



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:37 AM GMT

PDB ID : 3EXG  
Title : Crystal structure of the pyruvate dehydrogenase (E1p) component of human pyruvate dehydrogenase complex  
Authors : Kato, M.; Wynn, R.M.; Chuang, J.L.; Tso, S.-C.; Machius, M.; Li, J.; Chuang, D.T.  
Deposited on : 2008-10-16  
Resolution : 3.01 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

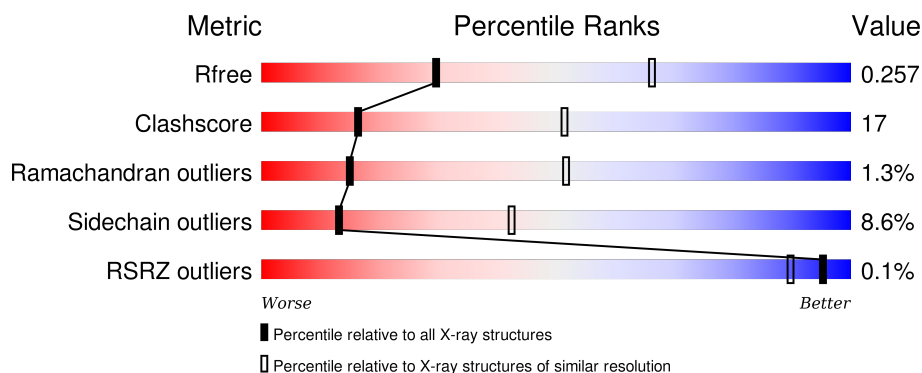
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	1	382	<div> <div>54%</div> <div>29%</div> <div>• • 12%</div> </div>
1	3	382	<div> <div>55%</div> <div>28%</div> <div>6% • 10%</div> </div>
1	5	382	<div> <div>61%</div> <div>22%</div> <div>7% • 9%</div> </div>
1	A	382	<div> <div>53%</div> <div>31%</div> <div>5% • 10%</div> </div>
1	C	382	<div> <div>51%</div> <div>34%</div> <div>• • 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	382	
1	G	382	
1	I	382	
1	K	382	
1	M	382	
1	O	382	
1	Q	382	
1	S	382	
1	U	382	
1	W	382	
1	Y	382	
2	2	329	
2	4	329	
2	6	329	
2	B	329	
2	D	329	
2	F	329	
2	H	329	
2	J	329	
2	L	329	
2	N	329	
2	P	329	
2	R	329	
2	T	329	
2	V	329	

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Mol	Chain	Length	Quality of chain
2	X	329	<div><div></div><div>71%</div><div>24%</div><div>5%</div><div></div></div>
2	Z	329	<div><div></div><div>73%</div><div>24%</div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 83339 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 dehydrogenase E1 component subunit alpha, somatic form, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2677	1684	471	500	22			
1	C	342	Total	C	N	O	S	0	0	0
			2677	1684	471	500	22			
1	E	349	Total	C	N	O	S	0	0	0
			2728	1717	481	508	22			
1	G	346	Total	C	N	O	S	0	0	0
			2712	1707	478	505	22			
1	I	344	Total	C	N	O	S	0	0	0
			2693	1694	473	504	22			
1	K	347	Total	C	N	O	S	0	0	0
			2712	1708	476	506	22			
1	M	349	Total	C	N	O	S	0	0	0
			2728	1717	481	508	22			
1	O	332	Total	C	N	O	S	0	0	0
			2580	1626	449	483	22			
1	Q	344	Total	C	N	O	S	0	0	0
			2693	1694	473	504	22			
1	S	340	Total	C	N	O	S	0	0	0
			2661	1675	466	498	22			
1	U	348	Total	C	N	O	S	0	0	0
			2723	1714	480	507	22			
1	W	345	Total	C	N	O	S	0	0	0
			2705	1702	477	504	22			
1	Y	349	Total	C	N	O	S	0	0	0
			2728	1717	481	508	22			
1	1	335	Total	C	N	O	S	0	0	0
			2614	1647	458	487	22			
1	3	342	Total	C	N	O	S	0	0	0
			2676	1683	469	502	22			
1	5	347	Total	C	N	O	S	0	0	0
			2712	1708	476	506	22			

