



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 16, 2018 – 08:13 PM EST

PDB ID : 1Y9E  
Title : Crystal structure of Bacillus subtilis protein yhfP with NAD bound  
Authors : Min, T.; Gorman, J.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2004-12-15  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

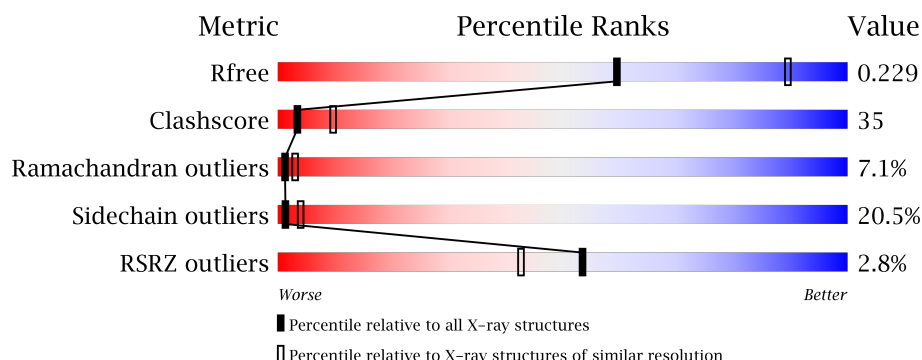
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



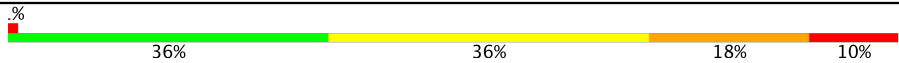
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>34%</div> <div>17%</div> <div>7%</div> </div> </div>
1	B	330	<div> <div>3%</div> <div> <div></div> <div>34%</div> <div>40%</div> <div>16%</div> <div>10%</div> </div> </div>
1	C	330	<div> <div>5%</div> <div> <div></div> <div>35%</div> <div>36%</div> <div>21%</div> <div>8%</div> </div> </div>
1	D	330	<div> <div>3%</div> <div> <div></div> <div>34%</div> <div>39%</div> <div>19%</div> <div>8%</div> </div> </div>
1	E	330	<div> <div>2%</div> <div> <div></div> <div>37%</div> <div>40%</div> <div>13%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	330	

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
2	NAD	E	5255	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14982 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 protein yhfP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	Se	0	0	0
			2429	1529	414	481	1	4			
1	B	329	Total	C	N	O	S	Se	0	0	0
			2421	1525	406	485	1	4			
1	C	329	Total	C	N	O	S	Se	0	0	0
			2412	1516	408	483	1	4			
1	D	329	Total	C	N	O	S	Se	0	0	0
			2431	1527	414	485	1	4			
1	E	329	Total	C	N	O	S	Se	0	0	0
			2433	1531	414	483	1	4			
1	F	329	Total	C	N	O	S	Se	0	0	0
			2437	1533	414	485	1	4			

There are 24 discrepancies between the modelled and reference sequences:

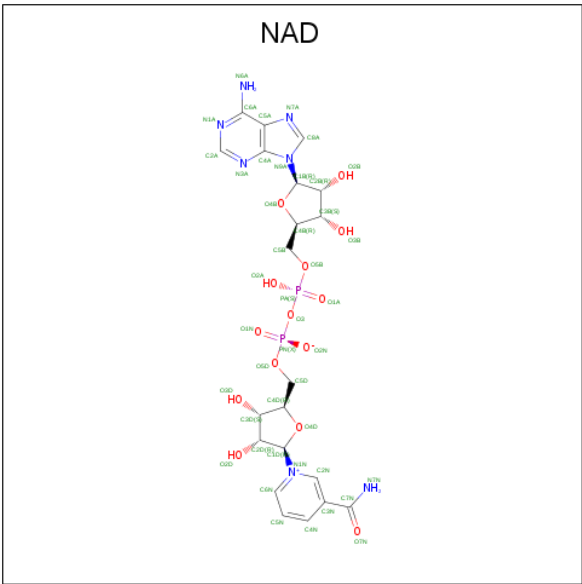
Chain	Residue	Modelled	Actual	Comment	Reference
A	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
A	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
A	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
A	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
B	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
B	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
B	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
B	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
C	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
C	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
C	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
C	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
D	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
D	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
D	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
D	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
E	126	MSE	MET	MODIFIED RESIDUE	UNP O07615

