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 (i)) were used in the production of this report:

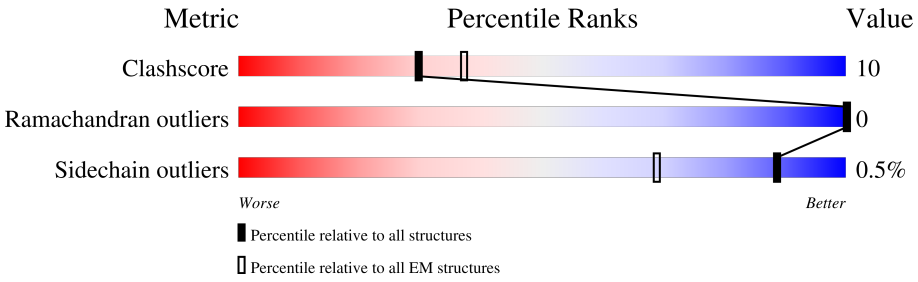
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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	Whole archive (#Entries)	EM structures (#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 >=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 <=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	A	348	57% 18% · 25%
1	B	348	56% 18% · 25%
1	C	348	56% 18% · 25%
1	D	348	57% 17% · 25%
1	E	348	57% 17% · 25%
1	F	348	56% 18% · 25%
1	G	348	57% 17% · 25%
1	H	348	57% 17% · 25%

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Mol	Chain	Length	Quality of chain
1	I	348	55% 19% 25%
1	J	348	57% 18% 25%
1	K	348	57% 18% 25%
1	L	348	57% 17% 25%
2	M	338	61% 17% 22%
2	N	338	56% 22% 22%
2	O	338	57% 20% 22%
2	P	338	63% 15% 22%
2	Q	338	57% 21% 22%
2	R	338	59% 19% 22%
2	S	338	60% 18% 22%
2	T	338	60% 18% 22%
2	U	338	58% 20% 22%
2	V	338	62% 16% 22%
2	W	338	58% 20% 22%
2	X	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.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	B	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	C	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	D	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	E	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	F	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	G	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	H	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	I	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	J	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	K	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		
1	L	260	Total	C	N	O	S	260	0
			1968	1231	353	371	13		

There are 420 discrepancies between the modelled and reference sequences:

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	478	ASP	-	expression tag	UNP Q9ZNR6
C	479	ASP	-	expression tag	UNP Q9ZNR6
C	480	LYS	-	expression tag	UNP Q9ZNR6
C	481	LEU	-	expression tag	UNP Q9ZNR6
C	482	ALA	-	expression tag	UNP Q9ZNR6
C	483	GLY	-	expression tag	UNP Q9ZNR6
C	484	GLY	-	expression tag	UNP Q9ZNR6
C	485	GLY	-	expression tag	UNP Q9ZNR6
C	486	GLY	-	expression tag	UNP Q9ZNR6
C	487	SER	-	expression tag	UNP Q9ZNR6
C	488	GLY	-	expression tag	UNP Q9ZNR6
C	489	GLY	-	expression tag	UNP Q9ZNR6
C	490	GLY	-	expression tag	UNP Q9ZNR6
C	491	GLY	-	expression tag	UNP Q9ZNR6
C	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
E	978	MET	-	expression tag	UNP Q9ZNR6
E	979	ASP	-	expression tag	UNP Q9ZNR6
E	980	TYR	-	expression tag	UNP Q9ZNR6
E	981	LYS	-	expression tag	UNP Q9ZNR6
E	982	ASP	-	expression tag	UNP Q9ZNR6
E	983	HIS	-	expression tag	UNP Q9ZNR6
E	984	ASP	-	expression tag	UNP Q9ZNR6
E	985	GLY	-	expression tag	UNP Q9ZNR6
E	986	ASP	-	expression tag	UNP Q9ZNR6
E	987	TYR	-	expression tag	UNP Q9ZNR6
E	988	LYS	-	expression tag	UNP Q9ZNR6
E	989	ASP	-	expression tag	UNP Q9ZNR6
E	990	HIS	-	expression tag	UNP Q9ZNR6
E	991	ASP	-	expression tag	UNP Q9ZNR6
E	992	ILE	-	expression tag	UNP Q9ZNR6
E	993	ASP	-	expression tag	UNP Q9ZNR6
E	994	TYR	-	expression tag	UNP Q9ZNR6
E	995	LYS	-	expression tag	UNP Q9ZNR6
E	996	ASP	-	expression tag	UNP Q9ZNR6
E	997	ASP	-	expression tag	UNP Q9ZNR6
E	998	ASP	-	expression tag	UNP Q9ZNR6
E	999	ASP	-	expression tag	UNP Q9ZNR6
E	1000	LYS	-	expression tag	UNP Q9ZNR6
E	1001	LEU	-	expression tag	UNP Q9ZNR6
E	1002	ALA	-	expression tag	UNP Q9ZNR6
E	1003	GLY	-	expression tag	UNP Q9ZNR6
E	1004	GLY	-	expression tag	UNP Q9ZNR6
E	1005	GLY	-	expression tag	UNP Q9ZNR6
E	1006	GLY	-	expression tag	UNP Q9ZNR6
E	1007	SER	-	expression tag	UNP Q9ZNR6
E	1008	GLY	-	expression tag	UNP Q9ZNR6
E	1009	GLY	-	expression tag	UNP Q9ZNR6
E	1010	GLY	-	expression tag	UNP Q9ZNR6
E	1011	GLY	-	expression tag	UNP Q9ZNR6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	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
H	1758	MET	-	expression tag	UNP Q9ZNR6
H	1759	ASP	-	expression tag	UNP Q9ZNR6
H	1760	TYR	-	expression tag	UNP Q9ZNR6
H	1761	LYS	-	expression tag	UNP Q9ZNR6
H	1762	ASP	-	expression tag	UNP Q9ZNR6
H	1763	HIS	-	expression tag	UNP Q9ZNR6
H	1764	ASP	-	expression tag	UNP Q9ZNR6
H	1765	GLY	-	expression tag	UNP Q9ZNR6
H	1766	ASP	-	expression tag	UNP Q9ZNR6
H	1767	TYR	-	expression tag	UNP Q9ZNR6
H	1768	LYS	-	expression tag	UNP Q9ZNR6
H	1769	ASP	-	expression tag	UNP Q9ZNR6
H	1770	HIS	-	expression tag	UNP Q9ZNR6

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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	2038	ASP	-	expression tag	UNP Q9ZNR6
I	2039	ASP	-	expression tag	UNP Q9ZNR6
I	2040	LYS	-	expression tag	UNP Q9ZNR6
I	2041	LEU	-	expression tag	UNP Q9ZNR6
I	2042	ALA	-	expression tag	UNP Q9ZNR6
I	2043	GLY	-	expression tag	UNP Q9ZNR6
I	2044	GLY	-	expression tag	UNP Q9ZNR6
I	2045	GLY	-	expression tag	UNP Q9ZNR6
I	2046	GLY	-	expression tag	UNP Q9ZNR6
I	2047	SER	-	expression tag	UNP Q9ZNR6
I	2048	GLY	-	expression tag	UNP Q9ZNR6
I	2049	GLY	-	expression tag	UNP Q9ZNR6
I	2050	GLY	-	expression tag	UNP Q9ZNR6
I	2051	GLY	-	expression tag	UNP Q9ZNR6
I	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
K	2544	ASP	-	expression tag	UNP Q9ZNR6
K	2545	GLY	-	expression tag	UNP Q9ZNR6
K	2546	ASP	-	expression tag	UNP Q9ZNR6
K	2547	TYR	-	expression tag	UNP Q9ZNR6
K	2548	LYS	-	expression tag	UNP Q9ZNR6
K	2549	ASP	-	expression tag	UNP Q9ZNR6
K	2550	HIS	-	expression tag	UNP Q9ZNR6
K	2551	ASP	-	expression tag	UNP Q9ZNR6
K	2552	ILE	-	expression tag	UNP Q9ZNR6
K	2553	ASP	-	expression tag	UNP Q9ZNR6
K	2554	TYR	-	expression tag	UNP Q9ZNR6
K	2555	LYS	-	expression tag	UNP Q9ZNR6
K	2556	ASP	-	expression tag	UNP Q9ZNR6
K	2557	ASP	-	expression tag	UNP Q9ZNR6
K	2558	ASP	-	expression tag	UNP Q9ZNR6
K	2559	ASP	-	expression tag	UNP Q9ZNR6
K	2560	LYS	-	expression tag	UNP Q9ZNR6
K	2561	LEU	-	expression tag	UNP Q9ZNR6
K	2562	ALA	-	expression tag	UNP Q9ZNR6
K	2563	GLY	-	expression tag	UNP Q9ZNR6
K	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

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	O	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	P	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	Q	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	R	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	S	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	T	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	U	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	V	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	W	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		
2	X	263	Total	C	N	O	S	263	0
			2012	1257	370	369	16		

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-49	MET	-	expression tag	UNP Q8L940
M	-48	ASP	-	expression tag	UNP Q8L940
M	-47	TYR	-	expression tag	UNP Q8L940
M	-46	LYS	-	expression tag	UNP Q8L940
M	-45	ASP	-	expression tag	UNP Q8L940
M	-44	HIS	-	expression tag	UNP Q8L940
M	-43	ASP	-	expression tag	UNP Q8L940
M	-42	GLY	-	expression tag	UNP Q8L940
M	-41	ASP	-	expression tag	UNP Q8L940
M	-40	TYR	-	expression tag	UNP Q8L940
M	-39	LYS	-	expression tag	UNP Q8L940
M	-38	ASP	-	expression tag	UNP Q8L940
M	-37	HIS	-	expression tag	UNP Q8L940
M	-36	ASP	-	expression tag	UNP Q8L940
M	-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
M	-29	ASP	-	expression tag	UNP Q8L940
M	-28	ASP	-	expression tag	UNP Q8L940
M	-27	LYS	-	expression tag	UNP Q8L940
M	-26	LEU	-	expression tag	UNP Q8L940
M	-25	ALA	-	expression tag	UNP Q8L940
M	-24	GLY	-	expression tag	UNP Q8L940
M	-23	GLY	-	expression tag	UNP Q8L940
M	-22	GLY	-	expression tag	UNP Q8L940
M	-21	GLY	-	expression tag	UNP Q8L940
M	-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 Q8L940

