



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:27 AM UTC

PDB ID : 1S20 / pdb_00001s20
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

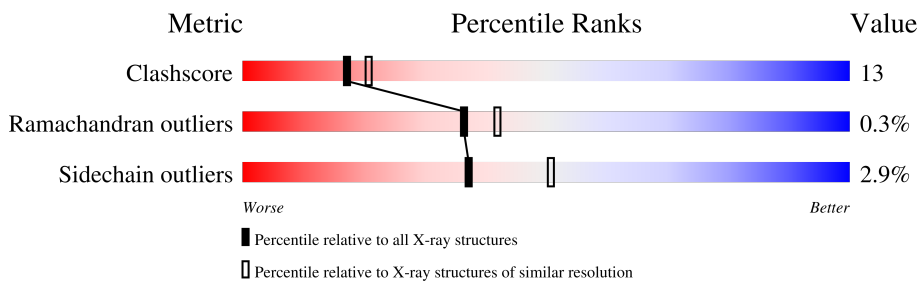
1 Overall quality at a glance

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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

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	
1	H	340	

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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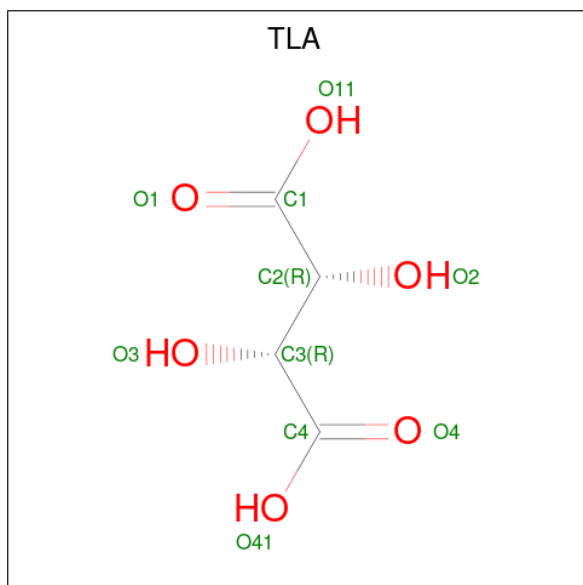
Chain	Residue	Modelled	Actual	Comment	Reference
G	32	MSE	MET	modified residue	UNP P37672
G	93	MSE	MET	modified residue	UNP P37672
G	94	MSE	MET	modified residue	UNP P37672
G	118	MSE	MET	modified residue	UNP P37672
G	144	MSE	MET	modified residue	UNP P37672
G	170	MSE	MET	modified residue	UNP P37672
G	173	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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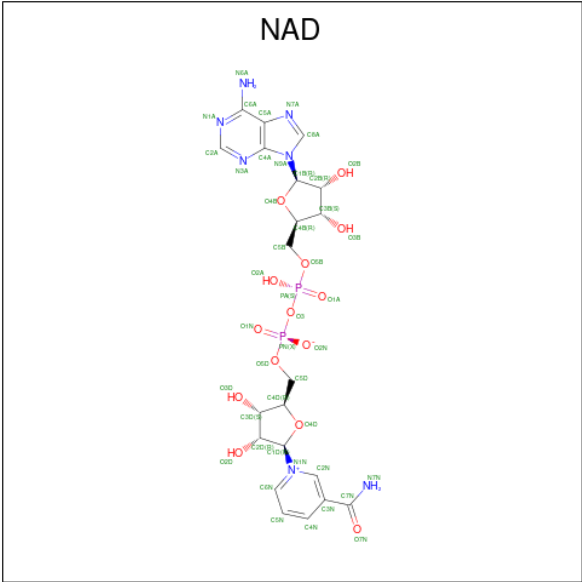
Chain	Residue	Modelled	Actual	Comment	Reference
H	338	HIS	-	expression tag	UNP P37672
H	339	HIS	-	expression tag	UNP P37672
H	340	HIS	-	expression tag	UNP P37672

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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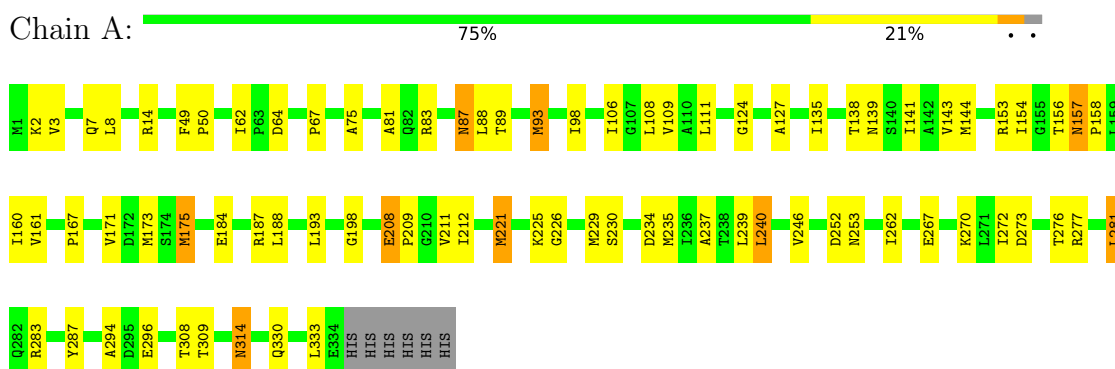
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	186	Total 186	O 186	0	0
4	H	168	Total 168	O 168	0	0

