



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 6, 2016 – 09:13 PM EST

PDB ID : 5D4W  
Title : Crystal structure of Hsp104  
Authors : Heuck, A.; Schitter-Sollner, S.; Clausen, T.  
Deposited on : 2015-08-09  
Resolution : 3.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

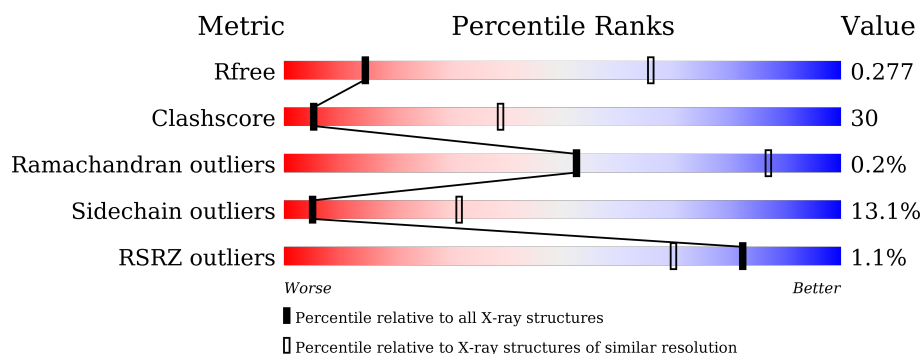
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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. 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	926	<div> <div>%</div> <div> <div></div> <div>33%</div> <div>35%</div> <div>6%</div> <div>26%</div> </div> </div>
1	B	926	<div> <div></div> <div>32%</div> <div>37%</div> <div>6%</div> <div>26%</div> </div>
1	C	926	<div> <div>%</div> <div> <div></div> <div>34%</div> <div>34%</div> <div>6%</div> <div>26%</div> </div> </div>

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	ADP	A	1001	-	-	X	-
2	ADP	B	1001	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16269 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 Putative heat shock protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	688	Total	C	N	O	S	Se	0	0	0
			5369	3354	985	1009	5	16			
1	B	688	Total	C	N	O	S	Se	0	0	0
			5369	3354	985	1009	5	16			
1	C	688	Total	C	N	O	S	Se	0	0	0
			5369	3354	985	1009	5	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP G0S4G4
A	296	ALA	GLU	engineered mutation	UNP G0S4G4
A	707	ALA	GLU	engineered mutation	UNP G0S4G4
B	1	MSE	-	initiating methionine	UNP G0S4G4
B	296	ALA	GLU	engineered mutation	UNP G0S4G4
B	707	ALA	GLU	engineered mutation	UNP G0S4G4
C	1	MSE	-	initiating methionine	UNP G0S4G4
C	296	ALA	GLU	engineered mutation	UNP G0S4G4
C	707	ALA	GLU	engineered mutation	UNP G0S4G4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

