wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:49 PM GMT

PDB ID	:	1V9L
Title	:	L-glutamate dehydrogenase from Pyrobaculum islandicum complexed with NAD
Authors	:	Bhuiya, M.W.; Sakuraba, H.; Ohshima, T.; Imagawa, T.; Katunuma, N.; Tsuge, H.
Deposited on	:	2004-01-26
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

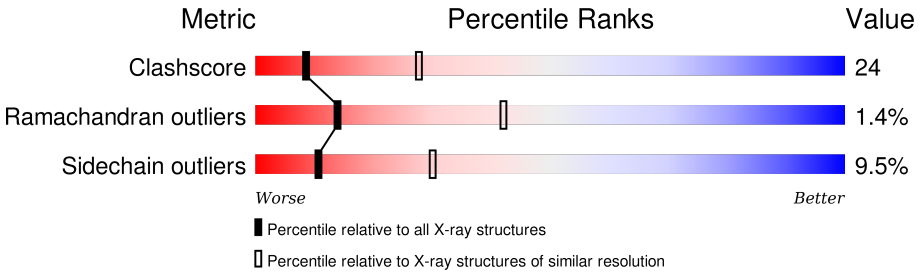
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	57% 38%
1	B	421	47% 46% 6%
1	C	421	51% 42% 6%
1	D	421	55% 38% 5%
1	E	421	51% 43% 5%
1	F	421	56% 38% 5%

2 Entry composition (i)

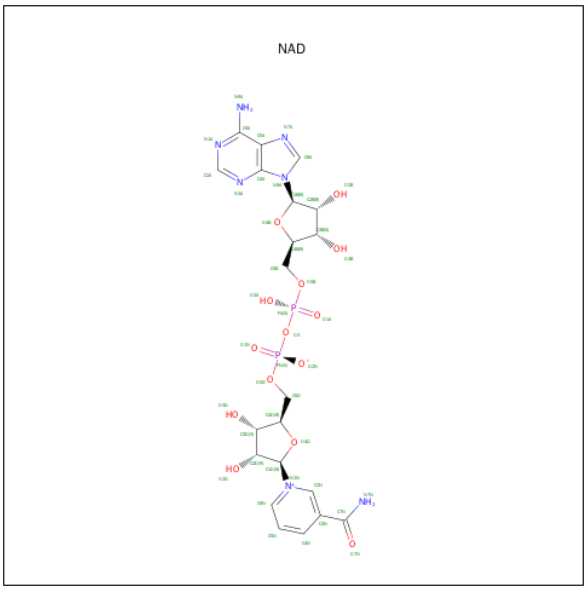
There are 3 unique types of molecules in this entry. The entry contains 20087 atoms, of which 1 is hydrogen and 0 are deuteriums.

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 glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3282	2112	566	593	11			
1	B	418	Total	C	N	O	S	0	0	0
			3282	2112	566	593	11			
1	C	418	Total	C	N	O	S	0	0	0
			3282	2112	566	593	11			
1	D	418	Total	C	N	O	S	0	0	0
			3282	2112	566	593	11			
1	E	418	Total	C	N	O	S	0	0	0
			3282	2112	566	593	11			
1	F	418	Total	C	H	N	O	S	0	0	0
			3283	2112	1	566	593	11			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	17	Total	O	0	0
			17	17		
3	C	16	Total	O	0	0
			16	16		
3	D	24	Total	O	0	0
			24	24		
3	E	31	Total	O	0	0
			31	31		
3	F	25	Total	O	0	0
			25	25		