There are 368 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP P08559
A	-19	GLY	-	EXPRESSION TAG	UNP P08559
A	-18	SER	-	EXPRESSION TAG	UNP P08559
A	-17	SER	-	EXPRESSION TAG	UNP P08559
A	-16	HIS	-	EXPRESSION TAG	UNP P08559
A	-15	HIS	-	EXPRESSION TAG	UNP P08559
A	-14	HIS	-	EXPRESSION TAG	UNP P08559
A	-13	HIS	-	EXPRESSION TAG	UNP P08559
A	-12	HIS	-	EXPRESSION TAG	UNP P08559
A	-11	HIS	-	EXPRESSION TAG	UNP P08559
A	-10	SER	-	EXPRESSION TAG	UNP P08559
A	-9	SER	-	EXPRESSION TAG	UNP P08559
A	-8	GLY	-	EXPRESSION TAG	UNP P08559
A	-7	LEU	-	EXPRESSION TAG	UNP P08559
A	-6	VAL	-	EXPRESSION TAG	UNP P08559
A	-5	PRO	-	EXPRESSION TAG	UNP P08559
A	-4	ARG	-	EXPRESSION TAG	UNP P08559
A	-3	GLY	-	EXPRESSION TAG	UNP P08559
A	-2	SER	-	EXPRESSION TAG	UNP P08559
A	-1	HIS	-	EXPRESSION TAG	UNP P08559
A	0	MET	-	EXPRESSION TAG	UNP P08559
A	203	ALA	SER	ENGINEERED	UNP P08559
A	271	ALA	SER	ENGINEERED	UNP P08559
C	-20	MET	-	EXPRESSION TAG	UNP P08559
C	-19	GLY	-	EXPRESSION TAG	UNP P08559
C	-18	SER	-	EXPRESSION TAG	UNP P08559
C	-17	SER	-	EXPRESSION TAG	UNP P08559
C	-16	HIS	-	EXPRESSION TAG	UNP P08559
C	-15	HIS	-	EXPRESSION TAG	UNP P08559
C	-14	HIS	-	EXPRESSION TAG	UNP P08559
C	-13	HIS	-	EXPRESSION TAG	UNP P08559
C	-12	HIS	-	EXPRESSION TAG	UNP P08559
C	-11	HIS	-	EXPRESSION TAG	UNP P08559
C	-10	SER	-	EXPRESSION TAG	UNP P08559
C	-9	SER	-	EXPRESSION TAG	UNP P08559
C	-8	GLY	-	EXPRESSION TAG	UNP P08559
C	-7	LEU	-	EXPRESSION TAG	UNP P08559
C	-6	VAL	-	EXPRESSION TAG	UNP P08559
C	-5	PRO	-	EXPRESSION TAG	UNP P08559
C	-4	ARG	-	EXPRESSION TAG	UNP P08559
C	-3	GLY	-	EXPRESSION TAG	UNP P08559
C	-2	SER	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	EXPRESSION TAG	UNP P08559
C	0	MET	-	EXPRESSION TAG	UNP P08559
C	203	ALA	SER	ENGINEERED	UNP P08559
C	271	ALA	SER	ENGINEERED	UNP P08559
E	-20	MET	-	EXPRESSION TAG	UNP P08559
E	-19	GLY	-	EXPRESSION TAG	UNP P08559
E	-18	SER	-	EXPRESSION TAG	UNP P08559
E	-17	SER	-	EXPRESSION TAG	UNP P08559
E	-16	HIS	-	EXPRESSION TAG	UNP P08559
E	-15	HIS	-	EXPRESSION TAG	UNP P08559
E	-14	HIS	-	EXPRESSION TAG	UNP P08559
E	-13	HIS	-	EXPRESSION TAG	UNP P08559
E	-12	HIS	-	EXPRESSION TAG	UNP P08559
E	-11	HIS	-	EXPRESSION TAG	UNP P08559
E	-10	SER	-	EXPRESSION TAG	UNP P08559
E	-9	SER	-	EXPRESSION TAG	UNP P08559
E	-8	GLY	-	EXPRESSION TAG	UNP P08559
E	-7	LEU	-	EXPRESSION TAG	UNP P08559
E	-6	VAL	-	EXPRESSION TAG	UNP P08559
E	-5	PRO	-	EXPRESSION TAG	UNP P08559
E	-4	ARG	-	EXPRESSION TAG	UNP P08559
E	-3	GLY	-	EXPRESSION TAG	UNP P08559
E	-2	SER	-	EXPRESSION TAG	UNP P08559
E	-1	HIS	-	EXPRESSION TAG	UNP P08559
E	0	MET	-	EXPRESSION TAG	UNP P08559
E	203	ALA	SER	ENGINEERED	UNP P08559
E	271	ALA	SER	ENGINEERED	UNP P08559
G	-20	MET	-	EXPRESSION TAG	UNP P08559
G	-19	GLY	-	EXPRESSION TAG	UNP P08559
G	-18	SER	-	EXPRESSION TAG	UNP P08559
G	-17	SER	-	EXPRESSION TAG	UNP P08559
G	-16	HIS	-	EXPRESSION TAG	UNP P08559
G	-15	HIS	-	EXPRESSION TAG	UNP P08559
G	-14	HIS	-	EXPRESSION TAG	UNP P08559
G	-13	HIS	-	EXPRESSION TAG	UNP P08559
G	-12	HIS	-	EXPRESSION TAG	UNP P08559
G	-11	HIS	-	EXPRESSION TAG	UNP P08559
G	-10	SER	-	EXPRESSION TAG	UNP P08559
G	-9	SER	-	EXPRESSION TAG	UNP P08559
G	-8	GLY	-	EXPRESSION TAG	UNP P08559
G	-7	LEU	-	EXPRESSION TAG	UNP P08559
G	-6	VAL	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	PRO	-	EXPRESSION TAG	UNP P08559
G	-4	ARG	-	EXPRESSION TAG	UNP P08559
G	-3	GLY	-	EXPRESSION TAG	UNP P08559
G	-2	SER	-	EXPRESSION TAG	UNP P08559
G	-1	HIS	-	EXPRESSION TAG	UNP P08559
G	0	MET	-	EXPRESSION TAG	UNP P08559
G	203	ALA	SER	ENGINEERED	UNP P08559
G	271	ALA	SER	ENGINEERED	UNP P08559
I	-20	MET	-	EXPRESSION TAG	UNP P08559
I	-19	GLY	-	EXPRESSION TAG	UNP P08559
I	-18	SER	-	EXPRESSION TAG	UNP P08559
I	-17	SER	-	EXPRESSION TAG	UNP P08559
I	-16	HIS	-	EXPRESSION TAG	UNP P08559
I	-15	HIS	-	EXPRESSION TAG	UNP P08559
I	-14	HIS	-	EXPRESSION TAG	UNP P08559
I	-13	HIS	-	EXPRESSION TAG	UNP P08559
I	-12	HIS	-	EXPRESSION TAG	UNP P08559
I	-11	HIS	-	EXPRESSION TAG	UNP P08559
I	-10	SER	-	EXPRESSION TAG	UNP P08559
I	-9	SER	-	EXPRESSION TAG	UNP P08559
I	-8	GLY	-	EXPRESSION TAG	UNP P08559
I	-7	LEU	-	EXPRESSION TAG	UNP P08559
I	-6	VAL	-	EXPRESSION TAG	UNP P08559
I	-5	PRO	-	EXPRESSION TAG	UNP P08559
I	-4	ARG	-	EXPRESSION TAG	UNP P08559
I	-3	GLY	-	EXPRESSION TAG	UNP P08559
I	-2	SER	-	EXPRESSION TAG	UNP P08559
I	-1	HIS	-	EXPRESSION TAG	UNP P08559
I	0	MET	-	EXPRESSION TAG	UNP P08559
I	203	ALA	SER	ENGINEERED	UNP P08559
I	271	ALA	SER	ENGINEERED	UNP P08559
K	-20	MET	-	EXPRESSION TAG	UNP P08559
K	-19	GLY	-	EXPRESSION TAG	UNP P08559
K	-18	SER	-	EXPRESSION TAG	UNP P08559
K	-17	SER	-	EXPRESSION TAG	UNP P08559
K	-16	HIS	-	EXPRESSION TAG	UNP P08559
K	-15	HIS	-	EXPRESSION TAG	UNP P08559
K	-14	HIS	-	EXPRESSION TAG	UNP P08559
K	-13	HIS	-	EXPRESSION TAG	UNP P08559
K	-12	HIS	-	EXPRESSION TAG	UNP P08559
K	-11	HIS	-	EXPRESSION TAG	UNP P08559
K	-10	SER	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	EXPRESSION TAG	UNP P08559
K	-8	GLY	-	EXPRESSION TAG	UNP P08559
K	-7	LEU	-	EXPRESSION TAG	UNP P08559
K	-6	VAL	-	EXPRESSION TAG	UNP P08559
K	-5	PRO	-	EXPRESSION TAG	UNP P08559
K	-4	ARG	-	EXPRESSION TAG	UNP P08559
K	-3	GLY	-	EXPRESSION TAG	UNP P08559
K	-2	SER	-	EXPRESSION TAG	UNP P08559
K	-1	HIS	-	EXPRESSION TAG	UNP P08559
K	0	MET	-	EXPRESSION TAG	UNP P08559
K	203	ALA	SER	ENGINEERED	UNP P08559
K	271	ALA	SER	ENGINEERED	UNP P08559
M	-20	MET	-	EXPRESSION TAG	UNP P08559
M	-19	GLY	-	EXPRESSION TAG	UNP P08559
M	-18	SER	-	EXPRESSION TAG	UNP P08559
M	-17	SER	-	EXPRESSION TAG	UNP P08559
M	-16	HIS	-	EXPRESSION TAG	UNP P08559
M	-15	HIS	-	EXPRESSION TAG	UNP P08559
M	-14	HIS	-	EXPRESSION TAG	UNP P08559
M	-13	HIS	-	EXPRESSION TAG	UNP P08559
M	-12	HIS	-	EXPRESSION TAG	UNP P08559
M	-11	HIS	-	EXPRESSION TAG	UNP P08559
M	-10	SER	-	EXPRESSION TAG	UNP P08559
M	-9	SER	-	EXPRESSION TAG	UNP P08559
M	-8	GLY	-	EXPRESSION TAG	UNP P08559
M	-7	LEU	-	EXPRESSION TAG	UNP P08559
M	-6	VAL	-	EXPRESSION TAG	UNP P08559
M	-5	PRO	-	EXPRESSION TAG	UNP P08559
M	-4	ARG	-	EXPRESSION TAG	UNP P08559
M	-3	GLY	-	EXPRESSION TAG	UNP P08559
M	-2	SER	-	EXPRESSION TAG	UNP P08559
M	-1	HIS	-	EXPRESSION TAG	UNP P08559
M	0	MET	-	EXPRESSION TAG	UNP P08559
M	203	ALA	SER	ENGINEERED	UNP P08559
M	271	ALA	SER	ENGINEERED	UNP P08559
O	-20	MET	-	EXPRESSION TAG	UNP P08559
O	-19	GLY	-	EXPRESSION TAG	UNP P08559
O	-18	SER	-	EXPRESSION TAG	UNP P08559
O	-17	SER	-	EXPRESSION TAG	UNP P08559
O	-16	HIS	-	EXPRESSION TAG	UNP P08559
O	-15	HIS	-	EXPRESSION TAG	UNP P08559
O	-14	HIS	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-13	HIS	-	EXPRESSION TAG	UNP P08559
O	-12	HIS	-	EXPRESSION TAG	UNP P08559
O	-11	HIS	-	EXPRESSION TAG	UNP P08559
O	-10	SER	-	EXPRESSION TAG	UNP P08559
O	-9	SER	-	EXPRESSION TAG	UNP P08559
O	-8	GLY	-	EXPRESSION TAG	UNP P08559
O	-7	LEU	-	EXPRESSION TAG	UNP P08559
O	-6	VAL	-	EXPRESSION TAG	UNP P08559
O	-5	PRO	-	EXPRESSION TAG	UNP P08559
O	-4	ARG	-	EXPRESSION TAG	UNP P08559
O	-3	GLY	-	EXPRESSION TAG	UNP P08559
O	-2	SER	-	EXPRESSION TAG	UNP P08559
O	-1	HIS	-	EXPRESSION TAG	UNP P08559
O	0	MET	-	EXPRESSION TAG	UNP P08559
O	203	ALA	SER	ENGINEERED	UNP P08559
O	271	ALA	SER	ENGINEERED	UNP P08559
