



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:28 am BST

PDB ID : 5XZQ  
Title : Hydroxynitrile lyase from Passiflora edulis (PeHNL)  
Authors : Motojima, F.; Nuykert, A.; Asano, Y.  
Deposited on : 2017-07-13  
Resolution : 2.80 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

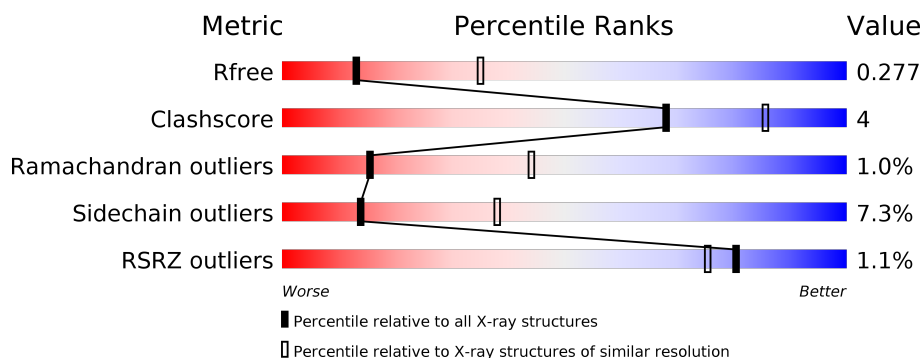
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 69%, grey 23%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>69%</span> <span>7%</span> <span>23%</span> </div> </div>
1	B	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 61%, grey 24%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>61%</span> <span>13%</span> <span>24%</span> </div> </div>
1	C	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 69%, grey 23%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>69%</span> <span>8%</span> <span>23%</span> </div> </div>
1	D	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 65%, grey 23%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>65%</span> <span>11%</span> <span>23%</span> </div> </div>
1	E	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 60%, grey 24%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>60%</span> <span>14%</span> <span>24%</span> </div> </div>
1	F	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 61%, grey 26%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>61%</span> <span>11%</span> <span>26%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	140	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>61%14%25%</div></div></div>
1	H	140	<div><div><div></div><div></div><div></div></div><div>63%13%24%</div></div>
1	I	140	<div><div><div></div><div></div><div></div></div><div>63%13%24%</div></div>
1	J	140	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>64%13%23%</div></div></div>
1	K	140	<div><div><div></div><div></div><div></div></div><div>61%13%26%</div></div>
1	L	140	<div><div><div></div><div></div><div></div></div><div>64%11%24%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10599 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 Hydroxynitrile lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			893	585	142	164	2			
1	B	107	Total	C	N	O	S	0	0	0
			881	576	141	162	2			
1	C	108	Total	C	N	O	S	0	0	0
			888	581	142	163	2			
1	D	108	Total	C	N	O	S	0	0	0
			888	581	142	163	2			
1	E	106	Total	C	N	O	S	0	0	0
			874	571	140	161	2			
1	F	103	Total	C	N	O	S	0	0	0
			849	553	137	157	2			
1	G	105	Total	C	N	O	S	0	0	0
			863	562	139	160	2			
1	H	107	Total	C	N	O	S	0	0	0
			881	576	141	162	2			
1	I	107	Total	C	N	O	S	0	1	0
			888	581	143	162	2			
1	J	108	Total	C	N	O	S	0	1	0
			894	585	142	165	2			
1	K	104	Total	C	N	O	S	0	0	0
			856	558	138	158	2			
1	L	107	Total	C	N	O	S	0	0	0
			881	576	141	162	2			

