

wwPDB EM Validation Summary Report (i)

Nov 28, 2022 – 06:30 AM EST

PDB ID	:	7LB6
EMDB ID	:	EMD-23264
Title	:	PDX1.2/PDX1.3 co-expression complex
Authors	:	Novikova, I.V.; Evans, J.E.
Deposited on	:	2021-01-07
Resolution	:	3.16 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

:	0.0.1. dev 43
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.31.2
	: : : : :

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.16 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain				
1	А	348	• 57%	18%	•	25%	
1	В	348	• 56%	18%	•	25%	
1	С	348	56%	18%	·	25%	
1	D	348	• 57%	17%	•	25%	
1	Е	348	• 57%	17%	•	25%	
1	F	348	• 56%	18%	•	25%	
1	G	348	• 57%	17%	•	25%	
1	Н	348	• 57%	17%	•	25%	



Mol	Chain	Length	Quality of chain				
1	Ι	348	55%	19% •	25%		
1	J	348	57%	18% •	25%		
1	Κ	348	57%	18% •	25%		
1	L	348	57%	17% •	25%		
2	М	338	61%	17%	22%		
2	Ν	338	56%	22%	22%		
2	Ο	338	57%	20%	22%		
2	Р	338	63%	15%	22%		
2	Q	338	57%	21%	22%		
2	R	338	59%	19%	22%		
2	S	338	60%	18%	22%		
2	Т	338	60%	18%	22%		
2	U	338	58%	20%	22%		
2	V	338	62%	16%	22%		
2	W	338	58%	20%	22%		
2	Х	338	59%	19%	22%		



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 47760 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	Δ	260	Total	С	Ν	0	S	260	0
1	A	200	1968	1231	353	371	13	200	0
1	D	260	Total	С	Ν	0	S	260	0
1	D	200	1968	1231	353	371	13	200	0
1	C	260	Total	С	Ν	0	S	260	0
1	U	200	1968	1231	353	371	13	200	0
1	П	260	Total	С	Ν	0	S	260	0
1	D	200	1968	1231	353	371	13	200	0
1	F	260	Total	С	Ν	0	S	260	0
1		200	1968	1231	353	371	13	200	0
1	Б	260	Total	С	Ν	0	S	260	0
1	Г	200	1968	1231	353	371	13		0
1	С	260	Total	С	Ν	0	S	260	0
1	G	200	1968	1231	353	371	13	200	0
1	ц	260	Total	С	Ν	0	S	260	0
1	11	200	1968	1231	353	371	13	200	0
1	т	260	Total	С	Ν	0	S	260	0
1	L	200	1968	1231	353	371	13	200	0
1	Т	260	Total	С	Ν	Ο	\mathbf{S}	260	0
1	J	200	1968	1231	353	371	13	200	0
1	K	260	Total	С	Ν	0	S	260	0
	IX	200	1968	1231	353	371	13	200	U
1	т	260	Total	С	Ν	0	S	260	0
1		200	1968	1231	353	371	13	200	U

• Molecule 1 is a protein called Pyridoxal 5'-phosphate synthase-like subunit PDX1.2.

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-62	MET	-	expression tag	UNP Q9ZNR6
А	-61	ASP	-	expression tag	UNP Q9ZNR6
А	-60	TYR	-	expression tag	UNP Q9ZNR6
А	-59	LYS	-	expression tag	UNP Q9ZNR6
А	-58	ASP	-	expression tag	UNP Q9ZNR6
А	-57	HIS	-	expression tag	UNP Q9ZNR6



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Chain	Residue	Modelled	Actual	Comment	Reference
А	-56	ASP	-	expression tag	UNP Q9ZNR6
А	-55	GLY	-	expression tag	UNP Q9ZNR6
A	-54	ASP	-	expression tag	UNP Q9ZNR6
А	-53	TYR	-	expression tag	UNP Q9ZNR6
А	-52	LYS	-	expression tag	UNP Q9ZNR6
А	-51	ASP	-	expression tag	UNP Q9ZNR6
А	-50	HIS	-	expression tag	UNP Q9ZNR6
А	-49	ASP	-	expression tag	UNP Q9ZNR6
A	-48	ILE	-	expression tag	UNP Q9ZNR6
А	-47	ASP	-	expression tag	UNP Q9ZNR6
А	-46	TYR	-	expression tag	UNP Q9ZNR6
А	-45	LYS	-	expression tag	UNP Q9ZNR6
А	-44	ASP	-	expression tag	UNP Q9ZNR6
А	-43	ASP	-	expression tag	UNP Q9ZNR6
А	-42	ASP	-	expression tag	UNP Q9ZNR6
А	-41	ASP	-	expression tag	UNP Q9ZNR6
А	-40	LYS	-	expression tag	UNP Q9ZNR6
А	-39	LEU	-	expression tag	UNP Q9ZNR6
А	-38	ALA	-	expression tag	UNP Q9ZNR6
А	-37	GLY	-	expression tag	UNP Q9ZNR6
А	-36	GLY	-	expression tag	UNP Q9ZNR6
А	-35	GLY	-	expression tag	UNP Q9ZNR6
А	-34	GLY	-	expression tag	UNP Q9ZNR6
А	-33	SER	-	expression tag	UNP Q9ZNR6
А	-32	GLY	-	expression tag	UNP Q9ZNR6
А	-31	GLY	-	expression tag	UNP Q9ZNR6
А	-30	GLY	-	expression tag	UNP Q9ZNR6
А	-29	GLY	-	expression tag	UNP Q9ZNR6
А	-28	SER	-	expression tag	UNP Q9ZNR6
В	198	MET	-	expression tag	UNP Q9ZNR6
В	199	ASP	-	expression tag	UNP Q9ZNR6
В	200	TYR	-	expression tag	UNP Q9ZNR6
В	201	LYS	-	expression tag	UNP Q9ZNR6
В	202	ASP	-	expression tag	UNP Q9ZNR6
В	203	HIS	-	expression tag	UNP Q9ZNR6
В	204	ASP	-	expression tag	UNP Q9ZNR6
В	205	GLY	-	expression tag	UNP Q9ZNR6
В	206	ASP	-	expression tag	UNP Q9ZNR6
В	207	TYR	-	expression tag	UNP Q9ZNR6
В	208	LYS	-	expression tag	UNP Q9ZNR6
В	209	ASP	-	expression tag	UNP Q9ZNR6
В	210	HIS	-	expression tag	UNP Q9ZNR6

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Chain	Residue	Modelled	Actual	Comment	Reference
В	211	ASP	-	expression tag	UNP Q9ZNR6
В	212	ILE	-	expression tag	UNP Q9ZNR6
В	213	ASP	-	expression tag	UNP Q9ZNR6
В	214	TYR	-	expression tag	UNP Q9ZNR6
В	215	LYS	-	expression tag	UNP Q9ZNR6
В	216	ASP	-	expression tag	UNP Q9ZNR6
В	217	ASP	-	expression tag	UNP Q9ZNR6
В	218	ASP	-	expression tag	UNP Q9ZNR6
В	219	ASP	-	expression tag	UNP Q9ZNR6
В	220	LYS	-	expression tag	UNP Q9ZNR6
В	221	LEU	-	expression tag	UNP Q9ZNR6
В	222	ALA	-	expression tag	UNP Q9ZNR6
В	223	GLY	-	expression tag	UNP Q9ZNR6
В	224	GLY	-	expression tag	UNP Q9ZNR6
В	225	GLY	-	expression tag	UNP Q9ZNR6
В	226	GLY	-	expression tag	UNP Q9ZNR6
В	227	SER	-	expression tag	UNP Q9ZNR6
В	228	GLY	-	expression tag	UNP Q9ZNR6
В	229	GLY	-	expression tag	UNP Q9ZNR6
В	230	GLY	-	expression tag	UNP Q9ZNR6
В	231	GLY	-	expression tag	UNP Q9ZNR6
В	232	SER	-	expression tag	UNP Q9ZNR6
С	458	MET	-	expression tag	UNP Q9ZNR6
С	459	ASP	-	expression tag	UNP Q9ZNR6
С	460	TYR	-	expression tag	UNP Q9ZNR6
С	461	LYS	-	expression tag	UNP Q9ZNR6
С	462	ASP	-	expression tag	UNP Q9ZNR6
С	463	HIS	-	expression tag	UNP Q9ZNR6
С	464	ASP	-	expression tag	UNP Q9ZNR6
С	465	GLY	_	expression tag	UNP Q9ZNR6
С	466	ASP	_	expression tag	UNP Q9ZNR6
С	467	TYR	-	expression tag	UNP Q9ZNR6
С	468	LYS	-	expression tag	UNP Q9ZNR6
С	469	ASP	-	expression tag	UNP Q9ZNR6
С	470	HIS	-	expression tag	UNP Q9ZNR6
С	471	ASP	-	expression tag	UNP Q9ZNR6
С	472	ILE	-	expression tag	UNP Q9ZNR6
С	473	ASP	-	expression tag	UNP Q9ZNR6
С	474	TYR	-	expression tag	UNP Q9ZNR6
С	475	LYS	-	expression tag	UNP Q9ZNR6
С	476	ASP	-	expression tag	UNP Q9ZNR6
С	477	ASP	-	expression tag	UNP Q9ZNR6

