wwPDB X-ray Structure Validation Summary Report (i)

Oct 19, 2023 – 08:54 AM EDT

PDB ID	:	2NV2
Title	:	Structure of the PLP synthase complex Pdx1/2 (YaaD/E) from Bacillus subtilis
Authors	:	Strohmeier, M.; Tews, I.; Sinning, I.
Deposited on	:	2006-11-10
Resolution	:	2.12 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
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:

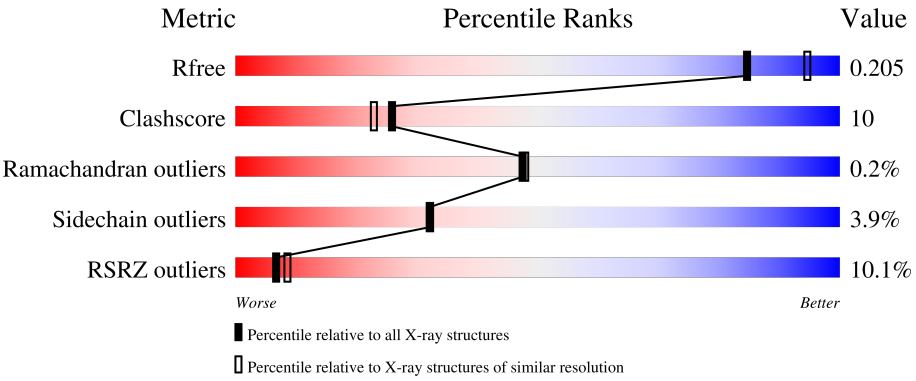
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	294	4% 78% 13% • 9%
1	C	294	4% 80% 11% • 9%
1	E	294	4% 76% 14% • 9%
1	G	294	4% 78% 13% • 9%
1	I	294	4% 77% 14% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	294	5% 78% 12% • 8%
1	M	294	3% 82% 9% 9%
1	O	294	4% 79% 11% • 9%
1	Q	294	6% 79% 12% • 8%
1	S	294	5% 79% 12% • 8%
1	U	294	5% 78% 14% 8%
1	W	294	4% 78% 12% • 8%
2	B	204	19% 78% 13% • 5%
2	D	204	18% 80% 13% • 5%
2	F	204	24% 72% 20% • 6%
2	H	204	9% 82% 10% • 5%
2	J	204	10% 86% 8% • •
2	L	204	14% 80% 13% • 6%
2	N	204	5% 82% 10% • 5%
2	P	204	9% 76% 16% • 5%
2	R	204	13% 80% 13% • 5%
2	T	204	25% 77% 16% • 5%
2	V	204	39% 76% 18% • 5%
2	X	204	10% 76% 16% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	6001	-	-	X	-
3	CL	C	6005	-	-	X	-
3	CL	E	6009	-	-	X	-
3	CL	I	6017	-	-	X	-
3	CL	Q	6033	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	S	6037	-	-	X	-
3	CL	U	6041	-	-	X	-
3	CL	W	6045	-	-	X	-
4	EDO	A	6031	-	-	X	-
4	EDO	E	6047	-	-	X	-
4	EDO	G	6043	-	-	X	-
4	EDO	I	6039	-	-	X	-
4	EDO	M	6007	-	-	X	-
4	EDO	Q	6035	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 48293 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyridoxal biosynthesis lyase pdxS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	6	0
			2028	1270	354	388	16			
1	C	269	Total	C	N	O	S	0	5	0
			2037	1273	355	393	16			
1	E	269	Total	C	N	O	S	0	5	0
			2037	1273	356	392	16			
1	G	268	Total	C	N	O	S	0	3	0
			2007	1255	348	388	16			
1	I	271	Total	C	N	O	S	0	4	0
			2042	1276	357	393	16			
1	K	270	Total	C	N	O	S	0	4	0
			2032	1272	356	388	16			
1	M	269	Total	C	N	O	S	0	5	0
			2036	1273	356	391	16			
1	O	268	Total	C	N	O	S	0	4	0
			2024	1265	357	386	16			
1	Q	270	Total	C	N	O	S	0	3	0
			2028	1268	356	388	16			
1	S	270	Total	C	N	O	S	0	3	0
			2028	1267	355	390	16			
1	U	271	Total	C	N	O	S	0	4	0
			2034	1271	356	391	16			
1	W	270	Total	C	N	O	S	0	6	0
			2044	1280	357	391	16			

- Molecule 2 is a protein called Glutamine amidotransferase subunit pdxT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	2	0
			1500	948	264	280	8			
2	D	194	Total	C	N	O	S	0	1	0
			1497	946	262	281	8			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	191	Total	C	N	O	S	0	1	0
			1474	932	257	277	8			
2	H	193	Total	C	N	O	S	0	2	0
			1494	944	260	282	8			
2	J	196	Total	C	N	O	S	0	1	0
			1512	957	264	283	8			
2	L	192	Total	C	N	O	S	0	1	0
			1483	937	259	279	8			
2	N	193	Total	C	N	O	S	0	1	0
			1488	940	260	280	8			
2	P	193	Total	C	N	O	S	0	2	0
			1496	947	261	280	8			
2	R	193	Total	C	N	O	S	0	2	0
			1500	948	264	280	8			
2	T	194	Total	C	N	O	S	0	1	0
			1493	944	262	279	8			
2	V	194	Total	C	N	O	S	0	1	0
			1497	946	262	281	8			
2	X	195	Total	C	N	O	S	0	1	0
			1505	952	263	282	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	170	ASN	HIS	engineered mutation	UNP P37528
B	197	LEU	-	expression tag	UNP P37528
B	198	GLU	-	expression tag	UNP P37528
B	199	HIS	-	expression tag	UNP P37528
B	200	HIS	-	expression tag	UNP P37528
B	201	HIS	-	expression tag	UNP P37528
B	202	HIS	-	expression tag	UNP P37528
B	203	HIS	-	expression tag	UNP P37528
B	204	HIS	-	expression tag	UNP P37528
D	170	ASN	HIS	engineered mutation	UNP P37528
D	197	LEU	-	expression tag	UNP P37528
D	198	GLU	-	expression tag	UNP P37528
D	199	HIS	-	expression tag	UNP P37528
D	200	HIS	-	expression tag	UNP P37528
D	201	HIS	-	expression tag	UNP P37528
D	202	HIS	-	expression tag	UNP P37528
D	203	HIS	-	expression tag	UNP P37528
D	204	HIS	-	expression tag	UNP P37528
F	170	ASN	HIS	engineered mutation	UNP P37528

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	197	LEU	-	expression tag	UNP P37528
F	198	GLU	-	expression tag	UNP P37528
F	199	HIS	-	expression tag	UNP P37528
F	200	HIS	-	expression tag	UNP P37528
F	201	HIS	-	expression tag	UNP P37528
F	202	HIS	-	expression tag	UNP P37528
F	203	HIS	-	expression tag	UNP P37528
F	204	HIS	-	expression tag	UNP P37528
H	170	ASN	HIS	engineered mutation	UNP P37528
H	197	LEU	-	expression tag	UNP P37528
H	198	GLU	-	expression tag	UNP P37528
H	199	HIS	-	expression tag	UNP P37528
H	200	HIS	-	expression tag	UNP P37528
H	201	HIS	-	expression tag	UNP P37528
H	202	HIS	-	expression tag	UNP P37528
H	203	HIS	-	expression tag	UNP P37528
H	204	HIS	-	expression tag	UNP P37528
J	170	ASN	HIS	engineered mutation	UNP P37528
J	197	LEU	-	expression tag	UNP P37528
J	198	GLU	-	expression tag	UNP P37528
J	199	HIS	-	expression tag	UNP P37528
J	200	HIS	-	expression tag	UNP P37528
J	201	HIS	-	expression tag	UNP P37528
J	202	HIS	-	expression tag	UNP P37528
J	203	HIS	-	expression tag	UNP P37528
J	204	HIS	-	expression tag	UNP P37528
L	170	ASN	HIS	engineered mutation	UNP P37528
L	197	LEU	-	expression tag	UNP P37528
L	198	GLU	-	expression tag	UNP P37528
L	199	HIS	-	expression tag	UNP P37528
L	200	HIS	-	expression tag	UNP P37528
L	201	HIS	-	expression tag	UNP P37528
L	202	HIS	-	expression tag	UNP P37528
L	203	HIS	-	expression tag	UNP P37528
L	204	HIS	-	expression tag	UNP P37528
N	170	ASN	HIS	engineered mutation	UNP P37528
N	197	LEU	-	expression tag	UNP P37528
N	198	GLU	-	expression tag	UNP P37528
N	199	HIS	-	expression tag	UNP P37528
N	200	HIS	-	expression tag	UNP P37528
N	201	HIS	-	expression tag	UNP P37528
N	202	HIS	-	expression tag	UNP P37528

