



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:11 PM GMT

PDB ID : 4WXY
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

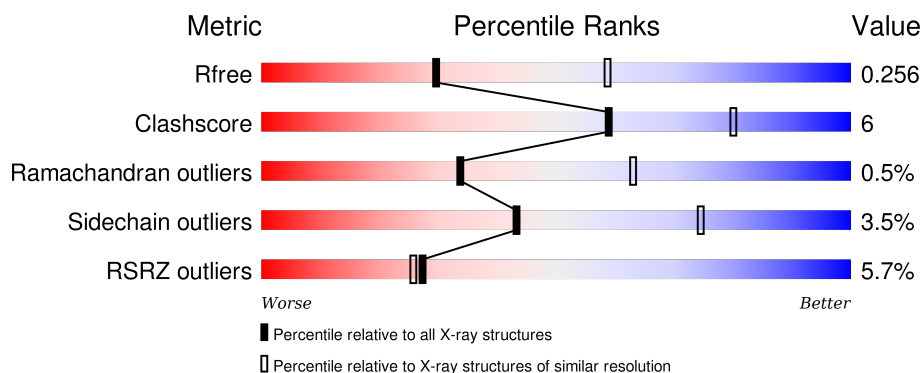
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	C	304	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	E	304	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	G	304	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	I	304	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 5%</div> </div> </div>

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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

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

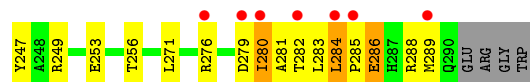
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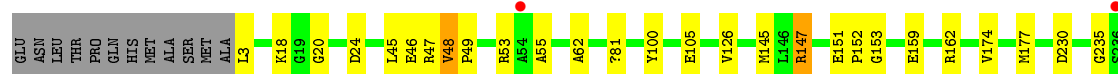
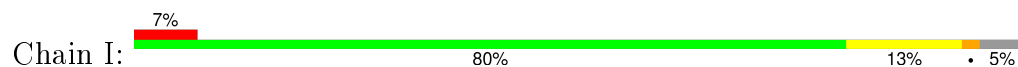
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	9	Total 9	O 9	0	0
3	J	10	Total 10	O 10	0	0
3	L	11	Total 11	O 11	0	0

- Molecule 1: Pyridoxal biosynthesis lyase PdxS

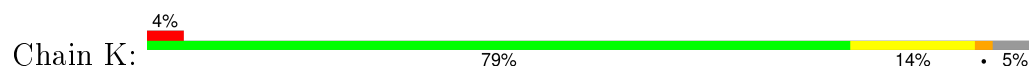




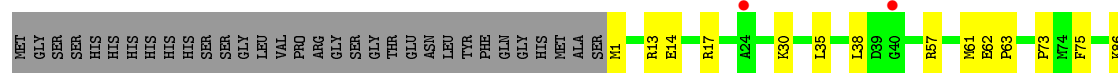
- Molecule 1: Pyridoxal biosynthesis lyase PdxS



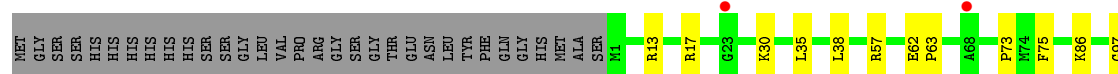
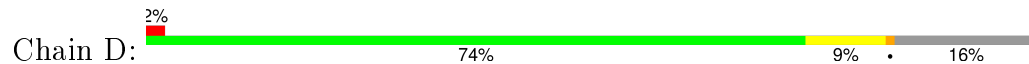
- Molecule 1: Pyridoxal biosynthesis lyase PdxS



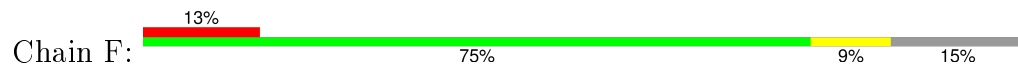
- Molecule 2: Glutamine amidotransferase subunit PdxT

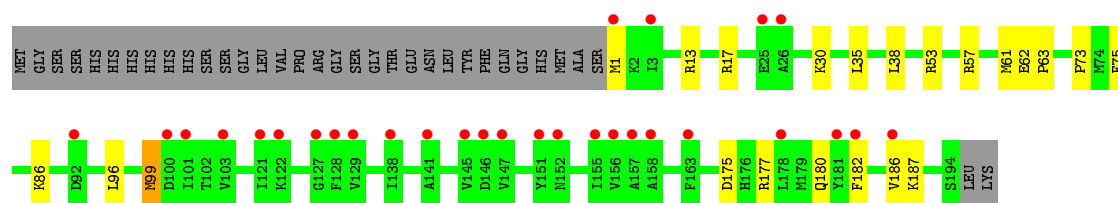


- Molecule 2: Glutamine amidotransferase subunit PdxT

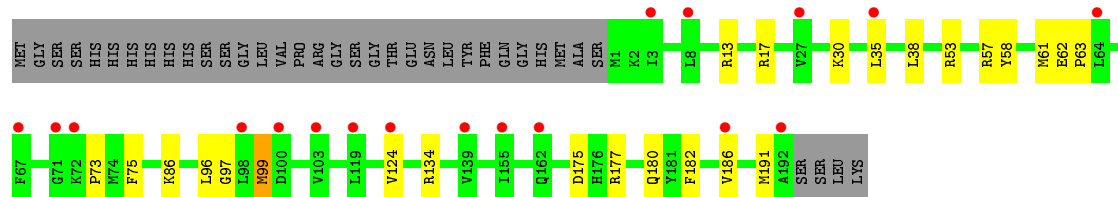
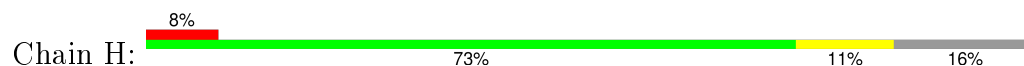