3 Residue-property plots

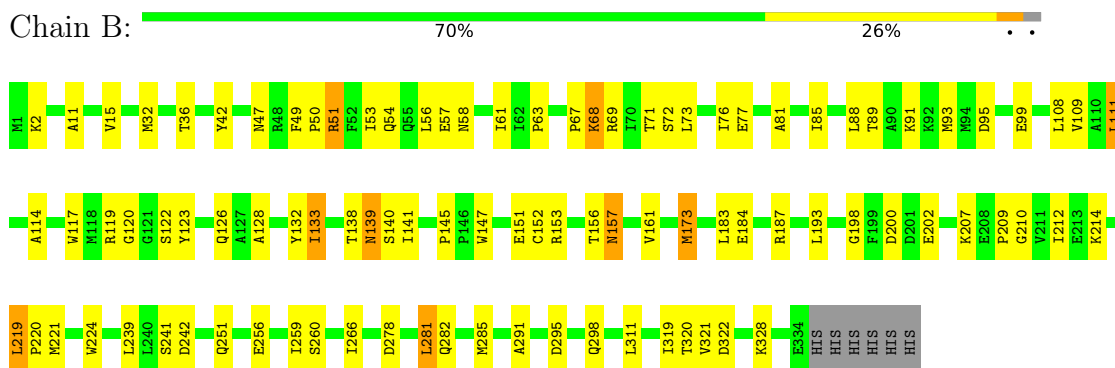
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

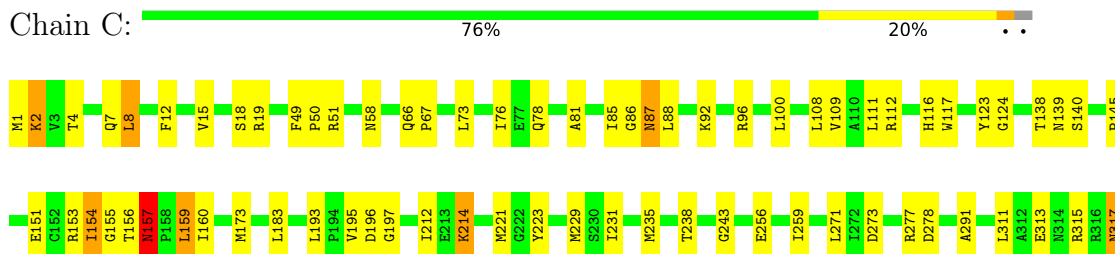
• Molecule 1: Hypothetical oxidoreductase yiaK



• Molecule 1: Hypothetical oxidoreductase yiaK



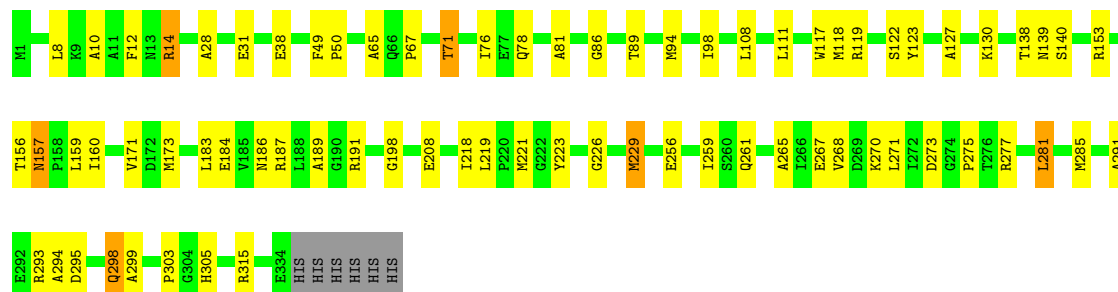
• Molecule 1: Hypothetical oxidoreductase yiaK





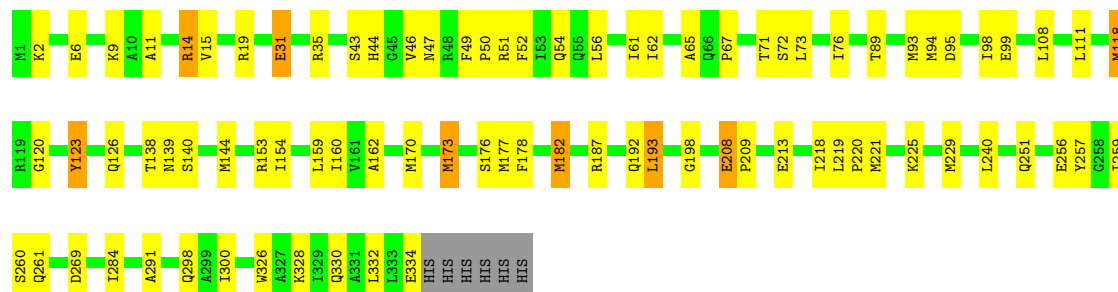
• Molecule 1: Hypothetical oxidoreductase yiaK

Chain D: 76% 20% ..



