



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:46 am BST

PDB ID : 6M7G
Title : Crystal structure of ArsN, N-acetyltransferase with substrate phosphinothricin from *Pseudomonas putida* KT2440
Authors : Venkadesh, S.; Dheeman, D.S.; Yoshinaga, M.; Kandavelu, P.; Rosen, B.P.
Deposited on : 2018-08-20
Resolution : 2.66 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
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

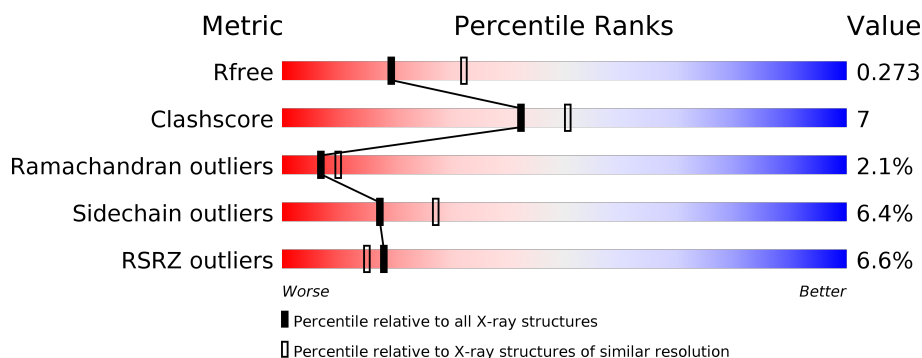
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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	207	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	207	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div></div> <div>15%</div> </div> </div>
1	C	207	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>13%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	207	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>•</div> <div>15%</div> </div> </div>
1	E	207	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>19%</div> <div></div> <div>15%</div> </div> </div>
1	F	207	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>19%</div> <div>•</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	207	
1	H	207	
1	I	207	
1	J	207	
1	K	207	
1	L	207	

