



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2017 – 07:26 PM EDT

PDB ID : 5UDR  
Title : LarE, a sulfur transferase involved in synthesis of the cofactor for lactate racemase in complex with nicotinamide mononucleotide NMN  
Authors : Fellner, M.; Desguin, B.; Hausinger, R.P.; Hu, J.  
Deposited on : unknown  
Resolution : 2.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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-20029824  
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-20029824

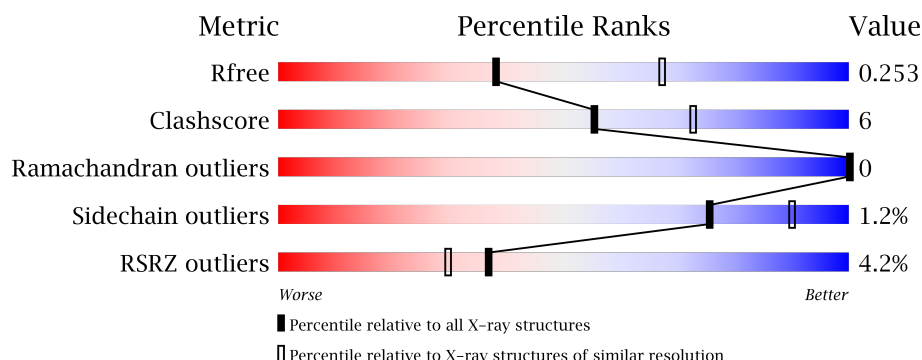
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (2.64-2.60)

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	286	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>10%</div> </div> </div>
1	B	286	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>11%</div> <div>15%</div> </div> </div>
1	C	286	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>14%</div> </div> </div>
1	D	286	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>9%</div> <div>19%</div> </div> </div>
1	E	286	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	286	

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	NMN	C	501	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11391 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 ATP-utilizing enzyme of the PP-loopsuperfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1934	1219	336	372	7			
1	B	243	Total	C	N	O	S	0	0	0
			1863	1174	324	360	5			
1	C	247	Total	C	N	O	S	0	0	0
			1871	1176	325	364	6			
1	D	232	Total	C	N	O	S	0	0	0
			1631	1017	292	318	4			
1	E	260	Total	C	N	O	S	0	0	0
			1923	1211	332	373	7			
1	F	249	Total	C	N	O	S	0	0	0
			1899	1196	329	368	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	ALA	-	expression tag	UNP A0A0G9FES3
A	278	SER	-	expression tag	UNP A0A0G9FES3
A	279	TRP	-	expression tag	UNP A0A0G9FES3
A	280	SER	-	expression tag	UNP A0A0G9FES3
A	281	HIS	-	expression tag	UNP A0A0G9FES3
A	282	PRO	-	expression tag	UNP A0A0G9FES3
A	283	GLN	-	expression tag	UNP A0A0G9FES3
A	284	PHE	-	expression tag	UNP A0A0G9FES3
A	285	GLU	-	expression tag	UNP A0A0G9FES3
A	286	LYS	-	expression tag	UNP A0A0G9FES3
B	277	ALA	-	expression tag	UNP A0A0G9FES3
B	278	SER	-	expression tag	UNP A0A0G9FES3
B	279	TRP	-	expression tag	UNP A0A0G9FES3
B	280	SER	-	expression tag	UNP A0A0G9FES3
B	281	HIS	-	expression tag	UNP A0A0G9FES3
B	282	PRO	-	expression tag	UNP A0A0G9FES3
B	283	GLN	-	expression tag	UNP A0A0G9FES3