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	203	HIS	-	expression tag	UNP P37528
N	204	HIS	-	expression tag	UNP P37528
P	170	ASN	HIS	engineered mutation	UNP P37528
P	197	LEU	-	expression tag	UNP P37528
P	198	GLU	-	expression tag	UNP P37528
P	199	HIS	-	expression tag	UNP P37528
P	200	HIS	-	expression tag	UNP P37528
P	201	HIS	-	expression tag	UNP P37528
P	202	HIS	-	expression tag	UNP P37528
P	203	HIS	-	expression tag	UNP P37528
P	204	HIS	-	expression tag	UNP P37528
R	170	ASN	HIS	engineered mutation	UNP P37528
R	197	LEU	-	expression tag	UNP P37528
R	198	GLU	-	expression tag	UNP P37528
R	199	HIS	-	expression tag	UNP P37528
R	200	HIS	-	expression tag	UNP P37528
R	201	HIS	-	expression tag	UNP P37528
R	202	HIS	-	expression tag	UNP P37528
R	203	HIS	-	expression tag	UNP P37528
R	204	HIS	-	expression tag	UNP P37528
T	170	ASN	HIS	engineered mutation	UNP P37528
T	197	LEU	-	expression tag	UNP P37528
T	198	GLU	-	expression tag	UNP P37528
T	199	HIS	-	expression tag	UNP P37528
T	200	HIS	-	expression tag	UNP P37528
T	201	HIS	-	expression tag	UNP P37528
T	202	HIS	-	expression tag	UNP P37528
T	203	HIS	-	expression tag	UNP P37528
T	204	HIS	-	expression tag	UNP P37528
V	170	ASN	HIS	engineered mutation	UNP P37528
V	197	LEU	-	expression tag	UNP P37528
V	198	GLU	-	expression tag	UNP P37528
V	199	HIS	-	expression tag	UNP P37528
V	200	HIS	-	expression tag	UNP P37528
V	201	HIS	-	expression tag	UNP P37528
V	202	HIS	-	expression tag	UNP P37528
V	203	HIS	-	expression tag	UNP P37528
V	204	HIS	-	expression tag	UNP P37528
X	170	ASN	HIS	engineered mutation	UNP P37528
X	197	LEU	-	expression tag	UNP P37528
X	198	GLU	-	expression tag	UNP P37528
X	199	HIS	-	expression tag	UNP P37528

Continued on next page...

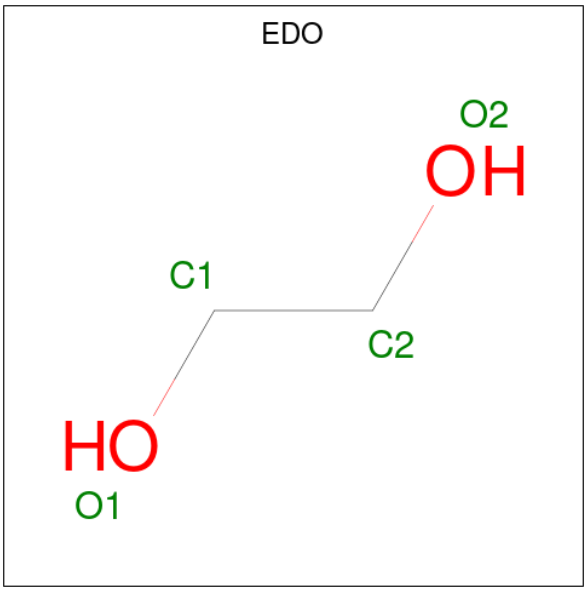
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	200	HIS	-	expression tag	UNP P37528
X	201	HIS	-	expression tag	UNP P37528
X	202	HIS	-	expression tag	UNP P37528
X	203	HIS	-	expression tag	UNP P37528
X	204	HIS	-	expression tag	UNP P37528

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	G	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0
3	M	1	Total Cl 1 1	0	0
3	O	1	Total Cl 1 1	0	0
3	Q	1	Total Cl 1 1	0	0
3	S	1	Total Cl 1 1	0	0
3	U	1	Total Cl 1 1	0	0
3	W	1	Total Cl 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



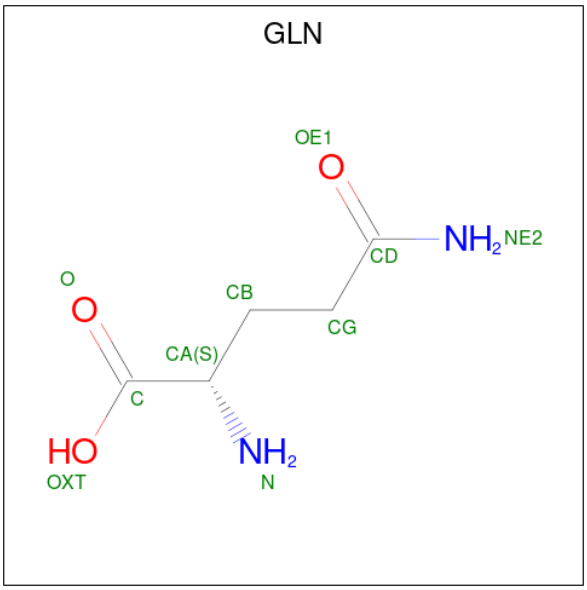
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Q	1	Total C O 4 2 2	0	0
4	U	1	Total C O 4 2 2	0	0
4	U	1	Total C O 4 2 2	0	0
4	W	1	Total C O 4 2 2	0	0

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 10 5 2 3	0	0
5	D	1	Total C N O 10 5 2 3	0	0
5	F	1	Total C N O 10 5 2 3	0	0
5	H	1	Total C N O 10 5 2 3	0	0
5	J	1	Total C N O 10 5 2 3	0	0
5	L	1	Total C N O 10 5 2 3	0	0
5	N	1	Total C N O 10 5 2 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total C N O 10 5 2 3	0	0
5	R	1	Total C N O 10 5 2 3	0	0
5	T	1	Total C N O 10 5 2 3	0	0
5	V	1	Total C N O 10 5 2 3	0	0
5	X	1	Total C N O 9 5 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	295	Total O 295 295	0	0
6	B	120	Total O 120 120	0	0
6	C	348	Total O 348 348	0	0
6	D	142	Total O 142 142	0	0
6	E	335	Total O 335 335	0	0
6	F	115	Total O 115 115	0	0
6	G	330	Total O 330 330	0	0
6	H	164	Total O 164 164	0	0
6	I	330	Total O 330 330	0	0
6	J	204	Total O 204 204	0	0
6	K	303	Total O 303 303	0	0
6	L	153	Total O 153 153	0	0
6	M	334	Total O 334 334	0	0
6	N	198	Total O 198 198	0	0

Continued on next page...

Continued from previous page...

