wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:36 AM GMT

PDB ID	:	3BG3
Title	:	Crystal Structure of Human Pyruvate Carboxylase (missing the biotin carboxylase domain at the N-terminus)
Authors	:	Xiang, S.; Tong, L.
Deposited on	:	2007-11-26
Resolution	:	2.80 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:

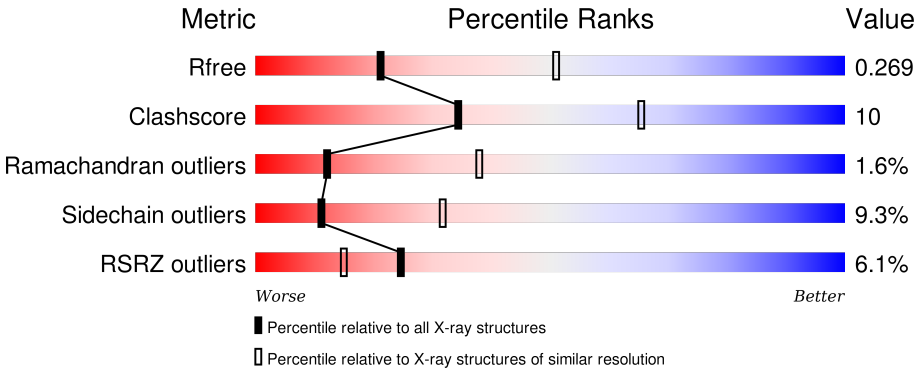
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	718	8% 66% 23% 5% 5%
1	B	718	3% 60% 22% • 16%
1	C	718	2% 58% 23% • 16%
1	D	718	8% 68% 24% • • 5%

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
3	PYR	C	2000	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19813 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 Pyruvate carboxylase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	680	Total	C	N	O	S	0	0	0
			5222	3314	895	978	35			
1	B	604	Total	C	N	O	S	0	0	0
			4663	2960	802	872	29			
1	C	604	Total	C	N	O	S	0	0	0
			4663	2960	802	872	29			
1	D	680	Total	C	N	O	S	0	0	0
			5222	3314	895	978	35			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	MET	-	EXPRESSION TAG	UNP P11498
A	462	GLY	-	EXPRESSION TAG	UNP P11498
A	463	SER	-	EXPRESSION TAG	UNP P11498
A	464	SER	-	EXPRESSION TAG	UNP P11498
A	465	HIS	-	EXPRESSION TAG	UNP P11498
A	466	HIS	-	EXPRESSION TAG	UNP P11498
A	467	HIS	-	EXPRESSION TAG	UNP P11498
A	468	HIS	-	EXPRESSION TAG	UNP P11498
A	469	HIS	-	EXPRESSION TAG	UNP P11498
A	470	HIS	-	EXPRESSION TAG	UNP P11498
A	471	SER	-	EXPRESSION TAG	UNP P11498
A	472	SER	-	EXPRESSION TAG	UNP P11498
A	473	GLY	-	EXPRESSION TAG	UNP P11498
A	474	LEU	-	EXPRESSION TAG	UNP P11498
A	475	VAL	-	EXPRESSION TAG	UNP P11498
A	476	PRO	-	EXPRESSION TAG	UNP P11498
A	477	ARG	-	EXPRESSION TAG	UNP P11498
A	478	GLY	-	EXPRESSION TAG	UNP P11498
A	479	SER	-	EXPRESSION TAG	UNP P11498
A	480	HIS	-	EXPRESSION TAG	UNP P11498
A	481	MET	-	EXPRESSION TAG	UNP P11498