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Chain	Residue	Modelled	Actual	Comment	Reference	
С	478	ASP	-	expression tag	UNP Q9ZNR6	
С	479	ASP	-	expression tag	UNP Q9ZNR6	
С	480	LYS	-	expression tag	UNP Q9ZNR6	
С	481	LEU	-	expression tag	UNP Q9ZNR6	
С	482	ALA	-	expression tag	UNP Q9ZNR6	
С	483	GLY	-	expression tag	UNP Q9ZNR6	
С	484	GLY	-	expression tag	UNP Q9ZNR6	
С	485	GLY	-	expression tag	UNP Q9ZNR6	
С	486	GLY	-	expression tag	UNP Q9ZNR6	
С	487	SER	-	expression tag	UNP Q9ZNR6	
С	488	GLY	-	expression tag	UNP Q9ZNR6	
С	489	GLY	-	expression tag	UNP Q9ZNR6	
С	490	GLY	-	expression tag	UNP Q9ZNR6	
С	491	GLY	-	expression tag	UNP Q9ZNR6	
С	492	SER	-	expression tag	UNP Q9ZNR6	
D	718	MET	-	expression tag	UNP Q9ZNR6	
D	719	ASP	-	expression tag	UNP Q9ZNR6	
D	720	TYR	-	expression tag	UNP Q9ZNR6	
D	721	LYS	-	expression tag	UNP Q9ZNR6	
D	722	ASP	-	expression tag	UNP Q9ZNR6	
D	723	HIS	-	expression tag	UNP Q9ZNR6	
D	724	ASP	-	expression tag	UNP Q9ZNR6	
D	725	GLY	-	expression tag	UNP Q9ZNR6	
D	726	ASP	-	expression tag	UNP Q9ZNR6	
D	727	TYR	-	expression tag	UNP Q9ZNR6	
D	728	LYS	-	expression tag	UNP Q9ZNR6	
D	729	ASP	-	expression tag	UNP Q9ZNR6	
D	730	HIS	-	expression tag	UNP Q9ZNR6	
D	731	ASP	-	expression tag	UNP Q9ZNR6	
D	732	ILE	-	expression tag	UNP Q9ZNR6	
D	733	ASP	-	expression tag	UNP Q9ZNR6	
D	734	TYR	-	expression tag	UNP Q9ZNR6	
D	735	LYS	-	expression tag	UNP Q9ZNR6	
D	736	ASP	-	expression tag	UNP Q9ZNR6	
D	737	ASP	-	expression tag	UNP Q9ZNR6	
D	738	ASP	-	expression tag	UNP Q9ZNR6	
D	739	ASP	-	expression tag	UNP Q9ZNR6	
D	740	LYS	-	expression tag	UNP Q9ZNR6	
D	741	LEU	-	expression tag	UNP Q9ZNR6	
D	742	ALA	-	expression tag	UNP Q9ZNR6	
D	743	GLY	-	expression tag	UNP Q9ZNR6	
D	744	GLY	-	expression tag	UNP Q9ZNR6	

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Chain	Residue	Modelled	Actual	Comment	Reference	
D	745	GLY	-	expression tag	UNP Q9ZNR6	
D	746	GLY	-	expression tag	UNP Q9ZNR6	
D	747	SER	-	expression tag	UNP Q9ZNR6	
D	748	GLY	-	expression tag	UNP Q9ZNR6	
D	749	GLY	-	expression tag	UNP Q9ZNR6	
D	750	GLY	-	expression tag	UNP Q9ZNR6	
D	751	GLY	-	expression tag	UNP Q9ZNR6	
D	752	SER	-	expression tag	UNP Q9ZNR6	
Е	978	MET	-	expression tag	UNP Q9ZNR6	
Е	979	ASP	-	expression tag	UNP Q9ZNR6	
Е	980	TYR	-	expression tag	UNP Q9ZNR6	
Е	981	LYS	-	expression tag	UNP Q9ZNR6	
Е	982	ASP	-	expression tag	UNP Q9ZNR6	
Е	983	HIS	-	expression tag	UNP Q9ZNR6	
Е	984	ASP	-	expression tag	UNP Q9ZNR6	
Е	985	GLY	-	expression tag	UNP Q9ZNR6	
Е	986	ASP	-	expression tag	UNP Q9ZNR6	
Е	987	TYR	-	expression tag	UNP Q9ZNR6	
Е	988	LYS	-	expression tag	UNP Q9ZNR6	
Е	989	ASP	-	expression tag	UNP Q9ZNR6	
Е	990	HIS	-	expression tag	UNP Q9ZNR6	
Е	991	ASP	-	expression tag	UNP Q9ZNR6	
Е	992	ILE	-	expression tag	UNP Q9ZNR6	
Е	993	ASP	-	expression tag	UNP Q9ZNR6	
Е	994	TYR	-	expression tag	UNP Q9ZNR6	
Е	995	LYS	-	expression tag	UNP Q9ZNR6	
Е	996	ASP	-	expression tag	UNP Q9ZNR6	
Е	997	ASP	-	expression tag	UNP Q9ZNR6	
Е	998	ASP	-	expression tag	UNP Q9ZNR6	
Е	999	ASP	-	expression tag	UNP Q9ZNR6	
Е	1000	LYS	-	expression tag	UNP Q9ZNR6	
Е	1001	LEU	-	expression tag	UNP Q9ZNR6	
Е	1002	ALA	-	expression tag	UNP Q9ZNR6	
Е	1003	GLY	-	expression tag	UNP Q9ZNR6	
Е	1004	GLY	-	expression tag	UNP Q9ZNR6	
Е	1005	GLY	-	expression tag	UNP Q9ZNR6	
Е	1006	GLY	-	expression tag	UNP Q9ZNR6	
Е	1007	SER	-	expression tag	UNP Q9ZNR6	
Е	1008	GLY	-	expression tag	UNP Q9ZNR6	
Е	1009	GLY	-	expression tag	UNP Q9ZNR6	
Е	1010	GLY	-	expression tag	UNP Q9ZNR6	
Е	1011	GLY	-	expression tag	UNP Q9ZNR6	

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Chain	Residue	Modelled	Actual	Comment	Reference
Ε	1012	SER	-	expression tag	UNP Q9ZNR6
F	1238	MET	-	expression tag	UNP Q9ZNR6
F	1239	ASP	-	expression tag	UNP Q9ZNR6
F	1240	TYR	-	expression tag	UNP Q9ZNR6
F	1241	LYS	-	expression tag	UNP Q9ZNR6
F	1242	ASP	-	expression tag	UNP Q9ZNR6
F	1243	HIS	-	expression tag	UNP Q9ZNR6
F	1244	ASP	-	expression tag	UNP Q9ZNR6
F	1245	GLY	-	expression tag	UNP Q9ZNR6
F	1246	ASP	-	expression tag	UNP Q9ZNR6
F	1247	TYR	-	expression tag	UNP Q9ZNR6
F	1248	LYS	-	expression tag	UNP Q9ZNR6
F	1249	ASP	-	expression tag	UNP Q9ZNR6
F	1250	HIS	-	expression tag	UNP Q9ZNR6
F	1251	ASP	-	expression tag	UNP Q9ZNR6
F	1252	ILE	-	expression tag	UNP Q9ZNR6
F	1253	ASP	-	expression tag	UNP Q9ZNR6
F	1254	TYR	-	expression tag	UNP Q9ZNR6
F	1255	LYS	-	expression tag	UNP Q9ZNR6
F	1256	ASP	-	expression tag	UNP Q9ZNR6
F	1257	ASP	-	expression tag	UNP Q9ZNR6
F	1258	ASP	-	expression tag	UNP Q9ZNR6
F	1259	ASP	-	expression tag	UNP Q9ZNR6
F	1260	LYS	-	expression tag	UNP Q9ZNR6
F	1261	LEU	-	expression tag	UNP Q9ZNR6
F	1262	ALA	-	expression tag	UNP Q9ZNR6
F	1263	GLY	-	expression tag	UNP Q9ZNR6
F	1264	GLY	-	expression tag	UNP Q9ZNR6
F	1265	GLY	-	expression tag	UNP Q9ZNR6
F	1266	GLY	-	expression tag	UNP Q9ZNR6
F	1267	SER	-	expression tag	UNP Q9ZNR6
F	1268	GLY	-	expression tag	UNP Q9ZNR6
F	1269	GLY	-	expression tag	UNP Q9ZNR6
F	1270	GLY	-	expression tag	UNP Q9ZNR6
F	1271	GLY	-	expression tag	UNP Q9ZNR6
F	1272	SER	-	expression tag	UNP Q9ZNR6
G	1498	MET	-	expression tag	UNP Q9ZNR6
G	1499	ASP	-	expression tag	UNP Q9ZNR6
G	1500	TYR	-	expression tag	UNP Q9ZNR6
G	1501	LYS	-	expression tag	UNP Q9ZNR6
G	1502	ASP	-	expression tag	UNP Q9ZNR6
G	1503	HIS	-	expression tag	UNP Q9ZNR6

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Chain	Residue	Modelled	Actual	Comment	Reference	
G	1504	ASP	-	expression tag	UNP Q9ZNR6	
G	1505	GLY	-	expression tag	UNP Q9ZNR6	
G	1506	ASP	-	expression tag	UNP Q9ZNR6	
G	1507	TYR	-	expression tag	UNP Q9ZNR6	
G	1508	LYS	-	expression tag	UNP Q9ZNR6	
G	1509	ASP	-	expression tag	UNP Q9ZNR6	
G	1510	HIS	-	expression tag	UNP Q9ZNR6	
G	1511	ASP	-	expression tag	UNP Q9ZNR6	
G	1512	ILE	-	expression tag	UNP Q9ZNR6	
G	1513	ASP	-	expression tag	UNP Q9ZNR6	
G	1514	TYR	-	expression tag	UNP Q9ZNR6	
G	1515	LYS	-	expression tag	UNP Q9ZNR6	
G	1516	ASP	-	expression tag	UNP Q9ZNR6	
G	1517	ASP	-	expression tag	UNP Q9ZNR6	
G	1518	ASP	-	expression tag	UNP Q9ZNR6	
G	1519	ASP	-	expression tag	UNP Q9ZNR6	
G	1520	LYS	-	expression tag	UNP Q9ZNR6	
G	1521	LEU	-	expression tag	UNP Q9ZNR6	
G	1522	ALA	-	expression tag	UNP Q9ZNR6	
G	1523	GLY	-	expression tag	UNP Q9ZNR6	
G	1524	GLY	-	expression tag	UNP Q9ZNR6	
G	1525	GLY	-	expression tag	UNP Q9ZNR6	
G	1526	GLY	-	expression tag	UNP Q9ZNR6	
G	1527	SER	-	expression tag	UNP Q9ZNR6	
G	1528	GLY	-	expression tag	UNP Q9ZNR6	
G	1529	GLY	-	expression tag	UNP Q9ZNR6	
G	1530	GLY	-	expression tag	UNP Q9ZNR6	
G	1531	GLY	-	expression tag	UNP Q9ZNR6	
G	1532	SER	-	expression tag	UNP Q9ZNR6	
Н	1758	MET	-	expression tag	UNP Q9ZNR6	
Н	1759	ASP	-	expression tag	UNP Q9ZNR6	
Н	1760	TYR	-	expression tag	UNP Q9ZNR6	
Н	1761	LYS	-	expression tag	UNP Q9ZNR6	
Н	1762	ASP	-	expression tag	UNP Q9ZNR6	
Н	1763	HIS	-	expression tag	UNP Q9ZNR6	
Н	1764	ASP	-	expression tag	UNP Q9ZNR6	
Н	1765	GLY	-	expression tag	UNP Q9ZNR6	
Н	1766	ASP	-	expression tag	UNP Q9ZNR6	
Н	1767	TYR	-	expression tag	UNP Q9ZNR6	
Н	1768	LYS	-	expression tag	UNP Q9ZNR6	
Н	1769	ASP	-	expression tag	UNP Q9ZNR6	
Н	1770	HIS	_	expression tag	UNP Q9ZNR6	