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP A0A1L7NZN4
A	-17	ASN	-	expression tag	UNP A0A1L7NZN4
A	-16	HIS	-	expression tag	UNP A0A1L7NZN4
A	-15	LYS	-	expression tag	UNP A0A1L7NZN4
A	-14	VAL	-	expression tag	UNP A0A1L7NZN4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP A0A1L7NZN4
A	-12	HIS	-	expression tag	UNP A0A1L7NZN4
A	-11	HIS	-	expression tag	UNP A0A1L7NZN4
A	-10	HIS	-	expression tag	UNP A0A1L7NZN4
A	-9	HIS	-	expression tag	UNP A0A1L7NZN4
A	-8	HIS	-	expression tag	UNP A0A1L7NZN4
A	-7	ILE	-	expression tag	UNP A0A1L7NZN4
A	-6	GLU	-	expression tag	UNP A0A1L7NZN4
A	-5	GLY	-	expression tag	UNP A0A1L7NZN4
A	-4	ARG	-	expression tag	UNP A0A1L7NZN4
A	-3	HIS	-	expression tag	UNP A0A1L7NZN4
A	-2	MET	-	expression tag	UNP A0A1L7NZN4
A	-1	GLU	-	expression tag	UNP A0A1L7NZN4
A	0	LEU	-	expression tag	UNP A0A1L7NZN4
B	-18	MET	-	expression tag	UNP A0A1L7NZN4
B	-17	ASN	-	expression tag	UNP A0A1L7NZN4
B	-16	HIS	-	expression tag	UNP A0A1L7NZN4
B	-15	LYS	-	expression tag	UNP A0A1L7NZN4
B	-14	VAL	-	expression tag	UNP A0A1L7NZN4
B	-13	HIS	-	expression tag	UNP A0A1L7NZN4
B	-12	HIS	-	expression tag	UNP A0A1L7NZN4
B	-11	HIS	-	expression tag	UNP A0A1L7NZN4
B	-10	HIS	-	expression tag	UNP A0A1L7NZN4
B	-9	HIS	-	expression tag	UNP A0A1L7NZN4
B	-8	HIS	-	expression tag	UNP A0A1L7NZN4
B	-7	ILE	-	expression tag	UNP A0A1L7NZN4
B	-6	GLU	-	expression tag	UNP A0A1L7NZN4
B	-5	GLY	-	expression tag	UNP A0A1L7NZN4
B	-4	ARG	-	expression tag	UNP A0A1L7NZN4
B	-3	HIS	-	expression tag	UNP A0A1L7NZN4
B	-2	MET	-	expression tag	UNP A0A1L7NZN4
B	-1	GLU	-	expression tag	UNP A0A1L7NZN4
B	0	LEU	-	expression tag	UNP A0A1L7NZN4
C	-18	MET	-	expression tag	UNP A0A1L7NZN4
C	-17	ASN	-	expression tag	UNP A0A1L7NZN4
C	-16	HIS	-	expression tag	UNP A0A1L7NZN4
C	-15	LYS	-	expression tag	UNP A0A1L7NZN4
C	-14	VAL	-	expression tag	UNP A0A1L7NZN4
C	-13	HIS	-	expression tag	UNP A0A1L7NZN4
C	-12	HIS	-	expression tag	UNP A0A1L7NZN4
C	-11	HIS	-	expression tag	UNP A0A1L7NZN4
C	-10	HIS	-	expression tag	UNP A0A1L7NZN4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	HIS	-	expression tag	UNP A0A1L7NZN4
C	-8	HIS	-	expression tag	UNP A0A1L7NZN4
C	-7	ILE	-	expression tag	UNP A0A1L7NZN4
C	-6	GLU	-	expression tag	UNP A0A1L7NZN4
C	-5	GLY	-	expression tag	UNP A0A1L7NZN4
C	-4	ARG	-	expression tag	UNP A0A1L7NZN4
C	-3	HIS	-	expression tag	UNP A0A1L7NZN4
C	-2	MET	-	expression tag	UNP A0A1L7NZN4
C	-1	GLU	-	expression tag	UNP A0A1L7NZN4
C	0	LEU	-	expression tag	UNP A0A1L7NZN4
D	-18	MET	-	expression tag	UNP A0A1L7NZN4
D	-17	ASN	-	expression tag	UNP A0A1L7NZN4
D	-16	HIS	-	expression tag	UNP A0A1L7NZN4
D	-15	LYS	-	expression tag	UNP A0A1L7NZN4
D	-14	VAL	-	expression tag	UNP A0A1L7NZN4
D	-13	HIS	-	expression tag	UNP A0A1L7NZN4
D	-12	HIS	-	expression tag	UNP A0A1L7NZN4
D	-11	HIS	-	expression tag	UNP A0A1L7NZN4
D	-10	HIS	-	expression tag	UNP A0A1L7NZN4
D	-9	HIS	-	expression tag	UNP A0A1L7NZN4
D	-8	HIS	-	expression tag	UNP A0A1L7NZN4
D	-7	ILE	-	expression tag	UNP A0A1L7NZN4
D	-6	GLU	-	expression tag	UNP A0A1L7NZN4
D	-5	GLY	-	expression tag	UNP A0A1L7NZN4