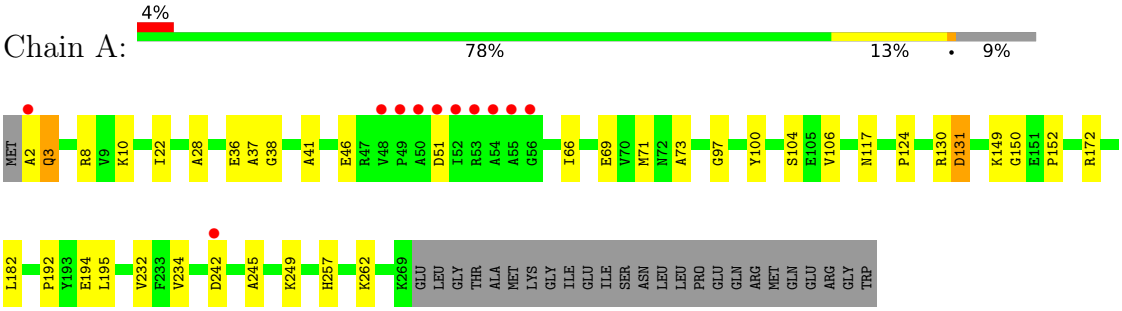
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	O	343	Total O 343 343	0	0
6	P	177	Total O 177 177	0	0
6	Q	323	Total O 323 323	0	0
6	R	173	Total O 173 173	0	0
6	S	311	Total O 311 311	0	0
6	T	134	Total O 134 134	0	0
6	U	285	Total O 285 285	0	0
6	V	104	Total O 104 104	0	0
6	W	334	Total O 334 334	0	0
6	X	219	Total O 219 219	0	0

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

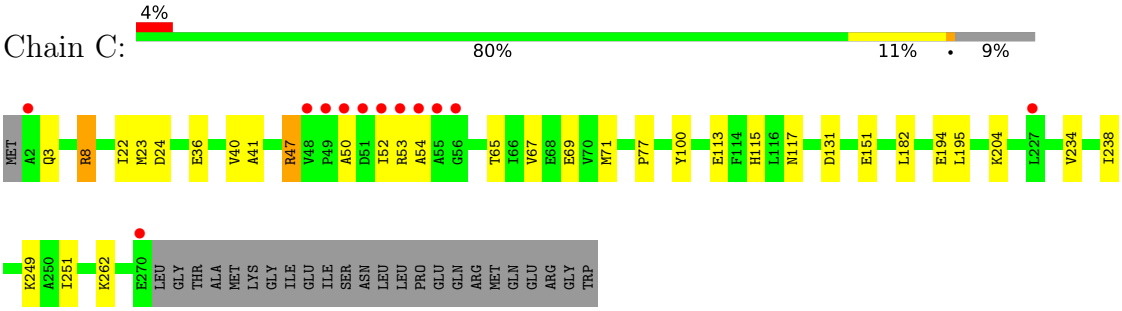
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain A:



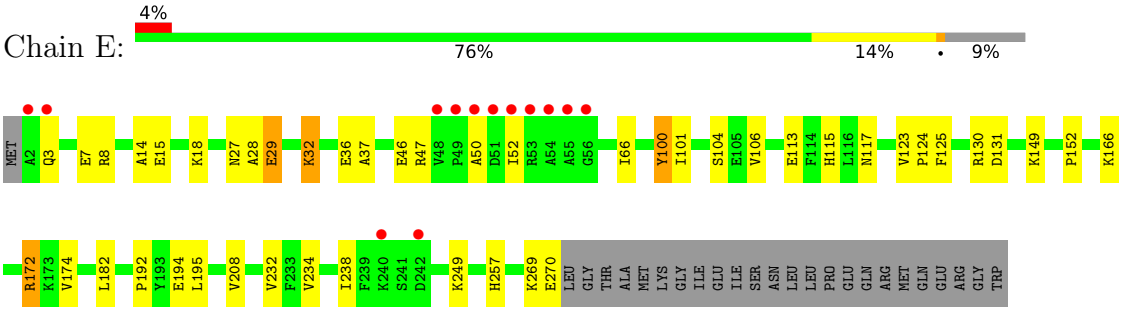
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain C:



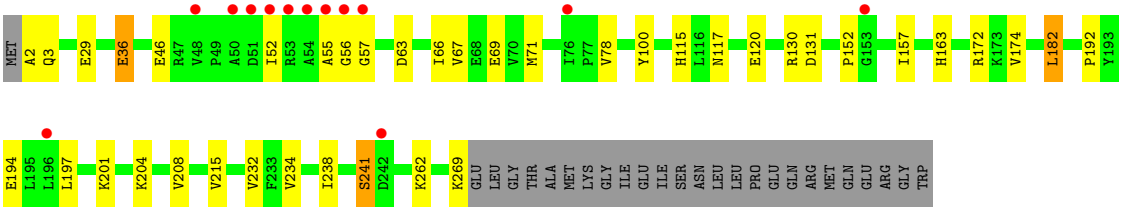
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain E:



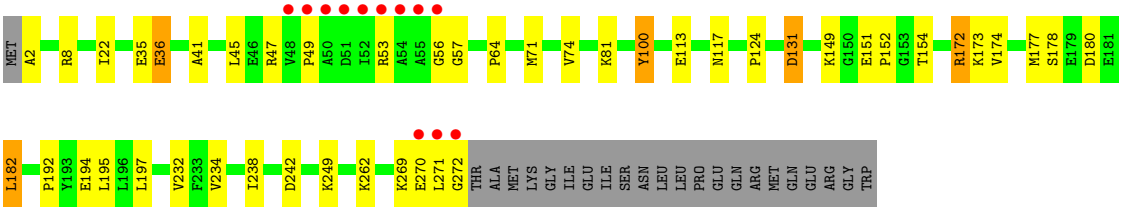
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain G:



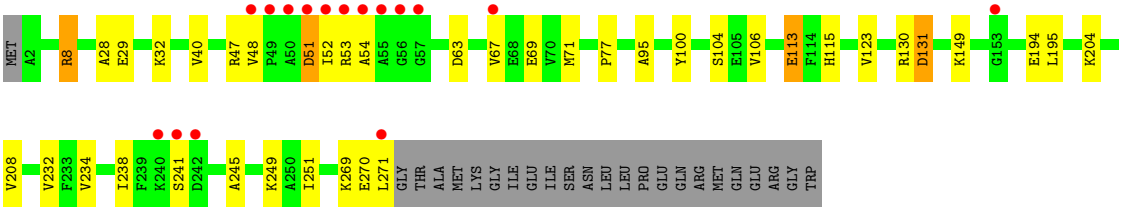
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain I:



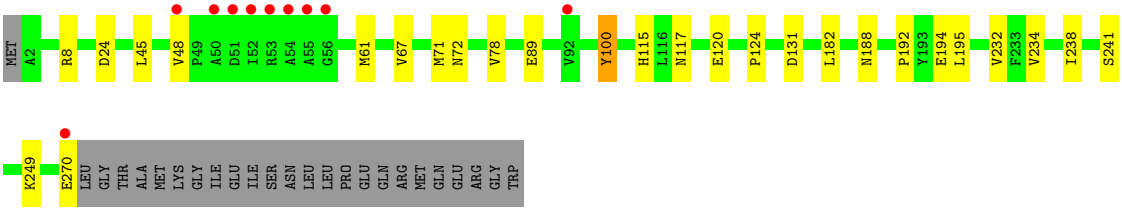
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain K:



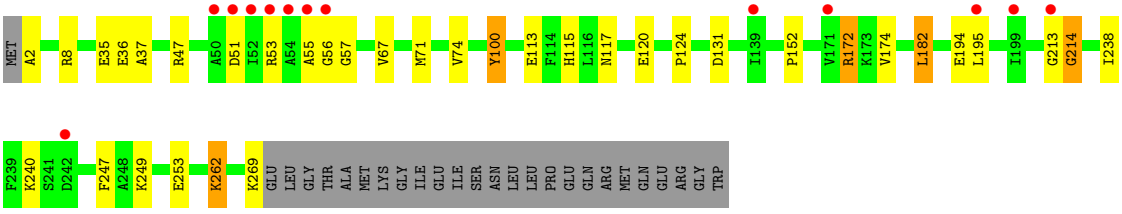
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain M:



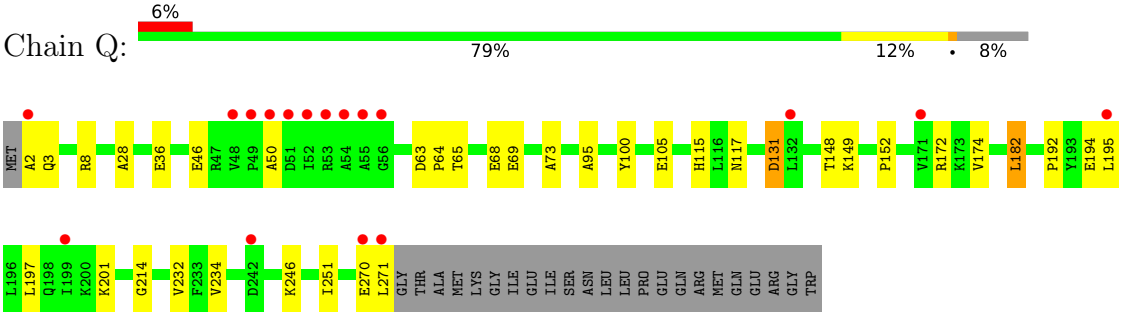
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain O:



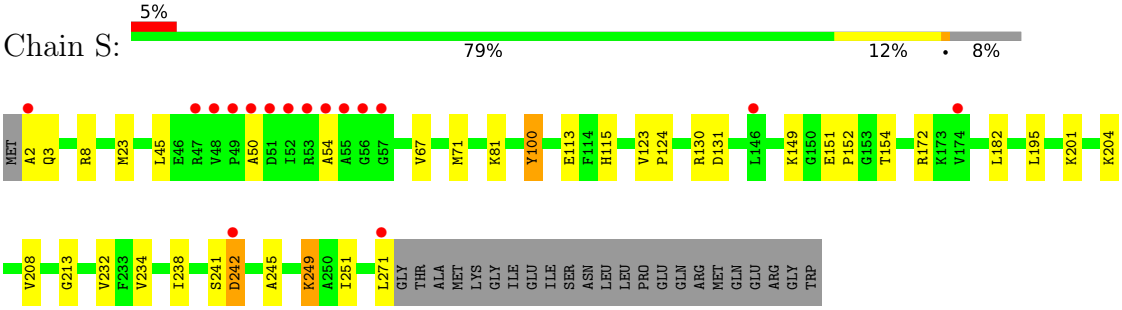
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain Q:



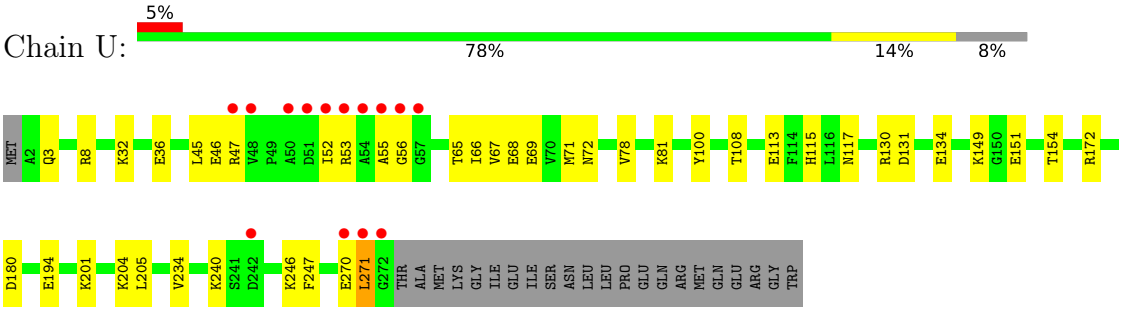
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain S:



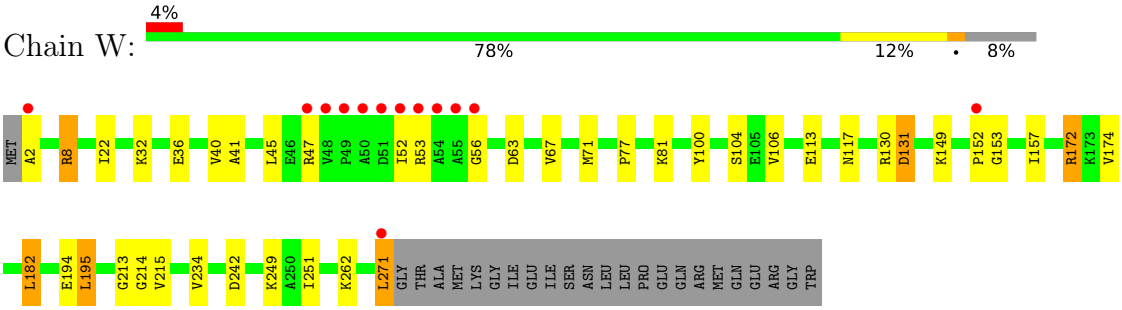
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain U:



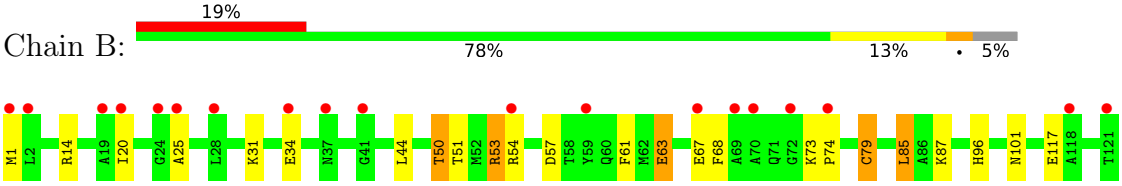
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

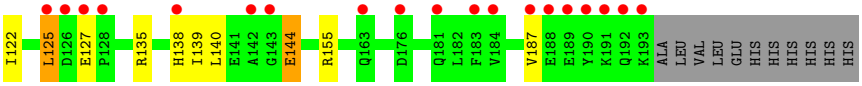
Chain W:



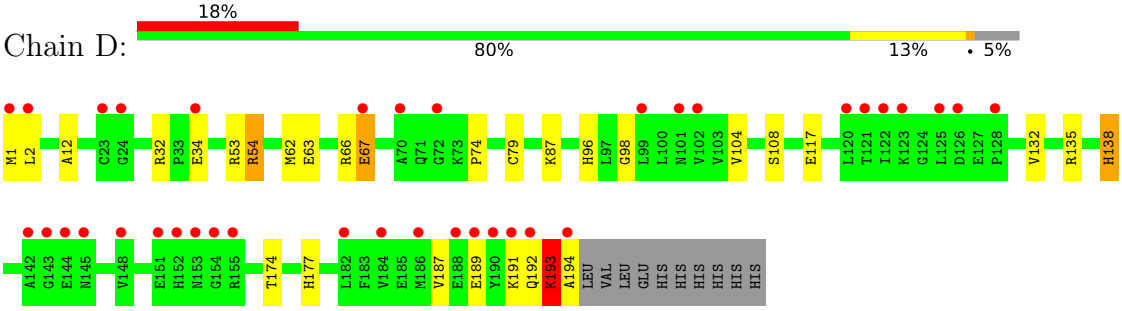
• Molecule 2: Glutamine amidotransferase subunit pdxT

Chain B:

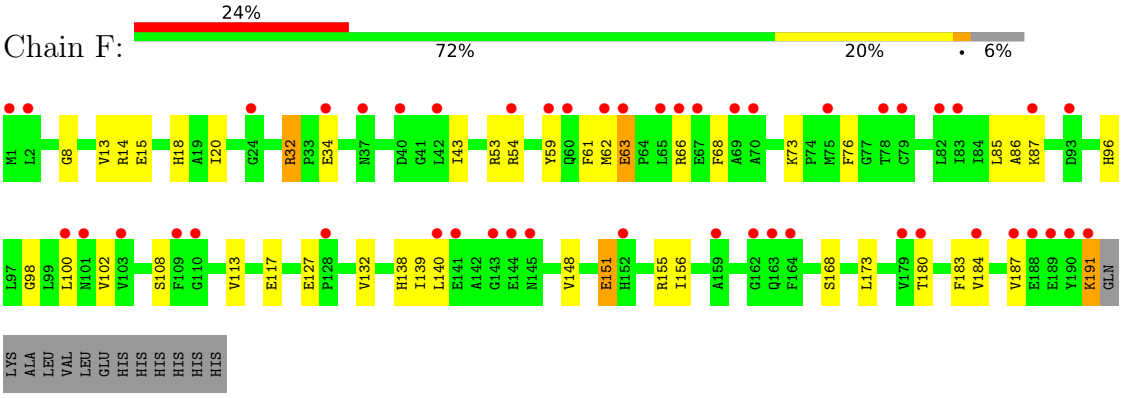




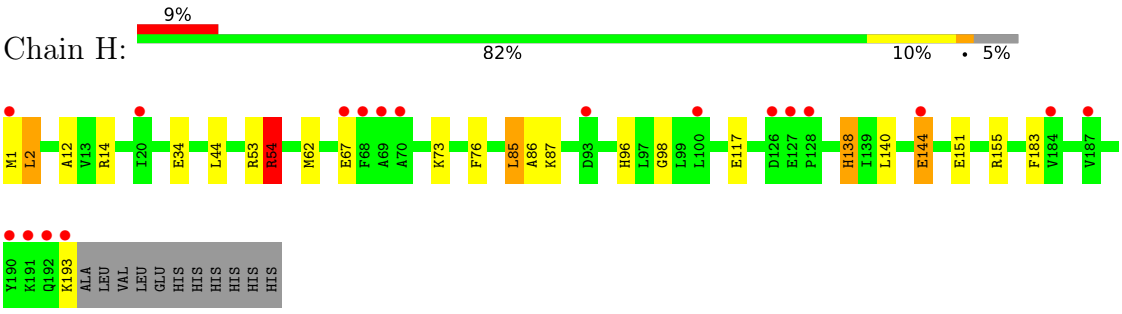
• Molecule 2: Glutamine amidotransferase subunit pdxT



