WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 04:22 am GMT

PDB ID	:	4R82
Title	:	Streptomyces globisporus C-1027 NADH:FAD oxidoreductase SgcE6 in complex with NAD and FAD fragments
Authors	:	Tan, K.; Bigelow, L.; Clancy, S.; Babnigg, G.; Bingman, C.A.; Yennamalli, R.; Lohman, J.R.; Ma, M.; Shen, B.; Phillips Jr., G.N.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG); Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on	:	2014-08-29
Resolution	:	1.66 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:
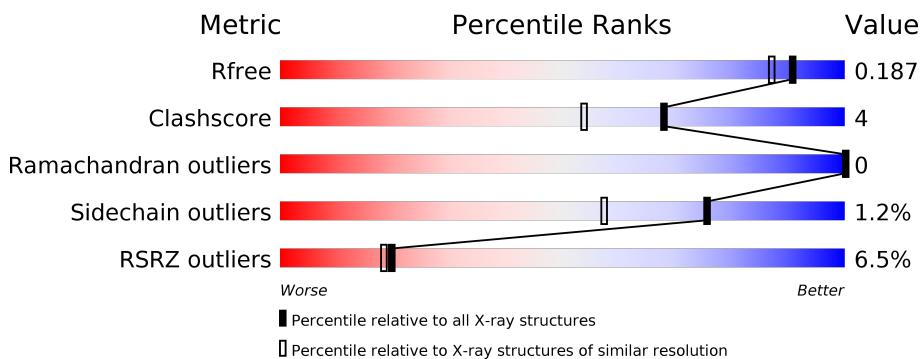
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
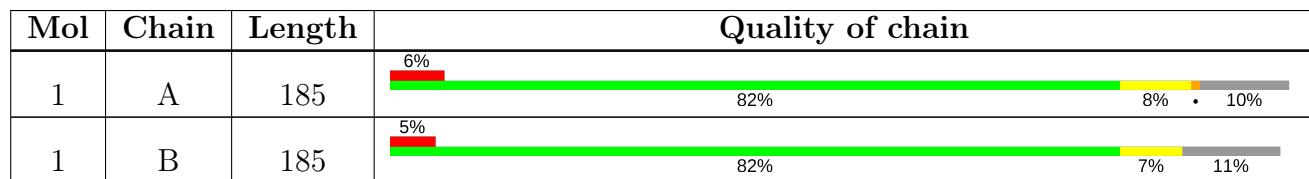
The reported resolution of this entry is 1.66 Å.

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	Percentile Ranks	Value
Rfree		0.187
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		6.5%

Worse ——— Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

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.

Mol	Chain	Length	Quality of chain
1	A	185	6% / 82% / 8% · 10%
1	B	185	5% / 82% / 7% 11%

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
5	ACT	A	205	-	-	X	X
5	ACT	A	206	-	-	-	X
5	ACT	A	207	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 2931 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.
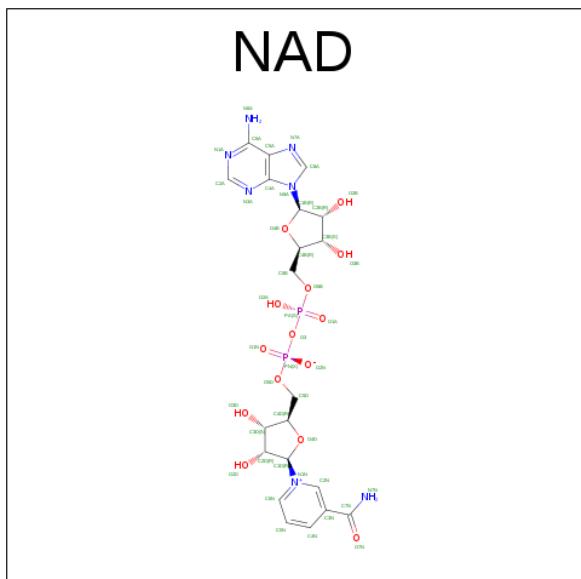
- Molecule 1 is a protein called Oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	Se	0	6	0
			1273	810	227	231	2	3			
1	B	165	Total	C	N	O	S	Se	0	2	0
			1242	788	221	228	2	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8GME2
A	-1	ASN	-	EXPRESSION TAG	UNP Q8GME2
A	0	ALA	-	EXPRESSION TAG	UNP Q8GME2
B	-2	SER	-	EXPRESSION TAG	UNP Q8GME2
B	-1	ASN	-	EXPRESSION TAG	UNP Q8GME2
B	0	ALA	-	EXPRESSION TAG	UNP Q8GME2