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Chain	Residue	Modelled	Actual	Comment	Reference
E	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
E	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
E	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
F	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
F	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
F	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
F	288	MSE	MET	MODIFIED RESIDUE	UNP O07615

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 11 6 5	0	0
2	B	1	Total C N 11 6 5	0	0
2	C	1	Total C N 11 6 5	0	0
2	D	1	Total C N 11 6 5	0	0
2	E	1	Total C N 11 6 5	0	0
2	F	1	Total C N 11 6 5	0	0

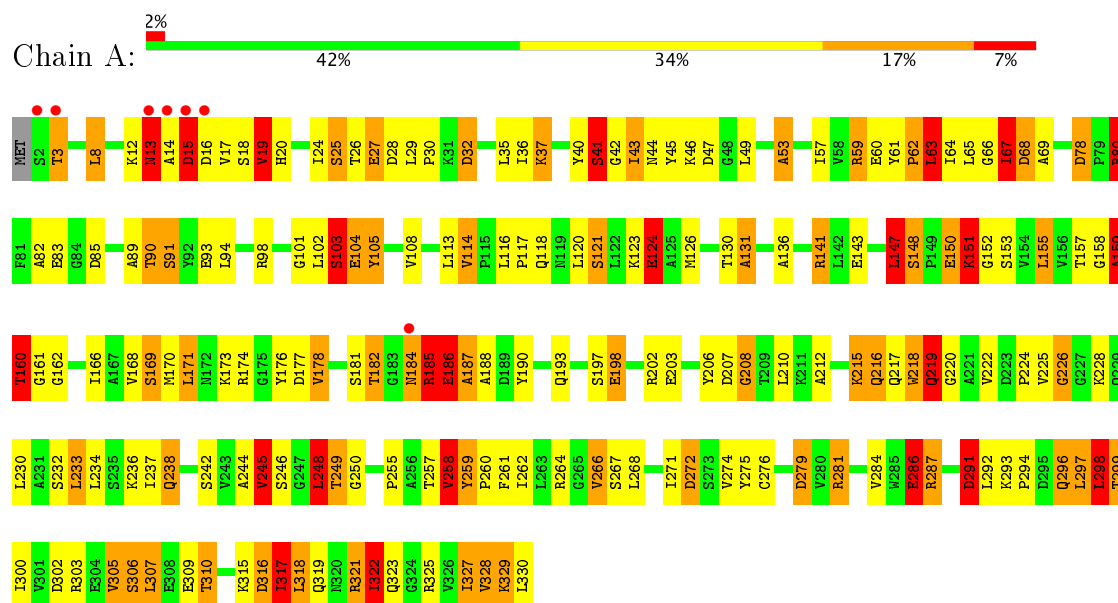
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total 65	O 65	0	0
3	B	56	Total 56	O 56	0	0
3	C	57	Total 57	O 57	0	0
3	D	53	Total 53	O 53	0	0
3	E	60	Total 60	O 60	0	0
3	F	62	Total 62	O 62	0	0

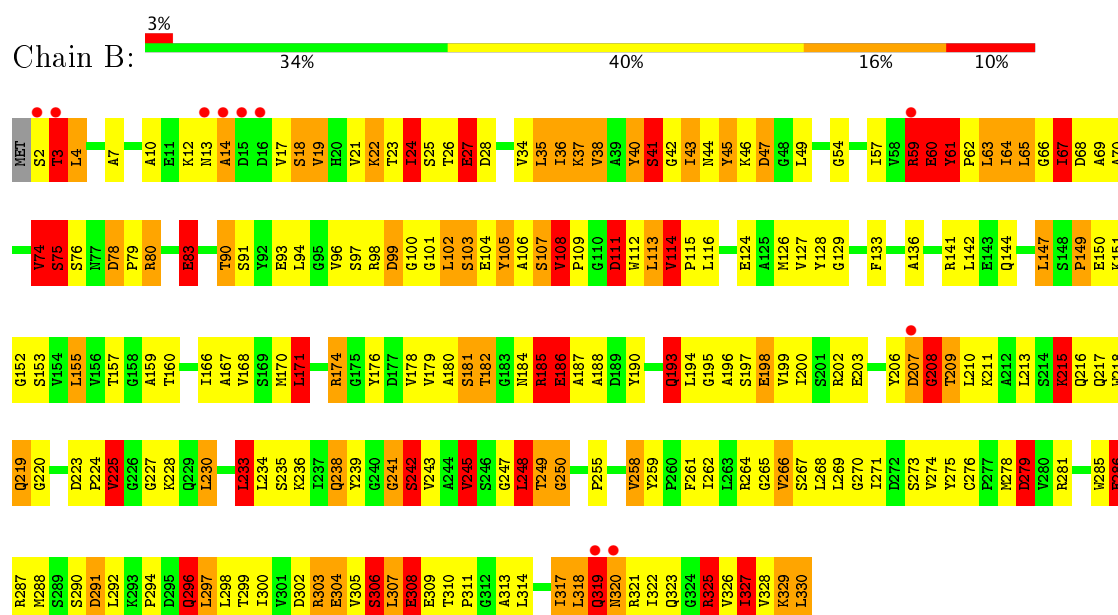
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