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
2	PPQ	F	801	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16138 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 Phosphinothricin N-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1320	852	235	232	1			
1	B	175	Total	C	N	O	S	0	0	0
			1315	849	234	231	1			
1	C	176	Total	C	N	O	S	0	0	0
			1320	852	235	232	1			
1	D	176	Total	C	N	O	S	0	0	0
			1320	852	235	232	1			
1	E	176	Total	C	N	O	S	0	0	0
			1320	852	235	232	1			
1	F	176	Total	C	N	O	S	0	0	0
			1320	852	235	232	1			
1	G	176	Total	C	N	O	S	0	0	0
			1324	854	235	234	1			
1	H	174	Total	C	N	O	S	0	0	0
			1310	846	233	230	1			
1	I	176	Total	C	N	O	S	0	0	0
			1320	852	235	232	1			
1	J	176	Total	C	N	O	S	0	0	0
			1320	852	235	232	1			
1	K	176	Total	C	N	O	S	0	0	0
			1320	852	235	232	1			
1	L	176	Total	C	N	O	S	0	0	0
			1320	852	235	232	1			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	LEU	-	expression tag	UNP Q88LK7
A	185	GLY	-	expression tag	UNP Q88LK7
A	186	PRO	-	expression tag	UNP Q88LK7
A	187	GLU	-	expression tag	UNP Q88LK7
A	188	GLN	-	expression tag	UNP Q88LK7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	189	LYS	-	expression tag	UNP Q88LK7
A	190	LEU	-	expression tag	UNP Q88LK7
A	191	ILE	-	expression tag	UNP Q88LK7
A	192	SER	-	expression tag	UNP Q88LK7
A	193	GLU	-	expression tag	UNP Q88LK7
A	194	GLU	-	expression tag	UNP Q88LK7
A	195	ASP	-	expression tag	UNP Q88LK7
A	196	LEU	-	expression tag	UNP Q88LK7
A	197	ASN	-	expression tag	UNP Q88LK7
A	198	SER	-	expression tag	UNP Q88LK7
A	199	ALA	-	expression tag	UNP Q88LK7
A	200	VAL	-	expression tag	UNP Q88LK7
A	201	ASP	-	expression tag	UNP Q88LK7
A	202	HIS	-	expression tag	UNP Q88LK7
A	203	HIS	-	expression tag	UNP Q88LK7
A	204	HIS	-	expression tag	UNP Q88LK7
A	205	HIS	-	expression tag	UNP Q88LK7
A	206	HIS	-	expression tag	UNP Q88LK7
A	207	HIS	-	expression tag	UNP Q88LK7
B	184	LEU	-	expression tag	UNP Q88LK7
B	185	GLY	-	expression tag	UNP Q88LK7
B	186	PRO	-	expression tag	UNP Q88LK7
B	187	GLU	-	expression tag	UNP Q88LK7
B	188	GLN	-	expression tag	UNP Q88LK7
B	189	LYS	-	expression tag	UNP Q88LK7
B	190	LEU	-	expression tag	UNP Q88LK7
B	191	ILE	-	expression tag	UNP Q88LK7
B	192	SER	-	expression tag	UNP Q88LK7
B	193	GLU	-	expression tag	UNP Q88LK7
B	194	GLU	-	expression tag	UNP Q88LK7
B	195	ASP	-	expression tag	UNP Q88LK7
B	196	LEU	-	expression tag	UNP Q88LK7
B	197	ASN	-	expression tag	UNP Q88LK7
B	198	SER	-	expression tag	UNP Q88LK7
B	199	ALA	-	expression tag	UNP Q88LK7
B	200	VAL	-	expression tag	UNP Q88LK7
B	201	ASP	-	expression tag	UNP Q88LK7
B	202	HIS	-	expression tag	UNP Q88LK7
B	203	HIS	-	expression tag	UNP Q88LK7
B	204	HIS	-	expression tag	UNP Q88LK7
B	205	HIS	-	expression tag	UNP Q88LK7
B	206	HIS	-	expression tag	UNP Q88LK7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	207	HIS	-	expression tag	UNP Q88LK7
C	184	LEU	-	expression tag	UNP Q88LK7
C	185	GLY	-	expression tag	UNP Q88LK7
C	186	PRO	-	expression tag	UNP Q88LK7
C	187	GLU	-	expression tag	UNP Q88LK7
C	188	GLN	-	expression tag	UNP Q88LK7
C	189	LYS	-	expression tag	UNP Q88LK7
C	190	LEU	-	expression tag	UNP Q88LK7
C	191	ILE	-	expression tag	UNP Q88LK7
C	192	SER	-	expression tag	UNP Q88LK7
C	193	GLU	-	expression tag	UNP Q88LK7
C	194	GLU	-	expression tag	UNP Q88LK7
C	195	ASP	-	expression tag	UNP Q88LK7
C	196	LEU	-	expression tag	UNP Q88LK7
C	197	ASN	-	expression tag	UNP Q88LK7
C	198	SER	-	expression tag	UNP Q88LK7
C	199	ALA	-	expression tag	UNP Q88LK7
C	200	VAL	-	expression tag	UNP Q88LK7
C	201	ASP	-	expression tag	UNP Q88LK7
C	202	HIS	-	expression tag	UNP Q88LK7
C	203	HIS	-	expression tag	UNP Q88LK7
C	204	HIS	-	expression tag	UNP Q88LK7
C	205	HIS	-	expression tag	UNP Q88LK7
C	206	HIS	-	expression tag	UNP Q88LK7
C	207	HIS	-	expression tag	UNP Q88LK7
D	184	LEU	-	expression tag	UNP Q88LK7
D	185	GLY	-	expression tag	UNP Q88LK7
D	186	PRO	-	expression tag	UNP Q88LK7
D	187	GLU	-	expression tag	UNP Q88LK7
D	188	GLN	-	expression tag	UNP Q88LK7
D	189	LYS	-	expression tag	UNP Q88LK7
D	190	LEU	-	expression tag	UNP Q88LK7
D	191	ILE	-	expression tag	UNP Q88LK7
D	192	SER	-	expression tag	UNP Q88LK7
D	193	GLU	-	expression tag	UNP Q88LK7
D	194	GLU	-	expression tag	UNP Q88LK7
D	195	ASP	-	expression tag	UNP Q88LK7
D	196	LEU	-	expression tag	UNP Q88LK7
D	197	ASN	-	expression tag	UNP Q88LK7
D	198	SER	-	expression tag	UNP Q88LK7
D	199	ALA	-	expression tag	UNP Q88LK7
D	200	VAL	-	expression tag	UNP Q88LK7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	201	ASP	-	expression tag	UNP Q88LK7
D	202	HIS	-	expression tag	UNP Q88LK7
D	203	HIS	-	expression tag	UNP Q88LK7
D	204	HIS	-	expression tag	UNP Q88LK7
D	205	HIS	-	expression tag	UNP Q88LK7
D	206	HIS	-	expression tag	UNP Q88LK7
D	207	HIS	-	expression tag	UNP Q88LK7
E	184	LEU	-	expression tag	UNP Q88LK7
E	185	GLY	-	expression tag	UNP Q88LK7
E	186	PRO	-	expression tag	UNP Q88LK7
E	187	GLU	-	expression tag	UNP Q88LK7
E	188	GLN	-	expression tag	UNP Q88LK7
E	189	LYS	-	expression tag	UNP Q88LK7
E	190	LEU	-	expression tag	UNP Q88LK7
E	191	ILE	-	expression tag	UNP Q88LK7
E	192	SER	-	expression tag	UNP Q88LK7
E	193	GLU	-	expression tag	UNP Q88LK7
E	194	GLU	-	expression tag	UNP Q88LK7
E	195	ASP	-	expression tag	UNP Q88LK7
E	196	LEU	-	expression tag	UNP Q88LK7
E	197	ASN	-	expression tag	UNP Q88LK7
E	198	SER	-	expression tag	UNP Q88LK7
E	199	ALA	-	expression tag	UNP Q88LK7
E	200	VAL	-	expression tag	UNP Q88LK7
E	201	ASP	-	expression tag	UNP Q88LK7
E	202	HIS	-	expression tag	UNP Q88LK7
E	203	HIS	-	expression tag	UNP Q88LK7
E	204	HIS	-	expression tag	UNP Q88LK7
E	205	HIS	-	expression tag	UNP Q88LK7
E	206	HIS	-	expression tag	UNP Q88LK7
E	207	HIS	-	expression tag	UNP Q88LK7
F	184	LEU	-	expression tag	UNP Q88LK7
F	185	GLY	-	expression tag	UNP Q88LK7
F	186	PRO	-	expression tag	UNP Q88LK7
F	187	GLU	-	expression tag	UNP Q88LK7
F	188	GLN	-	expression tag	UNP Q88LK7
F	189	LYS	-	expression tag	UNP Q88LK7
F	190	LEU	-	expression tag	UNP Q88LK7
F	191	ILE	-	expression tag	UNP Q88LK7
F	192	SER	-	expression tag	UNP Q88LK7
F	193	GLU	-	expression tag	UNP Q88LK7
F	194	GLU	-	expression tag	UNP Q88LK7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	195	ASP	-	expression tag	UNP Q88LK7
F	196	LEU	-	expression tag	UNP Q88LK7
F	197	ASN	-	expression tag	UNP Q88LK7
F	198	SER	-	expression tag	UNP Q88LK7
F	199	ALA	-	expression tag	UNP Q88LK7
F	200	VAL	-	expression tag	UNP Q88LK7
F	201	ASP	-	expression tag	UNP Q88LK7
F	202	HIS	-	expression tag	UNP Q88LK7
F	203	HIS	-	expression tag	UNP Q88LK7
F	204	HIS	-	expression tag	UNP Q88LK7
F	205	HIS	-	expression tag	UNP Q88LK7
F	206	HIS	-	expression tag	UNP Q88LK7
F	207	HIS	-	expression tag	UNP Q88LK7
G	184	LEU	-	expression tag	UNP Q88LK7
G	185	GLY	-	expression tag	UNP Q88LK7
G	186	PRO	-	expression tag	UNP Q88LK7
G	187	GLU	-	expression tag	UNP Q88LK7
G	188	GLN	-	expression tag	UNP Q88LK7
G	189	LYS	-	expression tag	UNP Q88LK7
G	190	LEU	-	expression tag	UNP Q88LK7
G	191	ILE	-	expression tag	UNP Q88LK7
G	192	SER	-	expression tag	UNP Q88LK7
G	193	GLU	-	expression tag	UNP Q88LK7
G	194	GLU	-	expression tag	UNP Q88LK7
G	195	ASP	-	expression tag	UNP Q88LK7
G	196	LEU	-	expression tag	UNP Q88LK7
G	197	ASN	-	expression tag	UNP Q88LK7
G	198	SER	-	expression tag	UNP Q88LK7
G	199	ALA	-	expression tag	UNP Q88LK7
G	200	VAL	-	expression tag	UNP Q88LK7
G	201	ASP	-	expression tag	UNP Q88LK7
G	202	HIS	-	expression tag	UNP Q88LK7
G	203	HIS	-	expression tag	UNP Q88LK7
G	204	HIS	-	expression tag	UNP Q88LK7
G	205	HIS	-	expression tag	UNP Q88LK7
G	206	HIS	-	expression tag	UNP Q88LK7
G	207	HIS	-	expression tag	UNP Q88LK7
H	184	LEU	-	expression tag	UNP Q88LK7
H	185	GLY	-	expression tag	UNP Q88LK7
H	186	PRO	-	expression tag	UNP Q88LK7
H	187	GLU	-	expression tag	UNP Q88LK7
H	188	GLN	-	expression tag	UNP Q88LK7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	189	LYS	-	expression tag	UNP Q88LK7
H	190	LEU	-	expression tag	UNP Q88LK7
H	191	ILE	-	expression tag	UNP Q88LK7
H	192	SER	-	expression tag	UNP Q88LK7
H	193	GLU	-	expression tag	UNP Q88LK7
H	194	GLU	-	expression tag	UNP Q88LK7
H	195	ASP	-	expression tag	UNP Q88LK7
H	196	LEU	-	expression tag	UNP Q88LK7
H	197	ASN	-	expression tag	UNP Q88LK7
H	198	SER	-	expression tag	UNP Q88LK7
H	199	ALA	-	expression tag	UNP Q88LK7
H	200	VAL	-	expression tag	UNP Q88LK7
H	201	ASP	-	expression tag	UNP Q88LK7
H	202	HIS	-	expression tag	UNP Q88LK7
H	203	HIS	-	expression tag	UNP Q88LK7
H	204	HIS	-	expression tag	UNP Q88LK7
H	205	HIS	-	expression tag	UNP Q88LK7
H	206	HIS	-	expression tag	UNP Q88LK7
H	207	HIS	-	expression tag	UNP Q88LK7
I	184	LEU	-	expression tag	UNP Q88LK7
I	185	GLY	-	expression tag	UNP Q88LK7
I	186	PRO	-	expression tag	UNP Q88LK7
I	187	GLU	-	expression tag	UNP Q88LK7
I	188	GLN	-	expression tag	UNP Q88LK7
I	189	LYS	-	expression tag	UNP Q88LK7
I	190	LEU	-	expression tag	UNP Q88LK7
I	191	ILE	-	expression tag	UNP Q88LK7
I	192	SER	-	expression tag	UNP Q88LK7
I	193	GLU	-	expression tag	UNP Q88LK7
I	194	GLU	-	expression tag	UNP Q88LK7
I	195	ASP	-	expression tag	UNP Q88LK7
I	196	LEU	-	expression tag	UNP Q88LK7
I	197	ASN	-	expression tag	UNP Q88LK7
I	198	SER	-	expression tag	UNP Q88LK7
I	199	ALA	-	expression tag	UNP Q88LK7
I	200	VAL	-	expression tag	UNP Q88LK7
I	201	ASP	-	expression tag	UNP Q88LK7
I	202	HIS	-	expression tag	UNP Q88LK7
I	203	HIS	-	expression tag	UNP Q88LK7
I	204	HIS	-	expression tag	UNP Q88LK7
I	205	HIS	-	expression tag	UNP Q88LK7
I	206	HIS	-	expression tag	UNP Q88LK7