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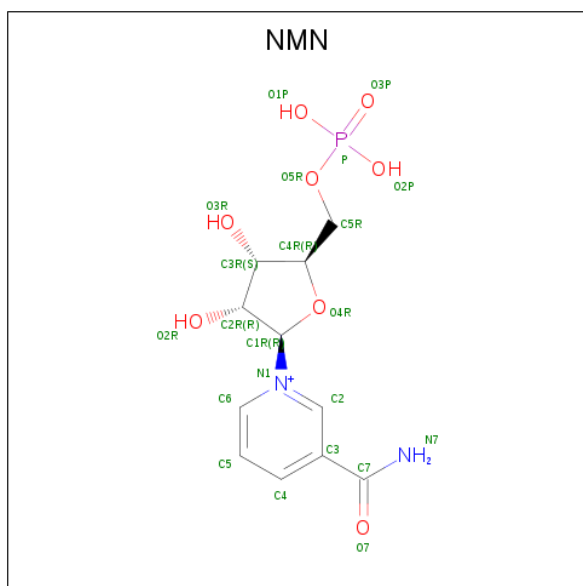
Chain	Residue	Modelled	Actual	Comment	Reference
B	284	PHE	-	expression tag	UNP A0A0G9FES3
B	285	GLU	-	expression tag	UNP A0A0G9FES3
B	286	LYS	-	expression tag	UNP A0A0G9FES3
C	277	ALA	-	expression tag	UNP A0A0G9FES3
C	278	SER	-	expression tag	UNP A0A0G9FES3
C	279	TRP	-	expression tag	UNP A0A0G9FES3
C	280	SER	-	expression tag	UNP A0A0G9FES3
C	281	HIS	-	expression tag	UNP A0A0G9FES3
C	282	PRO	-	expression tag	UNP A0A0G9FES3
C	283	GLN	-	expression tag	UNP A0A0G9FES3
C	284	PHE	-	expression tag	UNP A0A0G9FES3
C	285	GLU	-	expression tag	UNP A0A0G9FES3
C	286	LYS	-	expression tag	UNP A0A0G9FES3
D	277	ALA	-	expression tag	UNP A0A0G9FES3
D	278	SER	-	expression tag	UNP A0A0G9FES3
D	279	TRP	-	expression tag	UNP A0A0G9FES3
D	280	SER	-	expression tag	UNP A0A0G9FES3
D	281	HIS	-	expression tag	UNP A0A0G9FES3
D	282	PRO	-	expression tag	UNP A0A0G9FES3
D	283	GLN	-	expression tag	UNP A0A0G9FES3
D	284	PHE	-	expression tag	UNP A0A0G9FES3
D	285	GLU	-	expression tag	UNP A0A0G9FES3
D	286	LYS	-	expression tag	UNP A0A0G9FES3
E	277	ALA	-	expression tag	UNP A0A0G9FES3
E	278	SER	-	expression tag	UNP A0A0G9FES3
E	279	TRP	-	expression tag	UNP A0A0G9FES3
E	280	SER	-	expression tag	UNP A0A0G9FES3
E	281	HIS	-	expression tag	UNP A0A0G9FES3
E	282	PRO	-	expression tag	UNP A0A0G9FES3
E	283	GLN	-	expression tag	UNP A0A0G9FES3
E	284	PHE	-	expression tag	UNP A0A0G9FES3
E	285	GLU	-	expression tag	UNP A0A0G9FES3
E	286	LYS	-	expression tag	UNP A0A0G9FES3
F	277	ALA	-	expression tag	UNP A0A0G9FES3
F	278	SER	-	expression tag	UNP A0A0G9FES3
F	279	TRP	-	expression tag	UNP A0A0G9FES3
F	280	SER	-	expression tag	UNP A0A0G9FES3
F	281	HIS	-	expression tag	UNP A0A0G9FES3
F	282	PRO	-	expression tag	UNP A0A0G9FES3
F	283	GLN	-	expression tag	UNP A0A0G9FES3
F	284	PHE	-	expression tag	UNP A0A0G9FES3
F	285	GLU	-	expression tag	UNP A0A0G9FES3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	286	LYS	-	expression tag	UNP A0A0G9FES3

- Molecule 2 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (three-letter code: NMN) (formula:  $C_{11}H_{16}N_2O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	F	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

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

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

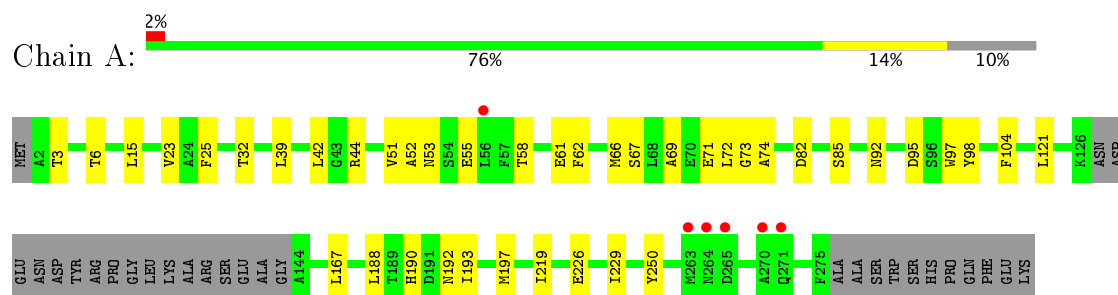
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total 19	O 19	0	0
4	B	51	Total 51	O 51	0	0
4	C	15	Total 15	O 15	0	0
4	D	14	Total 14	O 14	0	0
4	E	17	Total 17	O 17	0	0
4	F	20	Total 20	O 20	0	0

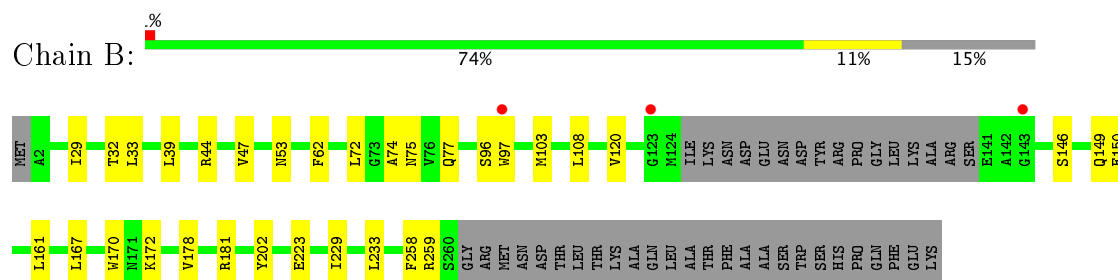
### 3 Residue-property plots [i](#)