- Molecule 2: Glutamine amidotransferase subunit PdxT

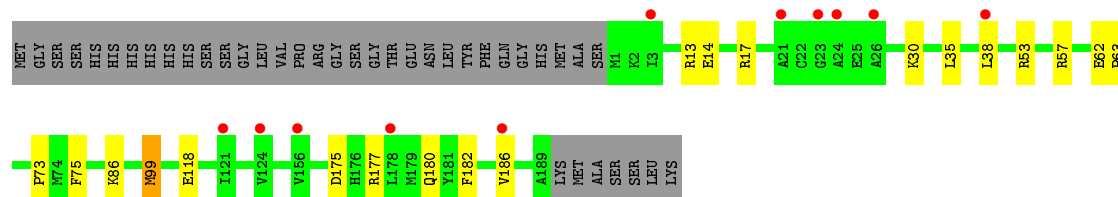
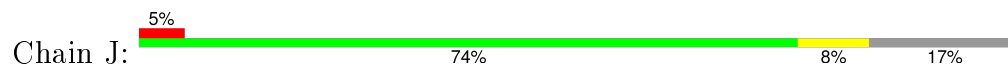




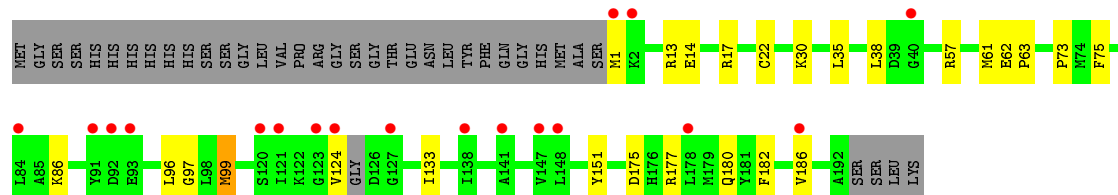
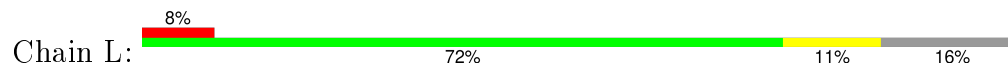
• Molecule 2: Glutamine amidotransferase subunit PdxT



• 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 46.19 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.70) 98.3 (46.19-2.69)	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	Depositor
R, R_{free}	0.209 , 0.257 0.209 , 0.256	Depositor DCC
R_{free} test set	4307 reflections (5.30%)	DCC
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 , 46.5	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 86273 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.62	0/2181	0.75	0/2943
1	C	0.62	0/2194	0.76	0/2960
1	E	0.63	0/2186	0.74	0/2950
1	G	0.63	0/2194	0.75	0/2960
1	I	0.66	0/2181	0.76	0/2943
1	K	0.64	0/2194	0.76	0/2960
2	B	0.54	0/1453	0.67	0/1951
2	D	0.52	0/1480	0.65	0/1987
2	F	0.48	0/1492	0.64	0/2003
2	H	0.47	0/1480	0.67	0/1987
2	J	0.52	0/1458	0.67	0/1959
2	L	0.52	0/1475	0.67	0/1979
All	All	0.59	0/21968	0.72	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

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	2207	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2189	0	2224	26	0
1	E	2181	0	2213	40	2
1	G	2189	0	2224	33	2
1	I	2176	0	2207	30	0
1	K	2189	0	2224	30	0
2	B	1448	0	1462	17	0
2	D	1474	0	1493	13	2
2	F	1486	0	1503	11	0
2	H	1474	0	1493	20	0
2	J	1452	0	1466	10	2
2	L	1470	0	1489	16	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	22205	255	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 6.