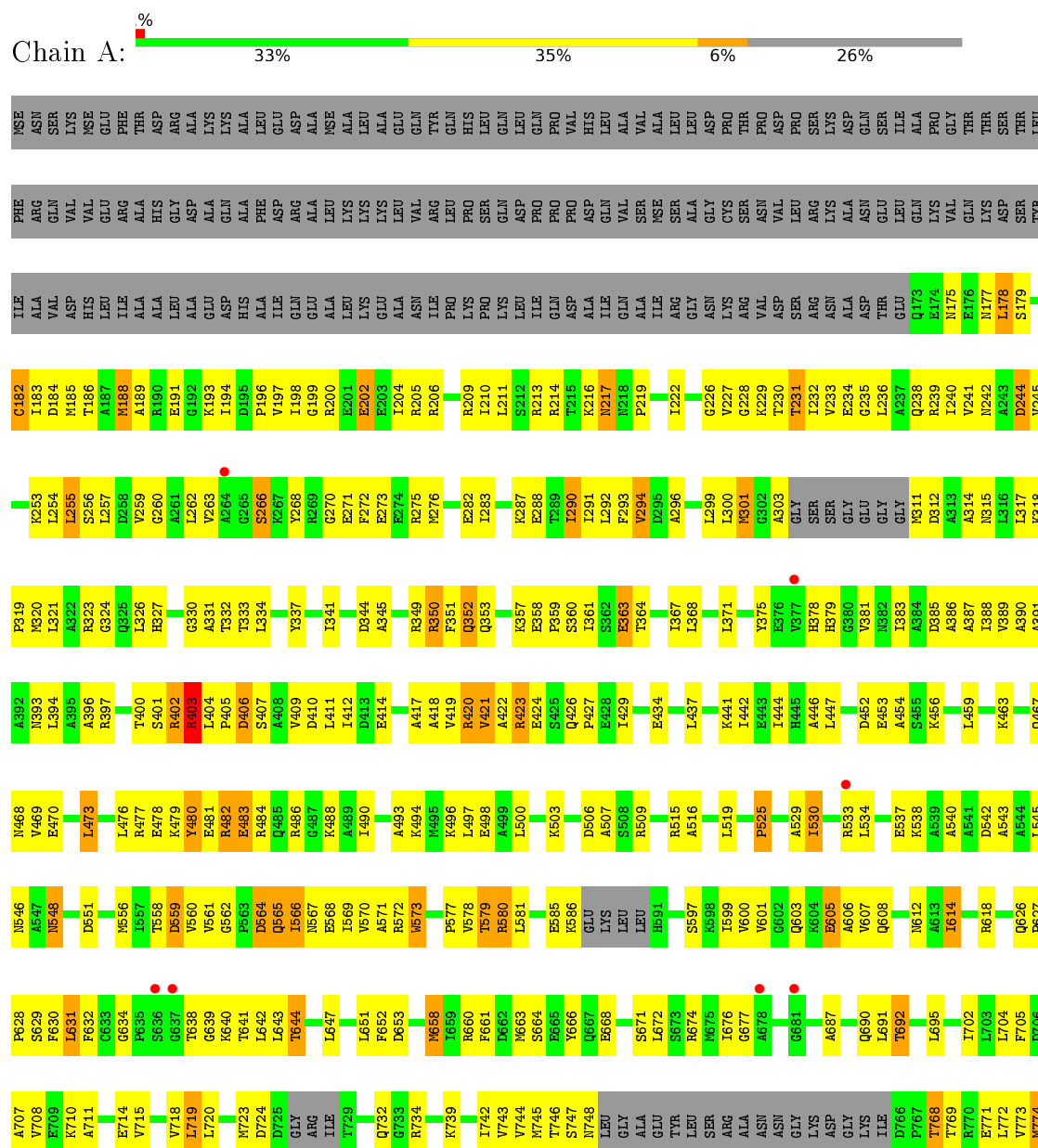


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Putative heat shock protein



N775	R849	F781	L860	L789	R801	R810	I814	Q815	Q816	R817	L818	T819	N821	D822	N824	V825	I826	I827	K828	E832	A833	K834	D835	K836	L837	G838	Q840	G841	Y842	S843	P844	V845	Y846
ALA	PRO	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ALA	PRO	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP

● Molecule 1: Putative heat shock protein

Chain B: 32% 37% 6% 26%

NSE	ASN	LYS	NSE	PHE	GLU	THR	ALA	ASP	ALA	LYS	LYS	ALA	LYS	ALA	GLN	TYR	GLN	HIS	LEU	GLN	LEU	GLN	VAL	HIS	LEU	LEU	GLN	VAL	ALA	VAL	LEU	ASP	VAL	ASP	ASP	PRO	PRO	VAL	HIS	LEU	LEU	ALA	ALA	VAL	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN	HIS	LEU	GLN	VAL	ASN	GLN	TYR	GLN</
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------