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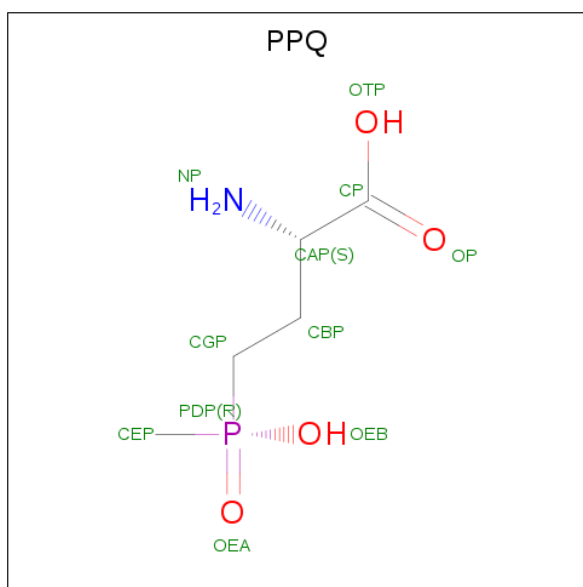
Chain	Residue	Modelled	Actual	Comment	Reference
I	207	HIS	-	expression tag	UNP Q88LK7
J	184	LEU	-	expression tag	UNP Q88LK7
J	185	GLY	-	expression tag	UNP Q88LK7
J	186	PRO	-	expression tag	UNP Q88LK7
J	187	GLU	-	expression tag	UNP Q88LK7
J	188	GLN	-	expression tag	UNP Q88LK7
J	189	LYS	-	expression tag	UNP Q88LK7
J	190	LEU	-	expression tag	UNP Q88LK7
J	191	ILE	-	expression tag	UNP Q88LK7
J	192	SER	-	expression tag	UNP Q88LK7
J	193	GLU	-	expression tag	UNP Q88LK7
J	194	GLU	-	expression tag	UNP Q88LK7
J	195	ASP	-	expression tag	UNP Q88LK7
J	196	LEU	-	expression tag	UNP Q88LK7
J	197	ASN	-	expression tag	UNP Q88LK7
J	198	SER	-	expression tag	UNP Q88LK7
J	199	ALA	-	expression tag	UNP Q88LK7
J	200	VAL	-	expression tag	UNP Q88LK7
J	201	ASP	-	expression tag	UNP Q88LK7
J	202	HIS	-	expression tag	UNP Q88LK7
J	203	HIS	-	expression tag	UNP Q88LK7
J	204	HIS	-	expression tag	UNP Q88LK7
J	205	HIS	-	expression tag	UNP Q88LK7
J	206	HIS	-	expression tag	UNP Q88LK7
J	207	HIS	-	expression tag	UNP Q88LK7
K	184	LEU	-	expression tag	UNP Q88LK7
K	185	GLY	-	expression tag	UNP Q88LK7
K	186	PRO	-	expression tag	UNP Q88LK7
K	187	GLU	-	expression tag	UNP Q88LK7
K	188	GLN	-	expression tag	UNP Q88LK7
K	189	LYS	-	expression tag	UNP Q88LK7
K	190	LEU	-	expression tag	UNP Q88LK7
K	191	ILE	-	expression tag	UNP Q88LK7
K	192	SER	-	expression tag	UNP Q88LK7
K	193	GLU	-	expression tag	UNP Q88LK7
K	194	GLU	-	expression tag	UNP Q88LK7
K	195	ASP	-	expression tag	UNP Q88LK7
K	196	LEU	-	expression tag	UNP Q88LK7
K	197	ASN	-	expression tag	UNP Q88LK7
K	198	SER	-	expression tag	UNP Q88LK7
K	199	ALA	-	expression tag	UNP Q88LK7
K	200	VAL	-	expression tag	UNP Q88LK7

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Chain	Residue	Modelled	Actual	Comment	Reference
K	201	ASP	-	expression tag	UNP Q88LK7
K	202	HIS	-	expression tag	UNP Q88LK7
K	203	HIS	-	expression tag	UNP Q88LK7
K	204	HIS	-	expression tag	UNP Q88LK7
K	205	HIS	-	expression tag	UNP Q88LK7
K	206	HIS	-	expression tag	UNP Q88LK7
K	207	HIS	-	expression tag	UNP Q88LK7
L	184	LEU	-	expression tag	UNP Q88LK7
L	185	GLY	-	expression tag	UNP Q88LK7
L	186	PRO	-	expression tag	UNP Q88LK7
L	187	GLU	-	expression tag	UNP Q88LK7
L	188	GLN	-	expression tag	UNP Q88LK7
L	189	LYS	-	expression tag	UNP Q88LK7
L	190	LEU	-	expression tag	UNP Q88LK7
L	191	ILE	-	expression tag	UNP Q88LK7
L	192	SER	-	expression tag	UNP Q88LK7
L	193	GLU	-	expression tag	UNP Q88LK7
L	194	GLU	-	expression tag	UNP Q88LK7
L	195	ASP	-	expression tag	UNP Q88LK7
L	196	LEU	-	expression tag	UNP Q88LK7
L	197	ASN	-	expression tag	UNP Q88LK7
L	198	SER	-	expression tag	UNP Q88LK7
L	199	ALA	-	expression tag	UNP Q88LK7
L	200	VAL	-	expression tag	UNP Q88LK7
L	201	ASP	-	expression tag	UNP Q88LK7
L	202	HIS	-	expression tag	UNP Q88LK7
L	203	HIS	-	expression tag	UNP Q88LK7
L	204	HIS	-	expression tag	UNP Q88LK7
L	205	HIS	-	expression tag	UNP Q88LK7
L	206	HIS	-	expression tag	UNP Q88LK7
L	207	HIS	-	expression tag	UNP Q88LK7

- Molecule 2 is PHOSPHINOTHRICIN (three-letter code: PPQ) (formula: C₅H₁₂NO₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	D	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	E	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	F	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	H	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	L	1	Total	C	N	O	P	0	0
			11	5	1	4	1		

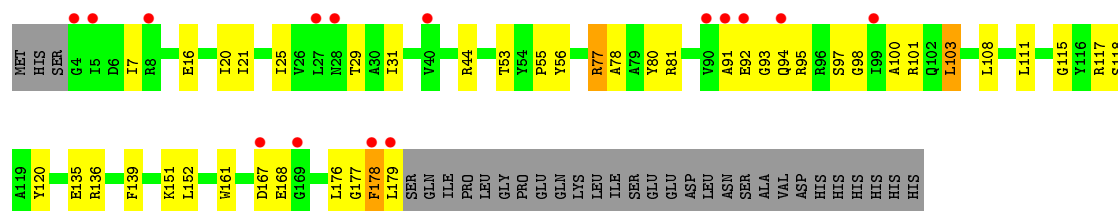
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	16	Total	O	0	0
			16	16		
3	C	17	Total	O	0	0
			17	17		
3	D	8	Total	O	0	0
			8	8		