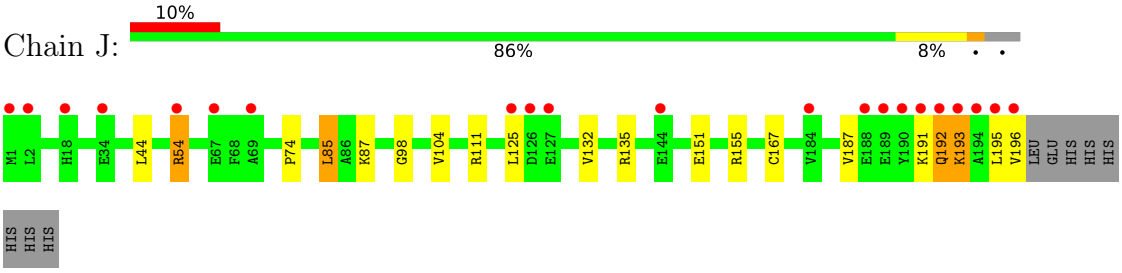
• Molecule 2: Glutamine amidotransferase subunit pdxT



• Molecule 2: Glutamine amidotransferase subunit pdxT

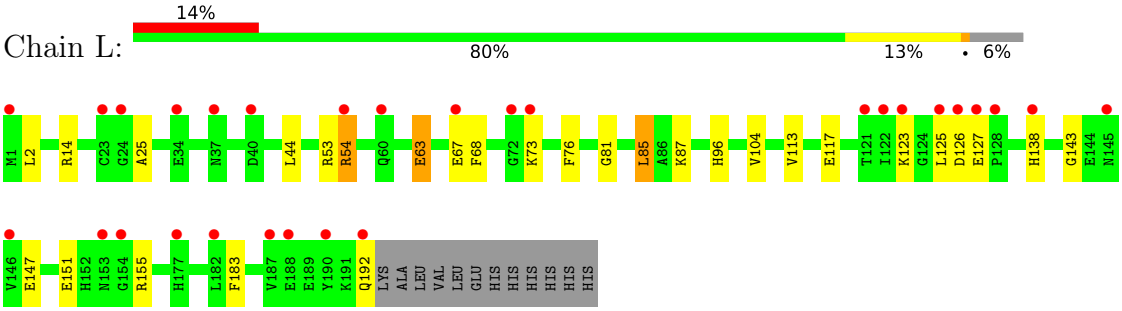


• Molecule 2: Glutamine amidotransferase subunit pdxT



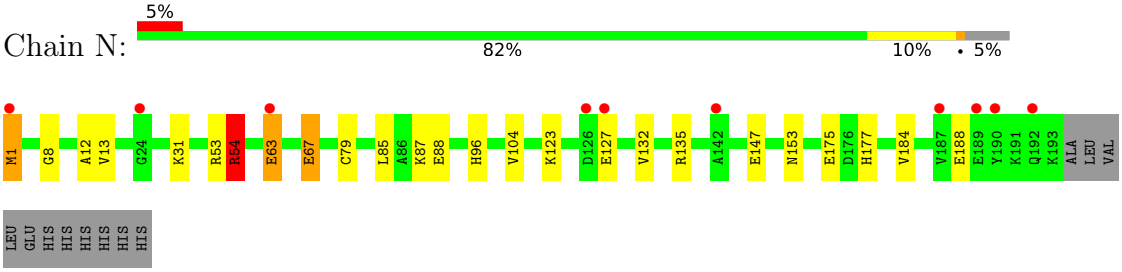
• Molecule 2: Glutamine amidotransferase subunit pdxT

Chain L:



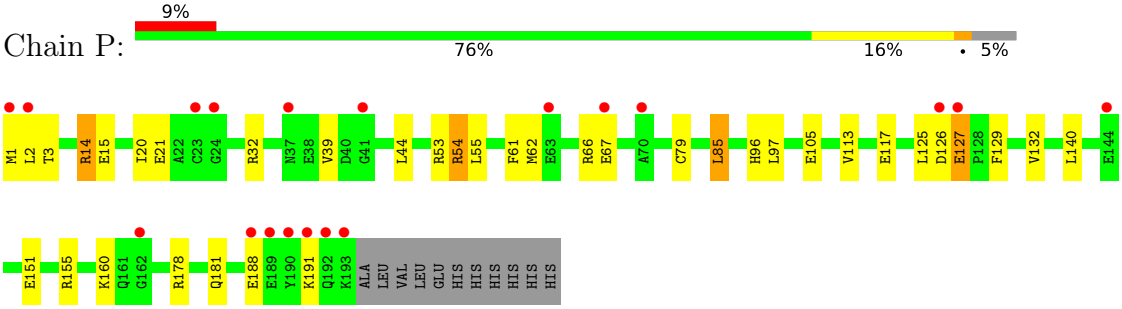
• Molecule 2: Glutamine amidotransferase subunit pdxT

Chain N:



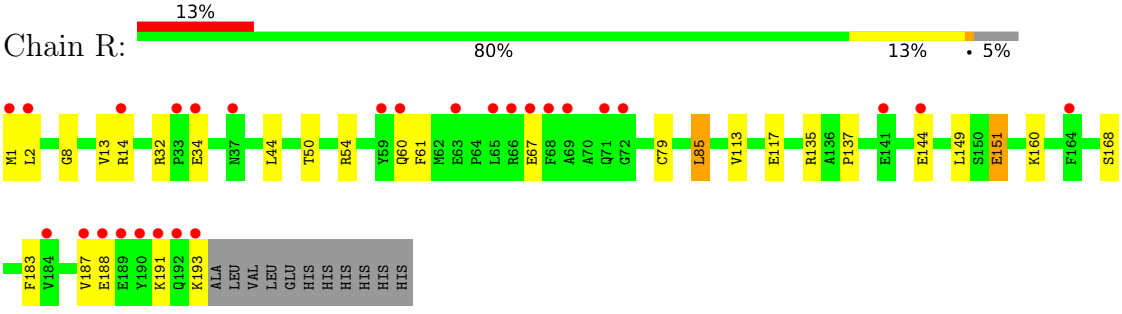
• Molecule 2: Glutamine amidotransferase subunit pdxT

Chain P:



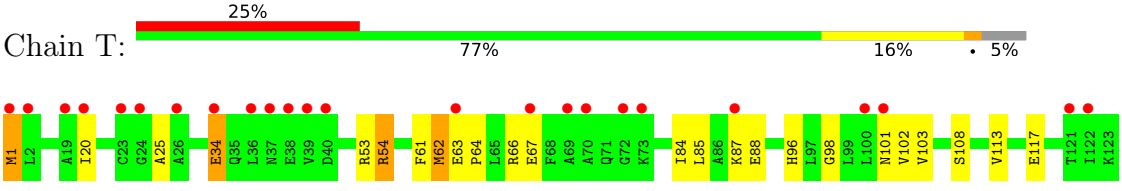
• Molecule 2: Glutamine amidotransferase subunit pdxT

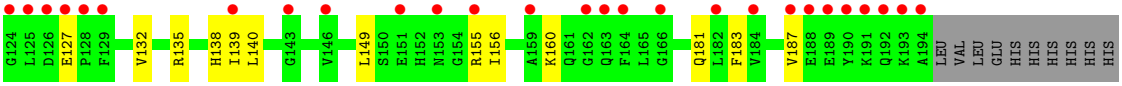
Chain R:



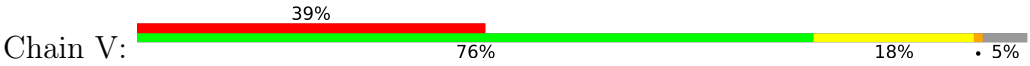
• Molecule 2: Glutamine amidotransferase subunit pdxT