Q	-20	MET	-	EXPRESSION TAG	UNP P08559
Q	-19	GLY	-	EXPRESSION TAG	UNP P08559
Q	-18	SER	-	EXPRESSION TAG	UNP P08559
Q	-17	SER	-	EXPRESSION TAG	UNP P08559
Q	-16	HIS	-	EXPRESSION TAG	UNP P08559
Q	-15	HIS	-	EXPRESSION TAG	UNP P08559
Q	-14	HIS	-	EXPRESSION TAG	UNP P08559
Q	-13	HIS	-	EXPRESSION TAG	UNP P08559
Q	-12	HIS	-	EXPRESSION TAG	UNP P08559
Q	-11	HIS	-	EXPRESSION TAG	UNP P08559
Q	-10	SER	-	EXPRESSION TAG	UNP P08559
Q	-9	SER	-	EXPRESSION TAG	UNP P08559
Q	-8	GLY	-	EXPRESSION TAG	UNP P08559
Q	-7	LEU	-	EXPRESSION TAG	UNP P08559
Q	-6	VAL	-	EXPRESSION TAG	UNP P08559
Q	-5	PRO	-	EXPRESSION TAG	UNP P08559
Q	-4	ARG	-	EXPRESSION TAG	UNP P08559
Q	-3	GLY	-	EXPRESSION TAG	UNP P08559
Q	-2	SER	-	EXPRESSION TAG	UNP P08559
Q	-1	HIS	-	EXPRESSION TAG	UNP P08559
Q	0	MET	-	EXPRESSION TAG	UNP P08559
Q	203	ALA	SER	ENGINEERED	UNP P08559
Q	271	ALA	SER	ENGINEERED	UNP P08559
S	-20	MET	-	EXPRESSION TAG	UNP P08559
S	-19	GLY	-	EXPRESSION TAG	UNP P08559
S	-18	SER	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-17	SER	-	EXPRESSION TAG	UNP P08559
S	-16	HIS	-	EXPRESSION TAG	UNP P08559
S	-15	HIS	-	EXPRESSION TAG	UNP P08559
S	-14	HIS	-	EXPRESSION TAG	UNP P08559
S	-13	HIS	-	EXPRESSION TAG	UNP P08559
S	-12	HIS	-	EXPRESSION TAG	UNP P08559
S	-11	HIS	-	EXPRESSION TAG	UNP P08559
S	-10	SER	-	EXPRESSION TAG	UNP P08559
S	-9	SER	-	EXPRESSION TAG	UNP P08559
S	-8	GLY	-	EXPRESSION TAG	UNP P08559
S	-7	LEU	-	EXPRESSION TAG	UNP P08559
S	-6	VAL	-	EXPRESSION TAG	UNP P08559
S	-5	PRO	-	EXPRESSION TAG	UNP P08559
S	-4	ARG	-	EXPRESSION TAG	UNP P08559
S	-3	GLY	-	EXPRESSION TAG	UNP P08559
S	-2	SER	-	EXPRESSION TAG	UNP P08559
S	-1	HIS	-	EXPRESSION TAG	UNP P08559
S	0	MET	-	EXPRESSION TAG	UNP P08559
S	203	ALA	SER	ENGINEERED	UNP P08559
S	271	ALA	SER	ENGINEERED	UNP P08559
U	-20	MET	-	EXPRESSION TAG	UNP P08559
U	-19	GLY	-	EXPRESSION TAG	UNP P08559
U	-18	SER	-	EXPRESSION TAG	UNP P08559
U	-17	SER	-	EXPRESSION TAG	UNP P08559
U	-16	HIS	-	EXPRESSION TAG	UNP P08559
U	-15	HIS	-	EXPRESSION TAG	UNP P08559
U	-14	HIS	-	EXPRESSION TAG	UNP P08559
U	-13	HIS	-	EXPRESSION TAG	UNP P08559
U	-12	HIS	-	EXPRESSION TAG	UNP P08559
U	-11	HIS	-	EXPRESSION TAG	UNP P08559
U	-10	SER	-	EXPRESSION TAG	UNP P08559
U	-9	SER	-	EXPRESSION TAG	UNP P08559
U	-8	GLY	-	EXPRESSION TAG	UNP P08559
U	-7	LEU	-	EXPRESSION TAG	UNP P08559
U	-6	VAL	-	EXPRESSION TAG	UNP P08559
U	-5	PRO	-	EXPRESSION TAG	UNP P08559
U	-4	ARG	-	EXPRESSION TAG	UNP P08559
U	-3	GLY	-	EXPRESSION TAG	UNP P08559
U	-2	SER	-	EXPRESSION TAG	UNP P08559
U	-1	HIS	-	EXPRESSION TAG	UNP P08559
U	0	MET	-	EXPRESSION TAG	UNP P08559
U	203	ALA	SER	ENGINEERED	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
U	271	ALA	SER	ENGINEERED	UNP P08559
W	-20	MET	-	EXPRESSION TAG	UNP P08559
W	-19	GLY	-	EXPRESSION TAG	UNP P08559
W	-18	SER	-	EXPRESSION TAG	UNP P08559
W	-17	SER	-	EXPRESSION TAG	UNP P08559
W	-16	HIS	-	EXPRESSION TAG	UNP P08559
W	-15	HIS	-	EXPRESSION TAG	UNP P08559
W	-14	HIS	-	EXPRESSION TAG	UNP P08559
W	-13	HIS	-	EXPRESSION TAG	UNP P08559
W	-12	HIS	-	EXPRESSION TAG	UNP P08559
W	-11	HIS	-	EXPRESSION TAG	UNP P08559
W	-10	SER	-	EXPRESSION TAG	UNP P08559
W	-9	SER	-	EXPRESSION TAG	UNP P08559
W	-8	GLY	-	EXPRESSION TAG	UNP P08559
W	-7	LEU	-	EXPRESSION TAG	UNP P08559
W	-6	VAL	-	EXPRESSION TAG	UNP P08559
W	-5	PRO	-	EXPRESSION TAG	UNP P08559
W	-4	ARG	-	EXPRESSION TAG	UNP P08559
W	-3	GLY	-	EXPRESSION TAG	UNP P08559
W	-2	SER	-	EXPRESSION TAG	UNP P08559
W	-1	HIS	-	EXPRESSION TAG	UNP P08559
W	0	MET	-	EXPRESSION TAG	UNP P08559
W	203	ALA	SER	ENGINEERED	UNP P08559
W	271	ALA	SER	ENGINEERED	UNP P08559
Y	-20	MET	-	EXPRESSION TAG	UNP P08559
Y	-19	GLY	-	EXPRESSION TAG	UNP P08559
Y	-18	SER	-	EXPRESSION TAG	UNP P08559
Y	-17	SER	-	EXPRESSION TAG	UNP P08559
Y	-16	HIS	-	EXPRESSION TAG	UNP P08559
Y	-15	HIS	-	EXPRESSION TAG	UNP P08559
Y	-14	HIS	-	EXPRESSION TAG	UNP P08559
Y	-13	HIS	-	EXPRESSION TAG	UNP P08559
Y	-12	HIS	-	EXPRESSION TAG	UNP P08559
Y	-11	HIS	-	EXPRESSION TAG	UNP P08559
Y	-10	SER	-	EXPRESSION TAG	UNP P08559
Y	-9	SER	-	EXPRESSION TAG	UNP P08559
Y	-8	GLY	-	EXPRESSION TAG	UNP P08559
Y	-7	LEU	-	EXPRESSION TAG	UNP P08559
Y	-6	VAL	-	EXPRESSION TAG	UNP P08559
Y	-5	PRO	-	EXPRESSION TAG	UNP P08559
Y	-4	ARG	-	EXPRESSION TAG	UNP P08559
Y	-3	GLY	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-2	SER	-	EXPRESSION TAG	UNP P08559
Y	-1	HIS	-	EXPRESSION TAG	UNP P08559
Y	0	MET	-	EXPRESSION TAG	UNP P08559
Y	203	ALA	SER	ENGINEERED	UNP P08559
Y	271	ALA	SER	ENGINEERED	UNP P08559
1	-20	MET	-	EXPRESSION TAG	UNP P08559
1	-19	GLY	-	EXPRESSION TAG	UNP P08559
1	-18	SER	-	EXPRESSION TAG	UNP P08559
1	-17	SER	-	EXPRESSION TAG	UNP P08559
1	-16	HIS	-	EXPRESSION TAG	UNP P08559
1	-15	HIS	-	EXPRESSION TAG	UNP P08559
1	-14	HIS	-	EXPRESSION TAG	UNP P08559
1	-13	HIS	-	EXPRESSION TAG	UNP P08559
1	-12	HIS	-	EXPRESSION TAG	UNP P08559
1	-11	HIS	-	EXPRESSION TAG	UNP P08559
1	-10	SER	-	EXPRESSION TAG	UNP P08559
1	-9	SER	-	EXPRESSION TAG	UNP P08559
1	-8	GLY	-	EXPRESSION TAG	UNP P08559
1	-7	LEU	-	EXPRESSION TAG	UNP P08559
1	-6	VAL	-	EXPRESSION TAG	UNP P08559
1	-5	PRO	-	EXPRESSION TAG	UNP P08559
1	-4	ARG	-	EXPRESSION TAG	UNP P08559
1	-3	GLY	-	EXPRESSION TAG	UNP P08559
1	-2	SER	-	EXPRESSION TAG	UNP P08559
1	-1	HIS	-	EXPRESSION TAG	UNP P08559
1	0	MET	-	EXPRESSION TAG	UNP P08559
1	203	ALA	SER	ENGINEERED	UNP P08559
1	271	ALA	SER	ENGINEERED	UNP P08559
3	-20	MET	-	EXPRESSION TAG	UNP P08559
3	-19	GLY	-	EXPRESSION TAG	UNP P08559
3	-18	SER	-	EXPRESSION TAG	UNP P08559
3	-17	SER	-	EXPRESSION TAG	UNP P08559
3	-16	HIS	-	EXPRESSION TAG	UNP P08559
3	-15	HIS	-	EXPRESSION TAG	UNP P08559
3	-14	HIS	-	EXPRESSION TAG	UNP P08559
3	-13	HIS	-	EXPRESSION TAG	UNP P08559
3	-12	HIS	-	EXPRESSION TAG	UNP P08559
3	-11	HIS	-	EXPRESSION TAG	UNP P08559
3	-10	SER	-	EXPRESSION TAG	UNP P08559
3	-9	SER	-	EXPRESSION TAG	UNP P08559
3	-8	GLY	-	EXPRESSION TAG	UNP P08559
3	-7	LEU	-	EXPRESSION TAG	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-6	VAL	-	EXPRESSION TAG	UNP P08559
3	-5	PRO	-	EXPRESSION TAG	UNP P08559
3	-4	ARG	-	EXPRESSION TAG	UNP P08559
3	-3	GLY	-	EXPRESSION TAG	UNP P08559
3	-2	SER	-	EXPRESSION TAG	UNP P08559
3	-1	HIS	-	EXPRESSION TAG	UNP P08559
3	0	MET	-	EXPRESSION TAG	UNP P08559
3	203	ALA	SER	ENGINEERED	UNP P08559
3	271	ALA	SER	ENGINEERED	UNP P08559
5	-20	MET	-	EXPRESSION TAG	UNP P08559
5	-19	GLY	-	EXPRESSION TAG	UNP P08559
5	-18	SER	-	EXPRESSION TAG	UNP P08559
5	-17	SER	-	EXPRESSION TAG	UNP P08559
5	-16	HIS	-	EXPRESSION TAG	UNP P08559
5	-15	HIS	-	EXPRESSION TAG	UNP P08559
5	-14	HIS	-	EXPRESSION TAG	UNP P08559
5	-13	HIS	-	EXPRESSION TAG	UNP P08559
5	-12	HIS	-	EXPRESSION TAG	UNP P08559
5	-11	HIS	-	EXPRESSION TAG	UNP P08559
5	-10	SER	-	EXPRESSION TAG	UNP P08559
5	-9	SER	-	EXPRESSION TAG	UNP P08559
5	-8	GLY	-	EXPRESSION TAG	UNP P08559
5	-7	LEU	-	EXPRESSION TAG	UNP P08559
5	-6	VAL	-	EXPRESSION TAG	UNP P08559
5	-5	PRO	-	EXPRESSION TAG	UNP P08559
5	-4	ARG	-	EXPRESSION TAG	UNP P08559
5	-3	GLY	-	EXPRESSION TAG	UNP P08559
5	-2	SER	-	EXPRESSION TAG	UNP P08559
5	-1	HIS	-	EXPRESSION TAG	UNP P08559
5	0	MET	-	EXPRESSION TAG	UNP P08559
5	203	ALA	SER	ENGINEERED	UNP P08559
5	271	ALA	SER	ENGINEERED	UNP P08559

