P37672
D	338	HIS	-	EXPRESSION TAG	UNP P37672
D	339	HIS	-	EXPRESSION TAG	UNP P37672
D	340	HIS	-	EXPRESSION TAG	UNP P37672
E	1	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	32	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	93	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	94	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	118	MSE	MET	MODIFIED RESIDUE	UNP P37672

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Chain	Residue	Modelled	Actual	Comment	Reference
E	144	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	170	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	173	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	175	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	177	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	182	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	221	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	229	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	235	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	285	MSE	MET	MODIFIED RESIDUE	UNP P37672
E	333	LEU	-	CLONING ARTIFACT	UNP P37672
E	334	GLU	-	CLONING ARTIFACT	UNP P37672
E	335	HIS	-	EXPRESSION TAG	UNP P37672
E	336	HIS	-	EXPRESSION TAG	UNP P37672
E	337	HIS	-	EXPRESSION TAG	UNP P37672
E	338	HIS	-	EXPRESSION TAG	UNP P37672
E	339	HIS	-	EXPRESSION TAG	UNP P37672
E	340	HIS	-	EXPRESSION TAG	UNP P37672
F	1	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	32	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	93	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	94	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	118	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	144	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	170	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	173	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	175	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	177	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	182	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	221	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	229	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	235	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	285	MSE	MET	MODIFIED RESIDUE	UNP P37672
F	333	LEU	-	CLONING ARTIFACT	UNP P37672
F	334	GLU	-	CLONING ARTIFACT	UNP P37672
F	335	HIS	-	EXPRESSION TAG	UNP P37672
F	336	HIS	-	EXPRESSION TAG	UNP P37672
F	337	HIS	-	EXPRESSION TAG	UNP P37672
F	338	HIS	-	EXPRESSION TAG	UNP P37672
F	339	HIS	-	EXPRESSION TAG	UNP P37672
F	340	HIS	-	EXPRESSION TAG	UNP P37672
G	1	MSE	MET	MODIFIED RESIDUE	UNP P37672

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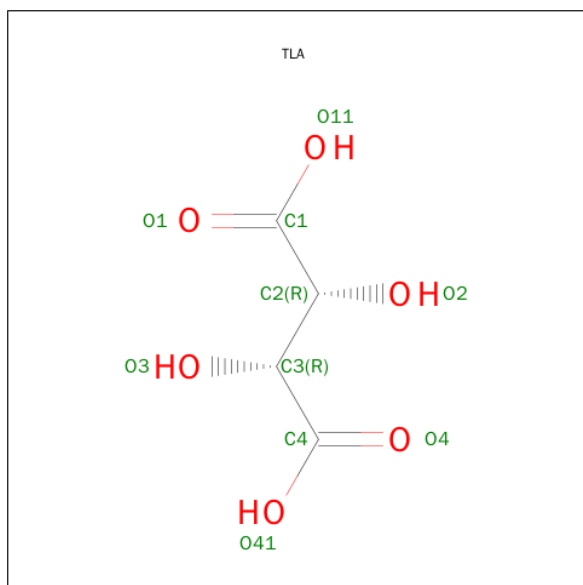
Chain	Residue	Modelled	Actual	Comment	Reference
G	32	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	93	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	94	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	118	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	144	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	170	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	173	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	175	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	177	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	182	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	221	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	229	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	235	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	285	MSE	MET	MODIFIED RESIDUE	UNP P37672
G	333	LEU	-	CLONING ARTIFACT	UNP P37672
G	334	GLU	-	CLONING ARTIFACT	UNP P37672
G	335	HIS	-	EXPRESSION TAG	UNP P37672
G	336	HIS	-	EXPRESSION TAG	UNP P37672
G	337	HIS	-	EXPRESSION TAG	UNP P37672
G	338	HIS	-	EXPRESSION TAG	UNP P37672
G	339	HIS	-	EXPRESSION TAG	UNP P37672
G	340	HIS	-	EXPRESSION TAG	UNP P37672
H	1	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	32	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	93	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	94	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	118	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	144	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	170	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	173	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	175	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	177	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	182	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	221	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	229	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	235	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	285	MSE	MET	MODIFIED RESIDUE	UNP P37672
H	333	LEU	-	CLONING ARTIFACT	UNP P37672
H	334	GLU	-	CLONING ARTIFACT	UNP P37672
H	335	HIS	-	EXPRESSION TAG	UNP P37672
H	336	HIS	-	EXPRESSION TAG	UNP P37672
H	337	HIS	-	EXPRESSION TAG	UNP P37672