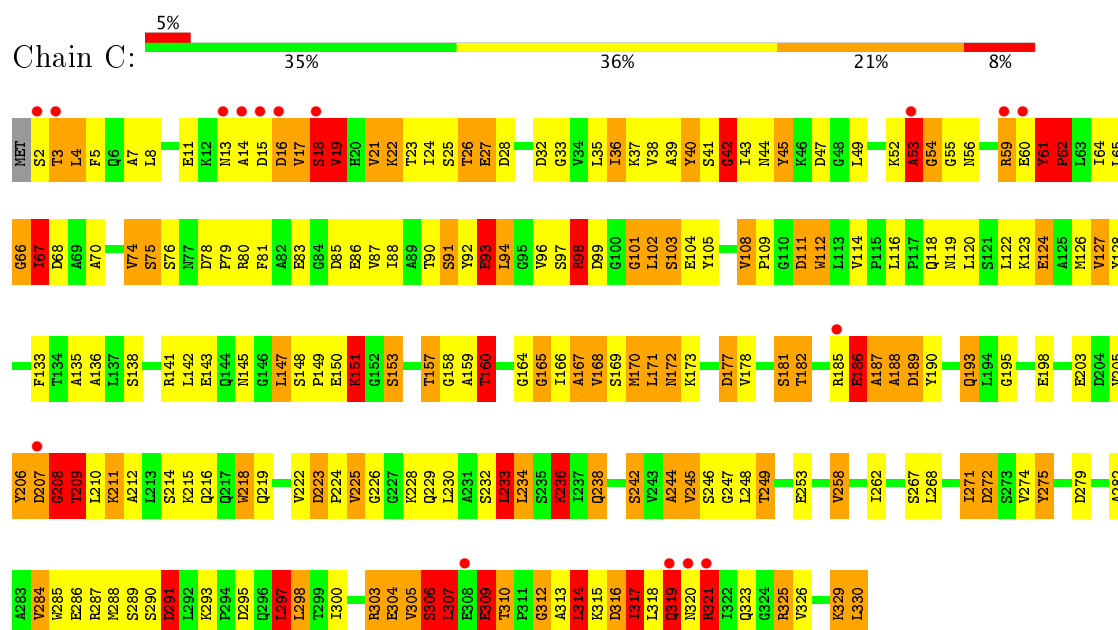
#### • Molecule 1: hypothetical protein yhfP



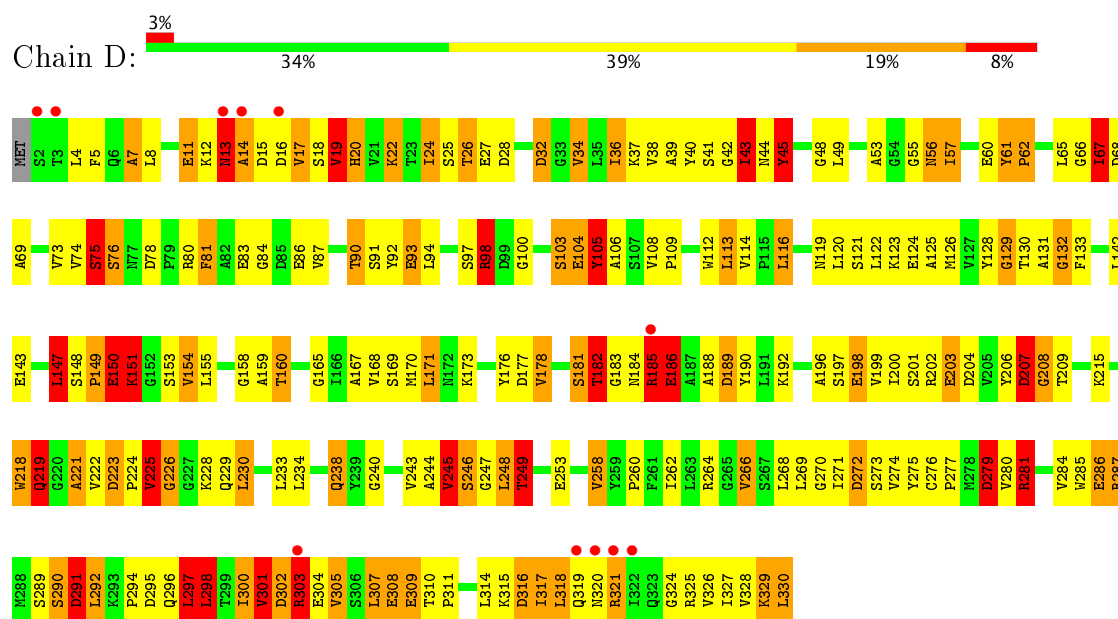
#### • Molecule 1: hypothetical protein yhfP



