wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 06:26 PM GMT

PDB ID	:	1GTH
Title	:	DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG, TERNARY COMPLEX WITH NADPH AND 5-IODOURACIL
Authors	:	Dobritzsch, D.; Ricagno, S.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on	:	2002-01-15
Resolution	:	2.25 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:

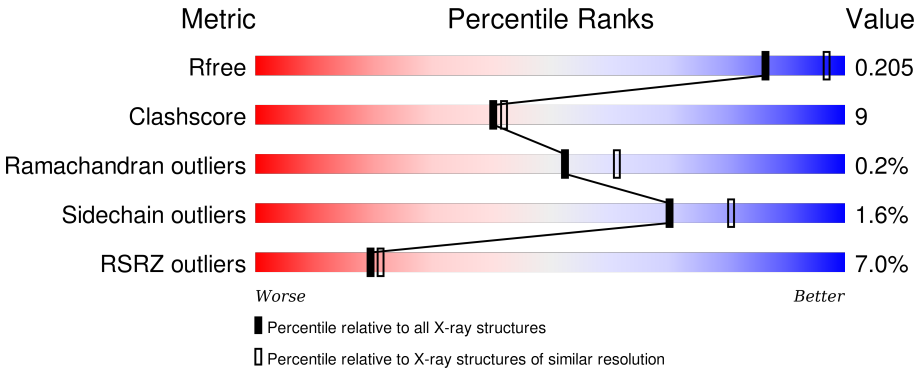
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	1025	5% 84% 15%
1	B	1025	5% 83% 15%
1	C	1025	7% 83% 16%
1	D	1025	10% 81% 17%

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	SF4	B	1027	-	-	X	-
2	SF4	C	1027	-	-	X	-
2	SF4	D	1027	-	-	X	-
6	IDH	B	1034	-	-	X	X
7	IUR	C	1034	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 34762 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.

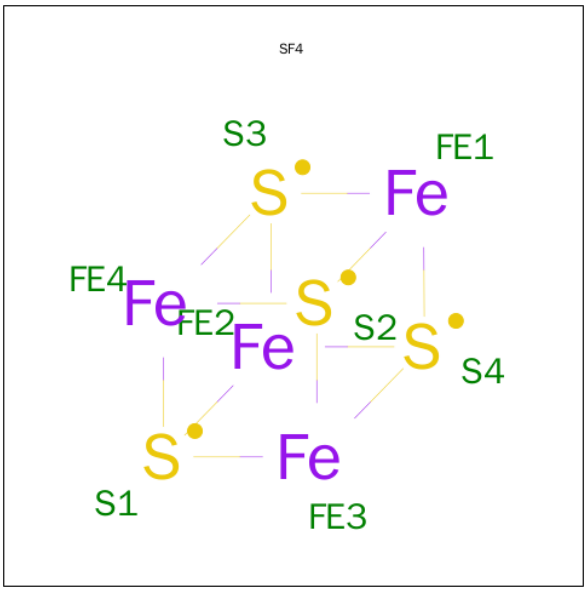
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1019	Total	C	N	O	S	0	0	0
			7770	4927	1317	1470	56			
1	B	1012	Total	C	N	O	S	0	0	0
			7719	4892	1309	1462	56			
1	C	1015	Total	C	N	O	S	0	0	0
			7740	4905	1313	1466	56			
1	D	1019	Total	C	N	O	S	0	0	0
			7770	4927	1317	1470	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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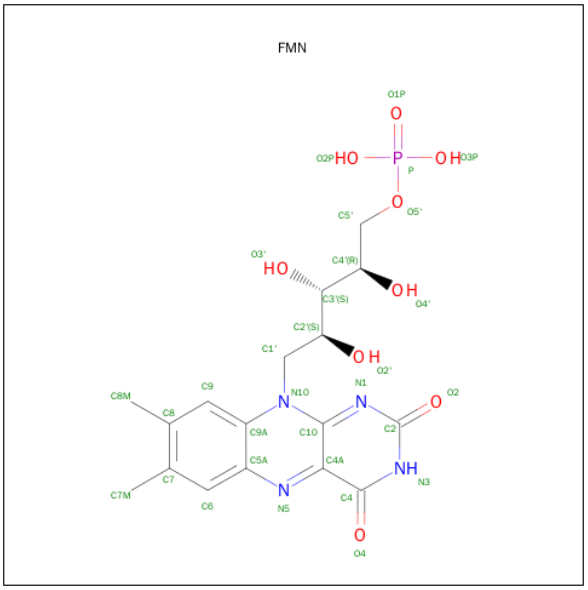
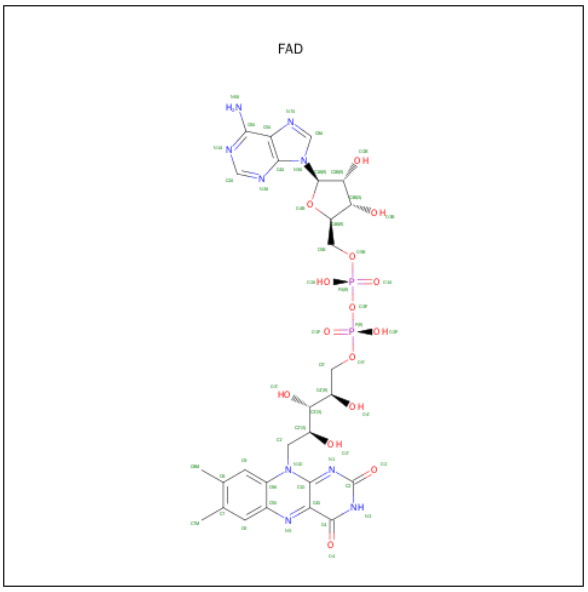
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