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	D	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	F	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	J	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	L	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	N	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	P	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	R	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	T	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	V	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	X	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	Z	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	2	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	4	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	6	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	K	0	0
			1	1		
3	J	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	H	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	V	1	Total	K	0	0
			1	1		

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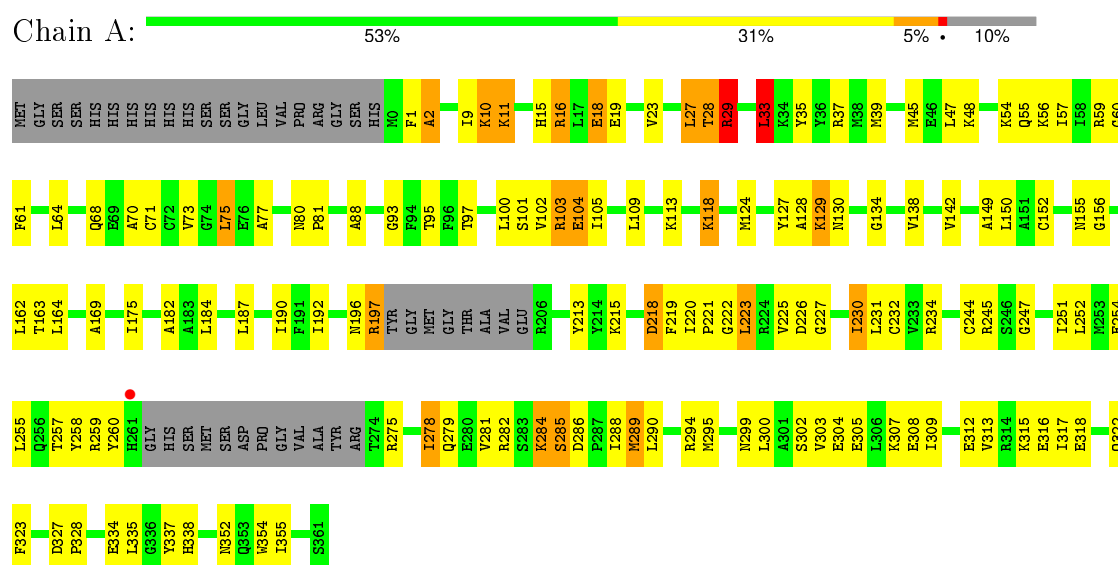
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Z	1	Total 1	K 1	0	0
3	T	1	Total 1	K 1	0	0
3	6	1	Total 1	K 1	0	0
3	N	1	Total 1	K 1	0	0
3	X	1	Total 1	K 1	0	0
3	4	1	Total 1	K 1	0	0
3	R	1	Total 1	K 1	0	0
3	L	1	Total 1	K 1	0	0
3	2	1	Total 1	K 1	0	0
3	F	1	Total 1	K 1	0	0



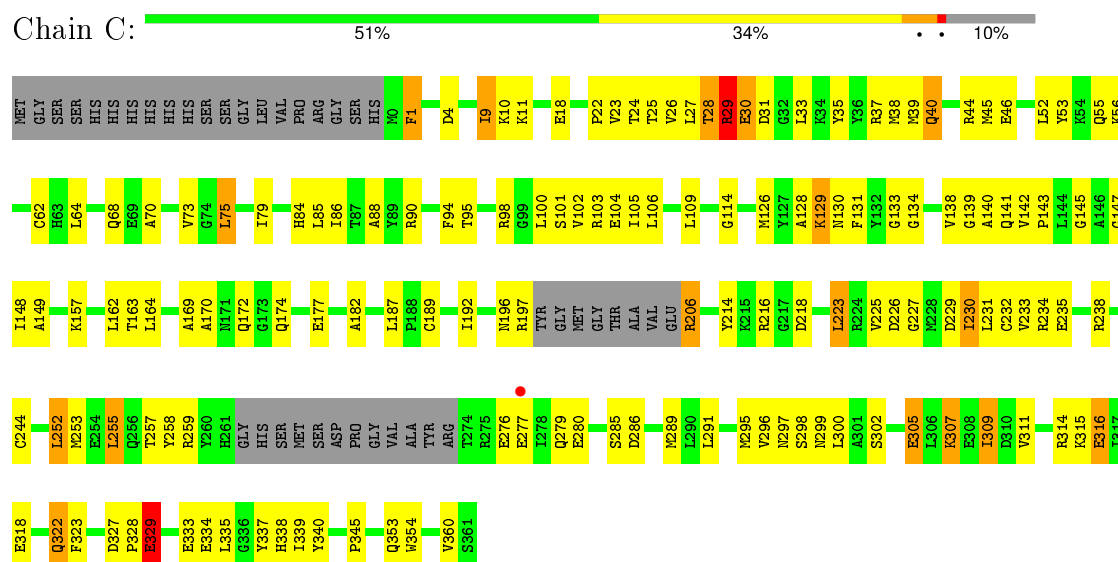
### 3 Residue-property plots

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 dehydrogenase E1 component subunit alpha, somatic form, mitochondrial



- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

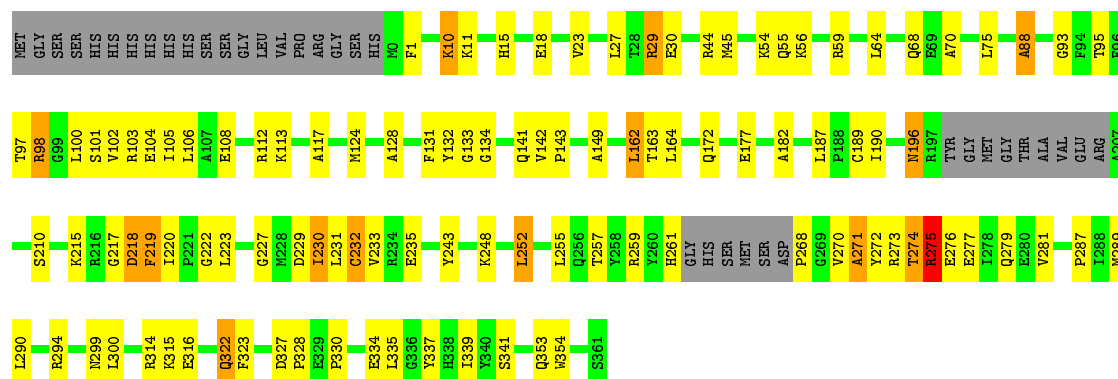


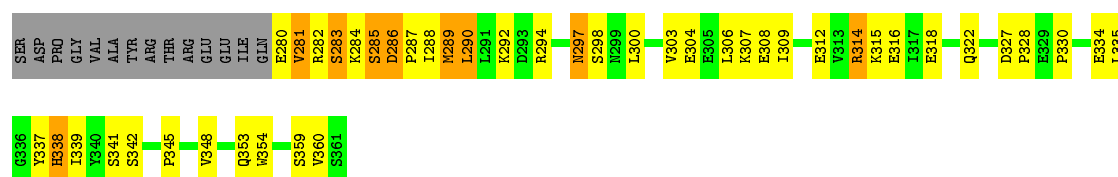


V360  
S361

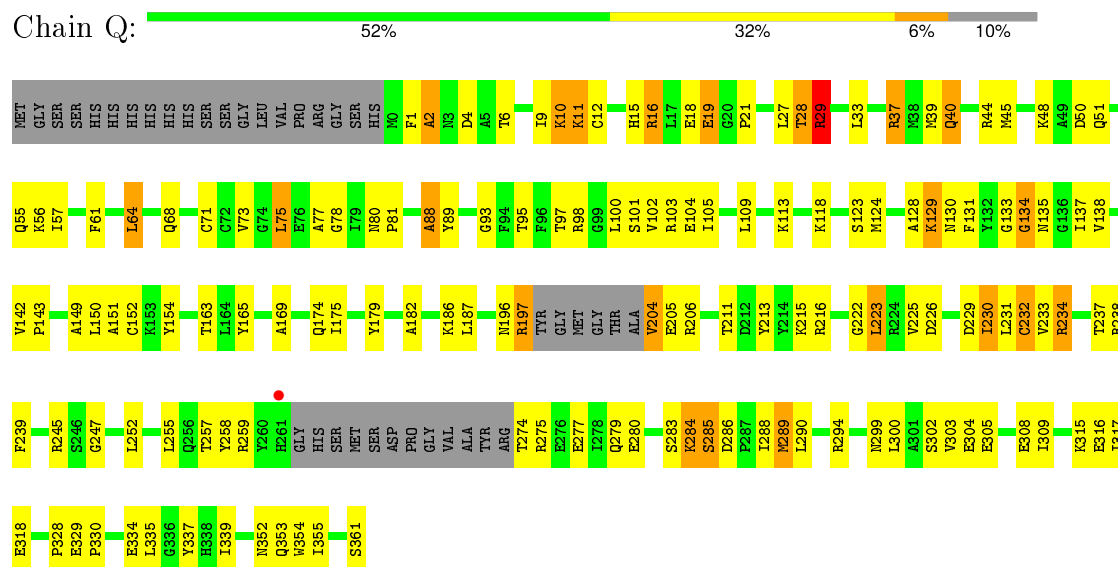
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain K: 62% 25% 9%

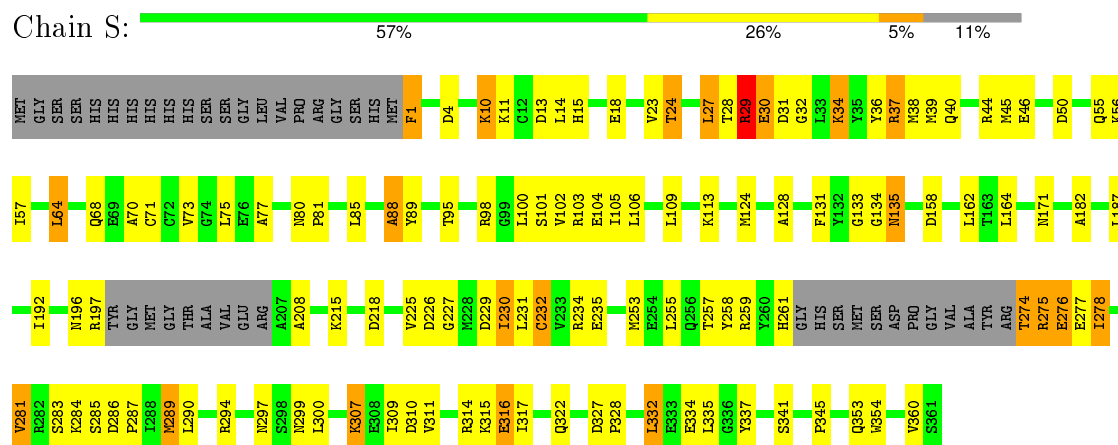




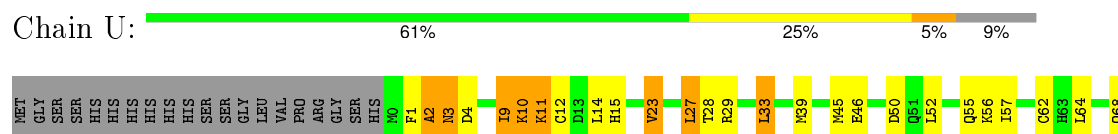
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

