



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:20 AM GMT

PDB ID : 3OQ0  
Title : Crystal Structure of motif N of Saccharomyces cerevisiae Dbf4  
Authors : Matthews, L.A.; Jones, D.R.; Prasad, A.A.; Duncker, B.P.; Guarne, A.  
Deposited on : 2010-09-02  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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.

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

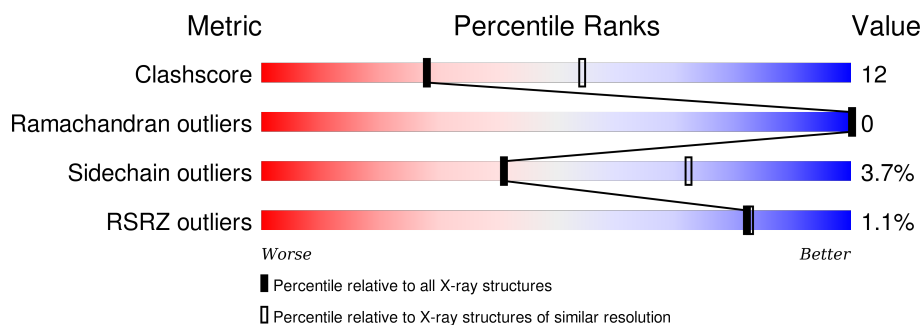
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	151	<div> <div></div> <div> <div></div> <div>54%</div> <div>11%</div> <div></div> <div>33%</div> </div> </div>
1	B	151	<div> <div></div> <div> <div></div> <div>45%</div> <div>17%</div> <div></div> <div>38%</div> </div> </div>
1	C	151	<div> <div></div> <div> <div></div> <div>48%</div> <div>17%</div> <div></div> <div>34%</div> </div> </div>
1	D	151	<div> <div></div> <div> <div></div> <div>50%</div> <div>17%</div> <div></div> <div>32%</div> </div> </div>
1	E	151	<div> <div></div> <div> <div></div> <div>48%</div> <div>15%</div> <div></div> <div>37%</div> </div> </div>
1	F	151	<div> <div></div> <div> <div></div> <div>55%</div> <div>11%</div> <div></div> <div>33%</div> </div> </div>
1	G	151	<div> <div></div> <div> <div></div> <div>44%</div> <div>17%</div> <div></div> <div>38%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	H	151	 50% 16% 34%
1	I	151	 48% 19% 32%
1	J	151	 48% 15% 37%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8369 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 DBF4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	Se	0	1	0
			855	543	149	159	4			
1	B	93	Total	C	N	O	Se	0	0	0
			780	497	135	145	3			
1	C	100	Total	C	N	O	Se	0	0	0
			834	531	144	156	3			
1	D	103	Total	C	N	O	Se	0	1	0
			868	551	151	163	3			
1	E	95	Total	C	N	O	Se	0	1	0
			801	510	137	151	3			
1	F	101	Total	C	N	O	Se	0	1	0
			855	543	149	159	4			
1	G	93	Total	C	N	O	Se	0	0	0
			780	497	135	145	3			
1	H	100	Total	C	N	O	Se	0	0	0
			834	531	144	156	3			
1	I	103	Total	C	N	O	Se	0	1	0
			868	551	151	163	3			
1	J	95	Total	C	N	O	Se	0	1	0
			801	510	137	151	3			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	MSE	-	EXPRESSION TAG	UNP P32325
A	101	GLY	-	EXPRESSION TAG	UNP P32325
A	102	SER	-	EXPRESSION TAG	UNP P32325
A	103	SER	-	EXPRESSION TAG	UNP P32325
A	104	HIS	-	EXPRESSION TAG	UNP P32325
A	105	HIS	-	EXPRESSION TAG	UNP P32325
A	106	HIS	-	EXPRESSION TAG	UNP P32325
A	107	HIS	-	EXPRESSION TAG	UNP P32325
A	108	HIS	-	EXPRESSION TAG	UNP P32325