All (255) 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:K:53:ARG:NH1	1:K:152:PRO:O	1.90	1.04
1:A:53:ARG:NH1	1:A:152:PRO:O	1.90	1.04
1:G:53:ARG:NH1	1:G:152:PRO:O	1.92	1.02
1:I:53:ARG:NH1	1:I:152:PRO:O	1.92	1.01
1:A:256:THR:O	2:B:30:LYS:NZ	1.95	0.98
1:K:256:THR:O	2:L:30:LYS:NZ	2.02	0.92
1:E:287:HIS:HA	3:E:323:HOH:O	1.69	0.92
1:C:243:ASN:HB2	3:C:311:HOH:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3:LEU:CD2	3:I:301:HOH:O	2.19	0.91
1:G:284:LEU:HD12	3:G:334:HOH:O	1.72	0.89
1:E:287:HIS:CB	3:E:323:HOH:O	2.22	0.87
1:I:3:LEU:HG	3:I:301:HOH:O	1.77	0.85
1:G:256:THR:O	2:H:30:LYS:NZ	2.08	0.85
2:D:175:ASP:OD2	2:D:177:ARG:NH2	2.10	0.84
1:E:81:L5P:H12	3:E:307:HOH:O	1.77	0.82
1:I:3:LEU:HD23	3:I:301:HOH:O	1.78	0.82
2:J:175:ASP:OD2	2:J:177:ARG:NH2	2.14	0.81
2:B:175:ASP:OD2	2:B:177:ARG:NH2	2.18	0.76
1:C:279:ASP:O	1:C:280:ILE:HG23	1.85	0.76
1:E:81:L5P:O10	1:E:152:PRO:HA	1.84	0.76
1:A:81:L5P:O10	1:A:153:GLY:N	2.19	0.75
1:E:279:ASP:O	1:E:280:ILE:HG23	1.86	0.75
1:I:256:THR:O	2:J:30:LYS:NZ	2.21	0.74
2:H:175:ASP:OD2	2:H:177:ARG:NH2	2.21	0.74
1:E:287:HIS:HB3	3:E:323:HOH:O	1.87	0.73
1:I:279:ASP:O	1:I:280:ILE:HG23	1.86	0.73
2:L:1:MET:N	3:L:204:HOH:O	2.21	0.73
1:E:287:HIS:CA	3:E:323:HOH:O	2.27	0.72
2:L:175:ASP:OD2	2:L:177:ARG:NH2	2.23	0.72
1:K:279:ASP:O	1:K:280:ILE:HG23	1.88	0.72
1:A:279:ASP:O	1:A:280:ILE:HG23	1.90	0.71
1:G:279:ASP:O	1:G:280:ILE:HG23	1.90	0.71
1:E:256:THR:O	2:F:30:LYS:NZ	2.25	0.70
1:G:284:LEU:CD1	3:G:334:HOH:O	2.36	0.69
1:G:249:ARG:HD2	2:H:53:ARG:NH2	2.07	0.69
1:E:288:ARG:NH2	3:E:313:HOH:O	2.11	0.68
1:C:152:PRO:HD2	1:C:286:GLU:HG2	1.76	0.68
1:E:81:L5P:O10	1:E:153:GLY:N	2.26	0.68
1:A:18:LYS:NZ	2:B:14:GLU:OE1	2.27	0.68
2:L:22:CYS:SG	3:L:211:HOH:O	2.51	0.67
1:I:152:PRO:HD2	1:I:286:GLU:HG2	1.77	0.67
1:C:81:L5P:O12	1:C:236:SER:N	2.24	0.66
1:K:198:GLU:HG2	3:K:308:HOH:O	1.94	0.66
1:E:152:PRO:HD2	1:E:286:GLU:HG2	1.76	0.65
1:I:3:LEU:CG	3:I:301:HOH:O	2.30	0.65
1:A:81:L5P:O11	1:A:236:SER:N	2.30	0.63
1:G:152:PRO:HD2	1:G:286:GLU:HG2	1.80	0.62
1:C:256:THR:O	2:D:30:LYS:NZ	2.32	0.62
2:F:175:ASP:OD2	2:F:177:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2:ALA:HB2	2:L:151:TYR:OH	2.00	0.62
1:K:152:PRO:HD2	1:K:286:GLU:HG2	1.81	0.62
2:B:140:GLU:HG2	3:B:204:HOH:O	1.99	0.61
2:H:61:MET:CB	3:H:201:HOH:O	2.50	0.59
1:E:81:L5P:O12	1:E:214:GLY:N	2.29	0.59
1:C:81:L5P:O10	1:C:153:GLY:N	2.35	0.58
1:C:287:HIS:HB2	3:C:313:HOH:O	2.02	0.58
2:H:13:ARG:HD3	2:H:17:ARG:HH12	1.69	0.58
2:B:1:MET:N	3:B:201:HOH:O	2.36	0.58
1:K:149:LYS:HZ1	1:K:289:MET:HB2	1.69	0.57
1:I:3:LEU:N	3:I:301:HOH:O	2.36	0.57
1:G:81:L5P:H23	1:G:152:PRO:HB3	1.86	0.57
1:G:81:L5P:O12	1:G:236:SER:N	2.38	0.57
1:A:152:PRO:HD2	1:A:286:GLU:HG2	1.87	0.56
1:I:81:L5P:O10	1:I:153:GLY:N	2.37	0.56
1:E:81:L5P:C2	3:E:307:HOH:O	2.51	0.56
2:B:171:GLU:OE2	3:B:213:HOH:O	2.18	0.56
2:L:13:ARG:HD3	2:L:17:ARG:HH12	1.69	0.56
1:E:174:VAL:HG22	1:E:177:MET:HE1	1.87	0.55
1:K:18:LYS:NZ	2:L:14:GLU:OE1	2.38	0.55
1:G:241:SER:HB2	1:G:247:TYR:CE2	2.42	0.55
1:C:276:ARG:NH1	3:C:323:HOH:O	2.37	0.55
2:D:191:MET:O	2:D:192:ALA:C	2.44	0.55
2:L:86:LYS:HB2	2:L:99:MET:O	2.07	0.54
2:J:13:ARG:HD3	2:J:17:ARG:HH12	1.72	0.54
2:F:13:ARG:HD3	2:F:17:ARG:HH12	1.73	0.54
1:G:249:ARG:HD2	2:H:53:ARG:HH21	1.71	0.54
2:B:13:ARG:HD3	2:B:17:ARG:HH12	1.71	0.54
1:K:81:L5P:O12	1:K:236:SER:N	2.33	0.54
2:D:13:ARG:HD3	2:D:17:ARG:HH12	1.71	0.54
2:H:61:MET:HB3	3:H:201:HOH:O	2.07	0.53
2:D:86:LYS:HB2	2:D:99:MET:O	2.09	0.53
1:A:290:GLN:HG3	3:A:318:HOH:O	2.09	0.53
1:E:81:L5P:H16	3:E:307:HOH:O	2.09	0.53
1:C:241:SER:HB2	1:C:247:TYR:CE2	2.44	0.52
1:G:249:ARG:CD	2:H:53:ARG:NH2	2.73	0.52
1:A:105:GLU:OE2	1:A:147:ARG:NH2	2.42	0.52
2:J:86:LYS:HB2	2:J:99:MET:O	2.10	0.51
1:E:149:LYS:NZ	1:E:289:MET:HB2	2.26	0.51
2:B:86:LYS:HB2	2:B:99:MET:O	2.10	0.51