D	-4	ARG	-	expression tag	UNP A0A1L7NZN4
D	-3	HIS	-	expression tag	UNP A0A1L7NZN4
D	-2	MET	-	expression tag	UNP A0A1L7NZN4
D	-1	GLU	-	expression tag	UNP A0A1L7NZN4
D	0	LEU	-	expression tag	UNP A0A1L7NZN4
E	-18	MET	-	expression tag	UNP A0A1L7NZN4
E	-17	ASN	-	expression tag	UNP A0A1L7NZN4
E	-16	HIS	-	expression tag	UNP A0A1L7NZN4
E	-15	LYS	-	expression tag	UNP A0A1L7NZN4
E	-14	VAL	-	expression tag	UNP A0A1L7NZN4
E	-13	HIS	-	expression tag	UNP A0A1L7NZN4
E	-12	HIS	-	expression tag	UNP A0A1L7NZN4
E	-11	HIS	-	expression tag	UNP A0A1L7NZN4
E	-10	HIS	-	expression tag	UNP A0A1L7NZN4
E	-9	HIS	-	expression tag	UNP A0A1L7NZN4
E	-8	HIS	-	expression tag	UNP A0A1L7NZN4
E	-7	ILE	-	expression tag	UNP A0A1L7NZN4
E	-6	GLU	-	expression tag	UNP A0A1L7NZN4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	GLY	-	expression tag	UNP A0A1L7NZN4
E	-4	ARG	-	expression tag	UNP A0A1L7NZN4
E	-3	HIS	-	expression tag	UNP A0A1L7NZN4
E	-2	MET	-	expression tag	UNP A0A1L7NZN4
E	-1	GLU	-	expression tag	UNP A0A1L7NZN4
E	0	LEU	-	expression tag	UNP A0A1L7NZN4
F	-18	MET	-	expression tag	UNP A0A1L7NZN4
F	-17	ASN	-	expression tag	UNP A0A1L7NZN4
F	-16	HIS	-	expression tag	UNP A0A1L7NZN4
F	-15	LYS	-	expression tag	UNP A0A1L7NZN4
F	-14	VAL	-	expression tag	UNP A0A1L7NZN4
F	-13	HIS	-	expression tag	UNP A0A1L7NZN4
F	-12	HIS	-	expression tag	UNP A0A1L7NZN4
F	-11	HIS	-	expression tag	UNP A0A1L7NZN4
F	-10	HIS	-	expression tag	UNP A0A1L7NZN4
F	-9	HIS	-	expression tag	UNP A0A1L7NZN4
F	-8	HIS	-	expression tag	UNP A0A1L7NZN4
F	-7	ILE	-	expression tag	UNP A0A1L7NZN4
F	-6	GLU	-	expression tag	UNP A0A1L7NZN4
F	-5	GLY	-	expression tag	UNP A0A1L7NZN4
F	-4	ARG	-	expression tag	UNP A0A1L7NZN4
F	-3	HIS	-	expression tag	UNP A0A1L7NZN4
F	-2	MET	-	expression tag	UNP A0A1L7NZN4
F	-1	GLU	-	expression tag	UNP A0A1L7NZN4
F	0	LEU	-	expression tag	UNP A0A1L7NZN4
G	-18	MET	-	expression tag	UNP A0A1L7NZN4
G	-17	ASN	-	expression tag	UNP A0A1L7NZN4
G	-16	HIS	-	expression tag	UNP A0A1L7NZN4
G	-15	LYS	-	expression tag	UNP A0A1L7NZN4
G	-14	VAL	-	expression tag	UNP A0A1L7NZN4
G	-13	HIS	-	expression tag	UNP A0A1L7NZN4
G	-12	HIS	-	expression tag	UNP A0A1L7NZN4
G	-11	HIS	-	expression tag	UNP A0A1L7NZN4
G	-10	HIS	-	expression tag	UNP A0A1L7NZN4
G	-9	HIS	-	expression tag	UNP A0A1L7NZN4
G	-8	HIS	-	expression tag	UNP A0A1L7NZN4
G	-7	ILE	-	expression tag	UNP A0A1L7NZN4
G	-6	GLU	-	expression tag	UNP A0A1L7NZN4
G	-5	GLY	-	expression tag	UNP A0A1L7NZN4
G	-4	ARG	-	expression tag	UNP A0A1L7NZN4
G	-3	HIS	-	expression tag	UNP A0A1L7NZN4
G	-2	MET	-	expression tag	UNP A0A1L7NZN4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLU	-	expression tag	UNP A0A1L7NZN4
G	0	LEU	-	expression tag	UNP A0A1L7NZN4
H	-18	MET	-	expression tag	UNP A0A1L7NZN4
H	-17	ASN	-	expression tag	UNP A0A1L7NZN4
H	-16	HIS	-	expression tag	UNP A0A1L7NZN4
H	-15	LYS	-	expression tag	UNP A0A1L7NZN4
H	-14	VAL	-	expression tag	UNP A0A1L7NZN4
H	-13	HIS	-	expression tag	UNP A0A1L7NZN4
H	-12	HIS	-	expression tag	UNP A0A1L7NZN4
H	-11	HIS	-	expression tag	UNP A0A1L7NZN4
H	-10	HIS	-	expression tag	UNP A0A1L7NZN4
H	-9	HIS	-	expression tag	UNP A0A1L7NZN4
