wwPDB X-ray Structure Validation Summary Report (i)

Jan 28, 2018 – 11:48 AM EST

PDB ID	:	1H7W
Title	:	Dihydropyrimidine dehydrogenase (DPD) from pig
Authors	:	Dobritzsch, D.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on	:	2001-01-19
Resolution	:	1.90 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:

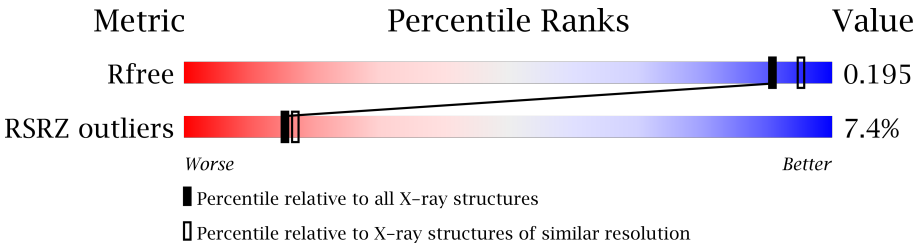
MolProbity	:	FAILED
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

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 1.90 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	5047 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36125 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.

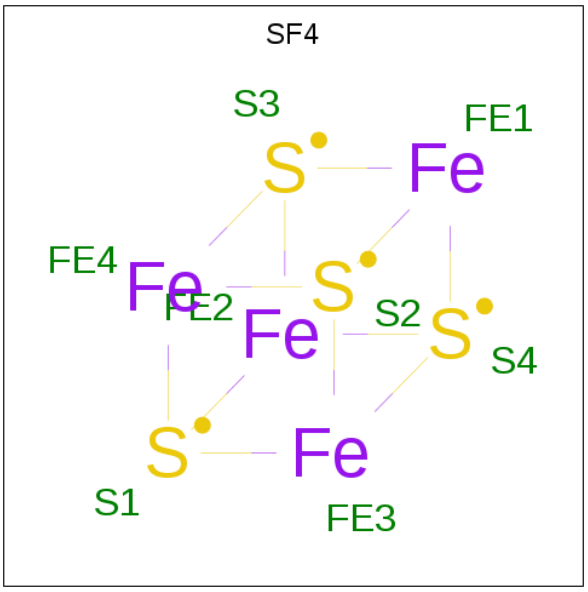
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	66	0	0
			7750	4913	1314	1467	56			
1	B	1017	Total	C	N	O	S	70	0	0
			7757	4918	1315	1468	56			
1	C	1016	Total	C	N	O	S	28	0	0
			7750	4913	1314	1467	56			
1	D	1018	Total	C	N	O	S	43	0	0
			7765	4924	1316	1469	56			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

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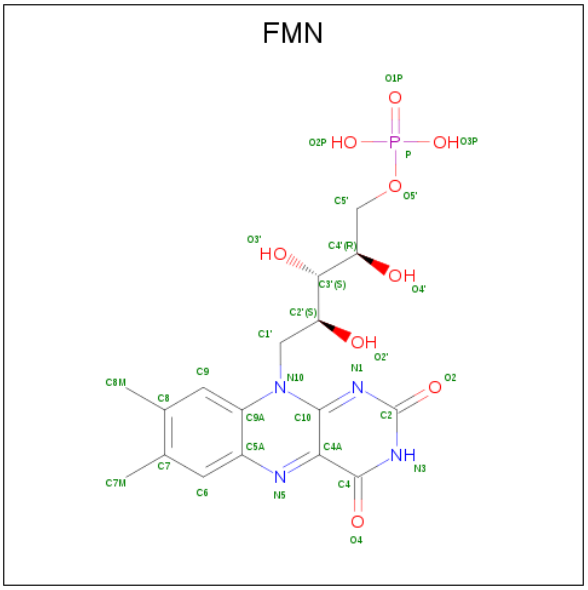
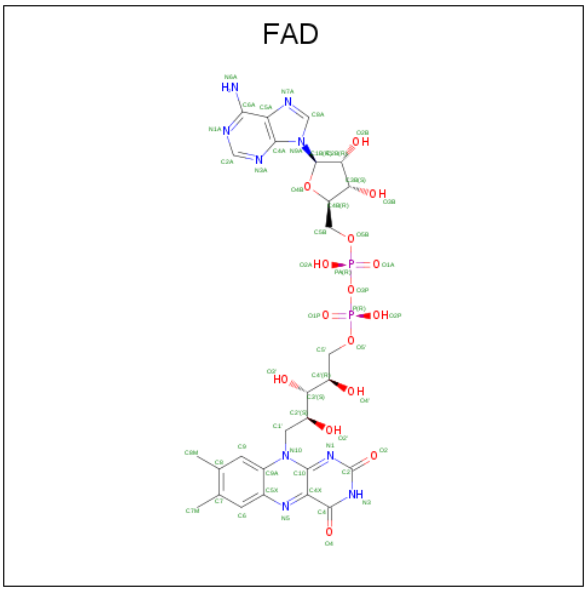
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

