wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 06:15 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

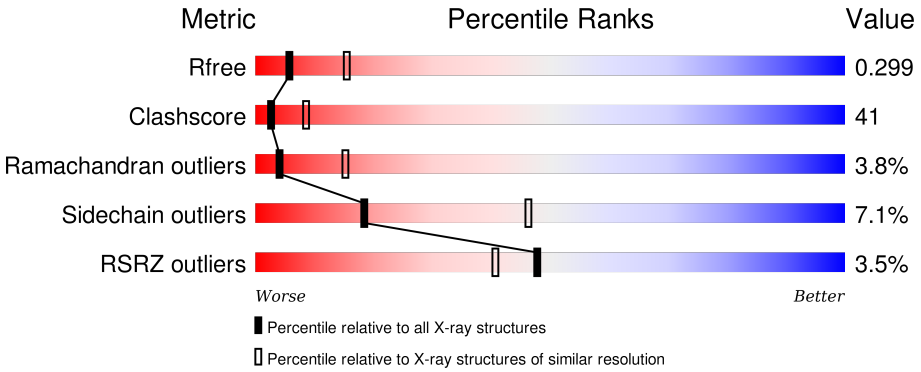
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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}	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (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 <=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	3% 40% 49% 6% 6%
1	B	682	4% 33% 55% 6% 6%

2 Entry composition

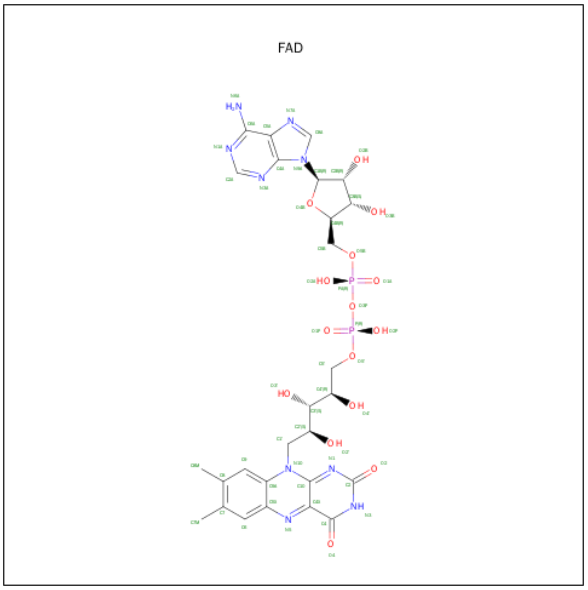
There are 5 unique types of molecules in this entry. The entry contains 10331 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

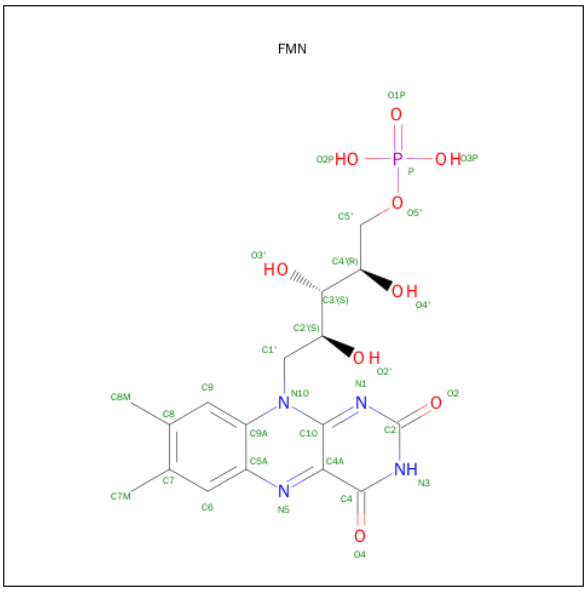
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	0	0
			5021	3202	827	977	15			
1	B	641	Total	C	N	O	S	0	0	0
			5007	3191	825	976	15			

