



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:53 pm GMT

PDB ID : 2BN4
Title : A SECOND FMN-BINDING SITE IN YEAST NADPH-CYTOCHROME P450 REDUCTASE SUGGESTS A NOVEL MECHANISM OF ELECTRON TRANSFER BY DIFLAVIN REDUCTASE
Authors : Podust, L.M.; Lepesheva, G.I.; Kim, Y.; Yermalitskaya, L.V.; Yermalitsky, V.N.; Lamb, D.C.; Kelly, S.L.; Waterman, M.R.
Deposited on : 2005-03-18
Resolution : 2.91 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 ⓘ symbol.

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 : trunk28620
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) : recalc28949

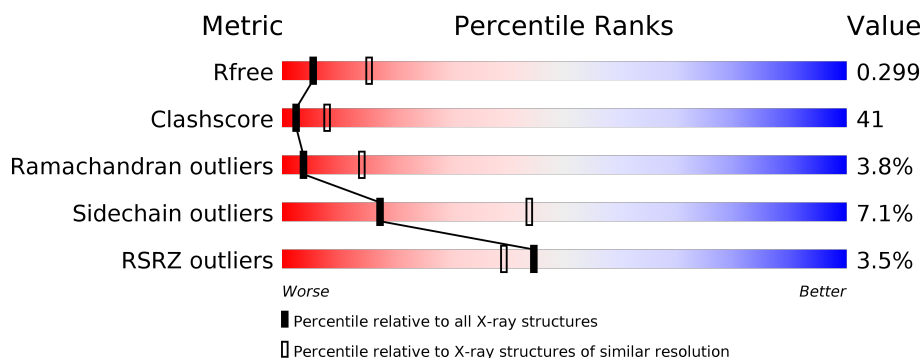
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	1813 (2.94-2.90)
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (2.94-2.90)

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 $\leq 5\%$. 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	682	<div> <div>3%</div> <div> <div></div> <div>40%</div> <div>49%</div> <div>6%</div> <div>6%</div> </div> </div>
1	B	682	<div> <div>4%</div> <div> <div></div> <div>33%</div> <div>55%</div> <div>6%</div> <div>6%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10331 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 NADPH CYTOCHROME P450 REDUCTASE.

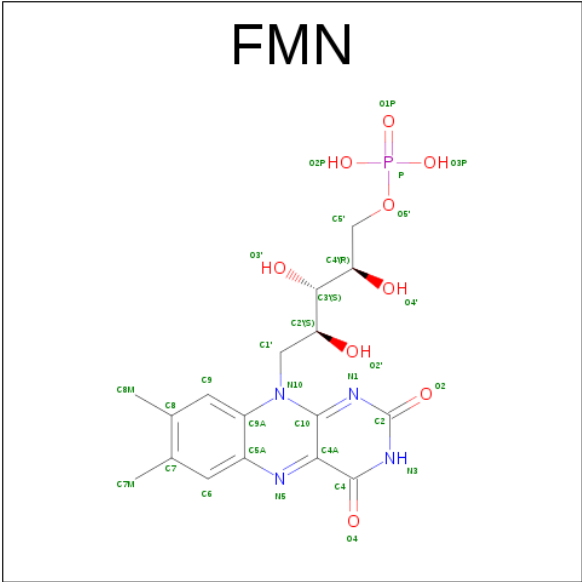
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	0	0
			5021	3202	827	977	15			
1	B	641	Total	C	N	O	S	0	0	0
			5007	3191	825	976	15			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



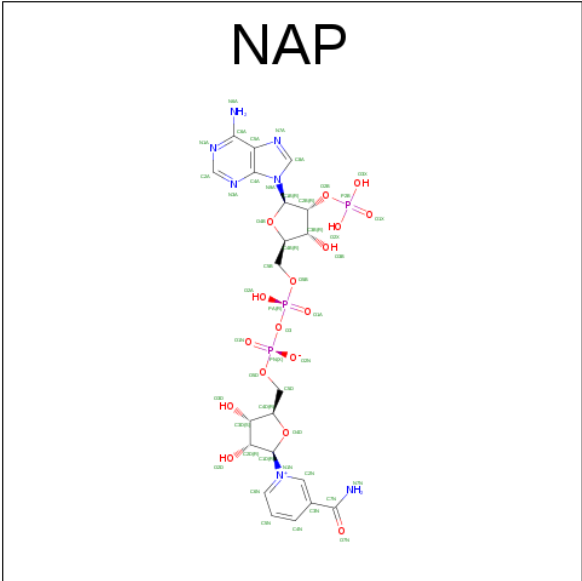
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