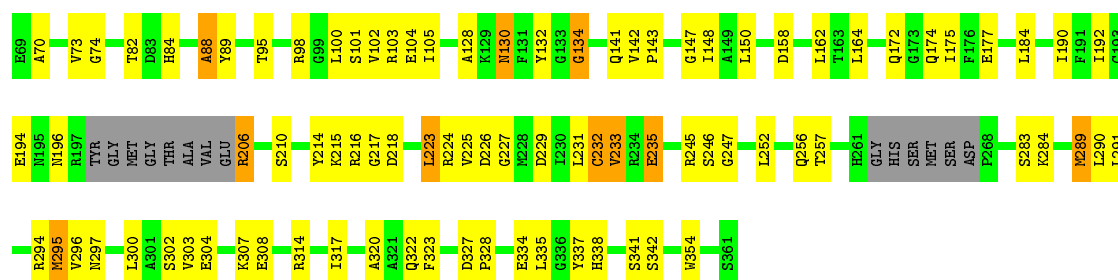


- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial



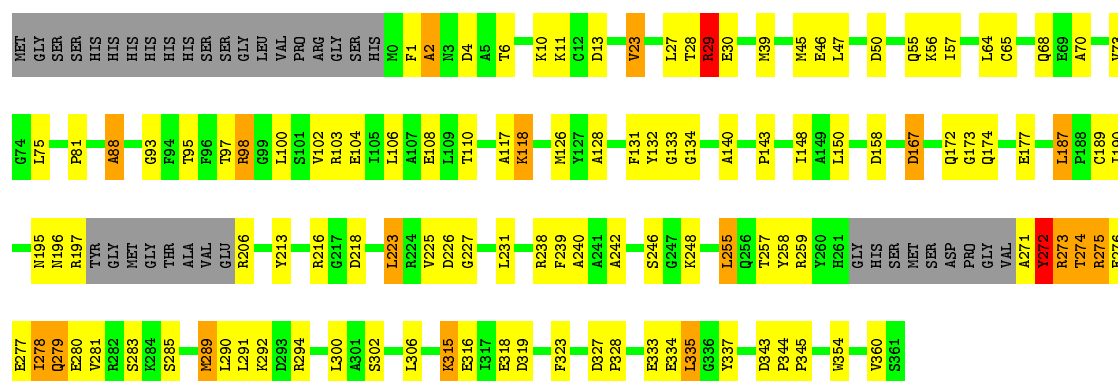
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial





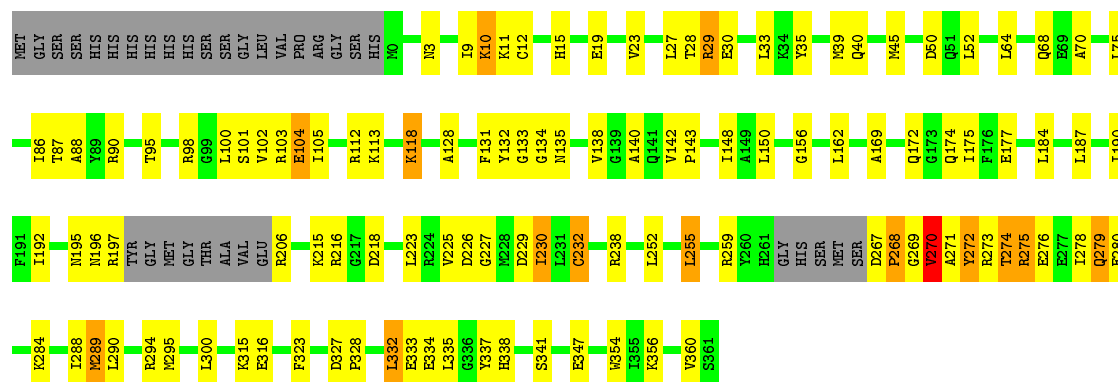
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain W: 59% 26% 10%



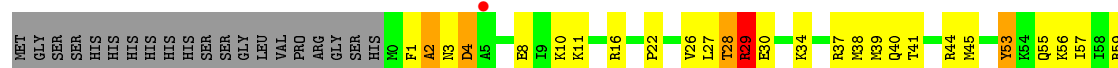
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain Y: 61% 26% 9%

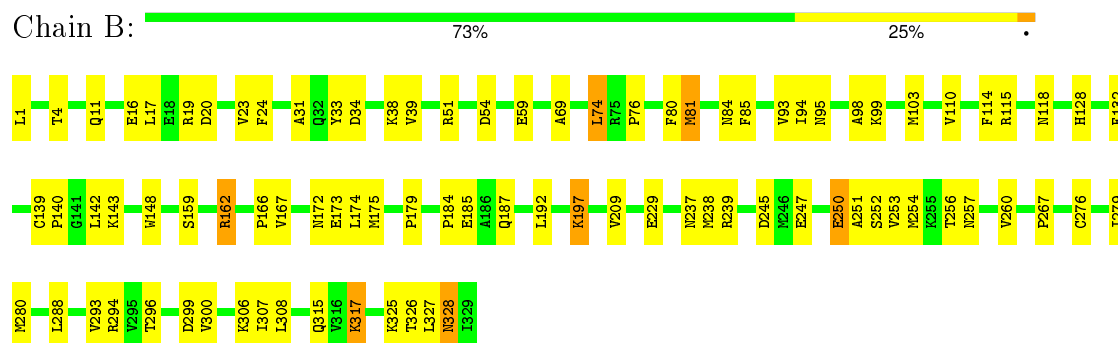


- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

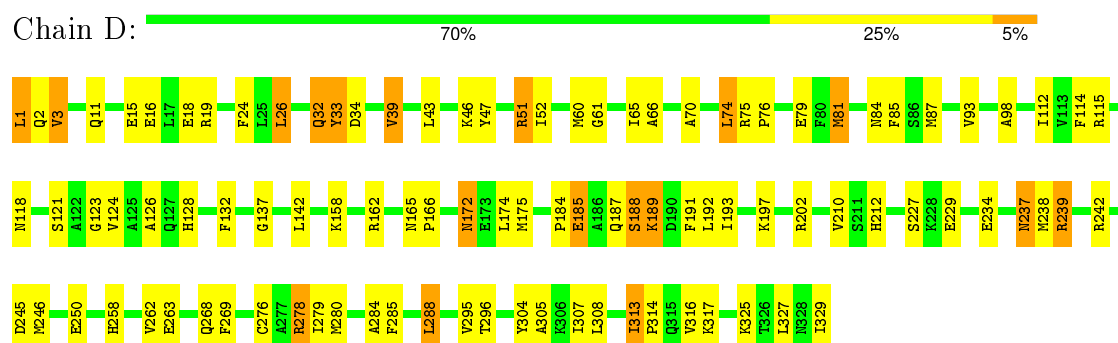
Chain 1: 54% 29% 12%



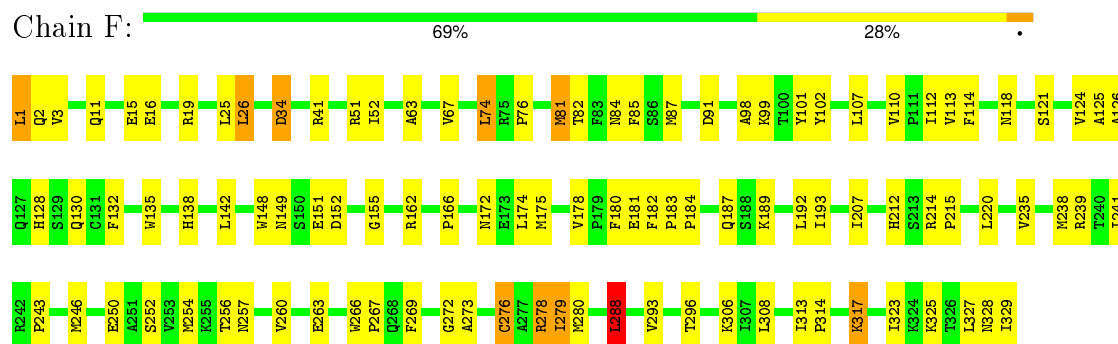




- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



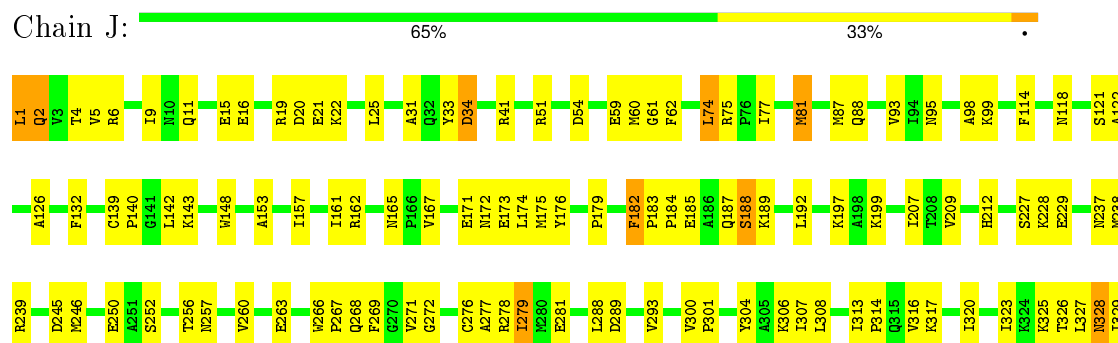
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