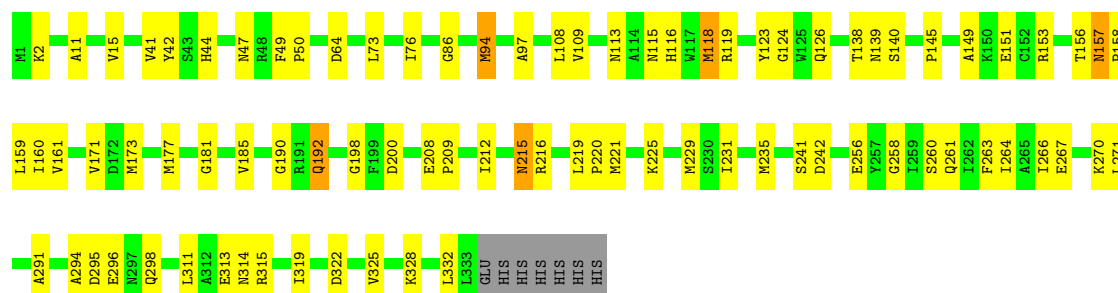
• Molecule 1: Hypothetical oxidoreductase yiaK

Chain E: 74% 22% ..



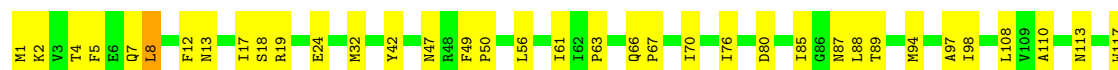
• Molecule 1: Hypothetical oxidoreductase yiaK

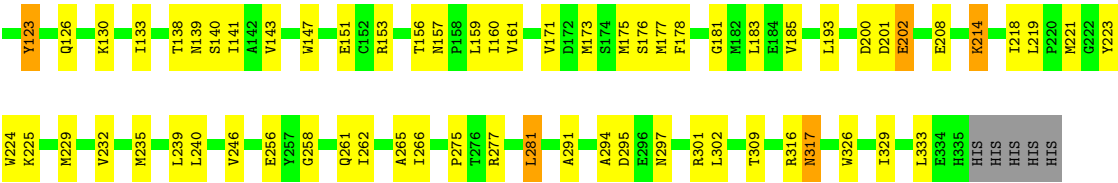
Chain F: 73% 24% ..



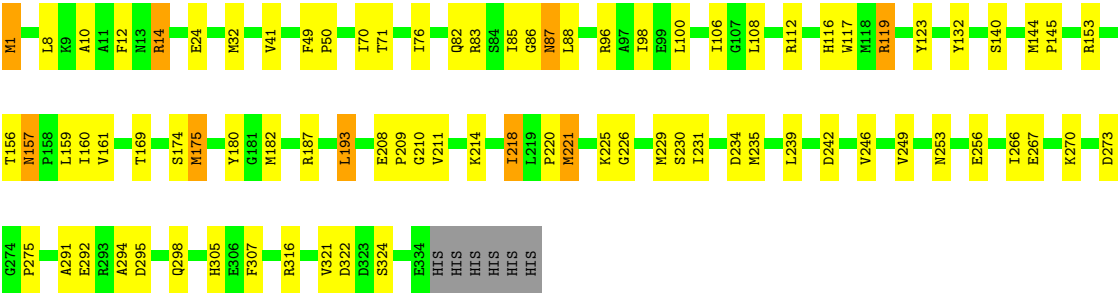
• Molecule 1: Hypothetical oxidoreductase yiaK

Chain G: 69% 28% ..





• Molecule 1: Hypothetical oxidoreductase yiaK



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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: NAD, TLA

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	0.43	0/2611	0.86	6/3510 (0.2%)
1	B	0.39	0/2611	0.82	3/3510 (0.1%)
1	C	0.41	0/2611	0.83	2/3510 (0.1%)
1	D	0.41	0/2611	0.83	3/3510 (0.1%)
1	E	0.41	0/2611	0.86	4/3510 (0.1%)
1	F	0.42	0/2602	0.85	2/3498 (0.1%)
1	G	0.42	0/2622	0.82	3/3525 (0.1%)
1	H	0.41	0/2611	0.81	1/3510 (0.0%)
All	All	0.41	0/20890	0.84	24/28083 (0.1%)

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.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ILE	N-CA-C	-6.88	99.86	109.21
1	A	124	GLY	N-CA-C	-6.67	104.23	112.77
1	D	86	GLY	N-CA-C	6.62	120.17	112.50
1	F	294	ALA	N-CA-C	-6.46	104.09	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	173	MSE	N-CA-C	6.16	118.95	108.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	123	TYR	Sidechain
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	75	0
1	B	2579	0	2562	83	0
1	C	2579	0	2562	68	0
1	D	2579	0	2562	60	0
1	E	2579	0	2562	67	0
1	F	2570	0	2556	76	0
1	G	2589	0	2569	81	0
1	H	2579	0	2562	70	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	526	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 13.

The worst 5 of 526 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%)	36	42
1	C	332/340 (98%)	314 (95%)	17 (5%)	1 (0%)	36	42
1	D	332/340 (98%)	321 (97%)	10 (3%)	1 (0%)	36	42
1	E	332/340 (98%)	317 (96%)	14 (4%)	1 (0%)	36	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	331/340 (97%)	317 (96%)	13 (4%)	1 (0%)	36	42
1	G	333/340 (98%)	316 (95%)	16 (5%)	1 (0%)	36	42
1	H	332/340 (98%)	318 (96%)	13 (4%)	1 (0%)	36	42
All	All	2656/2720 (98%)	2540 (96%)	109 (4%)	7 (0%)	36	42