1:K:241:SER:HB2	1:K:247:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:159:GLU:OE1	1:K:162:ARG:NH1	2.43	0.51
1:E:151:GLU:OE1	1:E:286:GLU:HB2	2.11	0.51
1:A:162:ARG:NH2	1:E:112:GLU:OE1	2.33	0.51
1:E:241:SER:HB2	1:E:247:TYR:CE2	2.46	0.51
2:H:61:MET:HB2	3:H:201:HOH:O	2.11	0.50
1:G:151:GLU:OE1	1:G:286:GLU:HB2	2.10	0.50
1:C:284:LEU:H	1:C:285:PRO:CD	2.24	0.50
2:H:75:PHE:HB2	2:H:182:PHE:CE1	2.47	0.50
1:A:241:SER:HB2	1:A:247:TYR:CE2	2.46	0.50
1:I:81:L5P:O10	1:I:152:PRO:HA	2.11	0.50
2:F:62:GLU:HB3	2:F:63:PRO:HD3	1.94	0.50
2:J:62:GLU:HB3	2:J:63:PRO:HD3	1.94	0.50
2:F:86:LYS:HB2	2:F:99:MET:O	2.12	0.50
1:K:1:MET:HA	3:K:303:HOH:O	2.11	0.50
2:H:62:GLU:HB3	2:H:63:PRO:HD3	1.94	0.49
1:G:112:GLU:OE1	1:K:162:ARG:NH2	2.36	0.49
1:A:284:LEU:H	1:A:285:PRO:CD	2.25	0.49
1:I:241:SER:HB2	1:I:247:TYR:CE2	2.47	0.49
2:H:73:PRO:HG2	2:H:186:VAL:HA	1.95	0.49
1:K:24:ASP:HB2	1:K:235:GLY:HA2	1.94	0.49
1:E:284:LEU:H	1:E:285:PRO:CD	2.25	0.49
1:K:280:ILE:HD12	1:K:281:ALA:N	2.28	0.49
1:C:247:TYR:OH	1:C:274:ALA:HB2	2.13	0.49
1:I:20:GLY:HA2	3:I:324:HOH:O	2.12	0.49
1:K:174:VAL:HG22	1:K:177:MET:HE1	1.95	0.49
2:D:73:PRO:HG2	2:D:186:VAL:HA	1.93	0.49
1:I:284:LEU:H	1:I:285:PRO:CD	2.26	0.49
1:I:280:ILE:HD12	1:I:281:ALA:N	2.28	0.49
1:G:149:LYS:HZ1	1:G:289:MET:HB2	1.78	0.49
1:C:24:ASP:HB2	1:C:235:GLY:HA2	1.95	0.48
1:C:151:GLU:HG2	1:C:159:GLU:HG3	1.95	0.48
1:A:174:VAL:HG22	1:A:177:MET:HE1	1.95	0.48
2:D:62:GLU:HB3	2:D:63:PRO:HD3	1.93	0.48
1:G:46:GLU:HA	3:G:321:HOH:O	2.14	0.48
2:J:73:PRO:HG2	2:J:186:VAL:HA	1.95	0.48
1:I:174:VAL:HG22	1:I:177:MET:HE1	1.96	0.48
1:K:46:GLU:HG2	1:K:62:ALA:HA	1.96	0.48
1:K:284:LEU:H	1:K:285:PRO:CD	2.26	0.48
1:E:100:TYR:CZ	1:E:124:PRO:HB2	2.49	0.48
1:G:284:LEU:H	1:G:285:PRO:CD	2.26	0.48
2:L:73:PRO:HG2	2:L:186:VAL:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:HIS:CG	3:E:323:HOH:O	2.62	0.47
2:L:62:GLU:HB3	2:L:63:PRO:HD3	1.97	0.47
1:I:18:LYS:NZ	2:J:14:GLU:OE1	2.44	0.47
2:F:73:PRO:HG2	2:F:186:VAL:HA	1.95	0.47
1:K:18:LYS:HG2	1:K:230:ASP:HB3	1.96	0.47
1:G:81:L5P:O10	1:G:153:GLY:N	2.42	0.47
1:E:151:GLU:HG2	1:E:159:GLU:HG3	1.95	0.47
2:B:73:PRO:HG2	2:B:186:VAL:HA	1.95	0.47
1:C:280:ILE:HD12	1:C:281:ALA:N	2.28	0.47
1:E:280:ILE:HD12	1:E:281:ALA:N	2.30	0.47
1:A:159:GLU:OE1	1:A:162:ARG:NH1	2.47	0.47
1:A:280:ILE:HD12	1:A:281:ALA:N	2.30	0.47
2:B:62:GLU:HB3	2:B:63:PRO:HD3	1.96	0.47
2:H:86:LYS:HB2	2:H:99:MET:O	2.14	0.46
1:G:151:GLU:HG2	1:G:159:GLU:HG3	1.97	0.46
1:K:81:L5P:O10	1:K:153:GLY:N	2.45	0.46
1:G:80:ALA:HB3	1:G:93:LEU:HD13	1.98	0.46
2:F:75:PHE:HB2	2:F:182:PHE:CE1	2.51	0.46
1:G:174:VAL:HG22	1:G:177:MET:HE1	1.96	0.46
1:I:159:GLU:OE2	1:I:162:ARG:NH1	2.48	0.46
1:I:24:ASP:HB2	1:I:235:GLY:HA2	1.97	0.46
1:G:149:LYS:NZ	1:G:289:MET:HB2	2.31	0.46
1:C:149:LYS:HZ1	1:C:289:MET:HB2	1.81	0.46
2:B:61:MET:SD	2:B:96:LEU:HD23	2.55	0.46
1:C:174:VAL:HG22	1:C:177:MET:HE1	1.97	0.46
1:K:105:GLU:OE2	1:K:147:ARG:NH2	2.48	0.46
1:K:102:ASP:OD1	1:K:147:ARG:NH1	2.49	0.46
1:G:280:ILE:HD12	1:G:281:ALA:N	2.31	0.45
1:A:84:ILE:HD11	1:A:289:MET:HG2	1.99	0.45
1:K:13:MET:HA	2:L:133:ILE:HG21	1.99	0.45
1:A:45:LEU:HD23	1:A:81:L5P:H10	1.99	0.45
1:E:249:ARG:HD2	2:F:53:ARG:NH2	2.31	0.45
1:E:24:ASP:HB2	1:E:235:GLY:HA2	1.98	0.45
1:I:257:HIS:HD2	3:J:210:HOH:O	1.99	0.45
1:E:18:LYS:HG2	1:E:230:ASP:HB3	1.98	0.45
1:G:46:GLU:HG2	1:G:62:ALA:HA	1.97	0.45
2:L:35:LEU:HA	2:L:38:LEU:HD12	1.99	0.45
1:A:8:ARG:NH1	2:B:129:VAL:HG11	2.32	0.45
1:A:80:ALA:HB3	1:A:93:LEU:HD13	1.98	0.44
1:A:24:ASP:HB2	1:A:235:GLY:HA2	1.99	0.44
1:C:105:GLU:OE2	1:C:147:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:ARG:NH1	1:K:55:ALA:HB3	2.32	0.44
1:K:80:ALA:HB3	1:K:93:LEU:HD13	1.99	0.44
1:I:47:ARG:NH1	1:I:55:ALA:HB3	2.32	0.44
2:D:35:LEU:HA	2:D:38:LEU:HD12	1.98	0.44
1:A:48:VAL:HG22	1:A:49:PRO:HD2	2.00	0.44
1:E:159:GLU:OE1	1:E:162:ARG:NH1	2.51	0.44