H	-8	HIS	-	expression tag	UNP A0A1L7NZN4
H	-7	ILE	-	expression tag	UNP A0A1L7NZN4
H	-6	GLU	-	expression tag	UNP A0A1L7NZN4
H	-5	GLY	-	expression tag	UNP A0A1L7NZN4
H	-4	ARG	-	expression tag	UNP A0A1L7NZN4
H	-3	HIS	-	expression tag	UNP A0A1L7NZN4
H	-2	MET	-	expression tag	UNP A0A1L7NZN4
H	-1	GLU	-	expression tag	UNP A0A1L7NZN4
H	0	LEU	-	expression tag	UNP A0A1L7NZN4
I	-18	MET	-	expression tag	UNP A0A1L7NZN4
I	-17	ASN	-	expression tag	UNP A0A1L7NZN4
I	-16	HIS	-	expression tag	UNP A0A1L7NZN4
I	-15	LYS	-	expression tag	UNP A0A1L7NZN4
I	-14	VAL	-	expression tag	UNP A0A1L7NZN4
I	-13	HIS	-	expression tag	UNP A0A1L7NZN4
I	-12	HIS	-	expression tag	UNP A0A1L7NZN4
I	-11	HIS	-	expression tag	UNP A0A1L7NZN4
I	-10	HIS	-	expression tag	UNP A0A1L7NZN4
I	-9	HIS	-	expression tag	UNP A0A1L7NZN4
I	-8	HIS	-	expression tag	UNP A0A1L7NZN4
I	-7	ILE	-	expression tag	UNP A0A1L7NZN4
I	-6	GLU	-	expression tag	UNP A0A1L7NZN4
I	-5	GLY	-	expression tag	UNP A0A1L7NZN4
I	-4	ARG	-	expression tag	UNP A0A1L7NZN4
I	-3	HIS	-	expression tag	UNP A0A1L7NZN4
I	-2	MET	-	expression tag	UNP A0A1L7NZN4
I	-1	GLU	-	expression tag	UNP A0A1L7NZN4
I	0	LEU	-	expression tag	UNP A0A1L7NZN4
J	-18	MET	-	expression tag	UNP A0A1L7NZN4
J	-17	ASN	-	expression tag	UNP A0A1L7NZN4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-16	HIS	-	expression tag	UNP A0A1L7NZN4
J	-15	LYS	-	expression tag	UNP A0A1L7NZN4
J	-14	VAL	-	expression tag	UNP A0A1L7NZN4
J	-13	HIS	-	expression tag	UNP A0A1L7NZN4
J	-12	HIS	-	expression tag	UNP A0A1L7NZN4
J	-11	HIS	-	expression tag	UNP A0A1L7NZN4
J	-10	HIS	-	expression tag	UNP A0A1L7NZN4
J	-9	HIS	-	expression tag	UNP A0A1L7NZN4
J	-8	HIS	-	expression tag	UNP A0A1L7NZN4
J	-7	ILE	-	expression tag	UNP A0A1L7NZN4
J	-6	GLU	-	expression tag	UNP A0A1L7NZN4
J	-5	GLY	-	expression tag	UNP A0A1L7NZN4
J	-4	ARG	-	expression tag	UNP A0A1L7NZN4
J	-3	HIS	-	expression tag	UNP A0A1L7NZN4
J	-2	MET	-	expression tag	UNP A0A1L7NZN4
J	-1	GLU	-	expression tag	UNP A0A1L7NZN4
J	0	LEU	-	expression tag	UNP A0A1L7NZN4
K	-18	MET	-	expression tag	UNP A0A1L7NZN4
K	-17	ASN	-	expression tag	UNP A0A1L7NZN4
K	-16	HIS	-	expression tag	UNP A0A1L7NZN4
K	-15	LYS	-	expression tag	UNP A0A1L7NZN4
K	-14	VAL	-	expression tag	UNP A0A1L7NZN4
K	-13	HIS	-	expression tag	UNP A0A1L7NZN4
K	-12	HIS	-	expression tag	UNP A0A1L7NZN4
K	-11	HIS	-	expression tag	UNP A0A1L7NZN4
K	-10	HIS	-	expression tag	UNP A0A1L7NZN4
K	-9	HIS	-	expression tag	UNP A0A1L7NZN4
K	-8	HIS	-	expression tag	UNP A0A1L7NZN4
K	-7	ILE	-	expression tag	UNP A0A1L7NZN4
K	-6	GLU	-	expression tag	UNP A0A1L7NZN4
K	-5	GLY	-	expression tag	UNP A0A1L7NZN4
K	-4	ARG	-	expression tag	UNP A0A1L7NZN4
K	-3	HIS	-	expression tag	UNP A0A1L7NZN4
K	-2	MET	-	expression tag	UNP A0A1L7NZN4
K	-1	GLU	-	expression tag	UNP A0A1L7NZN4
K	0	LEU	-	expression tag	UNP A0A1L7NZN4
L	-18	MET	-	expression tag	UNP A0A1L7NZN4
L	-17	ASN	-	expression tag	UNP A0A1L7NZN4
L	-16	HIS	-	expression tag	UNP A0A1L7NZN4
L	-15	LYS	-	expression tag	UNP A0A1L7NZN4
L	-14	VAL	-	expression tag	UNP A0A1L7NZN4
L	-13	HIS	-	expression tag	UNP A0A1L7NZN4