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

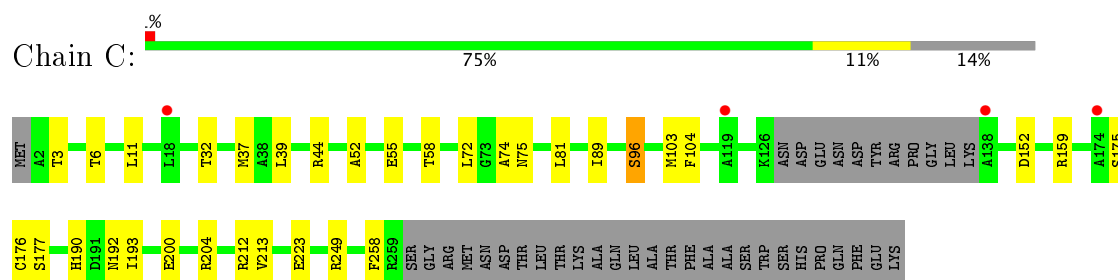
- Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily



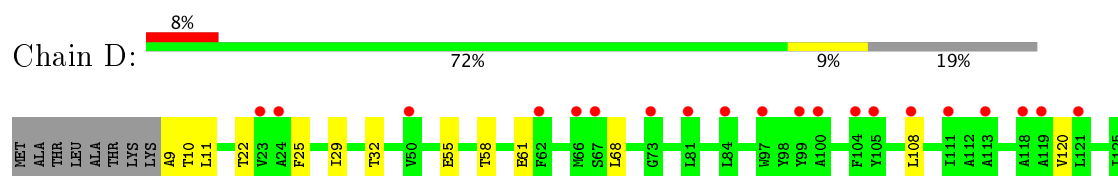
- Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily



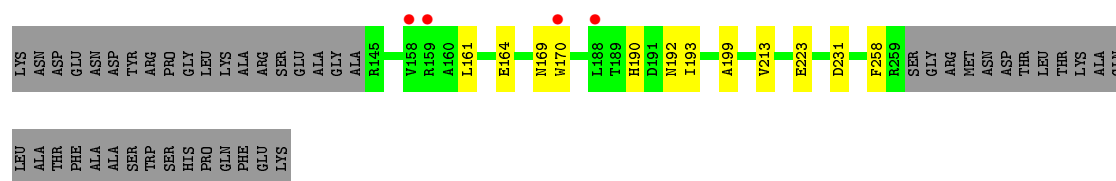
- Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily



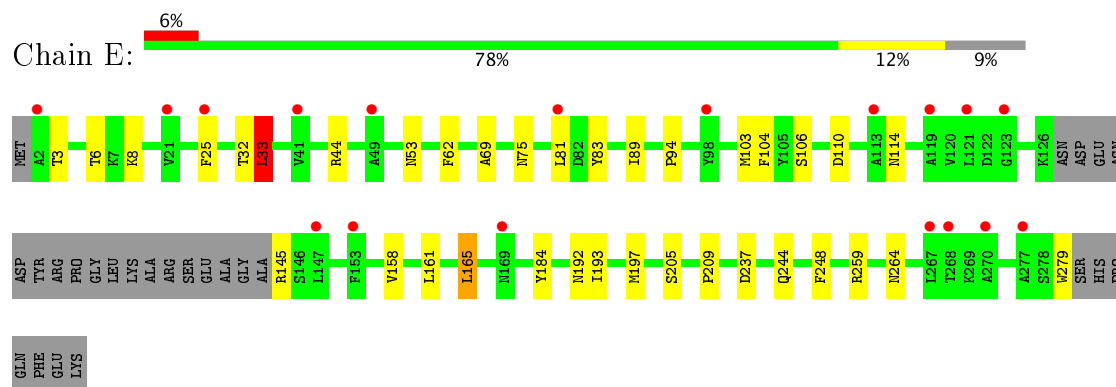
- Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily



