W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:26 PM GMT

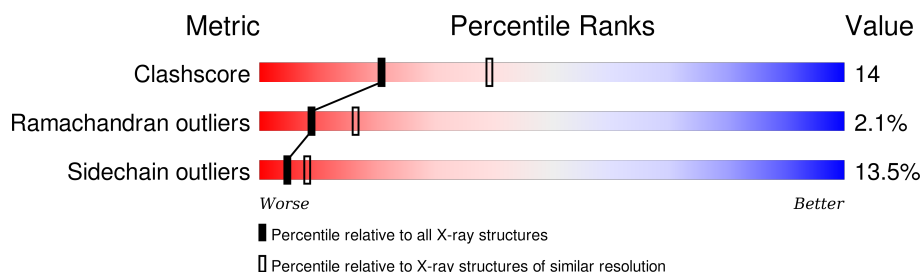|		
PDB ID	:	1FLG
Title	:	CRYSTAL STRUCTURE OF THE QUINOPROTEIN ETHANOL DEHYDROGENASE FROM PSEUDOMONAS AERUGINOSA
Authors	:	Keitel, T.; Diehl, A.; Knaute, T.; Stezowski, J.J.; Hohne, W.; Gorisch, H.
Deposited on	:	2000-08-14
Resolution	:	2.60 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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
Clashscore		14
Ramachandran outliers		2.1%
Sidechain outliers		13.5%