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Chain	Residue	Modelled	Actual	Comment	Reference	
Н	1771	ASP	-	expression tag	UNP Q9ZNR6	
Н	1772	ILE	-	expression tag	UNP Q9ZNR6	
Н	1773	ASP	-	expression tag	UNP Q9ZNR6	
Н	1774	TYR	-	expression tag	UNP Q9ZNR6	
Н	1775	LYS	-	expression tag	UNP Q9ZNR6	
Н	1776	ASP	-	expression tag	UNP Q9ZNR6	
Н	1777	ASP	-	expression tag	UNP Q9ZNR6	
Н	1778	ASP	-	expression tag	UNP Q9ZNR6	
Н	1779	ASP	-	expression tag	UNP Q9ZNR6	
Н	1780	LYS	-	expression tag	UNP Q9ZNR6	
Н	1781	LEU	-	expression tag	UNP Q9ZNR6	
Н	1782	ALA	-	expression tag	UNP Q9ZNR6	
Н	1783	GLY	-	expression tag	UNP Q9ZNR6	
Н	1784	GLY	-	expression tag	UNP Q9ZNR6	
Н	1785	GLY	-	expression tag	UNP Q9ZNR6	
Н	1786	GLY	-	expression tag	UNP Q9ZNR6	
Н	1787	SER	-	expression tag	UNP Q9ZNR6	
Н	1788	GLY	-	expression tag	UNP Q9ZNR6	
Н	1789	GLY	_	expression tag	UNP Q9ZNR6	
Н	1790	GLY	-	expression tag	UNP Q9ZNR6	
Н	1791	GLY	-	expression tag	UNP Q9ZNR6	
Н	1792	SER	-	expression tag	UNP Q9ZNR6	
Ι	2018	MET	-	expression tag	UNP Q9ZNR6	
Ι	2019	ASP	-	expression tag	UNP Q9ZNR6	
Ι	2020	TYR	-	expression tag	UNP Q9ZNR6	
Ι	2021	LYS	-	expression tag	UNP Q9ZNR6	
Ι	2022	ASP	-	expression tag	UNP Q9ZNR6	
Ι	2023	HIS	-	expression tag	UNP Q9ZNR6	
Ι	2024	ASP	-	expression tag	UNP Q9ZNR6	
Ι	2025	GLY	-	expression tag	UNP Q9ZNR6	
Ι	2026	ASP	-	expression tag	UNP Q9ZNR6	
Ι	2027	TYR	-	expression tag	UNP Q9ZNR6	
Ι	2028	LYS	-	expression tag	UNP Q9ZNR6	
Ι	2029	ASP	-	expression tag	UNP Q9ZNR6	
Ι	2030	HIS	-	expression tag	UNP Q9ZNR6	
Ι	2031	ASP	-	expression tag	UNP Q9ZNR6	
Ι	2032	ILE	-	expression tag	UNP Q9ZNR6	
Ι	2033	ASP	-	expression tag	UNP Q9ZNR6	
Ι	2034	TYR	-	expression tag	UNP Q9ZNR6	
Ι	2035	LYS	-	expression tag	UNP Q9ZNR6	
Ι	2036	ASP	-	expression tag	UNP Q9ZNR6	
Ι	2037	ASP	-	expression tag	UNP Q9ZNR6	

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Chain	Residue	Modelled	Actual	Comment	Reference
Ι	2038	ASP	_	expression tag	UNP Q9ZNR6
Ι	2039	ASP	-	expression tag	UNP Q9ZNR6
Ι	2040	LYS	-	expression tag	UNP Q9ZNR6
Ι	2041	LEU	-	expression tag	UNP Q9ZNR6
Ι	2042	ALA	_	expression tag	UNP Q9ZNR6
Ι	2043	GLY	-	expression tag	UNP Q9ZNR6
Ι	2044	GLY	_	expression tag	UNP Q9ZNR6
Ι	2045	GLY	-	expression tag	UNP Q9ZNR6
Ι	2046	GLY	-	expression tag	UNP Q9ZNR6
Ι	2047	SER	-	expression tag	UNP Q9ZNR6
Ι	2048	GLY	-	expression tag	UNP Q9ZNR6
Ι	2049	GLY	-	expression tag	UNP Q9ZNR6
Ι	2050	GLY	-	expression tag	UNP Q9ZNR6
Ι	2051	GLY	-	expression tag	UNP Q9ZNR6
Ι	2052	SER	-	expression tag	UNP Q9ZNR6
J	2278	MET	-	expression tag	UNP Q9ZNR6
J	2279	ASP	-	expression tag	UNP Q9ZNR6
J	2280	TYR	-	expression tag	UNP Q9ZNR6
J	2281	LYS	-	expression tag	UNP Q9ZNR6
J	2282	ASP	-	expression tag	UNP Q9ZNR6
J	2283	HIS	-	expression tag	UNP Q9ZNR6
J	2284	ASP	-	expression tag	UNP Q9ZNR6
J	2285	GLY	-	expression tag	UNP Q9ZNR6
J	2286	ASP	-	expression tag	UNP Q9ZNR6
J	2287	TYR	-	expression tag	UNP Q9ZNR6
J	2288	LYS	-	expression tag	UNP Q9ZNR6
J	2289	ASP	-	expression tag	UNP Q9ZNR6
J	2290	HIS	-	expression tag	UNP Q9ZNR6
J	2291	ASP	-	expression tag	UNP Q9ZNR6
J	2292	ILE	-	expression tag	UNP Q9ZNR6
J	2293	ASP	-	expression tag	UNP Q9ZNR6
J	2294	TYR	-	expression tag	UNP Q9ZNR6
J	2295	LYS	-	expression tag	UNP Q9ZNR6
J	2296	ASP	-	expression tag	UNP Q9ZNR6
J	2297	ASP	-	expression tag	UNP Q9ZNR6
J	2298	ASP	-	expression tag	UNP Q9ZNR6
J	2299	ASP	-	expression tag	UNP Q9ZNR6
J	2300	LYS	-	expression tag	UNP Q9ZNR6
J	2301	LEU	-	expression tag	UNP Q9ZNR6
J	2302	ALA	-	expression tag	UNP Q9ZNR6
J	2303	GLY	-	expression tag	UNP Q9ZNR6
J	2304	GLY	-	expression tag	UNP Q9ZNR6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	2305	GLY	-	expression tag	UNP Q9ZNR6
J	2306	GLY	-	expression tag	UNP Q9ZNR6
J	2307	SER	-	expression tag	UNP Q9ZNR6
J	2308	GLY	-	expression tag	UNP Q9ZNR6
J	2309	GLY	-	expression tag	UNP Q9ZNR6
J	2310	GLY	-	expression tag	UNP Q9ZNR6
J	2311	GLY	-	expression tag	UNP Q9ZNR6
J	2312	SER	-	expression tag	UNP Q9ZNR6
K	2538	MET	-	expression tag	UNP Q9ZNR6
K	2539	ASP	-	expression tag	UNP Q9ZNR6
K	2540	TYR	-	expression tag	UNP Q9ZNR6
K	2541	LYS	-	expression tag	UNP Q9ZNR6
K	2542	ASP	-	expression tag	UNP Q9ZNR6
K	2543	HIS	-	expression tag	UNP Q9ZNR6
К	2544	ASP	-	expression tag	UNP Q9ZNR6
К	2545	GLY	-	expression tag	UNP Q9ZNR6
К	2546	ASP	-	expression tag	UNP Q9ZNR6
К	2547	TYR	-	expression tag	UNP Q9ZNR6
K	2548	LYS	-	expression tag	UNP Q9ZNR6
К	2549	ASP	-	expression tag	UNP Q9ZNR6
K	2550	HIS	-	expression tag	UNP Q9ZNR6
К	2551	ASP	-	expression tag	UNP Q9ZNR6
К	2552	ILE	-	expression tag	UNP Q9ZNR6
К	2553	ASP	-	expression tag	UNP Q9ZNR6
К	2554	TYR	-	expression tag	UNP Q9ZNR6
K	2555	LYS	-	expression tag	UNP Q9ZNR6
K	2556	ASP	-	expression tag	UNP Q9ZNR6
К	2557	ASP	-	expression tag	UNP Q9ZNR6
K	2558	ASP	-	expression tag	UNP Q9ZNR6
К	2559	ASP	-	expression tag	UNP Q9ZNR6
K	2560	LYS	-	expression tag	UNP Q9ZNR6
К	2561	LEU	-	expression tag	UNP Q9ZNR6
K	2562	ALA	-	expression tag	UNP Q9ZNR6
К	2563	GLY	-	expression tag	UNP Q9ZNR6
К	2564	GLY	-	expression tag	UNP Q9ZNR6
K	2565	GLY	-	expression tag	UNP Q9ZNR6
K	2566	GLY	-	expression tag	UNP Q9ZNR6
K	2567	SER	-	expression tag	UNP Q9ZNR6
K	2568	GLY	-	expression tag	UNP Q9ZNR6
K	2569	GLY	-	expression tag	UNP Q9ZNR6
K	2570	GLY	-	expression tag	UNP Q9ZNR6
K	2571	GLY	-	expression tag	UNP Q9ZNR6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	2572	SER	-	expression tag	UNP Q9ZNR6
L	2798	MET	-	expression tag	UNP Q9ZNR6
L	2799	ASP	-	expression tag	UNP Q9ZNR6
L	2800	TYR	-	expression tag	UNP Q9ZNR6
L	2801	LYS	-	expression tag	UNP Q9ZNR6
L	2802	ASP	-	expression tag	UNP Q9ZNR6
L	2803	HIS	-	expression tag	UNP Q9ZNR6
L	2804	ASP	-	expression tag	UNP Q9ZNR6
L	2805	GLY	-	expression tag	UNP Q9ZNR6
L	2806	ASP	-	expression tag	UNP Q9ZNR6
L	2807	TYR	-	expression tag	UNP Q9ZNR6
L	2808	LYS	-	expression tag	UNP Q9ZNR6
L	2809	ASP	-	expression tag	UNP Q9ZNR6
L	2810	HIS	-	expression tag	UNP Q9ZNR6
L	2811	ASP	-	expression tag	UNP Q9ZNR6
L	2812	ILE	-	expression tag	UNP Q9ZNR6
L	2813	ASP	-	expression tag	UNP Q9ZNR6
L	2814	TYR	-	expression tag	UNP Q9ZNR6
L	2815	LYS	-	expression tag	UNP Q9ZNR6
L	2816	ASP	-	expression tag	UNP Q9ZNR6
L	2817	ASP	-	expression tag	UNP Q9ZNR6
L	2818	ASP	-	expression tag	UNP Q9ZNR6
L	2819	ASP	-	expression tag	UNP Q9ZNR6
L	2820	LYS	-	expression tag	UNP Q9ZNR6
L	2821	LEU	-	expression tag	UNP Q9ZNR6
L	2822	ALA	-	expression tag	UNP Q9ZNR6
L	2823	GLY	-	expression tag	UNP Q9ZNR6
L	2824	GLY	-	expression tag	UNP Q9ZNR6
L	2825	GLY	-	expression tag	UNP Q9ZNR6
L	2826	GLY	-	expression tag	UNP Q9ZNR6
L	2827	SER	-	expression tag	UNP Q9ZNR6
L	2828	GLY	-	expression tag	UNP Q9ZNR6
L	2829	GLY	-	expression tag	UNP Q9ZNR6
L	2830	GLY	-	expression tag	UNP Q9ZNR6
L	2831	GLY	-	expression tag	UNP Q9ZNR6
L	2832	SER	-	expression tag	UNP Q9ZNR6

