



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:38 PM GMT

PDB ID : 3PJE
Title : Structure of ENR G93S mutant-NAD⁺-triclosancomplex
Authors : Kim, H.T.; Shin, D.G.; Chang, H.J.
Deposited on : 2010-11-10
Resolution : 2.50 Å(reported)

This is a full wwPDB validation 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>

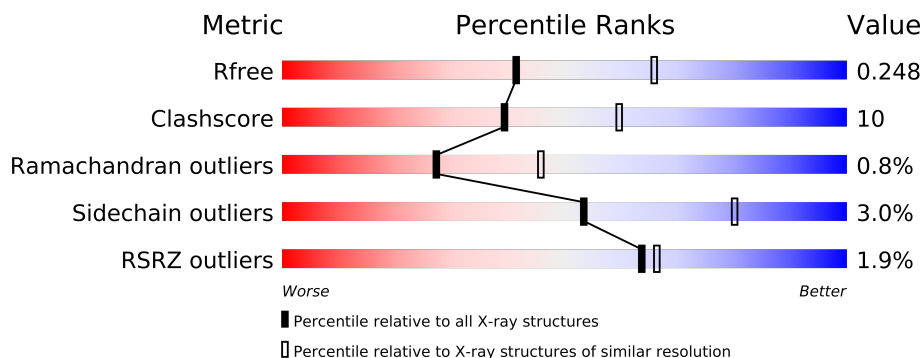
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	270	
1	B	270	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4029 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.

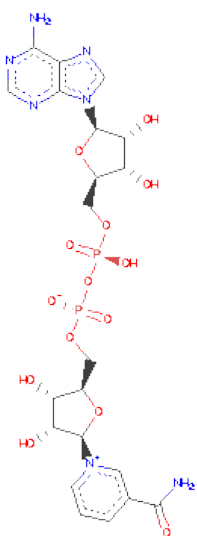
- Molecule 1 is a protein called Enoyl-[acyl-carrier-protein]reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1912	1204	330	365	13			
1	B	257	Total	C	N	O	S	0	0	0
			1912	1204	330	365	13			

There are 18 discrepancies between the modelled and reference sequences:

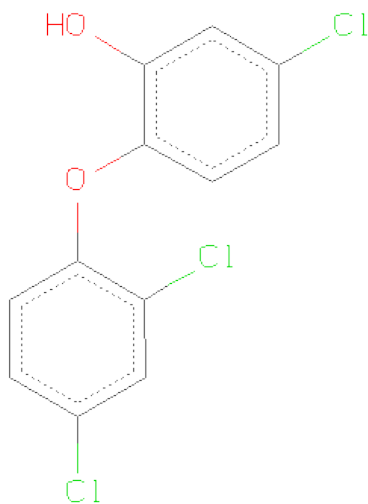
Chain	Residue	Modelled	Actual	Comment	Reference
A	93	SER	GLY	ENGINEERED MUTATION	UNP P0AEK4
A	263	LEU	-	EXPRESSION TAG	UNP P0AEK4
A	264	GLU	-	EXPRESSION TAG	UNP P0AEK4
A	265	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	266	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	267	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	268	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	269	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	270	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	93	SER	GLY	ENGINEERED MUTATION	UNP P0AEK4
B	263	LEU	-	EXPRESSION TAG	UNP P0AEK4
B	264	GLU	-	EXPRESSION TAG	UNP P0AEK4
B	265	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	266	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	267	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	268	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	269	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	270	HIS	-	EXPRESSION TAG	UNP P0AEK4

- 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		

- Molecule 3 is TRICLOSAN (three-letter code: TCL) (formula: C₁₂H₇Cl₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	B	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 4 is water.