- 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 31 17 4 9 1	0	0
3	B	1	Total C N O P 31 17 4 9 1	0	0
3	C	1	Total C N O P 31 17 4 9 1	0	0
3	D	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1148	Total	O	0	0
			1148	1148		
5	B	1125	Total	O	0	0
			1125	1125		
5	C	1176	Total	O	0	0
			1176	1176		
5	D	1190	Total	O	0	0
			1190	1190		

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3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.95Å 159.29Å 163.57Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	19.97 – 1.90 24.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.97-1.90) 99.0 (24.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	6.83 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.174 , 0.196 0.173 , 0.195	Depositor DCC
R_{free} test set	6435 reflections (2.03%)	DCC
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	36125	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no carbohydrates in this entry.

4.6 Ligand geometry

24 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	SF4	A	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	A	1030	-	31,33,33	2.84	11 (35%)	38,50,50	3.18	13 (34%)
4	FAD	A	1031	-	51,58,58	2.19	20 (39%)	54,89,89	1.76	9 (16%)
2	SF4	B	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	B	1030	-	31,33,33	2.75	11 (35%)	38,50,50	3.17	13 (34%)
4	FAD	B	1031	-	51,58,58	2.26	19 (37%)	54,89,89	1.75	9 (16%)
2	SF4	C	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	C	1030	-	31,33,33	2.90	11 (35%)	38,50,50	3.17	13 (34%)
4	FAD	C	1031	-	51,58,58	2.23	22 (43%)	54,89,89	1.76	9 (16%)
2	SF4	D	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	D	1030	-	31,33,33	2.83	11 (35%)	38,50,50	3.18	13 (34%)
4	FAD	D	1031	-	51,58,58	2.19	20 (39%)	54,89,89	1.78	9 (16%)

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	SF4	A	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	A	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	A	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	A	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	A	1030	-	-	0/16/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	1031	-	-	0/28/50/50	0/6/6/6
2	SF4	B	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	B	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	B	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	B	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	B	1030	-	-	0/16/18/18	0/3/3/3
4	FAD	B	1031	-	-	0/28/50/50	0/6/6/6
2	SF4	C	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	C	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	C	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	C	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	C	1030	-	-	0/16/18/18	0/3/3/3
4	FAD	C	1031	-	-	0/28/50/50	0/6/6/6
2	SF4	D	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	D	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	D	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	D	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	D	1030	-	-	0/16/18/18	0/3/3/3
4	FAD	D	1031	-	-	0/28/50/50	0/6/6/6

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1030	FMN	C1'-N10	-9.39	1.38	1.48
3	A	1030	FMN	C1'-N10	-9.32	1.38	1.48
3	D	1030	FMN	C1'-N10	-9.24	1.38	1.48
3	B	1030	FMN	C1'-N10	-8.89	1.39	1.48
4	D	1031	FAD	PA-O2A	-3.89	1.35	1.55

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1030	FMN	C4A-C4-N3	-7.79	112.40	123.48
3	A	1030	FMN	C4A-C4-N3	-7.76	112.43	123.48
3	B	1030	FMN	C4A-C4-N3	-7.69	112.54	123.48
3	C	1030	FMN	C4A-C4-N3	-7.67	112.57	123.48
4	D	1031	FAD	C4X-C4-N3	-4.50	117.08	123.48

There are no chirality outliers.