- Molecule 1: Putative heat shock protein



IE	ALA	VAL	ASP	HIS	ILE	ALA	ALA	ALA	ALA	GLU	GLN	GLU	LEU	LEU	LYS	LYS	LYS	LYS	ASN	IE	PRO	PRO	PRO	LEU	ILE	ILE	GLN	ALA	GLN	ILE	ILE	ARG	ARG	GLY	GLY	ASN	LYS	ARG	ASP	VAL	VAL	ARG	ASP	SER	SER	ARG	ASN	ALA	ALA	ASP	THR	THR	GLU	GLU	E173	E176	M177	L178	S179	K180	K181	K182	K183	K184	K185	K186	K187	K188	K189	K190	K191	K192	K193	K194	K195	K196	K197	K198	K199	K200	K201	K202	K203	K204	K205	K206	K207	K208	K209	K210	K211	K212	K213	K214	K215	K216	K217	K218	K219	K220	K221	K222	K223	K224	K225	K226	K227	K228	K229	K230	K231	K232	K233	K234	K235	K236	K237	K238	K239	K240	K241	K242	K243	K244	K245	K246	K247	K248	K249	K250	K251	K252	K253	K254	K255	K256	K257	K258	K259	K260	K261	K262	K263	K264	K265	K266	K267	K268	K269	K270	K271	K272	K273	K274	K275	K276	K277	K278	K279	K280	K281	K282	K283	K284	K285	K286	K287	K288	K289	K290	K291	K292	K293	K294	K295	K296	K297	K298	K299	K300	K301	K302	K303	K304	K305	K306	K307	K308	K309	K310	K311	K312	K313	K314	K315	K316	K317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500	K501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K525	K526	K527	K528	K529	K530	K531	K532	K533	K534	K535	K536	K537	K538	K539	K540	K541	K542	K543	K544	K545	K546	K547	K548	K549	K550	K551	K552	K553	K554	K555	K556	K557	K558	K559	K560	K561	K562	K563	K564	K565	K566	K567	K568	K569	K570	K571	K572	K573	K574	K575	K576	K577	K578	K579	K580	K581	K582	K583	K584	K585	K586	K587	K588	K589	K590	K591	K592	K593	K594	K595	K596	K597	K598	K599	K600	K601	K602	K603	K604	K605	K606	K607	K608	K609	K610	K611	K612	K613	K614	K615	K616	K617	K618	K619	K620	K621	K622	K623	K624	K625	K626	K627	K628	K629	K630	K631	K632	K633	K634	K635	K636	K637	K638	K639	K640	K641	K642	K643	K644
----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

G82	I183	D184	M185	T186	A187	M188	G189	K190	I191	I194	D195	P196	V197	I198	G199	R200	I204	R205	R206	R207	R208	R209	R210	R211	R212	R213	R214	R215	R216	R217	R218	R219	R220	R221	R222	R223	R224	R225	R226	R227	R228	R229	R230	R231	R232	R233	R234	R235	R236	R237	R238	R239	R240	R241	R242	R243	R244	R245	R246
-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

A250  
 A253  
 A254  
 A255  
 A256  
 A257  
 L262  
 G270  
 E271  
 F272  
 E273  
 E274  
 R275  
 M276  
 L280  
 A281  
 E282  
 L283  
 S286  
 K287  
 L290  
 L291  
 L292  
 V293  
 V294  
 L299  
 L300  
 M301  
 G302  
 A303  
 G317  
 SER  
 SER  
 G317  
 G317  
 G317  
 G317  
 M311  
 D312  
 A313  
 A314  
 M315  
 L316  
 L317  
 L318  
 F319  
 M320  
 L321  
 L326  
 E327  
 C328

I329	G330	A331	T332	T333	Y337	R338	K339	Y400	I341	E342	D344	K343	A345	A346	E348	R350	R350	F351	Q352	Q353	K357	E358	P359	S360	S361	S362	E363	T364	I365	S365	S366	L367	L368	R369	L370	L371	H379	G380	H381	H382	L383	L384	L385	L386	L387	L388	P389	A390	A391	A392	H393	L394	A395	A396	R397	T398
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

S401	R402	R403	L404	R405	R406	S407	A408	V409		I412		A417	A418	V419	R420	V421	A422	R423	A424	S425	Q426		I430	L433	A434	R435	R436	L437	R438		K441	I442	A443	I444		L447		K456	A457	R458	L459	A460	Q461	A462	K463	Q464		Q467	N468	V469		R475	L476	R477	E478	K479		Y480	Z481
------	------	------	------	------	------	------	------	------	--	------	--	------	------	------	------	------	------	------	------	------	------	--	------	------	------	------	------	------	------	--	------	------	------	------	--	------	--	------	------	------	------	------	------	------	------	------	--	------	------	------	--	------	------	------	------	------	--	------	------

A482	A483	A486	A490	A493	A496	A497	A498	A499	A500	D506	A507	S508	M509	M510	R515	A516	A517	D518	Y521	Y522	A523	I524	P525	E526	I530	I531	K532	K533	R534	I534	E535	A536	E537	A540	A541	D542	A543	A544	A545	I546	A547	M556	I557	T558	D559	V560	P563	D564	S565
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

