



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:31 AM GMT

PDB ID : 4GO4
Title : Crystal structure of PnpE in complex with Nicotinamide adenine dinucleotide
Authors : Su, J.; Zhang, C.; Liu, S.; Zhu, D.; Gu, L.
Deposited on : 2012-08-18
Resolution : 3.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

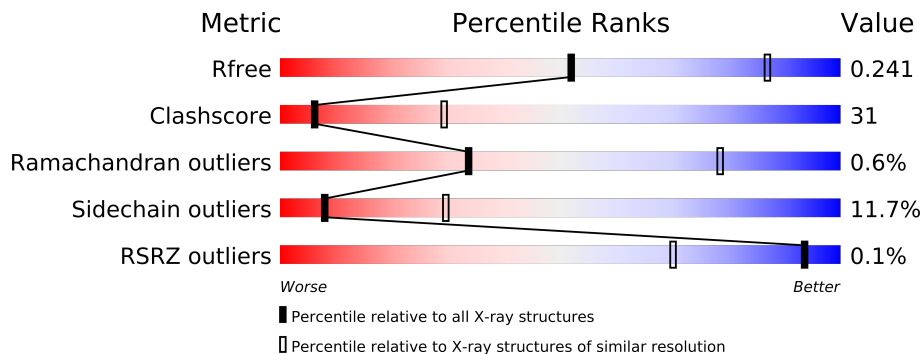
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	495	
1	B	495	
1	C	495	
1	D	495	
1	E	495	
1	F	495	
1	G	495	
1	H	495	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30071 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative gamma-hydroxymuconic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	B	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	C	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	D	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	E	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	F	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	G	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	H	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
A	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
A	488	LEU	-	EXPRESSION TAG	UNP C1I208
A	489	GLY	-	EXPRESSION TAG	UNP C1I208
A	490	HIS	-	EXPRESSION TAG	UNP C1I208
A	491	HIS	-	EXPRESSION TAG	UNP C1I208
A	492	HIS	-	EXPRESSION TAG	UNP C1I208
A	493	HIS	-	EXPRESSION TAG	UNP C1I208
A	494	HIS	-	EXPRESSION TAG	UNP C1I208
A	495	HIS	-	EXPRESSION TAG	UNP C1I208
B	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
B	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
B	488	LEU	-	EXPRESSION TAG	UNP C1I208

Continued on next page...

Continued from previous page...

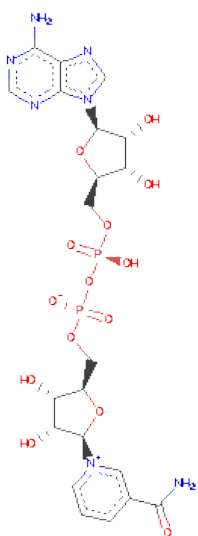
Chain	Residue	Modelled	Actual	Comment	Reference
B	489	GLY	-	EXPRESSION TAG	UNP C1I208
B	490	HIS	-	EXPRESSION TAG	UNP C1I208
B	491	HIS	-	EXPRESSION TAG	UNP C1I208
B	492	HIS	-	EXPRESSION TAG	UNP C1I208
B	493	HIS	-	EXPRESSION TAG	UNP C1I208
B	494	HIS	-	EXPRESSION TAG	UNP C1I208
B	495	HIS	-	EXPRESSION TAG	UNP C1I208
C	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
C	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
C	488	LEU	-	EXPRESSION TAG	UNP C1I208
C	489	GLY	-	EXPRESSION TAG	UNP C1I208
C	490	HIS	-	EXPRESSION TAG	UNP C1I208
C	491	HIS	-	EXPRESSION TAG	UNP C1I208
C	492	HIS	-	EXPRESSION TAG	UNP C1I208
C	493	HIS	-	EXPRESSION TAG	UNP C1I208
C	494	HIS	-	EXPRESSION TAG	UNP C1I208
C	495	HIS	-	EXPRESSION TAG	UNP C1I208
D	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
D	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
D	488	LEU	-	EXPRESSION TAG	UNP C1I208
D	489	GLY	-	EXPRESSION TAG	UNP C1I208
D	490	HIS	-	EXPRESSION TAG	UNP C1I208
D	491	HIS	-	EXPRESSION TAG	UNP C1I208
D	492	HIS	-	EXPRESSION TAG	UNP C1I208
D	493	HIS	-	EXPRESSION TAG	UNP C1I208
D	494	HIS	-	EXPRESSION TAG	UNP C1I208
D	495	HIS	-	EXPRESSION TAG	UNP C1I208
E	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
E	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
E	488	LEU	-	EXPRESSION TAG	UNP C1I208
E	489	GLY	-	EXPRESSION TAG	UNP C1I208
E	490	HIS	-	EXPRESSION TAG	UNP C1I208
E	491	HIS	-	EXPRESSION TAG	UNP C1I208
E	492	HIS	-	EXPRESSION TAG	UNP C1I208
E	493	HIS	-	EXPRESSION TAG	UNP C1I208
E	494	HIS	-	EXPRESSION TAG	UNP C1I208
E	495	HIS	-	EXPRESSION TAG	UNP C1I208
F	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
F	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
F	488	LEU	-	EXPRESSION TAG	UNP C1I208
F	489	GLY	-	EXPRESSION TAG	UNP C1I208
F	490	HIS	-	EXPRESSION TAG	UNP C1I208