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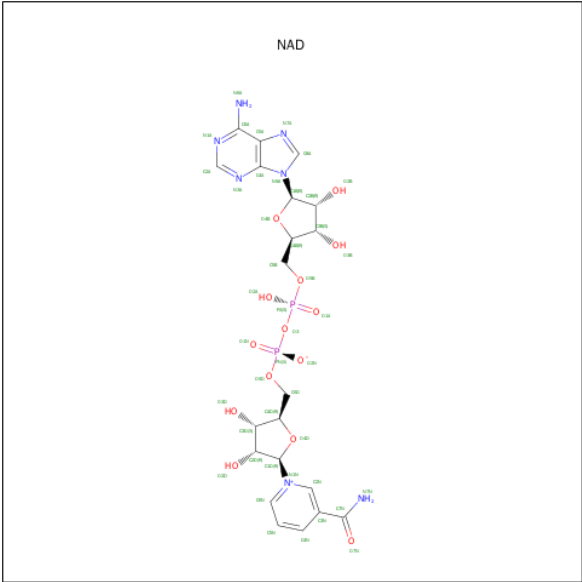
Chain	Residue	Modelled	Actual	Comment	Reference
H	338	HIS	-	EXPRESSION TAG	UNP P37672
H	339	HIS	-	EXPRESSION TAG	UNP P37672
H	340	HIS	-	EXPRESSION TAG	UNP P37672

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0
2	F	1	Total C O 10 4 6	0	0
2	G	1	Total C O 10 4 6	0	0
2	H	1	Total C O 10 4 6	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total	O	0	0
			203	203		
4	B	160	Total	O	0	0
			160	160		
4	C	177	Total	O	0	0
			177	177		
4	D	158	Total	O	0	0
			158	158		
4	E	159	Total	O	0	0
			159	159		
4	F	190	Total	O	0	0
			190	190		

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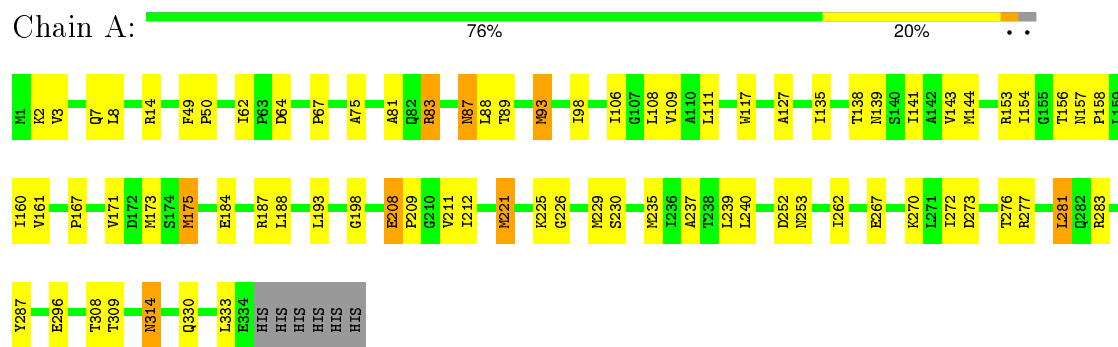
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	186	Total 186	O 186	0	0
4	H	168	Total 168	O 168	0	0