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	24	GLU
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%)	262 (96%)	11 (4%)	28	38
1	B	273/264 (103%)	264 (97%)	9 (3%)	33	45
1	C	273/264 (103%)	263 (96%)	10 (4%)	30	41
1	D	273/264 (103%)	267 (98%)	6 (2%)	45	61
1	E	273/264 (103%)	266 (97%)	7 (3%)	40	55
1	F	272/264 (103%)	267 (98%)	5 (2%)	51	68
1	G	274/264 (104%)	268 (98%)	6 (2%)	45	61
1	H	273/264 (103%)	264 (97%)	9 (3%)	33	45
All	All	2184/2112 (103%)	2121 (97%)	63 (3%)	37	51

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	273	ASP

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Mol	Chain	Res	Type
1	H	14	ARG
1	D	298	GLN
1	H	1	MSE
1	H	175	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	7	GLN
1	H	305	HIS
1	G	66	GLN
1	H	13	ASN
1	C	87	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 oligosaccharides 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
2	TLA	B	502	-	9,9,9	1.03	0	12,12,12	1.14	1 (8%)
2	TLA	F	506	-	9,9,9	1.17	0	12,12,12	1.19	1 (8%)
3	NAD	G	407	-	46,48,48	1.70	5 (10%)	64,73,73	1.92	12 (18%)
3	NAD	F	406	-	46,48,48	1.93	7 (15%)	64,73,73	1.97	12 (18%)
3	NAD	D	404	-	46,48,48	1.82	6 (13%)	64,73,73	1.93	12 (18%)
2	TLA	A	501	-	9,9,9	0.97	0	12,12,12	1.08	1 (8%)
3	NAD	A	401	-	46,48,48	1.74	7 (15%)	64,73,73	1.89	13 (20%)
3	NAD	H	408	-	46,48,48	1.80	5 (10%)	64,73,73	1.93	12 (18%)
2	TLA	D	504	-	9,9,9	1.14	0	12,12,12	1.12	1 (8%)
3	NAD	B	402	-	46,48,48	1.73	5 (10%)	64,73,73	1.90	11 (17%)
2	TLA	H	508	-	9,9,9	1.04	0	12,12,12	1.08	1 (8%)
2	TLA	G	507	-	9,9,9	1.05	0	12,12,12	1.20	1 (8%)

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	TLA	B	502	-	-	0/12/12/12	-
2	TLA	F	506	-	-	4/12/12/12	-
3	NAD	G	407	-	-	0/30/62/62	0/5/5/5
3	NAD	F	406	-	-	0/30/62/62	0/5/5/5
3	NAD	D	404	-	-	6/30/62/62	0/5/5/5
2	TLA	A	501	-	-	0/12/12/12	-
3	NAD	A	401	-	-	0/30/62/62	0/5/5/5
3	NAD	H	408	-	-	4/30/62/62	0/5/5/5
2	TLA	D	504	-	-	2/12/12/12	-
3	NAD	B	402	-	-	0/30/62/62	0/5/5/5
2	TLA	H	508	-	-	5/12/12/12	-
2	TLA	G	507	-	-	3/12/12/12	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	406	NAD	C2N-N1N	8.64	1.44	1.35
3	D	404	NAD	C2N-N1N	8.22	1.44	1.35
3	H	408	NAD	C2N-N1N	8.20	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAD	C2N-N1N	7.80	1.43	1.35
3	A	401	NAD	C2N-N1N	7.62	1.43	1.35

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	406	NAD	N3A-C2A-N1A	-6.88	118.17	128.58
3	H	408	NAD	N3A-C2A-N1A	-6.77	118.33	128.58
3	G	407	NAD	N3A-C2A-N1A	-6.76	118.34	128.58
3	B	402	NAD	N3A-C2A-N1A	-6.73	118.39	128.58
3	A	401	NAD	N3A-C2A-N1A	-6.72	118.41	128.58

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	404	NAD	C2N-C3N-C7N-O7N
3	D	404	NAD	C2N-C3N-C7N-N7N
3	D	404	NAD	C4N-C3N-C7N-O7N
3	D	404	NAD	C4N-C3N-C7N-N7N
3	H	408	NAD	C2N-C3N-C7N-O7N