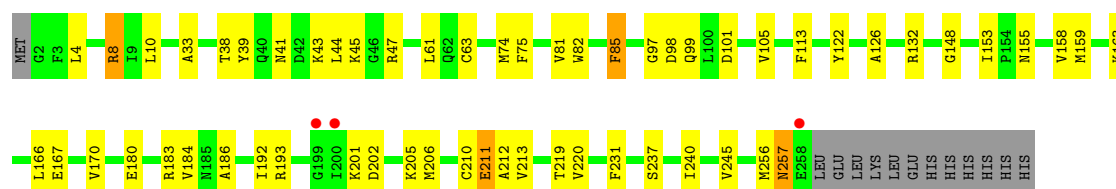
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total 37	O 37	0	0
4	B	46	Total 46	O 46	0	0

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 ($RSRZ > 2$). 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.

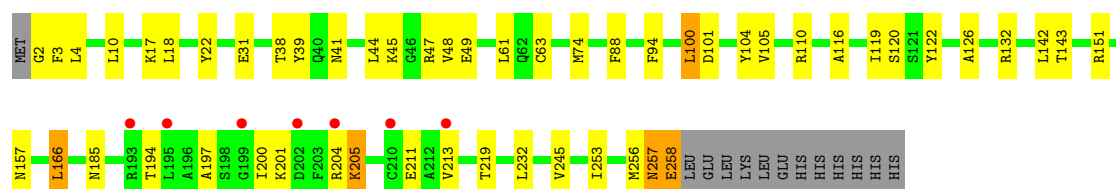
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH]

Chain A: 



- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH]

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	80.85Å 80.85Å 328.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.49 – 2.50 29.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (29.49-2.50) 95.2 (29.49-2.50)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.248 0.222 , 0.248	Depositor DCC
R_{free} test set	1072 reflections (4.88%)	DCC
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 22072 reflections (0.014%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4029	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: TCL, 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	0.38	0/1944	0.59	0/2626
1	B	0.38	0/1944	0.61	0/2626
All	All	0.38	0/3888	0.60	0/5252

There are no bond length outliers.

There are no bond angle outliers.

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	1912	0	1900	42	0
1	B	1912	0	1900	35	0
2	A	44	0	22	0	0
2	B	44	0	22	0	0
3	A	17	0	6	0	0
3	B	17	0	6	0	0
4	A	37	0	0	2	0
4	B	46	0	0	0	0
All	All	4029	0	3856	75	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 10.

