



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 06:23 PM UTC

PDB ID : 4WXY / pdb_00004wxy
Title : PLPS (inactive glutaminase mutant) co-crystallized with glutamine and R5P.
Authors : Smith, J.L.; Smith, A.M.
Deposited on : 2014-11-14
Resolution : 2.70 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

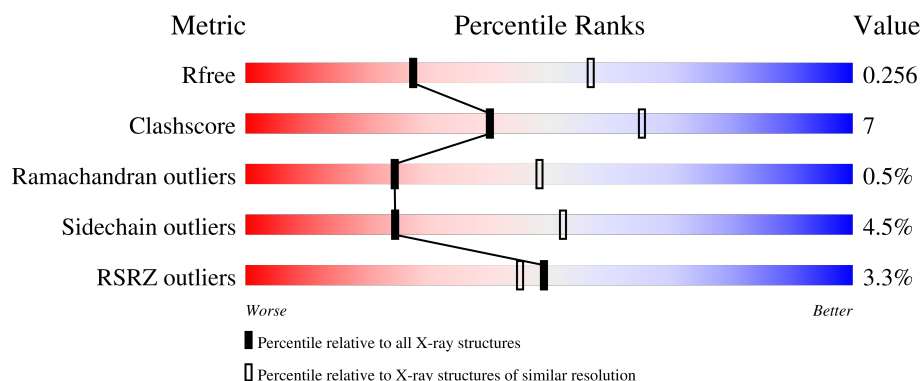
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	
1	C	304	
1	E	304	
1	G	304	
1	I	304	

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Mol	Chain	Length	Quality of chain
1	K	304	
2	B	228	
2	D	228	
2	F	228	
2	H	228	
2	J	228	
2	L	228	