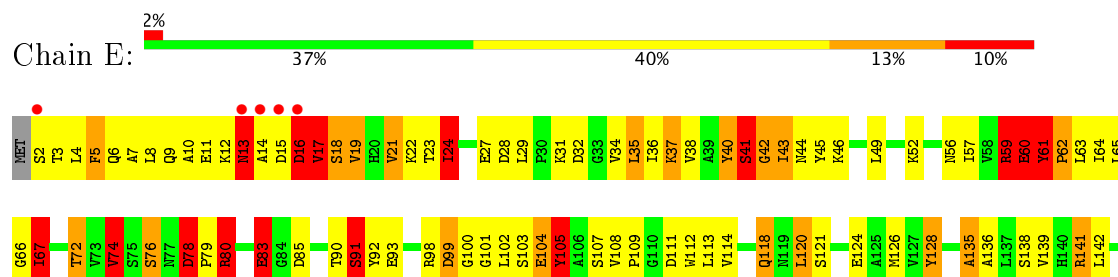
## • Molecule 1: hypothetical protein yhfP



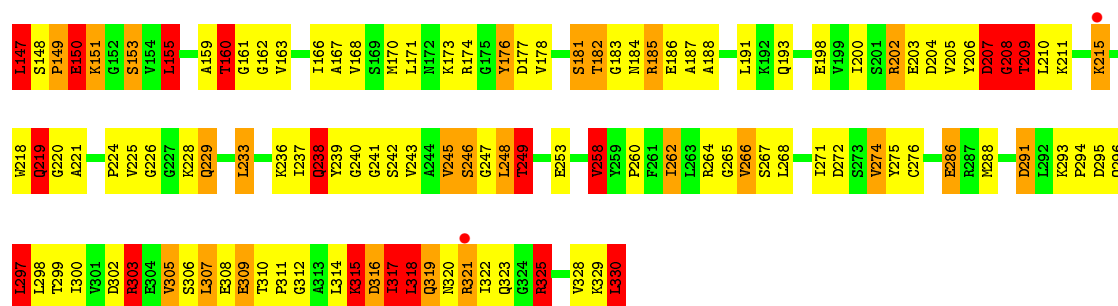
## • Molecule 1: hypothetical protein yhfP



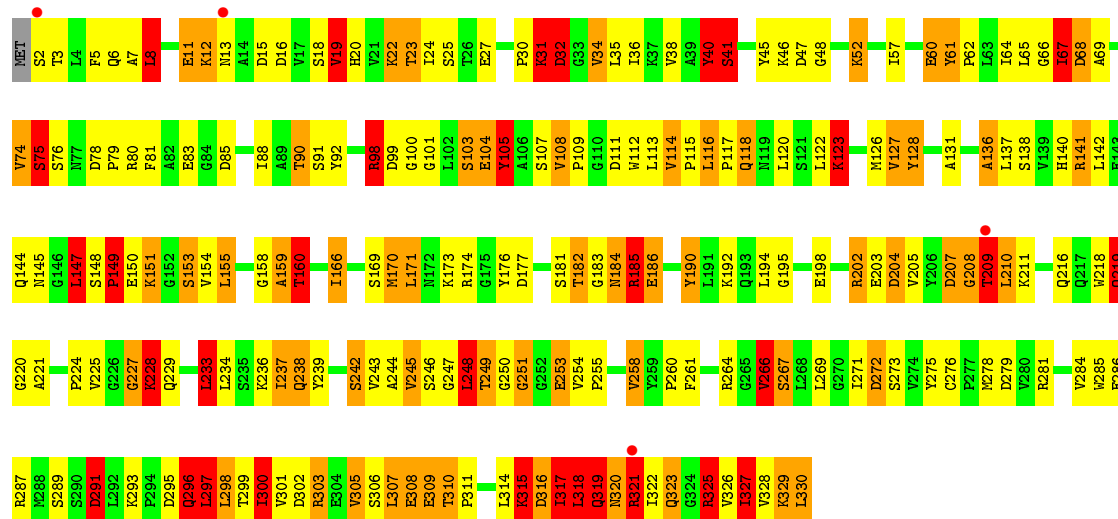
## • Molecule 1: hypothetical protein yhfP