All (75) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:75:PHE:HA	4:A:810:HOH:O	1.69	0.91
1:A:4:LEU:HB3	1:A:33:ALA:HB2	1.61	0.81
1:B:213:VAL:HG13	1:B:257:ASN:HB2	1.67	0.75
1:A:213:VAL:HG23	1:A:257:ASN:HB2	1.70	0.73
1:A:211:GLU:HB3	1:A:219:THR:HG23	1.71	0.73
1:A:159:MET:CE	1:A:163:LYS:HE2	2.21	0.70
1:A:10:LEU:HD11	1:A:38:THR:HG23	1.78	0.65
1:B:104:TYR:HD2	1:B:157:ASN:HB3	1.63	0.64
1:A:257:ASN:HD22	1:A:257:ASN:N	1.98	0.62
1:A:132:ARG:NH2	1:A:180:GLU:OE1	2.33	0.61
1:A:159:MET:HE3	1:A:163:LYS:HE2	1.84	0.59
1:B:143:THR:HG21	1:B:166:LEU:HD21	1.84	0.59
1:A:122:TYR:CE2	1:A:126:ALA:HB2	2.38	0.59
1:B:63:CYS:HB2	1:B:74:MET:HG3	1.85	0.58
1:A:41:ASN:OD1	1:A:43:LYS:HB3	2.04	0.57
1:B:253:ILE:C	1:B:253:ILE:HD12	2.26	0.56
1:B:17:LYS:HG2	1:B:22:TYR:CE1	2.42	0.55
1:A:159:MET:HE1	1:A:163:LYS:HE2	1.89	0.55
1:B:39:TYR:HB3	1:B:48:VAL:HG21	1.89	0.55
1:B:200:ILE:HD12	1:B:200:ILE:H	1.71	0.54
1:A:74:MET:SD	4:A:810:HOH:O	2.58	0.54
1:B:204:ARG:HB3	1:B:205:LYS:HE2	1.90	0.54
1:A:39:TYR:CE2	1:A:45:LYS:HB2	2.43	0.53
1:A:38:THR:HA	1:A:61:LEU:O	2.09	0.53
1:A:113:PHE:HA	1:A:158:VAL:HG21	1.89	0.53
1:A:101:ASP:OD1	1:A:201:LYS:HG3	2.08	0.53
1:A:44:LEU:HD23	1:A:47:ARG:NH1	2.23	0.53
1:B:100:LEU:HD22	1:B:100:LEU:N	2.24	0.52
1:A:81:VAL:HG23	1:A:82:TRP:N	2.24	0.52
1:A:105:VAL:HB	1:B:132:ARG:NH1	2.25	0.51
1:A:63:CYS:HB2	1:A:74:MET:HG3	1.93	0.51
1:B:256:MET:O	1:B:258:GLU:N	2.44	0.51
1:A:256:MET:C	1:A:257:ASN:HD22	2.15	0.50
1:B:101:ASP:OD1	1:B:201:LYS:HD3	2.11	0.49
1:B:45:LYS:HE2	1:B:49:GLU:OE1	2.12	0.49
1:B:41:ASN:OD1	1:B:44:LEU:HD23	2.12	0.49
1:B:200:ILE:HD12	1:B:200:ILE:N	2.28	0.48
1:A:163:LYS:O	1:A:167:GLU:HG3	2.14	0.47
1:A:170:VAL:HG13	1:A:184:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:CYS:C	1:A:212:ALA:H	2.18	0.47
1:A:8:ARG:HB3	1:A:82:TRP:CE3	2.50	0.46
1:B:143:THR:HG21	1:B:166:LEU:CD2	2.46	0.46
1:B:232:LEU:HD11	1:B:245:VAL:HG11	1.97	0.46
1:A:132:ARG:NH1	1:B:105:VAL:HB	2.31	0.46
1:B:122:TYR:CE2	1:B:126:ALA:HB2	2.51	0.45
1:A:202:ASP:O	1:A:206:MET:HG3	2.16	0.45
1:A:148:GLY:HA2	1:A:153:ILE:HD12	1.99	0.45
1:A:97:GLY:C	1:A:99:GLN:H	2.20	0.45
1:B:38:THR:HA	1:B:61:LEU:O	2.16	0.44
1:A:132:ARG:NE	1:A:180:GLU:OE1	2.49	0.44
1:A:202:ASP:HB3	1:A:205:LYS:HE3	1.98	0.44
1:A:183:ARG:HD2	1:A:240:ILE:O	2.17	0.44
1:A:231:PHE:CZ	1:A:237:SER:HB3	2.52	0.44
1:B:213:VAL:O	1:B:213:VAL:HG12	2.17	0.44
1:B:213:VAL:CG1	1:B:257:ASN:HB2	2.42	0.44
1:A:10:LEU:HD11	1:A:38:THR:CG2	2.46	0.43
1:B:10:LEU:HD11	1:B:38:THR:HG23	1.99	0.43
1:B:211:GLU:CG	1:B:219:THR:HG23	2.48	0.43
1:B:205:LYS:HE3	1:B:205:LYS:H	1.82	0.43
1:B:211:GLU:HG2	1:B:219:THR:HG23	1.99	0.43
1:B:94:PHE:HB3	1:B:119:ILE:HG21	2.00	0.43
1:B:142:LEU:HD12	1:B:185:ASN:O	2.19	0.43
1:A:257:ASN:ND2	1:A:257:ASN:N	2.66	0.42
1:B:3:PHE:CZ	1:B:31:GLU:HG3	2.54	0.42
1:B:2:GLY:C	1:B:4:LEU:H	2.23	0.42
1:A:192:ILE:HD11	1:A:220:VAL:HG23	2.01	0.42
1:B:10:LEU:HB3	1:B:88:PHE:HB3	2.02	0.42
1:A:213:VAL:HG22	1:A:213:VAL:O	2.20	0.42
1:A:193:ARG:NH1	1:A:193:ARG:HB2	2.35	0.42
1:B:151:ARG:HG3	1:B:151:ARG:NH1	2.33	0.42
1:B:116:ALA:O	1:B:120:SER:HB2	2.20	0.41
1:B:194:THR:H	1:B:197:ALA:HB3	1.85	0.41
1:A:85:PHE:CD2	1:A:85:PHE:N	2.89	0.41
1:A:231:PHE:CE1	1:A:237:SER:HB3	2.56	0.41
1:A:170:VAL:HG21	1:A:186:ALA:HB2	2.04	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	255/270 (94%)	236 (92%)	16 (6%)	3 (1%)	19	32
1	B	255/270 (94%)	234 (92%)	20 (8%)	1 (0%)	43	66
All	All	510/540 (94%)	470 (92%)	36 (7%)	4 (1%)	27	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	257	ASN
1	A	98	ASP
1	A	155	ASN
1	A	211	GLU