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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	48% 34% 15% •
1	B	582	50% 34% 13% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9232 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 PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total 4537	C 2891	N 783	O 852	S 11	0	0	0
1	B	582	Total 4537	C 2891	N 783	O 852	S 11	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: $C_{14}H_6N_2O_8$).
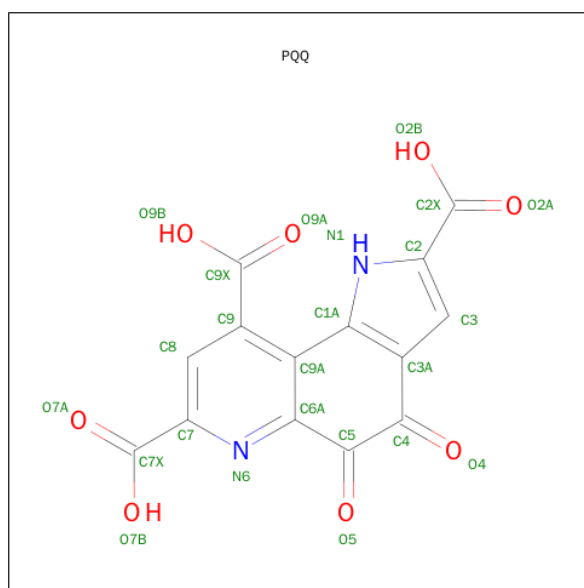
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 24	C 14	N 2	O 8	0	0
3	B	1	Total 24	C 14	N 2	O 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total 73	O 73	0	0
4	B	33	Total 33	O 33	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 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE)
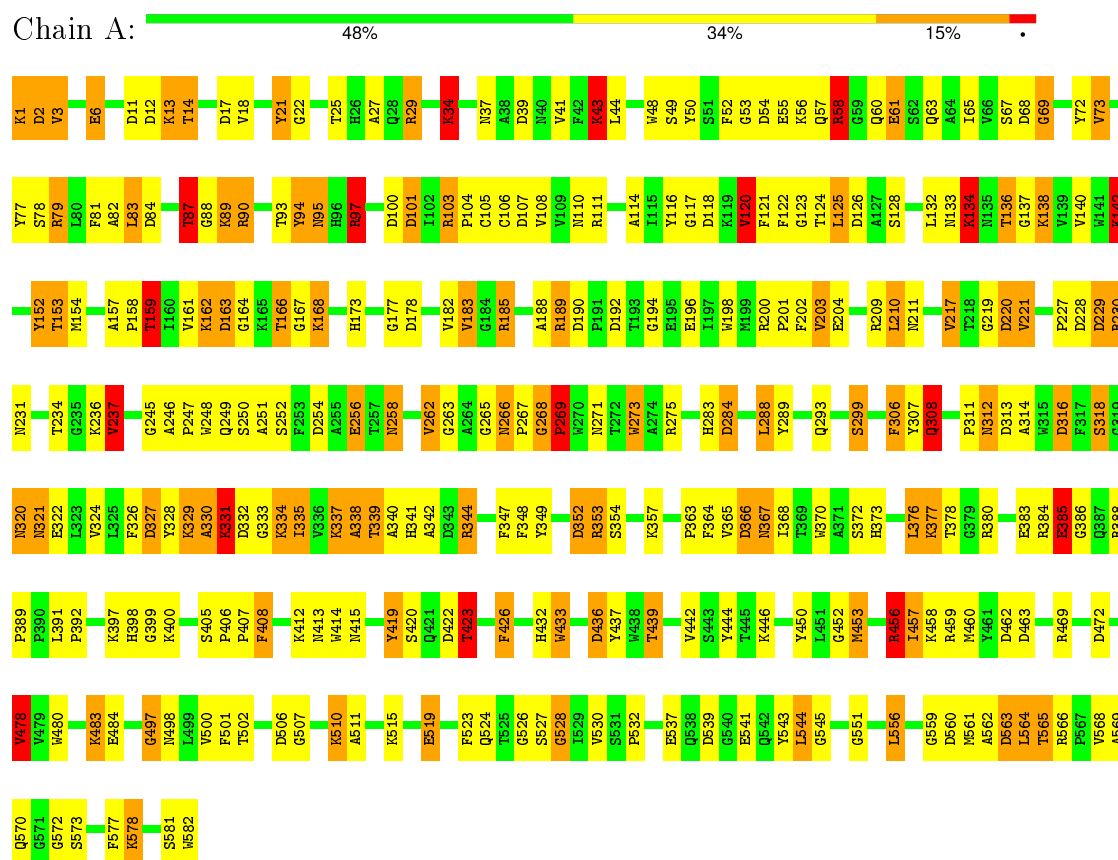
- Molecule 1: PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE)
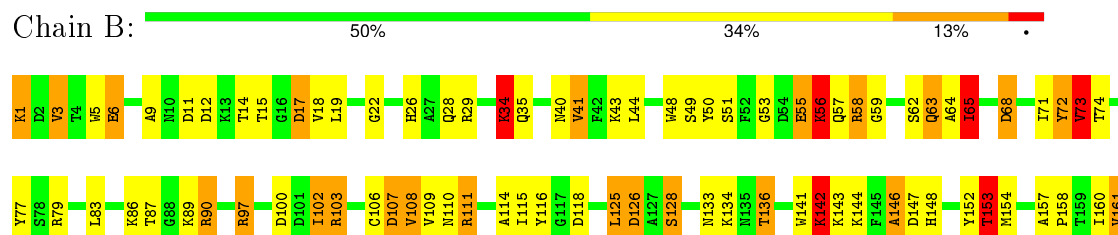
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	159.40Å　159.40Å　130.95Å 90.00°　90.00°　120.00°	Depositor
Resolution (Å)	12.50　−　2.60	Depositor
% Data completeness (in resolution range)	(Not available) (12.50-2.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.192　,　0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9232	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: PQQ, CA

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	1.05	8/4679 (0.2%)	2.69	315/6366 (4.9%)
1	B	0.82	0/4679	2.19	175/6366 (2.7%)
All	All	0.95	8/9358 (0.1%)	2.45	490/12732 (3.8%)

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	A	0	36
1	B	0	21
All	All	0	57

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	ASN	N-CA	11.72	1.69	1.46
1	A	386	GLY	N-CA	7.77	1.57	1.46
1	A	299	SER	CB-OG	-6.44	1.33	1.42
1	A	312	ASN	N-CA	6.12	1.58	1.46
1	A	88	GLY	N-CA	5.66	1.54	1.46