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	461	MET	-	EXPRESSION TAG	UNP P11498
B	462	GLY	-	EXPRESSION TAG	UNP P11498
B	463	SER	-	EXPRESSION TAG	UNP P11498
B	464	SER	-	EXPRESSION TAG	UNP P11498
B	465	HIS	-	EXPRESSION TAG	UNP P11498
B	466	HIS	-	EXPRESSION TAG	UNP P11498
B	467	HIS	-	EXPRESSION TAG	UNP P11498
B	468	HIS	-	EXPRESSION TAG	UNP P11498
B	469	HIS	-	EXPRESSION TAG	UNP P11498
B	470	HIS	-	EXPRESSION TAG	UNP P11498
B	471	SER	-	EXPRESSION TAG	UNP P11498
B	472	SER	-	EXPRESSION TAG	UNP P11498
B	473	GLY	-	EXPRESSION TAG	UNP P11498
B	474	LEU	-	EXPRESSION TAG	UNP P11498
B	475	VAL	-	EXPRESSION TAG	UNP P11498
B	476	PRO	-	EXPRESSION TAG	UNP P11498
B	477	ARG	-	EXPRESSION TAG	UNP P11498
B	478	GLY	-	EXPRESSION TAG	UNP P11498
B	479	SER	-	EXPRESSION TAG	UNP P11498
B	480	HIS	-	EXPRESSION TAG	UNP P11498
B	481	MET	-	EXPRESSION TAG	UNP P11498
C	461	MET	-	EXPRESSION TAG	UNP P11498
C	462	GLY	-	EXPRESSION TAG	UNP P11498
C	463	SER	-	EXPRESSION TAG	UNP P11498
C	464	SER	-	EXPRESSION TAG	UNP P11498
C	465	HIS	-	EXPRESSION TAG	UNP P11498
C	466	HIS	-	EXPRESSION TAG	UNP P11498
C	467	HIS	-	EXPRESSION TAG	UNP P11498
C	468	HIS	-	EXPRESSION TAG	UNP P11498
C	469	HIS	-	EXPRESSION TAG	UNP P11498
C	470	HIS	-	EXPRESSION TAG	UNP P11498
C	471	SER	-	EXPRESSION TAG	UNP P11498
C	472	SER	-	EXPRESSION TAG	UNP P11498
C	473	GLY	-	EXPRESSION TAG	UNP P11498
C	474	LEU	-	EXPRESSION TAG	UNP P11498
C	475	VAL	-	EXPRESSION TAG	UNP P11498
C	476	PRO	-	EXPRESSION TAG	UNP P11498
C	477	ARG	-	EXPRESSION TAG	UNP P11498
C	478	GLY	-	EXPRESSION TAG	UNP P11498
C	479	SER	-	EXPRESSION TAG	UNP P11498
C	480	HIS	-	EXPRESSION TAG	UNP P11498
C	481	MET	-	EXPRESSION TAG	UNP P11498

Continued on next page...

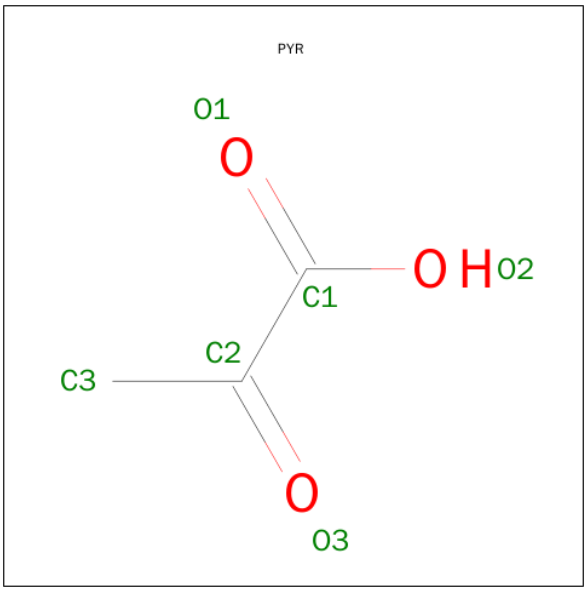
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	461	MET	-	EXPRESSION TAG	UNP P11498
D	462	GLY	-	EXPRESSION TAG	UNP P11498
D	463	SER	-	EXPRESSION TAG	UNP P11498
D	464	SER	-	EXPRESSION TAG	UNP P11498
D	465	HIS	-	EXPRESSION TAG	UNP P11498
D	466	HIS	-	EXPRESSION TAG	UNP P11498
D	467	HIS	-	EXPRESSION TAG	UNP P11498
D	468	HIS	-	EXPRESSION TAG	UNP P11498
D	469	HIS	-	EXPRESSION TAG	UNP P11498
D	470	HIS	-	EXPRESSION TAG	UNP P11498
D	471	SER	-	EXPRESSION TAG	UNP P11498
D	472	SER	-	EXPRESSION TAG	UNP P11498
D	473	GLY	-	EXPRESSION TAG	UNP P11498
D	474	LEU	-	EXPRESSION TAG	UNP P11498
D	475	VAL	-	EXPRESSION TAG	UNP P11498
D	476	PRO	-	EXPRESSION TAG	UNP P11498
D	477	ARG	-	EXPRESSION TAG	UNP P11498
D	478	GLY	-	EXPRESSION TAG	UNP P11498
D	479	SER	-	EXPRESSION TAG	UNP P11498
D	480	HIS	-	EXPRESSION TAG	UNP P11498
D	481	MET	-	EXPRESSION TAG	UNP P11498