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-12	HIS	-	expression tag	UNP A0A1L7NZN4
L	-11	HIS	-	expression tag	UNP A0A1L7NZN4
L	-10	HIS	-	expression tag	UNP A0A1L7NZN4
L	-9	HIS	-	expression tag	UNP A0A1L7NZN4
L	-8	HIS	-	expression tag	UNP A0A1L7NZN4
L	-7	ILE	-	expression tag	UNP A0A1L7NZN4
L	-6	GLU	-	expression tag	UNP A0A1L7NZN4
L	-5	GLY	-	expression tag	UNP A0A1L7NZN4
L	-4	ARG	-	expression tag	UNP A0A1L7NZN4
L	-3	HIS	-	expression tag	UNP A0A1L7NZN4
L	-2	MET	-	expression tag	UNP A0A1L7NZN4
L	-1	GLU	-	expression tag	UNP A0A1L7NZN4
L	0	LEU	-	expression tag	UNP A0A1L7NZN4

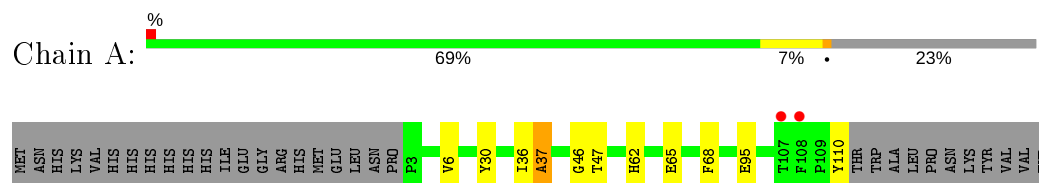
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	2	Total O 2 2	0	0
2	C	7	Total O 7 7	0	0
2	D	1	Total O 1 1	0	0
2	E	2	Total O 2 2	0	0
2	F	3	Total O 3 3	0	0
2	G	9	Total O 9 9	0	0
2	H	8	Total O 8 8	0	0
2	I	9	Total O 9 9	0	0
2	J	10	Total O 10 10	0	0
2	K	5	Total O 5 5	0	0
2	L	5	Total O 5 5	0	0

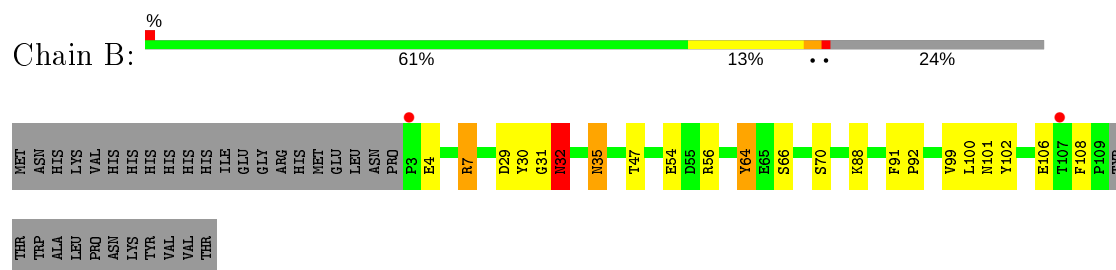
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