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Chain	Residue	Modelled	Actual	Comment	Reference
N	243	SER	-	expression tag	UNP Q8L940
O	477	MET	-	expression tag	UNP Q8L940
O	478	ASP	-	expression tag	UNP Q8L940
O	479	TYR	-	expression tag	UNP Q8L940
O	480	LYS	-	expression tag	UNP Q8L940
O	481	ASP	-	expression tag	UNP Q8L940
O	482	HIS	-	expression tag	UNP Q8L940
O	483	ASP	-	expression tag	UNP Q8L940
O	484	GLY	-	expression tag	UNP Q8L940
O	485	ASP	-	expression tag	UNP Q8L940
O	486	TYR	-	expression tag	UNP Q8L940
O	487	LYS	-	expression tag	UNP Q8L940
O	488	ASP	-	expression tag	UNP Q8L940
O	489	HIS	-	expression tag	UNP Q8L940
O	490	ASP	-	expression tag	UNP Q8L940
O	491	ILE	-	expression tag	UNP Q8L940
O	492	ASP	-	expression tag	UNP Q8L940
O	493	TYR	-	expression tag	UNP Q8L940
O	494	LYS	-	expression tag	UNP Q8L940
O	495	ASP	-	expression tag	UNP Q8L940
O	496	ASP	-	expression tag	UNP Q8L940
O	497	ASP	-	expression tag	UNP Q8L940
O	498	ASP	-	expression tag	UNP Q8L940
O	499	LYS	-	expression tag	UNP Q8L940
O	500	LEU	-	expression tag	UNP Q8L940
O	501	ALA	-	expression tag	UNP Q8L940
O	502	GLY	-	expression tag	UNP Q8L940
O	503	GLY	-	expression tag	UNP Q8L940
O	504	GLY	-	expression tag	UNP Q8L940
O	505	GLY	-	expression tag	UNP Q8L940
O	506	SER	-	expression tag	UNP Q8L940
P	740	MET	-	expression tag	UNP Q8L940
P	741	ASP	-	expression tag	UNP Q8L940
P	742	TYR	-	expression tag	UNP Q8L940
P	743	LYS	-	expression tag	UNP Q8L940
P	744	ASP	-	expression tag	UNP Q8L940
P	745	HIS	-	expression tag	UNP Q8L940
P	746	ASP	-	expression tag	UNP Q8L940
P	747	GLY	-	expression tag	UNP Q8L940
P	748	ASP	-	expression tag	UNP Q8L940
P	749	TYR	-	expression tag	UNP Q8L940
P	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
P	754	ILE	-	expression tag	UNP Q8L940
P	755	ASP	-	expression tag	UNP Q8L940
P	756	TYR	-	expression tag	UNP Q8L940
P	757	LYS	-	expression tag	UNP Q8L940
P	758	ASP	-	expression tag	UNP Q8L940
P	759	ASP	-	expression tag	UNP Q8L940
P	760	ASP	-	expression tag	UNP Q8L940
P	761	ASP	-	expression tag	UNP Q8L940
P	762	LYS	-	expression tag	UNP Q8L940
P	763	LEU	-	expression tag	UNP Q8L940
P	764	ALA	-	expression tag	UNP Q8L940
P	765	GLY	-	expression tag	UNP Q8L940
P	766	GLY	-	expression tag	UNP Q8L940
P	767	GLY	-	expression tag	UNP Q8L940
P	768	GLY	-	expression tag	UNP Q8L940
P	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
T	1792	MET	-	expression tag	UNP Q8L940
T	1793	ASP	-	expression tag	UNP Q8L940
T	1794	TYR	-	expression tag	UNP Q8L940
T	1795	LYS	-	expression tag	UNP Q8L940
T	1796	ASP	-	expression tag	UNP Q8L940
T	1797	HIS	-	expression tag	UNP Q8L940
T	1798	ASP	-	expression tag	UNP Q8L940
T	1799	GLY	-	expression tag	UNP Q8L940
T	1800	ASP	-	expression tag	UNP Q8L940
T	1801	TYR	-	expression tag	UNP Q8L940
T	1802	LYS	-	expression tag	UNP Q8L940
T	1803	ASP	-	expression tag	UNP Q8L940
T	1804	HIS	-	expression tag	UNP Q8L940
T	1805	ASP	-	expression tag	UNP Q8L940
T	1806	ILE	-	expression tag	UNP Q8L940
T	1807	ASP	-	expression tag	UNP Q8L940
T	1808	TYR	-	expression tag	UNP Q8L940

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Chain	Residue	Modelled	Actual	Comment	Reference
T	1809	LYS	-	expression tag	UNP Q8L940
T	1810	ASP	-	expression tag	UNP Q8L940
T	1811	ASP	-	expression tag	UNP Q8L940
T	1812	ASP	-	expression tag	UNP Q8L940
T	1813	ASP	-	expression tag	UNP Q8L940
T	1814	LYS	-	expression tag	UNP Q8L940
T	1815	LEU	-	expression tag	UNP Q8L940
T	1816	ALA	-	expression tag	UNP Q8L940
T	1817	GLY	-	expression tag	UNP Q8L940
T	1818	GLY	-	expression tag	UNP Q8L940
T	1819	GLY	-	expression tag	UNP Q8L940
T	1820	GLY	-	expression tag	UNP Q8L940
T	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
X	2844	MET	-	expression tag	UNP Q8L940
X	2845	ASP	-	expression tag	UNP Q8L940
X	2846	TYR	-	expression tag	UNP Q8L940
X	2847	LYS	-	expression tag	UNP Q8L940
X	2848	ASP	-	expression tag	UNP Q8L940
X	2849	HIS	-	expression tag	UNP Q8L940
X	2850	ASP	-	expression tag	UNP Q8L940
X	2851	GLY	-	expression tag	UNP Q8L940
X	2852	ASP	-	expression tag	UNP Q8L940
X	2853	TYR	-	expression tag	UNP Q8L940
X	2854	LYS	-	expression tag	UNP Q8L940
X	2855	ASP	-	expression tag	UNP Q8L940
X	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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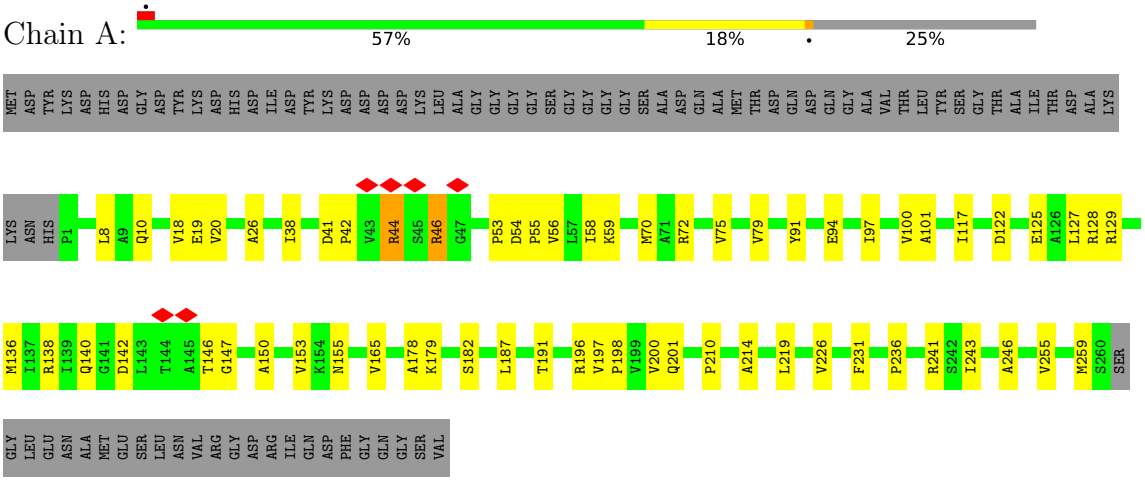
Chain	Residue	Modelled	Actual	Comment	Reference
X	2867	LEU	-	expression tag	UNP Q8L940
X	2868	ALA	-	expression tag	UNP Q8L940
X	2869	GLY	-	expression tag	UNP Q8L940
X	2870	GLY	-	expression tag	UNP Q8L940
X	2871	GLY	-	expression tag	UNP Q8L940
X	2872	GLY	-	expression tag	UNP Q8L940
X	2873	SER	-	expression 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.

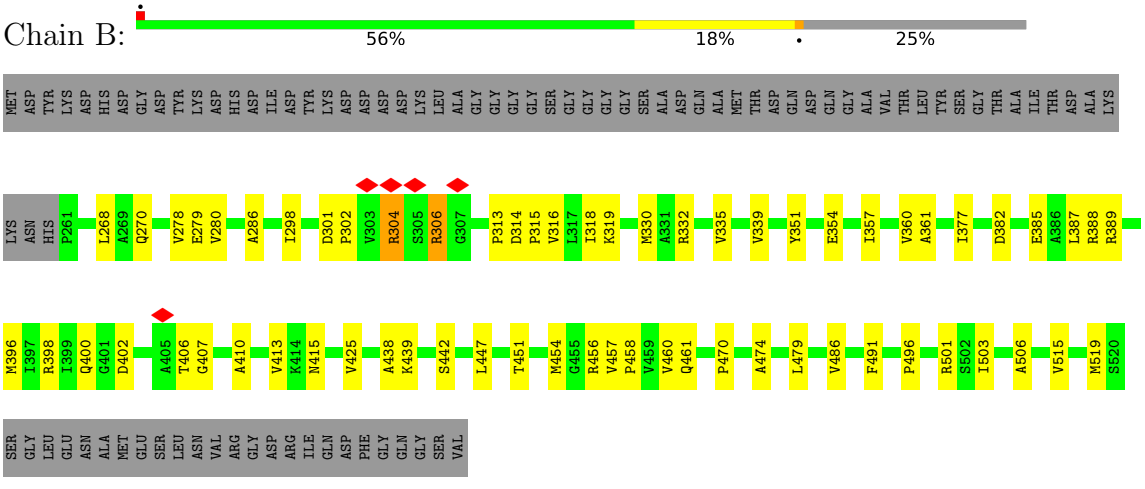
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

Chain A:



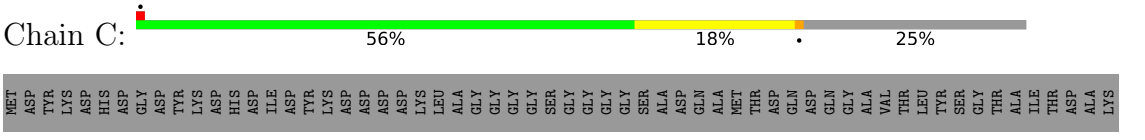
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

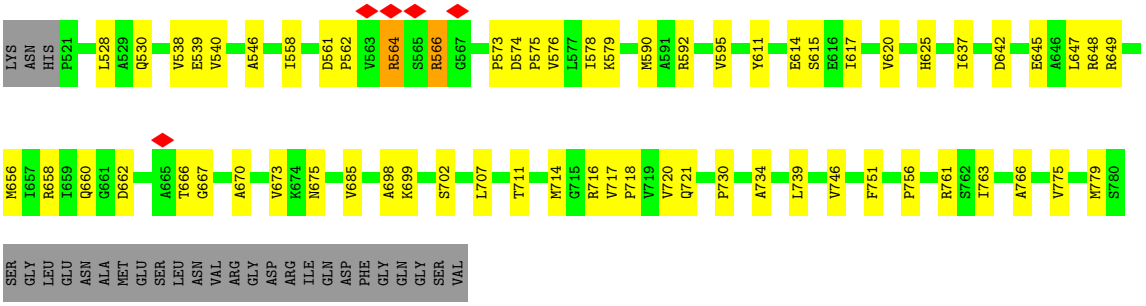
Chain B:



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

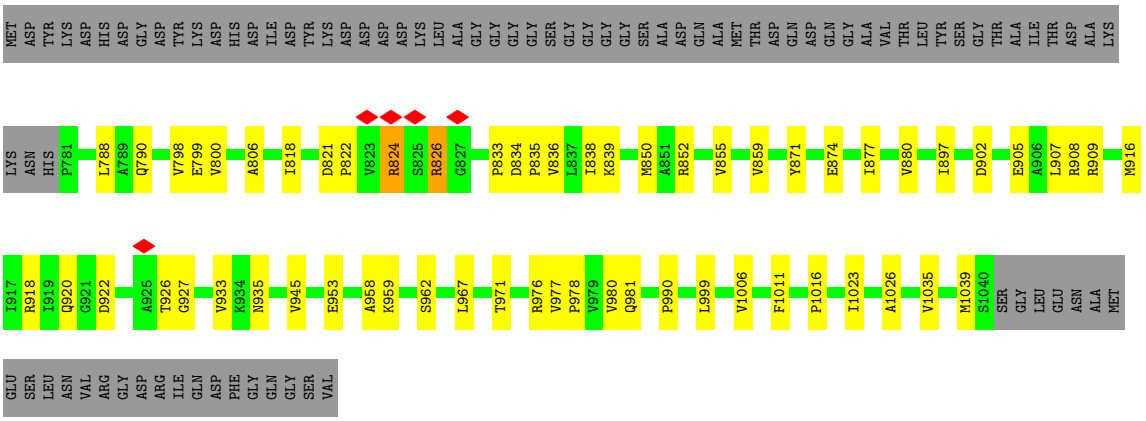
Chain C:





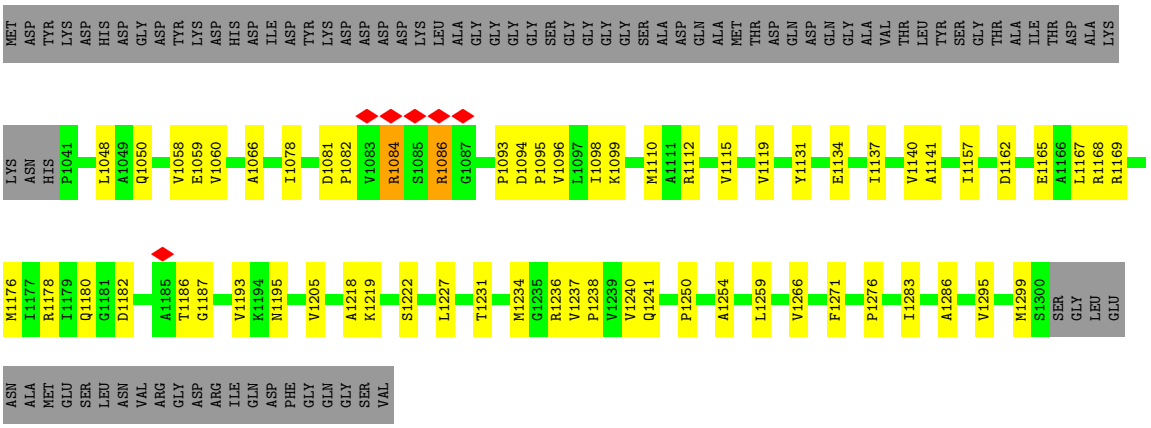
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

Chain D:



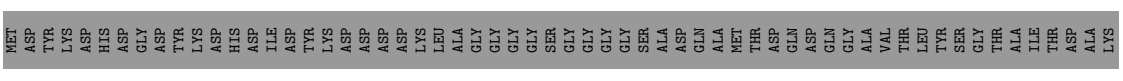
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

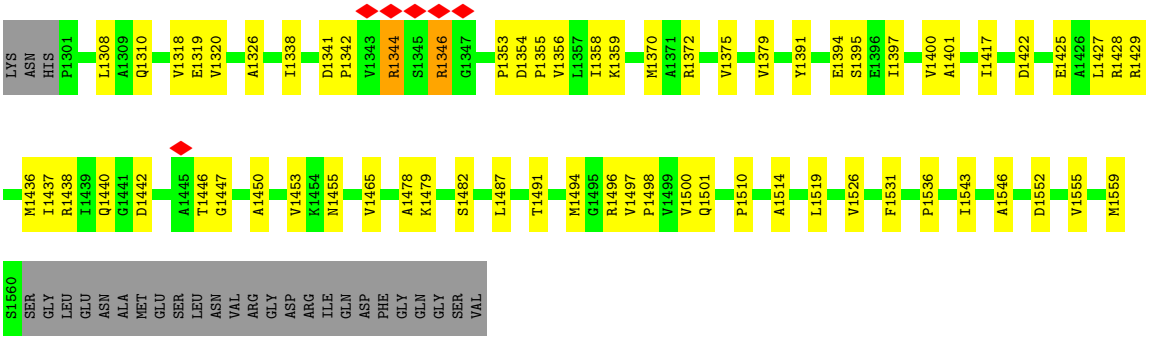
Chain E:



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

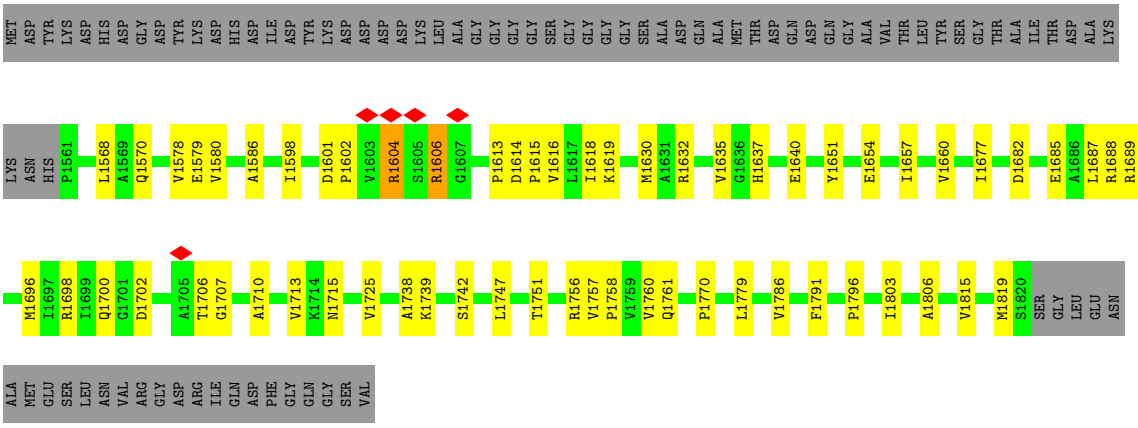
Chain F:





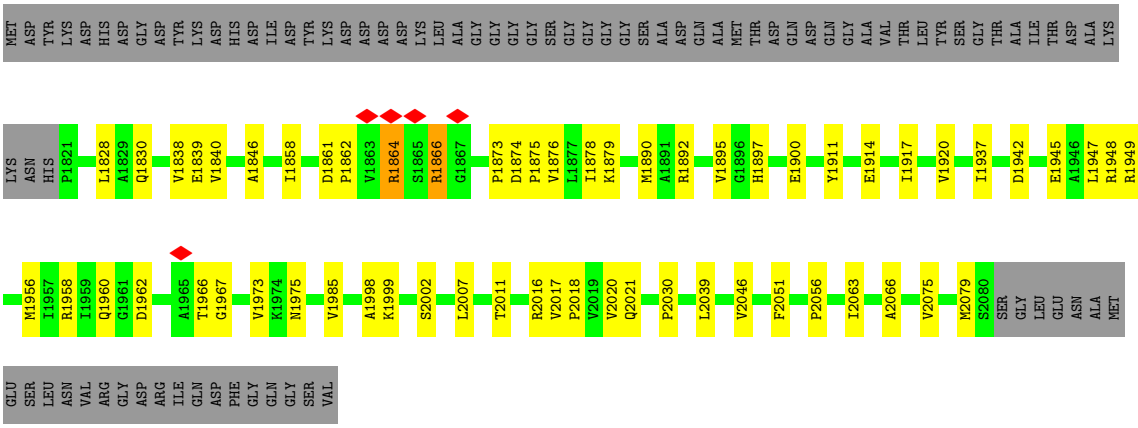
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

Chain G:



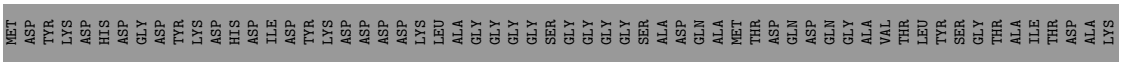
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

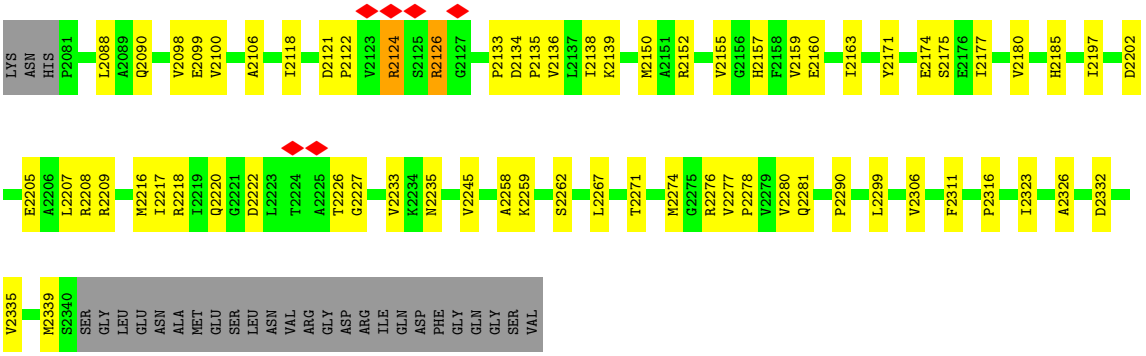
Chain H:



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

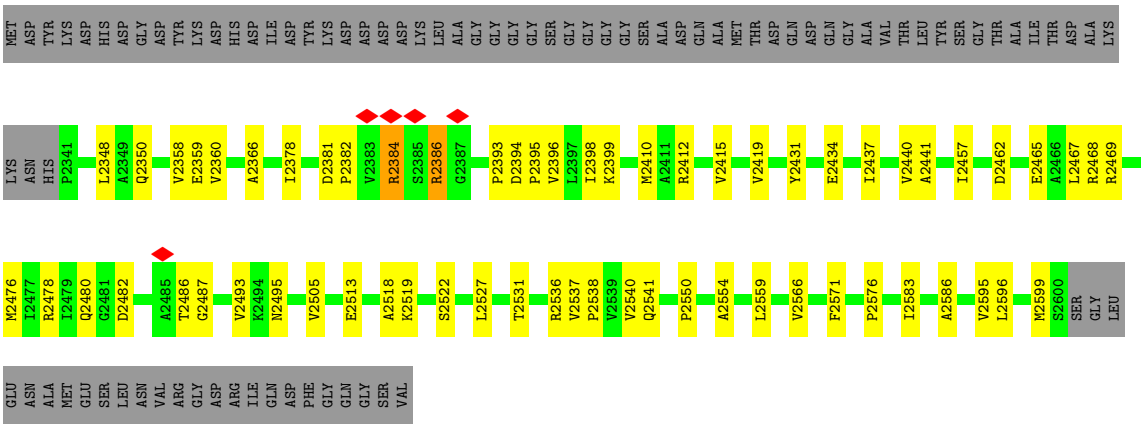
Chain I:





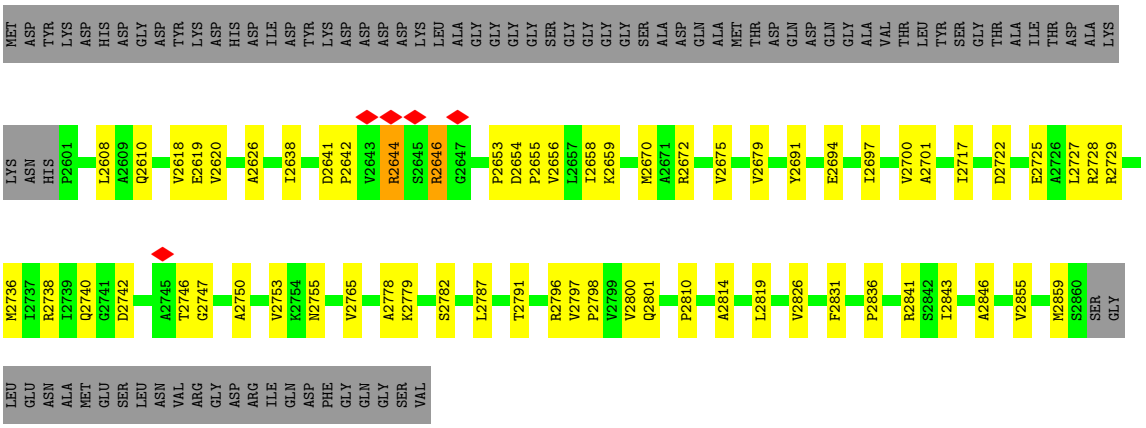
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

Chain J:



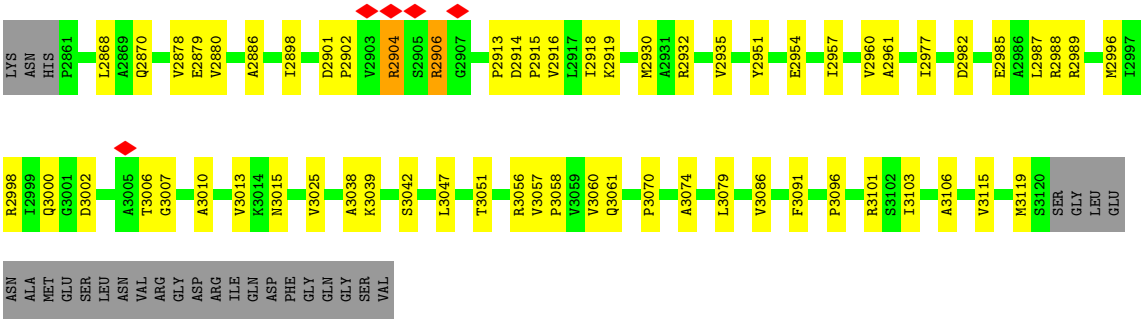
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

Chain K:



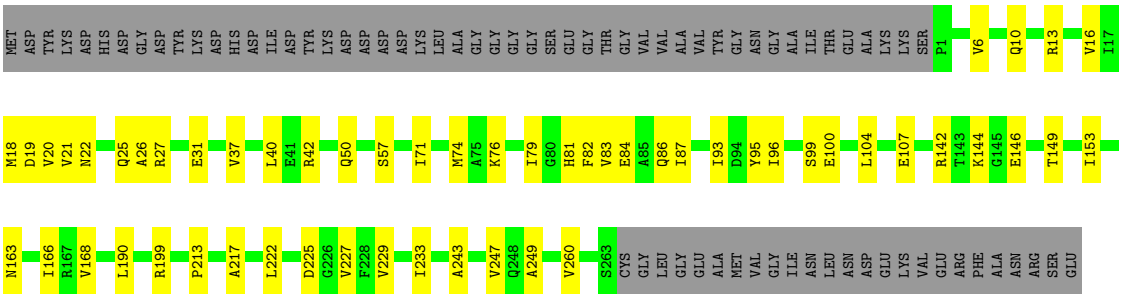
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2

Chain L:



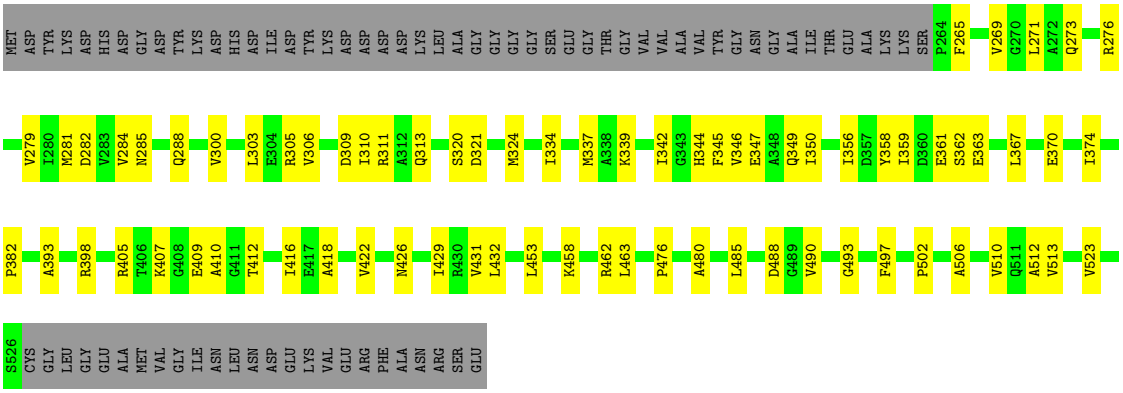
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain M:



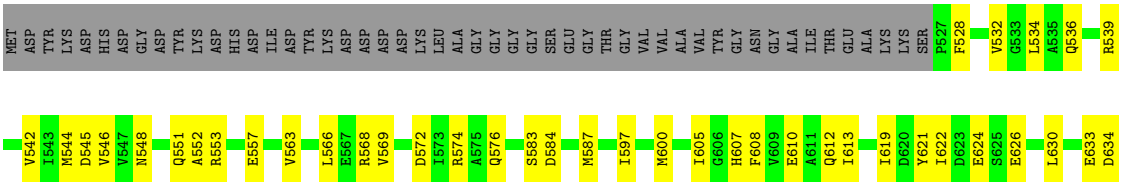
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

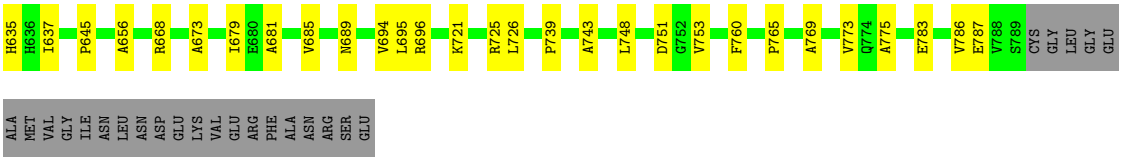
Chain N:



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

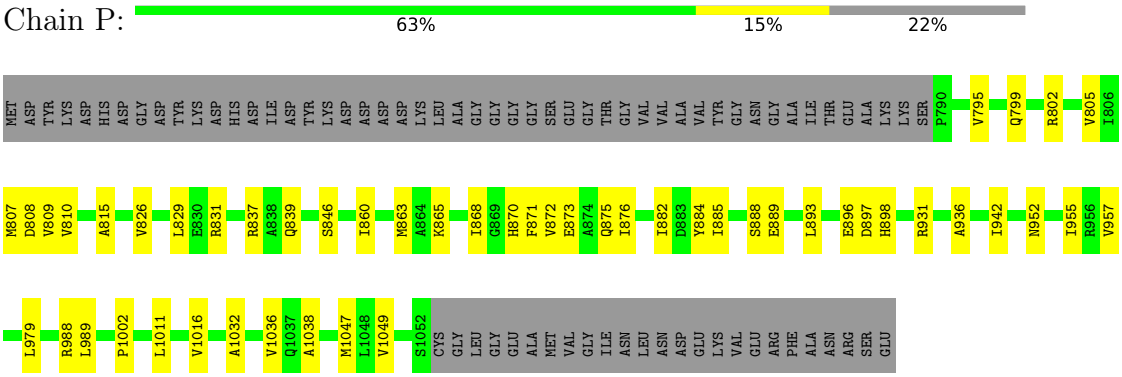
Chain O:





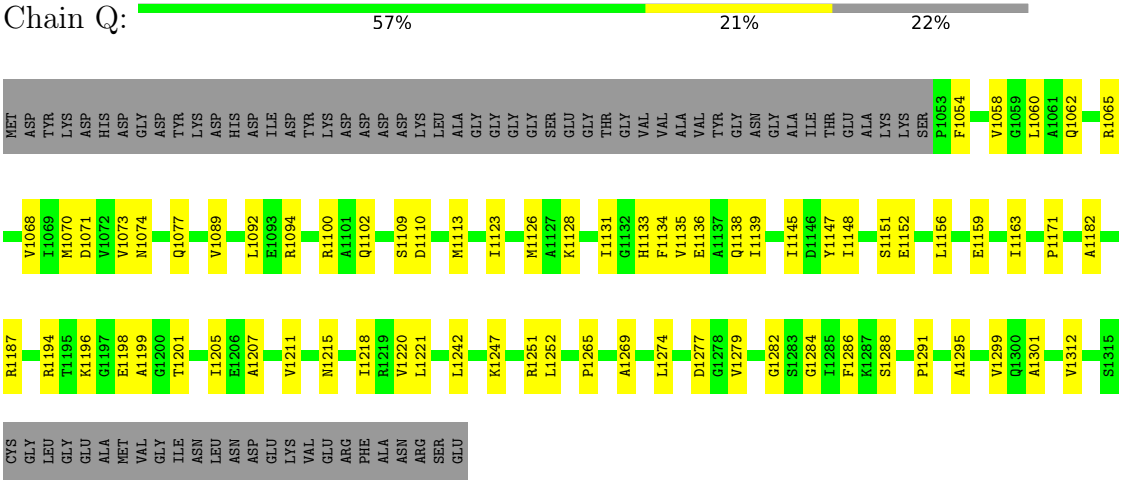
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain P:



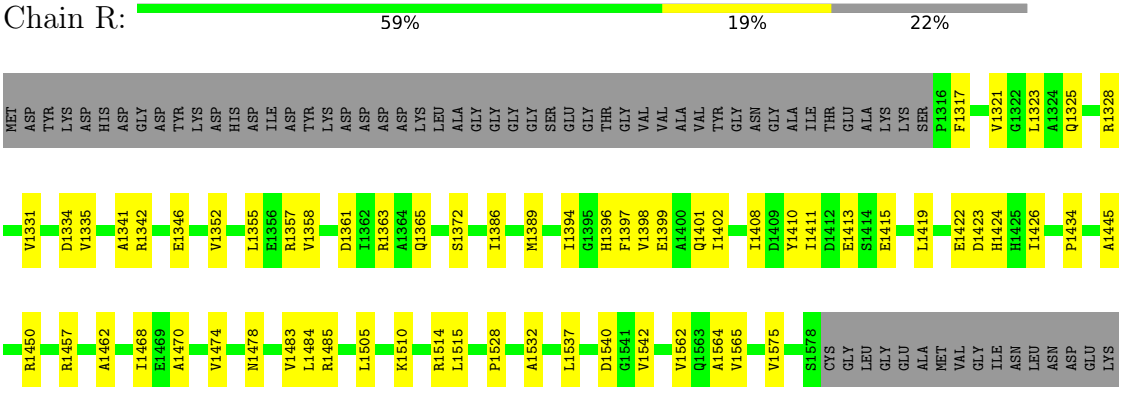
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain Q:



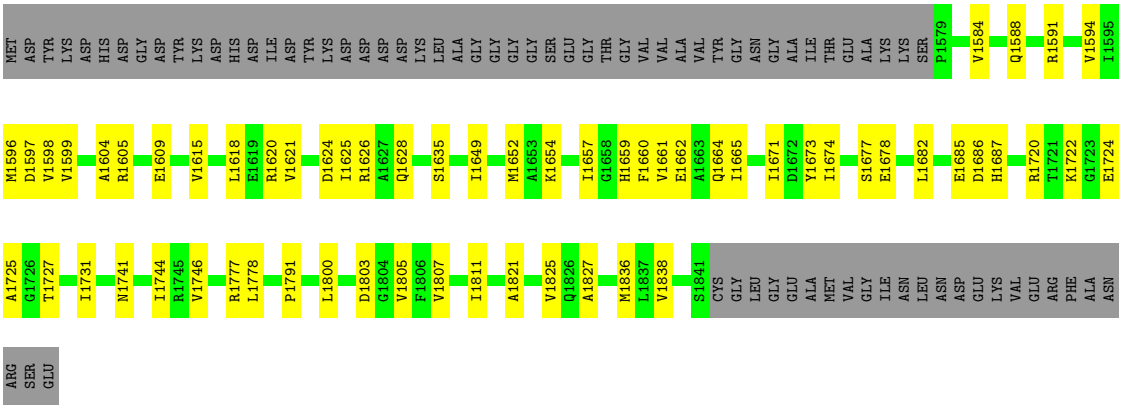
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain R:



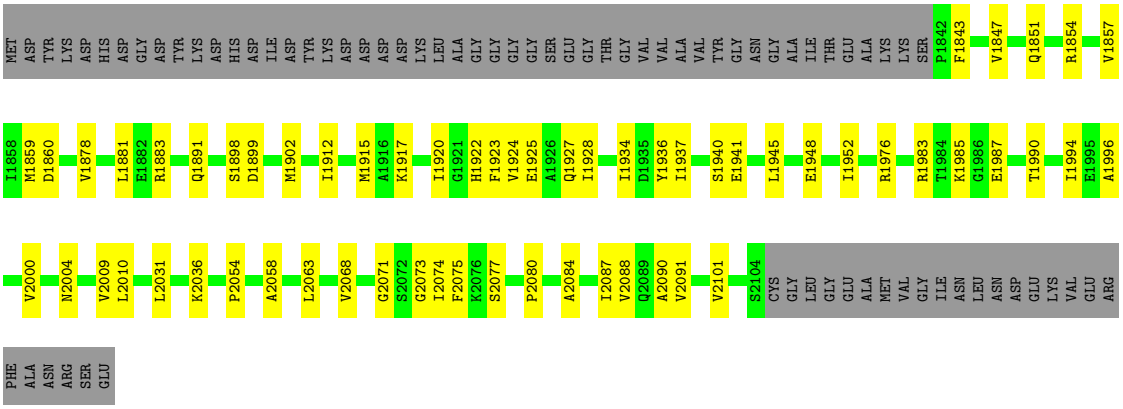
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain S:



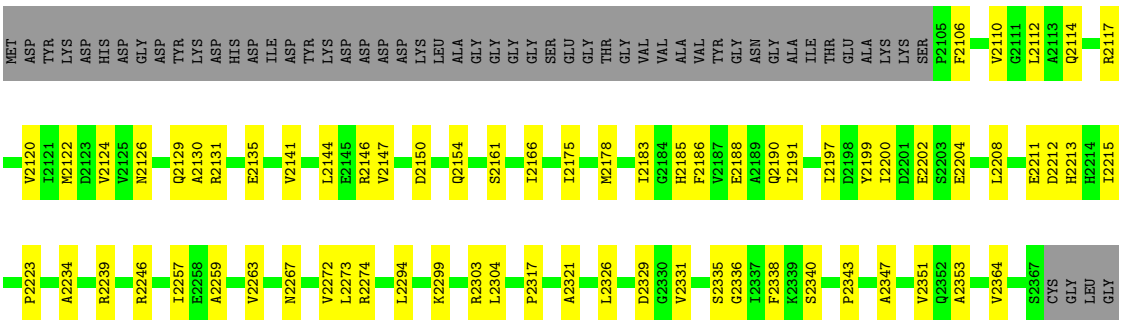
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain T:



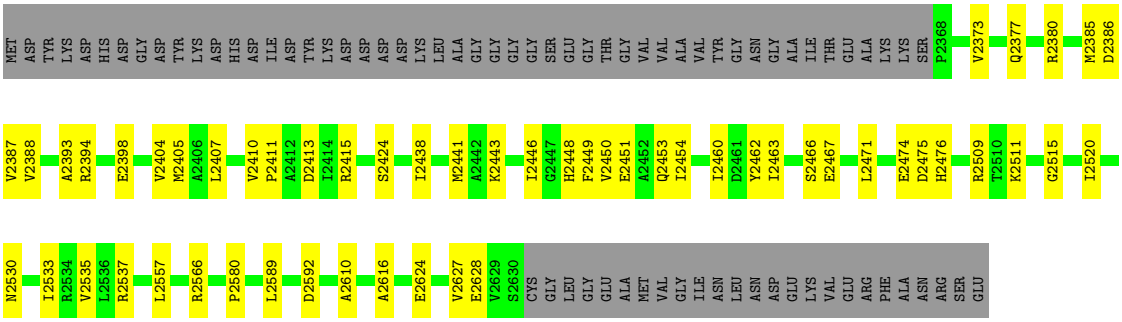
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain U:



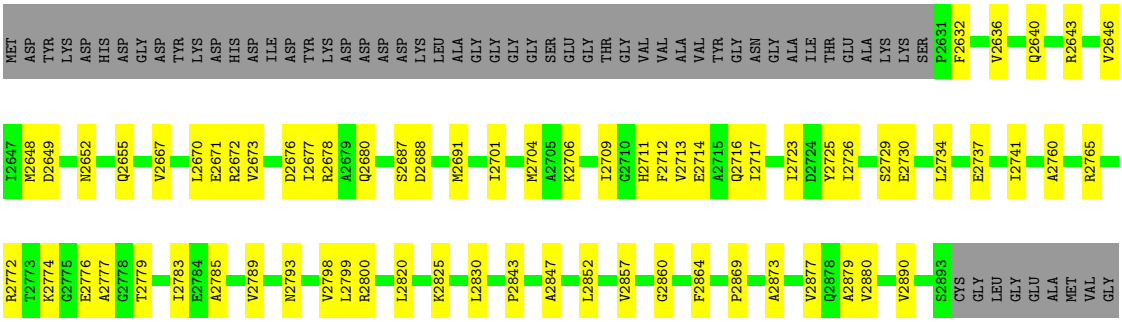
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain V:



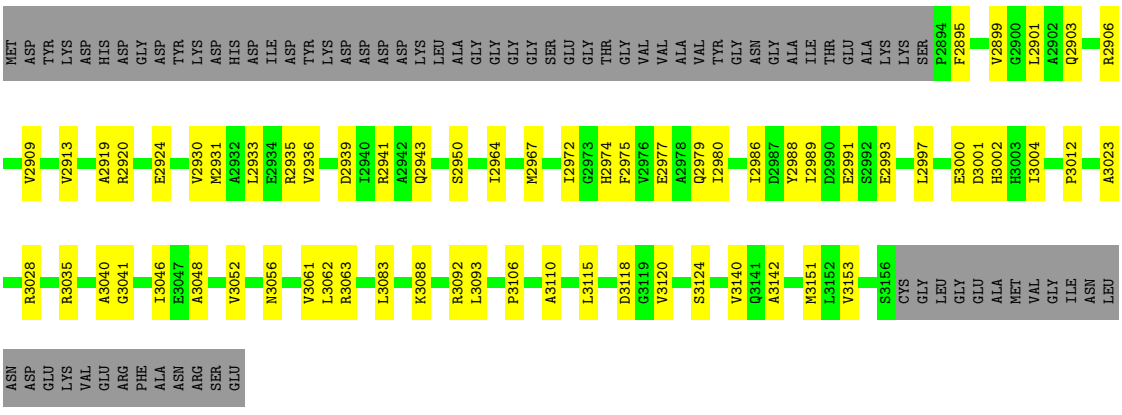
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

Chain W:



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

Chain X:



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 CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/1998	0.42	0/2701
1	B	0.26	0/1998	0.42	0/2701
1	C	0.26	0/1998	0.42	0/2701
1	D	0.26	0/1998	0.42	0/2701
1	E	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	H	0.26	0/1998	0.42	0/2701
1	I	0.26	0/1998	0.42	0/2701
1	J	0.26	0/1998	0.42	0/2701
1	K	0.26	0/1998	0.42	0/2701
1	L	0.26	0/1998	0.42	0/2701
2	M	0.28	0/2039	0.44	0/2749
2	N	0.29	0/2039	0.45	0/2749
2	O	0.29	0/2039	0.45	0/2749
2	P	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	T	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	X	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	A	1968	0	1856	42	0
1	B	1968	0	1851	43	0
1	C	1968	0	1852	43	0
1	D	1968	0	1856	39	0
1	E	1968	0	1853	43	0
1	F	1968	0	1850	46	0
1	G	1968	0	1835	39	0
1	H	1968	0	1851	39	0
1	I	1968	0	1845	47	0
1	J	1968	0	1854	42	0
1	K	1968	0	1847	41	0
1	L	1968	0	1834	41	0
2	M	2012	0	1918	36	0
2	N	2012	0	1925	52	0
2	O	2012	0	1926	45	0
2	P	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	T	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	X	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