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• Molecule 2 is a protein called Pyridoxal 5'-phosphate synthase subunit PDX1.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	М	263	Total 2012	C 1257	N 370	O 369	S 16	263	0



Mol	Chain	Residues		At	oms			AltConf	Trace	
0	N	262	Total	С	Ν	0	S	262	0	
	IN	203	2012	1257	370	369	16	203	0	
0	0	262	Total	С	Ν	0	S	262	0	
		203	2012	1257	370	369	16	203	0	
9	D	263	Total	С	Ν	0	S	263	0	
	1	203	2012	1257	370	369	16	203	0	
9	0	263	Total	С	Ν	0	S	263	0	
	Q	205	2012	1257	370	369	16	200	0	
9	В	263	Total	С	Ν	0	S	263	0	
	п	205	2012	1257	370	369	16		0	
2	S	S	263	Total	С	Ν	Ο	\mathbf{S}	263	0
2	G	205	2012	1257	370	369	16	205	0	
2	Т	263	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	263	0	
2	T	200	2012	1257	370	369	16	205	0	
2	II	263	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	263	0	
2	U	200	2012	1257	370	369	16	200	0	
2	V	263	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	263	0	
2	v	200	2012	1257	370	369	16	200	0	
2	W	263	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	263	0	
	vv	200	2012	1257	370	369	16	200	0	
2	x	263	Total	С	Ν	0	S	263	0	
		200	2012	1257	370	369	16	200	U	

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
М	-49	MET	-	expression tag	UNP Q8L940
М	-48	ASP	-	expression tag	UNP Q8L940
М	-47	TYR	-	expression tag	UNP Q8L940
М	-46	LYS	-	expression tag	UNP Q8L940
М	-45	ASP	-	expression tag	UNP Q8L940
М	-44	HIS	-	expression tag	UNP Q8L940
М	-43	ASP	-	expression tag	UNP Q8L940
М	-42	GLY	-	expression tag	UNP Q8L940
М	-41	ASP	-	expression tag	UNP Q8L940
М	-40	TYR	-	expression tag	UNP Q8L940
М	-39	LYS	-	expression tag	UNP Q8L940
М	-38	ASP	-	expression tag	UNP Q8L940
М	-37	HIS	-	expression tag	UNP Q8L940
М	-36	ASP	-	expression tag	UNP Q8L940
М	-35	ILE	-	expression tag	UNP Q8L940
M	-34	ASP	-	expression tag	UNP Q8L940
M	-33	TYR	-	expression tag	UNP Q8L940

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-32	LYS	-	expression tag	UNP Q8L940
M	-31	ASP	-	expression tag	UNP Q8L940
M	-30	ASP	-	expression tag	UNP Q8L940
М	-29	ASP	-	expression tag	UNP Q8L940
М	-28	ASP	-	expression tag	UNP Q8L940
М	-27	LYS	-	expression tag	UNP Q8L940
М	-26	LEU	-	expression tag	UNP Q8L940
М	-25	ALA	-	expression tag	UNP Q8L940
М	-24	GLY	-	expression tag	UNP Q8L940
М	-23	GLY	-	expression tag	UNP Q8L940
М	-22	GLY	-	expression tag	UNP Q8L940
М	-21	GLY	-	expression tag	UNP Q8L940
М	-20	SER	-	expression tag	UNP Q8L940
N	214	MET	-	expression tag	UNP Q8L940
N	215	ASP	-	expression tag	UNP Q8L940
N	216	TYR	-	expression tag	UNP Q8L940
N	217	LYS	-	expression tag	UNP Q8L940
N	218	ASP	-	expression tag	UNP Q8L940
N	219	HIS	-	expression tag	UNP Q8L940
N	220	ASP	-	expression tag	UNP Q8L940
N	221	GLY	-	expression tag	UNP Q8L940
N	222	ASP	-	expression tag	UNP Q8L940
N	223	TYR	-	expression tag	UNP Q8L940
N	224	LYS	-	expression tag	UNP Q8L940
N	225	ASP	-	expression tag	UNP Q8L940
N	226	HIS	-	expression tag	UNP Q8L940
N	227	ASP	-	expression tag	UNP Q8L940
N	228	ILE	-	expression tag	UNP Q8L940
N	229	ASP	-	expression tag	UNP Q8L940
N	230	TYR	-	expression tag	UNP Q8L940
N	231	LYS	-	expression tag	UNP Q8L940
N	232	ASP	-	expression tag	UNP Q8L940
N	233	ASP	-	expression tag	UNP Q8L940
N	234	ASP	-	expression tag	UNP Q8L940
N	235	ASP	-	expression tag	UNP Q8L940
N	236	LYS	-	expression tag	UNP Q8L940
N	237	LEU	-	expression tag	UNP Q8L940
N	238	ALA	-	expression tag	UNP Q8L940
N	239	GLY	-	expression tag	UNP Q8L940
N	240	GLY	-	expression tag	UNP Q8L940
N	241	GLY	-	expression tag	UNP Q8L940
N	242	GLY	_	expression tag	UNP Ø8L940

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Chain	Residue	Modelled	Actual	Comment	Reference
N	243	SER	-	expression tag	UNP Q8L940
0	477	MET	-	expression tag	UNP Q8L940
0	478	ASP	-	expression tag	UNP Q8L940
0	479	TYR	-	expression tag	UNP Q8L940
0	480	LYS	-	expression tag	UNP Q8L940
0	481	ASP	-	expression tag	UNP Q8L940
0	482	HIS	-	expression tag	UNP Q8L940
0	483	ASP	-	expression tag	UNP Q8L940
0	484	GLY	-	expression tag	UNP Q8L940
0	485	ASP	-	expression tag	UNP Q8L940
0	486	TYR	-	expression tag	UNP Q8L940
0	487	LYS	-	expression tag	UNP Q8L940
0	488	ASP	-	expression tag	UNP Q8L940
0	489	HIS	-	expression tag	UNP Q8L940
0	490	ASP	-	expression tag	UNP Q8L940
0	491	ILE	-	expression tag	UNP Q8L940
0	492	ASP	-	expression tag	UNP Q8L940
0	493	TYR	-	expression tag	UNP Q8L940
0	494	LYS	-	expression tag	UNP Q8L940
0	495	ASP	-	expression tag	UNP Q8L940
0	496	ASP	-	expression tag	UNP Q8L940
0	497	ASP	-	expression tag	UNP Q8L940
0	498	ASP	-	expression tag	UNP Q8L940
0	499	LYS	-	expression tag	UNP Q8L940
0	500	LEU	-	expression tag	UNP Q8L940
0	501	ALA	-	expression tag	UNP Q8L940
0	502	GLY	-	expression tag	UNP Q8L940
0	503	GLY	-	expression tag	UNP Q8L940
0	504	GLY	-	expression tag	UNP Q8L940
0	505	GLY	-	expression tag	UNP Q8L940
0	506	SER	-	expression tag	UNP Q8L940
Р	740	MET	-	expression tag	UNP Q8L940
Р	741	ASP	-	expression tag	UNP Q8L940
Р	742	TYR	-	expression tag	UNP Q8L940
Р	743	LYS	-	expression tag	UNP Q8L940
Р	744	ASP	-	expression tag	UNP Q8L940
Р	745	HIS	-	expression tag	UNP Q8L940
Р	746	ASP	-	expression tag	UNP Q8L940
Р	747	GLY	-	expression tag	UNP Q8L940
Р	748	ASP	-	expression tag	UNP Q8L940
Р	749	TYR	-	expression tag	UNP Q8L940
Р	750	LYS	-	expression tag	UNP Q8L940

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Chain	Residue	Modelled	Actual	Comment	Reference
P	751	ASP	-	expression tag	UNP Q8L940
P	752	HIS	-	expression tag	UNP Q8L940
P	753	ASP	-	expression tag	UNP Q8L940
Р	754	ILE	-	expression tag	UNP Q8L940
Р	755	ASP	-	expression tag	UNP Q8L940
Р	756	TYR	-	expression tag	UNP Q8L940
Р	757	LYS	-	expression tag	UNP Q8L940
Р	758	ASP	-	expression tag	UNP Q8L940
Р	759	ASP	-	expression tag	UNP Q8L940
Р	760	ASP	-	expression tag	UNP Q8L940
Р	761	ASP	-	expression tag	UNP Q8L940
Р	762	LYS	-	expression tag	UNP Q8L940
Р	763	LEU	-	expression tag	UNP Q8L940
Р	764	ALA	-	expression tag	UNP Q8L940
Р	765	GLY	-	expression tag	UNP Q8L940
Р	766	GLY	-	expression tag	UNP Q8L940
Р	767	GLY	-	expression tag	UNP Q8L940
Р	768	GLY	-	expression tag	UNP Q8L940
Р	769	SER	-	expression tag	UNP Q8L940
Q	1003	MET	-	expression tag	UNP Q8L940
Q	1004	ASP	-	expression tag	UNP Q8L940
Q	1005	TYR	-	expression tag	UNP Q8L940
Q	1006	LYS	-	expression tag	UNP Q8L940
Q	1007	ASP	-	expression tag	UNP Q8L940
Q	1008	HIS	-	expression tag	UNP Q8L940
Q	1009	ASP	-	expression tag	UNP Q8L940
Q	1010	GLY	-	expression tag	UNP Q8L940
Q	1011	ASP	-	expression tag	UNP Q8L940
Q	1012	TYR	-	expression tag	UNP Q8L940
Q	1013	LYS	-	expression tag	UNP Q8L940
Q	1014	ASP	-	expression tag	UNP Q8L940
Q	1015	HIS	-	expression tag	UNP Q8L940
Q	1016	ASP	-	expression tag	UNP Q8L940
Q	1017	ILE	-	expression tag	UNP Q8L940
Q	1018	ASP	-	expression tag	UNP Q8L940
Q	1019	TYR	-	expression tag	UNP Q8L940
Q	1020	LYS	-	expression tag	UNP Q8L940
Q	1021	ASP	-	expression tag	UNP Q8L940
Q	1022	ASP	-	expression tag	UNP Q8L940
Q	1023	ASP	-	expression tag	UNP Q8L940
Q	1024	ASP	-	expression tag	UNP Q8L940
Q	1025	LYS	-	expression tag	UNP Q8L940