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	197/210 (94%)	192 (98%)	5 (2%)	60	85
1	B	197/210 (94%)	190 (96%)	7 (4%)	47	73
All	All	394/420 (94%)	382 (97%)	12 (3%)	53	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	85	PHE
1	A	166	LEU
1	A	245	VAL
1	A	257	ASN

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Mol	Chain	Res	Type
1	B	18	LEU
1	B	47	ARG
1	B	100	LEU
1	B	110	ARG
1	B	166	LEU
1	B	205	LYS
1	B	258	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	B	40	GLN
1	B	54	GLN

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 ⓘ

4 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	701	-	48,48,48	3.53	30 (62%)	73,73,73	2.17	15 (20%)
3	TCL	A	801	-	18,18,18	2.12	10 (55%)	25,25,25	1.18	3 (12%)
2	NAD	B	702	-	48,48,48	3.56	29 (60%)	73,73,73	2.06	13 (17%)
3	TCL	B	802	-	18,18,18	2.11	9 (50%)	25,25,25	1.24	4 (16%)

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	701	-	-	0/30/62/62	0/3/5/5
3	TCL	A	801	-	-	0/4/4/4	0/2/2/2
2	NAD	B	702	-	-	0/30/62/62	0/3/5/5
3	TCL	B	802	-	-	0/4/4/4	0/2/2/2