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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	Percentiles	
1	A	258/348 (74%)	252 (98%)	6 (2%)	0	100	100
1	B	258/348 (74%)	252 (98%)	6 (2%)	0	100	100
1	C	258/348 (74%)	252 (98%)	6 (2%)	0	100	100
1	D	258/348 (74%)	252 (98%)	6 (2%)	0	100	100
1	E	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	H	258/348 (74%)	252 (98%)	6 (2%)	0	100	100
1	I	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	M	265/338 (78%)	257 (97%)	8 (3%)	0	100	100
2	N	265/338 (78%)	256 (97%)	9 (3%)	0	100	100
2	O	265/338 (78%)	255 (96%)	10 (4%)	0	100	100
2	P	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S	265/338 (78%)	258 (97%)	7 (3%)	0	100	100
2	T	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	X	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 sidechain 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	Percentiles	
1	A	214/280 (76%)	212 (99%)	2 (1%)	78	91
1	B	214/280 (76%)	212 (99%)	2 (1%)	78	91
1	C	214/280 (76%)	212 (99%)	2 (1%)	78	91
1	D	214/280 (76%)	212 (99%)	2 (1%)	78	91
1	E	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	H	214/280 (76%)	212 (99%)	2 (1%)	78	91
1	I	214/280 (76%)	212 (99%)	2 (1%)	78	91
1	J	214/280 (76%)	212 (99%)	2 (1%)	78	91
1	K	214/280 (76%)	212 (99%)	2 (1%)	78	91
1	L	214/280 (76%)	212 (99%)	2 (1%)	78	91
2	M	206/262 (79%)	206 (100%)	0	100	100
2	N	206/262 (79%)	206 (100%)	0	100	100
2	O	206/262 (79%)	206 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	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	T	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	X	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	H	1864[A]	ARG
1	I	2126[A]	ARG
1	I	2124[A]	ARG
1	J	2384[A]	ARG
1	D	824[A]	ARG

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

Mol	Chain	Res	Type
1	K	2711[A]	ASN
2	W	2878[B]	GLN
2	M	248[B]	GLN
2	W	2834[B]	GLN
2	T	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.

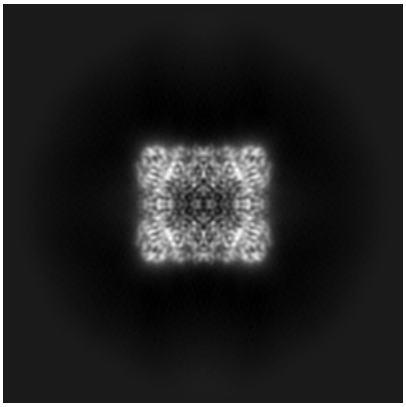
6 Map visualisation

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.

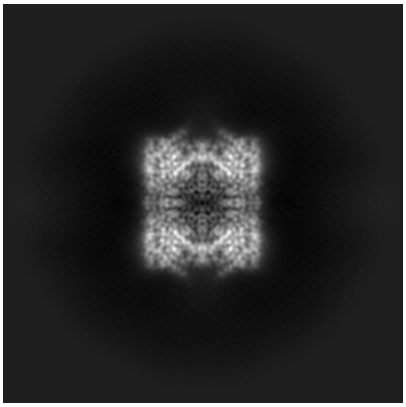
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

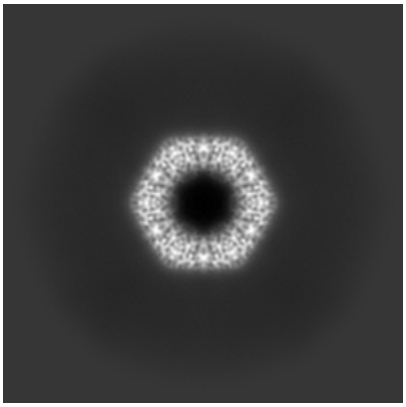
6.1.1 Primary map



X



Y

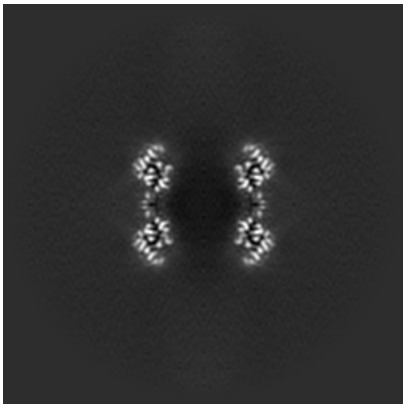


Z

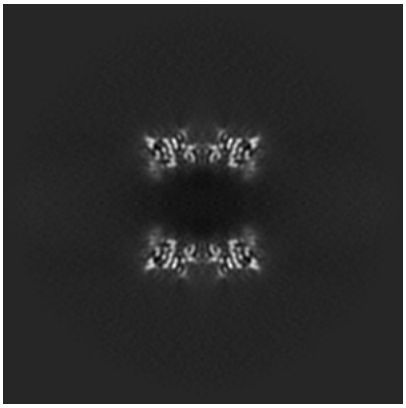
The images above show the map projected in three orthogonal directions.

6.2 Central slices

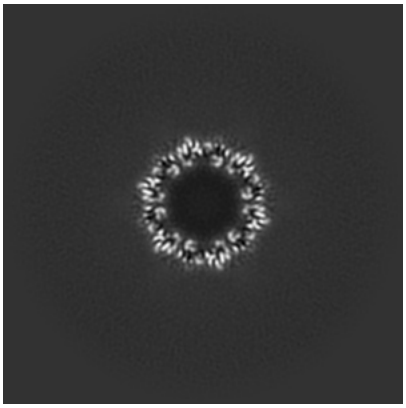
6.2.1 Primary map



X Index: 150



Y Index: 150

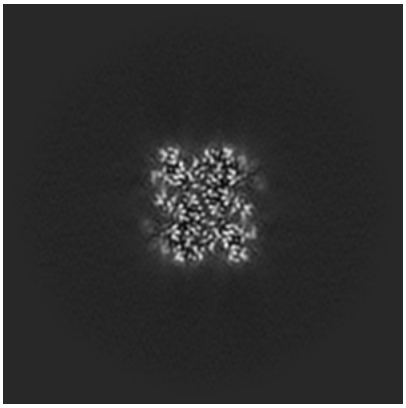


Z Index: 150

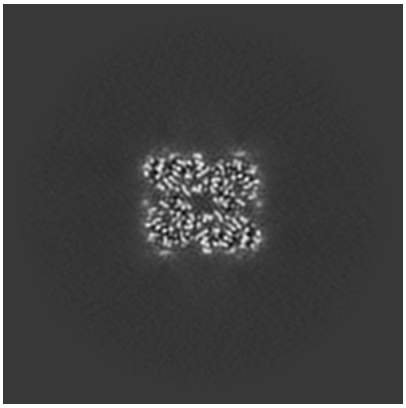
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

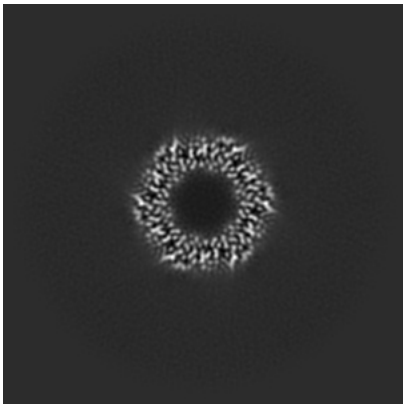
6.3.1 Primary map



X Index: 115



Y Index: 117

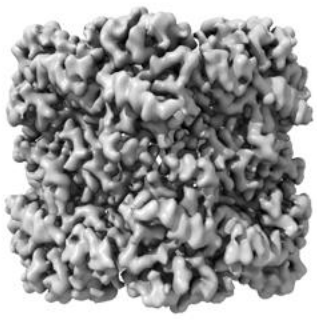


Z Index: 128

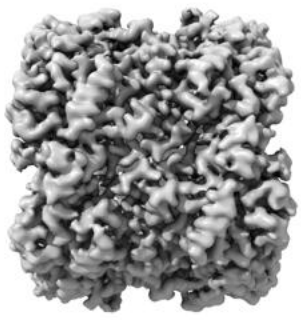
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

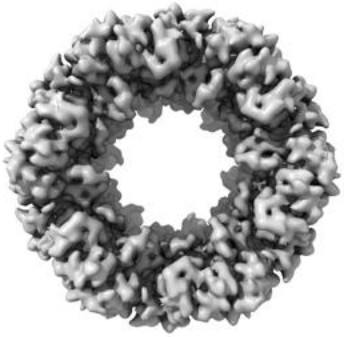
6.4.1 Primary map



X



Y



Z

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.

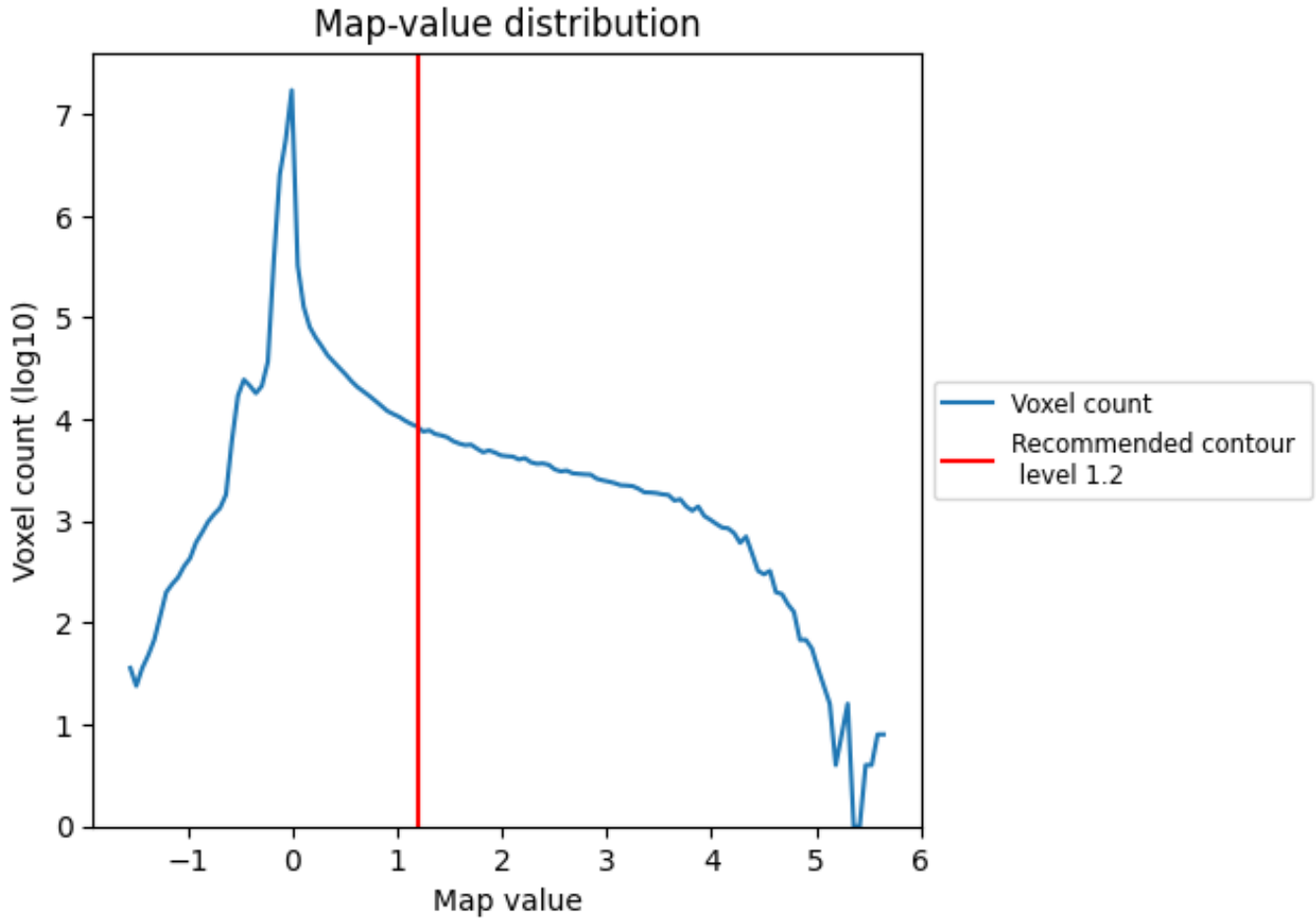
6.5 Mask visualisation (i)