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
1	L5P	E	81	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22167 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	288	Total	C	N	O	P	S	0	0	0
			2176	1354	391	414	1	16			
1	C	290	Total	C	N	O	P	S	0	0	0
			2189	1362	393	416	1	17			
1	E	289	Total	C	N	O	P	S	0	0	0
			2181	1357	392	415	1	16			
1	G	290	Total	C	N	O	P	S	0	0	0
			2189	1362	393	416	1	17			
1	I	288	Total	C	N	O	P	S	0	0	0
			2176	1354	391	414	1	16			
1	K	290	Total	C	N	O	P	S	0	0	0
			2189	1362	393	416	1	17			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLU	-	expression tag	UNP Q5L3Y2
A	-8	ASN	-	expression tag	UNP Q5L3Y2
A	-7	LEU	-	expression tag	UNP Q5L3Y2
A	-6	THR	-	expression tag	UNP Q5L3Y2
A	-5	PRO	-	expression tag	UNP Q5L3Y2
A	-4	GLN	-	expression tag	UNP Q5L3Y2
A	-3	HIS	-	expression tag	UNP Q5L3Y2
A	-2	MET	-	expression tag	UNP Q5L3Y2
A	-1	ALA	-	expression tag	UNP Q5L3Y2
A	0	SER	-	expression tag	UNP Q5L3Y2
A	216	THR	ALA	conflict	UNP Q5L3Y2
C	-9	GLU	-	expression tag	UNP Q5L3Y2
C	-8	ASN	-	expression tag	UNP Q5L3Y2
C	-7	LEU	-	expression tag	UNP Q5L3Y2
C	-6	THR	-	expression tag	UNP Q5L3Y2
C	-5	PRO	-	expression tag	UNP Q5L3Y2
C	-4	GLN	-	expression tag	UNP Q5L3Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP Q5L3Y2
C	-2	MET	-	expression tag	UNP Q5L3Y2
C	-1	ALA	-	expression tag	UNP Q5L3Y2
C	0	SER	-	expression tag	UNP Q5L3Y2
C	216	THR	ALA	conflict	UNP Q5L3Y2
E	-9	GLU	-	expression tag	UNP Q5L3Y2
E	-8	ASN	-	expression tag	UNP Q5L3Y2
E	-7	LEU	-	expression tag	UNP Q5L3Y2
E	-6	THR	-	expression tag	UNP Q5L3Y2
E	-5	PRO	-	expression tag	UNP Q5L3Y2
E	-4	GLN	-	expression tag	UNP Q5L3Y2
E	-3	HIS	-	expression tag	UNP Q5L3Y2
E	-2	MET	-	expression tag	UNP Q5L3Y2
E	-1	ALA	-	expression tag	UNP Q5L3Y2
E	0	SER	-	expression tag	UNP Q5L3Y2
E	216	THR	ALA	conflict	UNP Q5L3Y2
G	-9	GLU	-	expression tag	UNP Q5L3Y2
G	-8	ASN	-	expression tag	UNP Q5L3Y2
G	-7	LEU	-	expression tag	UNP Q5L3Y2
G	-6	THR	-	expression tag	UNP Q5L3Y2
G	-5	PRO	-	expression tag	UNP Q5L3Y2
G	-4	GLN	-	expression tag	UNP Q5L3Y2
G	-3	HIS	-	expression tag	UNP Q5L3Y2
G	-2	MET	-	expression tag	UNP Q5L3Y2
G	-1	ALA	-	expression tag	UNP Q5L3Y2
G	0	SER	-	expression tag	UNP Q5L3Y2
G	216	THR	ALA	conflict	UNP Q5L3Y2
I	-9	GLU	-	expression tag	UNP Q5L3Y2
I	-8	ASN	-	expression tag	UNP Q5L3Y2
I	-7	LEU	-	expression tag	UNP Q5L3Y2
I	-6	THR	-	expression tag	UNP Q5L3Y2
I	-5	PRO	-	expression tag	UNP Q5L3Y2
I	-4	GLN	-	expression tag	UNP Q5L3Y2
I	-3	HIS	-	expression tag	UNP Q5L3Y2
I	-2	MET	-	expression tag	UNP Q5L3Y2
I	-1	ALA	-	expression tag	UNP Q5L3Y2
I	0	SER	-	expression tag	UNP Q5L3Y2
I	216	THR	ALA	conflict	UNP Q5L3Y2
K	-9	GLU	-	expression tag	UNP Q5L3Y2
K	-8	ASN	-	expression tag	UNP Q5L3Y2
K	-7	LEU	-	expression tag	UNP Q5L3Y2
K	-6	THR	-	expression tag	UNP Q5L3Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	PRO	-	expression tag	UNP Q5L3Y2
K	-4	GLN	-	expression tag	UNP Q5L3Y2
K	-3	HIS	-	expression tag	UNP Q5L3Y2
K	-2	MET	-	expression tag	UNP Q5L3Y2
K	-1	ALA	-	expression tag	UNP Q5L3Y2
K	0	SER	-	expression tag	UNP Q5L3Y2
K	216	THR	ALA	conflict	UNP Q5L3Y2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1448	915	255	268	10			
2	D	192	Total	C	N	O	S	0	0	0
			1474	931	260	272	11			
2	F	194	Total	C	N	O	S	0	0	0
			1486	937	262	276	11			
2	H	192	Total	C	N	O	S	0	0	0
			1474	931	260	272	11			
2	J	189	Total	C	N	O	S	0	0	0
			1452	917	256	269	10			
2	L	191	Total	C	N	O	S	0	0	0
			1470	929	259	271	11			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-31	MET	-	initiating methionine	UNP Q5L3Y1
B	-30	GLY	-	expression tag	UNP Q5L3Y1
B	-29	SER	-	expression tag	UNP Q5L3Y1
B	-28	SER	-	expression tag	UNP Q5L3Y1
B	-27	HIS	-	expression tag	UNP Q5L3Y1
B	-26	HIS	-	expression tag	UNP Q5L3Y1
B	-25	HIS	-	expression tag	UNP Q5L3Y1
B	-24	HIS	-	expression tag	UNP Q5L3Y1
B	-23	HIS	-	expression tag	UNP Q5L3Y1
B	-22	HIS	-	expression tag	UNP Q5L3Y1
B	-21	SER	-	expression tag	UNP Q5L3Y1
B	-20	SER	-	expression tag	UNP Q5L3Y1
B	-19	GLY	-	expression tag	UNP Q5L3Y1
B	-18	LEU	-	expression tag	UNP Q5L3Y1
B	-17	VAL	-	expression tag	UNP Q5L3Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	PRO	-	expression tag	UNP Q5L3Y1
B	-15	ARG	-	expression tag	UNP Q5L3Y1
B	-14	GLY	-	expression tag	UNP Q5L3Y1
B	-13	SER	-	expression tag	UNP Q5L3Y1
B	-12	GLY	-	expression tag	UNP Q5L3Y1
B	-11	THR	-	expression tag	UNP Q5L3Y1
B	-10	GLU	-	expression tag	UNP Q5L3Y1
B	-9	ASN	-	expression tag	UNP Q5L3Y1
B	-8	LEU	-	expression tag	UNP Q5L3Y1
B	-7	TYR	-	expression tag	UNP Q5L3Y1
B	-6	PHE	-	expression tag	UNP Q5L3Y1
B	-5	GLN	-	expression tag	UNP Q5L3Y1
B	-4	GLY	-	expression tag	UNP Q5L3Y1
B	-3	HIS	-	expression tag	UNP Q5L3Y1
B	-2	MET	-	expression tag	UNP Q5L3Y1
B	-1	ALA	-	expression tag	UNP Q5L3Y1
B	0	SER	-	expression tag	UNP Q5L3Y1
B	32	SER	PRO	conflict	UNP Q5L3Y1
B	169	ASN	HIS	engineered mutation	UNP Q5L3Y1
D	-31	MET	-	initiating methionine	UNP Q5L3Y1
D	-30	GLY	-	expression tag	UNP Q5L3Y1
D	-29	SER	-	expression tag	UNP Q5L3Y1
D	-28	SER	-	expression tag	UNP Q5L3Y1
D	-27	HIS	-	expression tag	UNP Q5L3Y1
D	-26	HIS	-	expression tag	UNP Q5L3Y1
D	-25	HIS	-	expression tag	UNP Q5L3Y1
D	-24	HIS	-	expression tag	UNP Q5L3Y1
D	-23	HIS	-	expression tag	UNP Q5L3Y1
D	-22	HIS	-	expression tag	UNP Q5L3Y1
D	-21	SER	-	expression tag	UNP Q5L3Y1
D	-20	SER	-	expression tag	UNP Q5L3Y1
D	-19	GLY	-	expression tag	UNP Q5L3Y1
D	-18	LEU	-	expression tag	UNP Q5L3Y1
D	-17	VAL	-	expression tag	UNP Q5L3Y1
D	-16	PRO	-	expression tag	UNP Q5L3Y1
D	-15	ARG	-	expression tag	UNP Q5L3Y1
D	-14	GLY	-	expression tag	UNP Q5L3Y1
D	-13	SER	-	expression tag	UNP Q5L3Y1
D	-12	GLY	-	expression tag	UNP Q5L3Y1
D	-11	THR	-	expression tag	UNP Q5L3Y1
D	-10	GLU	-	expression tag	UNP Q5L3Y1
D	-9	ASN	-	expression tag	UNP Q5L3Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	LEU	-	expression tag	UNP Q5L3Y1
D	-7	TYR	-	expression tag	UNP Q5L3Y1
D	-6	PHE	-	expression tag	UNP Q5L3Y1