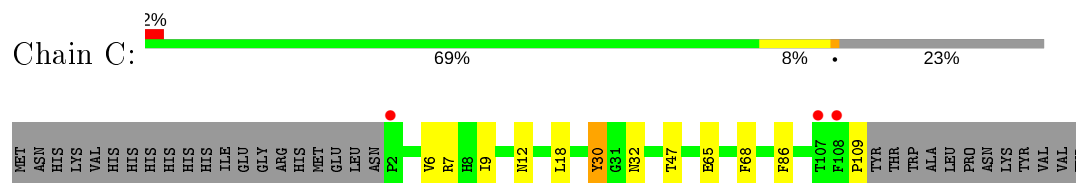
#### • Molecule 1: Hydroxynitrile lyase



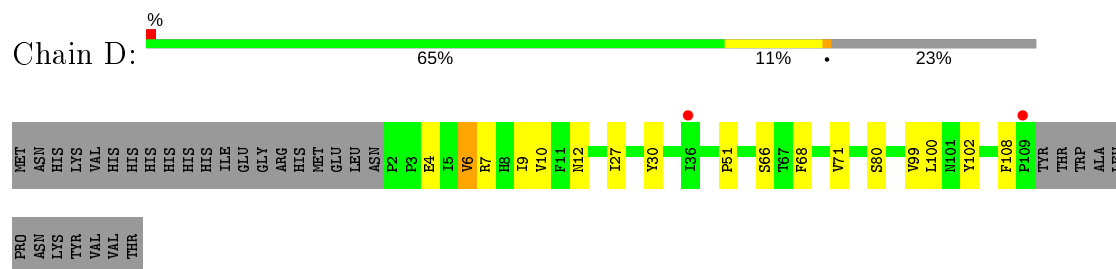
#### • Molecule 1: Hydroxynitrile lyase



#### • Molecule 1: Hydroxynitrile lyase

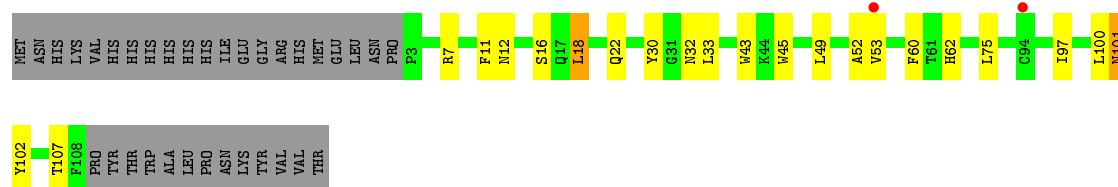


#### • Molecule 1: Hydroxynitrile lyase

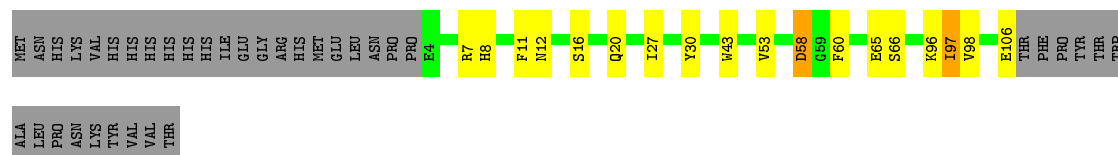


#### • Molecule 1: Hydroxynitrile lyase

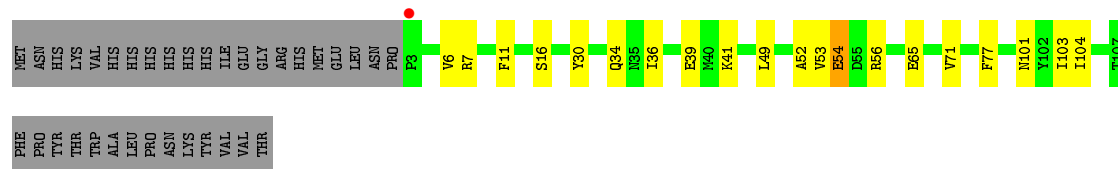




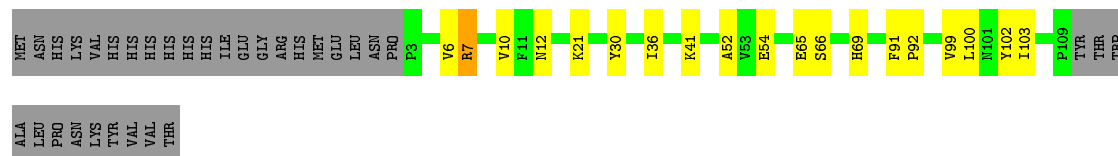
- Molecule 1: Hydroxynitrile lyase



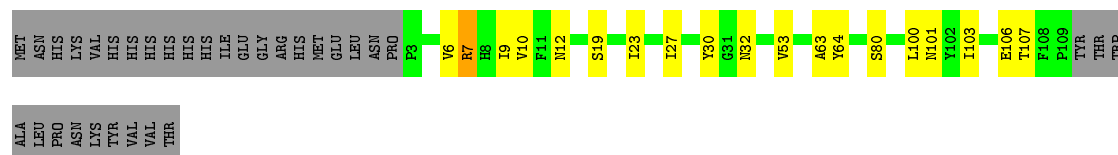
- Molecule 1: Hydroxynitrile lyase



- Molecule 1: Hydroxynitrile lyase

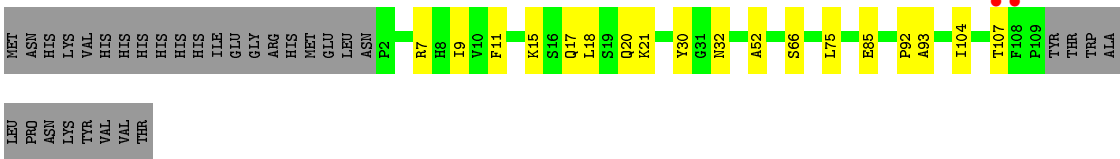


- Molecule 1: Hydroxynitrile lyase

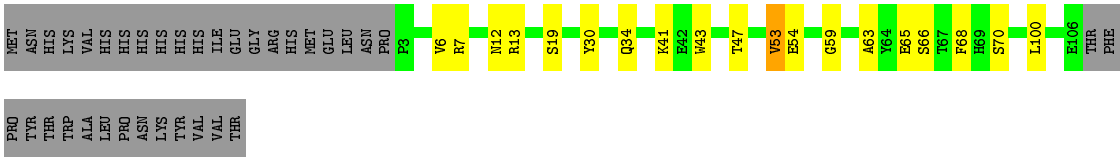


- Molecule 1: Hydroxynitrile lyase

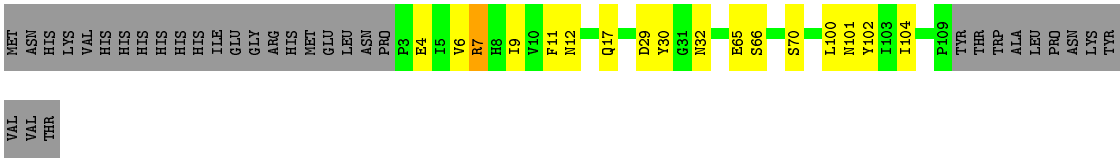




• Molecule 1: Hydroxynitrile lyase



• Molecule 1: Hydroxynitrile lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.45Å 88.57Å 104.57Å 90.00° 105.99° 90.00°	Depositor
Resolution (Å)	100.53 – 2.80 47.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (100.53-2.80) 99.1 (47.60-2.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.90 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.207 , 0.279 0.213 , 0.277	Depositor DCC
$R_{free}$ test set	1892 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.55	0/922	0.74	0/1253
1	B	0.63	0/909	0.78	0/1235
1	C	0.57	0/917	0.75	0/1247
1	D	0.56	0/917	0.75	0/1247
1	E	0.55	0/901	0.69	0/1223
1	F	0.53	0/874	0.75	0/1186
1	G	0.68	0/889	0.78	0/1207
1	H	0.65	0/909	0.79	0/1235
1	I	0.68	0/920	0.84	0/1250
1	J	0.65	0/926	0.82	0/1259
1	K	0.60	0/882	0.77	0/1197
1	L	0.57	0/909	0.71	0/1235
All	All	0.61	0/10875	0.77	0/14774