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

7 Map analysis

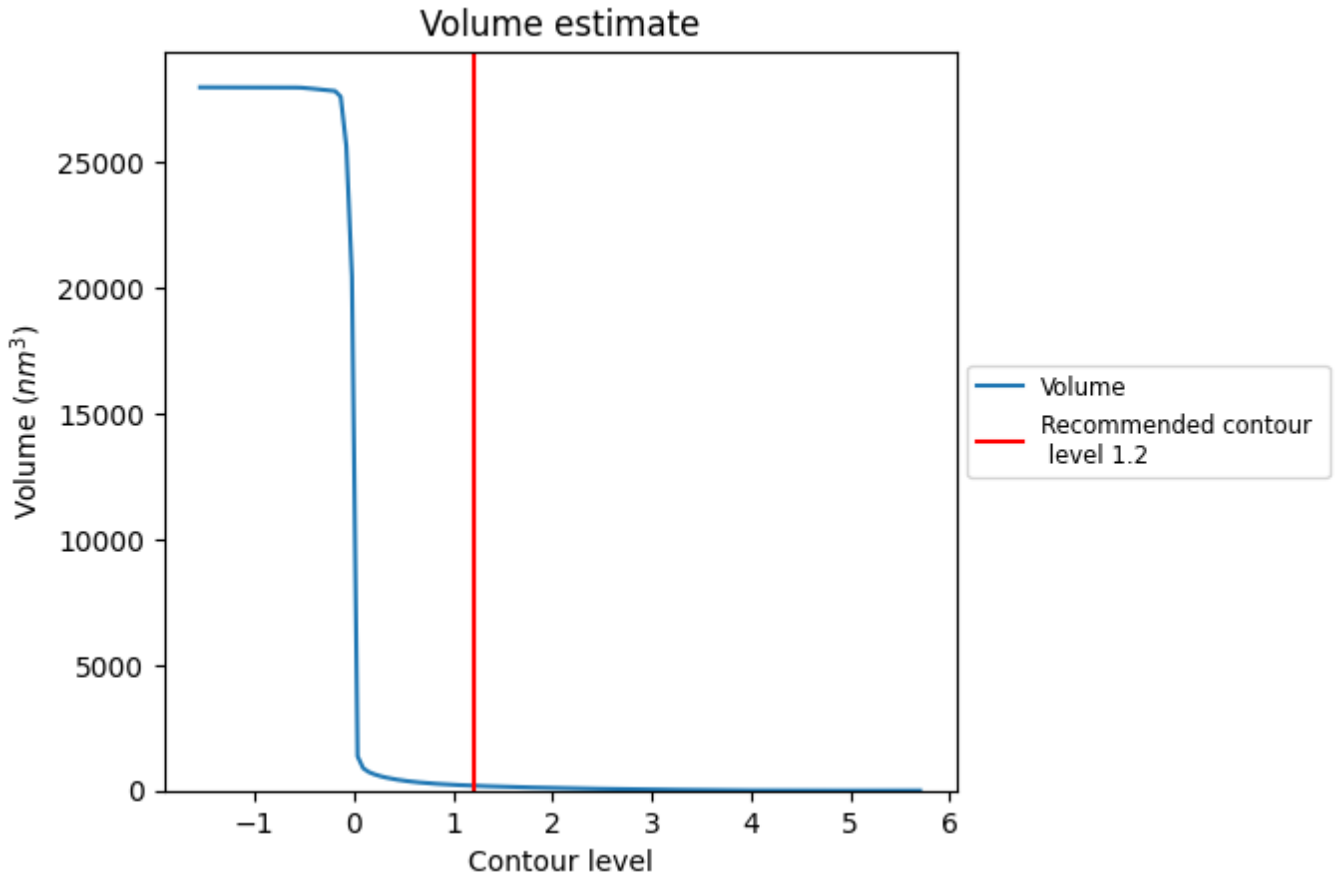
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

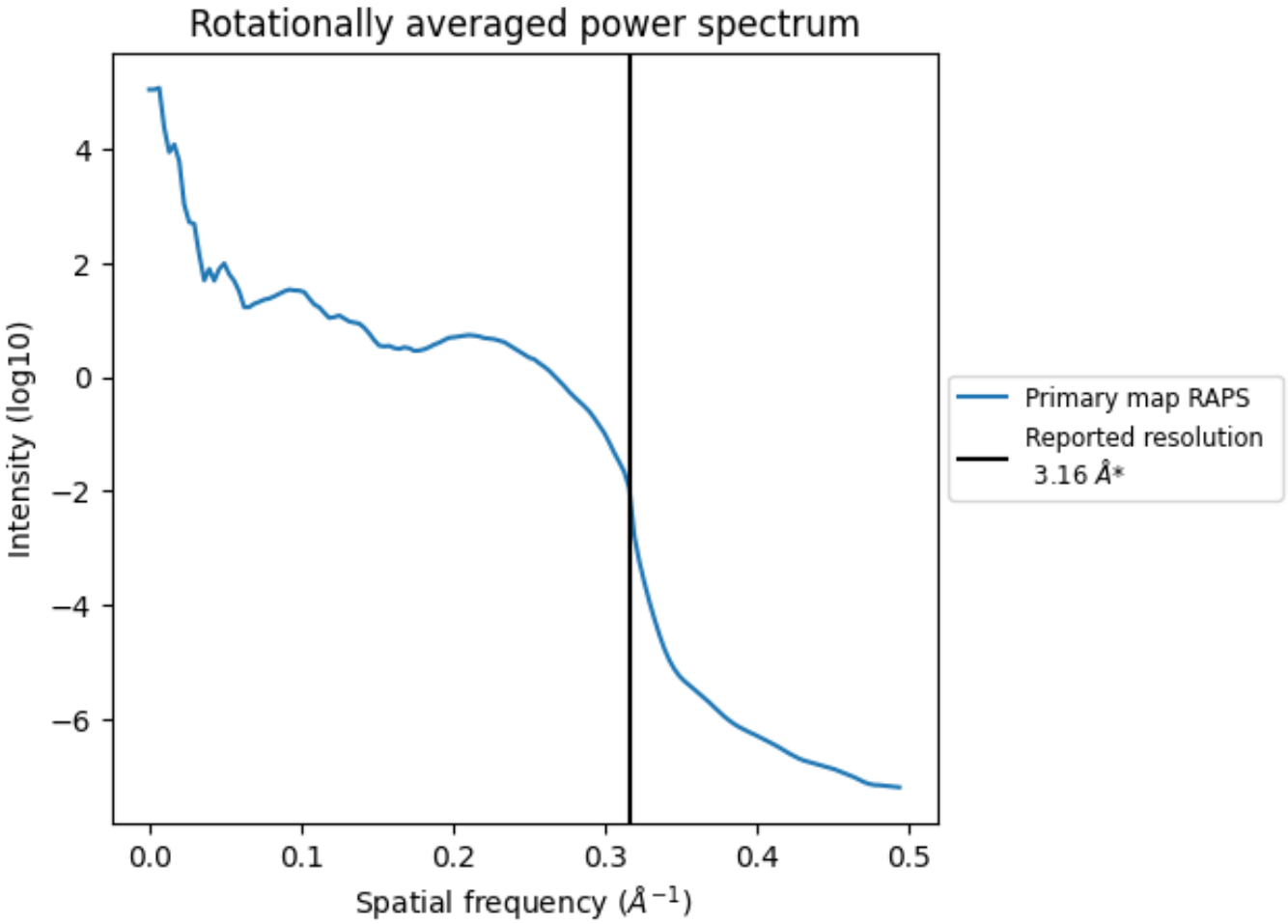
7.2 Volume estimate (i)



The volume at the recommended contour level is 194 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)