D	-5	GLN	-	expression tag	UNP Q5L3Y1
D	-4	GLY	-	expression tag	UNP Q5L3Y1
D	-3	HIS	-	expression tag	UNP Q5L3Y1
D	-2	MET	-	expression tag	UNP Q5L3Y1
D	-1	ALA	-	expression tag	UNP Q5L3Y1
D	0	SER	-	expression tag	UNP Q5L3Y1
D	32	SER	PRO	conflict	UNP Q5L3Y1
D	169	ASN	HIS	engineered mutation	UNP Q5L3Y1
F	-31	MET	-	initiating methionine	UNP Q5L3Y1
F	-30	GLY	-	expression tag	UNP Q5L3Y1
F	-29	SER	-	expression tag	UNP Q5L3Y1
F	-28	SER	-	expression tag	UNP Q5L3Y1
F	-27	HIS	-	expression tag	UNP Q5L3Y1
F	-26	HIS	-	expression tag	UNP Q5L3Y1
F	-25	HIS	-	expression tag	UNP Q5L3Y1
F	-24	HIS	-	expression tag	UNP Q5L3Y1
F	-23	HIS	-	expression tag	UNP Q5L3Y1
F	-22	HIS	-	expression tag	UNP Q5L3Y1
F	-21	SER	-	expression tag	UNP Q5L3Y1
F	-20	SER	-	expression tag	UNP Q5L3Y1
F	-19	GLY	-	expression tag	UNP Q5L3Y1
F	-18	LEU	-	expression tag	UNP Q5L3Y1
F	-17	VAL	-	expression tag	UNP Q5L3Y1
F	-16	PRO	-	expression tag	UNP Q5L3Y1
F	-15	ARG	-	expression tag	UNP Q5L3Y1
F	-14	GLY	-	expression tag	UNP Q5L3Y1
F	-13	SER	-	expression tag	UNP Q5L3Y1
F	-12	GLY	-	expression tag	UNP Q5L3Y1
F	-11	THR	-	expression tag	UNP Q5L3Y1
F	-10	GLU	-	expression tag	UNP Q5L3Y1
F	-9	ASN	-	expression tag	UNP Q5L3Y1
F	-8	LEU	-	expression tag	UNP Q5L3Y1
F	-7	TYR	-	expression tag	UNP Q5L3Y1
F	-6	PHE	-	expression tag	UNP Q5L3Y1
F	-5	GLN	-	expression tag	UNP Q5L3Y1
F	-4	GLY	-	expression tag	UNP Q5L3Y1
F	-3	HIS	-	expression tag	UNP Q5L3Y1
F	-2	MET	-	expression tag	UNP Q5L3Y1
F	-1	ALA	-	expression tag	UNP Q5L3Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP Q5L3Y1
F	32	SER	PRO	conflict	UNP Q5L3Y1
F	169	ASN	HIS	engineered mutation	UNP Q5L3Y1
H	-31	MET	-	initiating methionine	UNP Q5L3Y1
H	-30	GLY	-	expression tag	UNP Q5L3Y1
H	-29	SER	-	expression tag	UNP Q5L3Y1
H	-28	SER	-	expression tag	UNP Q5L3Y1
H	-27	HIS	-	expression tag	UNP Q5L3Y1
H	-26	HIS	-	expression tag	UNP Q5L3Y1
H	-25	HIS	-	expression tag	UNP Q5L3Y1
H	-24	HIS	-	expression tag	UNP Q5L3Y1
H	-23	HIS	-	expression tag	UNP Q5L3Y1
H	-22	HIS	-	expression tag	UNP Q5L3Y1
H	-21	SER	-	expression tag	UNP Q5L3Y1
H	-20	SER	-	expression tag	UNP Q5L3Y1
H	-19	GLY	-	expression tag	UNP Q5L3Y1
H	-18	LEU	-	expression tag	UNP Q5L3Y1
H	-17	VAL	-	expression tag	UNP Q5L3Y1
H	-16	PRO	-	expression tag	UNP Q5L3Y1
H	-15	ARG	-	expression tag	UNP Q5L3Y1
H	-14	GLY	-	expression tag	UNP Q5L3Y1
H	-13	SER	-	expression tag	UNP Q5L3Y1
H	-12	GLY	-	expression tag	UNP Q5L3Y1
H	-11	THR	-	expression tag	UNP Q5L3Y1
H	-10	GLU	-	expression tag	UNP Q5L3Y1
H	-9	ASN	-	expression tag	UNP Q5L3Y1
H	-8	LEU	-	expression tag	UNP Q5L3Y1
H	-7	TYR	-	expression tag	UNP Q5L3Y1
H	-6	PHE	-	expression tag	UNP Q5L3Y1
H	-5	GLN	-	expression tag	UNP Q5L3Y1
H	-4	GLY	-	expression tag	UNP Q5L3Y1
H	-3	HIS	-	expression tag	UNP Q5L3Y1
H	-2	MET	-	expression tag	UNP Q5L3Y1
H	-1	ALA	-	expression tag	UNP Q5L3Y1
H	0	SER	-	expression tag	UNP Q5L3Y1
H	32	SER	PRO	conflict	UNP Q5L3Y1
H	169	ASN	HIS	engineered mutation	UNP Q5L3Y1
J	-31	MET	-	initiating methionine	UNP Q5L3Y1
J	-30	GLY	-	expression tag	UNP Q5L3Y1
J	-29	SER	-	expression tag	UNP Q5L3Y1
J	-28	SER	-	expression tag	UNP Q5L3Y1
J	-27	HIS	-	expression tag	UNP Q5L3Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-26	HIS	-	expression tag	UNP Q5L3Y1
J	-25	HIS	-	expression tag	UNP Q5L3Y1
J	-24	HIS	-	expression tag	UNP Q5L3Y1
J	-23	HIS	-	expression tag	UNP Q5L3Y1
J	-22	HIS	-	expression tag	UNP Q5L3Y1
J	-21	SER	-	expression tag	UNP Q5L3Y1
J	-20	SER	-	expression tag	UNP Q5L3Y1
J	-19	GLY	-	expression tag	UNP Q5L3Y1
J	-18	LEU	-	expression tag	UNP Q5L3Y1
J	-17	VAL	-	expression tag	UNP Q5L3Y1
J	-16	PRO	-	expression tag	UNP Q5L3Y1
J	-15	ARG	-	expression tag	UNP Q5L3Y1
J	-14	GLY	-	expression tag	UNP Q5L3Y1
J	-13	SER	-	expression tag	UNP Q5L3Y1
J	-12	GLY	-	expression tag	UNP Q5L3Y1
J	-11	THR	-	expression tag	UNP Q5L3Y1
J	-10	GLU	-	expression tag	UNP Q5L3Y1
J	-9	ASN	-	expression tag	UNP Q5L3Y1
J	-8	LEU	-	expression tag	UNP Q5L3Y1
J	-7	TYR	-	expression tag	UNP Q5L3Y1
J	-6	PHE	-	expression tag	UNP Q5L3Y1
J	-5	GLN	-	expression tag	UNP Q5L3Y1
J	-4	GLY	-	expression tag	UNP Q5L3Y1
J	-3	HIS	-	expression tag	UNP Q5L3Y1
J	-2	MET	-	expression tag	UNP Q5L3Y1
J	-1	ALA	-	expression tag	UNP Q5L3Y1
J	0	SER	-	expression tag	UNP Q5L3Y1
J	32	SER	PRO	conflict	UNP Q5L3Y1
J	169	ASN	HIS	engineered mutation	UNP Q5L3Y1
L	-31	MET	-	initiating methionine	UNP Q5L3Y1
L	-30	GLY	-	expression tag	UNP Q5L3Y1
L	-29	SER	-	expression tag	UNP Q5L3Y1
L	-28	SER	-	expression tag	UNP Q5L3Y1
L	-27	HIS	-	expression tag	UNP Q5L3Y1
L	-26	HIS	-	expression tag	UNP Q5L3Y1
L	-25	HIS	-	expression tag	UNP Q5L3Y1
L	-24	HIS	-	expression tag	UNP Q5L3Y1
L	-23	HIS	-	expression tag	UNP Q5L3Y1
L	-22	HIS	-	expression tag	UNP Q5L3Y1
L	-21	SER	-	expression tag	UNP Q5L3Y1
L	-20	SER	-	expression tag	UNP Q5L3Y1
L	-19	GLY	-	expression tag	UNP Q5L3Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-18	LEU	-	expression tag	UNP Q5L3Y1
L	-17	VAL	-	expression tag	UNP Q5L3Y1
L	-16	PRO	-	expression tag	UNP Q5L3Y1
L	-15	ARG	-	expression tag	UNP Q5L3Y1
L	-14	GLY	-	expression tag	UNP Q5L3Y1
L	-13	SER	-	expression tag	UNP Q5L3Y1
L	-12	GLY	-	expression tag	UNP Q5L3Y1
L	-11	THR	-	expression tag	UNP Q5L3Y1
L	-10	GLU	-	expression tag	UNP Q5L3Y1
L	-9	ASN	-	expression tag	UNP Q5L3Y1
L	-8	LEU	-	expression tag	UNP Q5L3Y1
L	-7	TYR	-	expression tag	UNP Q5L3Y1
L	-6	PHE	-	expression tag	UNP Q5L3Y1
L	-5	GLN	-	expression tag	UNP Q5L3Y1
L	-4	GLY	-	expression tag	UNP Q5L3Y1
L	-3	HIS	-	expression tag	UNP Q5L3Y1
L	-2	MET	-	expression tag	UNP Q5L3Y1
L	-1	ALA	-	expression tag	UNP Q5L3Y1
L	0	SER	-	expression tag	UNP Q5L3Y1
L	32	SER	PRO	conflict	UNP Q5L3Y1
L	169	ASN	HIS	engineered mutation	UNP Q5L3Y1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	C	23	Total O 23 23	0	0
3	E	36	Total O 36 36	0	0
3	G	34	Total O 34 34	0	0
3	I	29	Total O 29 29	0	0
3	K	43	Total O 43 43	0	0
3	B	19	Total O 19 19	0	0
3	D	18	Total O 18 18	0	0
3	F	8	Total O 8 8	0	0