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Chain	Residue	Modelled	Actual	Comment	Reference
A	109	HIS	-	EXPRESSION TAG	UNP P32325
A	110	SER	-	EXPRESSION TAG	UNP P32325
A	111	SER	-	EXPRESSION TAG	UNP P32325
A	112	GLY	-	EXPRESSION TAG	UNP P32325
A	113	LEU	-	EXPRESSION TAG	UNP P32325
A	114	VAL	-	EXPRESSION TAG	UNP P32325
A	115	PRO	-	EXPRESSION TAG	UNP P32325
A	116	ARG	-	EXPRESSION TAG	UNP P32325
A	117	GLY	-	EXPRESSION TAG	UNP P32325
A	118	SER	-	EXPRESSION TAG	UNP P32325
A	119	HIS	-	EXPRESSION TAG	UNP P32325
B	100	MSE	-	EXPRESSION TAG	UNP P32325
B	101	GLY	-	EXPRESSION TAG	UNP P32325
B	102	SER	-	EXPRESSION TAG	UNP P32325
B	103	SER	-	EXPRESSION TAG	UNP P32325
B	104	HIS	-	EXPRESSION TAG	UNP P32325
B	105	HIS	-	EXPRESSION TAG	UNP P32325
B	106	HIS	-	EXPRESSION TAG	UNP P32325
B	107	HIS	-	EXPRESSION TAG	UNP P32325
B	108	HIS	-	EXPRESSION TAG	UNP P32325
B	109	HIS	-	EXPRESSION TAG	UNP P32325
B	110	SER	-	EXPRESSION TAG	UNP P32325
B	111	SER	-	EXPRESSION TAG	UNP P32325
B	112	GLY	-	EXPRESSION TAG	UNP P32325
B	113	LEU	-	EXPRESSION TAG	UNP P32325
B	114	VAL	-	EXPRESSION TAG	UNP P32325
B	115	PRO	-	EXPRESSION TAG	UNP P32325
B	116	ARG	-	EXPRESSION TAG	UNP P32325
B	117	GLY	-	EXPRESSION TAG	UNP P32325
B	118	SER	-	EXPRESSION TAG	UNP P32325
B	119	HIS	-	EXPRESSION TAG	UNP P32325
C	100	MSE	-	EXPRESSION TAG	UNP P32325
C	101	GLY	-	EXPRESSION TAG	UNP P32325
C	102	SER	-	EXPRESSION TAG	UNP P32325
C	103	SER	-	EXPRESSION TAG	UNP P32325
C	104	HIS	-	EXPRESSION TAG	UNP P32325
C	105	HIS	-	EXPRESSION TAG	UNP P32325
C	106	HIS	-	EXPRESSION TAG	UNP P32325
C	107	HIS	-	EXPRESSION TAG	UNP P32325
C	108	HIS	-	EXPRESSION TAG	UNP P32325
C	109	HIS	-	EXPRESSION TAG	UNP P32325
C	110	SER	-	EXPRESSION TAG	UNP P32325