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1026	LEU	-	expression tag	UNP Q8L940
Q	1027	ALA	-	expression tag	UNP Q8L940
Q	1028	GLY	-	expression tag	UNP Q8L940
Q	1029	GLY	-	expression tag	UNP Q8L940
Q	1030	GLY	-	expression tag	UNP Q8L940
Q	1031	GLY	-	expression tag	UNP Q8L940
Q	1032	SER	-	expression tag	UNP Q8L940
R	1266	MET	-	expression tag	UNP Q8L940
R	1267	ASP	-	expression tag	UNP Q8L940
R	1268	TYR	-	expression tag	UNP Q8L940
R	1269	LYS	-	expression tag	UNP Q8L940
R	1270	ASP	-	expression tag	UNP Q8L940
R	1271	HIS	-	expression tag	UNP Q8L940
R	1272	ASP	-	expression tag	UNP Q8L940
R	1273	GLY	-	expression tag	UNP Q8L940
R	1274	ASP	-	expression tag	UNP Q8L940
R	1275	TYR	-	expression tag	UNP Q8L940
R	1276	LYS	-	expression tag	UNP Q8L940
R	1277	ASP	-	expression tag	UNP Q8L940
R	1278	HIS	-	expression tag	UNP Q8L940
R	1279	ASP	-	expression tag	UNP Q8L940
R	1280	ILE	-	expression tag	UNP Q8L940
R	1281	ASP	-	expression tag	UNP Q8L940
R	1282	TYR	-	expression tag	UNP Q8L940
R	1283	LYS	-	expression tag	UNP Q8L940
R	1284	ASP	-	expression tag	UNP Q8L940
R	1285	ASP	-	expression tag	UNP Q8L940
R	1286	ASP	-	expression tag	UNP Q8L940
R	1287	ASP	-	expression tag	UNP Q8L940
R	1288	LYS	-	expression tag	UNP Q8L940
R	1289	LEU	-	expression tag	UNP Q8L940
R	1290	ALA	-	expression tag	UNP Q8L940
R	1291	GLY	-	expression tag	UNP Q8L940
R	1292	GLY	-	expression tag	UNP Q8L940
R	1293	GLY	-	expression tag	UNP Q8L940
R	1294	GLY	-	expression tag	UNP Q8L940
R	1295	SER	-	expression tag	UNP Q8L940
S	1529	MET	-	expression tag	UNP Q8L940
S	1530	ASP	-	expression tag	UNP Q8L940
S	1531	TYR	-	expression tag	UNP Q8L940
S	1532	LYS	-	expression tag	UNP Q8L940
S	1533	ASP	-	expression tag	UNP Q8L940



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Chain	Residue	Modelled	Actual	Comment	Reference	
S	1534	HIS	-	expression tag	UNP Q8L940	
S	1535	ASP	-	expression tag	UNP Q8L940	
S	1536	GLY	-	expression tag	UNP Q8L940	
S	1537	ASP	-	expression tag	UNP Q8L940	
S	1538	TYR	-	expression tag	UNP Q8L940	
S	1539	LYS	-	expression tag	UNP Q8L940	
S	1540	ASP	-	expression tag	UNP Q8L940	
S	1541	HIS	-	expression tag	UNP Q8L940	
S	1542	ASP	-	expression tag	UNP Q8L940	
S	1543	ILE	-	expression tag	UNP Q8L940	
S	1544	ASP	-	expression tag	UNP Q8L940	
S	1545	TYR	-	expression tag	UNP Q8L940	
S	1546	LYS	-	expression tag	UNP Q8L940	
S	1547	ASP	-	expression tag	UNP Q8L940	
S	1548	ASP	-	expression tag	UNP Q8L940	
S	1549	ASP	-	expression tag	UNP Q8L940	
S	1550	ASP	-	expression tag	UNP Q8L940	
S	1551	LYS	-	expression tag	UNP Q8L940	
S	1552	LEU	-	expression tag	UNP Q8L940	
S	1553	ALA	-	expression tag	UNP Q8L940	
S	1554	GLY	-	expression tag	UNP Q8L940	
S	1555	GLY	-	expression tag	UNP Q8L940	
S	1556	GLY	-	expression tag	UNP Q8L940	
S	1557	GLY	-	expression tag	UNP Q8L940	
S	1558	SER	-	expression tag	UNP Q8L940	
Т	1792	MET	-	expression tag	UNP Q8L940	
Т	1793	ASP	-	expression tag	UNP Q8L940	
Т	1794	TYR	-	expression tag	UNP Q8L940	
Т	1795	LYS	-	expression tag	UNP Q8L940	
Т	1796	ASP	-	expression tag	UNP Q8L940	
Т	1797	HIS	-	expression tag	UNP Q8L940	
Т	1798	ASP	-	expression tag	UNP Q8L940	
Т	1799	GLY	-	expression tag	UNP Q8L940	
Т	1800	ASP	-	expression tag	UNP Q8L940	
Т	1801	TYR	-	expression tag	UNP Q8L940	
Т	1802	LYS	-	expression tag	UNP Q8L940	
Т	1803	ASP	-	expression tag	UNP Q8L940	
Т	1804	HIS	-	expression tag	UNP Q8L940	
Т	1805	ASP	-	expression tag	UNP Q8L940	
Т	1806	ILE	-	expression tag	UNP Q8L940	
Т	1807	ASP	-	expression tag	UNP Q8L940	
Т	1808	TYR	-	expression tag	UNP Q8L940	

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Chain	Residue	Modelled	Actual	Comment	Reference
Т	1809	LYS	-	expression tag	UNP Q8L940
Т	1810	ASP	-	expression tag	UNP Q8L940
Т	1811	ASP	-	expression tag	UNP Q8L940
Т	1812	ASP	-	expression tag	UNP Q8L940
Т	1813	ASP	-	expression tag	UNP Q8L940
Т	1814	LYS	-	expression tag	UNP Q8L940
Т	1815	LEU	-	expression tag	UNP Q8L940
Т	1816	ALA	-	expression tag	UNP Q8L940
Т	1817	GLY	-	expression tag	UNP Q8L940
Т	1818	GLY	-	expression tag	UNP Q8L940
Т	1819	GLY	-	expression tag	UNP Q8L940
Т	1820	GLY	-	expression tag	UNP Q8L940
Т	1821	SER	-	expression tag	UNP Q8L940
U	2055	MET	-	expression tag	UNP Q8L940
U	2056	ASP	-	expression tag	UNP Q8L940
U	2057	TYR	-	expression tag	UNP Q8L940
U	2058	LYS	-	expression tag	UNP Q8L940
U	2059	ASP	-	expression tag	UNP Q8L940
U	2060	HIS	-	expression tag	UNP Q8L940
U	2061	ASP	-	expression tag	UNP Q8L940
U	2062	GLY	-	expression tag	UNP Q8L940
U	2063	ASP	-	expression tag	UNP Q8L940
U	2064	TYR	-	expression tag	UNP Q8L940
U	2065	LYS	-	expression tag	UNP Q8L940
U	2066	ASP	-	expression tag	UNP Q8L940
U	2067	HIS	-	expression tag	UNP Q8L940
U	2068	ASP	-	expression tag	UNP Q8L940
U	2069	ILE	-	expression tag	UNP Q8L940
U	2070	ASP	-	expression tag	UNP Q8L940
U	2071	TYR	-	expression tag	UNP Q8L940
U	2072	LYS	-	expression tag	UNP Q8L940
U	2073	ASP	-	expression tag	UNP Q8L940
U	2074	ASP	-	expression tag	UNP Q8L940
U	2075	ASP	-	expression tag	UNP Q8L940
U	2076	ASP	-	expression tag	UNP Q8L940
U	2077	LYS	-	expression tag	UNP Q8L940
U	2078	LEU	-	expression tag	UNP Q8L940
U	2079	ALA	-	expression tag	UNP Q8L940
U	2080	GLY	-	expression tag	UNP Q8L940
U	2081	GLY	-	expression tag	UNP Q8L940
U	2082	GLY	-	expression tag	UNP Q8L940
U	2083	GLY	-	expression tag	UNP Q8L940

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Chain	Residue	Modelled	Actual	Comment	Reference
U	2084	SER	-	expression tag	UNP Q8L940
V	2318	MET	-	expression tag	UNP Q8L940
V	2319	ASP	-	expression tag	UNP Q8L940
V	2320	TYR	-	expression tag	UNP Q8L940
V	2321	LYS	-	expression tag	UNP Q8L940
V	2322	ASP	-	expression tag	UNP Q8L940
V	2323	HIS	-	expression tag	UNP Q8L940
V	2324	ASP	-	expression tag	UNP Q8L940
V	2325	GLY	-	expression tag	UNP Q8L940
V	2326	ASP	-	expression tag	UNP Q8L940
V	2327	TYR	-	expression tag	UNP Q8L940
V	2328	LYS	-	expression tag	UNP Q8L940
V	2329	ASP	-	expression tag	UNP Q8L940
V	2330	HIS	-	expression tag	UNP Q8L940
V	2331	ASP	-	expression tag	UNP Q8L940
V	2332	ILE	-	expression tag	UNP Q8L940
V	2333	ASP	-	expression tag	UNP Q8L940
V	2334	TYR	-	expression tag	UNP Q8L940
V	2335	LYS	-	expression tag	UNP Q8L940
V	2336	ASP	-	expression tag	UNP Q8L940
V	2337	ASP	-	expression tag	UNP Q8L940
V	2338	ASP	-	expression tag	UNP Q8L940
V	2339	ASP	-	expression tag	UNP Q8L940
V	2340	LYS	-	expression tag	UNP Q8L940
V	2341	LEU	-	expression tag	UNP Q8L940
V	2342	ALA	-	expression tag	UNP Q8L940
V	2343	GLY	-	expression tag	UNP Q8L940
V	2344	GLY	-	expression tag	UNP Q8L940
V	2345	GLY	-	expression tag	UNP Q8L940
V	2346	GLY	-	expression tag	UNP Q8L940
V	2347	SER	-	expression tag	UNP Q8L940
W	2581	MET	-	expression tag	UNP Q8L940
W	2582	ASP	-	expression tag	UNP Q8L940
W	2583	TYR	-	expression tag	UNP Q8L940
W	2584	LYS	-	expression tag	UNP Q8L940
W	2585	ASP	-	expression tag	UNP Q8L940
W	2586	HIS	-	expression tag	UNP Q8L940
W	2587	ASP	-	expression tag	UNP Q8L940
W	2588	GLY	-	expression tag	UNP Q8L940
W	2589	ASP	-	expression tag	UNP Q8L940
W	2590	TYR	-	expression tag	UNP Q8L940
W	2591	LYS	-	expression tag	UNP Q8L940