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	491	HIS	-	EXPRESSION TAG	UNP C1I208
F	492	HIS	-	EXPRESSION TAG	UNP C1I208
F	493	HIS	-	EXPRESSION TAG	UNP C1I208
F	494	HIS	-	EXPRESSION TAG	UNP C1I208
F	495	HIS	-	EXPRESSION TAG	UNP C1I208
G	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
G	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
G	488	LEU	-	EXPRESSION TAG	UNP C1I208
G	489	GLY	-	EXPRESSION TAG	UNP C1I208
G	490	HIS	-	EXPRESSION TAG	UNP C1I208
G	491	HIS	-	EXPRESSION TAG	UNP C1I208
G	492	HIS	-	EXPRESSION TAG	UNP C1I208
G	493	HIS	-	EXPRESSION TAG	UNP C1I208
G	494	HIS	-	EXPRESSION TAG	UNP C1I208
G	495	HIS	-	EXPRESSION TAG	UNP C1I208
H	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
H	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
H	488	LEU	-	EXPRESSION TAG	UNP C1I208
H	489	GLY	-	EXPRESSION TAG	UNP C1I208
H	490	HIS	-	EXPRESSION TAG	UNP C1I208
H	491	HIS	-	EXPRESSION TAG	UNP C1I208
H	492	HIS	-	EXPRESSION TAG	UNP C1I208
H	493	HIS	-	EXPRESSION TAG	UNP C1I208
H	494	HIS	-	EXPRESSION TAG	UNP C1I208
H	495	HIS	-	EXPRESSION TAG	UNP C1I208

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	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	14	Total	O	0	0
			14	14		
3	B	20	Total	O	0	0
			20	20		
3	C	20	Total	O	0	0
			20	20		
3	D	15	Total	O	0	0
			15	15		

Continued on next page...

Continued from previous page...