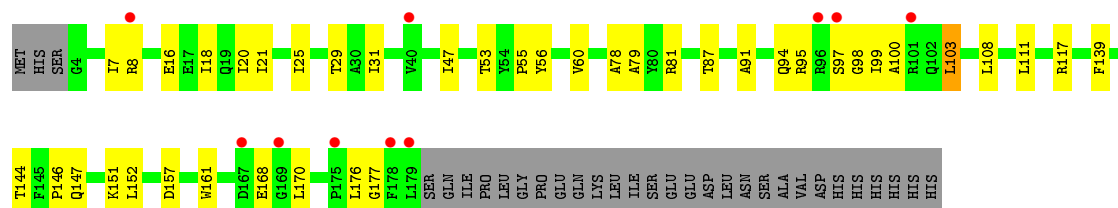
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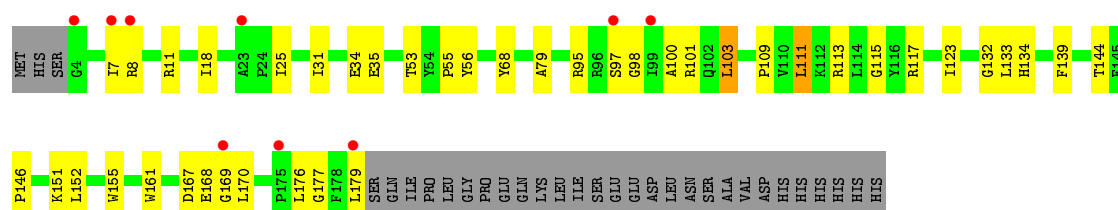
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	22	Total 22	O 22	0	0
3	F	21	Total 21	O 21	0	0
3	G	20	Total 20	O 20	0	0
3	H	10	Total 10	O 10	0	0
3	I	17	Total 17	O 17	0	0
3	J	24	Total 24	O 24	0	0
3	K	26	Total 26	O 26	0	0
3	L	19	Total 19	O 19	0	0



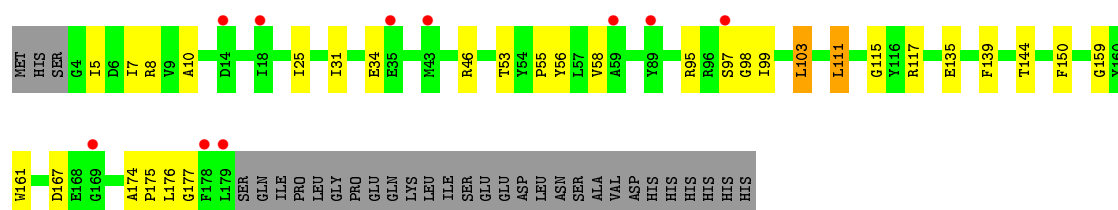
• Molecule 1: Phosphinothricin N-acetyltransferase



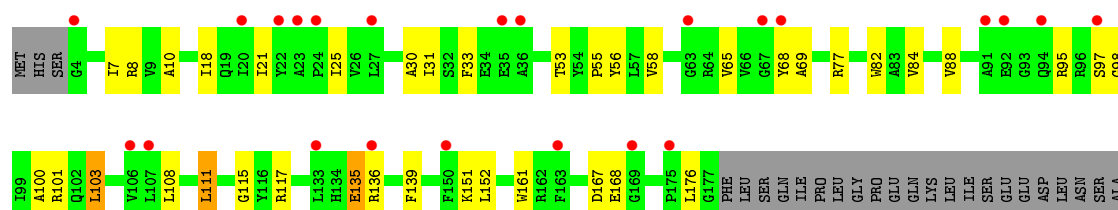
• Molecule 1: Phosphinothricin N-acetyltransferase



• Molecule 1: Phosphinothricin N-acetyltransferase



• Molecule 1: Phosphinothricin N-acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.84Å 142.69Å 178.31Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	39.91 – 2.66 39.91 – 2.66	Depositor EDS
% Data completeness (in resolution range)	91.3 (39.91-2.66) 91.5 (39.91-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.224 , 0.273 0.225 , 0.273	Depositor DCC
R_{free} test set	3560 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16138	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3968e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/1354	0.44	0/1851
1	B	0.26	0/1349	0.43	0/1844
1	C	0.27	0/1354	0.45	0/1851
1	D	0.26	0/1354	0.45	0/1851
1	E	0.28	0/1354	0.45	0/1851
1	F	0.27	0/1354	0.44	0/1851
1	G	0.27	0/1358	0.43	0/1856
1	H	0.27	0/1344	0.44	0/1837
1	I	0.27	0/1354	0.44	0/1851
1	J	0.27	0/1354	0.44	0/1851
1	K	0.28	0/1354	0.44	0/1851
1	L	0.28	0/1354	0.43	0/1851
All	All	0.27	0/16237	0.44	0/22196

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	1320	0	1250	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1315	0	1248	15	0
1	C	1320	0	1250	22	0
1	D	1320	0	1250	24	0
1	E	1320	0	1250	22	0
1	F	1320	0	1250	25	0
1	G	1324	0	1254	15	0
1	H	1310	0	1246	19	0
1	I	1320	0	1250	18	0
1	J	1320	0	1250	20	0
1	K	1320	0	1250	20	0
1	L	1320	0	1250	16	0
2	A	11	0	10	1	0
2	C	22	0	20	5	0
2	D	11	0	10	2	0
2	E	11	0	10	1	0
2	F	11	0	10	0	0
2	H	11	0	10	0	0
2	L	11	0	10	0	0
3	A	21	0	0	0	0
3	B	16	0	0	2	0
3	C	17	0	0	0	0
3	D	8	0	0	1	0
3	E	22	0	0	0	0
3	F	21	0	0	0	0
3	G	20	0	0	0	0
3	H	10	0	0	0	0
3	I	17	0	0	0	0
3	J	24	0	0	0	0
3	K	26	0	0	1	0
3	L	19	0	0	0	0
All	All	16138	0	15078	213	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 7.