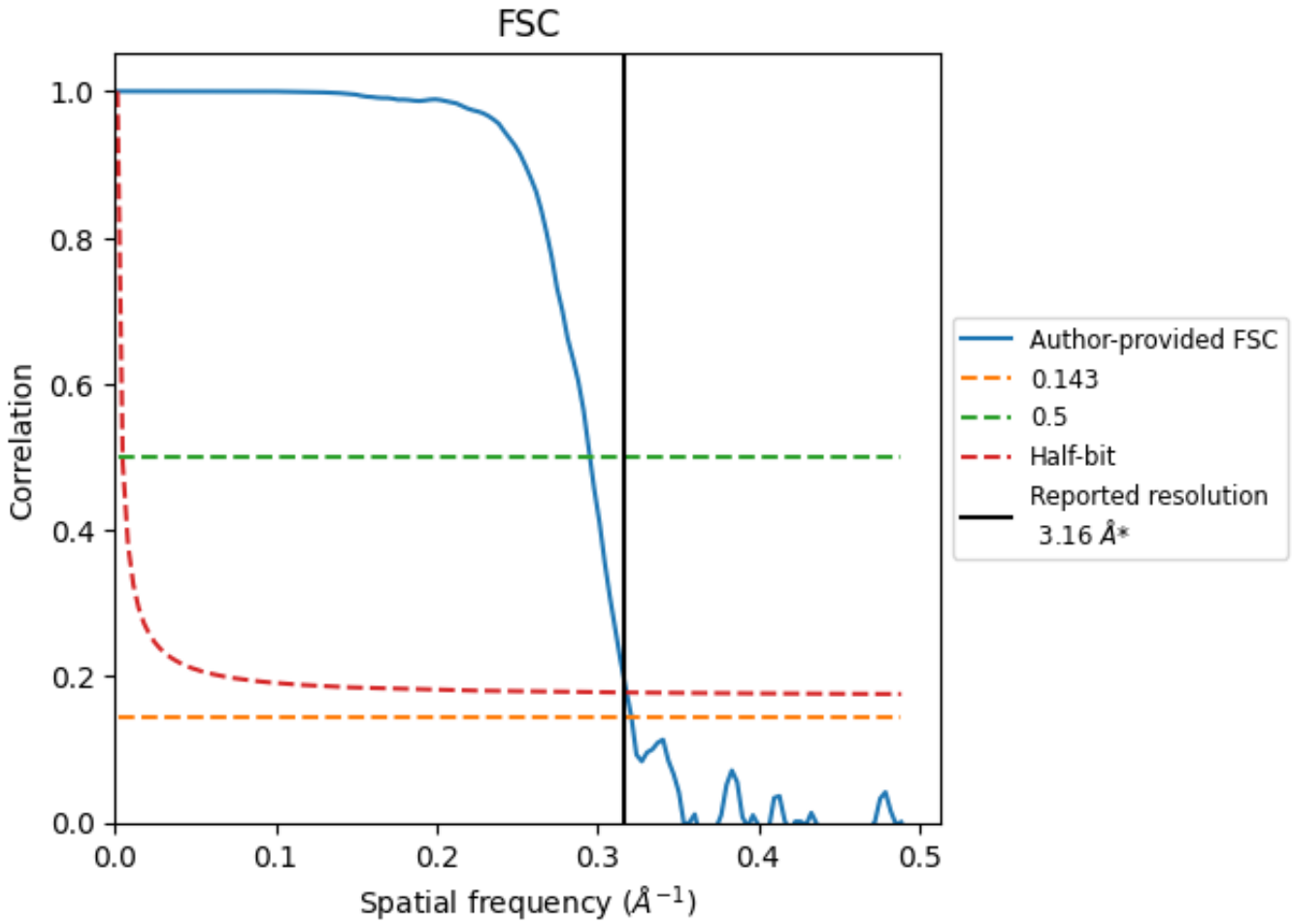


*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

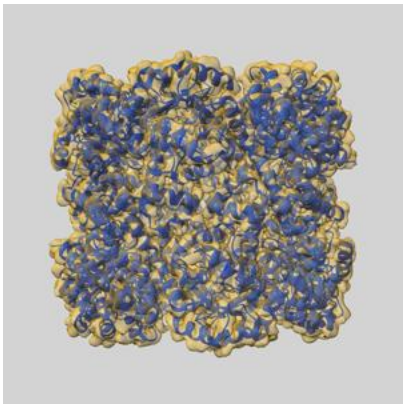
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.11	3.39	3.14
Unmasked-calculated*	-	-	-

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

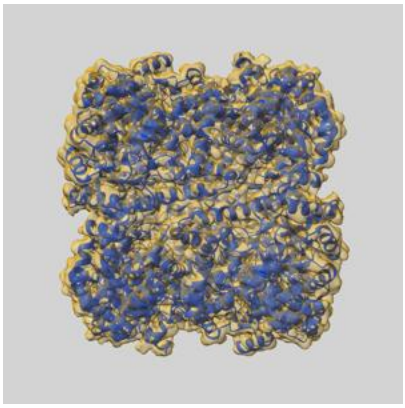
9 Map-model fit

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.

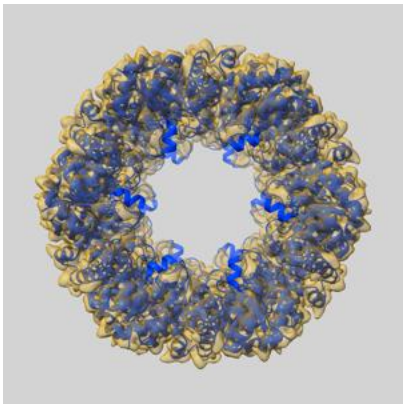
9.1 Map-model overlay



X



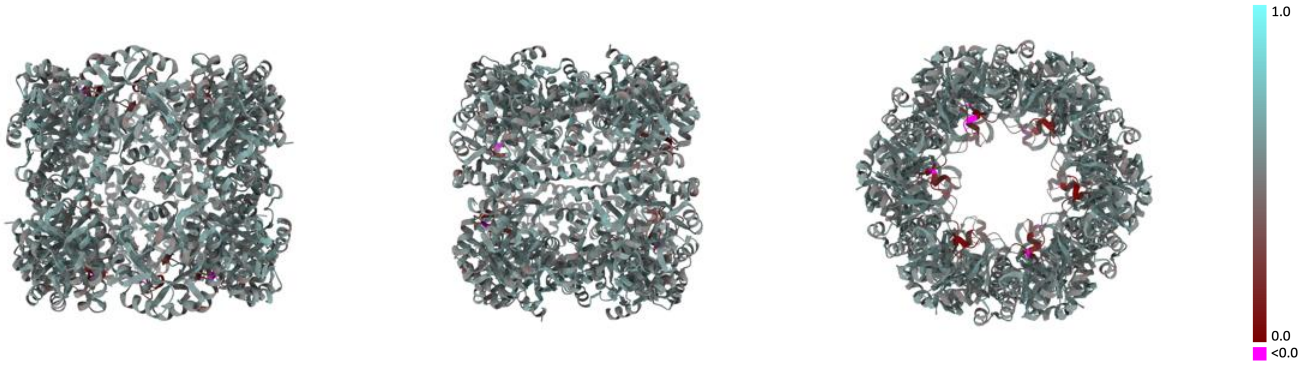
Y



Z

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.

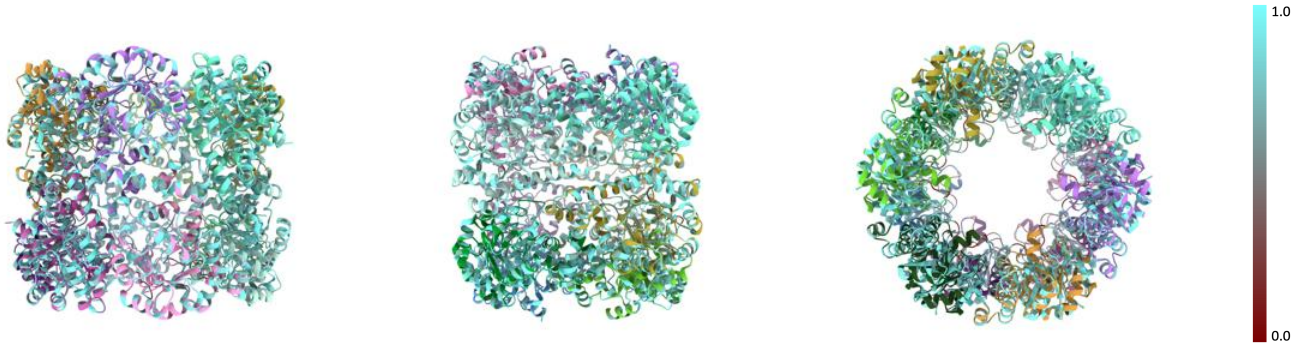
9.2 Q-score mapped to coordinate model



X Y Z

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.

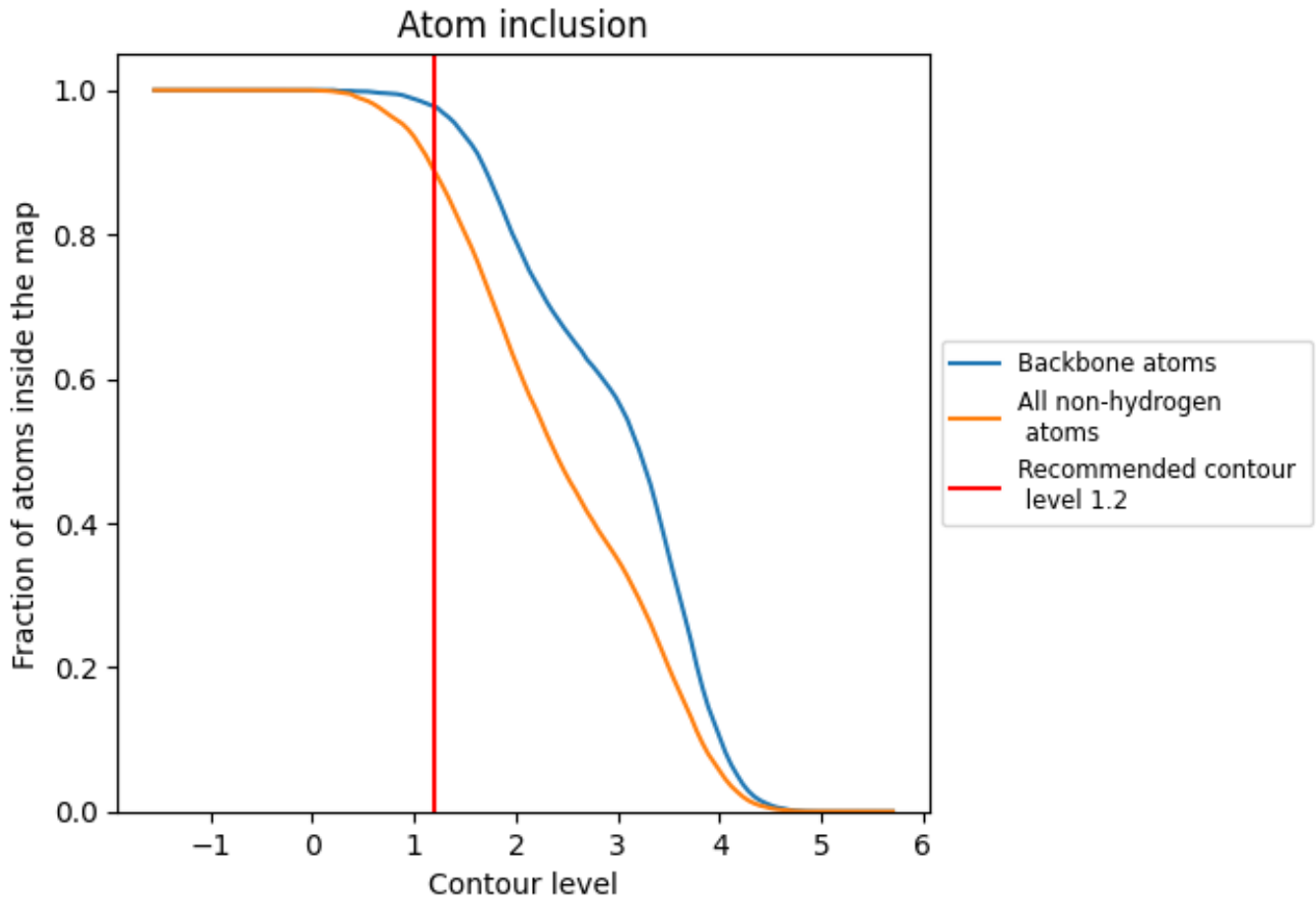
9.3 Atom inclusion mapped to coordinate model



X Y Z

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.

9.5 Map-model fit summary

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
A	0.8865	0.5300
B	0.8880	0.5310
C	0.8927	0.5310
D	0.8906	0.5300
E	0.8885	0.5310
F	0.8865	0.5320
G	0.8854	0.5300
H	0.8870	0.5320
I	0.8823	0.5320
J	0.8880	0.5320
K	0.8865	0.5300
L	0.8844	0.5310