1566 1567 1568 1569 1570 1571 1572 1573 1574 1575 1576 1577 1578 1579 1580 1581 1582 1583 1584 1585 1586 1587 1588 1589 1590 1591 1592 1593 1594 1595 1596 1597 1598 1599 1600 1601 1602 1603 1604 1605 1606 1607 1608 1609 1610 1611 1612 1613 1614 1615 1616 1617 1618 1619 1620 1621 1622 1623 1624 1625 1626 1627 1628 1629 1630 1631 1632 1633 1634 1635 1636 1637 1638 1639 1640 1641 1642 1643 1644 1645 1646 1647 1648 1649 1650 1651 1652 1653 1654 1655 1656 1657 1658 1659 1660 1661 1662 1663 1664 1665 1666 1667 1668 1669 1670 1671 1672 1673 1674 1675 1676 1677 1678 1679 1680 1681 1682 1683 1684 1685 1686 1687 1688 1689 1690 1691 1692 1693 1694 1695 1696 1697 1698 1699 1700 1701 1702 1703 1704 1705 1706 1707 1708 1709 1710 1711 1712 1713 1714 1715 1716 1717 1718 1719 1720 1721 1722 1723 1724 1725 1726 1727 1728 1729 1730 1731 1732 1733 1734 1735 1736 1737 1738 1739 1740 1741 1742 1743 1744 1745 1746 1747 1748 1749 1750 1751 1752 1753 1754 1755 1756 1757 1758 1759 1760 1761 1762 1763 1764 1765 1766 1767 1768 1769 1770 1771 1772 1773 1774 1775 1776 1777 1778 1779 1780 1781 1782 1783 1784 1785 1786 1787 1788 1789 1790 1791 1792 1793 1794 1795 1796 1797 1798 1799 1800 1801 1802 1803 1804 1805 1806 1807 1808 1809 1810 1811 1812 1813 1814 1815 1816 1817 1818 1819 1820 1821 1822 1823 1824 1825 1826 1827 1828 1829 1830 1831 1832 1833 1834 1835 1836 1837 1838 1839 1840 1841 1842 1843 1844 1845 1846 1847 1848 1849 1850 1851 1852 1853 1854 1855 1856 1857 1858 1859 1860 1861 1862 1863 1864 1865 1866 1867 1868 1869 1870 1871 1872 1873 1874 1875 1876 1877 1878 1879 1880 1881 1882 1883 1884 1885 1886 1887 1888 1889 1890 1891 1892 1893 1894 1895 1896 1897 1898 1899 1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910 1911 1912 1913 1914 1915 1916 1917 1918 1919 1920 1921 1922 1923 1924 1925 1926 1927 1928 1929 1930 1931 1932 1933 1934 1935 1936 1937 1938 1939 1940 1941 1942 1943 1944 1945 1946 1947 1948 1949 1950 1951 1952 1953 1954 1955 1956 1957 1958 1959 1960 1961 1962 1963 1964 1965 1966 1967 1968 1969 1970 1971 1972 1973 1974 1975 1976 1977 1978 1979 1980 1981 1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020 2021 2022 2023 2024 2025 2026 2027 2028 2029 2030 2031 2032 2033 2034 2035 2036 2037 2038 2039 2040 2041 2042 2043 2044 2045 2046 2047 2048 2049 2050 2051 2052 2053 2054 2055 2056 2057 2058 2059 2060 2061 2062 2063 2064 2065 2066 2067 2068 2069 2070 2071 2072 2073 2074 2075 2076 2077 2078 2079 2080 2081 2082 2083 2084 2085 2086 2087 2088 2089 2090 2091 2092 2093 2094 2095 2096 2097 2098 2099 2100 2101 2102 2103 2104 2105 2106 2107 2108 2109 2110 2111 2112 2113 2114 2115 2116 2117 2118 2119 2120 2121 2122 2123 2124 2125 2126 2127 2128 2129 2130 2131 2132 2133 2134 2135 2136 2137 2138 2139 2140 2141 2142 2143 2144 2145 2146 2147 2148 2149 2150 2151 2152 2153 2154 2155 2156 2157 2158 2159 2160 2161 2162 2163 2164 2165 2166 2167 2168 2169 2170 2171 2172 2173 2174 2175 2176 2177 2178 2179 2180 2181 2182 2183 2184 2185 2186 2187 2188 2189 2190 2191 2192 2193 2194 2195 2196 2197 2198 2199 2200 2201 2202 2203 2204 2205 2206 2207 2208 2209 2210 2211 2212 2213 2214 2215 2216 2217 2218 2219 2220 2221 2222 2223 2224 2225 2226 2227 2228 2229 2230 2231 2232 2233 2234 2235 2236 2237 2238 2239 2240 2241 2242 2243 2244 2245 2246 2247 2248 2249 2250 2251 2252 2253 2254 2255 2256 2257 2258 2259 2260 2261 2262 2263 2264 2265 2266 2267 2268 2269 2270 2271 2272 2273 2274 2275 2276 2277 2278 2279 2280 2281 2282 2283 2284 2285 2286 2287 2288 2289 2290 2291 2292 2293 2294 2295 2296 2297 2298 2299 2300 2301 2302 2303 2304 2305 2306 2307 2308 2309 2310 2311 2312 2313 2314 2315 2316 2317 2318 2319 2320 2321 2322 2323 2324 2325 2326 2327 2328 2329 2330 2331 2332 2333 2334 2335 2336 2337 2338 2339 2340 2341 2342 2343 2344 2345 2346 2347 2348 2349 2350 2351 2352 2353 2354 2355 2356 2357 2358 2359 2360 2361 2362 2363 2364 2365 2366 2367 2368 2369 2370 2371 2372 2373 2374 2375 2376 2377 2378 2379 2380 2381 2382 2383 2384