1:I:151:GLU:OE1	1:I:286:GLU:HB2	2.17	0.43
2:D:75:PHE:HB2	2:D:182:PHE:CE1	2.53	0.43
2:F:35:LEU:HA	2:F:38:LEU:HD12	1.99	0.43
1:I:46:GLU:HG2	1:I:62:ALA:HA	1.98	0.43
1:K:159:GLU:OE2	1:K:162:ARG:NH1	2.50	0.43
1:I:105:GLU:OE2	1:I:147:ARG:NH2	2.51	0.43
1:K:151:GLU:OE1	1:K:286:GLU:HB2	2.18	0.43
1:I:151:GLU:HG2	1:I:159:GLU:HG3	1.99	0.43
1:I:48:VAL:HG22	1:I:49:PRO:HD2	2.00	0.43
1:A:151:GLU:HG2	1:A:159:GLU:HG3	2.00	0.43
1:A:18:LYS:HG2	1:A:230:ASP:HB3	2.01	0.43
2:H:35:LEU:HA	2:H:38:LEU:HD12	1.99	0.43
1:A:47:ARG:NH1	1:A:55:ALA:HB3	2.32	0.43
1:A:46:GLU:HG2	1:A:62:ALA:HA	2.00	0.43
1:E:100:TYR:CE1	1:E:124:PRO:HB2	2.54	0.43
1:G:48:VAL:HG22	1:G:49:PRO:HD2	2.00	0.43
1:E:80:ALA:HB3	1:E:93:LEU:HD13	2.01	0.43
2:J:35:LEU:HA	2:J:38:LEU:HD12	2.00	0.43
2:J:75:PHE:HB2	2:J:182:PHE:CE1	2.54	0.43
1:A:149:LYS:NZ	1:A:289:MET:HB2	2.33	0.43
1:G:128:GLY:HA2	1:G:147:ARG:O	2.18	0.43
2:B:35:LEU:HA	2:B:38:LEU:HD12	2.00	0.43
2:L:86:LYS:HA	2:L:97:GLY:HA2	2.01	0.42
1:A:130:ARG:HG2	1:A:163:HIS:CE1	2.54	0.42
1:E:81:L5P:O10	1:E:152:PRO:CA	2.60	0.42
2:H:61:MET:SD	2:H:96:LEU:HD23	2.60	0.42
1:C:46:GLU:HG2	1:C:62:ALA:HA	2.00	0.42
1:C:128:GLY:HA2	1:C:147:ARG:O	2.20	0.42
1:E:46:GLU:HG2	1:E:62:ALA:HA	2.01	0.42
2:L:124:VAL:CG1	2:L:177:ARG:HB3	2.50	0.42
1:A:13:MET:HA	2:B:133:ILE:HG21	2.01	0.42
1:A:151:GLU:OE1	1:A:286:GLU:HB2	2.19	0.42
2:D:175:ASP:OD2	2:D:177:ARG:CZ	2.68	0.42
1:E:105:GLU:OE2	1:E:147:ARG:NH2	2.53	0.42
1:K:48:VAL:HG22	1:K:49:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:124:VAL:CG1	2:H:177:ARG:HB3	2.49	0.42
1:A:128:GLY:HA2	1:A:147:ARG:O	2.19	0.42
1:C:48:VAL:HG22	1:C:49:PRO:HD2	2.01	0.42
2:B:75:PHE:HB2	2:B:182:PHE:CE1	2.55	0.42
1:E:81:L5P:O11	1:E:236:SER:HB2	2.20	0.41
1:K:247:TYR:CE1	1:K:271:LEU:HD12	2.54	0.41
1:I:247:TYR:OH	1:I:274:ALA:HB2	2.20	0.41
2:L:61:MET:SD	2:L:96:LEU:HD23	2.59	0.41
1:K:130:ARG:HG2	1:K:163:HIS:CE1	2.55	0.41
1:C:47:ARG:NH1	1:C:55:ALA:HB3	2.34	0.41
2:F:1:MET:HE1	2:F:187:LYS:N	2.35	0.41
1:G:24:ASP:HB2	1:G:235:GLY:HA2	2.02	0.41
1:E:45:LEU:HD23	1:E:81:L5P:H10	2.01	0.41
1:A:8:ARG:HD3	2:B:131:VAL:HG21	2.01	0.41
2:H:134:ARG:HD3	3:H:208:HOH:O	2.20	0.41
1:C:151:GLU:OE1	1:C:286:GLU:HB2	2.21	0.41
2:F:61:MET:SD	2:F:96:LEU:HD23	2.60	0.41
1:E:48:VAL:HG22	1:E:49:PRO:HD2	2.01	0.41
1:E:47:ARG:NH1	1:E:55:ALA:HB3	2.35	0.41
1:G:53:ARG:NH2	1:G:151:GLU:OE1	2.49	0.41
1:G:241:SER:HB2	1:G:247:TYR:CD2	2.54	0.41
1:G:47:ARG:NH1	1:G:55:ALA:HB3	2.34	0.41
1:G:36:ALA:O	2:H:53:ARG:HD3	2.21	0.41
1:I:18:LYS:HG2	1:I:230:ASP:HB3	2.02	0.41
1:A:8:ARG:HD3	2:B:131:VAL:CG2	2.51	0.41
1:E:130:ARG:HG2	1:E:163:HIS:CE1	2.56	0.41
1:I:126:VAL:HA	1:I:145:MET:O	2.21	0.41
1:A:81:L5P:P9	3:A:307:HOH:O	2.78	0.40
1:G:253:GLU:HG2	2:H:58:TYR:HE1	1.86	0.40
1:G:284:LEU:N	1:G:285:PRO:CD	2.85	0.40
2:H:86:LYS:HA	2:H:97:GLY:HA2	2.02	0.40
2:L:75:PHE:HB2	2:L:182:PHE:CE1	2.56	0.40
1:I:249:ARG:HD2	2:J:53:ARG:NH2	2.36	0.40
1:C:284:LEU:N	1:C:285:PRO:CD	2.84	0.40
1:C:18:LYS:HG2	1:C:230:ASP:HB3	2.02	0.40
1:A:238:ILE:O	1:A:241:SER:OG	2.35	0.40
1:C:2:ALA:HB2	2:D:151:TYR:OH	2.21	0.40
2:D:86:LYS:HA	2:D:97:GLY:HA2	2.03	0.40
1:E:284:LEU:N	1:E:285:PRO:CD	2.84	0.40
2:D:132:PHE:HA	3:D:206:HOH:O	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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%)	26	55
1	C	286/304 (94%)	277 (97%)	7 (2%)	2 (1%)	26	55
1	E	285/304 (94%)	277 (97%)	6 (2%)	2 (1%)	26	55
1	G	286/304 (94%)	276 (96%)	8 (3%)	2 (1%)	26	55
1	I	284/304 (93%)	276 (97%)	6 (2%)	2 (1%)	26	55
1	K	286/304 (94%)	279 (98%)	5 (2%)	2 (1%)	26	55
2	B	183/228 (80%)	174 (95%)	9 (5%)	0	100	100
2	D	189/228 (83%)	181 (96%)	7 (4%)	1 (0%)	34	63
2	F	191/228 (84%)	180 (94%)	11 (6%)	0	100	100
2	H	189/228 (83%)	179 (95%)	9 (5%)	1 (0%)	34	63
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%)	34	63