- 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 23	C 10	N 5	O 7	P 1	0	0
2	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
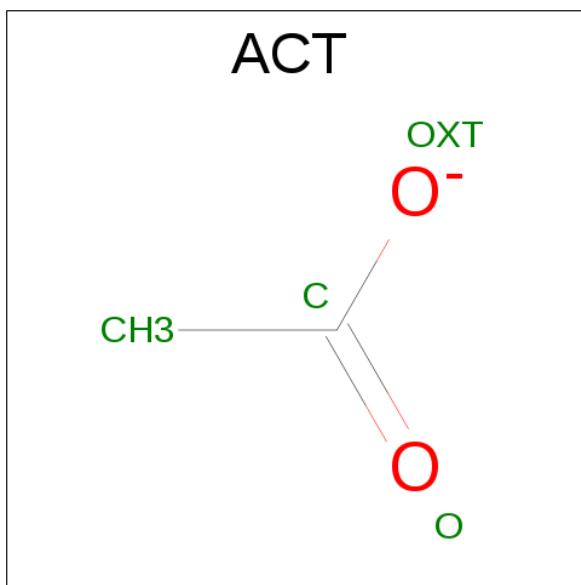
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Ca 2	0	0
3	A	1	Total 1	Ca 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	A	1	Total 1	Cl 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
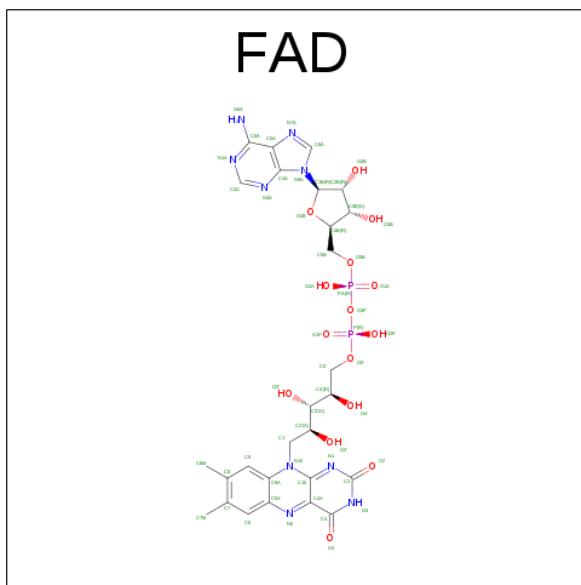
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total C O			0	0
			4	2	2		
5	A	1	Total C O			0	0
			4	2	2		
5	A	1	Total C O			0	0
			4	2	2		
5	B	1	Total C O			0	0
			4	2	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total Mg		0	0
			1	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
7	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
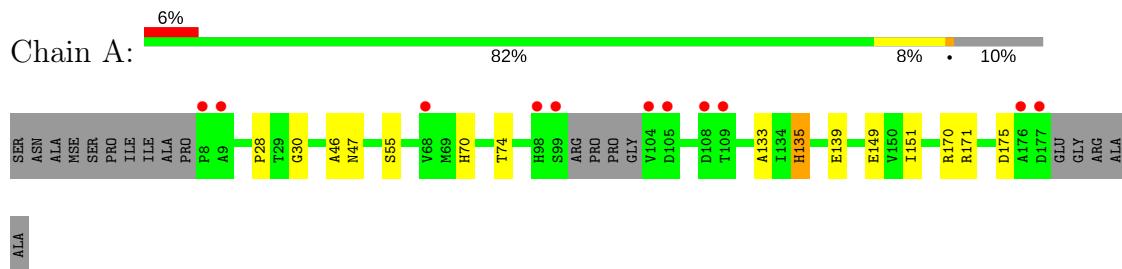
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	111	Total 112	O 112	0	1
8	B	125	Total 128	O 128	0	3
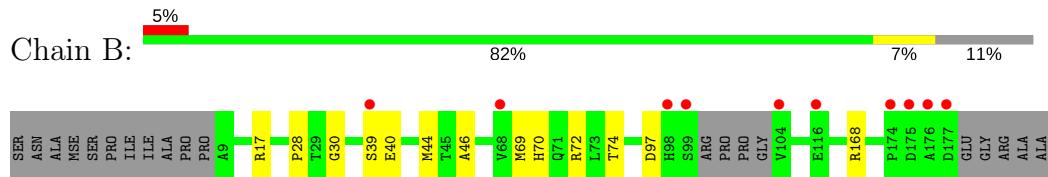
3 Residue-property plots (i)