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	NAD	C2B-C1B	-9.07	1.40	1.53
2	A	701	NAD	C2B-C1B	-8.98	1.40	1.53
2	B	702	NAD	C2D-C1D	-8.56	1.41	1.53
2	A	701	NAD	C2D-C1D	-8.50	1.41	1.53
2	B	702	NAD	O4D-C1D	-6.61	1.31	1.41
2	A	701	NAD	O4D-C1D	-6.25	1.31	1.41
2	A	701	NAD	PN-O2N	5.31	1.61	1.48
2	B	702	NAD	PN-O2N	5.11	1.60	1.48
2	B	702	NAD	C2D-C3D	-5.05	1.39	1.53
2	A	701	NAD	O2B-C2B	-4.99	1.30	1.43
2	B	702	NAD	O2B-C2B	-4.97	1.31	1.43
2	A	701	NAD	C2B-C3B	-4.95	1.39	1.53
2	B	702	NAD	O3B-C3B	-4.90	1.31	1.43
2	B	702	NAD	O2D-C2D	-4.88	1.31	1.43
2	B	702	NAD	O3D-C3D	-4.85	1.31	1.43
2	A	701	NAD	O3B-C3B	-4.84	1.31	1.43
2	A	701	NAD	O2D-C2D	-4.70	1.31	1.43
2	B	702	NAD	C2B-C3B	-4.67	1.40	1.53
2	A	701	NAD	C2D-C3D	-4.67	1.40	1.53
2	A	701	NAD	O4B-C1B	-4.62	1.34	1.41
2	B	702	NAD	O4B-C1B	-4.60	1.34	1.41
2	B	702	NAD	PN-O1N	4.59	1.60	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAD	O3D-C3D	-4.56	1.31	1.43
2	B	702	NAD	O4B-C4B	-4.46	1.34	1.45
2	A	701	NAD	PN-O1N	4.39	1.59	1.48
2	A	701	NAD	C3N-C7N	-4.28	1.43	1.50
2	B	702	NAD	O4D-C4D	-4.16	1.35	1.45
2	A	701	NAD	O4B-C4B	-4.15	1.35	1.45
2	B	702	NAD	C3N-C7N	-4.12	1.43	1.50
2	A	701	NAD	C2N-N1N	3.89	1.40	1.35
2	B	702	NAD	C2N-N1N	3.81	1.40	1.35
3	B	802	TCL	C1-C6	3.78	1.44	1.38
3	A	801	TCL	C1-C6	3.69	1.44	1.38
2	A	701	NAD	O4D-C4D	-3.60	1.36	1.45
2	B	702	NAD	O5D-C5D	-3.52	1.30	1.44
3	A	801	TCL	C10-C11	3.49	1.44	1.38
2	A	701	NAD	O5D-C5D	-3.38	1.30	1.44
2	A	701	NAD	C2A-N3A	3.22	1.38	1.32
2	B	702	NAD	C2A-N3A	3.22	1.38	1.32
2	B	702	NAD	C1D-N1N	-3.18	1.38	1.48
3	B	802	TCL	C1-C2	3.14	1.43	1.38
2	A	701	NAD	C1D-N1N	-3.08	1.39	1.48
3	B	802	TCL	C10-C11	3.06	1.43	1.38
2	B	702	NAD	O7N-C7N	3.05	1.31	1.24
2	A	701	NAD	C1B-N9A	-3.02	1.39	1.48
3	B	802	TCL	C13-C8	3.01	1.46	1.39
3	A	801	TCL	C12-C11	3.01	1.43	1.38
2	A	701	NAD	C3B-C4B	-3.00	1.44	1.53
2	B	702	NAD	C1B-N9A	-2.97	1.39	1.48
2	A	701	NAD	O5B-C5B	-2.96	1.32	1.44
2	B	702	NAD	O5B-C5B	-2.94	1.32	1.44
2	B	702	NAD	C3B-C4B	-2.88	1.45	1.53
2	A	701	NAD	O7N-C7N	2.84	1.30	1.24
2	A	701	NAD	C2A-N1A	2.82	1.39	1.33
2	A	701	NAD	C2N-C3N	2.80	1.42	1.38
2	B	702	NAD	C2N-C3N	2.72	1.42	1.38
2	B	702	NAD	C2A-N1A	2.71	1.39	1.33
2	A	701	NAD	C4N-C3N	2.60	1.43	1.39
3	A	801	TCL	C1-C2	2.53	1.42	1.38
3	B	802	TCL	C6-C5	2.51	1.44	1.40
3	A	801	TCL	C13-C8	2.51	1.45	1.39
3	A	801	TCL	C3-C2	2.49	1.42	1.38
2	A	701	NAD	PA-O1A	2.43	1.60	1.51
3	B	802	TCL	C4-C5	2.41	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	TCL	C12-C11	2.36	1.42	1.38
2	B	702	NAD	C4N-C3N	2.31	1.43	1.39
3	A	801	TCL	C8-C9	2.30	1.44	1.39
2	A	701	NAD	PA-O3	2.29	1.64	1.59
2	A	701	NAD	C5B-C4B	-2.27	1.44	1.51
3	B	802	TCL	C3-C2	2.27	1.42	1.38