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



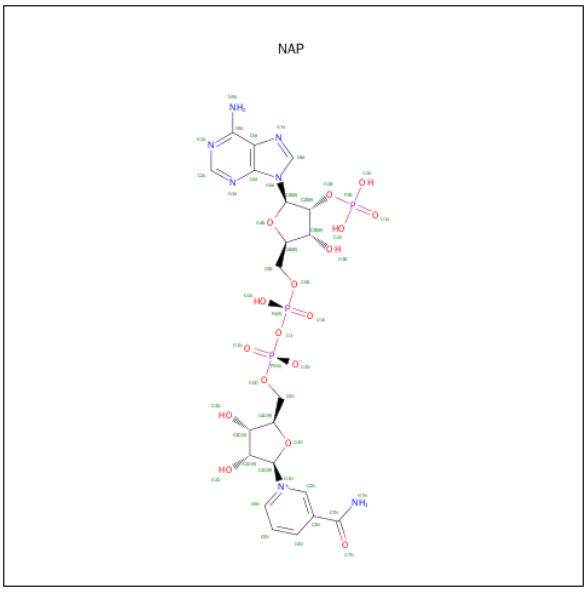
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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: $C_{21}H_{28}N_7O_{17}P_3$).



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

Continued on next page...

Continued from previous page...

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.

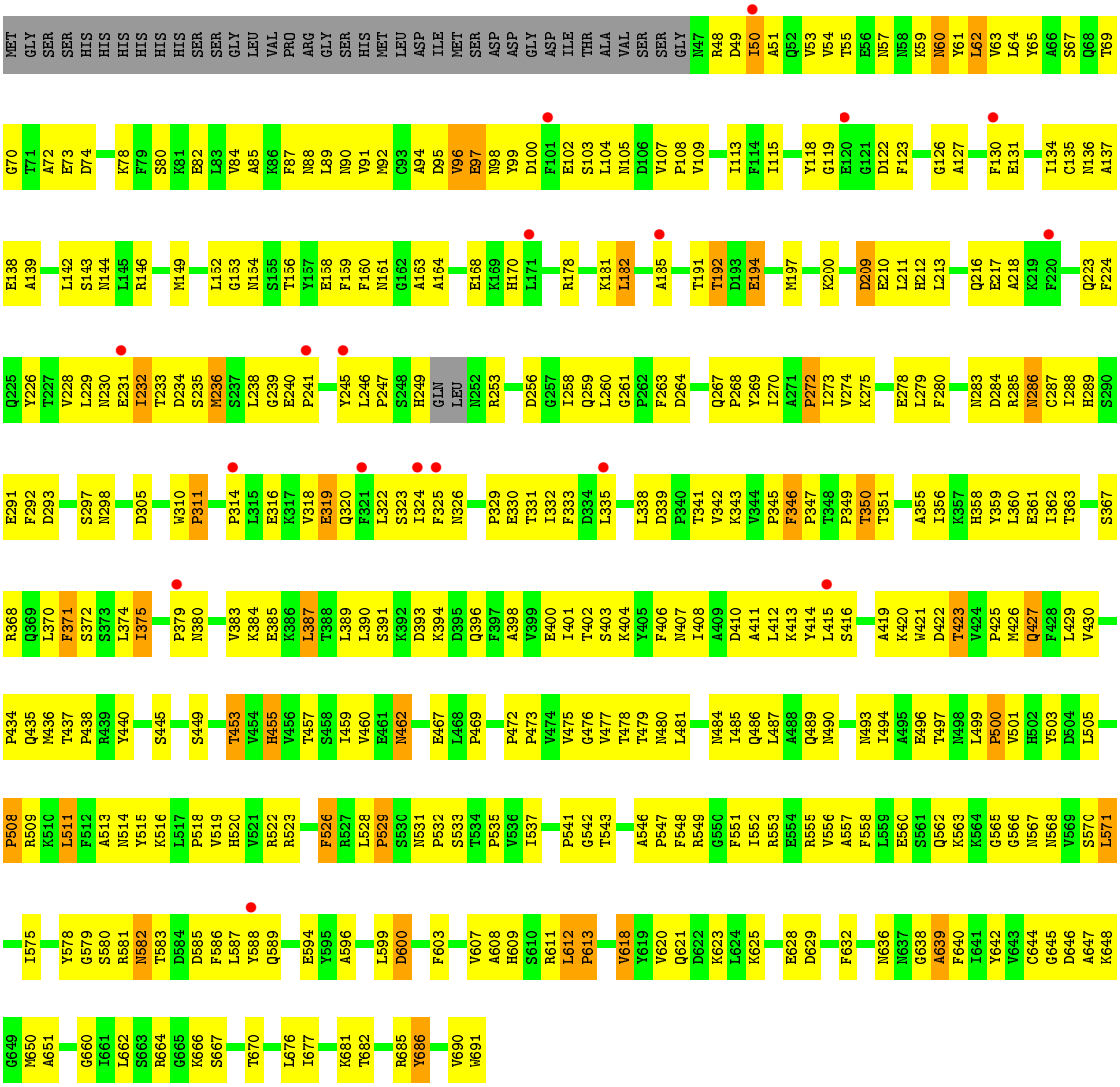
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total	O	0	0
			33	33		
5	B	22	Total	O	0	0
			22	22		