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: Oxidoreductase

Chain A:

• Molecule 1: Oxidoreductase

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.05Å 62.83Å 70.09Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	34.93 – 1.66 35.47 – 1.66	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.93-1.66) 99.5 (35.47-1.66)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 1.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.163 , 0.188 0.162 , 0.187	Depositor DCC
R_{free} test set	2166 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2931	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, NAD, CL, CA, ACT, FAD

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	0.34	0/1318	0.55	0/1787
1	B	0.34	0/1272	0.55	0/1725
All	All	0.34	0/2590	0.55	0/3512

There are no bond length outliers.

There are no bond angle outliers.

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	1273	0	1249	13	0
1	B	1242	0	1206	9	0
2	A	46	0	24	0	0
2	B	46	0	24	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	9	3	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	31	0	19	3	0
7	B	31	0	19	4	0
8	A	112	0	0	2	0
8	B	128	0	0	2	0
All	All	2931	0	2553	23	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 4.

All (23) 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:40:GLU:O	1:B:72:ARG:NH1	2.17	0.78
1:A:171:ARG:NH2	8:A:378:HOH:O	2.27	0.66
1:B:44:MSE:HE2	1:B:69:MSE:HG2	1.78	0.64
1:A:175:ASP:OD2	1:B:168:ARG:NE	2.29	0.63
1:A:139:GLU:HB3	5:A:207:ACT:H1	1.82	0.61
1:A:170:ARG:NH1	5:A:205:ACT:H3	2.22	0.55
1:A:133:ALA:HB2	1:A:151[B]:ILE:HD11	1.88	0.55
7:B:207:FAD:HO4'	7:B:207:FAD:P	2.35	0.50
1:A:135[A]:HIS:NE2	1:A:149:GLU:OE1	2.45	0.49
1:A:70:HIS:O	1:A:74:THR:HG23	2.13	0.48
1:B:72:ARG:NH1	8:B:325:HOH:O	2.47	0.48
1:A:55[B]:SER:OG	1:B:17[B]:ARG:NH2	2.47	0.47
7:A:209:FAD:O4'	7:A:209:FAD:P	2.72	0.47
1:A:28:PRO:HD2	1:B:30:GLY:HA3	1.96	0.46
7:B:207:FAD:O4'	7:B:207:FAD:P	2.74	0.46
1:A:46:ALA:HA	7:A:209:FAD:N5	2.31	0.45
1:A:47:ASN:ND2	8:A:381:HOH:O	2.49	0.45
7:A:209:FAD:O4'	7:A:209:FAD:O2P	2.34	0.44
1:B:46:ALA:HA	7:B:207:FAD:N5	2.32	0.44
1:A:170:ARG:HH12	5:A:205:ACT:H3	1.82	0.43
7:B:207:FAD:O3P	8:B:371:HOH:O	2.21	0.43
1:B:70:HIS:O	1:B:74:THR:HG23	2.19	0.43
1:A:30:GLY:HA3	1:B:28:PRO:HD2	2.02	0.42

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	168/185 (91%)	167 (99%)	1 (1%)	0	100	100
1	B	163/185 (88%)	162 (99%)	1 (1%)	0	100	100
All	All	331/370 (90%)	329 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	131/141 (93%)	129 (98%)	2 (2%)	70	48
1	B	125/141 (89%)	123 (98%)	2 (2%)	68	45
All	All	256/282 (91%)	252 (98%)	4 (2%)	75	45

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135[A]	HIS
1	A	135[B]	HIS
1	B	39	SER
1	B	97	ASP