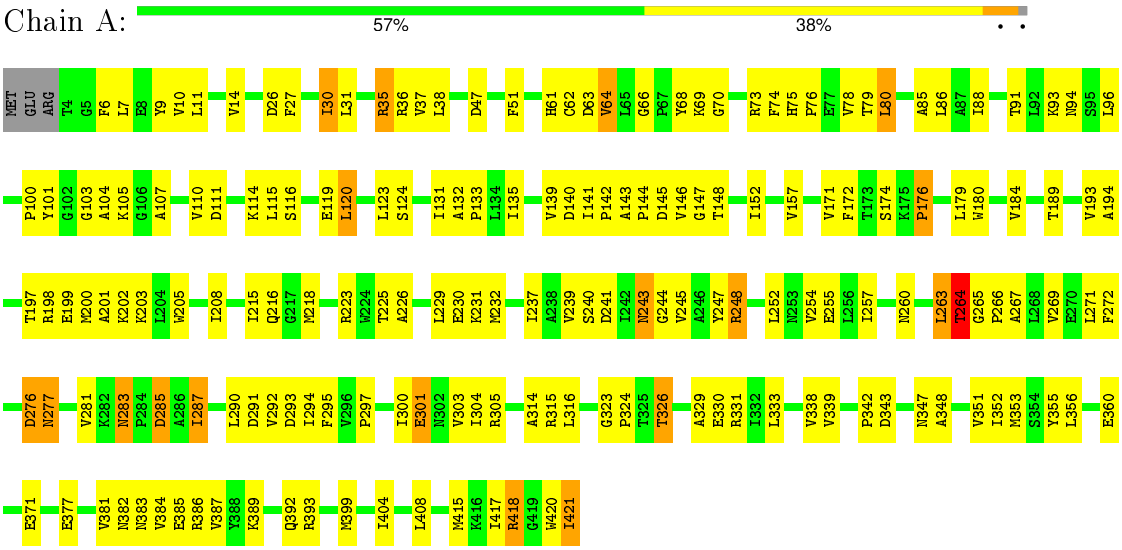
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

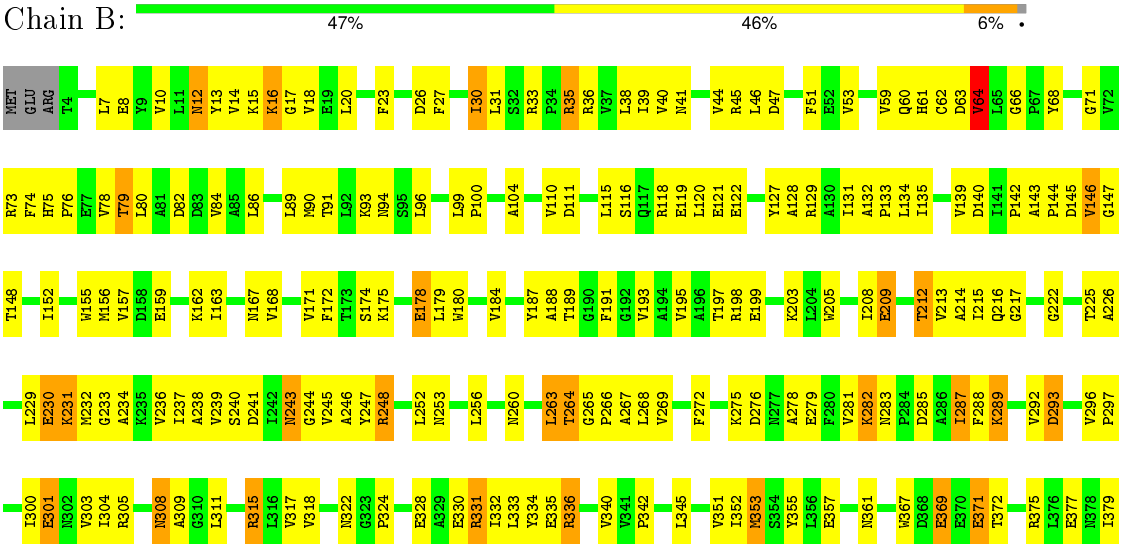
- Molecule 1: glutamate dehydrogenase

Chain A:



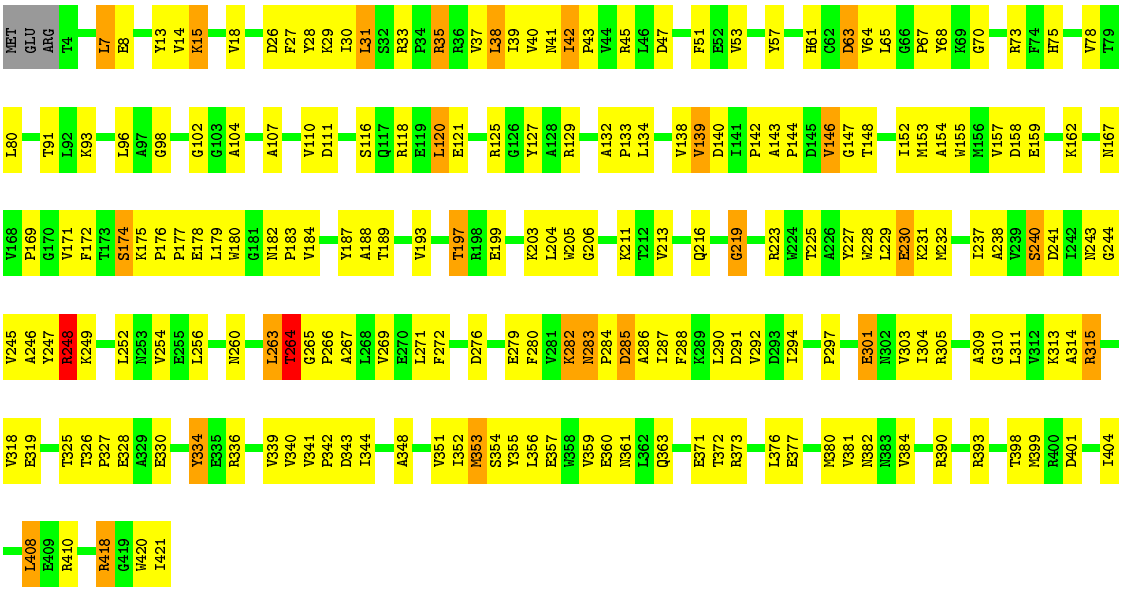
- Molecule 1: glutamate dehydrogenase

Chain B:



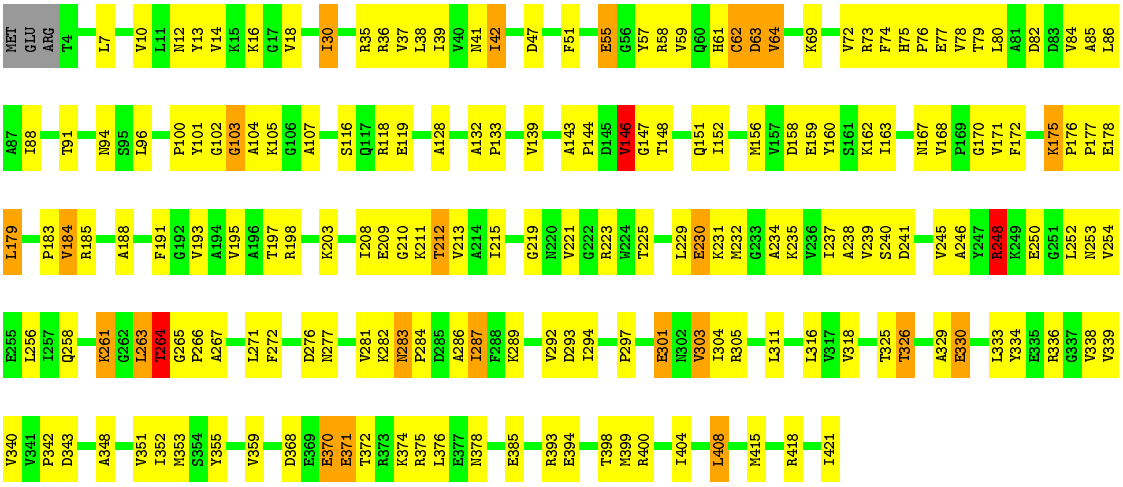
- Molecule 1: glutamate dehydrogenase

Chain C:



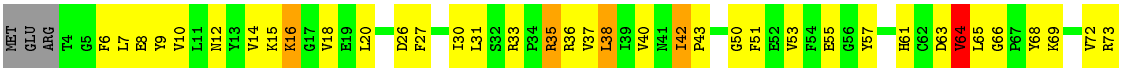
- Molecule 1: glutamate dehydrogenase

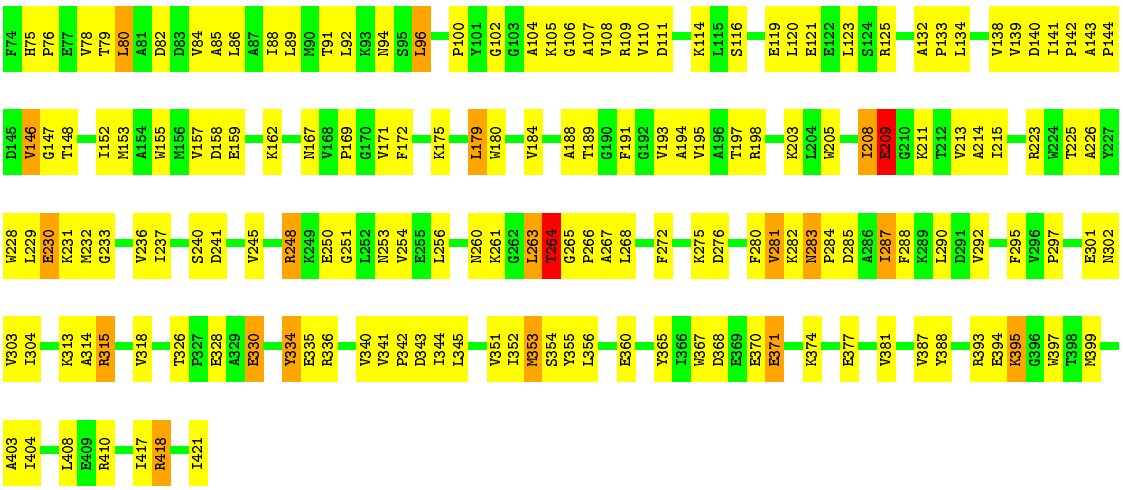
Chain D:



- Molecule 1: glutamate dehydrogenase

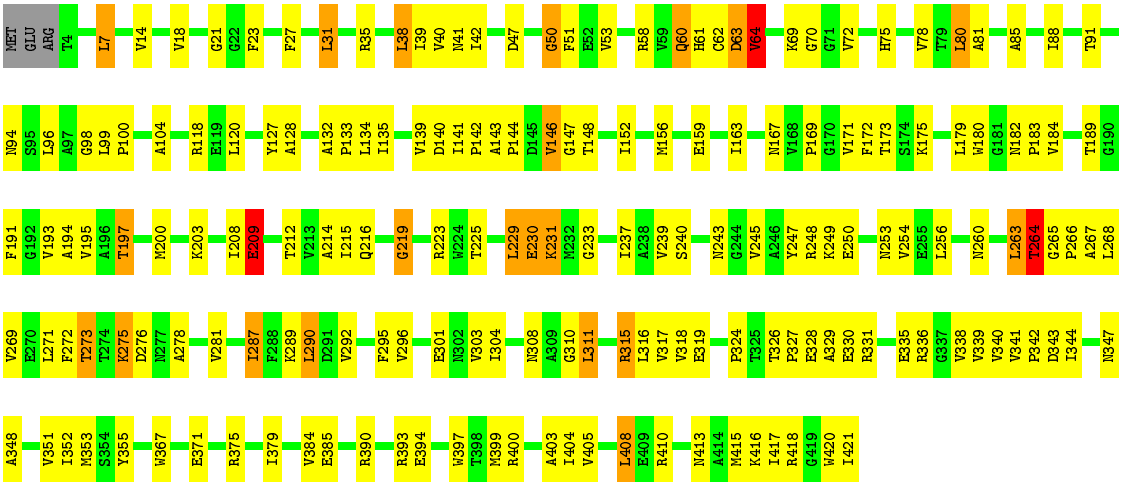
Chain E:





- Molecule 1: glutamate dehydrogenase

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.21Å 165.88Å 181.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20087	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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

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	0.45	0/3354	0.68	3/4549 (0.1%)
1	B	0.45	1/3354 (0.0%)	0.65	3/4549 (0.1%)
1	C	0.44	0/3354	0.62	0/4549
1	D	0.49	2/3354 (0.1%)	0.67	3/4549 (0.1%)
1	E	0.46	0/3354	0.68	3/4549 (0.1%)
1	F	0.49	2/3354 (0.1%)	0.72	5/4549 (0.1%)
All	All	0.46	5/20124 (0.0%)	0.67	17/27294 (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	A	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	263	LEU	C-N	-6.92	1.18	1.34
1	D	264	THR	C-N	-6.35	1.21	1.33
1	F	264	THR	C-N	5.67	1.43	1.33
1	F	209	GLU	C-O	-5.53	1.12	1.23
1	B	209	GLU	C-N	5.49	1.43	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	THR	O-C-N	-11.44	103.75	123.20
1	E	208	ILE	C-N-CA	-10.40	95.71	121.70
1	F	208	ILE	C-N-CA	-8.71	99.93	121.70
1	B	209	GLU	CA-C-N	-8.66	98.88	116.20
1	A	264	THR	CA-C-N	8.43	133.07	116.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	THR	Mainchain
1	D	101	TYR	Sidechain
1	E	209	GLU	Mainchain
1	F	264	THR	Mainchain

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	3282	0	3326	161	0
1	B	3282	0	3326	200	0
1	C	3282	0	3325	167	0
1	D	3282	0	3325	146	0
1	E	3282	0	3326	168	0
1	F	3282	1	3326	153	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	D	44	0	26	2	0
2	E	44	0	26	0	0
2	F	44	0	26	1	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0
3	C	16	0	0	1	0
3	D	24	0	0	0	0
3	E	31	0	0	1	0
3	F	25	0	0	0	0
All	All	20086	1	20110	955	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 24.