There are no torsion outliers.

5 of 32 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1029	SF4	FE1-FE2-S3-S4
2	B	1027	SF4	FE3-FE4-S1-S2
2	C	1029	SF4	FE1-FE2-S3-S4
2	B	1029	SF4	FE1-FE2-S3-S4
2	A	1029	SF4	FE1-FE2-S3-S4

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	1007/1025 (98%)	0.21	68 (6%)	18	20	7, 14, 36, 56	0
1	B	1007/1025 (98%)	0.23	77 (7%)	15	16	6, 14, 36, 55	0
1	C	1012/1025 (98%)	0.22	73 (7%)	16	18	6, 14, 38, 54	0
1	D	1012/1025 (98%)	0.24	82 (8%)	13	14	6, 14, 37, 55	0
All	All	4038/4100 (98%)	0.22	300 (7%)	15	17	6, 14, 37, 56	0

The worst 5 of 300 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	18.1
1	A	1017	LEU	16.1
1	D	2	ALA	16.0
1	C	1017	LEU	14.9
1	A	2	ALA	14.4

5.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates

There are no carbohydrates in this entry.

5.4 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
2	SF4	A	1027	8/8	0.97	0.10	0.63	8,9,11,12	0
2	SF4	B	1026	8/8	0.97	0.10	0.51	10,10,12,12	0
2	SF4	C	1027	8/8	0.97	0.10	0.42	8,9,11,11	0
3	FMN	A	1030	31/31	0.96	0.09	0.11	8,10,13,13	0
4	FAD	B	1031	53/53	0.97	0.10	0.10	9,12,14,15	0
2	SF4	A	1028	8/8	0.97	0.09	0.00	9,11,11,13	0
4	FAD	A	1031	53/53	0.96	0.10	-0.04	8,11,13,14	0
2	SF4	B	1029	8/8	0.97	0.09	-0.10	10,11,13,13	0
2	SF4	D	1028	8/8	0.97	0.09	-0.11	9,10,12,12	0
2	SF4	C	1026	8/8	0.97	0.09	-0.13	10,10,12,12	0
2	SF4	A	1026	8/8	0.97	0.09	-0.17	10,10,12,12	0
3	FMN	B	1030	31/31	0.97	0.09	-0.18	7,10,12,15	0
2	SF4	C	1029	8/8	0.97	0.09	-0.19	9,10,12,12	0
3	FMN	D	1030	31/31	0.97	0.08	-0.20	7,10,12,13	0
2	SF4	B	1028	8/8	0.97	0.09	-0.23	10,11,12,13	0
2	SF4	D	1027	8/8	0.97	0.09	-0.28	7,8,10,11	0
2	SF4	D	1029	8/8	0.97	0.09	-0.38	10,11,12,13	0
4	FAD	D	1031	53/53	0.97	0.09	-0.42	8,11,13,14	0
3	FMN	C	1030	31/31	0.97	0.09	-0.44	8,9,12,15	0
2	SF4	D	1026	8/8	0.97	0.09	-0.49	9,10,11,12	0
2	SF4	A	1029	8/8	0.97	0.09	-0.55	10,11,13,13	0
2	SF4	B	1027	8/8	0.97	0.09	-0.61	8,9,11,11	0
4	FAD	C	1031	53/53	0.97	0.08	-0.64	7,11,14,15	0
2	SF4	C	1028	8/8	0.97	0.09	-0.82	8,9,10,12	0

5.5 Other polymers (i)

There are no such residues in this entry.