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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	NAD	A	201	-	22,25,48	1.79	4 (18%)	24,38,73	2.25	4 (16%)
2	NAD	A	202	-	22,25,48	1.64	4 (18%)	24,38,73	2.70	5 (20%)
5	ACT	A	205	3	1,3,3	1.12	0	0,3,3	0.00	-
5	ACT	A	206	-	1,3,3	1.33	0	0,3,3	0.00	-
5	ACT	A	207	-	1,3,3	1.30	0	0,3,3	0.00	-
7	FAD	A	209	-	31,33,58	1.71	7 (22%)	38,50,89	1.63	4 (10%)
2	NAD	B	201	-	22,25,48	1.72	4 (18%)	24,38,73	2.57	4 (16%)
2	NAD	B	202	-	22,25,48	1.66	4 (18%)	24,38,73	2.63	5 (20%)
5	ACT	B	206	-	1,3,3	1.20	0	0,3,3	0.00	-
7	FAD	B	207	-	31,33,58	1.72	6 (19%)	38,50,89	1.65	5 (13%)

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	201	-	-	0/6/26/62	0/3/3/5
2	NAD	A	202	-	-	0/6/26/62	0/3/3/5
5	ACT	A	205	3	-	0/0/0/0	0/0/0/0
5	ACT	A	206	-	-	0/0/0/0	0/0/0/0
5	ACT	A	207	-	-	0/0/0/0	0/0/0/0
7	FAD	A	209	-	-	0/16/18/50	0/3/3/6
2	NAD	B	201	-	-	0/6/26/62	0/3/3/5
2	NAD	B	202	-	-	0/6/26/62	0/3/3/5
5	ACT	B	206	-	-	0/0/0/0	0/0/0/0
7	FAD	B	207	-	-	0/16/18/50	0/3/3/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	NAD	C2B-C1B	-4.79	1.46	1.53
2	B	201	NAD	C2B-C1B	-4.78	1.46	1.53
2	B	202	NAD	C2B-C1B	-4.28	1.46	1.53
2	A	202	NAD	C2B-C1B	-3.91	1.47	1.53
2	A	202	NAD	O4B-C4B	-2.81	1.38	1.45
2	B	202	NAD	O4B-C4B	-2.78	1.38	1.45
2	B	201	NAD	C2B-C3B	-2.73	1.46	1.53
7	A	209	FAD	C2-N1	-2.71	1.32	1.38
2	A	201	NAD	C2B-C3B	-2.69	1.46	1.53
7	B	207	FAD	C2-N1	-2.50	1.33	1.38
7	B	207	FAD	C2-N3	-2.44	1.33	1.38
2	B	202	NAD	C2B-C3B	-2.44	1.47	1.53
2	A	202	NAD	C2B-C3B	-2.42	1.47	1.53
7	A	209	FAD	C2-N3	-2.35	1.33	1.38
2	B	201	NAD	O4B-C4B	-2.22	1.40	1.45
2	A	201	NAD	C3B-C4B	-2.08	1.47	1.53
7	A	209	FAD	C7M-C7	2.04	1.55	1.51
7	B	207	FAD	C4X-N5	2.32	1.36	1.33
7	B	207	FAD	C10-N1	2.40	1.36	1.33
7	A	209	FAD	C5'-C4'	2.43	1.55	1.51
2	B	202	NAD	O4B-C1B	2.65	1.44	1.41
2	A	202	NAD	O4B-C1B	2.66	1.44	1.41
7	B	207	FAD	C5'-C4'	2.77	1.55	1.51
7	A	209	FAD	C4X-N5	2.82	1.37	1.33
2	B	201	NAD	O4B-C1B	3.15	1.45	1.41
7	A	209	FAD	C10-N1	3.39	1.38	1.33
2	A	201	NAD	O4B-C1B	3.89	1.46	1.41
7	A	209	FAD	O4-C4	5.59	1.38	1.24
7	B	207	FAD	O4-C4	6.12	1.39	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	NAD	N3A-C2A-N1A	-11.33	118.99	128.86
2	A	202	NAD	N3A-C2A-N1A	-10.81	119.44	128.86
2	B	202	NAD	N3A-C2A-N1A	-10.44	119.76	128.86
2	A	201	NAD	N3A-C2A-N1A	-9.29	120.76	128.86
2	A	202	NAD	C4B-O4B-C1B	-5.38	104.05	109.77
2	B	202	NAD	C4B-O4B-C1B	-4.79	104.67	109.77
7	B	207	FAD	C4X-C4-N3	-3.12	119.04	123.48
2	A	201	NAD	C4B-O4B-C1B	-2.73	106.86	109.77
7	A	209	FAD	C4X-C4-N3	-2.66	119.70	123.48
2	B	202	NAD	C4A-C5A-N7A	-2.63	106.87	109.41
7	B	207	FAD	O3'-C3'-C4'	-2.33	103.04	108.82
2	A	202	NAD	C1B-N9A-C4A	-2.01	123.17	126.64
2	B	201	NAD	O3-PA-O5B	2.09	112.29	106.73
2	A	202	NAD	C2A-N1A-C6A	2.12	122.48	118.77
2	A	201	NAD	PA-O5B-C5B	2.26	124.52	118.30
2	A	202	NAD	O5B-C5B-C4B	2.26	117.03	109.00
2	B	202	NAD	C2A-N1A-C6A	2.33	122.84	118.77
2	B	201	NAD	O5B-C5B-C4B	2.37	117.39	109.00
2	B	201	NAD	C2A-N1A-C6A	2.45	123.06	118.77
2	A	201	NAD	O3-PA-O5B	2.50	113.39	106.73
2	B	202	NAD	O5B-C5B-C4B	2.65	118.39	109.00
7	B	207	FAD	C1'-N10-C9A	3.78	121.81	118.35
7	B	207	FAD	C5X-C9A-N10	4.10	120.70	117.66
7	A	209	FAD	C5X-C9A-N10	4.43	120.95	117.66
7	A	209	FAD	C1'-N10-C9A	4.68	122.64	118.35
7	A	209	FAD	C4-N3-C2	4.83	119.38	115.16
7	B	207	FAD	C4-N3-C2	4.99	119.52	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	205	ACT	2	0
5	A	207	ACT	1	0
7	A	209	FAD	3	0
7	B	207	FAD	4	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, 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	163/185 (88%)	-0.02	11 (6%)	19	17	10, 16, 38, 62	0
1	B	162/185 (87%)	0.16	10 (6%)	21	19	10, 19, 46, 74	0
All	All	325/370 (87%)	0.07	21 (6%)	20	18	10, 17, 46, 74	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	VAL	6.8
1	B	104	VAL	5.8
1	B	99	SER	5.6
1	B	176	ALA	5.3
1	A	8	PRO	4.4
1	B	177	ASP	3.9
1	A	176	ALA	3.7
1	B	116	GLU	3.7
1	A	108	ASP	3.5
1	A	98	HIS	3.4
1	B	68	VAL	3.3
1	A	109	THR	3.2
1	A	177	ASP	3.1
1	A	105	ASP	2.9
1	A	99	SER	2.9
1	B	39	SER	2.8
1	B	174	PRO	2.6
1	A	68	VAL	2.5
1	B	98	HIS	2.4
1	B	175	ASP	2.2
1	A	9	ALA	2.1