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Chain	Residue	Modelled	Actual	Comment	Reference
W	2592	ASP	-	expression tag	UNP Q8L940
W	2593	HIS	-	expression tag	UNP Q8L940
W	2594	ASP	-	expression tag	UNP Q8L940
W	2595	ILE	-	expression tag	UNP Q8L940
W	2596	ASP	-	expression tag	UNP Q8L940
W	2597	TYR	-	expression tag	UNP Q8L940
W	2598	LYS	-	expression tag	UNP Q8L940
W	2599	ASP	-	expression tag	UNP Q8L940
W	2600	ASP	-	expression tag	UNP Q8L940
W	2601	ASP	-	expression tag	UNP Q8L940
W	2602	ASP	-	expression tag	UNP Q8L940
W	2603	LYS	-	expression tag	UNP Q8L940
W	2604	LEU	-	expression tag	UNP Q8L940
W	2605	ALA	-	expression tag	UNP Q8L940
W	2606	GLY	-	expression tag	UNP Q8L940
W	2607	GLY	-	expression tag	UNP Q8L940
W	2608	GLY	-	expression tag	UNP Q8L940
W	2609	GLY	-	expression tag	UNP Q8L940
W	2610	SER	-	expression tag	UNP Q8L940
Х	2844	MET	-	expression tag	UNP Q8L940
Х	2845	ASP	-	expression tag	UNP Q8L940
Х	2846	TYR	-	expression tag	UNP Q8L940
Х	2847	LYS	-	expression tag	UNP Q8L940
Х	2848	ASP	-	expression tag	UNP Q8L940
Х	2849	HIS	-	expression tag	UNP Q8L940
X	2850	ASP	-	expression tag	UNP Q8L940
Х	2851	GLY	-	expression tag	UNP Q8L940
X	2852	ASP	-	expression tag	UNP Q8L940
Х	2853	TYR	-	expression tag	UNP Q8L940
Х	2854	LYS	-	expression tag	UNP Q8L940
X	2855	ASP	-	expression tag	UNP Q8L940
Х	2856	HIS	-	expression tag	UNP Q8L940
X	2857	ASP	-	expression tag	UNP Q8L940
X	2858	ILE	-	expression tag	UNP Q8L940
X	2859	ASP	-	expression tag	UNP Q8L940
X	2860	TYR	-	expression tag	UNP Q8L940
X	2861	LYS	-	expression tag	UNP Q8L940
X	2862	ASP	-	expression tag	UNP Q8L940
X	2863	ASP	-	expression tag	UNP Q8L940
X	2864	ASP	-	expression tag	UNP Q8L940
X	2865	ASP	-	expression tag	UNP Q8L940
X	2866	LYS	-	expression tag	UNP Q8L940

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Chain	Residue	Modelled	Actual	Comment	Reference
Х	2867	LEU	-	expression tag	UNP Q8L940
Х	2868	ALA	-	expression tag	UNP Q8L940
Х	2869	GLY	-	expression tag	UNP Q8L940
Х	2870	GLY	-	expression tag	UNP Q8L940
Х	2871	GLY	-	expression tag	UNP Q8L940
Х	2872	GLY	-	expression tag	UNP Q8L940
Х	2873	SER	-	expression tag	UNP Q8L940



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2



LYS LYS LSS HIS HIS B52 B52 B530 C533 C533 C533 C533 C533 C533 C533 C	•
M666 M666 M668 M668 M668 M668 M668 M668	
SER SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2	
Chain D: 57% 17% • 25%	
MET MET ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	
LYS ASN HIS H15 H15 A306 A306 A306 A306 A306 A306 A306 A306	
1917 1917 1918 1918 1918 1918 1918 1922 1925 1922 1925 1922 1925 1922 1925 1925 1925 1925 1925 1925 1925 1925 1925 1925 1971 1971 1971 1971 1971 1971 1971 1971 1971 1971 1971 1971 1971 1971 1971 1971 1973 1976 1990 1990 1006 1990 1006 1016 1028 1028 1028 1028 1028 1028 1028 1028 1028 1028 1028 1028 1028 1028 1028 1028 1028 </td <td></td>	
SELU ASN VAL ASP ASP ASP ASP ASP ASP CLY CLN CLN CLN CLN CLN VAL	
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2	
Chain E: 57% 17% 25%	
MET MART TYR ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	
LYS LYS LSYS LSYS LIO448 LIO48	•
M1176 M1177 M1177 M1187 Q1180 Q1180 Q1187 Q1186 Q1187 Q1187 Q1186 M1196 M1196 M1196 M1234 Q1241 Q1241 Q1241 Q1241 Q1241 Q1241 Q1238 Q1238 Q1236 Q1241 Q1246 Q1241 Q1246 Q1241 Q1256 Q1241 Q1256 Q1241 Q1256 Q1241 Q1256 Q1241 Q1256 Q1241 Q1256 Q12888 Q12888 Q12888 Q1288 Q1288 Q1288 Q1288 Q1288 Q1288	
ALA ALA MET ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2	
Chain F: 56% 18% · 25%	
ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	



M1436 M1436 M138 M1436 M1436 M138 F1445 P1301 P1446 M1369 P1447 M1369 P1446 M1309 V1456 M1370 V1456 M1370 V1497 P1353 V1496 M1370 V1497 P1356 N1496 N1370 V1497 P1356 N1496 N1370 V1497 P1356 N1496 N1370 V1497 P1358 N1496 N1370 V1497 P1356 P1510 V1379 V1496 N1370 V1497 P1358 N1496 N1370 V1497 V1379 V1496 N1370 V1497 V1379 V1496 V1379 V1497 V1370 V1498 V1370 V1499 V1370 V1556 P1364

• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2





• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

Chain I:	55%	19%	•	25%	
MET ASP TYR LYS ASP ASP ASP ASP CLY	ASP TYR TYR ASP ASP ASP ASP TYR LYS ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	GLY GLY SER ALA ASP GLN MET THR ASP	GLN GLN GLY	ALA VAL THR LEU TYR SER GLY THR	ILE THR ASP ALA LYS





• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2





Y2903 72905 82905 82905 82905 82905 82905 82905 82905 82905 82905 82905 82905 82917 82916 82917 82918 82918 82918 82918 82918 82918 82918 82918 82930 82931 </th <th>V2935 Y2951 E2954 I2957 V2960</th> <th>A291 12977 12977 2985 2985 2986 12987 12989 82996 M2996</th>	V2935 Y2951 E2954 I2957 V2960	A291 12977 12977 2985 2985 2986 12987 12989 82996 M2996
K30339 K3039 S3042 F3051 F3055 V3055 V3055 V3055 P3056 Q3061 Q3061 P3070	L3079 V3086 F3091 P3096 R3101	I3102 I3103 A3106 V3115 S3120 S3120 SER GLY LEU GLU
VAL		
'-phosphate synthase sub	ounit PDX1.3	
61%	17%	22%
ASP ASP ASP ASP ASP ASP LLU ALA ALA CLY CLY CLY CLY CLY CLY CLY ALA ALA	VAL TYR GLY ASN GLY ALA THR GLU GLU	LAS SER SER PI PI PI PI PI PI TI3 TI3
L 12 17 17 17 17 17 17 17 17 17 17	193 194 196 196 899 8100 8100	E107 R142 R144 G145 E146 T149 T149
F228 V229 V229 V229 V247 A243 A243 A249 A249 A249 A249 A249 A249 A249 A249	GLU ALA MET VAL GLY GLY ASN ASN ASN	LYS LYS VAL ARC ARC ARA ARG SER SER CLU
'-phosphate synthase sub	ounit PDX1.3	
56%	22%	22%
ASP ASP ASP ASP ASP ASP ASP ALA CUU CUU CUU CUU CUU CUU CUU CUU CUU CU	VAL TYR GLY ASN CLZ ALZ THR THR GLU ALA	LYS LYS SER P264 P264 P266 C270 L271 L271 L271 L271 L271 L271 L271 L271
R311 R311 A312 C321 R320 R324 M324 M337 M337 K339 K339 K339 K339 K339 K339 K339 K	44 45 44 44 44 50 51 51 51 51 51 51 51 51 51 51 51 51 51	
	H3 F3 F3 F3 F3 F3 F3 F3 F3 F3 F3 F3 F3 F3	1350 1365 1365 1365 1367 1367 1367 1377 1377
V422 N426 1429 1429 1431 1433 1453 1453 1453 1463 1463 1463	A480 H80 H80 H80 H80 H80 H80 H80 H80 H80 H	P502 P502 A506 A506 B362 A510 B362 B362 B362 B362 B362 B362 B362 B362
ARG V422 PHE N426 ASN 1426 ASN 1429 SER 1429 SER 1429 CLU 1431 L453 L453 K452 L463 L463 P476	4480 4480 4480 4480 4480 4480 4480 4480	F502 F305 F502 1366 A506 5365 V510 5365 V510 1374 V513 1374
i'-phosphate synthase sub	ennit PDX1.3	F502 1350 F502 1366 F506 2366 F510 1366 M510 1367 M512 1374 V513 1374
Image: Second	ent PDX1.3	
South and the synthese subsets South and the synthe synthese subsets	8 2 8 <td>XER N 23 XER N</td>	XER N 23 XER N
	$ \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c}$	2000 20000 2000