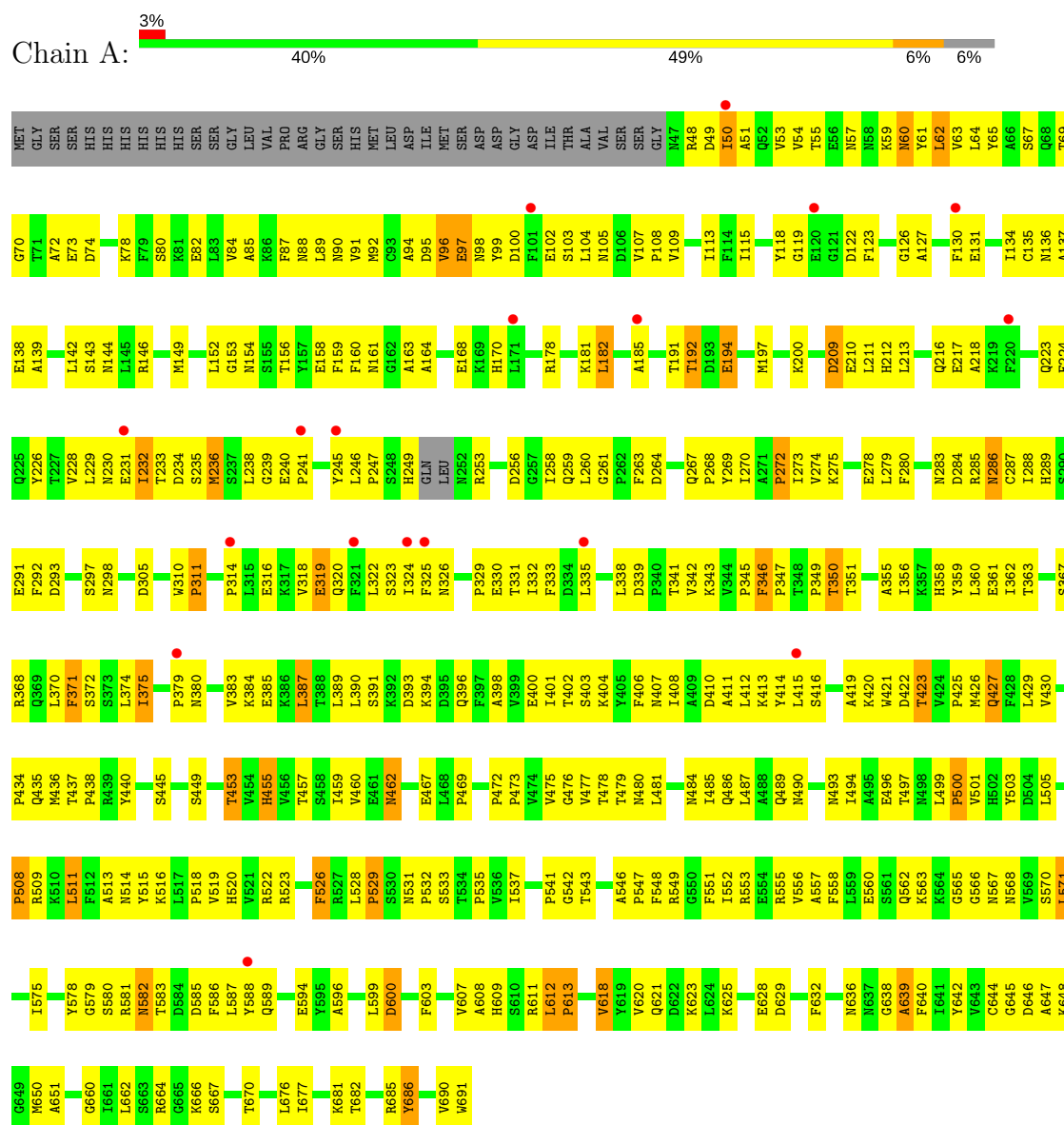
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total	O	0	0
			33	33		
5	B	22	Total	O	0	0
			22	22		

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 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: NADPH CYTOCHROME P450 REDUCTASE