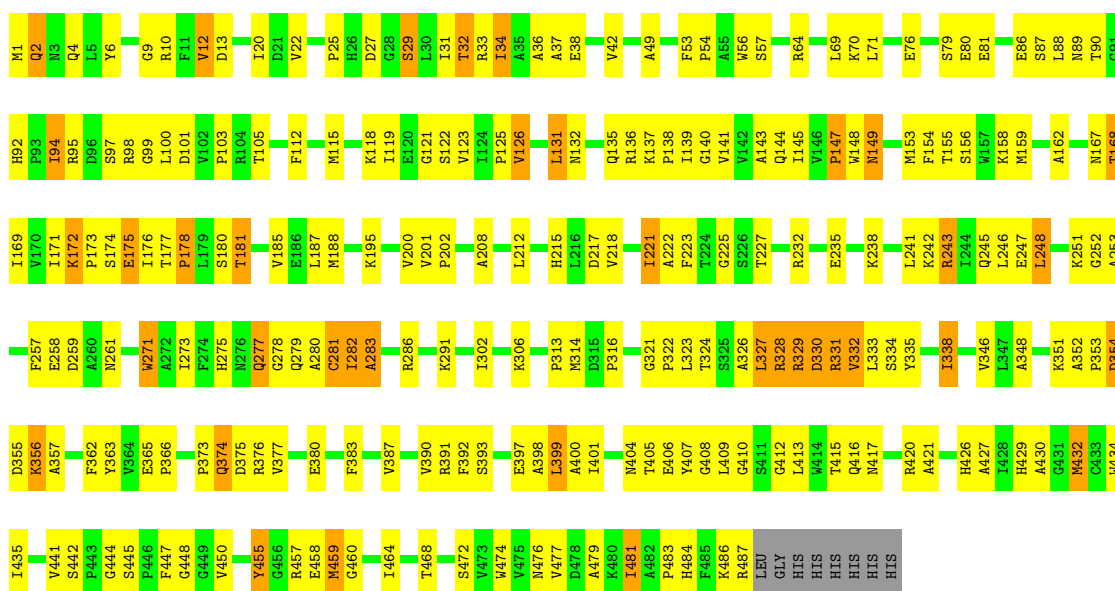
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	26	Total 26	O 26	0	0
3	F	12	Total 12	O 12	0	0
3	G	13	Total 13	O 13	0	0
3	H	15	Total 15	O 15	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

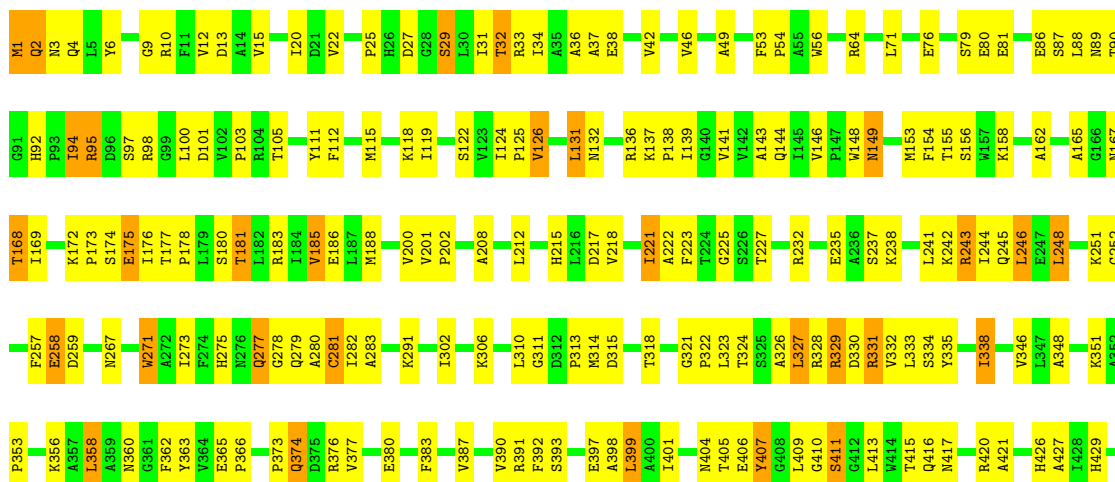
- Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain A:



- Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

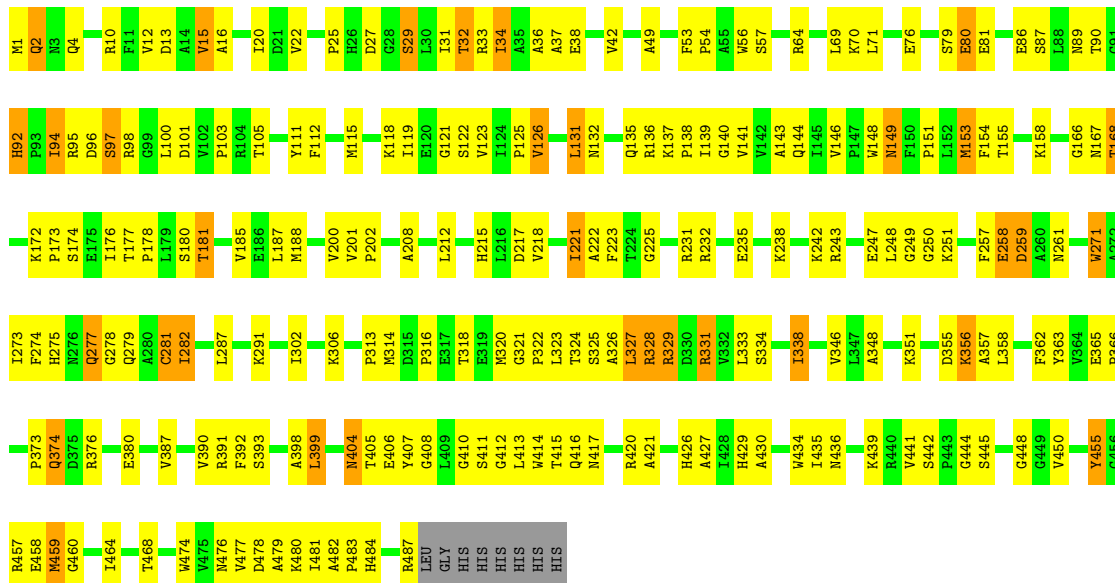
Chain B:





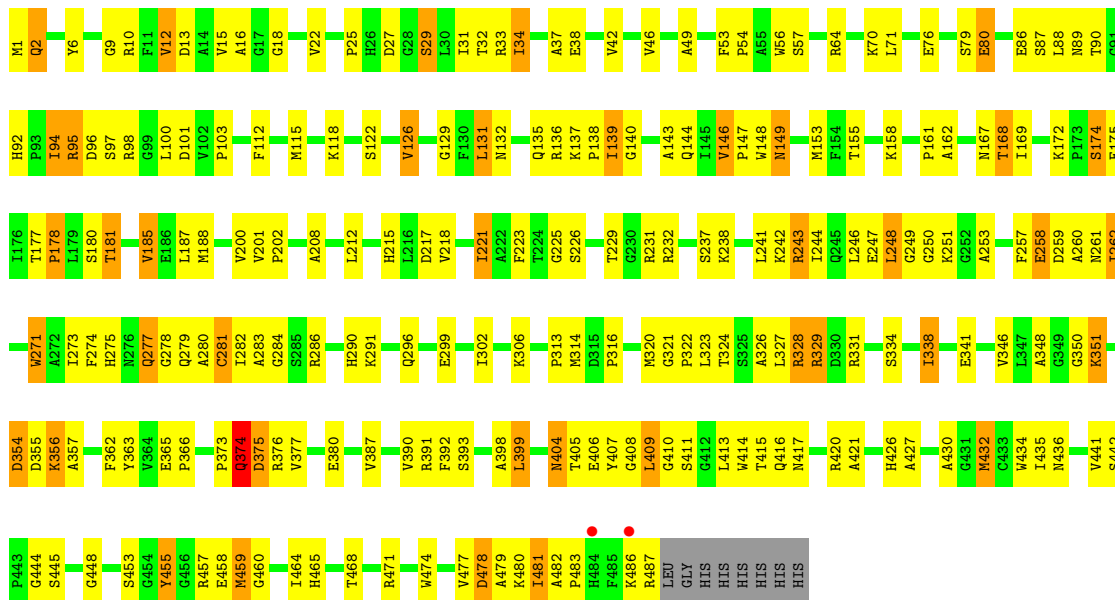
• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain C:



• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

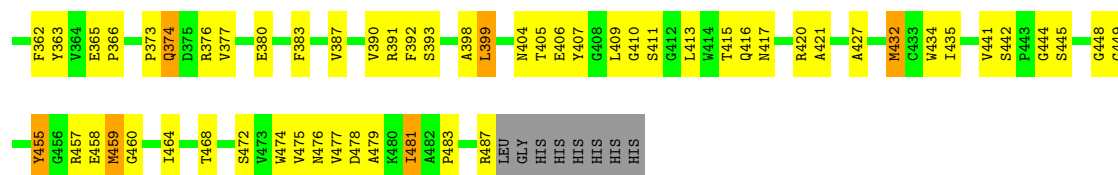
Chain D:



• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

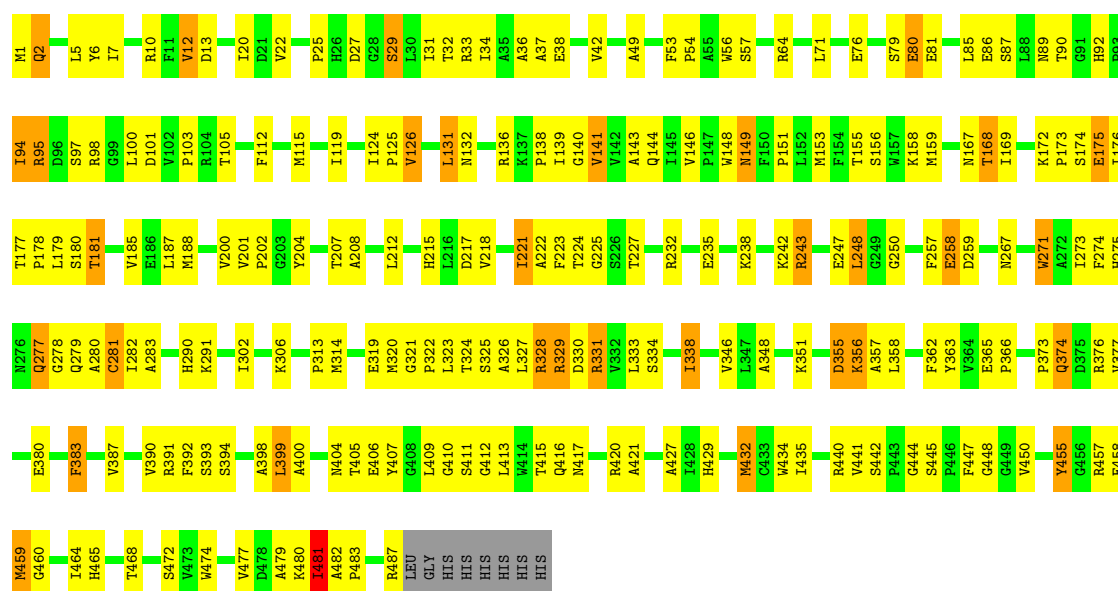
Chain E:





• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.91Å 154.54Å 143.44Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	37.24 – 3.10 48.46 – 3.10	Depositor EDS
% Data completeness (in resolution range)	88.6 (37.24-3.10) 92.1 (48.46-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.207 , 0.251 0.201 , 0.241	Depositor DCC
R_{free} test set	1820 reflections (2.89%)	DCC
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 7.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63060 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30071	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.47	0/3775	0.71	10/5119 (0.2%)
1	B	0.46	0/3775	0.60	2/5119 (0.0%)
1	C	0.46	0/3775	0.63	2/5119 (0.0%)
1	D	0.54	0/3775	0.67	6/5119 (0.1%)
1	E	0.49	0/3775	0.64	4/5119 (0.1%)
1	F	0.46	0/3775	0.63	2/5119 (0.0%)
1	G	0.47	0/3775	0.61	2/5119 (0.0%)
1	H	0.45	0/3775	0.62	3/5119 (0.1%)
All	All	0.48	0/30200	0.64	31/40952 (0.1%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ASP	CB-CA-C	-10.77	88.85	110.40
1	F	459	MET	CB-CA-C	-9.81	90.79	110.40
1	D	478	ASP	CB-CA-C	-9.65	91.11	110.40
1	D	479	ALA	N-CA-CB	-9.28	97.11	110.10
1	A	330	ASP	N-CA-C	9.12	135.62	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3698	0	3691	257	0
1	B	3698	0	3691	246	0
1	C	3698	0	3690	248	0
1	D	3698	0	3691	262	0
1	E	3698	0	3691	235	0
1	F	3698	0	3691	239	0
1	G	3698	0	3691	249	0
1	H	3698	0	3691	238	0
2	A	44	0	26	11	0
2	B	44	0	26	7	0
2	C	44	0	26	14	0
2	D	44	0	25	8	0
2	E	44	0	26	7	0
2	F	44	0	26	11	0
2	G	44	0	26	7	0
2	H	44	0	26	7	0
3	A	14	0	0	4	0
3	B	20	0	0	2	0
3	C	20	0	0	4	0
3	D	15	0	0	3	0
3	E	26	0	0	4	0
3	F	12	0	0	1	0
3	G	13	0	0	5	0
3	H	15	0	0	6	0
All	All	30071	0	29734	1824	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

The worst 5 of 1824 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:247:GLU:C	1:G:248:LEU:HD23	1.41	1.41
1:B:281:CYS:SG	1:B:409:LEU:HD21	1.61	1.39
1:F:325:SER:OG	1:F:328:ARG:CG	1.71	1.38
1:B:281:CYS:SG	1:B:409:LEU:CD2	2.14	1.35
1:G:325:SER:HB3	1:G:328:ARG:CZ	1.64	1.27

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	486/495 (98%)	446 (92%)	36 (7%)	4 (1%)	27	74
1	B	486/495 (98%)	443 (91%)	41 (8%)	2 (0%)	43	84
1	C	486/495 (98%)	445 (92%)	40 (8%)	1 (0%)	56	90
1	D	486/495 (98%)	448 (92%)	35 (7%)	3 (1%)	33	78
1	E	486/495 (98%)	450 (93%)	34 (7%)	2 (0%)	43	84
1	F	486/495 (98%)	444 (91%)	39 (8%)	3 (1%)	33	78
1	G	486/495 (98%)	447 (92%)	35 (7%)	4 (1%)	27	74
1	H	486/495 (98%)	446 (92%)	37 (8%)	3 (1%)	33	78
All	All	3888/3960 (98%)	3569 (92%)	297 (8%)	22 (1%)	33	78

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	459	MET
1	E	481	ILE
1	F	481	ILE
1	G	459	MET
1	H	481	ILE

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	377/383 (98%)	335 (89%)	42 (11%)	9	33
1	B	377/383 (98%)	331 (88%)	46 (12%)	7	26
1	C	377/383 (98%)	332 (88%)	45 (12%)	8	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	377/383 (98%)	329 (87%)	48 (13%)	6	24
1	E	377/383 (98%)	333 (88%)	44 (12%)	8	29
1	F	377/383 (98%)	335 (89%)	42 (11%)	9	33
1	G	377/383 (98%)	335 (89%)	42 (11%)	9	33
1	H	377/383 (98%)	334 (89%)	43 (11%)	8	31
All	All	3016/3064 (98%)	2664 (88%)	352 (12%)	8	29

5 of 352 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	277	GLN
1	E	185	VAL
1	H	221	ILE
1	D	329	ARG
1	D	477	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	404	ASN
1	E	374	GLN
1	H	277	GLN
1	D	416	GLN
1	E	132	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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