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Chain	Residue	Modelled	Actual	Comment	Reference
C	111	SER	-	EXPRESSION TAG	UNP P32325
C	112	GLY	-	EXPRESSION TAG	UNP P32325
C	113	LEU	-	EXPRESSION TAG	UNP P32325
C	114	VAL	-	EXPRESSION TAG	UNP P32325
C	115	PRO	-	EXPRESSION TAG	UNP P32325
C	116	ARG	-	EXPRESSION TAG	UNP P32325
C	117	GLY	-	EXPRESSION TAG	UNP P32325
C	118	SER	-	EXPRESSION TAG	UNP P32325
C	119	HIS	-	EXPRESSION TAG	UNP P32325
D	100	MSE	-	EXPRESSION TAG	UNP P32325
D	101	GLY	-	EXPRESSION TAG	UNP P32325
D	102	SER	-	EXPRESSION TAG	UNP P32325
D	103	SER	-	EXPRESSION TAG	UNP P32325
D	104	HIS	-	EXPRESSION TAG	UNP P32325
D	105	HIS	-	EXPRESSION TAG	UNP P32325
D	106	HIS	-	EXPRESSION TAG	UNP P32325
D	107	HIS	-	EXPRESSION TAG	UNP P32325
D	108	HIS	-	EXPRESSION TAG	UNP P32325
D	109	HIS	-	EXPRESSION TAG	UNP P32325
D	110	SER	-	EXPRESSION TAG	UNP P32325
D	111	SER	-	EXPRESSION TAG	UNP P32325
D	112	GLY	-	EXPRESSION TAG	UNP P32325
D	113	LEU	-	EXPRESSION TAG	UNP P32325
D	114	VAL	-	EXPRESSION TAG	UNP P32325
D	115	PRO	-	EXPRESSION TAG	UNP P32325
D	116	ARG	-	EXPRESSION TAG	UNP P32325
D	117	GLY	-	EXPRESSION TAG	UNP P32325
D	118	SER	-	EXPRESSION TAG	UNP P32325
D	119	HIS	-	EXPRESSION TAG	UNP P32325
E	100	MSE	-	EXPRESSION TAG	UNP P32325
E	101	GLY	-	EXPRESSION TAG	UNP P32325
E	102	SER	-	EXPRESSION TAG	UNP P32325
E	103	SER	-	EXPRESSION TAG	UNP P32325
E	104	HIS	-	EXPRESSION TAG	UNP P32325
E	105	HIS	-	EXPRESSION TAG	UNP P32325
E	106	HIS	-	EXPRESSION TAG	UNP P32325
E	107	HIS	-	EXPRESSION TAG	UNP P32325
E	108	HIS	-	EXPRESSION TAG	UNP P32325
E	109	HIS	-	EXPRESSION TAG	UNP P32325
E	110	SER	-	EXPRESSION TAG	UNP P32325
E	111	SER	-	EXPRESSION TAG	UNP P32325
E	112	GLY	-	EXPRESSION TAG	UNP P32325

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Chain	Residue	Modelled	Actual	Comment	Reference
E	113	LEU	-	EXPRESSION TAG	UNP P32325
E	114	VAL	-	EXPRESSION TAG	UNP P32325
E	115	PRO	-	EXPRESSION TAG	UNP P32325
E	116	ARG	-	EXPRESSION TAG	UNP P32325
E	117	GLY	-	EXPRESSION TAG	UNP P32325
E	118	SER	-	EXPRESSION TAG	UNP P32325
E	119	HIS	-	EXPRESSION TAG	UNP P32325
F	100	MSE	-	EXPRESSION TAG	UNP P32325
F	101	GLY	-	EXPRESSION TAG	UNP P32325
F	102	SER	-	EXPRESSION TAG	UNP P32325
F	103	SER	-	EXPRESSION TAG	UNP P32325
F	104	HIS	-	EXPRESSION TAG	UNP P32325
F	105	HIS	-	EXPRESSION TAG	UNP P32325
F	106	HIS	-	EXPRESSION TAG	UNP P32325
F	107	HIS	-	EXPRESSION TAG	UNP P32325
F	108	HIS	-	EXPRESSION TAG	UNP P32325
F	109	HIS	-	EXPRESSION TAG	UNP P32325
F	110	SER	-	EXPRESSION TAG	UNP P32325
F	111	SER	-	EXPRESSION TAG	UNP P32325
F	112	GLY	-	EXPRESSION TAG	UNP P32325
F	113	LEU	-	EXPRESSION TAG	UNP P32325
F	114	VAL	-	EXPRESSION TAG	UNP P32325
F	115	PRO	-	EXPRESSION TAG	UNP P32325
F	116	ARG	-	EXPRESSION TAG	UNP P32325
F	117	GLY	-	EXPRESSION TAG	UNP P32325
F	118	SER	-	EXPRESSION TAG	UNP P32325
F	119	HIS	-	EXPRESSION TAG	UNP P32325
G	100	MSE	-	EXPRESSION TAG	UNP P32325
G	101	GLY	-	EXPRESSION TAG	UNP P32325
G	102	SER	-	EXPRESSION TAG	UNP P32325
G	103	SER	-	EXPRESSION TAG	UNP P32325
G	104	HIS	-	EXPRESSION TAG	UNP P32325
G	105	HIS	-	EXPRESSION TAG	UNP P32325
G	106	HIS	-	EXPRESSION TAG	UNP P32325
G	107	HIS	-	EXPRESSION TAG	UNP P32325
G	108	HIS	-	EXPRESSION TAG	UNP P32325
G	109	HIS	-	EXPRESSION TAG	UNP P32325
G	110	SER	-	EXPRESSION TAG	UNP P32325
G	111	SER	-	EXPRESSION TAG	UNP P32325
G	112	GLY	-	EXPRESSION TAG	UNP P32325
G	113	LEU	-	EXPRESSION TAG	UNP P32325
G	114	VAL	-	EXPRESSION TAG	UNP P32325