All (213) 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:D:97:SER:HB2	1:D:100:ALA:H	1.35	0.91
1:B:97:SER:HB2	1:B:100:ALA:H	1.47	0.77
1:J:55:PRO:HA	1:J:176:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:PRO:HA	1:L:176:LEU:HD22	1.69	0.75
1:F:55:PRO:HA	1:F:176:LEU:HD22	1.68	0.75
1:E:55:PRO:HA	1:E:176:LEU:HD22	1.69	0.74
1:C:97:SER:HB2	1:C:100:ALA:H	1.51	0.73
1:G:7:ILE:HD12	1:G:103:LEU:HD13	1.71	0.72
1:I:97:SER:HB2	1:I:100:ALA:H	1.54	0.71
1:I:115:GLY:O	1:I:117:ARG:NH1	2.24	0.70
1:I:55:PRO:HA	1:I:176:LEU:HD22	1.73	0.70
1:A:55:PRO:HA	1:A:176:LEU:HD22	1.74	0.69
1:G:55:PRO:HA	1:G:176:LEU:HD22	1.74	0.68
1:J:97:SER:HB2	1:J:100:ALA:H	1.58	0.68
1:I:101:ARG:HD3	1:I:136:ARG:HH12	1.58	0.68
1:H:97:SER:HB2	1:H:100:ALA:H	1.57	0.67
1:L:55:PRO:HB3	1:L:176:LEU:HD13	1.76	0.67
1:K:55:PRO:HA	1:K:176:LEU:HD22	1.75	0.67
1:A:93:GLY:HA3	1:D:29:THR:HG22	1.75	0.67
1:C:55:PRO:HA	1:C:176:LEU:HD22	1.77	0.67
1:E:78:ALA:HB1	1:E:81:ARG:HH11	1.59	0.67
1:H:55:PRO:HA	1:H:176:LEU:HD22	1.76	0.67
1:F:97:SER:HB2	1:F:100:ALA:H	1.61	0.66
1:E:20:ILE:HD11	1:L:132:GLY:HA2	1.77	0.66
1:D:55:PRO:HA	1:D:176:LEU:HD22	1.78	0.66
1:J:7:ILE:HD12	1:J:103:LEU:HD13	1.78	0.65
1:D:7:ILE:HD12	1:D:103:LEU:HD13	1.78	0.64
1:H:139:PHE:HB3	1:H:161:TRP:HB3	1.79	0.64
1:F:139:PHE:HB3	1:F:161:TRP:HB3	1.80	0.64
1:K:139:PHE:HB3	1:K:161:TRP:HB3	1.80	0.64
1:I:7:ILE:HD12	1:I:103:LEU:HD13	1.80	0.64
1:C:139:PHE:HB3	1:C:161:TRP:HB3	1.81	0.63
1:F:101:ARG:HB2	1:F:133:LEU:HD11	1.80	0.63
1:K:78:ALA:HB1	1:K:81:ARG:HH11	1.64	0.63
1:B:151:LYS:HG2	1:B:152:LEU:HG	1.82	0.62
1:C:7:ILE:HD12	1:C:103:LEU:HD13	1.80	0.62
1:G:139:PHE:HB3	1:G:161:TRP:HB3	1.80	0.62
1:E:139:PHE:HB3	1:E:161:TRP:HB3	1.83	0.61
1:G:97:SER:HB2	1:G:99:ILE:H	1.66	0.61
1:A:7:ILE:HD12	1:A:103:LEU:HD13	1.83	0.60
1:A:117:ARG:HH21	1:A:170:LEU:H	1.49	0.60
1:I:24:PRO:HG3	1:J:20:ILE:HD11	1.82	0.60
1:J:25:ILE:HG23	1:J:31:ILE:HB	1.83	0.60
1:A:139:PHE:HB3	1:A:161:TRP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:10:ALA:HB2	1:J:58:VAL:HG13	1.83	0.60
1:D:139:PHE:HB3	1:D:161:TRP:HB3	1.82	0.59
1:A:97:SER:HB2	1:A:99:ILE:N	2.18	0.59
1:D:115:GLY:O	1:D:117:ARG:NH1	2.34	0.59
1:H:7:ILE:HD12	1:H:103:LEU:HD13	1.84	0.59
1:H:101:ARG:HD3	1:H:136:ARG:NH1	2.18	0.58
1:D:80:TYR:HE2	2:D:801:PPQ:HBP2	1.68	0.58
1:J:115:GLY:O	1:J:117:ARG:NH1	2.37	0.58
1:J:139:PHE:HB3	1:J:161:TRP:HB3	1.85	0.58
1:E:151:LYS:HG2	1:E:152:LEU:HG	1.86	0.57
1:A:151:LYS:HG2	1:A:152:LEU:HG	1.84	0.57
1:D:151:LYS:HG2	1:D:152:LEU:HG	1.86	0.57
1:B:139:PHE:HB3	1:B:161:TRP:HB3	1.85	0.57
1:E:7:ILE:HD12	1:E:103:LEU:HD13	1.86	0.57
1:A:28:ASN:HB3	1:D:94:GLN:HB2	1.86	0.57
1:K:97:SER:HB2	1:K:99:ILE:N	2.20	0.57
1:C:53:THR:HA	1:C:175:PRO:HB3	1.85	0.57
1:I:151:LYS:HG2	1:I:152:LEU:HG	1.86	0.57
1:F:151:LYS:HG2	1:F:152:LEU:HG	1.86	0.57
1:H:151:LYS:HG2	1:H:152:LEU:HG	1.87	0.56
1:D:176:LEU:O	1:D:178:PHE:N	2.38	0.56
1:E:97:SER:HB2	1:E:100:ALA:H	1.68	0.56
1:L:139:PHE:HB3	1:L:161:TRP:HB3	1.87	0.56
1:B:55:PRO:HA	1:B:176:LEU:HD22	1.86	0.56
1:B:98:GLY:N	3:B:301:HOH:O	2.35	0.56
1:K:55:PRO:HB3	1:K:176:LEU:HD13	1.87	0.56
1:G:25:ILE:HG23	1:G:31:ILE:HB	1.86	0.56
1:H:115:GLY:O	1:H:117:ARG:NH1	2.39	0.56
1:E:87:THR:HG23	2:E:801:PPQ:HNP2	1.71	0.56
1:H:25:ILE:HG23	1:H:31:ILE:HB	1.89	0.55
1:L:117:ARG:NE	1:L:167:ASP:HB2	2.22	0.55
1:F:7:ILE:HD12	1:F:103:LEU:HD13	1.88	0.55
1:G:10:ALA:HB2	1:G:58:VAL:HG13	1.89	0.55
1:G:97:SER:HB2	1:G:99:ILE:N	2.22	0.55
1:E:21:ILE:HG12	1:E:91:ALA:HB2	1.90	0.54
1:I:101:ARG:HD3	1:I:136:ARG:NH1	2.23	0.54
1:E:97:SER:HB2	1:E:99:ILE:N	2.23	0.54
1:B:7:ILE:HD12	1:B:103:LEU:HD13	1.89	0.54
1:F:34:GLU:O	1:F:151:LYS:NZ	2.35	0.53
1:B:101:ARG:HD3	1:B:136:ARG:HH12	1.74	0.53
1:B:21:ILE:HG23	1:B:91:ALA:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ALA:HB3	1:I:33:PHE:HB3	1.91	0.53
1:J:151:LYS:HG2	1:J:152:LEU:HG	1.89	0.53
1:B:115:GLY:O	1:B:117:ARG:NH1	2.41	0.53
1:C:117:ARG:HH21	1:C:170:LEU:H	1.55	0.52
1:D:25:ILE:HG23	1:D:31:ILE:HB	1.91	0.52
1:K:25:ILE:HG23	1:K:31:ILE:HB	1.92	0.52
1:A:27:LEU:HD12	1:D:20:ILE:HG21	1.91	0.52
1:D:101:ARG:HD3	1:D:136:ARG:HH12	1.75	0.52
1:F:35:GLU:OE1	1:J:81:ARG:NH1	2.33	0.51
1:H:82:TRP:HB3	1:H:117:ARG:HG2	1.93	0.51
1:L:101:ARG:HB2	1:L:133:LEU:HD11	1.91	0.51
1:H:101:ARG:HD3	1:H:136:ARG:HH12	1.75	0.51
1:B:155:TRP:CH2	1:C:117:ARG:HG3	2.46	0.51
1:I:59:ALA:N	1:I:67:GLY:O	2.36	0.51
1:K:21:ILE:HG12	1:K:91:ALA:HB2	1.93	0.51
1:F:115:GLY:O	1:F:117:ARG:NH1	2.43	0.50
1:D:91:ALA:O	1:D:93:GLY:N	2.45	0.50
1:E:117:ARG:HH21	1:E:170:LEU:H	1.58	0.50
1:D:21:ILE:HG23	1:D:91:ALA:HA	1.92	0.50
1:K:115:GLY:O	1:K:117:ARG:NH1	2.44	0.50
1:K:16:GLU:O	1:K:20:ILE:HD13	2.12	0.50
1:L:7:ILE:HD12	1:L:103:LEU:HD13	1.94	0.49
1:E:25:ILE:HG23	1:E:31:ILE:HB	1.93	0.49
1:G:115:GLY:O	1:G:117:ARG:NH1	2.45	0.49
1:G:117:ARG:HG3	1:L:155:TRP:CH2	2.48	0.49
1:G:144:THR:HA	1:G:159:GLY:HA2	1.94	0.49
1:L:109:PRO:O	1:L:113:ARG:HG3	2.12	0.49
1:A:55:PRO:HB3	1:A:176:LEU:HD13	1.95	0.49