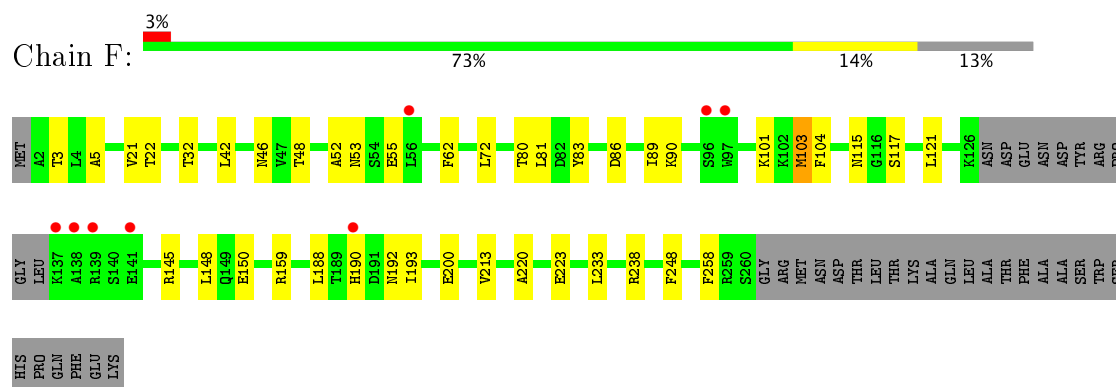




- Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily



- Molecule 1: ATP-utilizing enzyme of the PP-loopsuperfamily



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.09 Å   108.09 Å   324.96 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.42 – 2.62 48.42 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.42-2.62) 99.9 (48.42-2.62)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.61 Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575	Depositor
R, $R_{free}$	0.215   ,   0.246 0.216   ,   0.253	Depositor DCC
$R_{free}$ test set	2872 reflections (4.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.3	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	0.94	EDS
Total number of atoms	11391	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.36	0/1963	0.49	0/2666
1	B	0.31	0/1892	0.50	0/2566
1	C	0.30	0/1898	0.48	0/2574
1	D	0.30	0/1658	0.52	1/2260 (0.0%)
1	E	0.34	0/1953	0.52	2/2655 (0.1%)
1	F	0.33	0/1928	0.48	0/2613
All	All	0.32	0/11292	0.50	3/15334 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	165	LEU	CA-CB-CG	5.98	129.06	115.30
1	D	231	ASP	CB-CG-OD2	5.04	122.83	118.30
1	E	33	LEU	CA-CB-CG	5.04	126.88	115.30

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	1934	0	1855	25	0
1	B	1863	0	1819	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1871	0	1821	21	0
1	D	1631	0	1386	17	0
1	E	1923	0	1811	25	0
1	F	1899	0	1847	27	0
2	A	22	0	14	0	0
2	B	22	0	14	1	0
2	C	22	0	14	0	0
2	D	22	0	14	0	0
2	E	22	0	14	1	0
2	F	22	0	14	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	19	0	0	1	0
4	B	51	0	0	5	0
4	C	15	0	0	2	0
4	D	14	0	0	0	0
4	E	17	0	0	3	0
4	F	20	0	0	2	0
All	All	11391	0	10623	129	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 6.