• Molecule 1: NADPH CYTOCHROME P450 REDUCTASE



E633	Q562	L494	M426	L360	D293	R146	K77	MET
M634	K563	A495	Q427	E361	L294	Y147	K77	GLY
I635	E496	E496	F428	L362	F224	M148	S80	SER
N636	N568	T497	L429	T363	Q225	M149	K81	SER
G638	V569	N498	V430	G364	E231	F150	E82	HIS
A639	S570	L499	E431	Q369	I232	G151	L83	HIS
F640	L571	P500	S432	L370	T233	L152	V84	HIS
Y642	G572	H502	V433	F371	D234	G153	F87	HIS
V643	H574	Y503	Q435	S372	S235	N154	N88	HIS
C644	I575	P508	M436	S373	M236	T156	L89	SER
G645	L576	R509	T437	L374	L238	Y157	N90	SER
D646	F577	K510	P438	I375	G239	E158	V91	GLY
A647	G579	L511	R439	Q376	F159	F160	N92	LEU
K648	G580	P512	Y440	F377	E240	N161	C93	VAL
G649	R581	A513	A441	A378	P241	G162	A94	PRO
M650	R582	N514	S442	N313	Y245	A163	D95	ARG
A651	T583	Y515	I443	N380	L246	A164	V96	SER
K652	D584	K516	S444	A381	P247	K165	E97	HIS
G653	D585	L517	S445	D382	Q250	K166	N98	MET
V654	F586	P518	S446	V383	H249	K169	D100	LEU
S655	F586	V519	L448	E385	Q251	H170	F101	ASP
T656	Q589	H520	S449	K386	ASN	E102	E102	ILE
A657	D590	V521	E450	L387	ARG	A173	S103	MET
L658	E591	R522	K451	L390	ASN	A174	L104	SER
G659	E594	R527	Q452	S391	L327	G175	N105	ASP
G660	Y595	L528	T453	K392	D328	D256	D106	ASP
I661	A596	P529	V454	F397	P329	G257	V107	GLY
L662	A596	S530	H455	D395	E330	L179	P108	ASP
S663	K597	S530	V456	Q396	T331	E184	Y109	ILE
R664	K598	N531	V456	F397	L332	A185	I110	THR
G665	L599	P532	I459	A398	F333	G188	I113	ALA
K666	D600	T534	V460	E400	D334	A189	T117	SER
T669	G601	V536	M465	I401	L335	G190	T117	SER
E672	F603	V536	E467	T402	K336	L265	Y118	GLY
A673	E604	L537	L468	S403	P337	S266	G119	N47
T674	H609	P538	P469	K404	L338	Q267	E120	R48
E675	S610	G540	D470	Y405	P340	P268	P124	D49
L676	R611	P541	A471	F406	T341	Y269	D125	I50
I677	L612	G542	P472	N407	V342	P272	N129	Q62
L680	P613	T543	P473	I408	V343	I273	F133	A51
K681	K616	G544	V474	A409	V344	V274	I134	K59
T682	G617	V545	V475	D410	P345	K275	C135	N60
S683	V618	A546	G476	A411	F346	S202	L207	Y61
G684	G618	P547	V477	L412	P347	R277	E210	L62
R685	Y619	F548	T478	K413	T348	E278	L211	V63
Y686	V620	B549	T479	Y414	P349	L279	A137	L63
Q687	Q621	G550	M480	L415	T350	N283	E138	A66
V690	F551	L481	L482	S416	T351	D284	L213	S67
W691	L552	L482	R483	A419	G353	R285	G140	Q68
	R553	R483	M484	K420	A354	N286	A141	T69
	E554	E554	I485	W421	A355	C287	Q216	
	R555	R555	Q486	D422	I356	T288	E217	
	Y627	V556	L487	T423	K357	H289	A218	
	V631	A557	M493	V424	H358	F292	N144	A72
	F632	F558			Y359		L145	E73
								D74

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 77.84Å 261.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.41 – 2.91 43.41 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.1 (43.41-2.91) 91.3 (43.41-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.300 0.239 , 0.299	Depositor DCC
R_{free} test set	3256 reflections (9.89%)	DCC
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.135 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10331	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: FMN, NAP, 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	0.42	0/5137	0.69	1/6978 (0.0%)
1	B	0.42	0/5120	0.68	1/6952 (0.0%)
All	All	0.42	0/10257	0.69	2/13930 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ASN	N-CA-C	-6.79	92.66	111.00
1	B	312	SER	N-CA-C	-5.11	97.21	111.00

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	5021	0	4876	362	0
1	B	5007	0	4880	463	0
2	A	53	0	31	2	0
2	B	53	0	31	4	0
3	A	31	0	19	3	0
3	B	31	0	19	2	0
4	A	40	0	19	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	40	0	19	1	0
5	A	33	0	0	3	0
5	B	22	0	0	5	0
All	All	10331	0	9894	822	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 41.