3 Residue-property plots

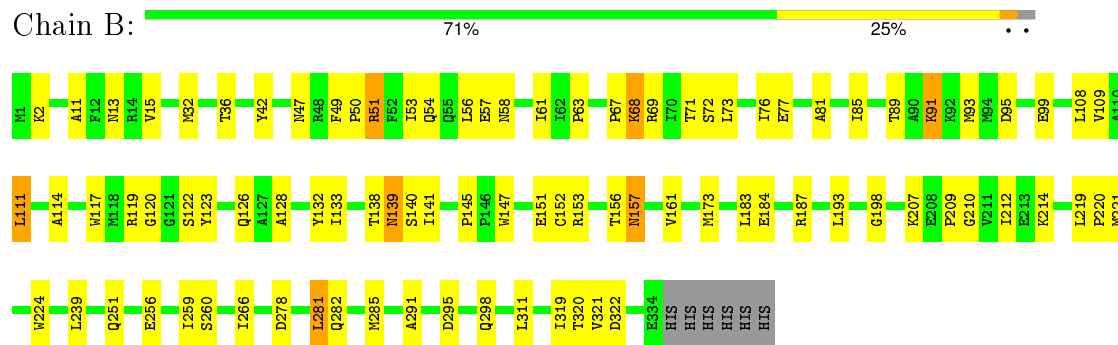
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

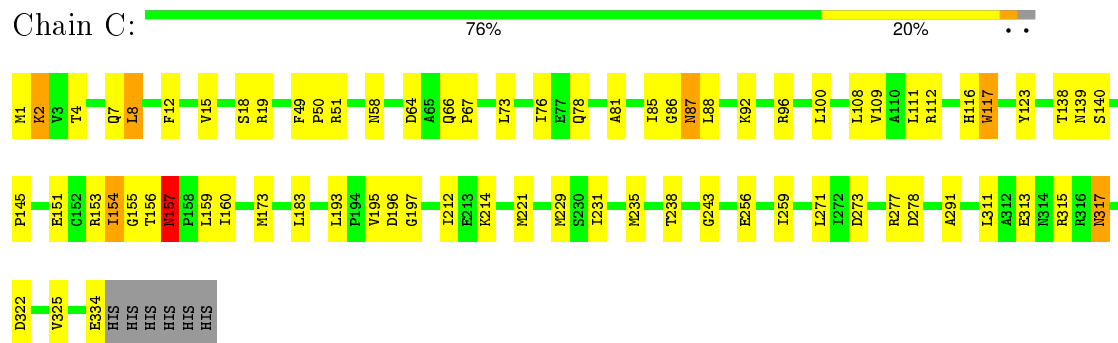
• Molecule 1: Hypothetical oxidoreductase yiaK



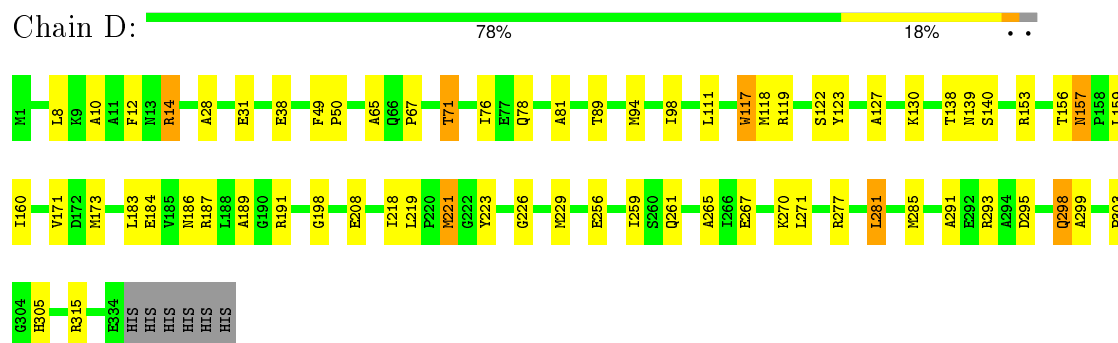
• Molecule 1: Hypothetical oxidoreductase yiaK