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Chain	Residue	Modelled	Actual	Comment	Reference
G	115	PRO	-	EXPRESSION TAG	UNP P32325
G	116	ARG	-	EXPRESSION TAG	UNP P32325
G	117	GLY	-	EXPRESSION TAG	UNP P32325
G	118	SER	-	EXPRESSION TAG	UNP P32325
G	119	HIS	-	EXPRESSION TAG	UNP P32325
H	100	MSE	-	EXPRESSION TAG	UNP P32325
H	101	GLY	-	EXPRESSION TAG	UNP P32325
H	102	SER	-	EXPRESSION TAG	UNP P32325
H	103	SER	-	EXPRESSION TAG	UNP P32325
H	104	HIS	-	EXPRESSION TAG	UNP P32325
H	105	HIS	-	EXPRESSION TAG	UNP P32325
H	106	HIS	-	EXPRESSION TAG	UNP P32325
H	107	HIS	-	EXPRESSION TAG	UNP P32325
H	108	HIS	-	EXPRESSION TAG	UNP P32325
H	109	HIS	-	EXPRESSION TAG	UNP P32325
H	110	SER	-	EXPRESSION TAG	UNP P32325
H	111	SER	-	EXPRESSION TAG	UNP P32325
H	112	GLY	-	EXPRESSION TAG	UNP P32325
H	113	LEU	-	EXPRESSION TAG	UNP P32325
H	114	VAL	-	EXPRESSION TAG	UNP P32325
H	115	PRO	-	EXPRESSION TAG	UNP P32325
H	116	ARG	-	EXPRESSION TAG	UNP P32325
H	117	GLY	-	EXPRESSION TAG	UNP P32325
H	118	SER	-	EXPRESSION TAG	UNP P32325
H	119	HIS	-	EXPRESSION TAG	UNP P32325
I	100	MSE	-	EXPRESSION TAG	UNP P32325
I	101	GLY	-	EXPRESSION TAG	UNP P32325
I	102	SER	-	EXPRESSION TAG	UNP P32325
I	103	SER	-	EXPRESSION TAG	UNP P32325
I	104	HIS	-	EXPRESSION TAG	UNP P32325
I	105	HIS	-	EXPRESSION TAG	UNP P32325
I	106	HIS	-	EXPRESSION TAG	UNP P32325
I	107	HIS	-	EXPRESSION TAG	UNP P32325
I	108	HIS	-	EXPRESSION TAG	UNP P32325
I	109	HIS	-	EXPRESSION TAG	UNP P32325
I	110	SER	-	EXPRESSION TAG	UNP P32325
I	111	SER	-	EXPRESSION TAG	UNP P32325
I	112	GLY	-	EXPRESSION TAG	UNP P32325
I	113	LEU	-	EXPRESSION TAG	UNP P32325
I	114	VAL	-	EXPRESSION TAG	UNP P32325
I	115	PRO	-	EXPRESSION TAG	UNP P32325
I	116	ARG	-	EXPRESSION TAG	UNP P32325