3 Residue-property plots (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.

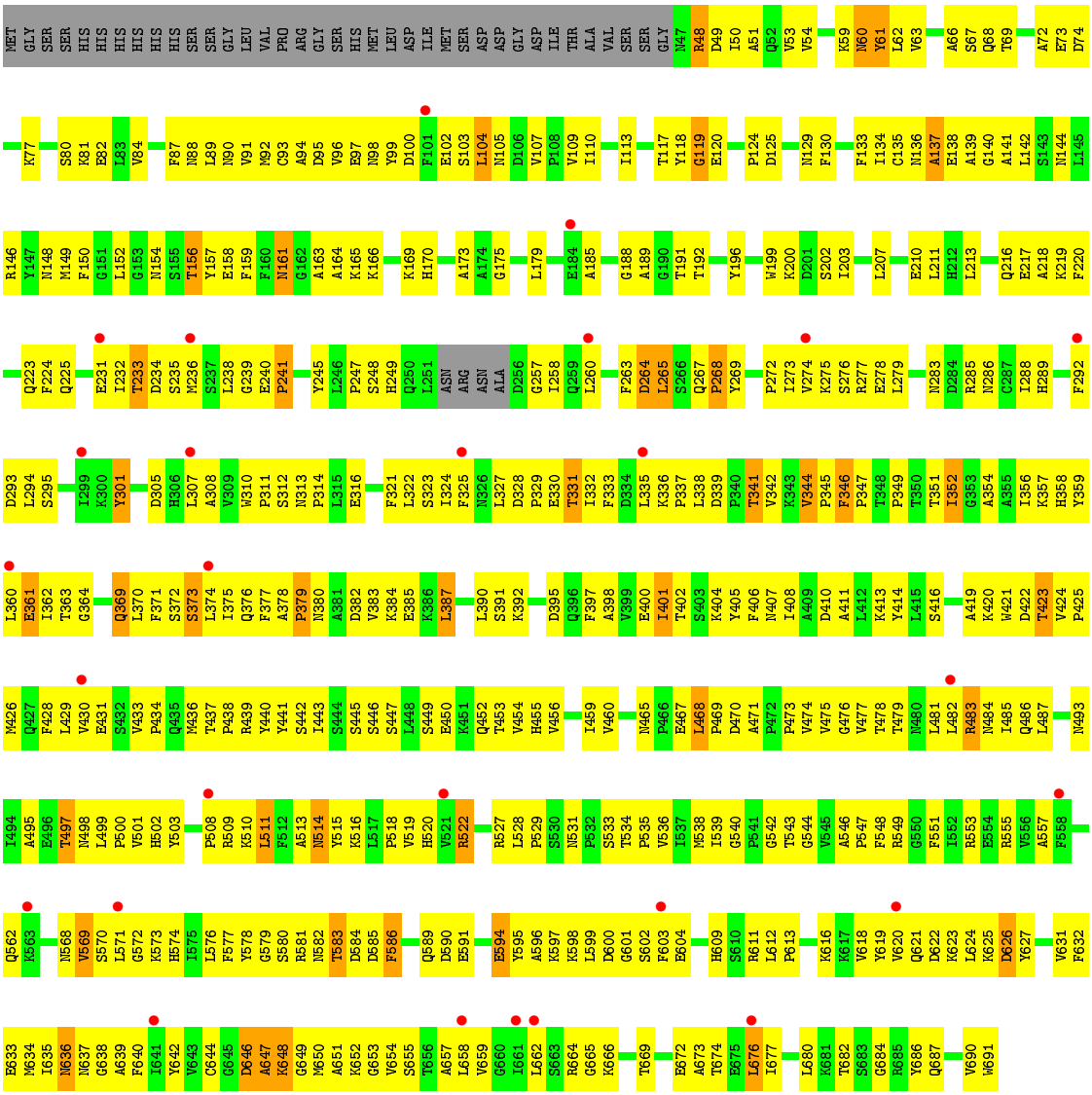
- Molecule 1: NADPH CYTOCHROME P450 REDUCTASE