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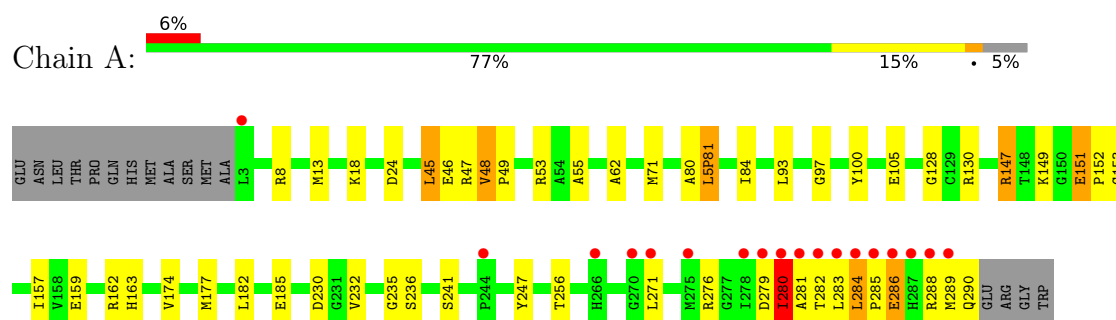
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	9	Total 9	O 9	0	0
3	J	10	Total 10	O 10	0	0
3	L	11	Total 11	O 11	0	0