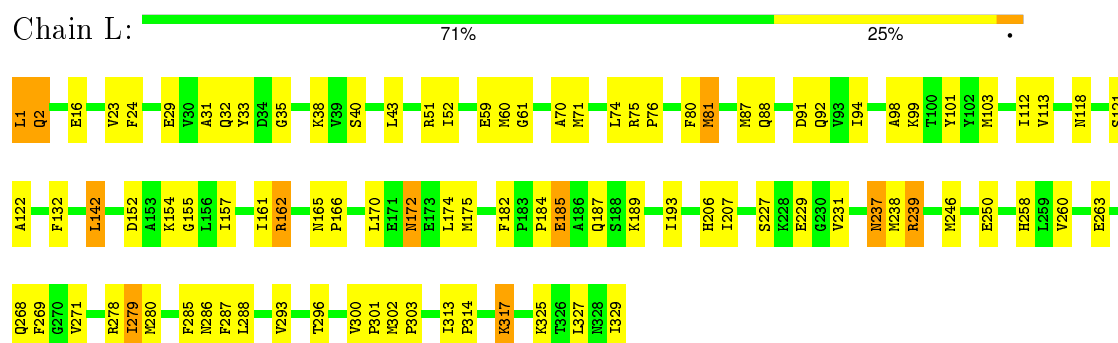
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



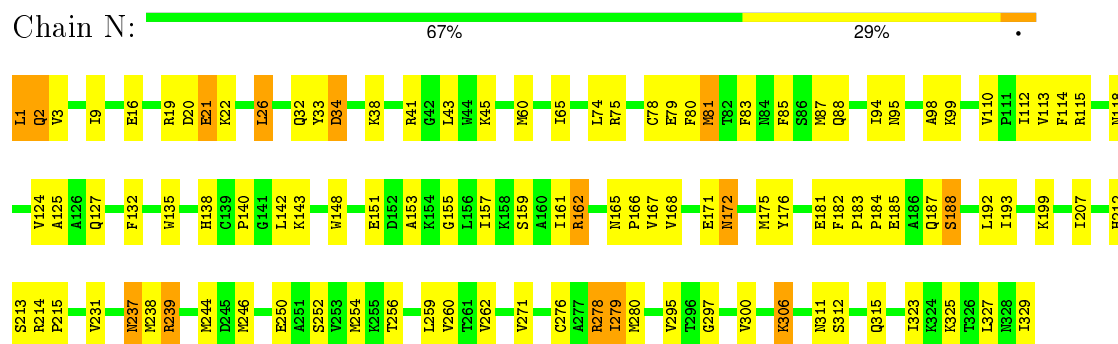
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



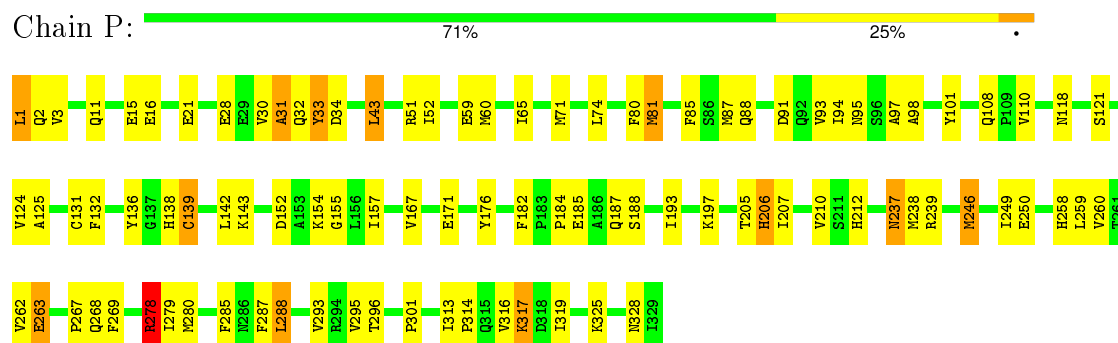
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



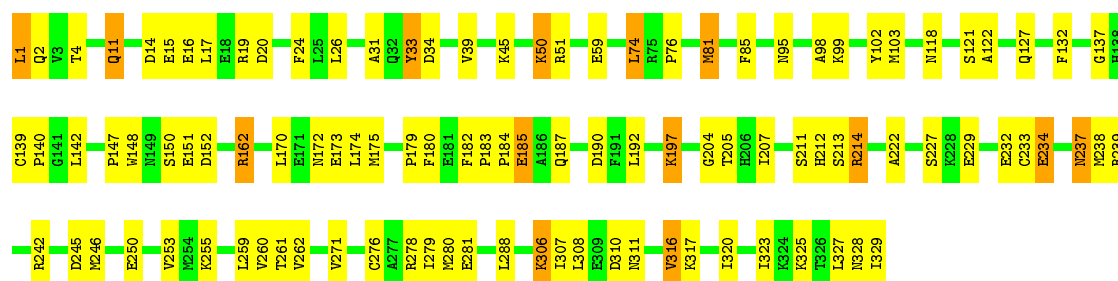
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

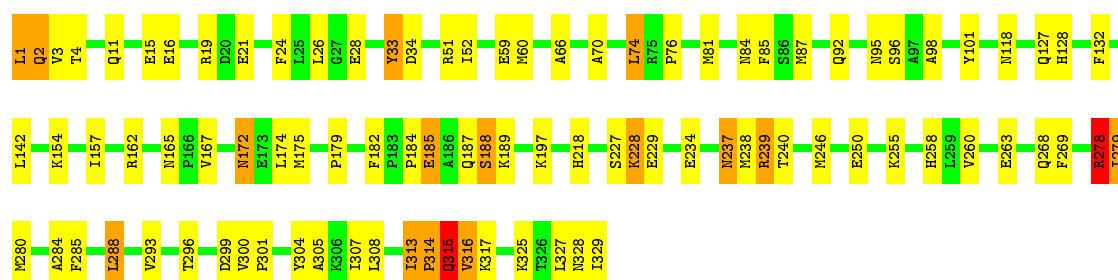


Chain R:  68% 28%



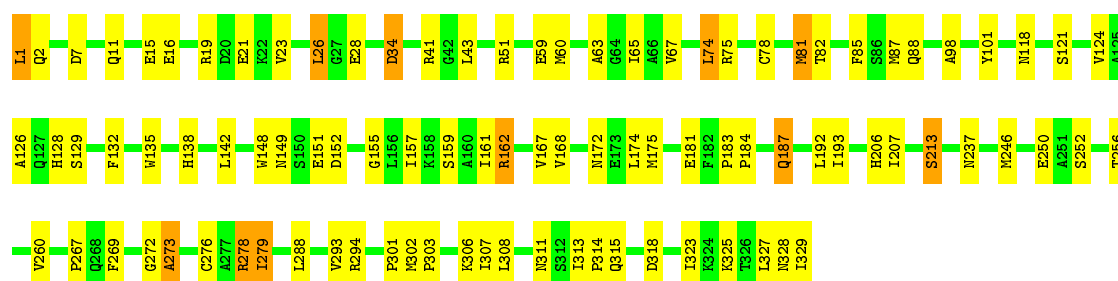
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain T:  72% 23% 5%



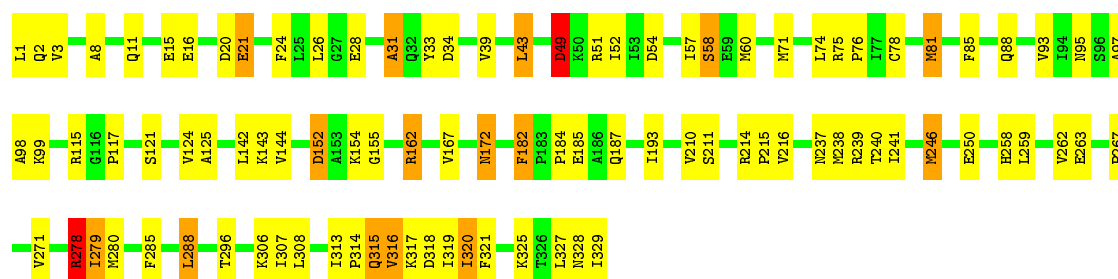
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain V:  71% 26%