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	893	0	848	6	0
1	B	881	0	839	11	0
1	C	888	0	846	5	0
1	D	888	0	846	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	874	0	832	10	0
1	F	849	0	808	7	0
1	G	863	0	823	15	0
1	H	881	0	839	9	0
1	I	888	0	846	8	0
1	J	894	0	852	9	0
1	K	856	0	816	8	0
1	L	881	0	839	8	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	7	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
2	G	9	0	0	0	0
2	H	8	0	0	0	0
2	I	9	0	0	0	0
2	J	10	0	0	0	0
2	K	5	0	0	1	0
2	L	5	0	0	0	0
All	All	10599	0	10034	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (79) 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:G:103:ILE:HD11	1:J:52:ALA:HB2	1.47	0.96
1:G:54:GLU:OE2	1:G:56:ARG:NH1	2.25	0.70
1:K:41:LYS:NZ	2:K:201:HOH:O	2.32	0.63
1:H:10:VAL:HG22	1:H:99:VAL:HG22	1.80	0.63
1:H:52:ALA:HB2	1:I:103:ILE:HD11	1.81	0.62
1:K:34:GLN:HE22	1:K:43:TRP:H	1.48	0.62
1:F:43:TRP:HA	1:F:65:GLU:O	1.99	0.62
1:C:65:GLU:OE1	1:D:102:TYR:OH	2.24	0.56
1:K:13:ARG:NH1	1:K:59:GLY:O	2.39	0.55
1:K:6:VAL:HG22	1:K:68:PHE:HB2	1.88	0.55
1:A:65:GLU:OE2	1:B:7:ARG:HD2	2.07	0.55
1:G:65:GLU:OE2	1:H:102:TYR:OH	2.25	0.54
1:G:65:GLU:OE2	1:H:7:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:ASP:O	1:F:96:LYS:NZ	2.41	0.54
1:L:9:ILE:HD13	1:L:65:GLU:HB3	1.89	0.53
1:B:88:LYS:O	1:B:92:PRO:HG2	2.09	0.52
1:A:6:VAL:HG22	1:A:68:PHE:HB2	1.92	0.51
1:F:11:PHE:HB2	1:F:98:VAL:HG13	1.92	0.51
1:D:6:VAL:HG22	1:D:68:PHE:HB2	1.93	0.50
1:E:12:ASN:OD1	1:E:62:HIS:HB2	2.11	0.50
1:F:97:ILE:HG23	1:F:97:ILE:O	2.11	0.50
1:L:7:ARG:O	1:L:101:ASN:HA	2.12	0.50
1:C:30:TYR:HB2	1:C:86:PHE:CZ	2.47	0.50
1:I:19:SER:HA	1:K:19:SER:HA	1.94	0.49
1:E:49:LEU:HB2	1:E:53:VAL:HG21	1.95	0.48
1:D:10:VAL:HG13	1:D:99:VAL:HG22	1.96	0.48
1:A:65:GLU:OE2	1:B:102:TYR:OH	2.27	0.48
1:D:99:VAL:O	1:D:100:LEU:HD12	2.13	0.47
1:J:7:ARG:HD3	1:J:104:ILE:HD11	1.95	0.47
1:B:54:GLU:OE2	1:B:56:ARG:NH1	2.47	0.47
1:G:71:VAL:HB	1:J:52:ALA:HB1	1.96	0.47
1:B:35:ASN:N	1:B:35:ASN:HD22	2.13	0.46
1:E:43:TRP:CH2	1:E:45:TRP:CD1	3.04	0.46
1:J:18:LEU:HD11	1:J:93:ALA:HB1	1.96	0.46
1:I:53:VAL:HG13	1:J:75:LEU:HD21	1.98	0.46
1:C:109:PRO:HG3	1:D:27:ILE:HB	1.97	0.46
1:C:6:VAL:HG22	1:C:68:PHE:HB2	1.97	0.45
1:E:101:ASN:N	1:E:101:ASN:ND2	2.64	0.45
1:G:39:GLU:HB2	1:G:77:PHE:HB2	1.99	0.45
1:E:49:LEU:CB	1:E:53:VAL:HG21	2.47	0.45
1:I:7:ARG:O	1:I:101:ASN:HA	2.17	0.45
1:G:34:GLN:NE2	1:G:41:LYS:O	2.50	0.45
1:H:41:LYS:HD3	1:H:69:HIS:CD2	2.53	0.44
1:G:36:ILE:CG1	1:G:36:ILE:O	2.66	0.44
1:G:101:ASN:ND2	1:H:54:GLU:OE1	2.47	0.44
1:E:75:LEU:HD21	1:F:53:VAL:HG13	2.00	0.43
1:I:23:ILE:O	1:I:27:ILE:HG12	2.17	0.43
1:L:29:ASP:HA	1:L:32:ASN:ND2	2.32	0.43
1:L:102:TYR:CE2	1:L:104:ILE:HD13	2.53	0.43
1:E:18:LEU:HD22	1:E:22:GLN:OE1	2.18	0.43
1:G:49:LEU:HD21	1:H:103:ILE:HG13	2.00	0.43
1:G:53:VAL:HG12	1:G:53:VAL:O	2.19	0.43
1:G:7:ARG:HE	1:G:104:ILE:HD11	1.84	0.42
1:I:10:VAL:O	1:I:63:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ARG:HB3	1:E:102:TYR:CZ	2.54	0.42
1:A:36:ILE:O	1:A:37:ALA:HB2	2.18	0.42
1:A:47:THR:HG22	1:A:62:HIS:CD2	2.55	0.42
1:E:11:PHE:HB3	1:E:60:PHE:CD2	2.55	0.42
1:J:15:LYS:HE2	1:J:92:PRO:O	2.19	0.42
1:H:91:PHE:N	1:H:92:PRO:CD	2.83	0.42
1:J:85[B]:GLU:HA	1:J:85[B]:GLU:OE1	2.20	0.42
1:K:100:LEU:HD22	1:L:11:PHE:CD1	2.54	0.42
1:B:7:ARG:O	1:B:101:ASN:HA	2.20	0.42
1:K:63:ALA:HB2	1:L:100:LEU:HD22	2.00	0.42
1:G:11:PHE:CD2	1:H:100:LEU:HD13	2.55	0.41
1:I:100:LEU:HD13	1:J:11:PHE:CD2	2.55	0.41
1:L:4:GLU:O	1:L:70:SER:HA	2.20	0.41
1:K:65:GLU:OE1	1:L:102:TYR:OH	2.38	0.41
1:I:9:ILE:HG21	1:J:9:ILE:HG21	2.01	0.41
1:B:29:ASP:HA	1:B:32:ASN:HD21	1.84	0.41
1:B:91:PHE:N	1:B:92:PRO:CD	2.84	0.41
1:F:8:HIS:HB3	1:F:66:SER:HB2	2.03	0.41
1:C:9:ILE:HG21	1:D:9:ILE:HG21	2.02	0.41
1:B:64:TYR:CD1	1:B:64:TYR:N	2.89	0.41
1:E:100:LEU:HD11	1:F:60:PHE:HB2	2.03	0.40
1:A:46:GLY:HA3	1:B:102:TYR:HB2	2.02	0.40
1:B:99:VAL:C	1:B:100:LEU:HD12	2.42	0.40
1:G:34:GLN:NE2	1:G:41:LYS:C	2.75	0.40
1:G:7:ARG:HD3	1:G:7:ARG:HA	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	106/140 (76%)	95 (90%)	10 (9%)	1 (1%)	17 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	105/140 (75%)	90 (86%)	12 (11%)	3 (3%)	4	15
1	C	106/140 (76%)	98 (92%)	8 (8%)	0	100	100
1	D	106/140 (76%)	93 (88%)	12 (11%)	1 (1%)	17	46
1	E	104/140 (74%)	92 (88%)	11 (11%)	1 (1%)	15	44
1	F	101/140 (72%)	90 (89%)	8 (8%)	3 (3%)	4	15
1	G	103/140 (74%)	96 (93%)	5 (5%)	2 (2%)	8	26
1	H	105/140 (75%)	101 (96%)	4 (4%)	0	100	100
1	I	106/140 (76%)	102 (96%)	4 (4%)	0	100	100
1	J	107/140 (76%)	103 (96%)	4 (4%)	0	100	100
1	K	102/140 (73%)	94 (92%)	6 (6%)	2 (2%)	7	24
1	L	105/140 (75%)	101 (96%)	4 (4%)	0	100	100
All	All	1256/1680 (75%)	1155 (92%)	88 (7%)	13 (1%)	15	44