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, 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
5	ACT	A	205	4/4	0.92	0.24	9.13	37,38,39,39	0
5	ACT	A	207	4/4	0.73	0.24	4.31	50,52,53,55	0
5	ACT	A	206	4/4	0.90	0.18	2.27	25,33,38,41	0
7	FAD	A	209	31/53	0.93	0.10	-0.04	9,12,49,58	0
7	FAD	B	207	31/53	0.93	0.11	-0.22	9,12,38,48	0
2	NAD	A	201	23/44	0.97	0.06	-0.38	12,14,24,33	0
2	NAD	B	202	23/44	0.92	0.10	-0.38	11,14,67,70	0
2	NAD	B	201	23/44	0.96	0.08	-0.99	12,14,26,35	0
3	CA	B	204	1/1	0.99	0.05	-1.80	25,25,25,25	0
4	CL	A	204	1/1	0.97	0.05	-2.16	26,26,26,26	0
4	CL	B	205	1/1	0.98	0.04	-3.50	24,24,24,24	0
6	MG	A	208	1/1	0.95	0.07	-3.51	30,30,30,30	0
2	NAD	A	202	23/44	0.94	0.08	-	10,14,68,94	0
3	CA	B	203	1/1	0.99	0.04	-	16,16,16,16	0
3	CA	A	203	1/1	1.00	0.03	-	16,16,16,16	0
5	ACT	B	206	4/4	0.91	0.22	-	36,39,40,41	0

6.5 Other polymers (i)

There are no such residues in this entry.