Chain A:



- Molecule 1: NADPH CYTOCHROME P450 REDUCTASE

Chain B:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET LEU ASP ILE MET SER ASP ASP GLY ASP ILE THR ALA VAL SER SER GLY N47 R48 D49 I50 A51 Q52 V53 V54 K59 N60 Y61 L62 V63 A66 S67 Q68 T69 A72 E73 D74
K77 S80 K81 E82 L83 V84 F87 N88 L89 N90 V91 M92 C93 A94 D95 V96 E97 N98 Y99 D100 F101 E102 S103 L104 N105 D106 V107 P108 V109 I110 I113 T117 Y118 G119 E120 P124 D125 N129 F130 F133 I134 C135 N136 A137 E138 A139 G140 A141 L142 S143 N144 L145
R146 Y147 N148 M149 F150 G151 L152 G153 N154 S155 T156 Y157 E158 F159 F160 N161 G162 A163 A164 K165 K166 K169 H170 A173 A174 G175 L179 E184 A185 G188 A189 G190 T191 T192 Y196 W199 K200 D201 S202 I203 L207 E210 L211 H212 L213 Q216 E217 A218 K219 F220
Q223 F224 Q225 E231 I232 T233 D234 S235 M236 S237 L238 G239 E240 P241 Y245 L246 P247 S248 H249 Q250 L251 ASN ARG ASN ALA D256 G257 I258 Q259 L260 F263 D264 L265 S266 Q267 P268 Y269 P272 I273 V274 K275 S276 R277 E278 L279 N283 D284 R285 N286 C287 I288 H289 F292
D293 L294 S295 I299 K300 Y301 D305 H306 L307 A308 V309 W310 P311 S312 N313 P314 L315 E316 F321 L322 S323 I324 F325 N326 L327 D328 P329 E330 T331 I332 F333 D334 L335 K336 P337 L338 D339 P340 T341 V342 K343 V344 P345 F346 P347 T348 P349 T350 T351 I352 G353 A354 A355 I356 K357 H358 Y359
L360 E361 I362 T363 G364 Q369 L370 F371 S372 S373 L374 I375 Q376 F377 A378 P379 N380 A381 D382 V383 K384 E385 K386 L387 L390 S391 K392 D395 Q396 F397 A398 V399 E400 I401 T402 S403 K404 Y405 F406 N407 I408 A409 D410 A411 L412 K413 Y414 L415 S416 A419 K420 W421 D422 T423 V424 P425
N426 Q427 F428 L429 V430 E431 S432 V433 P434 Q435 M436 T437 P438 R439 Y440 Y441 S442 I443 S444 S445 S446 S447 L448 S449 E450 K451 Q452 T453 V454 H455 V456 I459 V460 N465 P466 E467 L468 P469 D470 A471 P472 P473 V474 V475 G476 V477 T478 T479 N480 L481 L482 R483 N484 I485 Q486 L487 N493
I494 A495 E496 T497 N498 L499 P500 V501 H502 Y503 P508 R509 K510 L511 F512 A513 N514 Y515 K516 L517 P518 V519 H520 V521 R522 R527 L528 P529 S530 N531 P532 S533 T534 P535 V536 I537 M538 I539 G540 P541 G542 T543 G544 V545 A546 P547 F548 R549 G550 F551 I552 R553 E554 N555 V556 A557 P558
Q562 K563 N568 V569 S570 L571 G572 K573 H574 I575 L576 F577 Y578 G579 S580 R581 N582 T583 D584 D585 F586 Q589 D590 E591 E594 Y595 A596 K597 K598 L599 D600 G601 S602 F603 E604 H609 S610 R611 L612 P613 K616 K617 V618 Y619 V620 Q621 D622 K623 L624 K625 D626 Y627 V631 F632
E633 M634 I635 N636 N637 G638 A639 F640 I641 Y642 V643 G644 G645 D646 A647 K648 G649 M650 A651 K652 G653 V654 S655 T656 A657 L658 V659 G660 I661 L662 S663 R664 G665 K666 T669 E672 A673 T674 E675 L676 I677 L680 K681 T682 S683 G684 R685 Y686 Q687 V690 W691