8 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	601	-	48,48,48	2.71	17 (35%)	73,73,73	2.39	32 (43%)
2	NAD	B	601	-	48,48,48	2.62	16 (33%)	73,73,73	2.26	26 (35%)
2	NAD	C	601	-	48,48,48	2.70	16 (33%)	73,73,73	2.33	28 (38%)
2	NAD	D	601	-	48,48,48	2.72	15 (31%)	73,73,73	2.21	22 (30%)
2	NAD	E	601	-	48,48,48	2.86	19 (39%)	73,73,73	2.42	30 (41%)
2	NAD	F	601	-	48,48,48	2.63	16 (33%)	73,73,73	2.45	29 (39%)
2	NAD	G	601	-	48,48,48	2.77	19 (39%)	73,73,73	2.37	29 (39%)
2	NAD	H	601	-	48,48,48	2.71	16 (33%)	73,73,73	2.42	29 (39%)

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	601	-	-	0/30/62/62	0/3/5/5
2	NAD	B	601	-	-	0/30/62/62	0/3/5/5
2	NAD	C	601	-	-	0/30/62/62	0/3/5/5
2	NAD	D	601	-	-	0/30/62/62	0/3/5/5
2	NAD	E	601	-	-	0/30/62/62	0/3/5/5
2	NAD	F	601	-	-	0/30/62/62	0/3/5/5
2	NAD	G	601	-	-	0/30/62/62	0/3/5/5
2	NAD	H	601	-	-	0/30/62/62	0/3/5/5

The worst 5 of 134 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NAD	C2N-C3N	9.11	1.51	1.38
2	C	601	NAD	C2N-C3N	8.64	1.51	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	NAD	C2N-C3N	8.60	1.51	1.38
2	G	601	NAD	C2N-C3N	8.54	1.50	1.38
2	E	601	NAD	C2N-N1N	8.17	1.45	1.35

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	NAD	N3A-C2A-N1A	-10.69	119.77	128.71
2	E	601	NAD	N3A-C2A-N1A	-10.21	120.17	128.71
2	D	601	NAD	N3A-C2A-N1A	-9.90	120.43	128.71
2	H	601	NAD	N3A-C2A-N1A	-9.70	120.60	128.71
2	C	601	NAD	N3A-C2A-N1A	-9.47	120.79	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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(Å²)	Q<0.9	
1	A	487/495 (98%)	-0.15	0	100	100	33, 61, 91, 111	0
1	B	487/495 (98%)	-0.11	0	100	100	38, 60, 91, 115	0
1	C	487/495 (98%)	-0.22	0	100	100	31, 57, 90, 116	0
1	D	487/495 (98%)	-0.25	2 (0%)	90	45	30, 50, 83, 118	0
1	E	487/495 (98%)	-0.23	1 (0%)	93	61	32, 50, 85, 123	0
1	F	487/495 (98%)	-0.16	0	100	100	29, 62, 91, 120	0
1	G	487/495 (98%)	-0.17	0	100	100	29, 58, 89, 120	0
1	H	487/495 (98%)	-0.12	0	100	100	36, 62, 90, 124	0
All	All	3896/3960 (98%)	-0.18	3 (0%)	93	70	29, 57, 90, 124	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	486	LYS	2.9
1	E	378	CYS	2.7
1	D	484	HIS	2.2

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

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAD	D	601	44/44	0.22	0.70	45,66,90,95	0
2	NAD	E	601	44/44	0.20	0.41	37,60,82,85	0
2	NAD	A	601	44/44	0.21	0.13	48,77,102,113	0
2	NAD	G	601	44/44	0.23	0.10	48,74,90,103	0
2	NAD	C	601	44/44	0.19	-0.01	38,55,82,90	0
2	NAD	F	601	44/44	0.19	-0.12	49,68,83,101	0
2	NAD	H	601	44/44	0.21	-0.28	54,75,91,108	0
2	NAD	B	601	44/44	0.17	-0.75	45,67,89,100	0

6.5 Other polymers

There are no such residues in this entry.