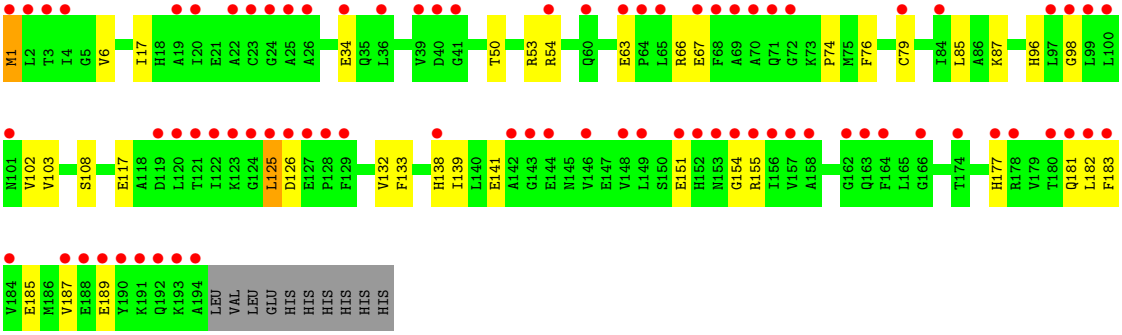
Chain T:



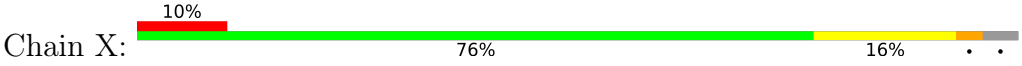


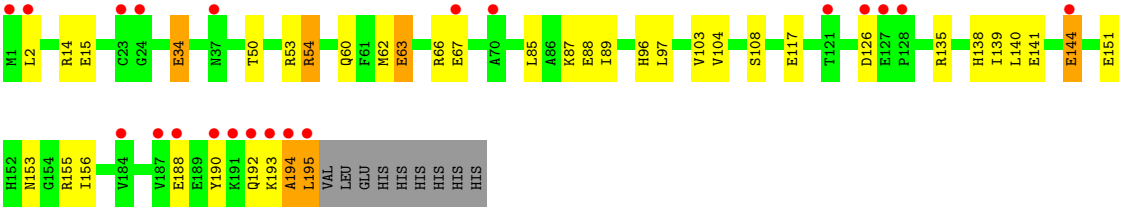
• Molecule 2: Glutamine amidotransferase subunit pdxT





• Molecule 2: Glutamine amidotransferase subunit pdxT





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.51Å 259.01Å 144.96Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	50.00 – 2.12 49.62 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.12) 98.2 (49.62-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.146 , 0.198 0.157 , 0.205	Depositor DCC
R_{free} test set	19065 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	48293	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO

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	0.72	0/2070	0.77	5/2792 (0.2%)
1	C	0.80	0/2076	0.80	2/2799 (0.1%)
1	E	0.76	0/2076	0.79	4/2799 (0.1%)
1	G	0.76	0/2040	0.81	3/2753 (0.1%)
1	I	0.77	0/2078	0.85	4/2802 (0.1%)
1	K	0.75	0/2068	0.78	3/2790 (0.1%)
1	M	0.78	0/2075	0.81	1/2797 (0.0%)
1	O	0.77	0/2060	0.85	4/2777 (0.1%)
1	Q	0.75	0/2061	0.80	5/2780 (0.2%)
1	S	0.73	0/2061	0.79	4/2781 (0.1%)
1	U	0.73	0/2070	0.77	4/2793 (0.1%)
1	W	0.83	0/2086	0.80	4/2814 (0.1%)
2	B	0.56	0/1531	0.71	2/2066 (0.1%)
2	D	0.54	0/1525	0.71	2/2059 (0.1%)
2	F	0.53	0/1502	0.63	0/2029
2	H	0.57	0/1525	0.72	1/2060 (0.0%)
2	J	0.62	1/1540 (0.1%)	0.75	1/2080 (0.0%)
2	L	0.54	0/1511	0.66	0/2041
2	N	0.66	0/1516	0.76	4/2048 (0.2%)
2	P	0.60	0/1527	0.70	0/2062
2	R	0.57	0/1531	0.69	2/2066 (0.1%)
2	T	0.53	0/1521	0.69	1/2054 (0.0%)
2	V	0.48	0/1525	0.69	0/2059
2	X	0.62	0/1533	0.73	2/2070 (0.1%)
All	All	0.69	1/43108 (0.0%)	0.76	58/58171 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	I	0	1
2	D	0	1
2	P	1	0
2	X	0	1
All	All	1	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	167	CYS	CB-SG	-5.57	1.72	1.81

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	8	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	O	172[A]	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	O	172[B]	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	Q	63	ASP	CB-CG-OD2	6.62	124.26	118.30
1	K	63	ASP	CB-CG-OD1	-6.62	112.35	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	P	54[B]	ARG	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	193	LYS	Peptide
1	G	56	GLY	Peptide
1	I	56	GLY	Peptide
2	X	194	ALA	Peptide

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	2028	0	2078	33	0
1	C	2037	0	2079	39	0
1	E	2037	0	2081	73	0
1	G	2007	0	2041	40	0
1	I	2042	0	2085	54	0
1	K	2032	0	2081	35	0
1	M	2036	0	2084	29	0
1	O	2024	0	2074	46	0
1	Q	2028	0	2072	37	0
1	S	2028	0	2065	34	0
1	U	2034	0	2070	43	0
1	W	2044	0	2095	51	0
2	B	1500	0	1512	35	0
2	D	1497	0	1504	33	0
2	F	1474	0	1478	36	0
2	H	1494	0	1494	21	0
2	J	1512	0	1524	10	0
2	L	1483	0	1486	28	1
2	N	1488	0	1488	28	0
2	P	1496	0	1508	48	0
2	R	1500	0	1512	28	0
2	T	1493	0	1500	57	0
2	V	1497	0	1504	39	0
2	X	1505	0	1515	43	1
3	A	1	0	0	2	0
3	C	1	0	0	2	0
3	E	1	0	0	2	0
3	G	1	0	0	1	0
3	I	1	0	0	2	0
3	K	1	0	0	1	0
3	M	1	0	0	0	0
3	O	1	0	0	1	0
3	Q	1	0	0	2	0
3	S	1	0	0	2	0
3	U	1	0	0	2	0
3	W	1	0	0	2	0
4	A	12	0	18	8	0
4	C	8	0	12	0	0
4	E	8	0	11	9	0
4	G	4	0	6	9	0
4	I	12	0	17	9	0
4	K	4	0	6	0	0
4	M	4	0	5	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	8	0	11	11	0
4	U	8	0	12	0	0
4	W	4	0	6	0	0
5	B	10	0	7	1	0
5	D	10	0	7	1	0
5	F	10	0	7	0	0
5	H	10	0	7	0	0
5	J	10	0	7	0	0
5	L	10	0	7	0	0
5	N	10	0	7	0	0
5	P	10	0	7	2	0
5	R	10	0	7	0	0
5	T	10	0	7	0	0
5	V	10	0	7	0	0
5	X	9	0	7	0	0
6	A	295	0	0	13	0
6	B	120	0	0	19	0
6	C	348	0	0	14	0
6	D	142	0	0	14	0
6	E	335	0	0	48	0
6	F	115	0	0	10	0
6	G	330	0	0	22	0
6	H	164	0	0	6	0
6	I	330	0	0	33	0
6	J	204	0	0	1	0
6	K	303	0	0	20	0
6	L	153	0	0	15	0
6	M	334	0	0	17	0
6	N	198	0	0	19	0
6	O	343	0	0	28	0
6	P	177	0	0	21	0
6	Q	323	0	0	21	0
6	R	173	0	0	14	1
6	S	311	0	0	25	0
6	T	134	0	0	32	0
6	U	285	0	0	22	0
6	V	104	0	0	16	0
6	W	334	0	0	35	1
6	X	219	0	0	24	0
All	All	48293	0	43118	897	2

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 897 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:R:54[B]:ARG:NH1	6:R:3257:HOH:O	1.57	1.31
1:S:234:VAL:HB	6:S:6294:HOH:O	1.32	1.28
1:E:172[B]:ARG:NH1	6:E:6234:HOH:O	1.67	1.28
1:C:36[B]:GLU:HG3	2:D:54[B]:ARG:NH2	1.48	1.27
6:A:6321:HOH:O	2:B:31:LYS:HB3	1.27	1.27