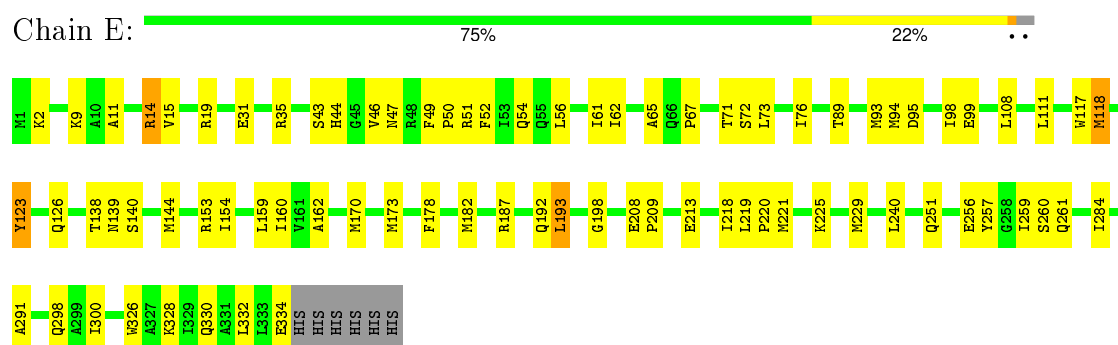
• Molecule 1: Hypothetical oxidoreductase yiaK



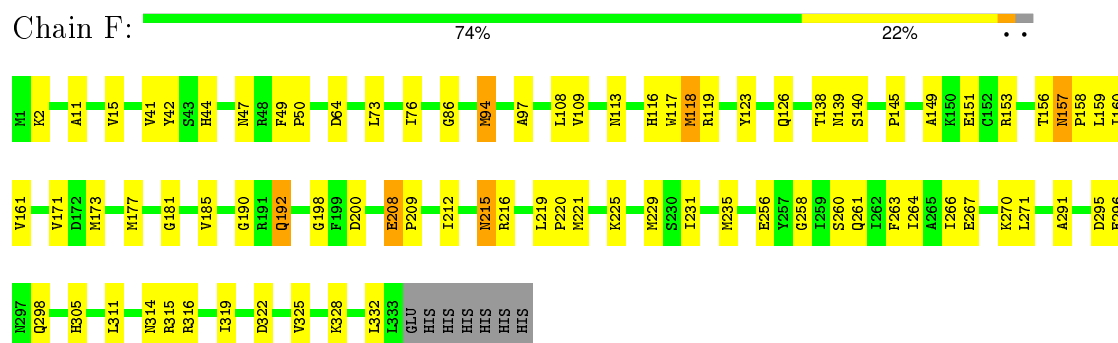
- Molecule 1: Hypothetical oxidoreductase *viaK*



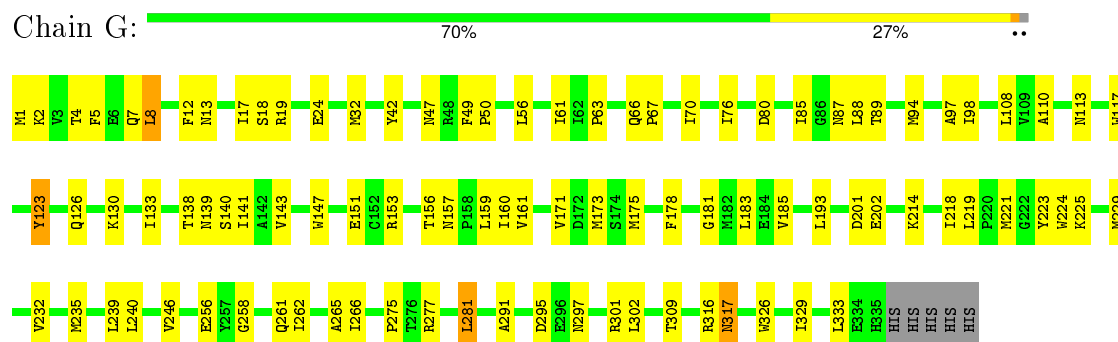
- Molecule 1: Hypothetical oxidoreductase *viaK*



