



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 02:33 pm GMT

PDB ID : 1QRD
Title : QUINONE REDUCTASE/FAD/CIBACRON BLUE/DUROQUINONE COMPLEX
Authors : Li, R.; Bianchet, M.A.; Talalay, P.; Amzel, L.M.
Deposited on : 1995-07-28
Resolution : 2.40 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

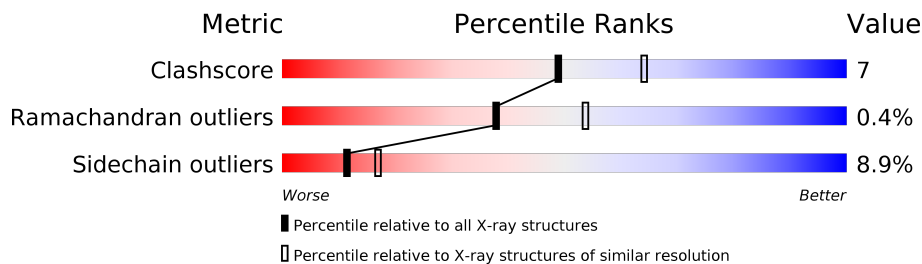
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	273	
1	B	273	

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
2	FAD	A	274	X	-	-	-
2	FAD	B	274	X	-	-	-
4	DQN	A	276	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DQN	B	276	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4642 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 QUINONE-REDUCTASE.

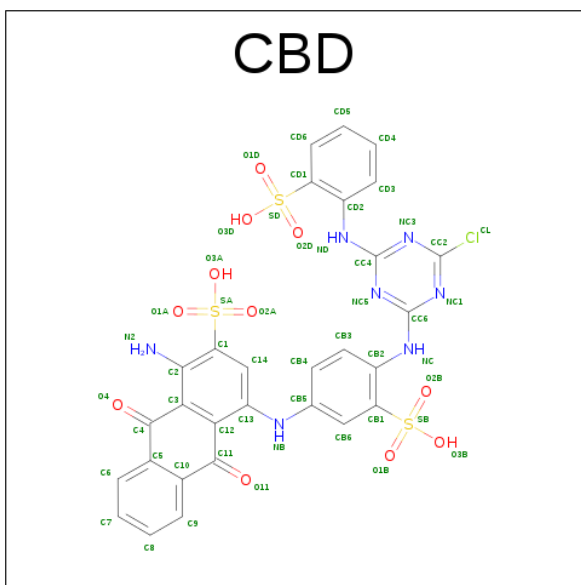
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2181	1416	364	395	6			
1	B	273	Total	C	N	O	S	0	0	0
			2181	1416	364	395	6			

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



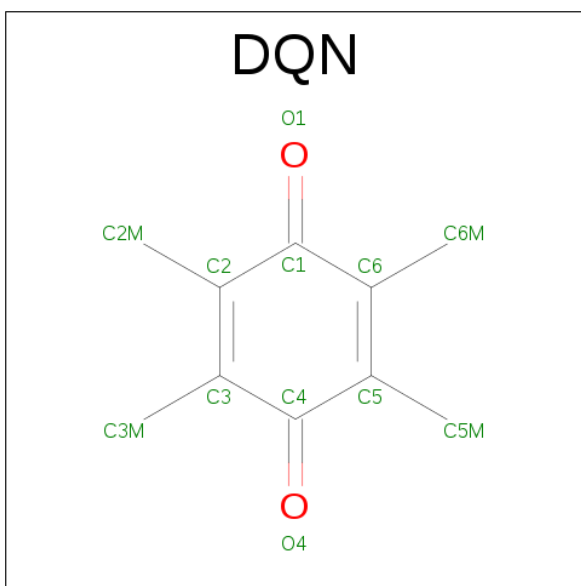
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is CIBACRON BLUE (three-letter code: CBD) (formula: $C_{29}H_{20}ClN_7O_{11}S_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 51	C 29	Cl 1	N 7	O 11	S 3	0	0
3	B	1	Total 51	C 29	Cl 1	N 7	O 11	S 3	0	0

- Molecule 4 is DUROQUINONE (three-letter code: DQN) (formula: $C_{10}H_{12}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 10 2	0	0
4	B	1	Total C O 12 10 2	0	0

- Molecule 5 is water.

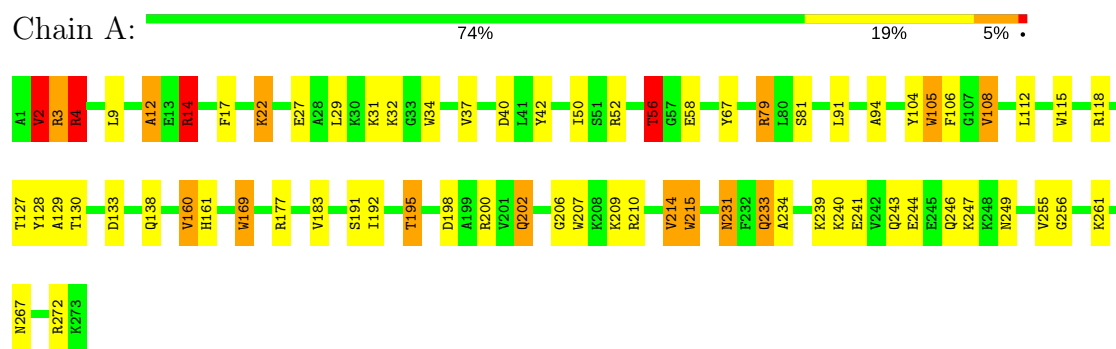
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total 25	O 25	0	0
5	B	23	Total 23	O 23	0	0