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



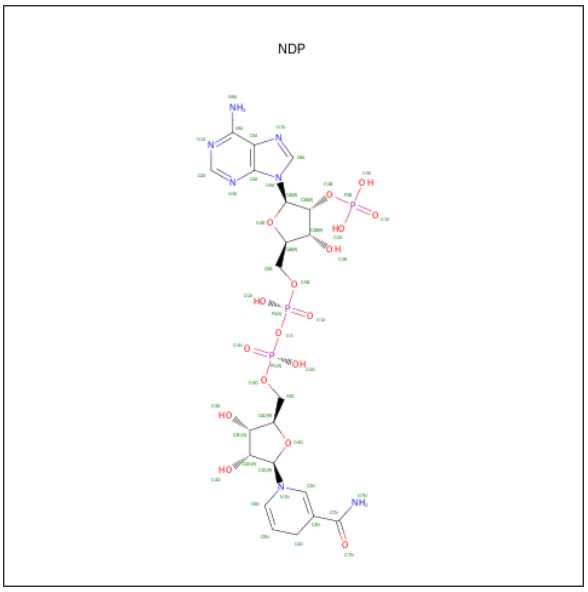
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 17 4 9 1	0	0
3	B	1	Total C N O P 31 17 4 9 1	0	0
3	C	1	Total C N O P 31 17 4 9 1	0	0
3	D	1	Total C N O P 31 17 4 9 1	0	0

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



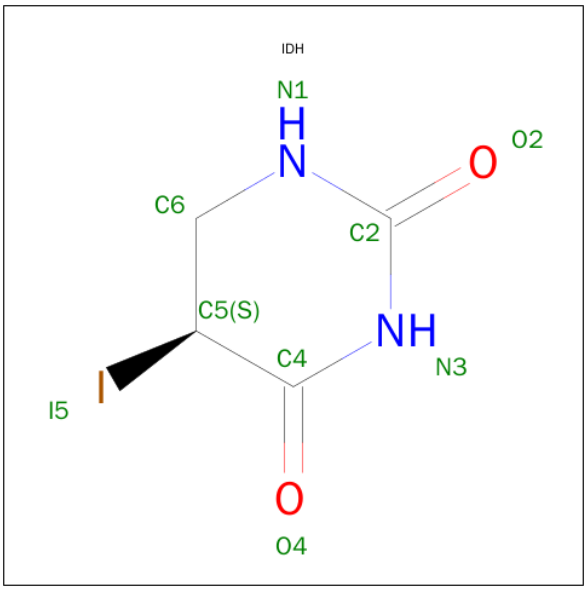
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



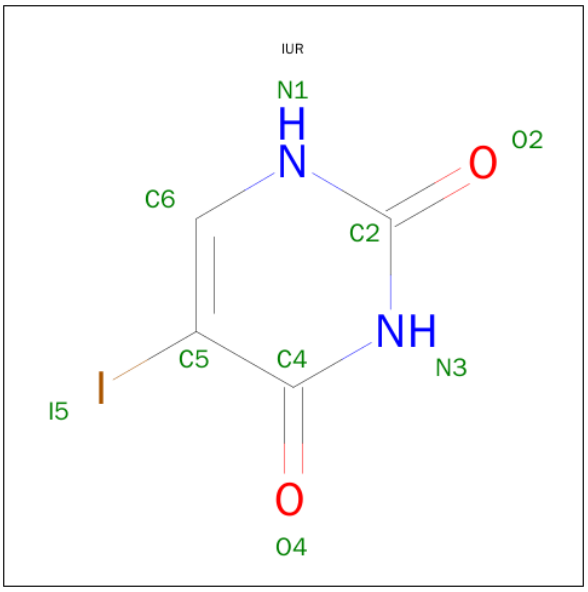
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 48 21 7 17 3	0	0
5	B	1	Total C N O P 48 21 7 17 3	0	0
5	C	1	Total C N O P 48 21 7 17 3	0	0
5	D	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 6 is (5S)-5-IODODIHYDRO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: IDH) (formula: $C_4H_5IN_2O_2$).