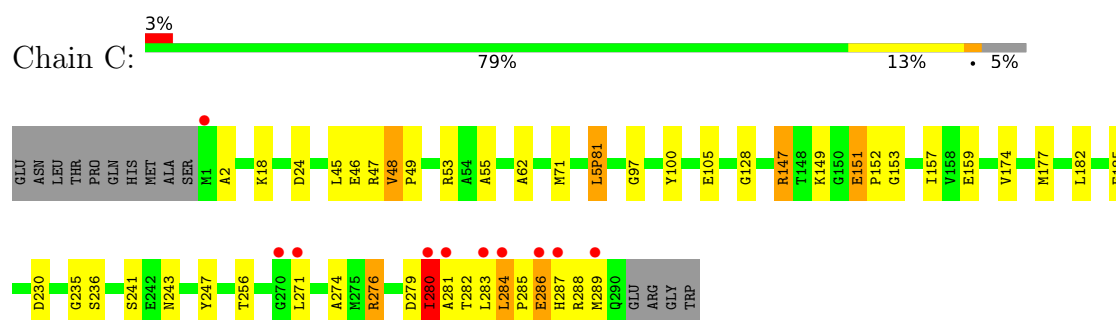
3 Residue-property plots [i](#)

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.

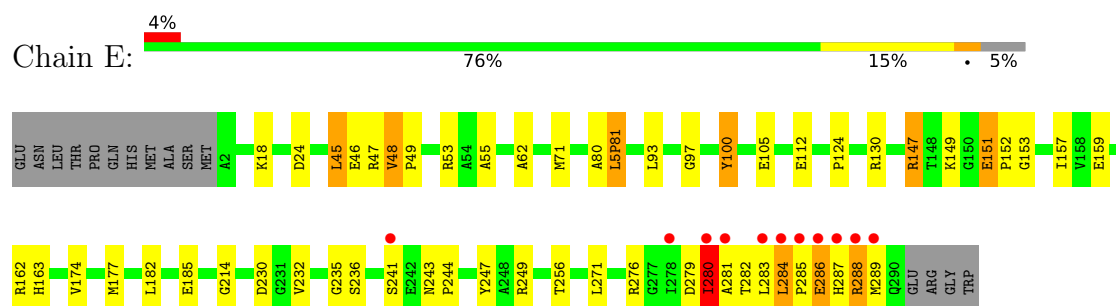
• Molecule 1: Pyridoxal biosynthesis lyase PdxS



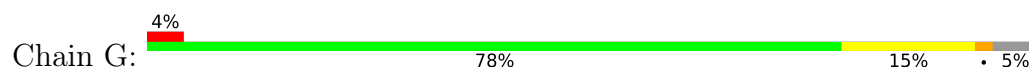
• Molecule 1: Pyridoxal biosynthesis lyase PdxS