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ILE

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Mol	Chain	Res	Type
1	C	280	ILE
1	E	280	ILE
1	G	280	ILE
1	I	280	ILE
1	K	280	ILE
2	H	191	MET
2	D	191	MET
1	A	284	LEU
1	C	284	LEU
1	E	284	LEU
1	G	284	LEU
1	I	284	LEU
1	K	284	LEU

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%)	210 (96%)	10 (4%)	34	65
1	C	221/233 (95%)	211 (96%)	10 (4%)	34	65
1	E	220/233 (94%)	210 (96%)	10 (4%)	34	65
1	G	221/233 (95%)	211 (96%)	10 (4%)	34	65
1	I	220/233 (94%)	210 (96%)	10 (4%)	34	65
1	K	221/233 (95%)	211 (96%)	10 (4%)	34	65
2	B	148/180 (82%)	145 (98%)	3 (2%)	63	87
2	D	150/180 (83%)	147 (98%)	3 (2%)	63	87
2	F	152/180 (84%)	149 (98%)	3 (2%)	63	87
2	H	150/180 (83%)	147 (98%)	3 (2%)	63	87
2	J	148/180 (82%)	145 (98%)	3 (2%)	63	87
2	L	150/180 (83%)	147 (98%)	3 (2%)	63	87
All	All	2221/2478 (90%)	2143 (96%)	78 (4%)	43	74

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	48	VAL
1	A	100	TYR
1	A	147	ARG
1	A	271	LEU
1	A	276	ARG
1	A	282	THR
1	A	283	LEU
1	A	286	GLU
1	A	288	ARG
1	C	45	LEU
1	C	48	VAL
1	C	100	TYR
1	C	147	ARG
1	C	271	LEU
1	C	276	ARG
1	C	282	THR
1	C	283	LEU
1	C	286	GLU
1	C	288	ARG
1	E	45	LEU
1	E	48	VAL
1	E	100	TYR
1	E	147	ARG
1	E	271	LEU
1	E	276	ARG
1	E	282	THR
1	E	283	LEU
1	E	286	GLU
1	E	288	ARG
1	G	45	LEU
1	G	48	VAL
1	G	100	TYR
1	G	147	ARG
1	G	271	LEU
1	G	276	ARG
1	G	282	THR
1	G	283	LEU
1	G	286	GLU
1	G	288	ARG
1	I	45	LEU
1	I	48	VAL

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Mol	Chain	Res	Type
1	I	100	TYR
1	I	147	ARG
1	I	271	LEU
1	I	276	ARG
1	I	282	THR
1	I	283	LEU
1	I	286	GLU
1	I	288	ARG
1	K	45	LEU
1	K	48	VAL
1	K	100	TYR
1	K	147	ARG
1	K	271	LEU
1	K	276	ARG
1	K	282	THR
1	K	283	LEU
1	K	286	GLU
1	K	288	ARG
2	B	57	ARG
2	B	99	MET
2	B	180	GLN
2	D	57	ARG
2	D	99	MET
2	D	180	GLN
2	F	57	ARG
2	F	99	MET
2	F	180	GLN
2	H	57	ARG
2	H	99	MET
2	H	180	GLN
2	J	57	ARG
2	J	99	MET
2	J	180	GLN
2	L	57	ARG
2	L	99	MET
2	L	180	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	257	HIS

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$
1	L5P	A	81	1	19,21,22	1.18	1 (5%)	15,27,29	1.57	5 (33%)
2	CYG	B	78	2	10,14,15	1.38	1 (10%)	6,17,19	8.32	5 (83%)
1	L5P	C	81	1	19,21,22	1.28	2 (10%)	15,27,29	1.70	6 (40%)
2	CYG	D	78	2	10,14,15	1.20	1 (10%)	6,17,19	9.60	5 (83%)
1	L5P	E	81	1	19,21,22	1.26	2 (10%)	15,27,29	1.73	4 (26%)
2	CYG	F	78	2	10,14,15	1.54	1 (10%)	6,17,19	9.11	5 (83%)
1	L5P	G	81	1	19,21,22	1.36	1 (5%)	15,27,29	1.40	3 (20%)
2	CYG	H	78	2	10,14,15	1.72	2 (20%)	6,17,19	8.68	4 (66%)
1	L5P	I	81	1	19,21,22	1.17	3 (15%)	15,27,29	1.66	5 (33%)
2	CYG	J	78	2	10,14,15	0.93	1 (10%)	6,17,19	10.63	5 (83%)
1	L5P	K	81	1	19,21,22	1.42	3 (15%)	15,27,29	1.57	4 (26%)
2	CYG	L	78	2	10,14,15	1.27	1 (10%)	6,17,19	9.19	5 (83%)

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
1	L5P	A	81	1	-	0/22/25/27	0/0/0/0
2	CYG	B	78	2	-	0/10/16/18	0/0/0/0
1	L5P	C	81	1	-	0/22/25/27	0/0/0/0
2	CYG	D	78	2	-	0/10/16/18	0/0/0/0
1	L5P	E	81	1	-	0/22/25/27	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CYG	F	78	2	-	0/10/16/18	0/0/0/0
1	L5P	G	81	1	-	0/22/25/27	0/0/0/0
2	CYG	H	78	2	-	0/10/16/18	0/0/0/0
1	L5P	I	81	1	-	0/22/25/27	0/0/0/0
2	CYG	J	78	2	-	0/10/16/18	0/0/0/0
1	L5P	K	81	1	-	0/22/25/27	0/0/0/0
2	CYG	L	78	2	-	0/10/16/18	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	78	CYG	CB-SG	-4.76	1.75	1.81
1	G	81	L5P	C6-C5	-4.51	1.49	1.53
2	B	78	CYG	CB-SG	-3.97	1.76	1.81
2	F	78	CYG	CB-SG	-3.93	1.76	1.81
1	E	81	L5P	C6-C5	-3.88	1.49	1.53
1	K	81	L5P	CB-CA	-3.63	1.50	1.53
1	A	81	L5P	C6-C5	-3.47	1.50	1.53
1	C	81	L5P	C6-C5	-3.33	1.50	1.53
2	D	78	CYG	CB-SG	-3.14	1.77	1.81
1	C	81	L5P	CB-CA	-2.96	1.50	1.53
1	I	81	L5P	C6-C5	-2.86	1.50	1.53
1	K	81	L5P	C6-C5	-2.84	1.50	1.53
1	K	81	L5P	P9-O10	-2.57	1.45	1.54
2	L	78	CYG	CB-SG	-2.57	1.78	1.81
2	J	78	CYG	CB-SG	-2.48	1.78	1.81
1	E	81	L5P	P9-O8	-2.06	1.53	1.60
1	I	81	L5P	CB-CA	-2.05	1.51	1.53
1	I	81	L5P	P9-O10	-2.00	1.47	1.54
2	H	78	CYG	CG1-CD1	2.26	1.53	1.50