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:87:LYS:NZ	2:X:141:GLU:OE1[1_656]	1.83	0.37
6:R:1160:HOH:O	6:W:6293:HOH:O[1_556]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/294 (92%)	269 (99%)	3 (1%)	0	100	100
1	C	272/294 (92%)	266 (98%)	6 (2%)	0	100	100
1	E	272/294 (92%)	266 (98%)	6 (2%)	0	100	100
1	G	269/294 (92%)	264 (98%)	4 (2%)	1 (0%)	34	32
1	I	273/294 (93%)	265 (97%)	7 (3%)	1 (0%)	34	32
1	K	272/294 (92%)	265 (97%)	7 (3%)	0	100	100
1	M	272/294 (92%)	270 (99%)	2 (1%)	0	100	100
1	O	270/294 (92%)	266 (98%)	2 (1%)	2 (1%)	22	17
1	Q	271/294 (92%)	266 (98%)	3 (1%)	2 (1%)	22	17
1	S	271/294 (92%)	265 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	273/294 (93%)	269 (98%)	4 (2%)	0	100	100
1	W	274/294 (93%)	269 (98%)	5 (2%)	0	100	100
2	B	193/204 (95%)	186 (96%)	6 (3%)	1 (0%)	29	25
2	D	193/204 (95%)	187 (97%)	5 (3%)	1 (0%)	29	25
2	F	190/204 (93%)	183 (96%)	7 (4%)	0	100	100
2	H	193/204 (95%)	187 (97%)	6 (3%)	0	100	100
2	J	195/204 (96%)	187 (96%)	7 (4%)	1 (0%)	29	25
2	L	191/204 (94%)	183 (96%)	8 (4%)	0	100	100
2	N	192/204 (94%)	185 (96%)	6 (3%)	1 (0%)	29	25
2	P	193/204 (95%)	188 (97%)	5 (3%)	0	100	100
2	R	193/204 (95%)	189 (98%)	3 (2%)	1 (0%)	29	25
2	T	193/204 (95%)	188 (97%)	5 (3%)	0	100	100
2	V	193/204 (95%)	183 (95%)	9 (5%)	1 (0%)	29	25
2	X	194/204 (95%)	186 (96%)	7 (4%)	1 (0%)	29	25
All	All	5574/5976 (93%)	5432 (98%)	129 (2%)	13 (0%)	47	48

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	193	LYS
1	G	57	GLY
1	I	57	GLY
1	O	57	GLY
2	J	192	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/227 (92%)	203 (97%)	7 (3%)	38	39
1	C	211/227 (93%)	204 (97%)	7 (3%)	38	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	211/227 (93%)	204 (97%)	7 (3%)	38	39
1	G	207/227 (91%)	198 (96%)	9 (4%)	29	28
1	I	211/227 (93%)	203 (96%)	8 (4%)	33	33
1	K	210/227 (92%)	203 (97%)	7 (3%)	38	39
1	M	211/227 (93%)	207 (98%)	4 (2%)	57	61
1	O	209/227 (92%)	203 (97%)	6 (3%)	42	44
1	Q	209/227 (92%)	202 (97%)	7 (3%)	38	39
1	S	209/227 (92%)	200 (96%)	9 (4%)	29	28
1	U	209/227 (92%)	203 (97%)	6 (3%)	42	44
1	W	212/227 (93%)	204 (96%)	8 (4%)	33	33
2	B	160/168 (95%)	151 (94%)	9 (6%)	21	18
2	D	159/168 (95%)	151 (95%)	8 (5%)	24	22
2	F	157/168 (94%)	147 (94%)	10 (6%)	17	14
2	H	159/168 (95%)	149 (94%)	10 (6%)	18	14
2	J	161/168 (96%)	152 (94%)	9 (6%)	21	18
2	L	158/168 (94%)	150 (95%)	8 (5%)	24	21
2	N	158/168 (94%)	150 (95%)	8 (5%)	24	21
2	P	160/168 (95%)	152 (95%)	8 (5%)	24	22
2	R	160/168 (95%)	150 (94%)	10 (6%)	18	14
2	T	158/168 (94%)	149 (94%)	9 (6%)	20	17
2	V	159/168 (95%)	152 (96%)	7 (4%)	28	27
2	X	160/168 (95%)	149 (93%)	11 (7%)	15	12
All	All	4428/4740 (93%)	4236 (96%)	192 (4%)	32	28

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	195	LEU
1	S	100	TYR
2	P	54[A]	ARG
1	Q	182	LEU
1	S	249	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	115	HIS
2	R	153	ASN
1	M	117	ASN
2	P	96	HIS
2	T	96	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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)

Of 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	M	6007	-	3,3,3	0.91	0	2,2,2	0.50	0
4	EDO	W	6046	-	3,3,3	0.24	0	2,2,2	0.05	0
5	GLN	N	6028	-	8,9,9	0.64	0	10,11,11	1.14	1 (10%)
4	EDO	I	6039	-	3,3,3	0.67	0	2,2,2	0.13	0
5	GLN	T	6040	-	8,9,9	0.77	0	10,11,11	1.05	2 (20%)
5	GLN	H	6016	-	8,9,9	0.80	1 (12%)	10,11,11	1.14	2 (20%)
5	GLN	J	6020	-	8,9,9	0.91	0	10,11,11	0.82	0
4	EDO	A	6030	-	3,3,3	0.27	0	2,2,2	0.76	0
5	GLN	V	6044	-	8,9,9	0.90	0	10,11,11	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	I	6018	-	3,3,3	0.29	0	2,2,2	0.88	0
5	GLN	F	6012	-	8,9,9	0.73	0	10,11,11	1.10	2 (20%)
4	EDO	U	6042	-	3,3,3	0.46	0	2,2,2	0.16	0
5	GLN	P	6032	-	8,9,9	1.00	1 (12%)	10,11,11	1.11	2 (20%)
4	EDO	E	6010	-	3,3,3	0.39	0	2,2,2	0.30	0
5	GLN	R	6036	-	8,9,9	0.83	0	10,11,11	0.93	1 (10%)
4	EDO	Q	6035	-	3,3,3	1.03	0	2,2,2	0.88	0
4	EDO	G	6043	-	3,3,3	0.61	0	2,2,2	0.09	0
4	EDO	A	6031	-	3,3,3	0.61	0	2,2,2	0.21	0
5	GLN	B	6004	-	8,9,9	0.72	0	10,11,11	1.07	1 (10%)
4	EDO	U	6014	-	3,3,3	0.22	0	2,2,2	0.41	0
4	EDO	C	6026	-	3,3,3	0.22	0	2,2,2	0.28	0
4	EDO	E	6047	-	3,3,3	0.77	0	2,2,2	0.27	0
5	GLN	D	6008	-	8,9,9	0.81	0	10,11,11	0.80	0
4	EDO	I	6038	-	3,3,3	0.26	0	2,2,2	0.30	0
5	GLN	X	6048	-	7,8,9	0.78	0	4,9,11	0.08	0
4	EDO	K	6022	-	3,3,3	0.27	0	2,2,2	0.27	0
4	EDO	A	6002	-	3,3,3	0.62	0	2,2,2	0.55	0
5	GLN	L	6024	-	8,9,9	0.93	1 (12%)	10,11,11	0.77	0
4	EDO	Q	6034	-	3,3,3	0.28	0	2,2,2	0.11	0
4	EDO	C	6006	-	3,3,3	0.28	0	2,2,2	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	M	6007	-	-	1/1/1/1	-
4	EDO	W	6046	-	-	0/1/1/1	-
5	GLN	N	6028	-	-	0/9/9/9	-
4	EDO	I	6039	-	-	0/1/1/1	-
5	GLN	T	6040	-	-	0/9/9/9	-
5	GLN	H	6016	-	-	0/9/9/9	-
5	GLN	J	6020	-	-	0/9/9/9	-
4	EDO	A	6030	-	-	1/1/1/1	-
5	GLN	V	6044	-	-	0/9/9/9	-
4	EDO	I	6018	-	-	1/1/1/1	-
5	GLN	F	6012	-	-	0/9/9/9	-
4	EDO	U	6042	-	-	0/1/1/1	-
5	GLN	P	6032	-	-	0/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	6010	-	-	1/1/1/1	-
5	GLN	R	6036	-	-	0/9/9/9	-
4	EDO	Q	6035	-	-	1/1/1/1	-
4	EDO	G	6043	-	-	1/1/1/1	-
4	EDO	A	6031	-	-	1/1/1/1	-
5	GLN	B	6004	-	-	0/9/9/9	-
4	EDO	U	6014	-	-	1/1/1/1	-
4	EDO	C	6026	-	-	1/1/1/1	-
4	EDO	E	6047	-	-	0/1/1/1	-
5	GLN	D	6008	-	-	0/9/9/9	-
4	EDO	I	6038	-	-	1/1/1/1	-
5	GLN	X	6048	-	-	0/6/7/9	-
4	EDO	K	6022	-	-	0/1/1/1	-
4	EDO	A	6002	-	-	0/1/1/1	-
5	GLN	L	6024	-	-	0/9/9/9	-
4	EDO	Q	6034	-	-	0/1/1/1	-
4	EDO	C	6006	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	6032	GLN	OXT-C	-2.62	1.22	1.30
5	L	6024	GLN	OXT-C	-2.24	1.23	1.30
5	H	6016	GLN	OXT-C	-2.04	1.23	1.30