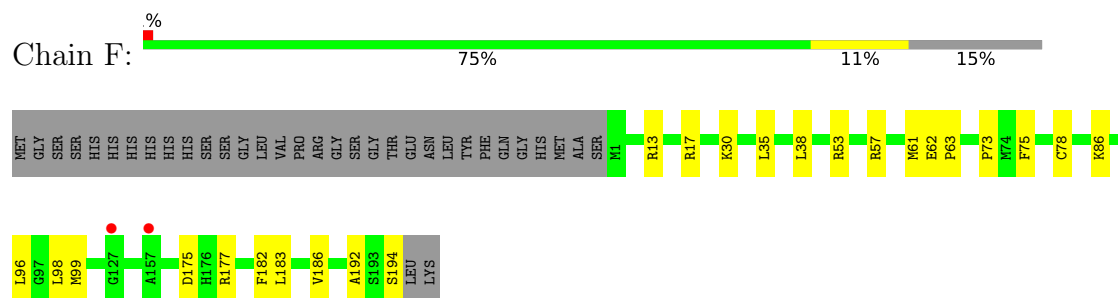
• Molecule 1: Pyridoxal biosynthesis lyase PdxS



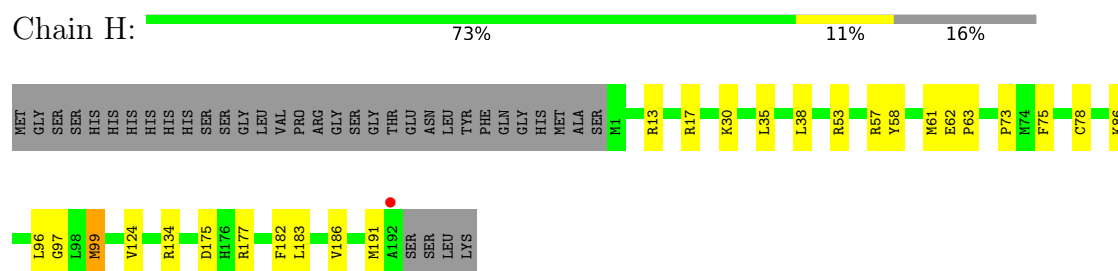
• Molecule 1: Pyridoxal biosynthesis lyase PdxS



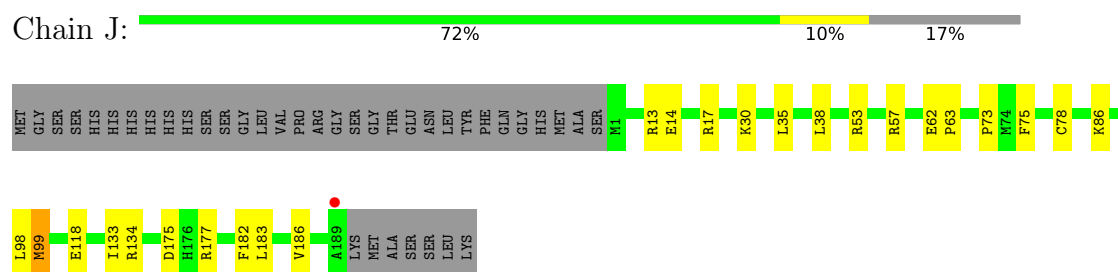
- Molecule 2: Glutamine amidotransferase subunit PdxT



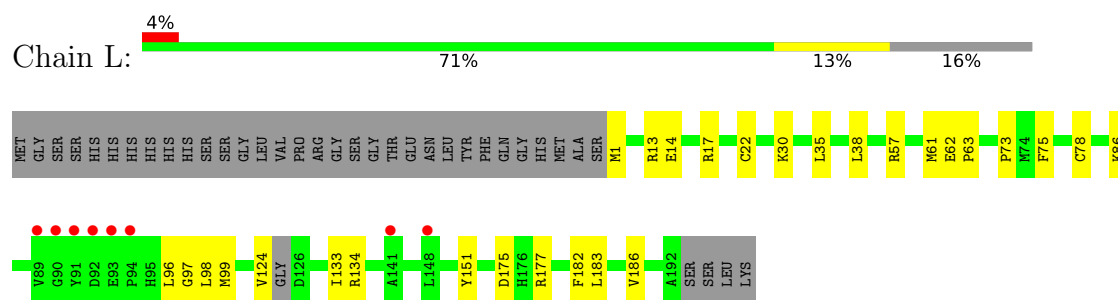
- Molecule 2: Glutamine amidotransferase subunit PdxT



- Molecule 2: Glutamine amidotransferase subunit PdxT



- Molecule 2: Glutamine amidotransferase subunit PdxT



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	141.02Å 249.14Å 179.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.70) 98.5 (50.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.257 0.209 , 0.256	Depositor DCC
R_{free} test set	4334 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22167	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: L5P, CYG

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	0.86	0/2181	0.97	0/2943
1	C	0.85	0/2194	0.97	0/2960
1	E	0.88	0/2186	0.97	0/2950
1	G	0.88	0/2194	0.94	0/2960
1	I	0.90	0/2181	0.98	0/2943
1	K	0.88	0/2194	0.96	0/2960
2	B	0.74	0/1453	0.90	0/1951
2	D	0.70	0/1480	0.87	0/1987
2	F	0.64	0/1492	0.86	0/2003
2	H	0.64	0/1480	0.87	0/1987
2	J	0.71	0/1458	0.91	0/1959
2	L	0.70	0/1475	0.88	0/1979
All	All	0.81	0/21968	0.93	0/29582