- Molecule 1: hypothetical protein yhfP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.27Å 136.92Å 167.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.98-2.80) 94.5 (20.00-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.227 , 0.233 0.225 , 0.229	Depositor DCC
$R_{free}$ test set	2568 reflections (4.72%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	14982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	2.12	70/2461 (2.8%)	2.05	88/3333 (2.6%)
1	B	2.16	86/2453 (3.5%)	1.85	60/3325 (1.8%)
1	C	2.09	72/2444 (2.9%)	1.87	55/3315 (1.7%)
1	D	2.18	81/2463 (3.3%)	1.83	56/3335 (1.7%)
1	E	2.20	82/2465 (3.3%)	1.92	70/3338 (2.1%)
1	F	2.22	89/2469 (3.6%)	1.99	85/3343 (2.5%)
All	All	2.16	480/14755 (3.3%)	1.92	414/19989 (2.1%)

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	A	0	9
1	B	0	9
1	C	1	8
1	D	1	5
1	E	0	5
1	F	0	4
All	All	2	40

The worst 5 of 480 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	198	GLU	CG-CD	18.13	1.79	1.51
1	B	286	GLU	CG-CD	17.69	1.78	1.51
1	E	286	GLU	CD-OE1	16.23	1.43	1.25
1	A	286	GLU	CG-CD	15.81	1.75	1.51
1	E	83	GLU	CG-CD	15.61	1.75	1.51

The worst 5 of 414 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	TYR	C-N-CD	-21.88	72.47	120.60
1	A	325	ARG	NE-CZ-NH1	-17.28	111.66	120.30
1	F	325	ARG	NE-CZ-NH1	-16.71	111.94	120.30
1	C	207	ASP	CB-CG-OD1	16.28	132.95	118.30
1	C	279	ASP	CB-CG-OD1	-13.84	105.84	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	43	ILE	CA
1	D	43	ILE	CA

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ASN	Peptide
1	A	131	ALA	Peptide
1	A	150	GLU	Peptide
1	A	41	SER	Mainchain,Peptide
1	A	62	PRO	Peptide

## 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	2429	0	2454	160	0
1	B	2421	0	2425	168	0
1	C	2412	0	2405	206	0
1	D	2431	0	2444	169	0
1	E	2433	0	2458	165	0
1	F	2437	0	2460	186	0
2	A	11	0	4	5	0
2	B	11	0	4	5	0
2	C	11	0	4	4	0
2	D	11	0	4	0	0
2	E	11	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	11	0	4	5	0
3	A	65	0	0	1	0
3	B	56	0	0	3	0
3	C	57	0	0	5	0
3	D	53	0	0	8	0
3	E	60	0	0	7	0
3	F	62	0	0	8	0
All	All	14982	0	14670	1037	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 35.

The worst 5 of 1037 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:B:3:THR:CG2	1:B:3:THR:CB	1.75	1.60
1:A:24:ILE:CG1	1:A:24:ILE:CD1	1.81	1.58
1:D:26:THR:CB	1:D:26:THR:CG2	1.76	1.57
1:B:303:ARG:CB	1:B:303:ARG:CG	1.75	1.57
1:B:215:LYS:CB	1:B:215:LYS:CG	1.81	1.57

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	327/330 (99%)	268 (82%)	38 (12%)	21 (6%)	1	4
1	B	327/330 (99%)	264 (81%)	37 (11%)	26 (8%)	1	2
1	C	327/330 (99%)	251 (77%)	43 (13%)	33 (10%)	1	1
1	D	327/330 (99%)	257 (79%)	43 (13%)	27 (8%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	327/330 (99%)	274 (84%)	37 (11%)	16 (5%)	2	8
1	F	327/330 (99%)	269 (82%)	41 (12%)	17 (5%)	2	7
All	All	1962/1980 (99%)	1583 (81%)	239 (12%)	140 (7%)	1	3