1:B:113:ARG:NH2	3:B:304:HOH:O	2.39	0.48
1:C:75:ARG:HB3	2:C:802:PPQ:OP	2.12	0.48
1:A:77:ARG:NH1	2:A:801:PPQ:OEA	2.43	0.48
1:E:16:GLU:O	1:E:20:ILE:HD13	2.14	0.48
1:F:132:GLY:HA2	1:K:20:ILE:HD11	1.95	0.48
1:D:44:ARG:NE	3:D:901:HOH:O	2.44	0.48
1:J:34:GLU:OE2	1:J:46:ARG:NH2	2.35	0.48
1:E:18:ILE:HD12	1:E:47:ILE:HD11	1.94	0.48
1:L:25:ILE:HG23	1:L:31:ILE:HB	1.96	0.48
1:D:97:SER:HA	1:D:98:GLY:HA3	1.61	0.48
1:F:97:SER:HA	1:F:98:GLY:HA3	1.59	0.48
1:C:117:ARG:NE	1:C:167:ASP:HB2	2.28	0.48
1:H:30:ALA:HB1	1:H:33:PHE:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:PRO:HB3	1:E:176:LEU:HD13	1.96	0.47
1:K:78:ALA:HB1	1:K:81:ARG:NH1	2.29	0.47
1:L:94:GLN:HG2	1:L:99:ILE:HD11	1.95	0.47
1:A:29:THR:HG22	1:D:93:GLY:HA3	1.96	0.47
1:D:77:ARG:HD3	2:D:801:PPQ:HBP1	1.96	0.47
1:F:55:PRO:HB3	1:F:176:LEU:HD13	1.97	0.47
1:H:135:GLU:HB3	1:J:136:ARG:HD3	1.95	0.47
1:J:97:SER:HA	1:J:98:GLY:HA3	1.66	0.47
1:L:97:SER:HB2	1:L:100:ALA:H	1.79	0.47
1:H:55:PRO:HB3	1:H:176:LEU:HD13	1.96	0.47
1:J:55:PRO:HB3	1:J:176:LEU:HD13	1.96	0.47
1:K:162:ARG:NH1	3:K:301:HOH:O	2.37	0.47
1:I:84:VAL:HG11	1:I:111:LEU:HG	1.95	0.47
1:C:10:ALA:HB2	1:C:58:VAL:HG13	1.97	0.46
1:B:117:ARG:NE	1:B:167:ASP:HB2	2.29	0.46
1:C:77:ARG:HH11	2:C:802:PPQ:HBP1	1.80	0.46
1:C:75:ARG:HD3	2:C:802:PPQ:OP	2.15	0.46
1:H:10:ALA:HB2	1:H:58:VAL:HG13	1.97	0.46
1:I:97:SER:HA	1:I:98:GLY:HA3	1.69	0.46
1:K:144:THR:O	1:K:146:PRO:HD3	2.16	0.46
1:F:132:GLY:CA	1:K:20:ILE:HD11	2.45	0.46
1:I:25:ILE:HG23	1:I:31:ILE:HB	1.96	0.46
1:K:18:ILE:HD12	1:K:47:ILE:HD11	1.98	0.46
1:J:144:THR:HA	1:J:159:GLY:HA2	1.97	0.46
1:D:117:ARG:NE	1:D:167:ASP:HB2	2.30	0.46
1:F:109:PRO:O	1:F:113:ARG:HG3	2.16	0.46
1:E:147:GLN:N	1:E:157:ASP:OD1	2.40	0.45
1:E:8:ARG:HH11	1:E:60:VAL:HG21	1.80	0.45
1:C:97:SER:HA	1:C:98:GLY:HA3	1.68	0.45
1:F:117:ARG:NE	1:F:167:ASP:HB2	2.30	0.45
1:H:97:SER:HA	1:H:98:GLY:HA3	1.64	0.45
1:C:55:PRO:HB3	1:C:176:LEU:HD13	1.98	0.45
1:C:77:ARG:NH1	2:C:802:PPQ:HBP1	2.31	0.45
1:C:78:ALA:HB1	1:C:81:ARG:NH1	2.31	0.45
1:E:97:SER:HA	1:E:98:GLY:HA3	1.68	0.44
1:F:168:GLU:HA	1:J:155:TRP:HE1	1.81	0.44
1:K:22:TYR:OH	1:K:34:GLU:OE1	2.31	0.44
1:E:20:ILE:HD11	1:L:132:GLY:CA	2.45	0.44
1:F:18:ILE:HG23	1:F:68:TYR:CE1	2.53	0.44
1:I:139:PHE:HB3	1:I:161:TRP:HB3	1.99	0.44
1:I:97:SER:HB2	1:I:100:ALA:N	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:NE	1:A:167:ASP:HB2	2.32	0.44
1:D:179:LEU:HA	1:E:7:ILE:O	2.17	0.44
1:A:78:ALA:HB1	1:A:81:ARG:NH1	2.33	0.44
1:G:34:GLU:OE2	1:G:46:ARG:NH2	2.43	0.44
1:G:97:SER:HA	1:G:98:GLY:HA3	1.68	0.44
1:D:78:ALA:HB1	1:D:81:ARG:NH1	2.34	0.43
1:C:9:VAL:O	1:F:11:ARG:NH2	2.51	0.43
1:H:18:ILE:HG23	1:H:68:TYR:CE1	2.52	0.43
1:K:34:GLU:O	1:K:151:LYS:NZ	2.40	0.43
1:A:10:ALA:HB2	1:A:58:VAL:HG13	2.01	0.43
1:D:118:SER:HG	1:D:120:TYR:HE2	1.65	0.43
1:C:117:ARG:HD2	1:C:166:GLY:O	2.17	0.43
1:K:97:SER:HB2	1:K:100:ALA:H	1.83	0.43
1:F:155:TRP:HE1	1:J:168:GLU:HA	1.84	0.42
1:G:150:PHE:HB3	1:L:82:TRP:CZ3	2.54	0.42
1:B:9:VAL:HA	1:B:57:LEU:HD23	2.01	0.42
1:B:91:ALA:O	1:B:93:GLY:N	2.53	0.42
1:C:75:ARG:NH2	2:C:802:PPQ:HNP2	2.16	0.42
1:F:25:ILE:HG23	1:F:31:ILE:HB	2.01	0.42
1:I:117:ARG:NE	1:I:167:ASP:HB2	2.34	0.42
1:I:21:ILE:HD11	1:I:65:VAL:HG12	2.01	0.42
1:J:68:TYR:HH	1:J:89:TYR:HD2	1.64	0.42
1:A:117:ARG:HD2	1:A:166:GLY:O	2.18	0.42
1:E:144:THR:O	1:E:146:PRO:HD3	2.20	0.42
1:C:7:ILE:H	1:F:179:LEU:C	2.23	0.42
1:K:21:ILE:HG23	1:K:91:ALA:HA	2.01	0.42
1:F:111:LEU:HA	1:F:111:LEU:HD12	1.95	0.42
1:G:111:LEU:HA	1:G:111:LEU:HD12	1.82	0.41
1:L:151:LYS:HG2	1:L:152:LEU:HG	2.01	0.41
1:D:16:GLU:O	1:D:20:ILE:HD13	2.19	0.41
1:H:84:VAL:HG11	1:H:111:LEU:HG	2.02	0.41
1:L:97:SER:HA	1:L:98:GLY:HA3	1.59	0.41
1:A:97:SER:HA	1:A:98:GLY:HA3	1.72	0.41
1:H:69:ALA:HB2	1:H:88:VAL:HG22	2.01	0.41
1:C:69:ALA:HB2	1:C:103:LEU:HG	2.01	0.41
1:F:123:ILE:HD11	1:F:134:HIS:ND1	2.36	0.41
1:B:97:SER:HA	1:B:98:GLY:HA3	1.65	0.41
1:C:47:ILE:HG12	1:C:56:TYR:CE2	2.55	0.41
1:F:79:ALA:HB3	1:J:33:PHE:HB3	2.03	0.41
1:F:144:THR:O	1:F:146:PRO:HD3	2.20	0.41
1:I:55:PRO:HB3	1:I:176:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:HA	1:A:175:PRO:HB3	2.02	0.40
1:G:174:ALA:HA	1:G:175:PRO:HD3	1.86	0.40
1:K:97:SER:HB2	1:K:99:ILE:H	1.87	0.40
1:J:78:ALA:HB1	1:J:81:ARG:NH1	2.37	0.40
1:H:21:ILE:HD11	1:H:65:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	174/207 (84%)	162 (93%)	7 (4%)	5 (3%)	4	6
1	B	173/207 (84%)	160 (92%)	8 (5%)	5 (3%)	4	6
1	C	174/207 (84%)	162 (93%)	9 (5%)	3 (2%)	9	13
1	D	174/207 (84%)	160 (92%)	9 (5%)	5 (3%)	4	6
1	E	174/207 (84%)	164 (94%)	7 (4%)	3 (2%)	9	13
1	F	174/207 (84%)	162 (93%)	8 (5%)	4 (2%)	6	8
1	G	174/207 (84%)	164 (94%)	7 (4%)	3 (2%)	9	13
1	H	172/207 (83%)	165 (96%)	5 (3%)	2 (1%)	13	19
1	I	174/207 (84%)	164 (94%)	6 (3%)	4 (2%)	6	8
1	J	174/207 (84%)	164 (94%)	7 (4%)	3 (2%)	9	13
1	K	174/207 (84%)	164 (94%)	6 (3%)	4 (2%)	6	8
1	L	174/207 (84%)	164 (94%)	8 (5%)	2 (1%)	14	21
All	All	2085/2484 (84%)	1955 (94%)	87 (4%)	43 (2%)	7	10