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	2176	0	2208	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2189	0	2224	31	0
1	E	2181	0	2213	45	2
1	G	2189	0	2224	39	2
1	I	2176	0	2207	35	0
1	K	2189	0	2224	36	0
2	B	1448	0	1462	18	0
2	D	1474	0	1493	14	2
2	F	1486	0	1503	11	0
2	H	1474	0	1493	20	0
2	J	1452	0	1466	11	2
2	L	1470	0	1489	17	0
3	A	23	0	0	2	0
3	B	19	0	0	3	0
3	C	23	0	0	3	0
3	D	18	0	0	1	1
3	E	36	0	0	9	0
3	F	8	0	0	0	0
3	G	34	0	0	3	0
3	H	9	0	0	4	0
3	I	29	0	0	6	1
3	J	10	0	0	1	0
3	K	43	0	0	2	0
3	L	11	0	0	2	0
All	All	22167	0	22206	290	5

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 7.

The worst 5 of 290 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ARG:NH1	1:E:152:PRO:O	1.80	1.13
1:C:53:ARG:NH1	1:C:152:PRO:O	1.84	1.11
1:A:53:ARG:NH1	1:A:152:PRO:O	1.90	1.04
1:K:53:ARG:NH1	1:K:152:PRO:O	1.90	1.04
1:G:53:ARG:NH1	1:G:152:PRO:O	1.92	1.02

All (5) 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)
1:E:243:ASN:ND2	1:G:29:GLU:OE1[6_554]	1.16	1.04
2:D:153:ASP:OD2	2:J:118:GLU:O[7_545]	1.78	0.42
1:E:243:ASN:ND2	1:G:29:GLU:CD[6_554]	1.92	0.28
3:I:301:HOH:O	3:D:203:HOH:O[7_555]	2.00	0.20
2:D:153:ASP:CG	2:J:118:GLU:O[7_545]	2.19	0.01

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	284/304 (93%)	276 (97%)	6 (2%)	2 (1%)	18	41
1	C	286/304 (94%)	277 (97%)	7 (2%)	2 (1%)	18	41
1	E	285/304 (94%)	277 (97%)	6 (2%)	2 (1%)	18	41
1	G	286/304 (94%)	276 (96%)	8 (3%)	2 (1%)	18	41
1	I	284/304 (93%)	276 (97%)	6 (2%)	2 (1%)	18	41
1	K	286/304 (94%)	279 (98%)	5 (2%)	2 (1%)	18	41
2	B	183/228 (80%)	174 (95%)	9 (5%)	0	100	100
2	D	189/228 (83%)	181 (96%)	7 (4%)	1 (0%)	24	48
2	F	191/228 (84%)	180 (94%)	11 (6%)	0	100	100
2	H	189/228 (83%)	179 (95%)	9 (5%)	1 (0%)	24	48
2	J	186/228 (82%)	178 (96%)	8 (4%)	0	100	100
2	L	186/228 (82%)	176 (95%)	10 (5%)	0	100	100
All	All	2835/3192 (89%)	2729 (96%)	92 (3%)	14 (0%)	24	48

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ILE
1	C	280	ILE
1	E	280	ILE

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Mol	Chain	Res	Type
1	G	280	ILE
1	I	280	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/233 (94%)	206 (94%)	14 (6%)	16	38
1	C	221/233 (95%)	208 (94%)	13 (6%)	18	42
1	E	220/233 (94%)	206 (94%)	14 (6%)	16	38
1	G	221/233 (95%)	208 (94%)	13 (6%)	18	42
1	I	220/233 (94%)	206 (94%)	14 (6%)	16	38
1	K	221/233 (95%)	207 (94%)	14 (6%)	16	39
2	B	148/180 (82%)	145 (98%)	3 (2%)	48	76
2	D	150/180 (83%)	147 (98%)	3 (2%)	48	76
2	F	152/180 (84%)	149 (98%)	3 (2%)	48	76
2	H	150/180 (83%)	147 (98%)	3 (2%)	48	76
2	J	148/180 (82%)	144 (97%)	4 (3%)	39	69
2	L	150/180 (83%)	147 (98%)	3 (2%)	48	76
All	All	2221/2478 (90%)	2120 (96%)	101 (4%)	24	52

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	147	ARG
1	K	147	ARG
2	L	98	LEU
1	I	157	ILE
1	I	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	290	GLN
2	J	66	GLN
2	L	66	GLN
2	J	106	ASN
1	E	290	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CYG	D	78	2	12,14,15	1.04	0	10,17,19	5.38	6 (60%)
2	CYG	F	78	2	12,14,15	1.26	2 (16%)	10,17,19	4.97	5 (50%)
1	L5P	K	81	1	20,21,22	1.16	2 (10%)	16,27,29	1.60	4 (25%)
2	CYG	J	78	2	12,14,15	0.84	0	10,17,19	5.83	6 (60%)
1	L5P	I	81	1	20,21,22	0.98	0	16,27,29	1.53	6 (37%)
1	L5P	C	81	1	20,21,22	1.02	1 (5%)	16,27,29	1.62	5 (31%)
1	L5P	A	81	1	20,21,22	1.01	1 (5%)	16,27,29	1.51	4 (25%)
1	L5P	E	81	1	20,21,22	1.16	2 (10%)	16,27,29	1.66	4 (25%)
1	L5P	G	81	1	20,21,22	1.09	1 (5%)	16,27,29	1.60	5 (31%)
2	CYG	H	78	2	12,14,15	1.22	2 (16%)	10,17,19	4.95	4 (40%)
2	CYG	L	78	2	12,14,15	1.22	1 (8%)	10,17,19	4.95	6 (60%)
2	CYG	B	78	2	12,14,15	1.02	1 (8%)	10,17,19	4.95	5 (50%)