3	A	801	TCL	C10-C9	2.17	1.42	1.38
3	A	801	TCL	C4-C5	2.16	1.44	1.39
2	A	701	NAD	C3D-C4D	-2.14	1.47	1.53
2	B	702	NAD	PA-O3	2.13	1.63	1.59
2	B	702	NAD	C3D-C4D	-2.02	1.47	1.53
3	A	801	TCL	C3-C4	2.02	1.42	1.38
2	B	702	NAD	PA-O1A	2.01	1.59	1.51
3	B	802	TCL	C8-C9	2.00	1.43	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAD	N3A-C2A-N1A	-10.06	120.30	128.71
2	B	702	NAD	N3A-C2A-N1A	-9.47	120.79	128.71
2	A	701	NAD	C4B-O4B-C1B	-5.89	103.36	109.75
2	B	702	NAD	O4B-C1B-C2B	-5.37	98.54	106.77
2	A	701	NAD	O4B-C1B-C2B	-5.30	98.64	106.77
2	B	702	NAD	C4B-O4B-C1B	-5.27	104.02	109.75
2	A	701	NAD	O4D-C1D-N1N	5.20	113.27	107.95
2	A	701	NAD	O4B-C1B-N9A	5.05	113.14	108.44
2	B	702	NAD	O4B-C1B-N9A	4.44	112.57	108.44
2	B	702	NAD	O4D-C1D-N1N	3.85	111.89	107.95
2	B	702	NAD	O2N-PN-O1N	-3.63	107.77	118.72
3	A	801	TCL	C8-O7-C5	3.55	126.67	117.93
2	A	701	NAD	O2N-PN-O1N	-3.37	108.55	118.72
2	B	702	NAD	O3-PA-O5B	3.37	118.47	103.41
2	A	701	NAD	O3-PA-O5B	3.21	117.77	103.41
2	A	701	NAD	C3N-C7N-N7N	2.96	121.14	117.77
3	B	802	TCL	C8-O7-C5	2.86	124.98	117.93
2	B	702	NAD	C3N-C7N-N7N	2.82	120.98	117.77
2	A	701	NAD	O7N-C7N-N7N	-2.73	118.64	122.59
2	B	702	NAD	O7N-C7N-N7N	-2.70	118.70	122.59
2	A	701	NAD	N3A-C4A-N9A	2.68	130.28	125.43
2	A	701	NAD	C4D-O4D-C1D	-2.66	106.86	109.75
2	B	702	NAD	N3A-C4A-N9A	2.65	130.22	125.43
2	A	701	NAD	PN-O3-PA	-2.65	121.57	132.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	NAD	PN-O3-PA	-2.64	121.60	132.95
2	B	702	NAD	C4D-O4D-C1D	-2.60	106.92	109.75
3	B	802	TCL	C3-C2-C1	2.55	125.07	121.54
2	A	701	NAD	C5N-C4N-C3N	-2.23	117.43	120.32
3	A	801	TCL	C4-C3-C2	-2.20	116.76	119.22
2	A	701	NAD	O4B-C4B-C5B	2.10	116.87	109.36
2	B	702	NAD	C5N-C4N-C3N	-2.10	117.59	120.32
2	A	701	NAD	O2D-C2D-C3D	2.10	118.66	111.83
3	A	801	TCL	C3-C2-C1	2.10	124.44	121.54
3	B	802	TCL	C4-C3-C2	-2.02	116.97	119.22
3	B	802	TCL	C8-C9-CL16	2.00	122.07	119.45

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(Å ²)	Q<0.9
1	A	257/270 (95%)	-0.14	3 (1%) 75 77	18, 31, 66, 93	0
1	B	257/270 (95%)	-0.14	7 (2%) 52 54	18, 29, 69, 92	0
All	All	514/540 (95%)	-0.14	10 (1%) 64 66	18, 30, 69, 93	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	ARG	3.5
1	A	258	GLU	3.4
1	B	193	ARG	3.4
1	B	202	ASP	3.3
1	B	195	LEU	3.0
1	B	199	GLY	2.4
1	B	210	CYS	2.3
1	A	200	ILE	2.3
1	A	199	GLY	2.1
1	B	213	VAL	2.0

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	B	702	44/44	0.12	-0.49	20,28,34,34	0
2	NAD	A	701	44/44	0.13	-0.50	19,33,39,43	0
3	TCL	B	802	17/17	0.13	-0.53	27,29,31,31	0
3	TCL	A	801	17/17	0.12	-0.80	29,34,40,40	0

6.5 Other polymers

There are no such residues in this entry.