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

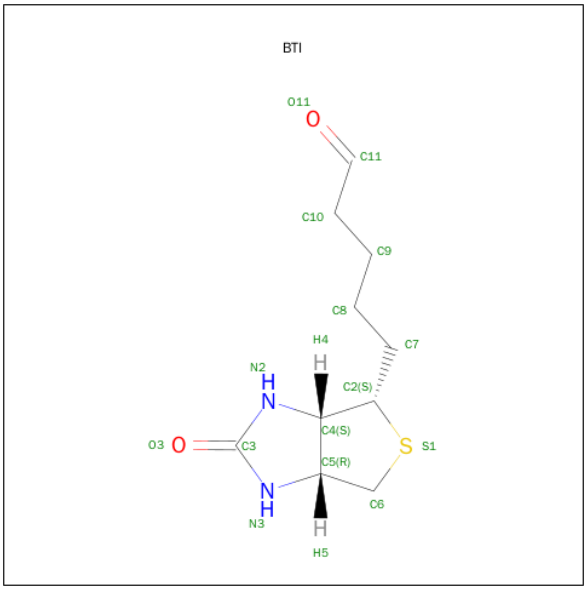
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).



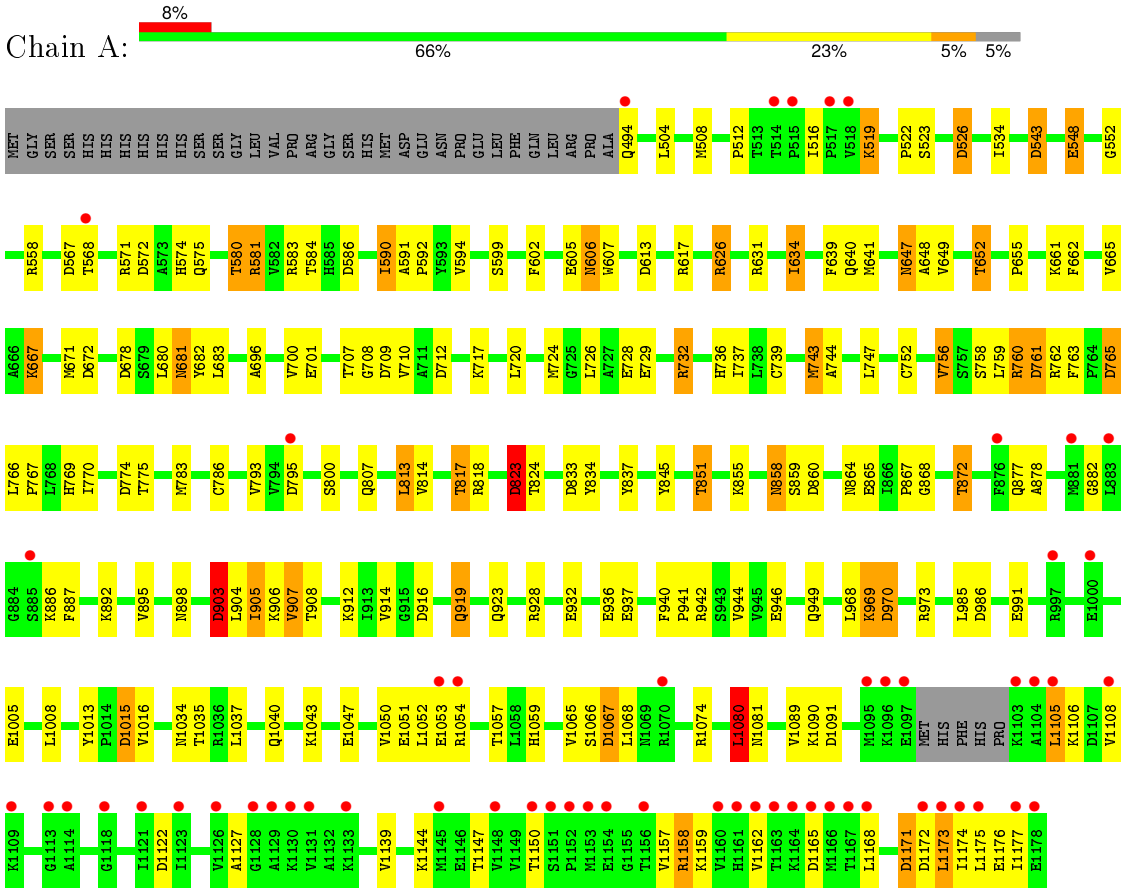
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	10	2	2	1	0	0