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	92	GLU
1	D	177	GLY
1	A	177	GLY
1	B	95	ARG
1	B	177	GLY
1	C	177	GLY
1	D	95	ARG
1	D	178	PHE
1	E	95	ARG
1	E	177	GLY
1	F	95	ARG
1	F	177	GLY
1	G	95	ARG
1	H	95	ARG
1	I	95	ARG
1	J	95	ARG
1	K	95	ARG
1	K	168	GLU
1	K	177	GLY
1	L	95	ARG
1	L	177	GLY
1	A	95	ARG
1	B	92	GLU
1	C	95	ARG
1	E	168	GLU
1	I	168	GLU
1	A	93	GLY
1	H	168	GLU
1	I	177	GLY
1	A	168	GLU
1	D	168	GLU
1	F	170	LEU
1	I	5	ILE
1	B	168	GLU
1	C	93	GLY
1	F	169	GLY
1	J	177	GLY
1	G	5	ILE
1	J	5	ILE
1	A	5	ILE
1	B	5	ILE
1	K	5	ILE
1	G	177	GLY

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	121/170 (71%)	114 (94%)	7 (6%)	20	31
1	B	121/170 (71%)	112 (93%)	9 (7%)	13	21
1	C	121/170 (71%)	112 (93%)	9 (7%)	13	21
1	D	121/170 (71%)	114 (94%)	7 (6%)	20	31
1	E	121/170 (71%)	114 (94%)	7 (6%)	20	31
1	F	121/170 (71%)	116 (96%)	5 (4%)	30	46
1	G	122/170 (72%)	115 (94%)	7 (6%)	20	31
1	H	121/170 (71%)	112 (93%)	9 (7%)	13	21
1	I	121/170 (71%)	111 (92%)	10 (8%)	11	16
1	J	121/170 (71%)	113 (93%)	8 (7%)	16	25
1	K	121/170 (71%)	114 (94%)	7 (6%)	20	31
1	L	121/170 (71%)	113 (93%)	8 (7%)	16	25
All	All	1453/2040 (71%)	1360 (94%)	93 (6%)	17	27

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	28	ASN
1	A	53	THR
1	A	56	TYR
1	A	103	LEU
1	A	111	LEU
1	A	135	GLU
1	B	53	THR
1	B	56	TYR
1	B	77	ARG
1	B	87	THR
1	B	103	LEU
1	B	104	TYR
1	B	108	LEU

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Mol	Chain	Res	Type
1	B	111	LEU
1	B	135	GLU
1	C	28	ASN
1	C	53	THR
1	C	56	TYR
1	C	77	ARG
1	C	90	VAL
1	C	94	GLN
1	C	103	LEU
1	C	111	LEU
1	C	167	ASP
1	D	53	THR
1	D	56	TYR
1	D	77	ARG
1	D	103	LEU
1	D	108	LEU
1	D	111	LEU
1	D	135	GLU
1	E	29	THR
1	E	53	THR
1	E	56	TYR
1	E	94	GLN
1	E	103	LEU
1	E	108	LEU
1	E	111	LEU
1	F	8	ARG
1	F	53	THR
1	F	56	TYR
1	F	103	LEU
1	F	111	LEU
1	G	8	ARG
1	G	53	THR
1	G	56	TYR
1	G	103	LEU
1	G	111	LEU
1	G	135	GLU
1	G	167	ASP
1	H	8	ARG
1	H	53	THR
1	H	56	TYR
1	H	77	ARG
1	H	103	LEU

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Mol	Chain	Res	Type
1	H	108	LEU
1	H	111	LEU
1	H	135	GLU
1	H	167	ASP
1	I	8	ARG
1	I	53	THR
1	I	56	TYR
1	I	77	ARG
1	I	103	LEU
1	I	108	LEU
1	I	111	LEU
1	I	133	LEU
1	I	135	GLU
1	I	167	ASP
1	J	8	ARG
1	J	53	THR
1	J	56	TYR
1	J	90	VAL
1	J	103	LEU
1	J	111	LEU
1	J	135	GLU
1	J	167	ASP
1	K	53	THR
1	K	56	TYR
1	K	103	LEU
1	K	108	LEU
1	K	111	LEU
1	K	135	GLU
1	K	167	ASP
1	L	8	ARG
1	L	53	THR
1	L	77	ARG
1	L	94	GLN
1	L	103	LEU
1	L	108	LEU
1	L	111	LEU
1	L	167	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN

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Mol	Chain	Res	Type
1	B	147	GLN
1	C	140	GLN
1	D	140	GLN
1	E	140	GLN
1	E	141	HIS
1	E	147	GLN
1	F	102	GLN
1	F	140	GLN
1	F	147	GLN
1	G	140	GLN
1	G	147	GLN
1	H	140	GLN
1	H	141	HIS
1	I	28	ASN
1	I	140	GLN
1	I	147	GLN
1	J	19	GLN
1	J	147	GLN
1	L	141	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands 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	PPQ	L	801	-	4,10,10	2.92	2 (50%)	2,14,14	2.11	1 (50%)
2	PPQ	H	801	-	4,10,10	2.89	2 (50%)	2,14,14	1.35	0
2	PPQ	A	801	-	4,10,10	1.91	1 (25%)	2,14,14	1.90	1 (50%)
2	PPQ	C	801	-	4,10,10	2.91	2 (50%)	2,14,14	1.90	1 (50%)
2	PPQ	F	801	-	4,10,10	1.76	1 (25%)	2,14,14	2.89	1 (50%)
2	PPQ	E	801	-	4,10,10	1.97	1 (25%)	2,14,14	1.71	1 (50%)
2	PPQ	D	801	-	4,10,10	2.76	2 (50%)	2,14,14	2.82	2 (100%)
2	PPQ	C	802	-	4,10,10	2.92	2 (50%)	2,14,14	2.31	1 (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	PPQ	L	801	-	-	4/6/10/10	-
2	PPQ	H	801	-	-	3/6/10/10	-
2	PPQ	A	801	-	-	0/6/10/10	-
2	PPQ	C	801	-	-	0/6/10/10	-
2	PPQ	F	801	-	-	0/6/10/10	-
2	PPQ	E	801	-	-	0/6/10/10	-
2	PPQ	D	801	-	-	4/6/10/10	-
2	PPQ	C	802	-	-	2/6/10/10	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	801	PPQ	PDP-OEA	4.58	1.58	1.50
2	C	801	PPQ	PDP-OEA	4.42	1.58	1.50
2	C	802	PPQ	PDP-OEA	4.40	1.58	1.50
2	H	801	PPQ	PDP-OEA	4.40	1.58	1.50
2	D	801	PPQ	PDP-OEA	4.32	1.58	1.50
2	H	801	PPQ	PDP-CGP	3.05	1.82	1.79
2	E	801	PPQ	PDP-CGP	2.92	1.82	1.79
2	C	801	PPQ	PDP-CGP	2.91	1.82	1.79
2	A	801	PPQ	PDP-CGP	2.87	1.82	1.79
2	C	802	PPQ	PDP-CGP	2.75	1.82	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	PPQ	PDP-CGP	2.72	1.82	1.79
2	L	801	PPQ	PDP-CGP	2.53	1.82	1.79
2	F	801	PPQ	PDP-CGP	2.45	1.82	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	801	PPQ	PDP-CGP-CBP	-3.94	107.33	114.53
2	D	801	PPQ	PDP-CGP-CBP	-3.43	108.26	114.53
2	C	802	PPQ	PDP-CGP-CBP	-3.16	108.74	114.53
2	L	801	PPQ	PDP-CGP-CBP	-2.95	109.13	114.53
2	C	801	PPQ	PDP-CGP-CBP	-2.54	109.88	114.53
2	A	801	PPQ	PDP-CGP-CBP	-2.41	110.13	114.53
2	E	801	PPQ	PDP-CGP-CBP	-2.18	110.54	114.53
2	D	801	PPQ	CEP-PDP-CGP	2.05	111.24	107.62