The worst 5 of 490 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH2	-36.92	101.84	120.30
1	B	29	ARG	NE-CZ-NH2	29.67	135.14	120.30
1	A	29	ARG	CD-NE-CZ	27.13	161.58	123.60
1	A	348	PHE	CB-CG-CD1	24.74	138.12	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	469	ARG	NE-CZ-NH1	-23.27	108.67	120.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASP	Mainchain
1	A	13	LYS	Mainchain
1	A	14	THR	Mainchain
1	A	58	ARG	Mainchain
1	A	6	GLU	Mainchain

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	4537	0	4311	123	6
1	B	4537	0	4311	143	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	24	0	3	1	0
3	B	24	0	3	0	0
4	A	73	0	0	4	0
4	B	33	0	0	1	0
All	All	9232	0	8628	255	6

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 14.

The worst 5 of 255 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:367:ASN:CA	1:A:367:ASN:N	1.69	1.51
1:A:366:ASP:O	1:A:367:ASN:HA	1.37	1.21
1:A:293:GLN:HE22	1:A:339:THR:HG21	0.95	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASP:O	1:A:367:ASN:CA	2.02	1.02
1:A:293:GLN:NE2	1:A:339:THR:HG21	1.77	0.98

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:HIS:CD2	1:A:456:ARG:NH2[2_665]	1.57	0.63
1:A:372:SER:OG	1:A:456:ARG:NH2[2_665]	1.92	0.28
1:A:372:SER:OG	1:A:456:ARG:NH1[2_665]	2.04	0.16
1:A:373:HIS:CG	1:A:456:ARG:NH2[2_665]	2.08	0.12
1:A:373:HIS:CD2	1:A:456:ARG:CZ[2_665]	2.13	0.07

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	580/582 (100%)	530 (91%)	45 (8%)	5 (1%)	21	42
1	B	580/582 (100%)	514 (89%)	47 (8%)	19 (3%)	5	7
All	All	1160/1164 (100%)	1044 (90%)	92 (8%)	24 (2%)	9	16

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ALA
1	A	385	GLU
1	B	217	VAL
1	B	289	TYR
1	B	330	ALA

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	469/469 (100%)	409 (87%)	60 (13%)	5	10
1	B	469/469 (100%)	402 (86%)	67 (14%)	4	7
All	All	938/938 (100%)	811 (86%)	127 (14%)	5	8

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	THR
1	B	86	LYS
1	B	493	LEU
1	A	581	SER
1	B	51	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	524	GLN
1	B	421	GLN
1	A	432	HIS
1	A	173	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)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	#$|Z| > 2$
3	PQQ	A	701	2	16,26,26	4.22	7 (43%)	17,40,40	6.29	13 (76%)
3	PQQ	B	702	2	16,26,26	3.61	6 (37%)	17,40,40	5.17	13 (76%)

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
3	PQQ	A	701	2	-	0/0/28/28	0/3/3/3
3	PQQ	B	702	2	-	0/0/28/28	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PQQ	C6A-C5	-8.75	1.39	1.49
3	B	702	PQQ	C6A-C5	-6.18	1.42	1.49
3	B	702	PQQ	C5-C4	-4.14	1.40	1.53
3	A	701	PQQ	C3A-C4	-3.98	1.40	1.48
3	A	701	PQQ	C5-C4	-3.82	1.41	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PQQ	C8-C7-N6	-14.01	106.05	122.39
3	B	702	PQQ	C8-C7-N6	-11.66	108.79	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	PQQ	O5-C5-C4	-9.01	105.53	119.29
3	A	701	PQQ	C9A-C6A-C5	-7.70	113.75	120.85
3	A	701	PQQ	O4-C4-C5	-7.41	107.97	119.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	PQQ	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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.