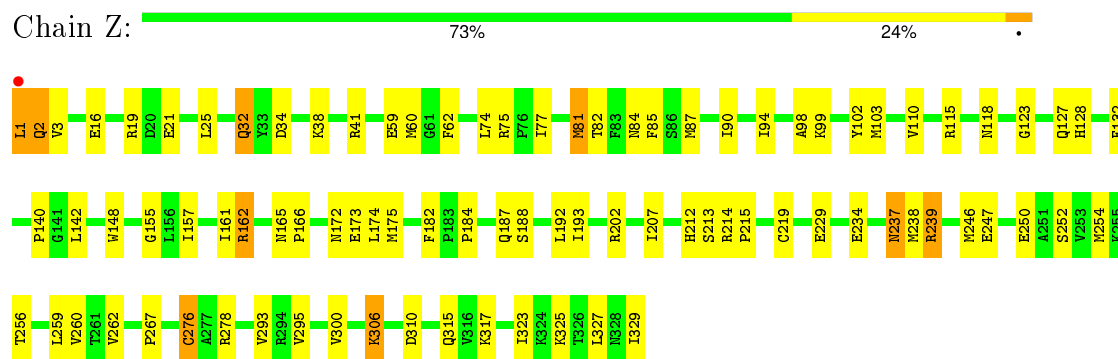


- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

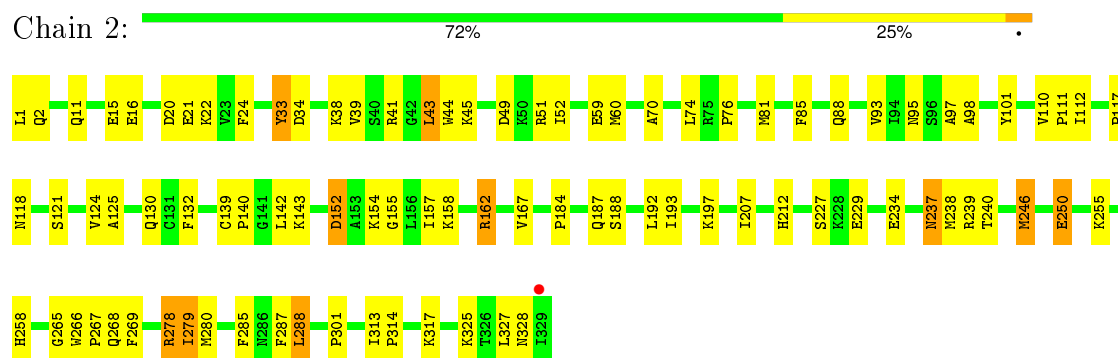
Chain X:  71% 24% 5%



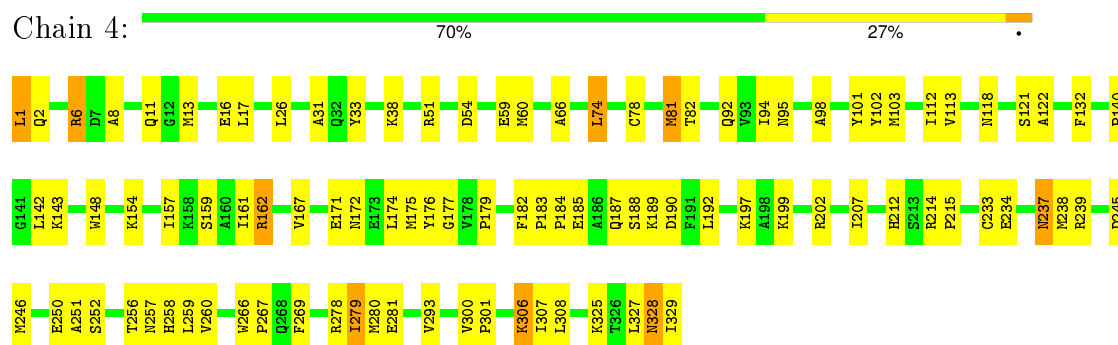
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



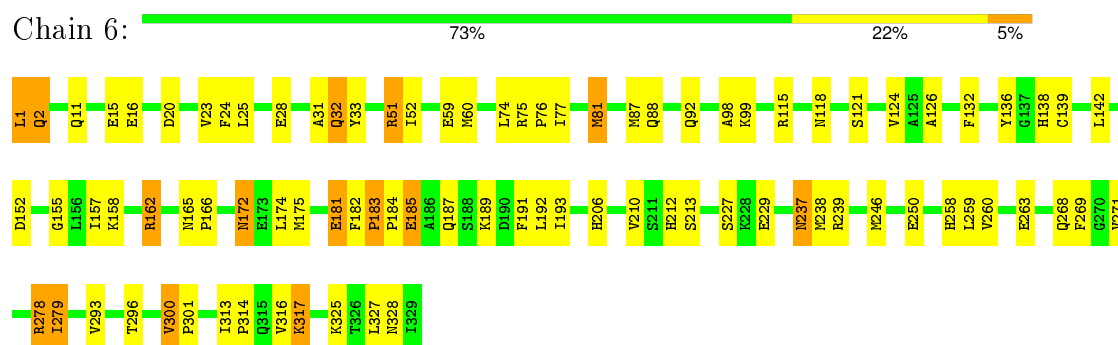
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.28Å 128.29Å 228.41Å 90.14° 90.05° 90.02°	Depositor
Resolution (Å)	50.00 – 3.01 49.11 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-3.01) 97.9 (49.11-3.01)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.4	Depositor
R, $R_{free}$	0.189 , 0.253 0.196 , 0.257	Depositor DCC
$R_{free}$ test set	13221 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.429 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 262510 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	83339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.55 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1273e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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:  
K

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	1	0.79	1/2663 (0.0%)	0.87	2/3583 (0.1%)
1	3	0.87	3/2725 (0.1%)	0.91	3/3666 (0.1%)
1	5	0.78	2/2764 (0.1%)	0.83	2/3720 (0.1%)
1	A	0.93	2/2727 (0.1%)	0.94	3/3669 (0.1%)
1	C	0.92	3/2727 (0.1%)	0.92	2/3669 (0.1%)
1	E	0.91	1/2780 (0.0%)	0.96	1/3742 (0.0%)
1	G	0.90	4/2763 (0.1%)	0.93	3/3718 (0.1%)
1	I	0.88	1/2743 (0.0%)	0.90	3/3691 (0.1%)
1	K	0.81	0/2764	0.85	1/3720 (0.0%)
1	M	0.90	3/2780 (0.1%)	0.93	2/3742 (0.1%)
1	O	0.81	0/2628	0.89	3/3537 (0.1%)
1	Q	0.86	1/2743 (0.0%)	0.93	5/3691 (0.1%)
1	S	0.86	0/2711	0.92	3/3648 (0.1%)
1	U	0.94	2/2775 (0.1%)	0.95	1/3734 (0.0%)
1	W	0.88	1/2756 (0.0%)	0.93	3/3708 (0.1%)
1	Y	0.93	2/2780 (0.1%)	0.93	1/3742 (0.0%)
2	2	0.90	2/2574 (0.1%)	0.93	2/3488 (0.1%)
2	4	0.87	1/2574 (0.0%)	0.93	1/3488 (0.0%)
2	6	0.90	2/2574 (0.1%)	0.94	7/3488 (0.2%)
2	B	1.00	3/2574 (0.1%)	0.98	3/3488 (0.1%)
2	D	0.95	0/2574	0.99	7/3488 (0.2%)
2	F	0.95	0/2574	0.94	3/3488 (0.1%)
2	H	0.93	1/2574 (0.0%)	0.93	1/3488 (0.0%)
2	J	0.89	1/2574 (0.0%)	0.92	2/3488 (0.1%)
2	L	0.90	0/2574	0.93	3/3488 (0.1%)
2	N	0.87	1/2574 (0.0%)	0.90	4/3488 (0.1%)
2	P	0.91	1/2574 (0.0%)	0.95	4/3488 (0.1%)
2	R	0.95	1/2574 (0.0%)	0.97	5/3488 (0.1%)
2	T	0.92	0/2574	0.96	5/3488 (0.1%)
2	V	0.91	1/2574 (0.0%)	0.94	1/3488 (0.0%)
2	X	0.90	0/2574	0.94	4/3488 (0.1%)
2	Z	0.87	2/2574 (0.1%)	0.88	3/3488 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.89	42/85013 (0.0%)	0.93	93/114788 (0.1%)

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	232	CYS	CB-SG	-10.74	1.64	1.82
1	5	232	CYS	CB-SG	-7.94	1.68	1.82
1	M	232	CYS	CB-SG	-7.92	1.68	1.82
2	B	276	CYS	CB-SG	-7.73	1.69	1.82
1	W	189	CYS	CB-SG	-7.02	1.70	1.82

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	ARG	NE-CZ-NH1	10.01	125.31	120.30
2	P	278	ARG	NE-CZ-NH2	-9.34	115.63	120.30
2	P	278	ARG	NE-CZ-NH1	9.10	124.85	120.30
2	2	278	ARG	NE-CZ-NH2	-8.95	115.83	120.30
2	D	278	ARG	NE-CZ-NH2	-8.14	116.23	120.30

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	1	2614	0	2587	120	0
1	3	2676	0	2644	123	0
1	5	2712	0	2679	115	0
1	A	2677	0	2645	136	0
1	C	2677	0	2645	116	0
1	E	2728	0	2693	93	0
1	G	2712	0	2681	103	0
1	I	2693	0	2660	88	0
1	K	2712	0	2679	97	0
1	M	2728	0	2693	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2580	0	2552	119	0
1	Q	2693	0	2660	122	0
1	S	2661	0	2630	130	0
1	U	2723	0	2692	87	0
1	W	2705	0	2672	95	0
1	Y	2728	0	2693	93	0
2	2	2519	0	2517	72	0
2	4	2519	0	2517	82	0
2	6	2519	0	2517	74	0
2	B	2519	0	2517	60	0
2	D	2519	0	2517	77	0
2	F	2519	0	2517	86	0
2	H	2519	0	2517	81	0
2	J	2519	0	2517	85	0
2	L	2519	0	2517	79	0
2	N	2519	0	2517	78	0
2	P	2519	0	2517	70	0
2	R	2519	0	2517	77	0
2	T	2519	0	2517	81	0
2	V	2519	0	2517	73	0
2	X	2519	0	2517	79	0
2	Z	2519	0	2517	70	0
3	2	1	0	0	0	0
3	4	1	0	0	0	0
3	6	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	T	1	0	0	0	0
3	V	1	0	0	0	0
3	X	1	0	0	0	0
3	Z	1	0	0	0	0
All	All	83339	0	82777	2778	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 17.