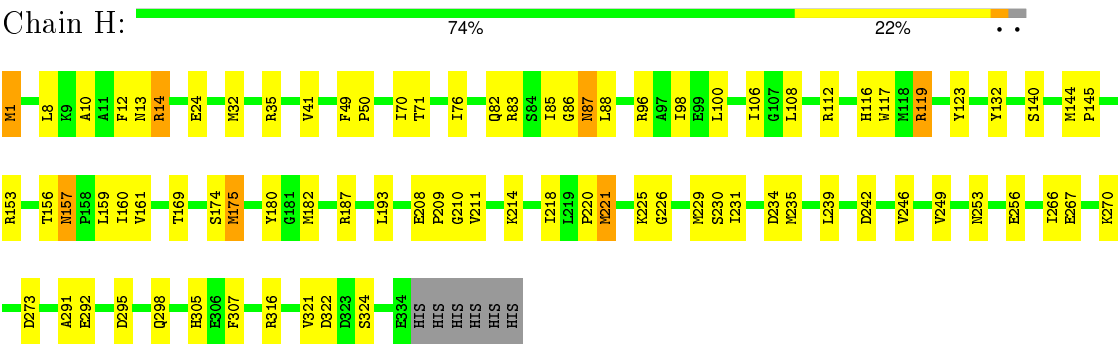
- Molecule 1: Hypothetical oxidoreductase *viaK*



- Molecule 1: Hypothetical oxidoreductase *viaK*



● Molecule 1: Hypothetical oxidoreductase yiaK



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.52Å 81.28Å 113.22Å 79.55° 77.22° 82.01°	Depositor
Resolution (Å)	24.02 – 2.20	Depositor
% Data completeness (in resolution range)	83.4 (24.02-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22358	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: TLA, 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	0.34	0/2611	0.56	0/3510
1	B	0.31	0/2611	0.53	0/3510
1	C	0.32	0/2611	0.54	0/3510
1	D	0.33	0/2611	0.54	0/3510
1	E	0.31	0/2611	0.55	0/3510
1	F	0.33	0/2602	0.54	0/3498
1	G	0.33	0/2622	0.53	0/3525
1	H	0.33	0/2611	0.53	0/3510
All	All	0.33	0/20890	0.54	0/28083

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	B	0	1
1	D	0	1
1	E	0	1
1	G	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	123	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	123	TYR	Sidechain
1	E	123	TYR	Sidechain
1	G	123	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	2579	0	2562	74	0
1	B	2579	0	2562	79	0
1	C	2579	0	2562	66	0
1	D	2579	0	2562	57	0
1	E	2579	0	2562	65	0
1	F	2570	0	2556	73	0
1	G	2589	0	2569	78	0
1	H	2579	0	2562	68	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	D	10	0	4	0	0
2	F	10	0	4	0	0
2	G	10	0	4	0	0
2	H	10	0	4	0	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
3	D	44	0	26	0	0
3	F	44	0	26	1	0
3	G	44	0	26	2	0
3	H	44	0	26	0	0
4	A	203	0	0	5	0
4	B	160	0	0	5	0
4	C	177	0	0	2	0
4	D	158	0	0	3	0
4	E	159	0	0	3	0
4	F	190	0	0	9	0
4	G	186	0	0	4	0
4	H	168	0	0	9	0
All	All	22358	0	20677	506	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 12.

The worst 5 of 506 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:G:94:MSE:HE1	1:G:265:ALA:HB2	1.39	1.03
1:A:173:MSE:HE3	1:A:175:MSE:HE1	1.46	0.95
1:B:184:GLU:HG3	1:B:187:ARG:HH21	1.34	0.93
1:D:94:MSE:HE1	1:D:265:ALA:HB2	1.51	0.92
1:B:139:ASN:HD21	1:B:260:SER:H	1.15	0.88

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	332/340 (98%)	319 (96%)	13 (4%)	0	100	100
1	B	332/340 (98%)	318 (96%)	13 (4%)	1 (0%)	46	50
1	C	332/340 (98%)	314 (95%)	17 (5%)	1 (0%)	46	50
1	D	332/340 (98%)	321 (97%)	10 (3%)	1 (0%)	46	50
1	E	332/340 (98%)	317 (96%)	14 (4%)	1 (0%)	46	50
1	F	331/340 (97%)	317 (96%)	13 (4%)	1 (0%)	46	50
1	G	333/340 (98%)	316 (95%)	16 (5%)	1 (0%)	46	50
1	H	332/340 (98%)	318 (96%)	13 (4%)	1 (0%)	46	50
All	All	2656/2720 (98%)	2540 (96%)	109 (4%)	7 (0%)	46	50

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	24	GLU

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Mol	Chain	Res	Type
1	D	157	ASN
1	E	118	MSE
1	F	118	MSE
1	C	157	ASN