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	801	PPQ	CAP-CBP-CGP-PDP
2	H	801	PPQ	CAP-CBP-CGP-PDP
2	D	801	PPQ	CBP-CGP-PDP-CEP
2	D	801	PPQ	CBP-CGP-PDP-OEA
2	D	801	PPQ	CBP-CGP-PDP-OEB
2	C	802	PPQ	NP-CAP-CBP-CGP
2	C	802	PPQ	CP-CAP-CBP-CGP
2	H	801	PPQ	NP-CAP-CBP-CGP
2	D	801	PPQ	NP-CAP-CBP-CGP
2	L	801	PPQ	CBP-CGP-PDP-OEA
2	L	801	PPQ	CBP-CGP-PDP-CEP
2	L	801	PPQ	NP-CAP-CBP-CGP
2	H	801	PPQ	CP-CAP-CBP-CGP

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PPQ	1	0
2	E	801	PPQ	1	0
2	D	801	PPQ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	802	PPQ	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	176/207 (85%)	0.44	4 (2%) 60 56	26, 39, 65, 80	0
1	B	175/207 (84%)	0.65	16 (9%) 9 7	29, 40, 67, 88	0
1	C	176/207 (85%)	0.57	9 (5%) 28 25	27, 40, 67, 77	0
1	D	176/207 (85%)	0.73	15 (8%) 10 8	27, 40, 67, 85	0
1	E	176/207 (85%)	0.61	10 (5%) 23 20	24, 36, 59, 82	0
1	F	176/207 (85%)	0.53	9 (5%) 28 25	23, 37, 61, 82	0
1	G	176/207 (85%)	0.62	10 (5%) 23 20	21, 35, 53, 71	0
1	H	174/207 (84%)	0.77	23 (13%) 3 2	27, 38, 64, 74	0
1	I	176/207 (85%)	0.67	17 (9%) 7 6	25, 37, 61, 76	0
1	J	176/207 (85%)	0.55	7 (3%) 38 34	25, 36, 56, 72	0
1	K	176/207 (85%)	0.58	14 (7%) 12 9	24, 37, 59, 82	0
1	L	176/207 (85%)	0.50	6 (3%) 45 41	22, 36, 60, 78	0
All	All	2109/2484 (84%)	0.60	140 (6%) 18 15	21, 38, 64, 88	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	GLY	8.8
1	G	178	PHE	7.7
1	L	179	LEU	7.4
1	D	4	GLY	7.1
1	L	178	PHE	6.5
1	D	178	PHE	5.9
1	K	97	SER	5.9
1	G	97	SER	5.6
1	I	97	SER	5.3
1	G	169	GLY	5.2
1	H	4	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	J	97	SER	5.0
1	K	179	LEU	4.9
1	E	169	GLY	4.9
1	H	91	ALA	4.8
1	F	4	GLY	4.6
1	D	28	ASN	4.4
1	B	28	ASN	4.3
1	B	95	ARG	4.2
1	K	178	PHE	4.2
1	J	178	PHE	4.1
1	D	5	ILE	4.1
1	B	92	GLU	3.9
1	H	97	SER	3.9
1	I	169	GLY	3.9
1	C	97	SER	3.8
1	E	97	SER	3.8
1	F	169	GLY	3.8
1	G	179	LEU	3.8
1	I	63	GLY	3.8
1	J	43	MET	3.8
1	D	179	LEU	3.7
1	E	179	LEU	3.7
1	E	178	PHE	3.7
1	H	94	GLN	3.7
1	G	43	MET	3.6
1	I	92	GLU	3.6
1	C	178	PHE	3.6
1	K	170	LEU	3.6
1	I	91	ALA	3.6
1	B	94	GLN	3.5
1	H	169	GLY	3.5
1	A	178	PHE	3.4
1	C	91	ALA	3.4
1	J	169	GLY	3.3
1	B	91	ALA	3.3
1	L	169	GLY	3.3
1	B	40	VAL	3.2
1	I	4	GLY	3.2
1	H	106	VAL	3.1
1	C	169	GLY	3.1
1	H	163	PHE	3.1
1	L	168	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	97	SER	3.1
1	I	94	GLN	3.1
1	I	179	LEU	3.0
1	A	94	GLN	3.0
1	H	107	LEU	3.0
1	D	91	ALA	3.0
1	K	167	ASP	3.0
1	H	27	LEU	2.9
1	E	8	ARG	2.9
1	D	169	GLY	2.8
1	G	14	ASP	2.8
1	I	23	ALA	2.8
1	D	40	VAL	2.8
1	H	175	PRO	2.8
1	J	175	PRO	2.8
1	K	90	VAL	2.8
1	K	8	ARG	2.8
1	H	68	TYR	2.8
1	B	169	GLY	2.7
1	H	67	GLY	2.7
1	B	27	LEU	2.7
1	H	23	ALA	2.7
1	J	35	GLU	2.7
1	E	167	ASP	2.7
1	D	27	LEU	2.7
1	D	94	GLN	2.6
1	H	92	GLU	2.6
1	G	59	ALA	2.6
1	H	63	GLY	2.6
1	D	8	ARG	2.5
1	K	175	PRO	2.5
1	H	136	ARG	2.5
1	C	28	ASN	2.5
1	K	96	ARG	2.5
1	I	175	PRO	2.5
1	K	169	GLY	2.4
1	B	178	PHE	2.4
1	E	101	ARG	2.4
1	C	4	GLY	2.4
1	I	178	PHE	2.4
1	B	153	ASP	2.4
1	F	179	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	36	ALA	2.3
1	B	66	VAL	2.3
1	I	110	VAL	2.3
1	C	104	TYR	2.3
1	G	35	GLU	2.3
1	K	101	ARG	2.3
1	H	24	PRO	2.3
1	E	96	ARG	2.3
1	H	35	GLU	2.3
1	C	167	ASP	2.3
1	D	92	GLU	2.3
1	D	167	ASP	2.2
1	K	37	VAL	2.2
1	B	8	ARG	2.2
1	H	20	ILE	2.2
1	K	158	VAL	2.2
1	I	35	GLU	2.2
1	B	7	ILE	2.2
1	L	20	ILE	2.2
1	E	175	PRO	2.2
1	I	68	TYR	2.2
1	G	89	TYR	2.1
1	H	22	TYR	2.1
1	D	99	ILE	2.1
1	H	150	PHE	2.1
1	F	99	ILE	2.1
1	L	8	ARG	2.1
1	F	8	ARG	2.1
1	A	28	ASN	2.1
1	J	40	VAL	2.1
1	E	40	VAL	2.1
1	F	175	PRO	2.1
1	B	100	ALA	2.1
1	F	23	ALA	2.1
1	B	90	VAL	2.0
1	D	90	VAL	2.0
1	A	91	ALA	2.0
1	C	40	VAL	2.0
1	F	7	ILE	2.0
1	I	24	PRO	2.0
1	H	133	LEU	2.0
1	K	40	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	18	ILE	2.0
1	I	18	ILE	2.0
1	I	22	TYR	2.0

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](#)

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	PPQ	F	801	11/11	0.72	0.42	46,57,68,84	0
2	PPQ	L	801	11/11	0.76	0.36	44,58,65,88	0
2	PPQ	A	801	11/11	0.86	0.26	34,51,64,65	0
2	PPQ	H	801	11/11	0.87	0.31	32,51,60,61	0
2	PPQ	E	801	11/11	0.90	0.29	34,52,60,62	0
2	PPQ	C	801	11/11	0.92	0.23	36,52,60,60	0
2	PPQ	D	801	11/11	0.92	0.29	40,48,61,67	0
2	PPQ	C	802	11/11	0.92	0.25	44,53,61,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.