All (129) 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:C:200:GLU:HG2	1:C:213:VAL:HG23	1.61	0.83
1:A:229:ILE:HG22	1:F:233:LEU:HD11	1.61	0.81
1:F:200:GLU:HG2	1:F:213:VAL:HG23	1.64	0.79
1:D:58:THR:OG1	1:D:61:GLU:HB2	1.87	0.75
1:F:55:GLU:OE2	1:F:190:HIS:ND1	2.21	0.71
1:B:44:ARG:NH1	1:B:75:ASN:OD1	2.23	0.70
1:F:42:LEU:O	1:F:46:ASN:ND2	2.22	0.69
1:C:212:ARG:HG2	1:C:258:PHE:HE2	1.58	0.69
1:B:47:VAL:O	4:B:602:HOH:O	2.11	0.68
1:A:55:GLU:OE2	1:A:190:HIS:ND1	2.22	0.68
1:A:39:LEU:HD11	1:A:74:ALA:HB2	1.75	0.67
1:D:9:ALA:O	1:D:10:THR:C	2.33	0.66
1:E:161:LEU:HD13	1:E:165:LEU:CD1	2.24	0.66
1:E:8:LYS:HD2	1:E:161:LEU:HD21	1.78	0.66
1:E:161:LEU:HD13	1:E:165:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG23	1:A:61:GLU:H	1.60	0.65
1:D:25:PHE:HE1	1:D:32:THR:HA	1.62	0.64
1:B:39:LEU:HD11	1:B:74:ALA:HB2	1.80	0.64
1:C:89:ILE:HA	1:C:96:SER:HB2	1.80	0.63
1:E:259:ARG:NH1	2:E:501:NMN:O3P	2.31	0.63
1:C:249:ARG:HD2	1:E:279:TRP:CD2	2.36	0.61
1:C:32:THR:HG23	1:C:72:LEU:HD11	1.83	0.61
1:A:32:THR:HG22	1:A:167:LEU:HD13	1.83	0.60
1:C:200:GLU:HG2	1:C:213:VAL:CG2	2.32	0.59
1:D:29:ILE:HD11	1:D:170:TRP:CE2	2.38	0.59
1:A:3:THR:HG23	1:A:6:THR:H	1.68	0.59
1:F:22:THR:HG22	1:F:48:THR:HB	1.84	0.58
1:C:204:ARG:NH1	4:C:601:HOH:O	2.37	0.57
1:F:148:LEU:HB2	4:F:611:HOH:O	2.04	0.57
1:C:3:THR:HG23	1:C:6:THR:H	1.69	0.57
1:A:197:MET:O	4:A:601:HOH:O	2.18	0.57
1:C:11:LEU:HD21	1:C:37:MET:HG3	1.86	0.57
1:B:33:LEU:HD11	1:B:161:LEU:HD23	1.87	0.55
1:D:161:LEU:HA	1:D:164:GLU:HB3	1.88	0.55
1:F:32:THR:HG23	1:F:72:LEU:HD11	1.87	0.55
1:D:9:ALA:O	1:D:11:LEU:N	2.40	0.55
1:E:25:PHE:HE2	1:E:32:THR:HA	1.73	0.53
1:C:81:LEU:HD11	1:C:104:PHE:HD2	1.72	0.53
1:C:52:ALA:HB2	1:C:104:PHE:CE2	2.43	0.53
1:E:110:ASP:O	1:E:114:ASN:ND2	2.34	0.53
1:E:33:LEU:HD23	1:E:158:VAL:HG13	1.90	0.53
1:F:22:THR:CG2	1:F:115:ASN:HD21	2.23	0.52
1:D:108:LEU:HB3	1:D:120:VAL:HG11	1.92	0.52
1:B:172:LYS:CB	4:B:603:HOH:O	2.59	0.51
1:F:53:ASN:O	1:F:80:THR:HA	2.11	0.51
1:B:178:VAL:O	1:B:181:ARG:HG2	2.11	0.51
1:F:223:GLU:HB3	1:F:258:PHE:HA	1.93	0.51
1:B:146:SER:O	1:B:150:GLU:HG3	2.11	0.50
1:E:33:LEU:HD11	1:E:161:LEU:HD12	1.94	0.50
1:C:212:ARG:HG2	1:C:258:PHE:CE2	2.43	0.50
1:E:81:LEU:HD11	1:E:104:PHE:HD2	1.77	0.50
1:C:212:ARG:CG	1:C:258:PHE:HE2	2.24	0.49
1:D:68:LEU:HD11	1:D:169:ASN:O	2.12	0.49
1:D:169:ASN:HD22	1:F:159:ARG:NE	2.10	0.49
1:B:32:THR:HG23	1:B:72:LEU:HD11	1.94	0.49
1:C:55:GLU:OE1	1:C:190:HIS:ND1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:THR:HG23	1:E:6:THR:H	1.78	0.49
1:B:32:THR:HG22	1:B:167:LEU:HD13	1.94	0.48
1:B:29:ILE:HD13	1:B:170:TRP:CZ2	2.48	0.48
1:D:29:ILE:HD11	1:D:170:TRP:CZ2	2.49	0.48
1:E:237:ASP:HB3	4:E:605:HOH:O	2.14	0.48
1:C:58:THR:HG23	4:C:614:HOH:O	2.13	0.48
1:A:52:ALA:HB2	1:A:104:PHE:HE2	1.79	0.48
1:B:77:GLN:CG	4:B:607:HOH:O	2.62	0.48
1:C:212:ARG:HB2	1:C:223:GLU:HB2	1.96	0.47
1:A:82:ASP:OD2	1:A:85:SER:HB3	2.15	0.47
1:B:172:LYS:N	4:B:603:HOH:O	2.12	0.47
1:F:3:THR:HG22	1:F:5:ALA:H	1.78	0.47
1:A:51:VAL:HG21	1:A:66:MET:HG2	1.96	0.47
1:C:223:GLU:HB3	1:C:258:PHE:HA	1.96	0.47
1:E:44:ARG:O	1:E:75:ASN:ND2	2.46	0.47
1:F:22:THR:HG23	1:F:117:SER:OG	2.14	0.47
1:A:229:ILE:CG2	1:F:233:LEU:HD11	2.39	0.47