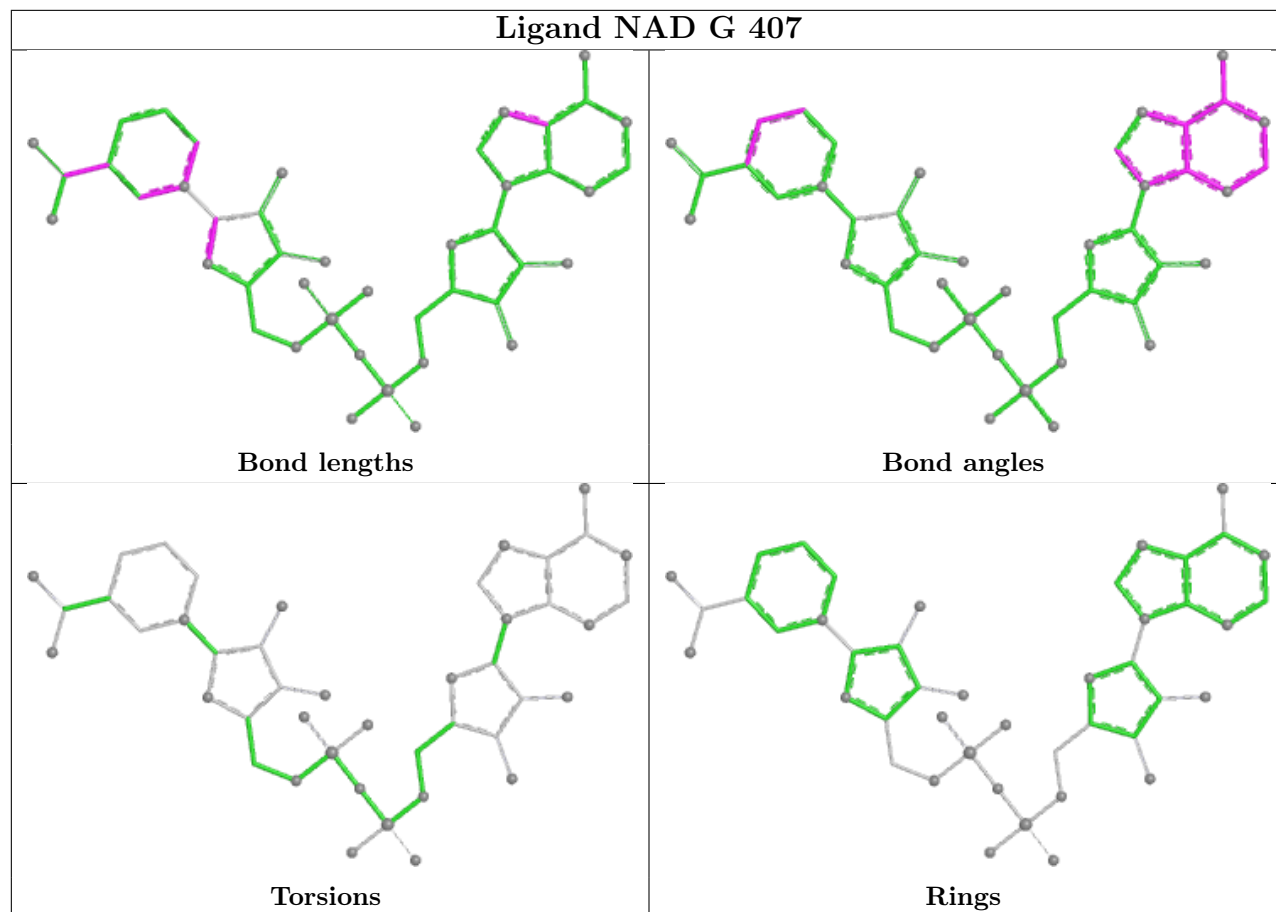
There are no ring outliers.

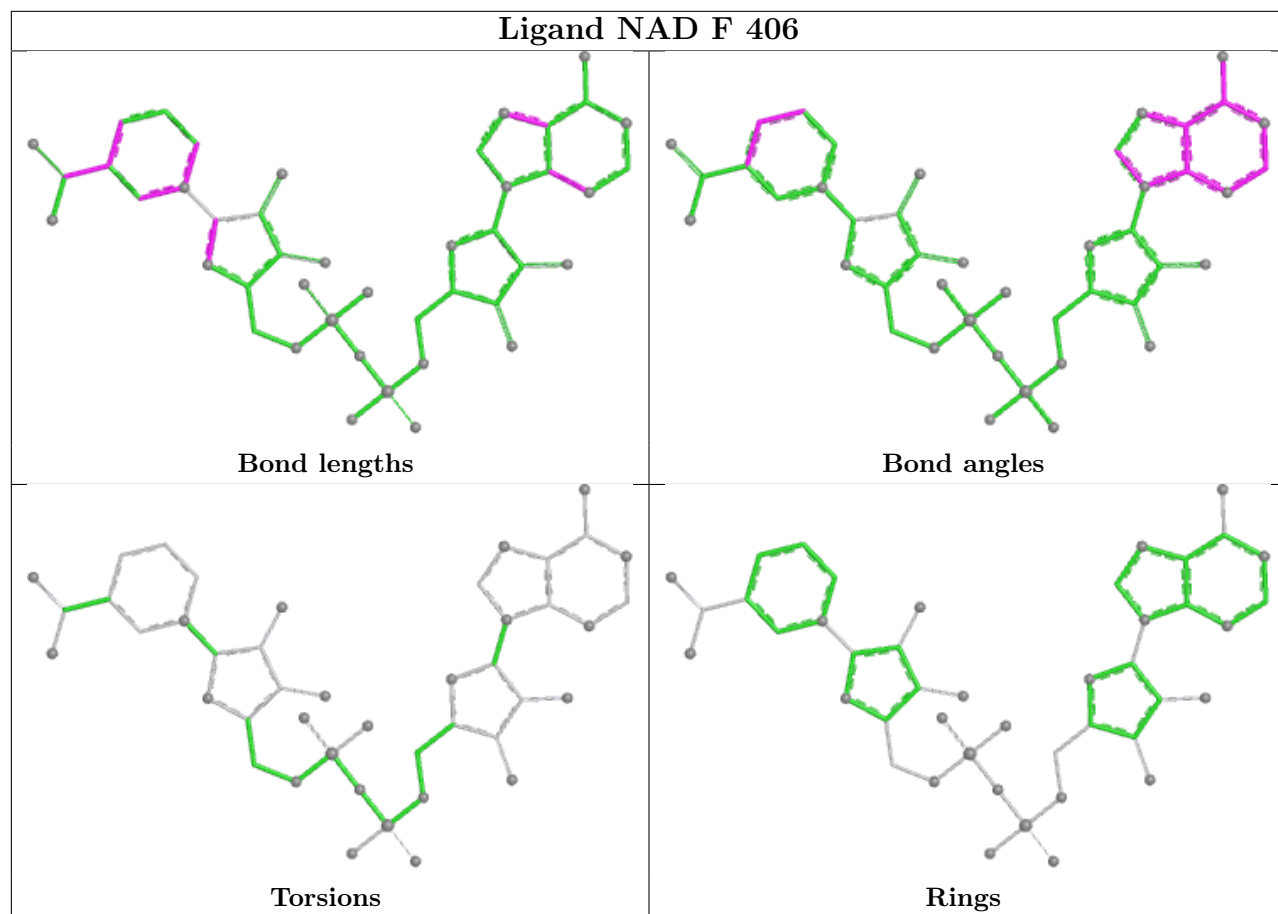
4 monomers are involved in 5 short contacts:

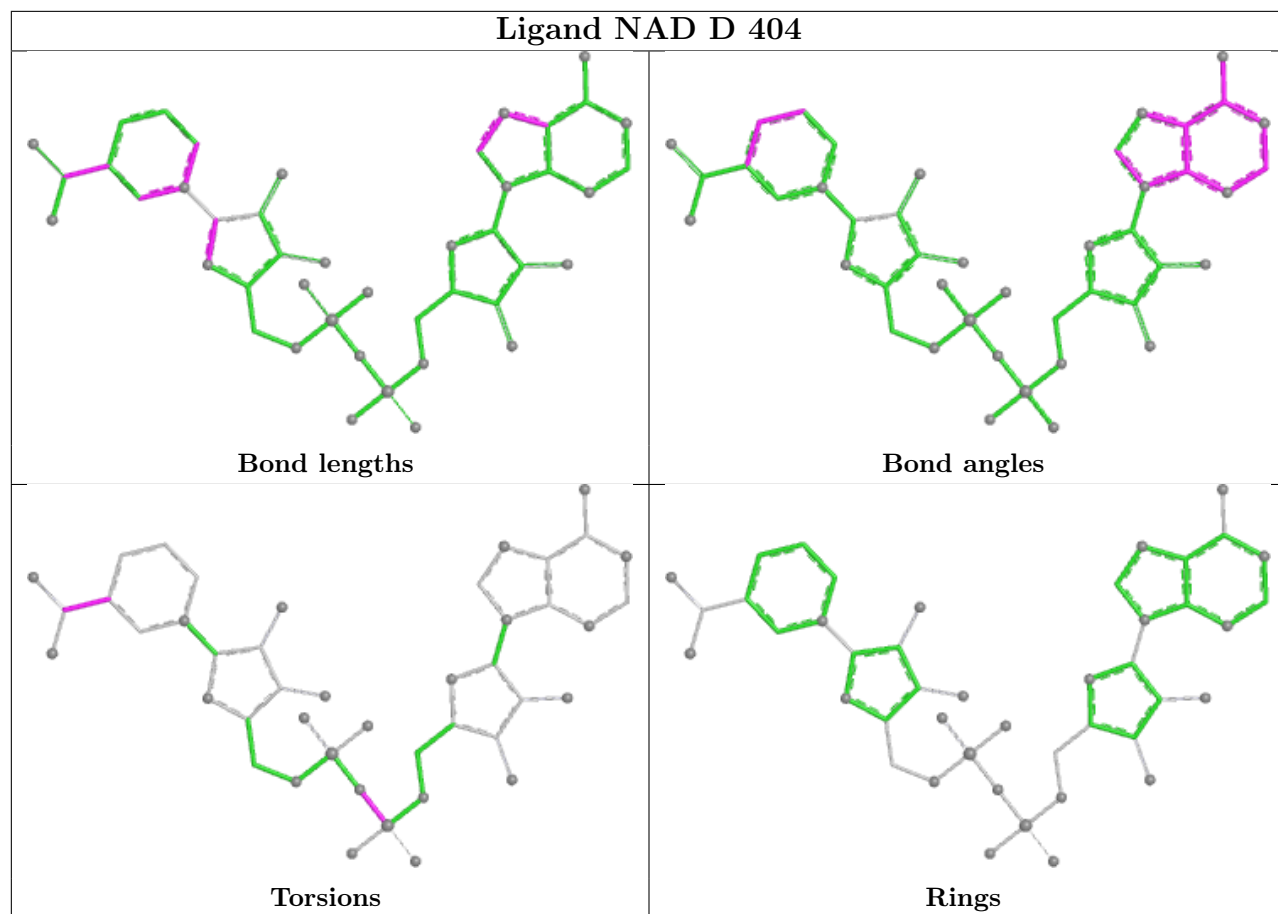
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	407	NAD	2	0
3	F	406	NAD	1	0
3	A	401	NAD	1	0
3	B	402	NAD	1	0