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
2	CYG	D	78	2	-	4/14/16/18	-
2	CYG	F	78	2	-	2/14/16/18	-
1	L5P	K	81	1	-	6/23/25/27	-
2	CYG	J	78	2	-	3/14/16/18	-
1	L5P	I	81	1	-	6/23/25/27	-
1	L5P	C	81	1	-	7/23/25/27	-
1	L5P	A	81	1	-	5/23/25/27	-
1	L5P	E	81	1	-	5/23/25/27	-
1	L5P	G	81	1	-	5/23/25/27	-
2	CYG	H	78	2	-	1/14/16/18	-
2	CYG	L	78	2	-	2/14/16/18	-
2	CYG	B	78	2	-	4/14/16/18	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	81	L5P	C6-C5	-3.10	1.49	1.53
1	E	81	L5P	C6-C5	-2.61	1.49	1.53
2	H	78	CYG	CB-SG	-2.60	1.75	1.81
1	K	81	L5P	P9-O10	-2.51	1.45	1.54
2	H	78	CYG	CG1-CD1	2.47	1.53	1.50

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	78	CYG	OE2-CD1-CG1	-13.27	108.67	123.98
2	D	78	CYG	OE2-CD1-CG1	-11.82	110.34	123.98
2	L	78	CYG	OE2-CD1-CG1	-11.28	110.97	123.98
2	F	78	CYG	OE2-CD1-CG1	-11.15	111.12	123.98
2	B	78	CYG	OE2-CD1-CG1	-10.02	112.42	123.98

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	81	L5P	O-C1-CA-CB
1	A	81	L5P	C3-C2-NZ-CE
1	C	81	L5P	O-C1-CA-CB

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Mol	Chain	Res	Type	Atoms
1	C	81	L5P	C3-C2-NZ-CE
1	C	81	L5P	C7-O8-P9-O12

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	K	81	L5P	2	0
1	I	81	L5P	2	0
1	C	81	L5P	2	0
1	A	81	L5P	4	0
1	E	81	L5P	9	0
1	G	81	L5P	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	287/304 (94%)	0.10	18 (6%)	26 23	32, 45, 113, 150	0
1	C	289/304 (95%)	0.10	10 (3%)	47 43	35, 47, 106, 130	0
1	E	288/304 (94%)	0.11	11 (3%)	44 40	31, 46, 100, 130	0
1	G	289/304 (95%)	0.07	11 (3%)	44 40	28, 45, 102, 137	0
1	I	287/304 (94%)	0.12	18 (6%)	26 23	29, 44, 112, 152	0
1	K	289/304 (95%)	0.03	12 (4%)	40 37	31, 43, 99, 147	0
2	B	187/228 (82%)	0.31	1 (0%)	87 86	40, 59, 85, 111	0
2	D	191/228 (83%)	0.17	1 (0%)	87 86	40, 63, 89, 121	0
2	F	193/228 (84%)	0.41	2 (1%)	79 78	42, 72, 104, 124	0
2	H	191/228 (83%)	0.29	1 (0%)	87 86	40, 71, 100, 117	0
2	J	188/228 (82%)	0.27	1 (0%)	87 86	37, 61, 84, 103	0
2	L	190/228 (83%)	0.36	8 (4%)	40 37	34, 66, 99, 134	0
All	All	2869/3192 (89%)	0.17	94 (3%)	49 45	28, 54, 101, 152	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	289	MET	4.7
1	A	280	ILE	4.3
1	E	283	LEU	4.2
1	K	289	MET	4.1
1	I	289	MET	4.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CYG	B	78	15/16	0.82	0.15	50,56,66,81	0
2	CYG	L	78	15/16	0.84	0.13	44,51,56,58	0
2	CYG	F	78	15/16	0.85	0.12	48,63,69,80	0
2	CYG	J	78	15/16	0.85	0.12	45,50,66,67	0
2	CYG	D	78	15/16	0.85	0.13	45,50,56,60	0
1	L5P	E	81	22/23	0.89	0.16	40,73,95,111	0
2	CYG	H	78	15/16	0.89	0.10	42,54,64,65	0
1	L5P	C	81	22/23	0.90	0.14	39,68,87,96	0
1	L5P	A	81	22/23	0.91	0.15	41,69,101,110	0
1	L5P	G	81	22/23	0.92	0.13	33,63,78,102	0
1	L5P	I	81	22/23	0.92	0.13	33,64,105,117	0
1	L5P	K	81	22/23	0.92	0.14	40,62,89,103	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.