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	273/264 (103%)	260 (95%)	13 (5%)	31	37
1	B	273/264 (103%)	264 (97%)	9 (3%)	45	56
1	C	273/264 (103%)	262 (96%)	11 (4%)	38	47
1	D	273/264 (103%)	266 (97%)	7 (3%)	54	66
1	E	273/264 (103%)	268 (98%)	5 (2%)	66	79
1	F	272/264 (103%)	263 (97%)	9 (3%)	45	56
1	G	274/264 (104%)	268 (98%)	6 (2%)	60	72
1	H	273/264 (103%)	263 (96%)	10 (4%)	41	50
All	All	2184/2112 (103%)	2114 (97%)	70 (3%)	46	57

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	273	ASP
1	D	298	GLN
1	H	35	ARG
1	C	317	ASN
1	D	117	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	314	ASN

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Mol	Chain	Res	Type
1	E	186	ASN
1	H	87	ASN
1	E	54	GLN
1	E	314	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](#)

12 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	$\# Z > 2$
3	NAD	A	401	-	38,48,48	1.29	5 (13%)	47,73,73	2.47	6 (12%)
2	TLA	A	501	-	3,9,9	0.58	0	6,12,12	1.29	1 (16%)
3	NAD	B	402	-	38,48,48	1.28	4 (10%)	47,73,73	2.51	6 (12%)
2	TLA	B	502	-	3,9,9	0.63	0	6,12,12	1.43	1 (16%)
3	NAD	D	404	-	38,48,48	1.35	4 (10%)	47,73,73	2.47	6 (12%)
2	TLA	D	504	-	3,9,9	0.59	0	6,12,12	1.55	1 (16%)
3	NAD	F	406	-	38,48,48	1.42	6 (15%)	47,73,73	2.54	6 (12%)
2	TLA	F	506	-	3,9,9	0.52	0	6,12,12	1.60	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	G	407	-	38,48,48	1.28	5 (13%)	47,73,73	2.51	6 (12%)
2	TLA	G	507	-	3,9,9	0.59	0	6,12,12	1.54	1 (16%)
3	NAD	H	408	-	38,48,48	1.34	4 (10%)	47,73,73	2.51	6 (12%)
2	TLA	H	508	-	3,9,9	0.67	0	6,12,12	1.46	2 (33%)

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
3	NAD	A	401	-	-	0/22/62/62	0/5/5/5
2	TLA	A	501	-	-	0/4/12/12	0/0/0/0
3	NAD	B	402	-	-	0/22/62/62	0/5/5/5
2	TLA	B	502	-	-	0/4/12/12	0/0/0/0
3	NAD	D	404	-	-	0/22/62/62	0/5/5/5
2	TLA	D	504	-	-	0/4/12/12	0/0/0/0
3	NAD	F	406	-	-	0/22/62/62	0/5/5/5
2	TLA	F	506	-	-	0/4/12/12	0/0/0/0
3	NAD	G	407	-	-	0/22/62/62	0/5/5/5
2	TLA	G	507	-	-	0/4/12/12	0/0/0/0
3	NAD	H	408	-	-	0/22/62/62	0/5/5/5
2	TLA	H	508	-	-	0/4/12/12	0/0/0/0

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	407	NAD	PA-O2A	-2.00	1.46	1.54
3	G	407	NAD	O4B-C1B	2.02	1.43	1.41
3	A	401	NAD	C4N-C3N	2.07	1.42	1.39
3	F	406	NAD	C2N-C3N	2.08	1.42	1.39
3	F	406	NAD	C4N-C3N	2.18	1.43	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	406	NAD	N3A-C2A-N1A	-14.01	118.17	128.89
3	H	408	NAD	N3A-C2A-N1A	-13.80	118.33	128.89
3	G	407	NAD	N3A-C2A-N1A	-13.78	118.34	128.89
3	B	402	NAD	N3A-C2A-N1A	-13.72	118.39	128.89
3	A	401	NAD	N3A-C2A-N1A	-13.69	118.41	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAD	1	0
3	B	402	NAD	1	0
3	F	406	NAD	1	0
3	G	407	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.