WORLDWIDE PROTEIN DATA BANK

ALA MET VAL GLY ILE ASN ASN ASN ASN CLU CLYS CLU GLU ARG ARG ARG ARG ARG ARG ARG CLU GLU CLU

• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain P:	63%	15%	22%
MET ASP TYR ASP ASP ASP ASP ASP TYR TYR TYR ASP TYR TYR ASP	ASP 11LE ASP 12VR ASP ASP ASP ASP ASP ASP ASP ASP ASP CUY CUY SER SER SER	THR THR CLY CLY CLY VAL ALA ALA CLY CLY THR CLY THR THR CLU	LYS LYS SER 858 790 799 7790 7799 7799 7799 7799 7799
M807 D808 V809 V809 V815 A815 A815 L829 L829 L829 L829 R831 R831	R837 4838 4838 4839 4839 4839 4864 4864 4864 4864 4864 4864 4864 4871 7871 7871 7871 7871 7872 7873 7873	A874 1875 1875 1882 1885 1885 1885 1885 1885 1885 188	1098 1098 1098 1098 1098 1098 1095 1095 1095 1095 1095 1095 1095 1095
L979 R988 L989 P1002 P1002 V1016 V1016	V1036 01037 01037 01037 01048 V1048 V1048 V1049 S1052 CVS CVS CVS CVS CVS CVS CVS CVS	111 1115 ASN ASN ASN ASP CJU CJU CJU CJU CJU ASN ASA ASA ASA ASA	SEA
• Molecule 2: Pyr	idoxal 5'-phosphate synt	hase subunit PDX1.3	}
Chain Q:	57%	21%	22%
MET ASP ASP LYR LYS ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	ASP ILLE ASP ASP LYS ASP ASP ASP ASP ASP ASP CUX GIX GIX SER SER SER SER CUX	THR THR OLY VAL VAL VAL VAL TYR ALA ALA ALA ALA ALA THR THR THR THR	LYS LYS SER SER F1064 F1064 C1060 L1060 L1060 C1060 R1061 R1065
V1068 11069 11070 11071 V1072 V1073 N1074 Q1077 V1089	L1092 E1094 R1004 A1100 A1100 A1102 A1102 M1113 M1113 M1128 M1128 K1128	11131 61132 F1133 F1133 F1135 F1135 E1135 01136 11139 11145 11145 11145	81151 E1152 L1156 E1159 T1163 P1171 P1171
R1187 R1194 R1196 R1196 R1196 E1198 A1199 A1199 A1200 C1200 C1200 E1206	A1207 V1211 N1215 N1216 11218 V1220 L1221 L1221 K1247 K1247 K1247	P1265 A1269 L1274 D1277 01277 01278 C1285 C1285 C1285 C1285 C1285 C1285 C1286	N1287 P1291 P1291 V1295 Q1300 Q1300 A1301 V1312 V1312 S1315
CYS GLY GLY GLY GLY GLY GLY GLY TLE ASN LEU ASN	ASP GLU LYS VAL CALU ARG PHE ALA ALA ARG SER CLU		
• Molecule 2: Pyr	idoxal 5'-phosphate synt	hase subunit PDX1.3	3
Chain R:	59%	19%	22%
MET ASP ASP LYR LYS ASP ASP GLY ASP ASP ASP ASP ASP HIS	ASP ILLE ASP ASP LLYS ASP ASP ASP ASP ASP ASP ASP CLY GLY SER SER SER CLY SER SER CLY	THR THR OLY VAL VAL VAL VAL TYR ALA ALA ALA ALA CLY THR THR THR THR	LAA LYS LYS SER F1317 F1317 F1317 C1322 C1322 C1322 C1323 C1323 C1323 C1323 C1323 C1323
V1331 D1334 V1335 A1341 R1342 E1346 E1346	L1355 E1356 R1357 V1356 R1365 A1364 Q1365 A1364 Q1365 A1366	H1395 H1397 F1397 V1398 F1397 V1398 F1398 F1398 F1400 F1400 F1410 F1411 F1411 F1411 F1413 F1413 F1413 F1413	E1415 E1415 E1422 E1422 E1424 H1424 H1426 F1426 F1426 F1434 A1445
R1450 R1457 A1462 A1462 E1468 A1470 A1470 V1474	M1478 V1483 L1484 R1485 K1505 K1510 K1510 F1528 P1528 A1532 A1532 L1537	D1540 C1541 V1542 V1542 A1564 A1564 V1566 S1565 C156 C15 C12 C12 C12 C12 C12 C12 C12 C12 C12 C12	LLU GLY GLU ALA MET MET MET ALA ASIN ASN ASN ASN CLU CLU LYS



VAL GLU ARG PHE ALA ASN ASN SER SER GLU

• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain S:	60%	18%	22%
MET ASP LYS LYS LYS LYS ASP ASP ASP ASP ASP TYS LYS ASP ASP ASP ASP	ASP ASP ASP ASP ASP ASP ASP ALA ALA CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	TYR GLY ASN ASN CLY ALA THR THR GLU ALA	LYS SER P1579 1579 01584 01588 R1591 V1594 11595
M1596 D1597 V1598 V1598 V1599 A1604 B1605 E1609 C1615 E1619 R1620 R1621 D1624 D1624 B1625 B1625 B1625 B1625 B1625	A1627 Q1628 Q1628 Q1628 S1635 C1669 M1652 A1653 H1657 C1660 C1666	11664 11665 11671 11672 11673 11673 11674 11674 11674 11674 11677	L1682 L1685 E1685 D1686 H1687 H1720 C1722 C1722 C1723 E1724
A1725 G1726 G1726 11731 11731 11741 N1741 N1745 N1745 N1777 L1178 P1791 P1791 P1791 N1809	C 1800 V1805 F 1806 V1807 V1805 V1805 A1821 A1821 A1821 A1821 A1825 A1826 V1838 A1826 A1836 A1826 A18366 A1836 A1836 A1836 A1836 A1836 A1836 A1836 A1836 A1836 A18	CYS GLY GLY GLV ALA ALA VAL VAL CLY	ASN LEU ASP GLU CVS CLV LVS CLV CVAL GLU ARG PHE ALA ASN
ARG SER GLU			
• Molecule 2: Pyridoxal 5'	-phosphate synthase subu	nit PDX1.3	
Chain T:	60%	18%	22%
MET ASP TYR LYR ASP ASP ASP ASP ASP ASP ASP TYR LYS ASP ASP ASP	ASP ASP ASP ASP LEV ALA ALA GLY GLY GLY GLY VAL ALA VAL	TYR GLY ASN GLY ALA ILE THR GLU ALA	LYS SER F1843 F1843 V1847 Q1851 R1854 V1854 V1854
I1858 M1859 D1860 D1860 D1861 E1881 R1878 R1878 R1883 E1881 R1883 R1883 R1883 E1883 R1883 R1883 R1883 R1883 R1883 R1883 R1883 R1883 R1893 R1893 R1992 R1992 R1912 R1912	A1916 K1917 11920 11921 H1922 F1923 V1924 A1926 A1926 A1926 A1926 11934 T1934 T1934 T1935	E1940 E1941 L1945 E1948 E1948 11952 R1976	R1993 T1984 K1985 G1986 E1987 T1990 T1995 A1995 A1996
V2000 N2004 V2009 L2010 L2010 K2036 P2054 A2058 L2063	62071 82073 12073 12073 12075 82076 82076 82076 82077 82076 82077 82078 82077 82078 82077 82078 82077 80077 800700	V22101 S2104 CYS CYS GLY GLY GLU GLU MALA MALA	VAL GLY TILE ASN ASN ASN ASN CLU CLU GLU ARG
PHE ALA ARSI SER SER GUU			
• Molecule 2: Pyridoxal 5'	-phosphate synthase subu	nit PDX1.3	
Chain U:	58%	20%	22%
MET ASP LYR LYR ASP ASP ASP ASP ASP ASP ASP TYR ASP ASP ASP	ASP ASP ASP LEU LEU ALA ALA GLY GLY GLY GLY VAL ALA VAL	TYR GLY GLY GLY ALA THR THR GLU CYS	LYS BER P2106 F2106 C2110 C2111 C2112 A2113 Q2114 Q2114 R2117
V2120 N2121 M2122 W2124 V2124 V2126 V2126 V2126 A2130 R2130 R2131 E2135 V2141 L2144 V2141	v2.447 v2.447 D2150 Q2154 Q2154 12166 12166 12175 N2178 N2178 12183 12185 H2185 H2185 H2186	2187 2188 2188 2190 2190 12191 2197 2198 72199 72199	D2201 E2202 E2203 E2204 E2211 D2212 H2213 H2213 H2213 H2214 12215
P223 A224 A224 R2239 R2239 R2239 A2259 A2259 V2263 V2263 V2263 V2263	L2294 L2294 K2299 R2303 L2304 L2320 D2329 D2329 C2330 V2331	22335 22335 72338 72338 82340 72340 72343 72343 72343	V2351 Q2353 A2353 V2364 V2364 V2364 CV3 GL7 GL7 GL7 GL7 GL7 GL7 GL7