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ALA
1	A	41	SER
1	A	62	PRO
1	A	105	TYR
1	A	159	ALA

### 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	259/258 (100%)	207 (80%)	52 (20%)	1	4
1	B	257/258 (100%)	203 (79%)	54 (21%)	1	4
1	C	255/258 (99%)	210 (82%)	45 (18%)	2	6
1	D	259/258 (100%)	204 (79%)	55 (21%)	1	3
1	E	260/258 (101%)	202 (78%)	58 (22%)	1	3
1	F	261/258 (101%)	207 (79%)	54 (21%)	1	4
All	All	1551/1548 (100%)	1233 (80%)	318 (20%)	1	4

5 of 318 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	309	GLU
1	D	182	THR
1	F	185	ARG
1	C	323	GLN
1	D	60	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	216	GLN
1	D	9	GLN
1	F	216	GLN
1	C	238	GLN
1	C	323	GLN

### 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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAD	A	1255	-	10,12,48	1.81	2 (20%)	8,17,73	4.60	4 (50%)
2	NAD	B	2255	-	10,12,48	1.28	2 (20%)	8,17,73	2.69	4 (50%)
2	NAD	C	3255	-	10,12,48	2.85	4 (40%)	8,17,73	2.13	4 (50%)
2	NAD	D	4255	-	10,12,48	1.96	3 (30%)	8,17,73	5.26	3 (37%)
2	NAD	E	5255	-	10,12,48	3.96	5 (50%)	8,17,73	5.24	6 (75%)
2	NAD	F	6255	-	10,12,48	2.87	4 (40%)	8,17,73	5.06	5 (62%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	1255	-	-	0/0/0/62	0/2/2/5
2	NAD	B	2255	-	-	0/0/0/62	0/2/2/5
2	NAD	C	3255	-	-	0/0/0/62	0/2/2/5
2	NAD	D	4255	-	-	0/0/0/62	0/2/2/5
2	NAD	E	5255	-	-	0/0/0/62	0/2/2/5
2	NAD	F	6255	-	-	0/0/0/62	0/2/2/5

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3255	NAD	C4A-N3A	-2.12	1.32	1.35
2	B	2255	NAD	C8A-N7A	2.07	1.38	1.34
2	B	2255	NAD	C2A-N3A	2.16	1.35	1.32
2	C	3255	NAD	C8A-N7A	2.52	1.39	1.34
2	A	1255	NAD	C2A-N1A	2.52	1.38	1.33

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4255	NAD	N3A-C2A-N1A	-14.40	116.31	128.86
2	F	6255	NAD	N3A-C2A-N1A	-12.38	118.08	128.86
2	E	5255	NAD	N3A-C2A-N1A	-9.82	120.31	128.86
2	E	5255	NAD	C5A-C6A-N6A	-7.38	105.43	120.47
2	A	1255	NAD	N3A-C2A-N1A	-6.66	123.06	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1255	NAD	5	0
2	B	2255	NAD	5	0
2	C	3255	NAD	4	0
2	F	6255	NAD	5	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	325/330 (98%)	-0.25	7 (2%) 62 52	18, 18, 18, 18	0
1	B	325/330 (98%)	-0.18	10 (3%) 49 38	18, 18, 18, 18	0
1	C	325/330 (98%)	-0.04	16 (4%) 30 20	18, 18, 18, 18	0
1	D	325/330 (98%)	-0.13	11 (3%) 46 34	18, 18, 18, 18	0
1	E	325/330 (98%)	-0.28	7 (2%) 62 52	18, 18, 18, 18	0
1	F	325/330 (98%)	-0.25	4 (1%) 79 72	18, 18, 18, 18	0
All	All	1950/1980 (98%)	-0.19	55 (2%) 53 43	18, 18, 18, 18	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	ALA	4.7
1	C	13	ASN	4.7
1	C	2	SER	4.3
1	D	13	ASN	3.6
1	A	2	SER	3.4

### 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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAD	E	5255	11/44	0.78	0.26	3.40	17,17,17,17	0
2	NAD	D	4255	11/44	0.91	0.18	1.82	17,17,17,17	0
2	NAD	F	6255	11/44	0.87	0.20	1.33	17,17,17,17	0
2	NAD	C	3255	11/44	0.92	0.18	1.24	17,17,17,17	0
2	NAD	A	1255	11/44	0.89	0.20	1.06	17,17,17,17	0
2	NAD	B	2255	11/44	0.90	0.18	0.60	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.