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.

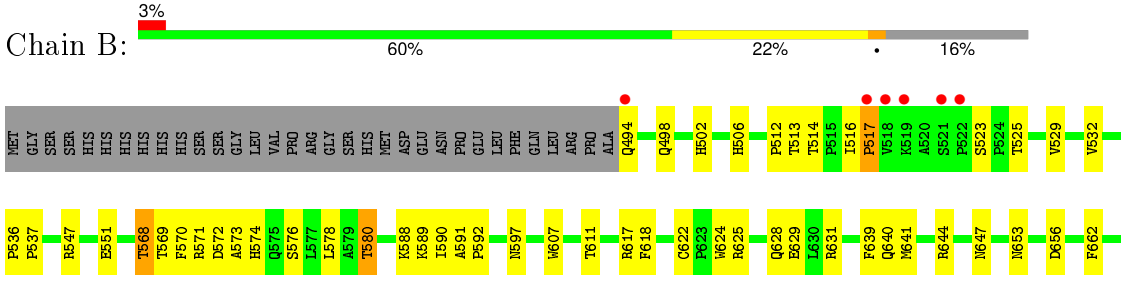
- Molecule 1: Pyruvate carboxylase, mitochondrial

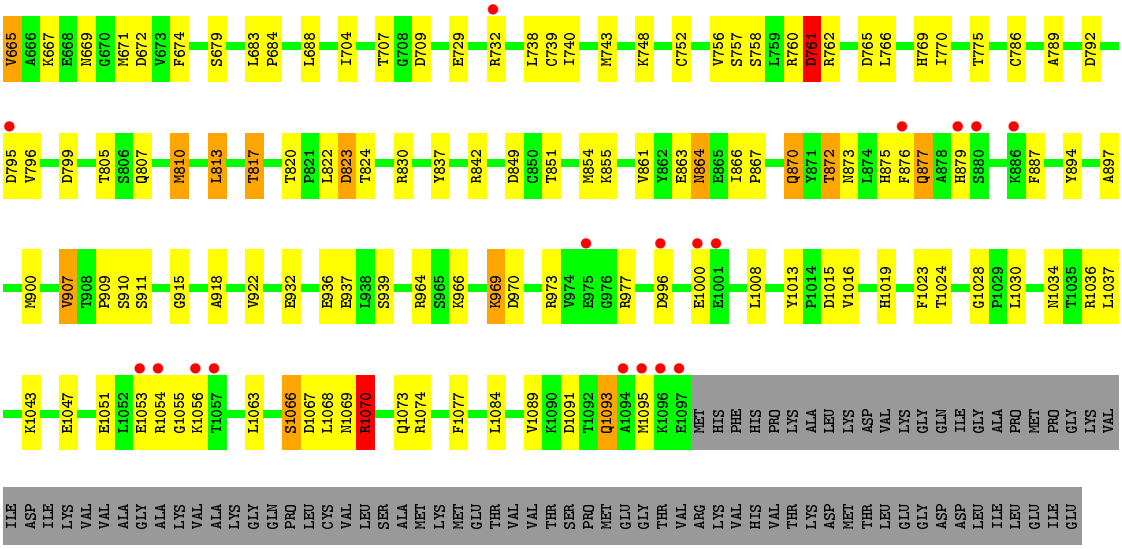
Chain A:



- Molecule 1: Pyruvate carboxylase, mitochondrial

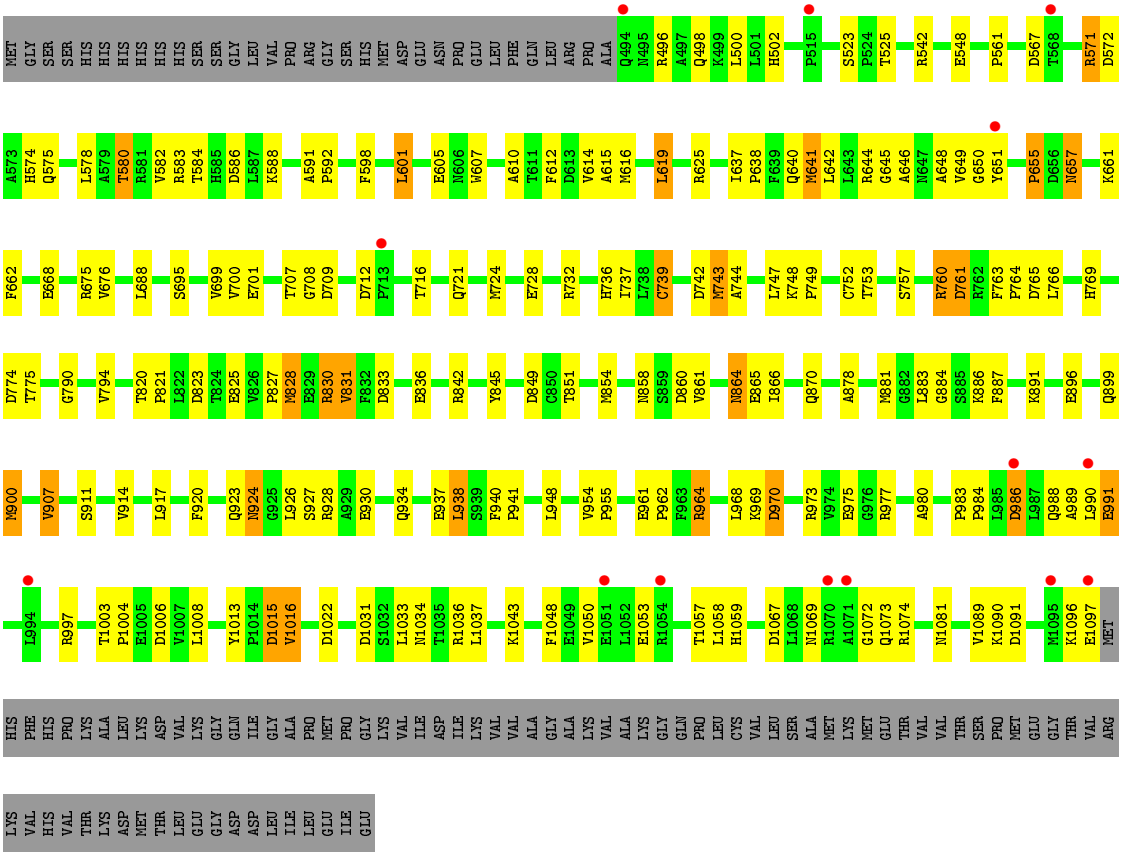
Chain B:





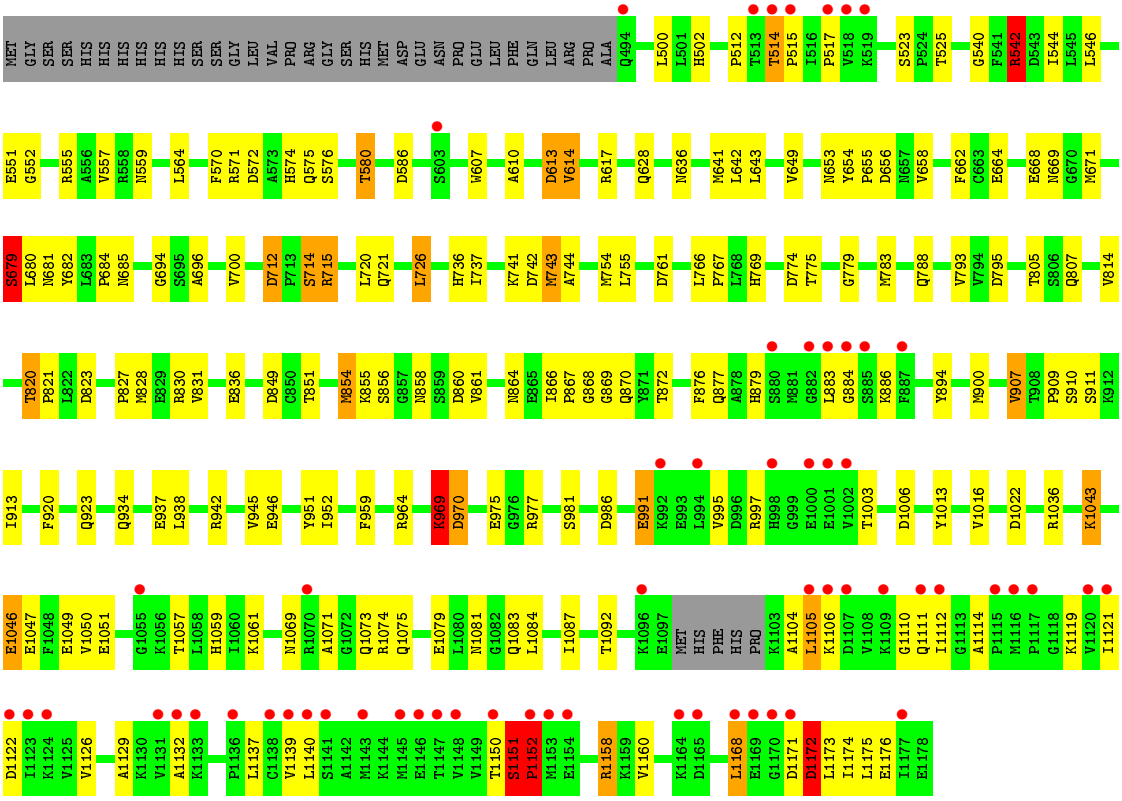
• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain C:



• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain D:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ASP GLU ASN PRO GLU LEU PHE GLN LEU ARG PRO ALA Q494 L500 L501 H502 P512 T513 T514 P515 I516 P517 V518 K519 S523 P524 T525 G540 F541 R542 D543 I544 L545 L546
E551 G552 R555 A556 V557 R558 N559 L564 F570 R571 D572 A573 H574 Q575 S576 T580 D586 S603 W607 A610 D613 V614 R617 Q628 N636 M641 L642 L643 V649 N653 Y654 P655 D656 N657 V658 F662 C663 E664 E668 N669 G670 M671
S679 L680 N681 Y682 L683 P684 N685 G694 S695 A696 V700 D712 P713 S714 R715 L720 Q721 L726 H736 I737 K741 D742 M743 A744 M754 L755 D761 L766 P767 L768 H769 D774 T775 G779 M783 Q788 V793 V794 D795 T805 S806 Q807 V814
T820 P821 L822 D823 P827 M828 E829 R830 V831 E836 D849 C850 T851 N854 K855 S856 G857 N858 S859 D860 V861 N864 E865 I866 P867 G868 G869 Q870 Y871 T872 F876 Q877 A878 H879 S880 H881 G882 L883 G884 S885 K886 F887 Y894 N900 Y907 T908 P909 S910 S911 K912
I913 F920 Q923 Q934 E937 L938 R942 V945 E946 Y951 I952 F959 R964 K969 D970 E975 G976 R977 S981 D986 E991 K992 E993 L994 V995 D996 R997 H998 G999 E1000 E1001 V1002 T1003 D1006 Y1013 V1016 D1022 R1036 K1043
E1046 E1047 F1048 E1049 V1050 E1051 G1055 K1056 T1057 L1058 H1059 I1060 K1061 N1069 R1070 A1071 G1072 Q1073 R1074 Q1075 E1079 L1080 N1081 G1082 Q1083 L1084 I1087 T1092 K1096 E1097 MET HIS PHE HIS PRO K1103 A1104 L1105 K1106 D1107 V1108 K1109 G1110 Q1111 I1112 G1113 A1114 P1115 M1116 P1117 G1118 K1119 V1120 I1121
D1122 I1123 K1124 V1125 V1126 A1129 K1130 V1131 A1132 K1133 P1136 L1137 C1138 V1139 L1140 S1141 A1142 M1143 K1144 M1145 E1146 T1147 V1148 V1149 T1150 S1151 P1152 M1153 E1154 R1158 K1159 V1160 K1164 D1165 L1168 E1169 G1170 D1171 D1172 L1173 I1174 L1175 E1176 I1177 E1178