The worst 5 of 822 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:A:361:GLU:HG2	1:A:436:MET:HA	1.30	1.13
1:A:528:LEU:HD23	1:A:529:PRO:HD2	1.28	1.11
1:B:59:LYS:HD3	1:B:92:MET:HB2	1.22	1.10
1:A:67:SER:HB2	1:A:72:ALA:HB3	1.39	1.05
1:B:482:LEU:HA	1:B:485:ILE:HD12	1.42	1.01

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	639/682 (94%)	513 (80%)	105 (16%)	21 (3%)	4	17
1	B	637/682 (93%)	504 (79%)	106 (17%)	27 (4%)	3	11
All	All	1276/1364 (94%)	1017 (80%)	211 (16%)	48 (4%)	4	14

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ASP

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Mol	Chain	Res	Type
1	A	508	PRO
1	A	566	GLY
1	B	233	THR
1	B	241	PRO

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	548/592 (93%)	508 (93%)	40 (7%)	16	42
1	B	549/592 (93%)	511 (93%)	38 (7%)	18	45
All	All	1097/1184 (93%)	1019 (93%)	78 (7%)	17	44

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	662	LEU
1	B	81	LYS
1	B	590	ASP
1	A	667	SER
1	A	686	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	637	ASN
1	B	161	ASN
1	B	567	ASN
1	B	90	ASN
1	B	170	HIS

5.3.3 RNA ⓘ

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	FAD	A	750	-	51,58,58	1.81	9 (17%)	54,89,89	2.01	5 (9%)
3	FMN	A	751	-	31,33,33	1.66	5 (16%)	38,50,50	3.17	11 (28%)
4	NAP	A	753	-	36,43,52	1.10	2 (5%)	42,67,80	1.97	4 (9%)
2	FAD	B	750	-	51,58,58	1.99	10 (19%)	54,89,89	2.08	4 (7%)
3	FMN	B	751	-	31,33,33	1.79	6 (19%)	38,50,50	3.14	13 (34%)
4	NAP	B	753	-	36,43,52	1.06	1 (2%)	42,67,80	2.03	9 (21%)

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	FAD	A	750	-	-	0/28/50/50	0/6/6/6
3	FMN	A	751	-	-	0/16/18/18	0/3/3/3
4	NAP	A	753	-	-	0/23/59/67	0/4/4/5
2	FAD	B	750	-	-	0/28/50/50	0/6/6/6
3	FMN	B	751	-	-	0/16/18/18	0/3/3/3
4	NAP	B	753	-	-	0/23/59/67	0/4/4/5

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	FAD	C5A-C4A	-2.22	1.35	1.40
4	A	753	NAP	C5A-N7A	-2.18	1.32	1.39
2	A	750	FAD	C5A-C4A	-2.17	1.35	1.40
3	B	751	FMN	P-O2P	-2.15	1.46	1.54
3	A	751	FMN	P-O2P	-2.03	1.46	1.54

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	753	NAP	N3A-C2A-N1A	-8.90	121.11	128.86
4	B	753	NAP	N3A-C2A-N1A	-8.58	121.39	128.86
3	B	751	FMN	C4A-C4-N3	-5.80	115.23	123.48
2	A	750	FAD	C4X-C4-N3	-5.70	115.36	123.48
3	A	751	FMN	C4A-C4-N3	-5.64	115.45	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	FAD	2	0
3	A	751	FMN	3	0
4	A	753	NAP	5	0
2	B	750	FAD	4	0
3	B	751	FMN	2	0
4	B	753	NAP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	643/682 (94%)	0.20	18 (2%) 53 49	35, 62, 89, 109	0
1	B	641/682 (93%)	0.20	27 (4%) 37 32	42, 69, 91, 118	0
All	All	1284/1364 (94%)	0.20	45 (3%) 44 39	35, 66, 90, 118	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	658	LEU	4.1
1	B	325	PHE	3.8
1	A	325	PHE	3.5
1	B	335	LEU	3.5
1	B	292	PHE	3.5

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(\AA^2)	Q<0.9
4	NAP	B	753	40/48	0.91	0.20	-0.06	88,92,112,112	0
4	NAP	A	753	40/48	0.95	0.20	-0.09	52,59,79,82	0
2	FAD	B	750	53/53	0.95	0.20	-0.13	49,60,67,69	0
3	FMN	B	751	31/31	0.95	0.17	-0.15	49,60,66,66	0
2	FAD	A	750	53/53	0.97	0.18	-0.23	29,47,58,60	0
3	FMN	A	751	31/31	0.97	0.17	-0.36	39,52,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.