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	6032	GLN	OXT-C-O	-2.76	117.83	124.09
5	N	6028	GLN	OXT-C-CA	2.57	122.15	113.38
5	B	6004	GLN	OXT-C-CA	2.54	122.04	113.38
5	H	6016	GLN	OXT-C-O	-2.40	118.64	124.09
5	F	6012	GLN	OXT-C-CA	2.37	121.45	113.38

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	6030	EDO	O1-C1-C2-O2
4	E	6010	EDO	O1-C1-C2-O2
4	U	6014	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	6038	EDO	O1-C1-C2-O2
4	Q	6035	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	6007	EDO	5	0
4	I	6039	EDO	9	0
5	P	6032	GLN	2	0
4	Q	6035	EDO	11	0
4	G	6043	EDO	9	0
4	A	6031	EDO	8	0
5	B	6004	GLN	1	0
4	E	6047	EDO	9	0
5	D	6008	GLN	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	268/294 (91%)	0.58	11 (4%)	37	43	29, 38, 55, 83	0
1	C	269/294 (91%)	0.74	12 (4%)	33	38	29, 34, 52, 81	0
1	E	269/294 (91%)	0.58	13 (4%)	30	35	30, 38, 54, 80	0
1	G	268/294 (91%)	0.54	13 (4%)	29	35	30, 36, 55, 87	0
1	I	271/294 (92%)	0.59	12 (4%)	34	40	28, 34, 57, 79	0
1	K	270/294 (91%)	0.65	16 (5%)	22	27	29, 36, 61, 79	0
1	M	269/294 (91%)	0.56	10 (3%)	41	48	28, 34, 52, 74	0
1	O	268/294 (91%)	0.62	13 (4%)	29	35	28, 35, 53, 73	0
1	Q	270/294 (91%)	0.70	17 (6%)	20	24	28, 36, 58, 76	0
1	S	270/294 (91%)	0.73	16 (5%)	22	27	30, 38, 62, 82	0
1	U	271/294 (92%)	0.62	14 (5%)	27	32	30, 39, 61, 82	0
1	W	270/294 (91%)	0.61	13 (4%)	30	35	28, 34, 53, 83	0
2	B	193/204 (94%)	1.17	38 (19%)	1	1	44, 55, 65, 83	0
2	D	194/204 (95%)	1.08	37 (19%)	1	1	40, 51, 60, 70	0
2	F	191/204 (93%)	1.47	48 (25%)	0	0	46, 60, 69, 78	0
2	H	193/204 (94%)	0.63	18 (9%)	8	11	37, 48, 58, 78	0
2	J	196/204 (96%)	0.48	21 (10%)	6	7	36, 45, 57, 63	0
2	L	192/204 (94%)	0.92	29 (15%)	2	3	40, 51, 60, 74	0
2	N	193/204 (94%)	0.46	10 (5%)	27	32	34, 44, 55, 76	0
2	P	193/204 (94%)	0.62	19 (9%)	7	9	38, 48, 59, 70	0
2	R	193/204 (94%)	0.82	27 (13%)	2	3	39, 49, 60, 82	0
2	T	194/204 (95%)	1.42	51 (26%)	0	0	46, 55, 65, 71	0
2	V	194/204 (95%)	1.97	80 (41%)	0	0	47, 62, 70, 78	0
2	X	195/204 (95%)	0.53	21 (10%)	5	7	35, 44, 57, 67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
All	All	5554/5976 (92%)	0.77	559 (10%)	7 8	28, 42, 64, 87	0

The worst 5 of 559 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	54	ALA	10.1
1	S	54	ALA	9.6
1	K	50	ALA	8.5
1	I	54	ALA	8.5
1	A	56	GLY	8.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	6001	1/1	0.75	0.08	73,73,73,73	0
3	CL	U	6041	1/1	0.79	0.08	80,80,80,80	0
3	CL	O	6029	1/1	0.81	0.13	83,83,83,83	0
3	CL	C	6005	1/1	0.85	0.08	75,75,75,75	0
3	CL	G	6013	1/1	0.85	0.11	74,74,74,74	0
4	EDO	A	6030	4/4	0.91	0.18	35,43,46,51	0
4	EDO	G	6043	4/4	0.91	0.25	31,37,44,50	0
4	EDO	M	6007	4/4	0.91	0.20	28,37,41,43	0
5	GLN	R	6036	10/10	0.91	0.17	36,37,39,40	0
3	CL	W	6045	1/1	0.92	0.05	65,65,65,65	0
4	EDO	A	6002	4/4	0.92	0.16	37,43,45,51	0
5	GLN	B	6004	10/10	0.92	0.12	43,44,45,46	0
3	CL	I	6017	1/1	0.92	0.09	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GLN	T	6040	10/10	0.92	0.13	41,42,43,43	0
5	GLN	V	6044	10/10	0.92	0.12	45,46,47,49	0
4	EDO	I	6039	4/4	0.93	0.22	34,39,46,49	0
3	CL	S	6037	1/1	0.93	0.07	72,72,72,72	0
4	EDO	Q	6035	4/4	0.93	0.19	32,34,43,46	0
3	CL	M	6025	1/1	0.93	0.07	65,65,65,65	0
5	GLN	L	6024	10/10	0.93	0.13	39,41,42,43	0
4	EDO	A	6031	4/4	0.93	0.19	32,39,44,49	0
4	EDO	E	6047	4/4	0.93	0.19	30,40,44,47	0
3	CL	E	6009	1/1	0.93	0.07	67,67,67,67	0
5	GLN	F	6012	10/10	0.94	0.17	43,46,47,49	0
5	GLN	H	6016	10/10	0.94	0.13	34,36,36,38	0
4	EDO	I	6018	4/4	0.94	0.14	35,40,44,49	0
4	EDO	I	6038	4/4	0.94	0.13	37,42,43,46	0
4	EDO	U	6042	4/4	0.94	0.12	38,43,46,51	0
4	EDO	C	6026	4/4	0.94	0.14	37,43,44,51	0
4	EDO	U	6014	4/4	0.95	0.13	38,42,44,46	0
3	CL	Q	6033	1/1	0.95	0.13	79,79,79,79	0
5	GLN	N	6028	10/10	0.95	0.10	32,32,34,34	0
5	GLN	X	6048	9/10	0.95	0.10	32,34,36,37	0
5	GLN	D	6008	10/10	0.96	0.10	33,35,35,35	0
5	GLN	P	6032	10/10	0.96	0.07	37,38,39,40	0
4	EDO	C	6006	4/4	0.96	0.12	38,41,43,50	0
4	EDO	W	6046	4/4	0.96	0.13	36,42,43,45	0
5	GLN	J	6020	10/10	0.96	0.07	33,34,35,35	0
4	EDO	E	6010	4/4	0.96	0.12	35,43,44,48	0
3	CL	K	6021	1/1	0.97	0.08	70,70,70,70	0
4	EDO	Q	6034	4/4	0.97	0.09	35,39,39,48	0
4	EDO	K	6022	4/4	0.97	0.10	33,39,39,45	0

6.5 Other polymers (i)

There are no such residues in this entry.