1:A:226:GLU:HA	1:A:229:ILE:HG13	1.96	0.47
1:B:53:ASN:HB2	1:B:62:PHE:CE2	2.50	0.47
1:E:193:ILE:O	1:E:197:MET:HG3	2.15	0.47
1:B:97:TRP:CE2	2:B:501:NMN:H1RC	2.50	0.46
1:C:39:LEU:HD11	1:C:74:ALA:HB2	1.96	0.46
1:D:9:ALA:C	1:D:11:LEU:N	2.67	0.46
1:D:192:ASN:OD1	1:D:193:ILE:N	2.49	0.46
1:E:83:TYR:HB3	1:E:89:ILE:HG21	1.98	0.46
1:A:53:ASN:HB2	1:A:62:PHE:CD2	2.51	0.46
1:E:259:ARG:N	4:E:602:HOH:O	2.00	0.46
1:D:55:GLU:OE2	1:D:190:HIS:ND1	2.40	0.45
1:E:25:PHE:CE1	1:E:69:ALA:HB2	2.51	0.45
1:B:202:TYR:OH	4:B:604:HOH:O	2.14	0.45
1:C:44:ARG:NH1	1:C:75:ASN:OD1	2.48	0.45
1:E:192:ASN:OD1	1:E:193:ILE:N	2.49	0.45
1:D:223:GLU:HB3	1:D:258:PHE:HA	1.97	0.45
1:F:81:LEU:HD11	1:F:104:PHE:HD2	1.82	0.45
1:A:44:ARG:NH1	1:A:73:GLY:O	2.49	0.45
1:B:223:GLU:HB3	1:B:258:PHE:HA	1.99	0.45
1:F:53:ASN:HB2	1:F:62:PHE:CE1	2.51	0.44
1:D:22:THR:O	1:D:120:VAL:HA	2.16	0.44
1:F:145:ARG:NH1	1:F:150:GLU:OE1	2.51	0.44
1:A:219:ILE:HG12	1:A:250:TYR:HB2	2.00	0.44
1:A:23:VAL:HG22	1:A:121:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:ASP:HB2	1:F:103:MET:HE1	1.99	0.44
1:A:92:ASN:HB2	1:A:188:LEU:CD1	2.48	0.44
1:B:108:LEU:HB3	1:B:120:VAL:HG11	2.00	0.44
1:E:53:ASN:HB2	1:E:62:PHE:CD1	2.52	0.44
1:A:67:SER:O	1:A:71:GLU:HG2	2.18	0.43
1:E:145:ARG:HA	1:E:145:ARG:HD2	1.79	0.43
1:F:52:ALA:HB2	1:F:104:PHE:CE2	2.53	0.43
1:A:53:ASN:HB2	1:A:62:PHE:CE2	2.53	0.43
1:F:21:VAL:HG11	1:F:121:LEU:HD11	2.01	0.43
1:B:146:SER:HB2	1:B:149:GLN:HG2	2.02	0.42
1:F:90:LYS:NZ	1:F:188:LEU:O	2.41	0.42
1:F:101:LYS:HA	1:F:101:LYS:HD3	1.86	0.42
1:A:95:ASP:HA	1:A:97:TRP:CD1	2.55	0.42
1:A:97:TRP:CG	1:A:98:TYR:N	2.87	0.42
1:E:264:ASN:HA	1:F:238:ARG:HD2	2.02	0.42
1:B:229:ILE:O	1:B:233:LEU:HD13	2.19	0.42
1:F:148:LEU:N	4:F:611:HOH:O	2.47	0.42
1:E:161:LEU:HD13	1:E:165:LEU:HD11	2.00	0.41
1:A:32:THR:HG23	1:A:72:LEU:HD11	2.02	0.41
1:A:25:PHE:CD2	1:A:69:ALA:HB2	2.55	0.41
1:A:15:LEU:O	1:A:42:LEU:HD21	2.21	0.41
1:A:192:ASN:OD1	1:A:193:ILE:N	2.53	0.41
1:D:199:ALA:HB3	1:D:213:VAL:HG21	2.01	0.41
1:F:83:TYR:HB3	1:F:89:ILE:HG21	2.02	0.41
1:E:244:GLN:HA	1:E:248:PHE:O	2.21	0.41
1:C:192:ASN:OD1	1:C:193:ILE:N	2.54	0.41
1:F:220:ALA:HB2	1:F:248:PHE:CG	2.55	0.41
1:E:94:PRO:HA	1:E:184:TYR:CE1	2.55	0.41
1:D:29:ILE:HA	1:D:29:ILE:HD13	1.99	0.40
1:C:176:CYS:SG	1:C:177:SER:N	2.94	0.40
1:E:209:PRO:O	4:E:604:HOH:O	2.22	0.40
1:F:192:ASN:OD1	1:F:193:ILE:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	253/286 (88%)	249 (98%)	4 (2%)	0	100	100
1	B	239/286 (84%)	234 (98%)	5 (2%)	0	100	100
1	C	243/286 (85%)	240 (99%)	3 (1%)	0	100	100
1	D	228/286 (80%)	223 (98%)	5 (2%)	0	100	100
1	E	256/286 (90%)	248 (97%)	8 (3%)	0	100	100
1	F	245/286 (86%)	242 (99%)	3 (1%)	0	100	100
All	All	1464/1716 (85%)	1436 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	193/236 (82%)	193 (100%)	0	100	100
1	B	193/236 (82%)	190 (98%)	3 (2%)	68	86
1	C	193/236 (82%)	188 (97%)	5 (3%)	51	77
1	D	135/236 (57%)	135 (100%)	0	100	100
1	E	188/236 (80%)	184 (98%)	4 (2%)	59	82
1	F	195/236 (83%)	194 (100%)	1 (0%)	91	97
All	All	1097/1416 (78%)	1084 (99%)	13 (1%)	75	90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	SER
1	B	103	MET
1	B	259	ARG