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.27Å 173.32Å 118.19Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.87 – 2.77	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.80) 92.4 (29.87-2.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.216 , 0.271 0.216 , 0.269	Depositor DCC
R_{free} test set	3915 reflections (5.46%)	DCC
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 76494 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19813	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: PYR, MN, BTI, KCX

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	0.51	6/5322 (0.1%)	0.77	22/7211 (0.3%)
1	B	0.59	5/4759 (0.1%)	0.76	14/6456 (0.2%)
1	C	0.50	1/4759 (0.0%)	0.75	17/6456 (0.3%)
1	D	0.57	6/5322 (0.1%)	0.78	16/7211 (0.2%)
All	All	0.54	18/20162 (0.1%)	0.76	69/27334 (0.3%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1066	SER	CB-OG	17.43	1.65	1.42
1	B	973	ARG	CZ-NH1	11.80	1.48	1.33
1	D	991	GLU	CD-OE2	11.34	1.38	1.25
1	A	937	GLU	CD-OE2	8.89	1.35	1.25
1	D	664	GLU	CD-OE2	8.78	1.35	1.25

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	973	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	973	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	D	613	ASP	CB-CG-OD2	7.90	125.41	118.30
1	D	860	ASP	CB-CG-OD2	7.80	125.32	118.30
1	D	774	ASP	CB-CG-OD2	7.69	125.22	118.30

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	5222	0	5215	106	0
1	B	4663	0	4608	101	0
1	C	4663	0	4608	95	0
1	D	5222	0	5217	101	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	3	1	0
3	B	6	0	3	0	0
3	C	6	0	3	0	0
3	D	6	0	3	0	0
4	A	15	0	15	0	0
All	All	19813	0	19675	395	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 10.

The worst 5 of 395 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:1066:SER:CB	1:B:1066:SER:OG	1.64	1.45
1:C:870:GLN:HE22	1:C:911:SER:HB2	1.17	1.07
1:B:568:THR:HG21	1:B:807:GLN:NE2	1.82	0.94
1:A:851:THR:HG21	1:D:855:LYS:HD2	1.47	0.94
1:C:870:GLN:NE2	1:C:911:SER:HB2	1.90	0.86

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	675/718 (94%)	612 (91%)	50 (7%)	13 (2%)	10 32
1	B	601/718 (84%)	542 (90%)	54 (9%)	5 (1%)	24 58
1	C	601/718 (84%)	543 (90%)	47 (8%)	11 (2%)	11 34
1	D	675/718 (94%)	603 (89%)	59 (9%)	13 (2%)	10 32
All	All	2552/2872 (89%)	2300 (90%)	210 (8%)	42 (2%)	12 38

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1165	ASP
1	B	1055	GLY
1	C	496	ARG
1	D	1110	GLY
1	D	1152	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	559/593 (94%)	495 (89%)	64 (11%)	7 21
1	B	496/593 (84%)	454 (92%)	42 (8%)	13 36
1	C	496/593 (84%)	447 (90%)	49 (10%)	10 28
1	D	559/593 (94%)	517 (92%)	42 (8%)	17 43
All	All	2110/2372 (89%)	1913 (91%)	197 (9%)	11 32