The worst 5 of 955 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:237:ILE:HD11	1:B:292:VAL:HG12	1.37	1.07
1:F:264:THR:CG2	1:F:267:ALA:H	1.70	1.04
1:B:47:ASP:HB3	1:B:118:ARG:HE	1.21	1.02
1:C:264:THR:HG23	1:C:266:PRO:HD2	1.42	0.99
1:A:237:ILE:HD11	1:A:292:VAL:HG12	1.44	0.98

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	416/421 (99%)	369 (89%)	41 (10%)	6 (1%)	14	42
1	B	416/421 (99%)	353 (85%)	56 (14%)	7 (2%)	11	36
1	C	416/421 (99%)	368 (88%)	42 (10%)	6 (1%)	14	42
1	D	416/421 (99%)	377 (91%)	32 (8%)	7 (2%)	11	36
1	E	416/421 (99%)	373 (90%)	38 (9%)	5 (1%)	16	47
1	F	416/421 (99%)	379 (91%)	32 (8%)	5 (1%)	16	47
All	All	2496/2526 (99%)	2219 (89%)	241 (10%)	36 (1%)	14	42

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	B	64	VAL
1	B	146	VAL

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Mol	Chain	Res	Type
1	C	47	ASP
1	C	248	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	339/342 (99%)	310 (91%)	29 (9%)	13 36
1	B	339/342 (99%)	306 (90%)	33 (10%)	10 29
1	C	339/342 (99%)	304 (90%)	35 (10%)	9 26
1	D	339/342 (99%)	308 (91%)	31 (9%)	12 33
1	E	339/342 (99%)	304 (90%)	35 (10%)	9 26
1	F	339/342 (99%)	309 (91%)	30 (9%)	12 35
All	All	2034/2052 (99%)	1841 (90%)	193 (10%)	11 30

5 of 193 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	315	ARG
1	D	175	LYS
1	F	250	GLU
1	C	330	GLU
1	D	38	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	392	GLN
1	D	302	ASN
1	F	302	ASN
1	C	413	ASN
1	D	151	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	430	-	38,48,48	2.40	10 (26%)	47,73,73	2.28	7 (14%)
2	NAD	B	1430	-	38,48,48	2.46	10 (26%)	47,73,73	2.23	9 (19%)
2	NAD	C	2430	-	38,48,48	2.27	10 (26%)	47,73,73	2.23	9 (19%)
2	NAD	D	3430	-	38,48,48	2.34	9 (23%)	47,73,73	2.25	8 (17%)
2	NAD	E	4430	-	38,48,48	2.40	7 (18%)	47,73,73	2.25	6 (12%)
2	NAD	F	5430	-	38,48,48	2.43	9 (23%)	47,73,73	2.22	6 (12%)

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	430	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1430	-	-	0/22/62/62	0/5/5/5
2	NAD	C	2430	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	3430	-	-	0/22/62/62	0/5/5/5
2	NAD	E	4430	-	-	0/22/62/62	0/5/5/5
2	NAD	F	5430	-	-	0/22/62/62	0/5/5/5

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4430	NAD	C2N-C3N	-2.92	1.34	1.39
2	D	3430	NAD	C2N-C3N	-2.90	1.34	1.39
2	B	1430	NAD	C2N-C3N	-2.82	1.34	1.39
2	C	2430	NAD	C2N-C3N	-2.78	1.34	1.39
2	A	430	NAD	C2N-C3N	-2.71	1.34	1.39

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	430	NAD	C5N-C4N-C3N	-9.41	108.50	120.33
2	C	2430	NAD	C5N-C4N-C3N	-9.21	108.75	120.33
2	B	1430	NAD	C5N-C4N-C3N	-9.16	108.81	120.33
2	F	5430	NAD	C5N-C4N-C3N	-9.07	108.93	120.33
2	A	430	NAD	N3A-C2A-N1A	-9.01	122.00	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
2	B	1430	NAD	1	0
2	C	2430	NAD	1	0
2	D	3430	NAD	2	0
2	F	5430	NAD	1	0

5.7 Other polymers (i)

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

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.