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Mol	Chain	Res	Type
1	C	96	SER
1	C	103	MET
1	C	152	ASP
1	C	159	ARG
1	C	175	SER
1	E	33	LEU
1	E	103	MET
1	E	106	SER
1	E	205	SER
1	F	103	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	NMN	A	501	-	21,23,23	4.06	11 (52%)	27,34,34	1.40	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NMN	B	501	-	21,23,23	4.09	11 (52%)	27,34,34	1.65	3 (11%)
2	NMN	C	501	-	21,23,23	4.07	11 (52%)	27,34,34	1.09	3 (11%)
2	NMN	D	501	-	21,23,23	4.08	11 (52%)	27,34,34	1.88	1 (3%)
2	NMN	E	501	-	21,23,23	4.09	11 (52%)	27,34,34	1.48	3 (11%)
2	NMN	F	501	-	21,23,23	4.07	11 (52%)	27,34,34	1.55	3 (11%)

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	NMN	A	501	-	-	0/10/30/30	0/2/2/2
2	NMN	B	501	-	-	0/10/30/30	0/2/2/2
2	NMN	C	501	-	-	0/10/30/30	0/2/2/2
2	NMN	D	501	-	-	0/10/30/30	0/2/2/2
2	NMN	E	501	-	-	0/10/30/30	0/2/2/2
2	NMN	F	501	-	-	0/10/30/30	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	NMN	C2R-C3R	-11.10	1.24	1.53
2	B	501	NMN	C2R-C3R	-11.02	1.24	1.53
2	F	501	NMN	C2R-C3R	-10.89	1.24	1.53
2	D	501	NMN	C2R-C3R	-10.84	1.24	1.53
2	C	501	NMN	C2R-C3R	-10.83	1.24	1.53
2	A	501	NMN	C2R-C3R	-10.80	1.24	1.53
2	C	501	NMN	O4R-C1R	-7.86	1.30	1.41
2	A	501	NMN	O4R-C1R	-7.72	1.30	1.41
2	B	501	NMN	O4R-C1R	-7.70	1.30	1.41
2	F	501	NMN	O4R-C1R	-7.54	1.30	1.41
2	D	501	NMN	O4R-C1R	-7.45	1.31	1.41
2	E	501	NMN	O4R-C1R	-7.35	1.31	1.41
2	E	501	NMN	C5R-C4R	-4.67	1.36	1.51
2	D	501	NMN	C5R-C4R	-4.65	1.36	1.51
2	B	501	NMN	C5R-C4R	-4.61	1.37	1.51
2	C	501	NMN	C5R-C4R	-4.48	1.37	1.51
2	F	501	NMN	C5R-C4R	-4.44	1.37	1.51
2	A	501	NMN	C5R-C4R	-4.43	1.37	1.51
2	F	501	NMN	C4-C3	-2.22	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NMN	C4-C3	-2.21	1.35	1.39
2	E	501	NMN	C4-C3	-2.19	1.35	1.39
2	B	501	NMN	C4-C3	-2.18	1.35	1.39
2	C	501	NMN	C4-C3	-2.16	1.35	1.39
2	D	501	NMN	C4-C3	-2.14	1.35	1.39
2	C	501	NMN	C3-C7	2.07	1.53	1.50
2	D	501	NMN	C3-C7	2.11	1.53	1.50
2	E	501	NMN	C3-C7	2.20	1.53	1.50
2	F	501	NMN	C3-C7	2.21	1.54	1.50
2	A	501	NMN	C3-C7	2.24	1.54	1.50
2	B	501	NMN	C3-C7	2.32	1.54	1.50
2	E	501	NMN	O4R-C4R	2.32	1.50	1.45
2	B	501	NMN	O2R-C2R	2.36	1.48	1.43
2	C	501	NMN	O2R-C2R	2.46	1.48	1.43
2	D	501	NMN	O4R-C4R	2.47	1.50	1.45
2	E	501	NMN	O2R-C2R	2.49	1.48	1.43
2	C	501	NMN	O4R-C4R	2.49	1.50	1.45
2	A	501	NMN	O2R-C2R	2.49	1.48	1.43
2	D	501	NMN	O2R-C2R	2.49	1.48	1.43
2	F	501	NMN	O2R-C2R	2.49	1.48	1.43
2	B	501	NMN	O4R-C4R	2.60	1.50	1.45
2	E	501	NMN	C3R-C4R	2.61	1.59	1.53
2	A	501	NMN	O4R-C4R	2.62	1.50	1.45
2	F	501	NMN	O4R-C4R	2.70	1.51	1.45
2	D	501	NMN	C3R-C4R	2.82	1.60	1.53
2	C	501	NMN	C3R-C4R	2.86	1.60	1.53
2	B	501	NMN	C3R-C4R	2.98	1.60	1.53
2	F	501	NMN	C3R-C4R	3.05	1.61	1.53
2	E	501	NMN	O3R-C3R	3.10	1.50	1.43
2	B	501	NMN	O3R-C3R	3.11	1.50	1.43
2	D	501	NMN	O3R-C3R	3.12	1.50	1.43
2	A	501	NMN	C3R-C4R	3.12	1.61	1.53
2	F	501	NMN	O3R-C3R	3.14	1.50	1.43
2	C	501	NMN	O3R-C3R	3.18	1.50	1.43
2	A	501	NMN	O3R-C3R	3.24	1.50	1.43
2	C	501	NMN	C7-N7	5.88	1.44	1.33
2	A	501	NMN	C7-N7	5.88	1.44	1.33
2	B	501	NMN	C7-N7	5.94	1.44	1.33
2	D	501	NMN	C7-N7	5.95	1.44	1.33
2	F	501	NMN	C7-N7	5.97	1.44	1.33
2	E	501	NMN	C7-N7	6.01	1.44	1.33
2	A	501	NMN	C2R-C1R	7.94	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NMN	C2R-C1R	8.04	1.66	1.53
2	F	501	NMN	C2R-C1R	8.04	1.66	1.53
2	C	501	NMN	C2R-C1R	8.11	1.66	1.53
2	E	501	NMN	C2R-C1R	8.38	1.67	1.53
2	D	501	NMN	C2R-C1R	8.39	1.67	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NMN	C4R-O4R-C1R	-8.51	100.71	109.77
2	B	501	NMN	C4R-O4R-C1R	-7.23	102.07	109.77
2	F	501	NMN	C4R-O4R-C1R	-6.32	103.04	109.77
2	E	501	NMN	C4R-O4R-C1R	-5.85	103.54	109.77
2	A	501	NMN	C4R-O4R-C1R	-5.39	104.03	109.77
2	C	501	NMN	C4R-O4R-C1R	-2.61	106.99	109.77
2	A	501	NMN	O7-C7-N7	-2.20	119.45	122.58
2	F	501	NMN	O7-C7-N7	-2.20	119.46	122.58
2	E	501	NMN	O7-C7-N7	-2.10	119.60	122.58
2	B	501	NMN	O7-C7-N7	-2.03	119.69	122.58
2	C	501	NMN	C3-C7-N7	2.05	120.12	117.77
2	E	501	NMN	C3-C7-N7	2.06	120.12	117.77
2	B	501	NMN	C3-C7-N7	2.07	120.14	117.77
2	C	501	NMN	C2R-C3R-C4R	2.09	106.70	102.62
2	F	501	NMN	C3-C7-N7	2.27	120.36	117.77
2	A	501	NMN	C3-C7-N7	2.36	120.47	117.77