5 of 197 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	870	GLN
1	C	571	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	969	LYS
1	B	877	GLN
1	B	1047	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	899	GLN
1	C	574	HIS
1	D	899	GLN
1	B	998	HIS
1	C	502	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KCX	A	741	2	7,11,12	0.94	1 (14%)	7,12,14	0.77	0
1	KCX	B	741	2	7,11,12	0.81	0	7,12,14	1.27	1 (14%)
1	KCX	C	741	2	7,11,12	0.72	0	7,12,14	0.85	0
1	KCX	D	741	2	7,11,12	0.64	0	7,12,14	1.05	0

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
1	KCX	A	741	2	-	0/6/10/12	0/0/0/0
1	KCX	B	741	2	-	0/6/10/12	0/0/0/0
1	KCX	C	741	2	-	0/6/10/12	0/0/0/0
1	KCX	D	741	2	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	741	KCX	CE-NZ	2.01	1.50	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	741	KCX	CE-NZ-CX	-2.25	120.94	123.49

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
1	D	741	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	PYR	A	2000	-	2,5,5	1.81	1 (50%)	2,6,6	0.14	0
4	BTI	A	2100	1	14,16,16	1.84	3 (21%)	13,21,21	1.23	1 (7%)
3	PYR	B	2000	-	2,5,5	1.94	1 (50%)	2,6,6	0.69	0
3	PYR	C	2000	-	2,5,5	1.86	1 (50%)	2,6,6	0.31	0
3	PYR	D	2000	-	2,5,5	2.07	1 (50%)	2,6,6	0.48	0

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	PYR	A	2000	-	-	0/0/4/4	0/0/0/0
4	BTI	A	2100	1	-	0/5/27/27	0/2/2/2
3	PYR	B	2000	-	-	0/0/4/4	0/0/0/0
3	PYR	C	2000	-	-	0/0/4/4	0/0/0/0
3	PYR	D	2000	-	-	0/0/4/4	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2100	BTI	C2-S1	-3.42	1.77	1.82
4	A	2100	BTI	C3-N3	-2.09	1.32	1.35
3	A	2000	PYR	O3-C2	2.54	1.31	1.22
3	C	2000	PYR	O3-C2	2.60	1.31	1.22
3	B	2000	PYR	O3-C2	2.72	1.32	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2100	BTI	N2-C3-N3	3.16	111.07	108.88

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	2000	PYR	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	679/718 (94%)	0.20	58 (8%)	13	6	49, 89, 174, 254	0
1	B	603/718 (83%)	0.02	24 (3%)	42	30	55, 89, 135, 163	0
1	C	603/718 (83%)	-0.08	14 (2%)	64	52	57, 91, 140, 165	0
1	D	679/718 (94%)	0.16	61 (8%)	12	6	51, 87, 159, 257	0
All	All	2564/2872 (89%)	0.08	157 (6%)	25	15	49, 89, 151, 257	0

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1173	LEU	7.1
1	A	1133	LYS	6.8
1	A	1129	ALA	6.4
1	A	1165	ASP	6.3
1	D	1140	LEU	6.2

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

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
1	KCX	B	741	12/13	0.98	0.23	-	64,66,68,68	0
1	KCX	A	741	12/13	0.97	0.23	-	66,69,70,70	0
1	KCX	D	741	12/13	0.98	0.23	-	54,60,63,64	0
1	KCX	C	741	12/13	0.98	0.24	-	70,72,74,75	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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
3	PYR	C	2000	6/6	0.78	0.40	2.31	88,89,91,91	0
3	PYR	B	2000	6/6	0.91	0.28	1.44	72,74,74,74	0
3	PYR	A	2000	6/6	0.93	0.21	0.30	75,76,77,79	0
3	PYR	D	2000	6/6	0.92	0.24	0.14	76,77,77,79	0
2	MN	B	2001	1/1	0.96	0.23	-0.35	68,68,68,68	0
2	MN	C	2001	1/1	0.98	0.21	-0.80	77,77,77,77	0
2	MN	D	2001	1/1	0.95	0.21	-0.97	68,68,68,68	0
2	MN	A	2001	1/1	0.95	0.22	-1.33	72,72,72,72	0
4	BTI	A	2100	15/15	0.96	0.13	-1.86	89,92,93,94	0

6.5 Other polymers (i)

There are no such residues in this entry.