GLU ALA MET VUAL CLAL ALA ASN ASN ASN ASN CLU CLVS CLU CLVS ASN ASN ASN ASN CLU CLVS CLU CLU SER CLU

• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain V:	62%	16%	22%	_
MET ASP ASP TYR LYS ASP GLY GLY CYS ASP ASP ASP ASP ASP ASP ASP	TYR LYS LYS ASP ASP ASP ASP LYS LLU LEU CLY GLY GLY	SER GLU GLU GLV CLL CLV VAL VAL VAL TYR CLV GLV GLV	ALA THE THE GLU GLU ALA LYS SER SER P2688	q2377 R2380 M2385 D2386
V2387 V2388 V2388 A2393 R2398 R2398 R2398 R2405 R2405 R2405 R2410 P2411 R2411 R2411	D2413 T2414 R2415 S2424 12438 M2441 M2441 A2443 R2443 R2443	H2447 H2447 F2448 F2450 E2451 A2451 12460 12460 12460 12462 12462 12462	22466 E2467 L2471 E2474 E2476 H2476 H2476 R2509	T2510 K2511 G2515 I2520
N2530 1253 R2535 R2535 R2536 R2536 R2536 R2566 R2566 R2566	D2592 A2610 A2616 E2624 E2624 E2629 V2629 S2629 S2629	LEU LEU GLV GLV GLV GLV ALA MET MET MET ASN LEU ASN ASP	GLU LYS VAL GLU GLU ARG ARG ASN ASN SER GLU GLU	
• Molecule 2: Pyridox	xal 5'-phosphate sy	vnthase subunit Pl	DX1.3	
Chain W:	58%	20%	22%	_
MET ASP TYR LYS LYS ASP ASP CLY GLY CYS ASP ASP ASP ASP ASP ASP ASP	TYR LYS ASP ASP ASP ASP LYS LEU ALA ALA ALA ALA GLY GLY	SER GLU GLU GLU GLY CLY CLY VAL VAL TYR GLY GLY	ILE THR THR GLU GLU GLU LYS LYS SER P2631 F2632	V2636 Q2640 R2643 V2646
12647 D2648 D2649 D2649 D2655 Q2655 C2657 L2670 E2671 R2677 R2677 C2677 D2676	12677 12677 A2678 A2678 Q2680 S2687 D2688 M2691 12701 M2704	A2705 K2706 12706 C2710 H2711 F2712 F2713 F2715 A2715 Q2716 12715	12723 12725 12725 12726 12726 52729 52730 12734 12734	12741 A2760 R2765
R2772 R2773 K2774 C2775 G2775 G2776 A2777 12779 T2779 C27789 A27783 A2785 A2785 A2785 A2785 A2785 A2785 A2785 A2785	V2798 L2799 L2200 L2220 K2825 K2825 L2830 L2830	A2847 L2852 V2857 V2857 C2860 F2864 P2869 P2869 A2873	V2877 Q2878 A2879 V2880 V2880 S2893 CYS GLY GLY	LEU GLY GLU ALA MET VAL CLY
11LE ASN 15SU 15SU 4SP 6LU 6LU 72AL 71KS 71A 71A 71A 71A 71A 71A 71A 71A 71A 71A				
• Molecule 2: Pyridox	xal 5'-phosphate sy	vnthase subunit P	DX1.3	
Chain X:	59%	19%	22%	_
MET ASP TYR LYS LYS ASP GLY CLY GLY CLYS ASP ASP ASP ASP ASP ASP ASP ASP	TYR LYS ASP ASP ASP ASP LY LEU CLY GLY GLY	SER GLU GLU GLV CLV CLV VAL VAL VAL TYR CLV GLV GLV	ILE ILE THE GLU ALA LYS LYS SER P2894 F2895	V2899 G2900 L2901 A2902 Q2903 R2903
V2909 V2913 V2913 A2919 R2920 R2930 M2931 M2933 L2933 R2933 R2933	V2336 D2399 I2940 R2941 R2941 R2943 R2943 R2943 R2943 I2964 I2964	12972 62973 H2974 F2975 F2975 22977 22976 12980 12986 12986	72988 72989 72990 82992 82992 82993 82993 82993 82993 82993 82993 82993 82930 8200 83001	H3002 H3003 I3004 P3012 A3023
R3028 R3025 R3035 A3040 G3041 13046 E3047 A3048 N3052 N3052	V3061 L3063 L3063 K3068 K3088 R3093 L3093 L3093	A3110 L3115 D3118 03119 V3120 V3120 S3124 V3140 C3141 V3141 V3141	Mais1 Lais2 Vais3 Sais6 CYS CYS CLY LEU CLY CLY CLY CLY CLY	ALA MET VAL GLY ILE ASN LEU
ASN ASP GLU CYS CYS CVAL GLU ALA ALA ASN ASN SER SER GLU				



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	286642	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	5.703	Depositor
Minimum map value	-1.552	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.222	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	303.59998, 303.59998, 303.59998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.012, 1.012, 1.012	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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	А	0.26	0/1998	0.42	0/2701	
1	В	0.26	0/1998	0.42	0/2701	
1	С	0.26	0/1998	0.42	0/2701	
1	D	0.26	0/1998	0.42	0/2701	
1	Е	0.26	0/1998	0.42	0/2701	
1	F	0.26	0/1998	0.42	0/2701	
1	G	0.26	0/1998	0.42	0/2701	
1	Н	0.26	0/1998	0.42	0/2701	
1	Ι	0.26	0/1998	0.42	0/2701	
1	J	0.26	0/1998	0.42	0/2701	
1	Κ	0.26	0/1998	0.42	0/2701	
1	L	0.26	0/1998	0.42	0/2701	
2	М	0.28	0/2039	0.44	0/2749	
2	N	0.29	0/2039	0.45	0/2749	
2	0	0.29	0/2039	0.45	0/2749	
2	Р	0.29	0/2039	0.45	0/2749	
2	Q	0.29	0/2039	0.45	0/2749	
2	R	0.29	0/2039	0.45	0/2749	
2	S	0.29	0/2039	0.44	0/2749	
2	Т	0.29	0/2039	0.45	0/2749	
2	U	0.29	0/2039	0.45	0/2749	
2	V	0.29	0/2039	0.45	0/2749	
2	W	0.29	0/2039	0.45	0/2749	
2	Х	0.29	0/2039	0.44	0/2749	
All	All	0.28	0/48444	0.43	0/65400	

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1968	0	1856	42	0
1	В	1968	0	1851	43	0
1	С	1968	0	1852	43	0
1	D	1968	0	1856	39	0
1	Е	1968	0	1853	43	0
1	F	1968	0	1850	46	0
1	G	1968	0	1835	39	0
1	Н	1968	0	1851	39	0
1	Ι	1968	0	1845	47	0
1	J	1968	0	1854	42	0
1	Κ	1968	0	1847	41	0
1	L	1968	0	1834	41	0
2	М	2012	0	1918	36	0
2	Ν	2012	0	1925	52	0
2	0	2012	0	1926	45	0
2	Р	2012	0	1922	33	0
2	Q	2012	0	1923	46	0
2	R	2012	0	1925	43	0
2	S	2012	0	1920	42	0
2	Т	2012	0	1924	40	0
2	U	2012	0	1909	44	0
2	V	2012	0	1931	37	0
2	W	2012	0	1924	47	0
2	Х	2012	0	1926	43	0
All	All	47760	0	45257	938	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 938 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)
2:P:837[B]:ARG:NH2	2:P:936[B]:ALA:O	2.11	0.84
2:W:2709[B]:ILE:HD11	2:W:2730[B]:GLU:HA	1.62	0.80
2:N:342[B]:ILE:HD11	2:N:363[B]:GLU:HA	1.62	0.80



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1131[B]:ILE:HD11	2:Q:1152[B]:GLU:HA	1.62	0.80
2:T:1920[B]:ILE:HD11	2:T:1941[B]:GLU:HA	1.63	0.80

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 PDB entries followed by that with respect to all EM entries.

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	Perce	entiles
1	А	258/348~(74%)	252~(98%)	6 (2%)	0	100	100
1	В	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
1	С	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
1	D	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
1	Е	258/348~(74%)	252~(98%)	6 (2%)	0	100	100
1	F	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
1	G	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
1	Н	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
1	Ι	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
1	J	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
1	K	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
1	L	258/348~(74%)	252 (98%)	6 (2%)	0	100	100
2	М	265/338~(78%)	257 (97%)	8 (3%)	0	100	100
2	Ν	265/338~(78%)	256 (97%)	9 (3%)	0	100	100
2	Ο	265/338~(78%)	255 (96%)	10 (4%)	0	100	100
2	Р	265/338 (78%)	256 (97%)	9 (3%)	0	100	100
2	Q	265/338~(78%)	257 (97%)	8 (3%)	0	100	100
2	R	265/338~(78%)	256 (97%)	9 (3%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	S	265/338~(78%)	258~(97%)	7(3%)	0	100	100
2	Т	265/338~(78%)	257~(97%)	8 (3%)	0	100	100
2	U	265/338~(78%)	257~(97%)	8 (3%)	0	100	100
2	V	265/338~(78%)	257~(97%)	8 (3%)	0	100	100
2	W	265/338~(78%)	258~(97%)	7 (3%)	0	100	100
2	Х	265/338~(78%)	256~(97%)	9(3%)	0	100	100
All	All	6276/8232~(76%)	6104 (97%)	172 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	Perce	ntiles
1	А	214/280~(76%)	212~(99%)	2(1%)	78	91
1	В	214/280~(76%)	212~(99%)	2(1%)	78	91
1	\mathbf{C}	214/280~(76%)	212~(99%)	2(1%)	78	91
1	D	214/280~(76%)	212 (99%)	2(1%)	78	91
1	Ε	214/280~(76%)	212 (99%)	2(1%)	78	91
1	F	214/280~(76%)	212 (99%)	2 (1%)	78	91
1	G	214/280~(76%)	212 (99%)	2(1%)	78	91
1	Н	214/280~(76%)	212 (99%)	2(1%)	78	91
1	Ι	214/280~(76%)	212 (99%)	2(1%)	78	91
1	J	214/280~(76%)	212 (99%)	2(1%)	78	91
1	Κ	214/280~(76%)	212 (99%)	2(1%)	78	91
1	L	214/280~(76%)	212 (99%)	2(1%)	78	91
2	М	206/262~(79%)	206 (100%)	0	100	100
2	Ν	206/262~(79%)	206 (100%)	0	100	100
2	О	206/262 (79%)	206 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	Р	206/262~(79%)	206 (100%)	0	100	100
2	Q	206/262~(79%)	206 (100%)	0	100	100
2	R	206/262~(79%)	206 (100%)	0	100	100
2	S	206/262~(79%)	206 (100%)	0	100	100
2	Т	206/262~(79%)	206 (100%)	0	100	100
2	U	206/262~(79%)	206 (100%)	0	100	100
2	V	206/262~(79%)	206 (100%)	0	100	100
2	W	206/262~(79%)	206 (100%)	0	100	100
2	Х	206/262~(79%)	206 (100%)	0	100	100
All	All	5040/6504~(78%)	5016 (100%)	24(0%)	89	95

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Н	1864[A]	ARG
1	Ι	2126[A]	ARG
1	Ι	2124[A]	ARG
1	J	2384[A]	ARG
1	D	824[A]	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such side chains are listed below:

Mol	Chain	Res	Type
1	K	2711[A]	ASN
2	W	2878[B]	GLN
2	М	248[B]	GLN
2	W	2834[B]	GLN
2	Т	2089[B]	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23264. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 150

Y Index: 150



Z Index: 150

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 115

Y Index: 117

Z Index: 128

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 194 $\rm nm^3;$ this corresponds to an approximate mass of 175 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.316 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.316 \AA^{-1}



8.2 Resolution estimates (i)

$\mathbf{Bosolution ostimato}(\mathbf{\hat{A}})$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.16	-	-	
Author-provided FSC curve	3.11	3.39	3.14	
Unmasked-calculated*	-	-	-	

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23264 and PDB model 7LB6. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.2).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.



Map-model fit summary (i) 9.5

The table lists the average atom inclusion at the recommended contour level (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.8872	0.5290	_ 10
А	0.8865	0.5300	1.0
В	0.8880	0.5310	
С	0.8927	0.5310	
D	0.8906	0.5300	
E	0.8885	0.5310	
F	0.8865	0.5320	
G	0.8854	0.5300	
Н	0.8870	0.5320	
Ι	0.8823	0.5320	0.0
J	0.8880	0.5320	<0.0
K	0.8865	0.5300	
L	0.8844	0.5310	