Year	Number of people (in thousands)
1980	3600
1981	3550
1982	3500
1983	3450
1984	3400
1985	3350
1986	3300
1987	3250
1988	3200
1989	3150
1990	3100
1991	3050
1992	3000
1993	2950
1994	2900
1995	2850
1996	2800
1997	2750
1998	2700
1999	2650
2000	2600
2001	2550
2002	2500
2003	2450
2004	2400
2005	2350
2006	2300
2007	2250
2008	2200
2009	2150
2010	2100
2011	2050
2012	2000
2013	1950
2014	1900
2015	1850
2016	1800
2017	1750
2018	1700
2019	1750
2020	1700

16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----

874  
875  
876  
877  
878  
879  
880  
881  
882  
883  
884  
885  
886  
887  
888  
889  
890  
891  
892  
893  
894  
895  
896  
897  
898  
899  
900  
901  
902  
903  
904  
905  
906  
907  
908  
909  
910  
911  
912  
913  
914  
915  
916  
917  
918  
919  
920  
921  
922  
923  
924  
925  
926  
927  
928  
929  
930  
931  
932  
933  
934  
935  
936  
937  
938  
939  
940  
941  
942  
943  
944  
945  
946  
947  
948  
949  
950  
951  
952  
953  
954  
955  
956  
957  
958  
959  
960  
961  
962  
963  
964  
965  
966  
967  
968  
969  
970  
971  
972  
973  
974  
975  
976  
977  
978  
979  
980  
981  
982  
983  
984  
985  
986  
987  
988  
989  
990  
991  
992  
993  
994  
995  
996  
997  
998  
999  
1000

Number of Children	Percentage of Families
0	35
1	25
2	15
3	10
4	8
5	6
6	4
7	3
8	2
9	1
10	1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.92Å 93.17Å 144.42Å 90.00° 119.72° 90.00°	Depositor
Resolution (Å)	47.58 – 3.70 47.58 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.58-3.70) 97.0 (47.58-3.60)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 3.57Å)	Xtriage
Refinement program	PHENIX (dev_2356: ???)	Depositor
R, $R_{free}$	0.237 , 0.277 0.237 , 0.277	Depositor DCC
$R_{free}$ test set	1778 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	116.6	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.259 for l,k,-h-l 0.259 for -h-l,k,h 0.167 for -h-l,-k,l 0.157 for h,-k,-h-l 0.166 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16269	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	210.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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](#)

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

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	0.31	0/5414	0.54	2/7262 (0.0%)
1	B	0.38	0/5414	0.61	3/7262 (0.0%)
1	C	0.32	0/5414	0.55	1/7262 (0.0%)
All	All	0.34	0/16242	0.57	6/21786 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	653	ASP	C-N-CA	-6.95	104.33	121.70
1	B	368	LEU	CA-CB-CG	6.87	131.10	115.30
1	B	653	ASP	C-N-CA	-6.72	104.90	121.70
1	B	195	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	653	ASP	C-N-CA	-5.50	107.96	121.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	SER	Peptide
1	A	402	ARG	Peptide
1	B	243	ALA	Peptide
1	B	385	ASP	Peptide
1	B	402	ARG	Peptide

## 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	5369	0	5537	323	0
1	B	5369	0	5537	397	0
1	C	5369	0	5537	331	0
2	A	54	0	24	11	0
2	B	54	0	24	18	0
2	C	54	0	24	4	0
All	All	16269	0	16683	994	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 30.