3 Residue-property plots [i](#)

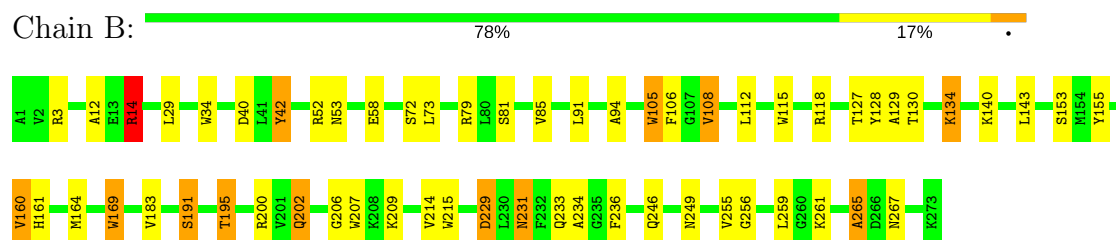
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: QUINONE-REDUCTASE



• Molecule 1: QUINONE-REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.00Å 107.00Å 88.40Å 90.00° 92.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	88.8 (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4642	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

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: DQN, FAD, CBD

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	0.99	1/2238 (0.0%)	1.75	54/3027 (1.8%)
1	B	0.96	0/2238	1.74	43/3027 (1.4%)
All	All	0.98	1/4476 (0.0%)	1.75	97/6054 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	VAL	CA-CB	6.98	1.69	1.54

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	NE-CZ-NH1	20.24	130.42	120.30
1	B	118	ARG	NE-CZ-NH2	-19.74	110.43	120.30
1	A	118	ARG	NE-CZ-NH1	12.89	126.74	120.30
1	A	177	ARG	NE-CZ-NH2	-11.69	114.46	120.30
1	A	52	ARG	NE-CZ-NH1	10.08	125.34	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	42	TYR	Sidechain

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	2181	0	2182	32	0
1	B	2181	0	2182	23	0
2	A	53	0	30	1	0
2	B	53	0	29	1	0
3	A	51	0	20	4	0
3	B	51	0	20	4	0
4	A	12	0	12	11	0
4	B	12	0	12	11	0
5	A	25	0	0	0	0
5	B	23	0	0	0	0
All	All	4642	0	4487	62	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 7.

The worst 5 of 62 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:127:THR:HG22	1:B:129:ALA:H	1.50	0.75
1:B:127:THR:HB	1:B:130:THR:OG1	1.90	0.71
3:A:275:CBD:CL	4:A:276:DQN:H5M1	2.28	0.70
1:A:231:ASN:ND2	1:A:234:ALA:H	1.91	0.69
1:B:231:ASN:ND2	1:B:234:ALA:H	1.91	0.68

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	271/273 (99%)	258 (95%)	12 (4%)	1 (0%)	38	54
1	B	271/273 (99%)	256 (94%)	14 (5%)	1 (0%)	38	54
All	All	542/546 (99%)	514 (95%)	26 (5%)	2 (0%)	38	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	ALA
1	A	272	ARG

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	231/231 (100%)	209 (90%)	22 (10%)	10	14
1	B	231/231 (100%)	212 (92%)	19 (8%)	13	20
All	All	462/462 (100%)	421 (91%)	41 (9%)	11	17

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	LYS
1	B	3	ARG
1	B	214	VAL
1	A	241	GLU

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Mol	Chain	Res	Type
1	A	244	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	268	GLN
1	B	231	ASN
1	A	249	ASN
1	B	202	GLN

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	274	-	51,58,58	2.46	9 (17%)	54,89,89	3.01	18 (33%)
3	CBD	A	275	-	56,56,56	2.04	13 (23%)	78,87,87	3.24	31 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DQN	A	276	-	12,12,12	0.86	0	18,18,18	0.94	0
2	FAD	B	274	-	51,58,58	2.30	9 (17%)	54,89,89	2.99	20 (37%)
3	CBD	B	275	-	56,56,56	2.25	12 (21%)	78,87,87	3.47	29 (37%)
4	DQN	B	276	-	12,12,12	1.03	0	18,18,18	0.96	1 (5%)

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	274	-	3/3/9/9	0/28/50/50	0/6/6/6
3	CBD	A	275	-	-	0/30/46/46	0/6/6/6
4	DQN	A	276	-	-	0/0/24/24	0/1/1/1
2	FAD	B	274	-	3/3/9/9	0/28/50/50	0/6/6/6
3	CBD	B	275	-	-	0/30/46/46	0/6/6/6
4	DQN	B	276	-	-	0/0/24/24	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	274	FAD	C1'-N10	-12.74	1.35	1.48
2	B	274	FAD	C1'-N10	-11.97	1.36	1.48
2	B	274	FAD	C6-C5X	-2.83	1.37	1.41
3	A	275	CBD	C1-SA	-2.49	1.75	1.78
3	B	275	CBD	C10-C11	-2.37	1.43	1.48

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	275	CBD	NC3-CC2-NC1	-11.61	113.82	129.76
3	A	275	CBD	NC3-CC2-NC1	-9.46	116.77	129.76
2	A	274	FAD	N3A-C2A-N1A	-9.41	120.67	128.86
2	B	274	FAD	N3A-C2A-N1A	-8.97	121.05	128.86
3	A	275	CBD	CB1-CB2-NC	-8.31	114.11	121.63

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	274	FAD	C4'
2	A	274	FAD	C2'

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Mol	Chain	Res	Type	Atom
2	A	274	FAD	C3'
2	B	274	FAD	C4'
2	B	274	FAD	C2'

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	274	FAD	1	0
3	A	275	CBD	4	0
4	A	276	DQN	11	0
2	B	274	FAD	1	0
3	B	275	CBD	4	0
4	B	276	DQN	11	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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.