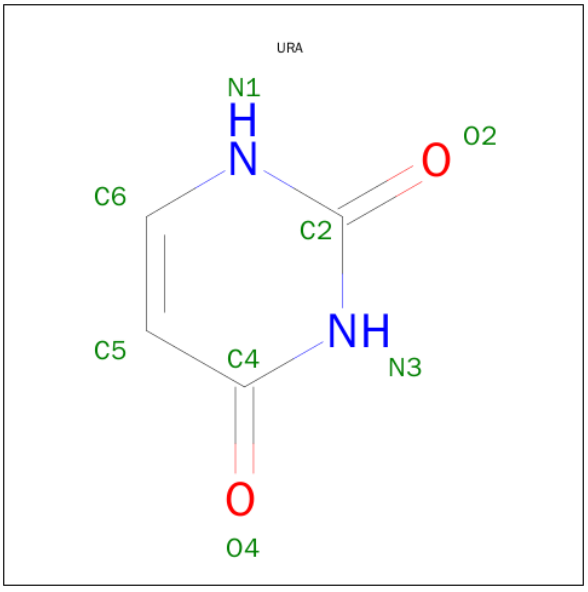
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 8 4 2 2	0	0
6	B	1	Total C I N O 9 4 1 2 2	0	0

- Molecule 7 is 5-IODOURACIL (three-letter code: IUR) (formula: $C_4H_3IN_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	I	N	O	0	0
			9	4	1	2	2		

- Molecule 8 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 9 is water.

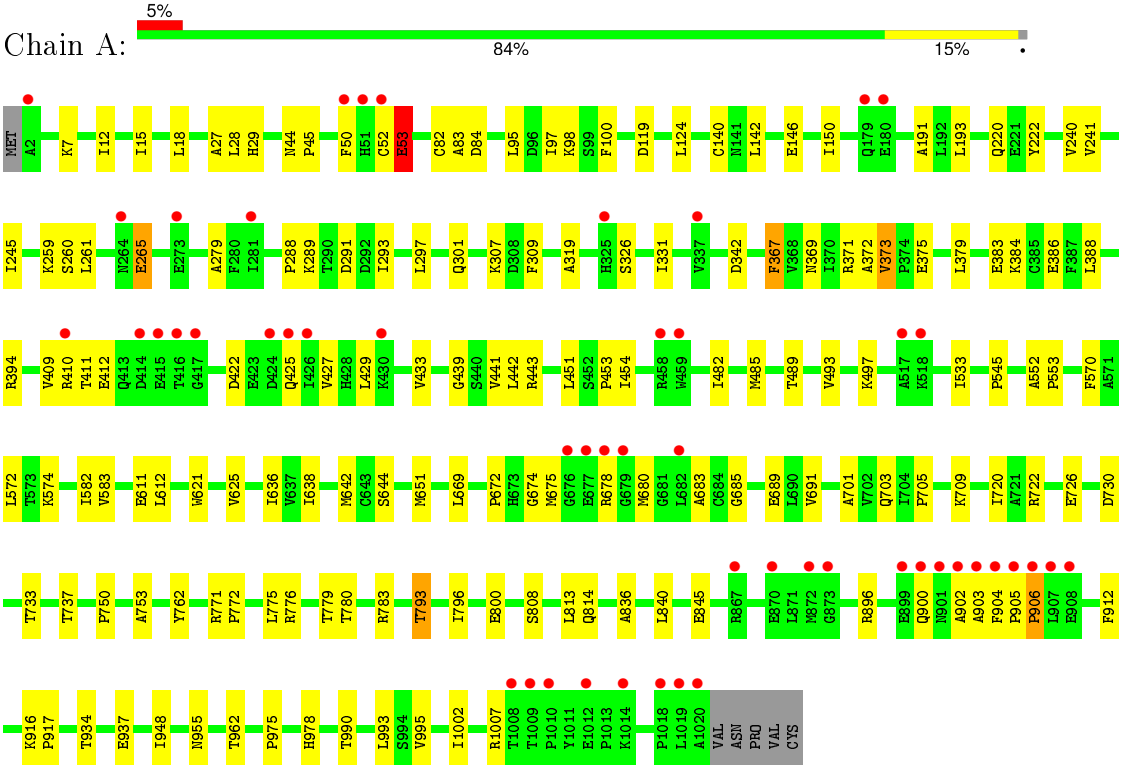
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	839	Total O 839 839	0	0
9	B	869	Total O 869 869	0	0
9	C	701	Total O 701 701	0	0
9	D	664	Total O 664 664	0	0

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.