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	78	CYG	OE2-CD1-CG1	-22.20	108.67	123.94
2	D	78	CYG	OE2-CD1-CG1	-19.76	110.34	123.94
2	L	78	CYG	OE2-CD1-CG1	-18.85	110.97	123.94
2	F	78	CYG	OE2-CD1-CG1	-18.63	111.12	123.94
2	B	78	CYG	OE2-CD1-CG1	-16.73	112.42	123.94
2	H	78	CYG	OE2-CD1-CG1	-16.71	112.44	123.94
2	B	78	CYG	CB1-CG1-CD1	-4.30	106.77	113.12
2	J	78	CYG	CB1-CG1-CD1	-4.07	107.11	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	81	L5P	O8-P9-O11	-3.64	97.87	107.14
2	L	78	CYG	CB1-CG1-CD1	-3.56	107.85	113.12
2	F	78	CYG	CB1-CG1-CD1	-3.40	108.09	113.12
2	D	78	CYG	CB1-CG1-CD1	-3.21	108.38	113.12
2	H	78	CYG	CB1-CG1-CD1	-3.18	108.42	113.12
1	E	81	L5P	O-C1-CA	-3.17	117.24	125.49
1	C	81	L5P	O8-P9-O11	-2.68	100.33	107.14
1	A	81	L5P	O8-P9-O11	-2.63	100.44	107.14
1	C	81	L5P	CG-CD-CE	-2.59	101.30	113.69
1	A	81	L5P	CG-CD-CE	-2.49	101.77	113.69
1	K	81	L5P	CG-CB-CA	-2.41	104.01	114.16
1	I	81	L5P	O8-P9-O11	-2.41	101.01	107.14
1	I	81	L5P	CG-CD-CE	-2.37	102.37	113.69
1	I	81	L5P	CG-CB-CA	-2.32	104.39	114.16
2	H	78	CYG	O-C-CA	-2.32	119.44	125.49
1	G	81	L5P	CG-CB-CA	-2.32	104.43	114.16
2	F	78	CYG	O-C-CA	-2.26	119.60	125.49
1	G	81	L5P	CG-CD-CE	-2.25	102.91	113.69
1	C	81	L5P	O12-P9-O8	-2.23	100.14	106.56
1	K	81	L5P	O12-P9-O8	-2.21	100.20	106.56
2	D	78	CYG	O-C-CA	-2.20	119.76	125.49
1	E	81	L5P	CG-CD-CE	-2.20	103.17	113.69
1	K	81	L5P	CG-CD-CE	-2.19	103.23	113.69
2	J	78	CYG	O-C-CA	-2.18	119.82	125.49
2	B	78	CYG	O-C-CA	-2.08	120.08	125.49
1	C	81	L5P	CG-CB-CA	-2.07	105.47	114.16
1	A	81	L5P	O-C1-CA	-2.06	120.12	125.49
1	K	81	L5P	O8-P9-O11	-2.03	101.98	107.14
1	G	81	L5P	O12-P9-O8	-2.01	100.77	106.56
1	A	81	L5P	O12-P9-O11	2.02	117.10	110.58
1	A	81	L5P	CD-CE-NZ	2.07	117.14	111.96
2	L	78	CYG	CB1-CA1-N1	2.12	116.56	110.52
1	I	81	L5P	O12-P9-O10	2.12	115.47	107.38
1	C	81	L5P	CD-CE-NZ	2.17	117.39	111.96
1	E	81	L5P	O12-P9-O11	2.68	119.21	110.58
1	C	81	L5P	O12-P9-O11	2.71	119.31	110.58
2	B	78	CYG	OE2-CD1-SG	2.86	125.10	122.83
1	I	81	L5P	O12-P9-O11	2.93	120.03	110.58
2	F	78	CYG	OE2-CD1-SG	3.58	125.67	122.83
2	L	78	CYG	OE2-CD1-SG	3.98	125.99	122.83
2	D	78	CYG	OE2-CD1-SG	4.25	126.20	122.83
2	J	78	CYG	OE2-CD1-SG	7.37	128.68	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	CYG	CG1-CD1-SG	10.11	122.45	113.36
2	J	78	CYG	CG1-CD1-SG	10.33	122.65	113.36
2	L	78	CYG	CG1-CD1-SG	10.74	123.02	113.36
2	F	78	CYG	CG1-CD1-SG	10.90	123.16	113.36
2	D	78	CYG	CG1-CD1-SG	11.22	123.45	113.36
2	H	78	CYG	CG1-CD1-SG	12.42	124.53	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 22 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