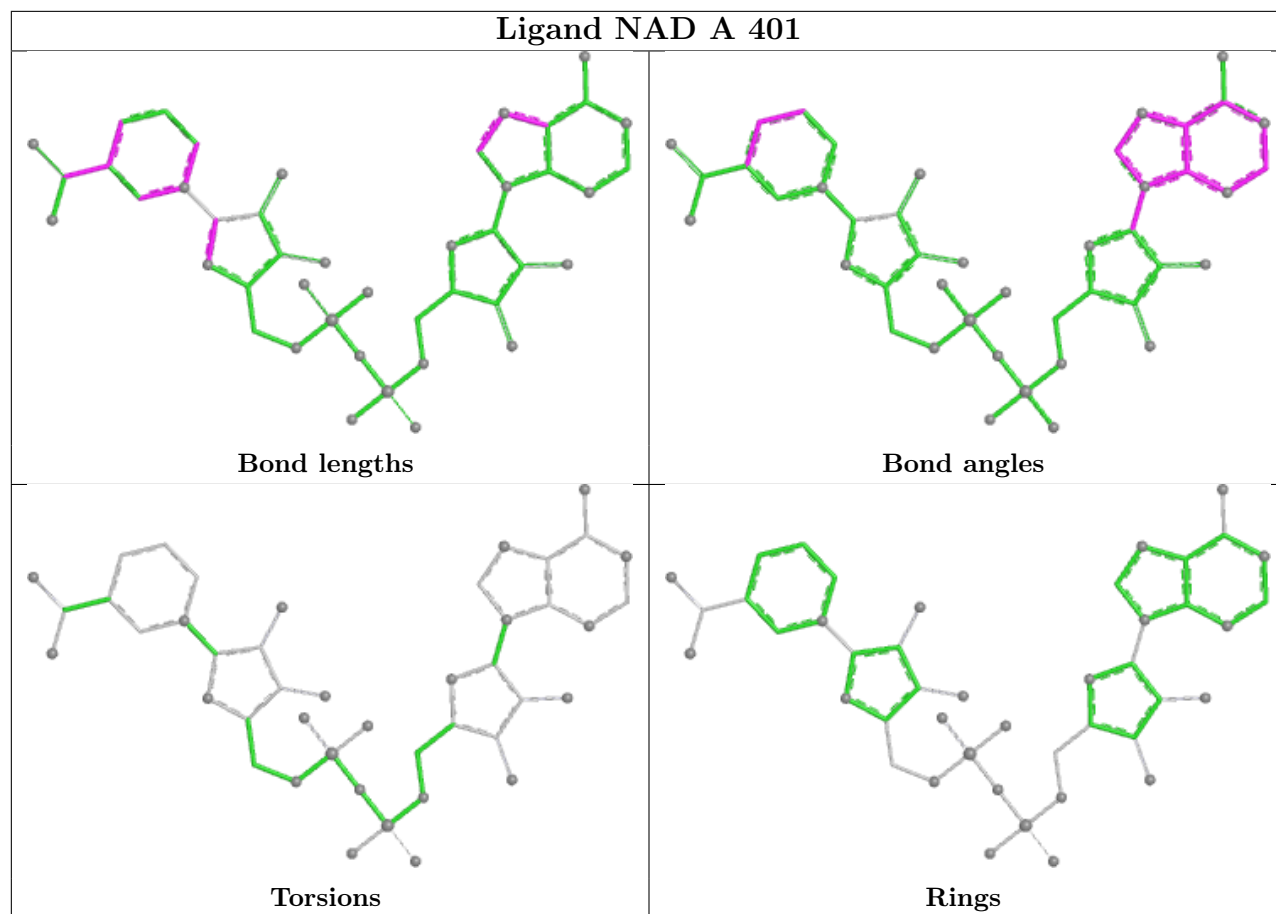
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

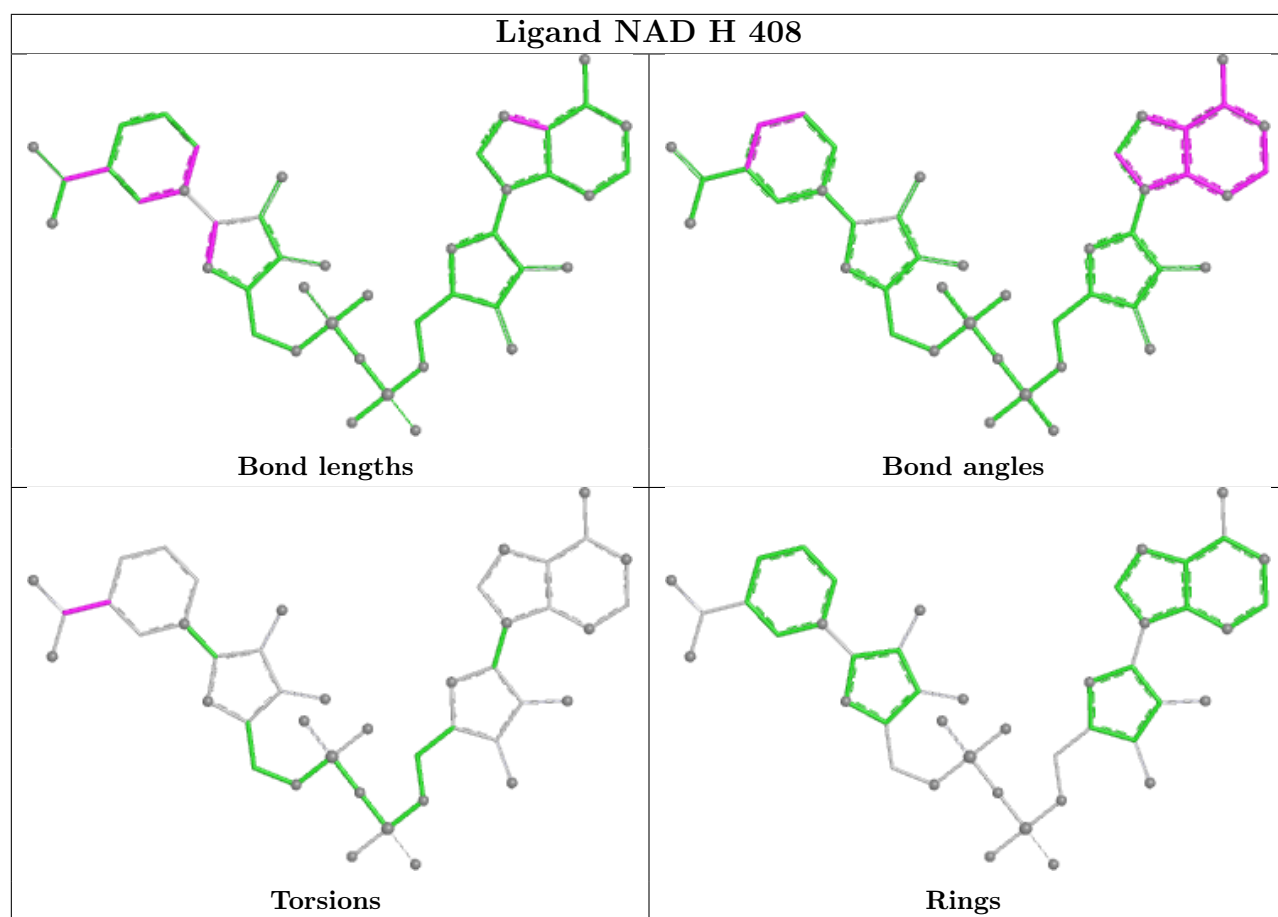
equivalents in the CSD to analyse the geometry.