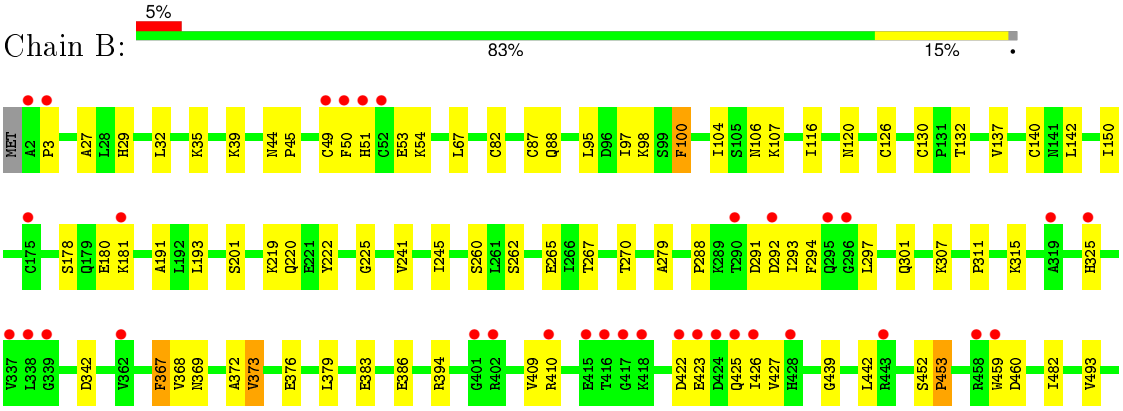
- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

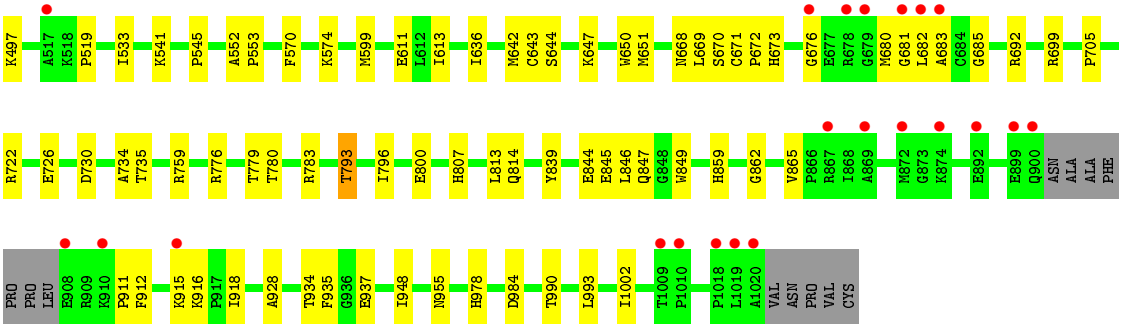
Chain A:



- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

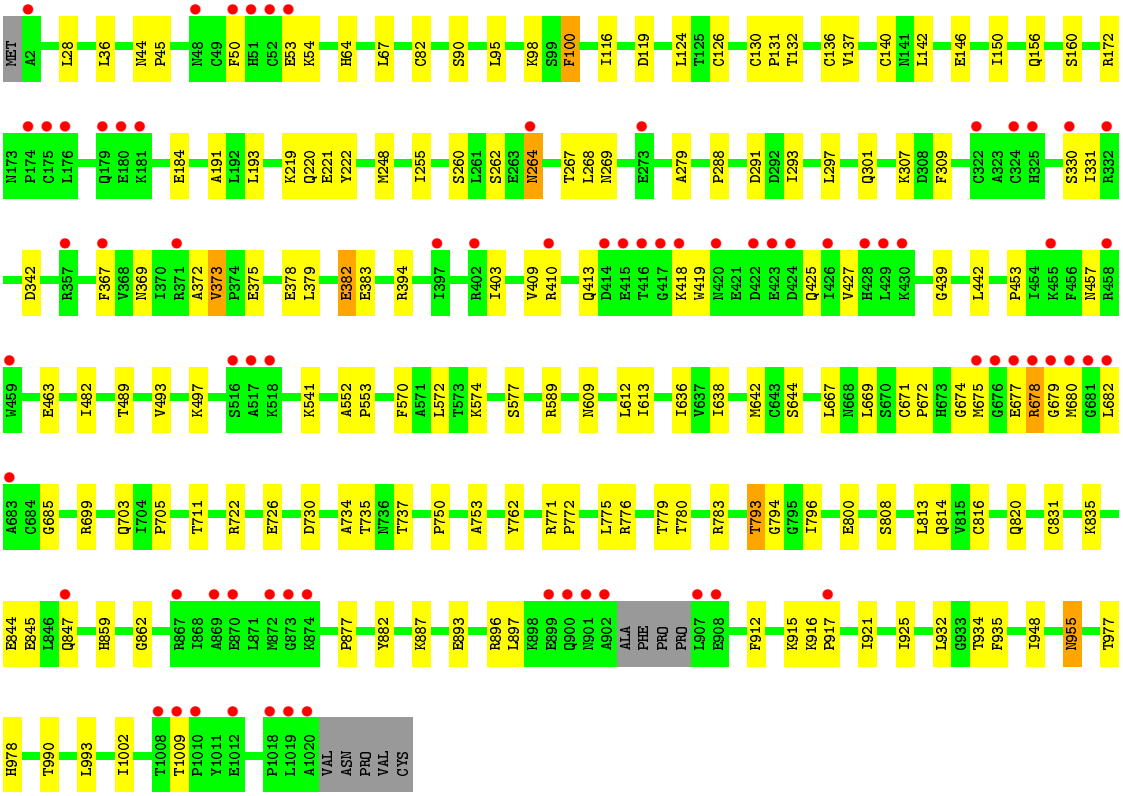
Chain B:





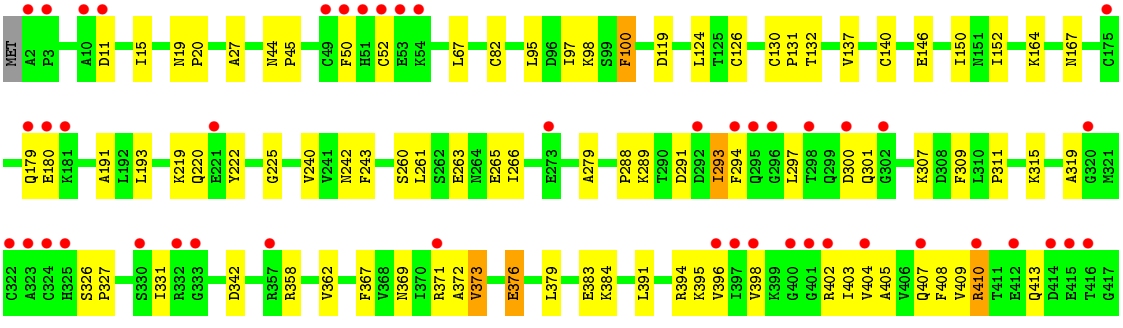
• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

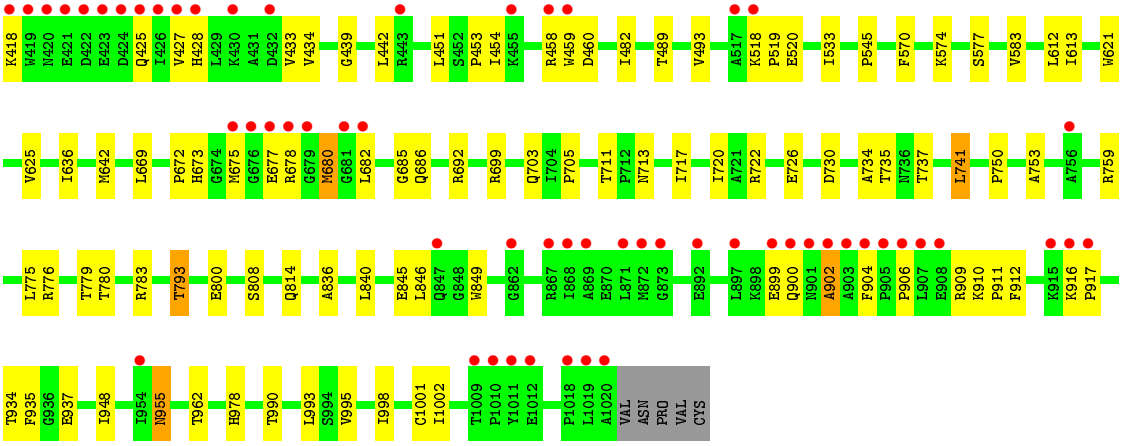
Chain C:



• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain D:




K418 W419 N420 E421 D422 E423 D424 Q425 I426 V427 H428 L429 K430 A431 D432 V433 V434 G439 L442 R443 L451 S452 P453 I454 K455 R458 W459 D460 I482 T489 V493 A517 K518 P519 E520 I533 P545 F570 K574 S577 V583 L612 I613 W621
V625 I636 M642 L669 P672 H673 G674 M675 G676 E677 R678 G679 M680 G681 L682 G685 Q686 R692 R699 Q703 I704 P705 T711 P712 N713 I717 I720 A721 R722 E726 D730 A734 T735 N736 T737 L741 P750 A753 A756 R759
L775 R776 T779 T780 R783 T793 E800 S808 Q814 A836 L840 E845 L846 Q847 G848 W849 G862 R867 I868 A869 E870 L871 M872 G873 E892 L897 K898 E899 Q900 N901 A902 A903 F904 P905 P906 L907 E908 R909 K910 P911 F912 K915 K916 P917
T934 F935 G936 E937 I948 I954 N955 T962 H978 T990 L993 S994 V995 I998 C1001 I1002 T1009 P1010 Y1011 E1012 P1018 L1019 A1020 VAL ASN PRO VAL CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.21Å 159.69Å 167.59Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	25.00 – 2.25 25.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-2.25) 98.3 (25.00-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.16 (at 2.26Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.209 0.175 , 0.205	Depositor DCC
R_{free} test set	3984 reflections (2.04%)	DCC
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 199145 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34762	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: URA, SF4, FMN, IDH, NDP, IUR, 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	0.34	0/7932	0.58	0/10751
1	B	0.34	0/7877	0.59	0/10672
1	C	0.33	0/7898	0.58	0/10701
1	D	0.33	0/7932	0.59	0/10751
All	All	0.34	0/31639	0.58	0/42875

There are no bond length outliers.

There are no bond angle outliers.

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	7770	0	7797	131	0
1	B	7719	0	7747	139	0
1	C	7740	0	7769	163	0
1	D	7770	0	7798	190	0
2	A	32	0	0	2	0
2	B	32	0	0	2	0
2	C	32	0	0	2	0
2	D	32	0	0	3	0
3	A	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	19	1	0
3	C	31	0	19	1	0
3	D	31	0	19	0	0
4	A	53	0	31	0	0
4	B	53	0	31	1	0
4	C	53	0	31	0	0
4	D	53	0	31	1	0
5	A	48	0	26	6	0
5	B	48	0	26	5	0
5	C	48	0	26	6	0
5	D	48	0	26	5	0
6	A	8	0	4	1	0
6	B	9	0	5	4	0
7	C	9	0	3	4	0
8	D	8	0	3	0	0
9	A	839	0	0	16	0
9	B	869	0	0	21	0
9	C	701	0	0	15	0
9	D	664	0	0	21	0
All	All	34762	0	31430	551	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 9.

The worst 5 of 551 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:C:427:VAL:HG21	1:D:410:ARG:HH21	1.25	1.02
1:C:264:ASN:H	1:C:264:ASN:HD22	1.17	0.91
1:D:904:PHE:O	1:D:906:PRO:HD3	1.70	0.90
1:C:410:ARG:NH1	1:D:427:VAL:HG13	1.87	0.89
1:C:410:ARG:HH12	1:D:427:VAL:HG22	1.36	0.88

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	1017/1025 (99%)	974 (96%)	40 (4%)	3 (0%)	46	52
1	B	1008/1025 (98%)	961 (95%)	45 (4%)	2 (0%)	52	61
1	C	1011/1025 (99%)	973 (96%)	36 (4%)	2 (0%)	52	61
1	D	1017/1025 (99%)	968 (95%)	48 (5%)	1 (0%)	56	66
All	All	4053/4100 (99%)	3876 (96%)	169 (4%)	8 (0%)	52	61

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	GLU
1	A	53	GLU
1	A	906	PRO
1	C	674	GLY
1	B	3	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	848/854 (99%)	840 (99%)	8 (1%)	84	91
1	B	843/854 (99%)	830 (98%)	13 (2%)	72	82
1	C	845/854 (99%)	830 (98%)	15 (2%)	66	77
1	D	848/854 (99%)	830 (98%)	18 (2%)	61	71
All	All	3384/3416 (99%)	3330 (98%)	54 (2%)	70	81

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	330	SER
1	C	678	ARG
1	D	680	MET
1	C	367	PHE
1	C	382	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	673	HIS
1	B	859	HIS
1	C	859	HIS
1	B	487	ASN
1	D	269	ASN

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)