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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
Estimated twinning fraction	0.135 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 33796 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

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

Continued on next page...

Continued from previous page...

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%)	5 19
1	B	637/682 (93%)	504 (79%)	106 (17%)	27 (4%)	3 12
All	All	1276/1364 (94%)	1017 (80%)	211 (16%)	48 (4%)	4 15

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ASP

Continued on next page...

Continued from previous page...

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 (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	548/592 (93%)	508 (93%)	40 (7%)	17 45
1	B	549/592 (93%)	511 (93%)	38 (7%)	19 48
All	All	1097/1184 (93%)	1019 (93%)	78 (7%)	18 46

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 (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	FAD	A	750	-	52,58,58	1.67	8 (15%)	52,89,89	2.15	5 (9%)
3	FMN	A	751	-	32,33,33	1.82	7 (21%)	34,50,50	3.48	9 (26%)
4	NAP	A	753	-	37,43,52	1.25	4 (10%)	45,67,80	2.25	6 (13%)
2	FAD	B	750	-	52,58,58	1.84	8 (15%)	52,89,89	2.22	6 (11%)
3	FMN	B	751	-	32,33,33	1.92	8 (25%)	34,50,50	3.40	10 (29%)
4	NAP	B	753	-	37,43,52	1.21	4 (10%)	45,67,80	2.19	9 (20%)

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	-	-	0/30/50/50	0/6/6/6
3	FMN	A	751	-	-	0/18/18/18	0/3/3/3
4	NAP	A	753	-	-	0/23/59/67	0/4/4/5
2	FAD	B	750	-	-	0/30/50/50	0/6/6/6
3	FMN	B	751	-	-	0/18/18/18	0/3/3/3
4	NAP	B	753	-	-	0/23/59/67	0/4/4/5

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	753	NAP	C2B-C1B	-3.14	1.44	1.53
4	B	753	NAP	C2B-C1B	-3.13	1.44	1.53
3	B	751	FMN	P-O2P	-2.55	1.46	1.54
3	A	751	FMN	P-O2P	-2.40	1.46	1.54
3	B	751	FMN	P-O3P	-2.32	1.46	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	753	NAP	N3A-C2A-N1A	-9.89	121.11	128.87
4	B	753	NAP	N3A-C2A-N1A	-9.53	121.39	128.87
4	A	753	NAP	C1B-N9A-C4A	-7.91	117.97	126.81
3	A	751	FMN	N3-C2-N1	-7.50	115.06	127.69
4	B	753	NAP	C1B-N9A-C4A	-7.18	118.79	126.81

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

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, 95^{th} 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%) 56 50	35, 62, 89, 109	0
1	B	641/682 (93%)	0.20	27 (4%) 40 34	42, 69, 91, 118	0
All	All	1284/1364 (94%)	0.20	45 (3%) 48 41	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

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, 95^{th} 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
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.