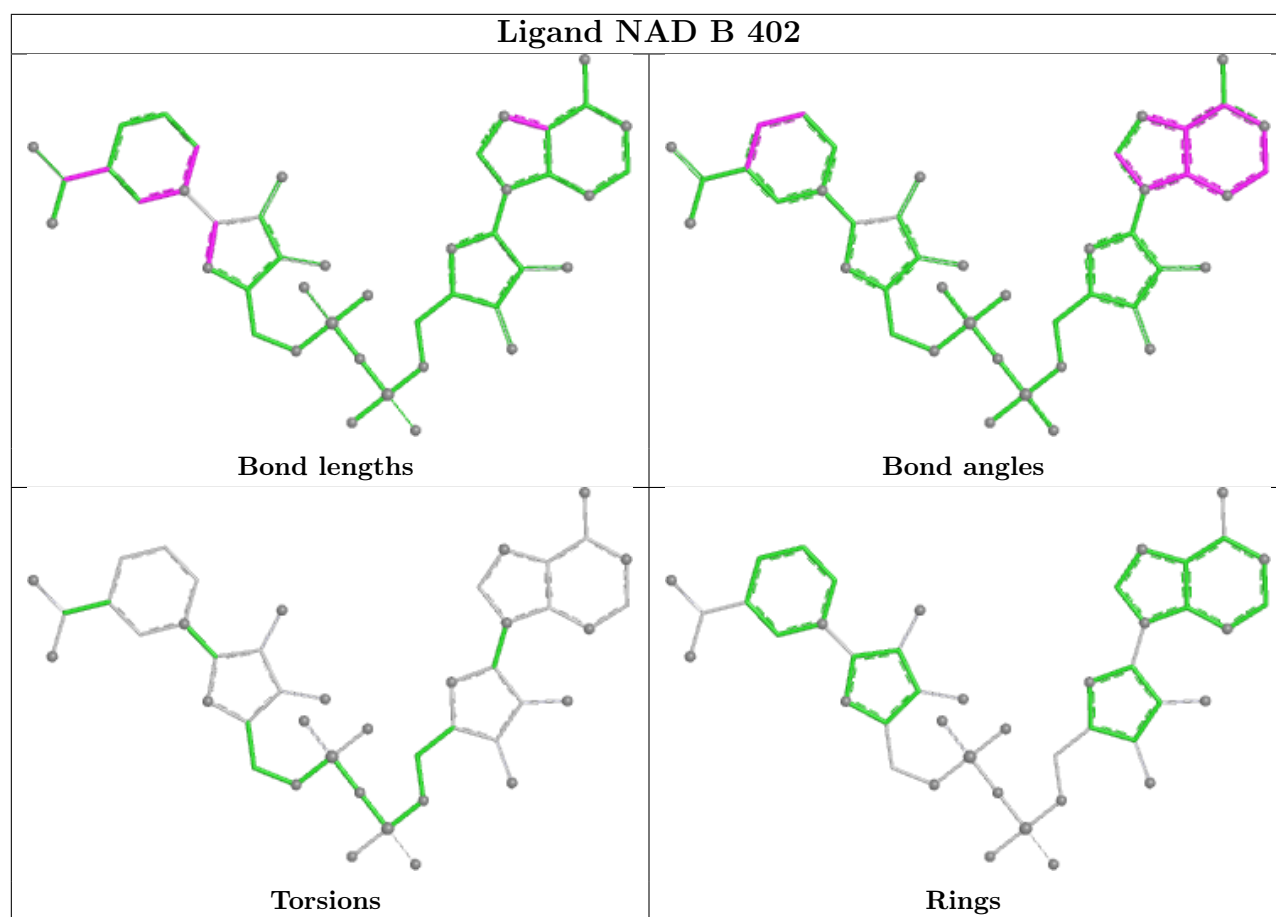












5.7 Other polymers [i](#)

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.