32 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	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1027	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1028	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1029	-	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	A	1030	-	32,33,33	2.70	9 (28%)	34,50,50	4.00	12 (35%)
4	FAD	A	1031	-	52,58,58	2.14	19 (36%)	52,89,89	1.98	11 (21%)
5	NDP	A	1032	-	44,52,52	1.53	6 (13%)	55,80,80	1.76	14 (25%)
6	IDH	A	1033	1	8,8,9	2.17	3 (37%)	8,10,12	1.01	0
2	SF4	B	1026	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1027	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1028	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1029	-	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	B	1030	-	32,33,33	2.70	9 (28%)	34,50,50	4.05	12 (35%)
4	FAD	B	1031	-	52,58,58	2.17	17 (32%)	52,89,89	2.02	11 (21%)
5	NDP	B	1032	-	44,52,52	1.52	7 (15%)	55,80,80	1.74	12 (21%)
6	IDH	B	1034	-	6,9,9	1.87	2 (33%)	7,12,12	3.07	2 (28%)
2	SF4	C	1026	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1027	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1028	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1029	-	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	C	1030	-	32,33,33	2.72	9 (28%)	34,50,50	3.98	12 (35%)
4	FAD	C	1031	-	52,58,58	2.16	17 (32%)	52,89,89	1.99	11 (21%)
5	NDP	C	1032	-	44,52,52	1.54	6 (13%)	55,80,80	1.75	14 (25%)
7	IUR	C	1034	-	7,9,9	1.49	1 (14%)	3,12,12	10.24	2 (66%)
2	SF4	D	1026	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1027	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1028	-	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1029	-	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	D	1030	-	32,33,33	2.68	9 (28%)	34,50,50	3.99	12 (35%)
4	FAD	D	1031	-	52,58,58	2.18	17 (32%)	52,89,89	2.03	11 (21%)
5	NDP	D	1032	-	44,52,52	1.55	6 (13%)	55,80,80	1.75	13 (23%)
8	URA	D	1034	-	6,8,8	2.17	1 (16%)	5,10,10	10.53	4 (80%)

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	-	-	0/0/48/48	2/6/5/5
2	SF4	A	1027	-	-	0/0/48/48	2/6/5/5
2	SF4	A	1028	-	-	0/0/48/48	2/6/5/5
2	SF4	A	1029	-	-	0/0/48/48	2/6/5/5
3	FMN	A	1030	-	-	0/18/18/18	0/3/3/3
4	FAD	A	1031	-	-	0/30/50/50	0/6/6/6
5	NDP	A	1032	-	-	0/30/77/77	0/5/5/5
6	IDH	A	1033	1	-	0/0/10/13	0/1/1/1
2	SF4	B	1026	-	-	0/0/48/48	2/6/5/5
2	SF4	B	1027	-	-	0/0/48/48	2/6/5/5
2	SF4	B	1028	-	-	0/0/48/48	2/6/5/5
2	SF4	B	1029	-	-	0/0/48/48	2/6/5/5
3	FMN	B	1030	-	-	0/18/18/18	0/3/3/3
4	FAD	B	1031	-	-	0/30/50/50	0/6/6/6
5	NDP	B	1032	-	-	0/30/77/77	0/5/5/5
6	IDH	B	1034	-	-	0/0/13/13	0/1/1/1
2	SF4	C	1026	-	-	0/0/48/48	2/6/5/5
2	SF4	C	1027	-	-	0/0/48/48	2/6/5/5
2	SF4	C	1028	-	-	0/0/48/48	2/6/5/5
2	SF4	C	1029	-	-	0/0/48/48	2/6/5/5
3	FMN	C	1030	-	-	0/18/18/18	0/3/3/3
4	FAD	C	1031	-	-	0/30/50/50	0/6/6/6
5	NDP	C	1032	-	-	0/30/77/77	0/5/5/5
7	IUR	C	1034	-	-	0/0/0/0	0/1/1/1
2	SF4	D	1026	-	-	0/0/48/48	2/6/5/5
2	SF4	D	1027	-	-	0/0/48/48	2/6/5/5
2	SF4	D	1028	-	-	0/0/48/48	2/6/5/5
2	SF4	D	1029	-	-	0/0/48/48	2/6/5/5
3	FMN	D	1030	-	-	0/18/18/18	0/3/3/3
4	FAD	D	1031	-	-	0/30/50/50	0/6/6/6
5	NDP	D	1032	-	-	0/30/77/77	0/5/5/5
8	URA	D	1034	-	-	0/0/0/0	0/1/1/1

The worst 5 of 138 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1030	FMN	C1'-N10	-9.08	1.38	1.48
3	A	1030	FMN	C1'-N10	-8.86	1.39	1.48
3	D	1030	FMN	C1'-N10	-8.56	1.39	1.48
3	C	1030	FMN	C1'-N10	-8.53	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1032	NDP	C4N-C5N	-5.19	1.37	1.49

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1030	FMN	C4A-C4-N3	-10.12	110.30	123.52
3	A	1030	FMN	C4A-C4-N3	-10.06	110.37	123.52
3	C	1030	FMN	C4A-C4-N3	-10.03	110.41	123.52
3	D	1030	FMN	C4A-C4-N3	-9.92	110.55	123.52
3	D	1030	FMN	N3-C2-N1	-7.59	114.90	127.69

There are no chirality outliers.

There are no torsion outliers.