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	SER
1	G	54	GLU
1	F	97	ILE
1	G	52	ALA
1	K	70	SER
1	A	37	ALA
1	B	31	GLY
1	B	32	ASN
1	E	52	ALA
1	F	58	ASP
1	F	16	SER
1	K	53	VAL
1	D	51	PRO

### 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	95/125 (76%)	92 (97%)	3 (3%)	39	73
1	B	94/125 (75%)	84 (89%)	10 (11%)	6	20
1	C	95/125 (76%)	89 (94%)	6 (6%)	18	46
1	D	95/125 (76%)	86 (90%)	9 (10%)	8	25
1	E	93/125 (74%)	85 (91%)	8 (9%)	10	30
1	F	90/125 (72%)	84 (93%)	6 (7%)	16	43
1	G	92/125 (74%)	89 (97%)	3 (3%)	38	72
1	H	94/125 (75%)	86 (92%)	8 (8%)	10	31
1	I	95/125 (76%)	86 (90%)	9 (10%)	8	25
1	J	96/125 (77%)	89 (93%)	7 (7%)	14	38
1	K	91/125 (73%)	84 (92%)	7 (8%)	13	35
1	L	94/125 (75%)	88 (94%)	6 (6%)	17	45
All	All	1124/1500 (75%)	1042 (93%)	82 (7%)	14	38

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
1	A	95	GLU
1	A	110	TYR
1	B	4	GLU
1	B	7	ARG
1	B	30	TYR
1	B	32	ASN
1	B	35	ASN
1	B	47	THR
1	B	64	TYR
1	B	66	SER
1	B	106	GLU
1	B	108	PHE
1	C	7	ARG
1	C	12	ASN
1	C	18	LEU
1	C	30	TYR
1	C	32	ASN
1	C	47	THR
1	D	4	GLU
1	D	6	VAL
1	D	7	ARG

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Mol	Chain	Res	Type
1	D	12	ASN
1	D	30	TYR
1	D	66	SER
1	D	71	VAL
1	D	80	SER
1	D	108	PHE
1	E	16	SER
1	E	18	LEU
1	E	30	TYR
1	E	32	ASN
1	E	33	LEU
1	E	97	ILE
1	E	101	ASN
1	E	107	THR
1	F	7	ARG
1	F	12	ASN
1	F	20	GLN
1	F	27	ILE
1	F	30	TYR
1	F	106	GLU
1	G	6	VAL
1	G	16	SER
1	G	30	TYR
1	H	6	VAL
1	H	7	ARG
1	H	12	ASN
1	H	21	LYS
1	H	30	TYR
1	H	36	ILE
1	H	65	GLU
1	H	66	SER
1	I	6	VAL
1	I	7	ARG
1	I	12	ASN
1	I	30	TYR
1	I	32	ASN
1	I	64	TYR
1	I	80	SER
1	I	106	GLU
1	I	107	THR
1	J	17	GLN
1	J	20	GLN

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Mol	Chain	Res	Type
1	J	21	LYS
1	J	30	TYR
1	J	32	ASN
1	J	66	SER
1	J	107	THR
1	K	7	ARG
1	K	12	ASN
1	K	30	TYR
1	K	47	THR
1	K	53	VAL
1	K	54	GLU
1	K	66	SER
1	L	6	VAL
1	L	7	ARG
1	L	12	ASN
1	L	17	GLN
1	L	30	TYR
1	L	66	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	ASN
1	B	35	ASN
1	C	17	GLN
1	E	32	ASN
1	E	101	ASN
1	F	34	GLN
1	G	34	GLN
1	H	69	HIS
1	I	32	ASN
1	J	25	GLN
1	J	34	GLN
1	K	34	GLN
1	K	69	HIS
1	L	32	ASN

### 5.3.3 RNA ⓘ

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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	108/140 (77%)	0.21	2 (1%) 66 59	47, 73, 102, 131	0
1	B	107/140 (76%)	0.01	2 (1%) 66 59	45, 65, 89, 127	0
1	C	108/140 (77%)	-0.02	3 (2%) 53 43	39, 62, 95, 127	0
1	D	108/140 (77%)	0.06	2 (1%) 66 59	45, 78, 99, 110	0
1	E	106/140 (75%)	0.30	2 (1%) 66 59	55, 91, 112, 120	0
1	F	103/140 (73%)	0.06	0 100 100	52, 67, 99, 105	0
1	G	105/140 (75%)	-0.09	1 (0%) 82 77	27, 50, 84, 99	0
1	H	107/140 (76%)	-0.11	0 100 100	23, 48, 80, 102	0
1	I	107/140 (76%)	-0.02	0 100 100	21, 53, 79, 112	0
1	J	108/140 (77%)	-0.15	2 (1%) 66 59	25, 43, 88, 117	0
1	K	104/140 (74%)	-0.12	0 100 100	30, 53, 84, 105	0
1	L	107/140 (76%)	-0.03	0 100 100	39, 71, 92, 101	0
All	All	1278/1680 (76%)	0.01	14 (1%) 80 75	21, 62, 99, 131	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	PRO	3.2
1	J	108	PHE	3.2
1	A	107	THR	3.1
1	D	36	ILE	2.7
1	C	107	THR	2.3
1	A	108	PHE	2.3
1	E	53	VAL	2.3
1	J	107	THR	2.3
1	B	107	THR	2.3
1	C	108	PHE	2.2
1	E	94	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	2	PRO	2.2
1	G	3	PRO	2.1
1	D	109	PRO	2.1

## 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 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.