The worst 5 of 2778 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:O:231:LEU:HD12	1:O:294:ARG:NH1	1.20	1.50
1:A:289:MET:CE	1:A:290:LEU:HD23	1.60	1.30
1:G:270:VAL:HG12	1:G:273:ARG:NH2	1.51	1.22
1:M:268:PRO:HB2	1:M:270:VAL:HG23	1.21	1.17
1:1:280:GLU:HG2	1:1:281:VAL:N	1.55	1.17

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	1	329/382 (86%)	295 (90%)	25 (8%)	9 (3%)	6	30
1	3	336/382 (88%)	305 (91%)	25 (7%)	6 (2%)	11	43
1	5	341/382 (89%)	306 (90%)	22 (6%)	13 (4%)	4	21
1	A	336/382 (88%)	311 (93%)	20 (6%)	5 (2%)	13	48
1	C	336/382 (88%)	303 (90%)	28 (8%)	5 (2%)	13	48
1	E	343/382 (90%)	313 (91%)	23 (7%)	7 (2%)	9	39
1	G	340/382 (89%)	305 (90%)	29 (8%)	6 (2%)	11	43
1	I	338/382 (88%)	309 (91%)	24 (7%)	5 (2%)	13	48
1	K	341/382 (89%)	304 (89%)	31 (9%)	6 (2%)	11	43
1	M	343/382 (90%)	311 (91%)	24 (7%)	8 (2%)	8	35
1	O	326/382 (85%)	286 (88%)	32 (10%)	8 (2%)	7	32
1	Q	338/382 (88%)	314 (93%)	19 (6%)	5 (2%)	13	48
1	S	334/382 (87%)	301 (90%)	25 (8%)	8 (2%)	7	34
1	U	342/382 (90%)	313 (92%)	23 (7%)	6 (2%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	339/382 (89%)	312 (92%)	22 (6%)	5 (2%)	13	48
1	Y	343/382 (90%)	319 (93%)	19 (6%)	5 (2%)	13	48
2	2	327/329 (99%)	297 (91%)	26 (8%)	4 (1%)	16	54
2	4	327/329 (99%)	304 (93%)	23 (7%)	0	100	100
2	6	327/329 (99%)	300 (92%)	24 (7%)	3 (1%)	21	62
2	B	327/329 (99%)	307 (94%)	19 (6%)	1 (0%)	46	82
2	D	327/329 (99%)	306 (94%)	19 (6%)	2 (1%)	30	71
2	F	327/329 (99%)	304 (93%)	22 (7%)	1 (0%)	46	82
2	H	327/329 (99%)	300 (92%)	24 (7%)	3 (1%)	21	62
2	J	327/329 (99%)	302 (92%)	25 (8%)	0	100	100
2	L	327/329 (99%)	302 (92%)	24 (7%)	1 (0%)	46	82
2	N	327/329 (99%)	307 (94%)	20 (6%)	0	100	100
2	P	327/329 (99%)	292 (89%)	30 (9%)	5 (2%)	13	48
2	R	327/329 (99%)	310 (95%)	16 (5%)	1 (0%)	46	82
2	T	327/329 (99%)	308 (94%)	16 (5%)	3 (1%)	21	62
2	V	327/329 (99%)	294 (90%)	30 (9%)	3 (1%)	21	62
2	X	327/329 (99%)	294 (90%)	30 (9%)	3 (1%)	21	62
2	Z	327/329 (99%)	306 (94%)	20 (6%)	1 (0%)	46	82
All	All	10637/11376 (94%)	9740 (92%)	759 (7%)	138 (1%)	15	52

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	285	SER
1	E	268	PRO
1	I	2	ALA
1	K	274	THR

### 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	1	271/310 (87%)	243 (90%)	28 (10%)	9	32
1	3	278/310 (90%)	250 (90%)	28 (10%)	9	33
1	5	281/310 (91%)	254 (90%)	27 (10%)	10	36
1	A	278/310 (90%)	250 (90%)	28 (10%)	9	33
1	C	278/310 (90%)	249 (90%)	29 (10%)	9	31
1	E	282/310 (91%)	258 (92%)	24 (8%)	13	43
1	G	281/310 (91%)	255 (91%)	26 (9%)	11	38
1	I	280/310 (90%)	255 (91%)	25 (9%)	12	41
1	K	281/310 (91%)	258 (92%)	23 (8%)	14	45
1	M	282/310 (91%)	251 (89%)	31 (11%)	8	29
1	O	268/310 (86%)	239 (89%)	29 (11%)	8	29
1	Q	280/310 (90%)	249 (89%)	31 (11%)	8	28
1	S	277/310 (89%)	249 (90%)	28 (10%)	9	33
1	U	282/310 (91%)	251 (89%)	31 (11%)	8	29
1	W	280/310 (90%)	248 (89%)	32 (11%)	7	27
1	Y	282/310 (91%)	253 (90%)	29 (10%)	9	32
2	2	268/268 (100%)	252 (94%)	16 (6%)	24	60
2	4	268/268 (100%)	253 (94%)	15 (6%)	26	64
2	6	268/268 (100%)	251 (94%)	17 (6%)	22	58
2	B	268/268 (100%)	253 (94%)	15 (6%)	26	64
2	D	268/268 (100%)	249 (93%)	19 (7%)	18	53
2	F	268/268 (100%)	251 (94%)	17 (6%)	22	58
2	H	268/268 (100%)	244 (91%)	24 (9%)	12	40
2	J	268/268 (100%)	247 (92%)	21 (8%)	16	48
2	L	268/268 (100%)	251 (94%)	17 (6%)	22	58
2	N	268/268 (100%)	245 (91%)	23 (9%)	13	42
2	P	268/268 (100%)	248 (92%)	20 (8%)	17	50
2	R	268/268 (100%)	245 (91%)	23 (9%)	13	42
2	T	268/268 (100%)	247 (92%)	21 (8%)	16	48
2	V	268/268 (100%)	249 (93%)	19 (7%)	18	53
2	X	268/268 (100%)	245 (91%)	23 (9%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	268/268 (100%)	251 (94%)	17 (6%)	22	58
All	All	8749/9248 (95%)	7993 (91%)	756 (9%)	13	42

5 of 756 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	297	ASN
2	R	317	LYS
2	4	11	GLN
2	P	3	VAL
1	Q	57	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 231 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	88	GLN
1	S	80	ASN
2	4	95	ASN
2	P	187	GLN
1	Q	299	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](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	335/382 (87%)	-0.27	1 (0%) 94 84	46, 56, 67, 88	0
1	3	342/382 (89%)	-0.36	0 100 100	45, 55, 72, 101	0
1	5	347/382 (90%)	-0.38	0 100 100	45, 56, 69, 92	0
1	A	342/382 (89%)	-0.40	1 (0%) 94 84	44, 55, 70, 101	0
1	C	342/382 (89%)	-0.31	1 (0%) 94 84	47, 56, 72, 100	0
1	E	349/382 (91%)	-0.45	0 100 100	45, 55, 67, 86	0
1	G	346/382 (90%)	-0.38	0 100 100	42, 55, 69, 86	0
1	I	344/382 (90%)	-0.35	0 100 100	44, 56, 75, 103	0
1	K	347/382 (90%)	-0.37	0 100 100	45, 56, 69, 86	0
1	M	349/382 (91%)	-0.47	0 100 100	45, 55, 66, 85	0
1	O	332/382 (86%)	-0.30	1 (0%) 94 84	45, 57, 66, 86	0
1	Q	344/382 (90%)	-0.41	1 (0%) 94 84	43, 56, 74, 98	0
1	S	340/382 (89%)	-0.32	0 100 100	47, 55, 73, 105	0
1	U	348/382 (91%)	-0.46	0 100 100	42, 55, 66, 84	0
1	W	345/382 (90%)	-0.42	0 100 100	43, 55, 70, 84	0
1	Y	349/382 (91%)	-0.43	0 100 100	46, 55, 66, 87	0
2	2	329/329 (100%)	-0.50	1 (0%) 94 84	45, 54, 63, 73	0
2	4	329/329 (100%)	-0.44	0 100 100	44, 54, 63, 73	0
2	6	329/329 (100%)	-0.47	0 100 100	45, 53, 63, 73	0
2	B	329/329 (100%)	-0.49	0 100 100	46, 53, 62, 72	0
2	D	329/329 (100%)	-0.49	0 100 100	44, 53, 61, 73	0
2	F	329/329 (100%)	-0.46	0 100 100	45, 54, 64, 76	0
2	H	329/329 (100%)	-0.46	0 100 100	45, 53, 63, 75	0
2	J	329/329 (100%)	-0.48	0 100 100	46, 54, 63, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
2	L	329/329 (100%)	-0.46	0	100	100	45, 53, 62, 72	0
2	N	329/329 (100%)	-0.46	0	100	100	47, 54, 63, 73	0
2	P	329/329 (100%)	-0.51	0	100	100	44, 53, 63, 74	0
2	R	329/329 (100%)	-0.49	0	100	100	45, 53, 62, 71	0
2	T	329/329 (100%)	-0.49	0	100	100	45, 53, 62, 73	0
2	V	329/329 (100%)	-0.46	0	100	100	47, 54, 64, 77	0
2	X	329/329 (100%)	-0.46	0	100	100	45, 54, 63, 75	0
2	Z	329/329 (100%)	-0.44	1 (0%)	94	84	45, 54, 62, 73	0
All	All	10765/11376 (94%)	-0.43	7 (0%)	95	90	42, 54, 65, 105	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	261	HIS	4.2
1	1	5	ALA	3.5
1	A	261	HIS	3.4
2	2	329	ILE	2.9
2	Z	1	LEU	2.4

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

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

## 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	K	4	1016	1/1	0.97	0.18	0.08	80,80,80,80	0
3	K	6	1007	1/1	0.97	0.09	-2.35	69,69,69,69	0
3	K	J	1014	1/1	0.96	0.10	-2.68	78,78,78,78	0
3	K	D	1002	1/1	0.95	0.05	-3.15	72,72,72,72	0
3	K	F	1008	1/1	0.96	0.06	-3.20	75,75,75,75	0
3	K	V	1004	1/1	0.93	0.07	-3.27	70,70,70,70	0
3	K	N	1009	1/1	0.97	0.07	-3.45	79,79,79,79	0
3	K	H	1013	1/1	0.93	0.07	-3.71	79,79,79,79	0
3	K	T	1006	1/1	0.90	0.08	-3.74	76,76,76,76	0
3	K	L	1011	1/1	0.98	0.06	-3.76	69,69,69,69	0
3	K	B	1003	1/1	0.97	0.06	-3.77	65,65,65,65	0
3	K	X	1005	1/1	0.97	0.10	-3.96	67,67,67,67	0
3	K	2	1015	1/1	0.96	0.06	-4.15	88,88,88,88	0
3	K	R	1001	1/1	0.95	0.06	-5.49	70,70,70,70	0
3	K	P	1012	1/1	0.97	0.05	-5.70	84,84,84,84	0
3	K	Z	1010	1/1	0.97	0.07	-5.82	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.