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, 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%)	-0.02	14 (4%) 33 32	32, 45, 113, 150	0
1	C	289/304 (95%)	0.01	11 (3%) 44 44	35, 47, 106, 130	0
1	E	288/304 (94%)	0.07	12 (4%) 40 39	31, 46, 100, 130	0
1	G	289/304 (95%)	-0.04	7 (2%) 62 62	28, 45, 102, 137	0
1	I	287/304 (94%)	0.19	20 (6%) 19 17	29, 44, 112, 152	0
1	K	289/304 (95%)	-0.00	11 (3%) 44 44	31, 43, 99, 147	0
2	B	187/228 (82%)	0.28	7 (3%) 45 45	40, 59, 85, 111	0
2	D	191/228 (83%)	0.29	5 (2%) 59 59	40, 63, 89, 121	0
2	F	193/228 (84%)	0.82	29 (15%) 3 2	42, 72, 104, 124	0
2	H	191/228 (83%)	0.52	18 (9%) 11 8	40, 71, 100, 117	0
2	J	188/228 (82%)	0.40	11 (5%) 26 24	37, 61, 84, 103	0
2	L	190/228 (83%)	0.59	18 (9%) 10 8	34, 66, 99, 134	0
All	All	2869/3192 (89%)	0.21	163 (5%) 27 26	28, 54, 101, 152	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	283	LEU	9.9
1	I	282	THR	8.2
1	I	276	ARG	7.7
1	I	283	LEU	7.7
1	K	282	THR	7.2
1	I	278	ILE	6.1
1	I	284	LEU	5.7
1	K	285	PRO	5.6
2	H	186	VAL	5.4
1	A	285	PRO	5.4
1	K	289	MET	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	287	HIS	5.2
2	F	157	ALA	5.1
1	K	287	HIS	5.0
1	A	279	ASP	5.0
1	I	279	ASP	5.0
1	I	54	ALA	5.0
2	F	141	ALA	4.9
1	E	288	ARG	4.6
1	A	283	LEU	4.5
1	G	282	THR	4.4
1	E	289	MET	4.4
2	D	153	ASP	4.4
2	F	1	MET	4.4
1	I	242	GLU	4.3
1	A	281	ALA	4.2
1	I	237	GLY	4.2
1	G	280	ILE	4.1
2	B	187	LYS	4.1
2	F	156	VAL	4.0
1	K	288	ARG	4.0
1	G	289	MET	3.9
2	H	192	ALA	3.9
2	L	92	ASP	3.9
1	A	286	GLU	3.9
2	F	147	VAL	3.8
1	A	289	MET	3.8
2	L	148	LEU	3.8
1	A	288	ARG	3.7
1	C	281	ALA	3.7
2	J	124	VAL	3.7
2	F	155	ILE	3.7
1	A	280	ILE	3.7
1	I	281	ALA	3.6
2	L	124	VAL	3.6
1	I	289	MET	3.6
2	F	121	ILE	3.5
1	E	286	GLU	3.5
1	K	281	ALA	3.5
1	C	283	LEU	3.5
1	I	287	HIS	3.5
2	F	122	LYS	3.5
2	F	178	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	J	23	GLY	3.4
1	E	281	ALA	3.4
1	A	287	HIS	3.4
1	I	277	GLY	3.3
1	C	279	ASP	3.3
2	L	1	MET	3.2
2	F	129	VAL	3.2
1	K	284	LEU	3.2
1	I	275	MET	3.1
2	D	23	GLY	3.1
1	K	1	MET	3.1
1	C	282	THR	3.1
2	B	121	ILE	3.1
2	F	3	ILE	3.1
2	F	182	PHE	3.1
1	C	54	ALA	3.0
2	L	141	ALA	3.0
1	E	276	ARG	3.0
2	H	139	VAL	3.0
1	E	287	HIS	3.0
2	L	186	VAL	3.0
2	L	123	GLY	3.0
1	A	284	LEU	3.0
2	F	163	PHE	3.0
1	E	278	ILE	3.0
2	F	181	TYR	2.9
1	A	276	ARG	2.9
1	I	288	ARG	2.9
2	L	93	GLU	2.8
2	L	127	GLY	2.8
2	B	120	SER	2.8
2	F	158	ALA	2.8
2	L	121	ILE	2.7
2	H	72	LYS	2.7
2	J	24	ALA	2.7
2	L	138	ILE	2.7
1	I	285	PRO	2.7
2	L	178	LEU	2.7
2	J	21	ALA	2.6
1	E	284	LEU	2.6
1	I	280	ILE	2.6
1	G	285	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	241	SER	2.6
2	H	3	ILE	2.6
2	J	156	VAL	2.6
2	F	146	ASP	2.6
2	L	120	SER	2.6
1	G	279	ASP	2.5
1	K	286	GLU	2.5
1	I	236	SER	2.5
2	L	2	LYS	2.5
1	C	289	MET	2.5
1	I	286	GLU	2.5
2	J	3	ILE	2.5
2	F	26	ALA	2.5
1	E	2	ALA	2.5
2	J	121	ILE	2.5
2	H	98	LEU	2.4
2	B	40	GLY	2.4
1	K	242	GLU	2.4
2	D	98	LEU	2.4
1	G	284	LEU	2.4
1	A	278	ILE	2.4
2	B	127	GLY	2.4
2	F	100	ASP	2.4
1	G	276	ARG	2.3
2	J	186	VAL	2.3
2	J	26	ALA	2.3
2	B	124	VAL	2.3
1	C	280	ILE	2.3
2	F	127	GLY	2.3
2	H	35	LEU	2.3
2	J	38	LEU	2.3
1	E	285	PRO	2.3
2	L	40	GLY	2.3
2	H	119	LEU	2.2
2	H	103	VAL	2.2
1	A	270	GLY	2.2
1	C	286	GLU	2.2
2	H	155	ILE	2.2
2	L	91	TYR	2.2
1	A	273	GLY	2.2
2	L	147	VAL	2.2
2	F	25	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	84	LEU	2.1
2	J	178	LEU	2.1
2	D	68	ALA	2.1
2	F	138	ILE	2.1
2	F	151	TYR	2.1
2	F	101	ILE	2.1
2	F	152	ASN	2.1
2	F	128	PHE	2.1
2	F	92	ASP	2.1
1	E	270	GLY	2.1
2	F	103	VAL	2.1
2	H	124	VAL	2.1
1	C	1	MET	2.1
2	F	145	VAL	2.1
2	H	27	VAL	2.1
1	C	275	MET	2.1
2	D	121	ILE	2.1
2	H	71	GLY	2.1
2	B	24	ALA	2.1
2	H	8	LEU	2.0
2	H	162	GLN	2.0
1	E	283	LEU	2.0
2	H	67	PHE	2.0
2	H	64	LEU	2.0
2	F	186	VAL	2.0
2	H	100	ASP	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	CYG	J	78	15/16	0.89	0.19	-	45,50,66,67	0
2	CYG	L	78	15/16	0.88	0.13	-	44,51,56,58	0
1	L5P	I	81	22/23	0.96	0.21	-	33,64,105,117	0
2	CYG	H	78	15/16	0.92	0.14	-	42,54,64,65	0
1	L5P	K	81	22/23	0.95	0.21	-	40,62,89,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CYG	B	78	15/16	0.85	0.20	-	50,56,66,81	0
1	L5P	E	81	22/23	0.90	0.27	-	40,73,95,111	0
2	CYG	D	78	15/16	0.85	0.21	-	45,50,56,60	0
1	L5P	G	81	22/23	0.95	0.23	-	33,63,78,102	0
1	L5P	A	81	22/23	0.95	0.20	-	41,69,101,110	0
1	L5P	C	81	22/23	0.94	0.20	-	39,68,87,96	0
2	CYG	F	78	15/16	0.85	0.19	-	48,63,69,80	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.