The worst 5 of 994 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:C:216:LYS:HB3	1:C:352:GLN:HB3	1.46	0.97
1:A:216:LYS:HB3	1:A:352:GLN:HB3	1.46	0.97
1:B:562:GLY:H	1:B:565:GLN:HB2	1.29	0.96
1:B:379:HIS:HA	1:B:420:ARG:HH12	1.31	0.91
1:B:200:ARG:HG3	1:B:232:ILE:HD11	1.55	0.89

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	678/926 (73%)	585 (86%)	91 (13%)	2 (0%)	46	83
1	B	678/926 (73%)	594 (88%)	83 (12%)	1 (0%)	56	90
1	C	678/926 (73%)	587 (87%)	89 (13%)	2 (0%)	46	83
All	All	2034/2778 (73%)	1766 (87%)	263 (13%)	5 (0%)	52	87

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	403	ARG
1	A	403	ARG
1	A	525	PRO
1	C	359	PRO
1	B	426	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	571/751 (76%)	501 (88%)	70 (12%)	6	34
1	B	571/751 (76%)	494 (86%)	77 (14%)	5	31
1	C	571/751 (76%)	493 (86%)	78 (14%)	4	30
All	All	1713/2253 (76%)	1488 (87%)	225 (13%)	5	31

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	410	ASP
1	B	644	THR
1	C	706	ASP
1	B	441	LYS
1	B	542	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	690	GLN
1	C	871	GLN
1	B	871	GLN
1	A	775	ASN
1	B	852	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	ADP	A	1001	-	24,29,29	1.07	2 (8%)	23,45,45	1.66	3 (13%)
2	ADP	A	1002	-	24,29,29	1.01	1 (4%)	23,45,45	1.60	1 (4%)
2	ADP	B	1001	-	24,29,29	1.51	2 (8%)	23,45,45	2.93	11 (47%)
2	ADP	B	1002	-	24,29,29	1.02	1 (4%)	23,45,45	1.65	2 (8%)
2	ADP	C	1001	-	24,29,29	1.13	2 (8%)	23,45,45	1.70	1 (4%)
2	ADP	C	1002	-	24,29,29	1.03	1 (4%)	23,45,45	1.67	3 (13%)

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	ADP	A	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	A	1002	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1002	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1002	-	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	O4'-C1'	2.05	1.44	1.41
2	C	1001	ADP	O4'-C1'	2.33	1.44	1.41
2	A	1002	ADP	C5-C4	3.22	1.47	1.40
2	B	1002	ADP	C5-C4	3.24	1.47	1.40
2	C	1002	ADP	C5-C4	3.31	1.48	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ADP	N3-C2-N1	-9.38	121.51	128.87
2	C	1001	ADP	N3-C2-N1	-6.45	123.81	128.87
2	A	1001	ADP	N3-C2-N1	-6.23	123.97	128.87
2	A	1002	ADP	N3-C2-N1	-6.15	124.04	128.87
2	B	1002	ADP	N3-C2-N1	-6.00	124.16	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ADP	10	0
2	A	1002	ADP	1	0
2	B	1001	ADP	16	0
2	B	1002	ADP	2	0
2	C	1001	ADP	3	0
2	C	1002	ADP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	672/926 (72%)	-0.67	12 (1%) 71 57	133, 225, 282, 313	10 (1%)
1	B	672/926 (72%)	-0.82	4 (0%) 90 83	1, 205, 268, 309	10 (1%)
1	C	672/926 (72%)	-0.85	6 (0%) 85 75	38, 219, 272, 294	10 (1%)
All	All	2016/2778 (72%)	-0.78	22 (1%) 82 70	1, 218, 275, 313	30 (1%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	825	VAL	4.1
1	A	681	GLY	3.8
1	B	671	SER	3.4
1	A	636	SER	3.2
1	C	883	VAL	2.9

### 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. 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	ADP	B	1001	27/27	0.99	0.15	-0.29	2,6,13,16	0
2	ADP	A	1001	27/27	0.94	0.15	-0.49	173,225,244,252	0
2	ADP	C	1001	27/27	0.96	0.15	-0.50	169,220,243,244	0
2	ADP	B	1002	27/27	0.96	0.12	-0.66	214,240,243,245	0
2	ADP	A	1002	27/27	0.95	0.12	-0.69	197,248,253,257	0
2	ADP	C	1002	27/27	0.94	0.11	-0.76	198,227,236,239	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.