5 of 32 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1027	SF4	FE3-FE4-S1-S2
2	C	1027	SF4	FE3-FE4-S1-S2
2	D	1026	SF4	FE1-FE2-S3-S4
2	D	1027	SF4	FE3-FE4-S1-S2
2	B	1026	SF4	FE1-FE2-S3-S4

16 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1026	SF4	1	0
2	A	1027	SF4	1	0
5	A	1032	NDP	6	0
6	A	1033	IDH	1	0
2	B	1027	SF4	2	0
3	B	1030	FMN	1	0
4	B	1031	FAD	1	0
5	B	1032	NDP	5	0
6	B	1034	IDH	4	0
2	C	1027	SF4	2	0
3	C	1030	FMN	1	0
5	C	1032	NDP	6	0
7	C	1034	IUR	4	0
2	D	1027	SF4	3	0
4	D	1031	FAD	1	0
5	D	1032	NDP	5	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	1019/1025 (99%)	-0.01	51 (5%)	32	36	14, 27, 63, 83	0
1	B	1012/1025 (98%)	0.01	56 (5%)	29	32	15, 27, 61, 83	0
1	C	1015/1025 (99%)	0.08	74 (7%)	18	19	17, 29, 63, 85	0
1	D	1019/1025 (99%)	0.23	104 (10%)	9	9	17, 29, 67, 87	0
All	All	4065/4100 (99%)	0.08	285 (7%)	19	21	14, 28, 64, 87	0

The worst 5 of 285 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	10.8
1	D	2	ALA	10.6
1	D	904	PHE	10.3
1	D	682	LEU	10.0
1	C	679	GLY	9.8

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
6	IDH	B	1034	9/9	0.90	0.24	3.42	39,42,45,52	1
6	IDH	A	1033	8/9	0.93	0.16	1.07	23,28,32,32	0
2	SF4	D	1026	8/8	0.96	0.12	0.94	26,28,28,28	0
2	SF4	C	1026	8/8	0.94	0.13	0.79	26,28,29,29	0
8	URA	D	1034	8/8	0.95	0.14	0.37	28,30,31,32	0
2	SF4	B	1027	8/8	0.96	0.13	0.32	18,19,21,21	0
2	SF4	C	1027	8/8	0.96	0.13	0.20	24,26,26,26	0
5	NDP	D	1032	48/48	0.92	0.17	0.09	40,47,57,58	0
4	FAD	C	1031	53/53	0.95	0.13	0.06	26,31,33,34	0
3	FMN	B	1030	31/31	0.97	0.12	0.02	17,19,21,22	0
5	NDP	C	1032	48/48	0.93	0.15	-0.01	39,46,56,57	0
5	NDP	A	1032	48/48	0.94	0.15	-0.06	36,42,56,56	0
2	SF4	A	1026	8/8	0.95	0.12	-0.07	21,23,23,24	0
4	FAD	D	1031	53/53	0.95	0.13	-0.15	25,28,35,37	0
5	NDP	B	1032	48/48	0.94	0.15	-0.21	36,44,56,57	0
7	IUR	C	1034	9/9	0.93	0.13	-0.21	27,28,32,38	1
2	SF4	B	1029	8/8	0.96	0.11	-0.22	22,23,24,24	0
3	FMN	A	1030	31/31	0.98	0.11	-0.22	16,19,21,22	0
2	SF4	D	1029	8/8	0.97	0.11	-0.23	29,30,31,31	0
2	SF4	D	1028	8/8	0.96	0.11	-0.25	28,29,30,31	0
2	SF4	D	1027	8/8	0.97	0.13	-0.25	22,23,24,24	0
2	SF4	B	1028	8/8	0.96	0.11	-0.35	20,22,23,23	0
2	SF4	A	1027	8/8	0.95	0.12	-0.35	17,20,20,21	0
4	FAD	A	1031	53/53	0.97	0.11	-0.52	21,26,32,33	0
3	FMN	C	1030	31/31	0.97	0.10	-0.53	16,20,22,22	0
2	SF4	A	1029	8/8	0.97	0.12	-0.59	21,22,23,23	0
2	SF4	C	1028	8/8	0.97	0.10	-0.63	23,25,26,26	0
4	FAD	B	1031	53/53	0.97	0.12	-0.65	22,26,32,34	0
2	SF4	A	1028	8/8	0.97	0.12	-0.66	21,23,24,24	0
2	SF4	B	1026	8/8	0.97	0.11	-1.00	19,23,24,24	0
2	SF4	C	1029	8/8	0.98	0.10	-1.03	24,25,27,27	0
3	FMN	D	1030	31/31	0.98	0.08	-1.11	16,20,22,23	0

6.5 Other polymers (i)

There are no such residues in this entry.