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	B	501	NMN	1	0
2	E	501	NMN	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	257/286 (89%)	0.21	6 (2%) 61 54	40, 63, 81, 96	0
1	B	243/286 (84%)	0.14	3 (1%) 79 75	34, 47, 67, 82	0
1	C	247/286 (86%)	0.17	4 (1%) 72 67	37, 58, 80, 102	0
1	D	232/286 (81%)	0.57	24 (10%) 7 4	39, 79, 107, 113	0
1	E	260/286 (90%)	0.46	18 (6%) 18 13	38, 75, 94, 102	0
1	F	249/286 (87%)	0.26	8 (3%) 48 41	37, 63, 87, 109	0
All	All	1488/1716 (86%)	0.30	63 (4%) 37 30	34, 61, 96, 113	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	138	ALA	6.9
1	D	119	ALA	5.8
1	A	263	MET	4.3
1	D	158	VAL	4.2
1	D	118	ALA	4.0
1	D	105	TYR	3.9
1	A	264	ASN	3.6
1	E	153	PHE	3.6
1	F	97	TRP	3.4
1	E	21	VAL	3.4
1	E	268	THR	3.4
1	E	277	ALA	3.4
1	E	98	TYR	3.4
1	A	270	ALA	3.3
1	D	111	ILE	3.3
1	B	97	TRP	3.3
1	D	159	ARG	3.3
1	E	113	ALA	3.2
1	E	119	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLY	3.1
1	D	100	ALA	3.0
1	F	139	ARG	3.0
1	C	174	ALA	3.0
1	D	84	LEU	3.0
1	F	56	LEU	3.0
1	E	270	ALA	3.0
1	D	62	PHE	2.9
1	E	267	LEU	2.9
1	D	23	VAL	2.8
1	F	141	GLU	2.7
1	D	97	TRP	2.6
1	E	25	PHE	2.6
1	E	123	GLY	2.6
1	D	66	MET	2.5
1	C	138	ALA	2.5
1	D	81	LEU	2.5
1	F	96	SER	2.5
1	C	119	ALA	2.5
1	A	265	ASP	2.5
1	D	188	LEU	2.5
1	B	143	GLY	2.4
1	E	2	ALA	2.4
1	F	137	LYS	2.4
1	D	121	LEU	2.3
1	D	73	GLY	2.3
1	D	24	ALA	2.3
1	E	169	ASN	2.3
1	D	50	VAL	2.3
1	E	121	LEU	2.3
1	D	67	SER	2.3
1	F	190	HIS	2.3
1	E	41	VAL	2.3
1	E	49	ALA	2.2
1	A	271	GLN	2.2
1	D	104	PHE	2.2
1	A	56	LEU	2.2
1	E	81	LEU	2.2
1	E	147	LEU	2.2
1	C	18	LEU	2.1
1	D	113	ALA	2.1
1	D	108	LEU	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	D	99	TYR	2.0
1	D	170	TRP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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<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	NMN	C	501	22/22	0.89	0.25	2.25	60,98,108,108	0
2	NMN	E	501	22/22	0.90	0.21	1.85	54,96,118,126	0
2	NMN	B	501	22/22	0.89	0.25	0.71	49,71,78,79	0
2	NMN	F	501	22/22	0.84	0.24	0.36	61,99,105,107	0
2	NMN	D	501	22/22	0.91	0.23	0.26	54,93,99,100	0
2	NMN	A	501	22/22	0.92	0.21	-0.05	56,92,100,101	0
3	MN	D	502	1/1	0.58	0.13	-	50,50,50,50	1
3	MN	A	502	1/1	0.85	0.10	-	47,47,47,47	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.