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Chain	Residue	Modelled	Actual	Comment	Reference
I	117	GLY	-	EXPRESSION TAG	UNP P32325
I	118	SER	-	EXPRESSION TAG	UNP P32325
I	119	HIS	-	EXPRESSION TAG	UNP P32325
J	100	MSE	-	EXPRESSION TAG	UNP P32325
J	101	GLY	-	EXPRESSION TAG	UNP P32325
J	102	SER	-	EXPRESSION TAG	UNP P32325
J	103	SER	-	EXPRESSION TAG	UNP P32325
J	104	HIS	-	EXPRESSION TAG	UNP P32325
J	105	HIS	-	EXPRESSION TAG	UNP P32325
J	106	HIS	-	EXPRESSION TAG	UNP P32325
J	107	HIS	-	EXPRESSION TAG	UNP P32325
J	108	HIS	-	EXPRESSION TAG	UNP P32325
J	109	HIS	-	EXPRESSION TAG	UNP P32325
J	110	SER	-	EXPRESSION TAG	UNP P32325
J	111	SER	-	EXPRESSION TAG	UNP P32325
J	112	GLY	-	EXPRESSION TAG	UNP P32325
J	113	LEU	-	EXPRESSION TAG	UNP P32325
J	114	VAL	-	EXPRESSION TAG	UNP P32325
J	115	PRO	-	EXPRESSION TAG	UNP P32325
J	116	ARG	-	EXPRESSION TAG	UNP P32325
J	117	GLY	-	EXPRESSION TAG	UNP P32325
J	118	SER	-	EXPRESSION TAG	UNP P32325
J	119	HIS	-	EXPRESSION TAG	UNP P32325

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	10	Total O 10 10	0	0
2	C	4	Total O 4 4	0	0
2	D	5	Total O 5 5	0	0
2	E	14	Total O 14 14	0	0
2	F	13	Total O 13 13	0	0
2	G	3	Total O 3 3	0	0
2	H	2	Total O 2 2	0	0

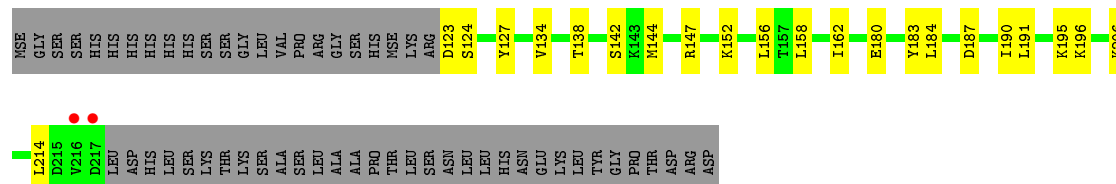
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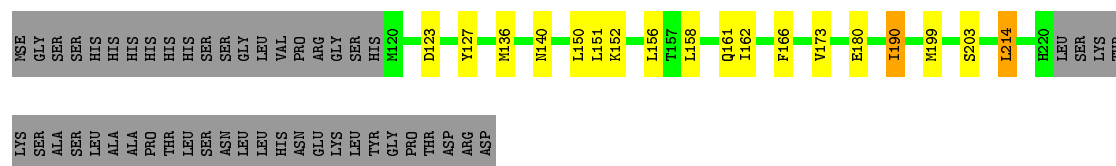
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	8	Total	O	0	0
			8	8		
2	J	14	Total	O	0	0
			14	14		



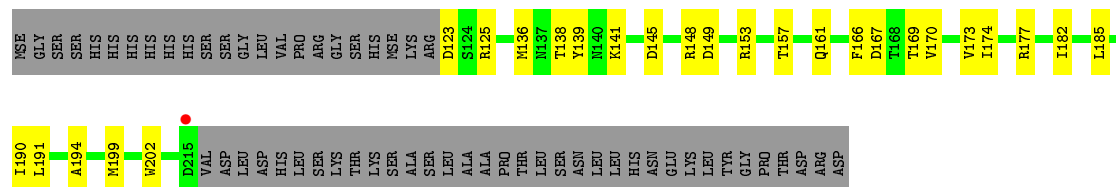
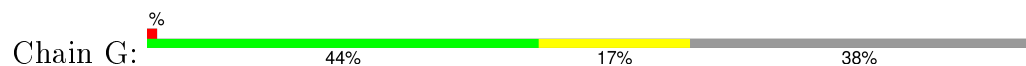
- Molecule 1: DBF4



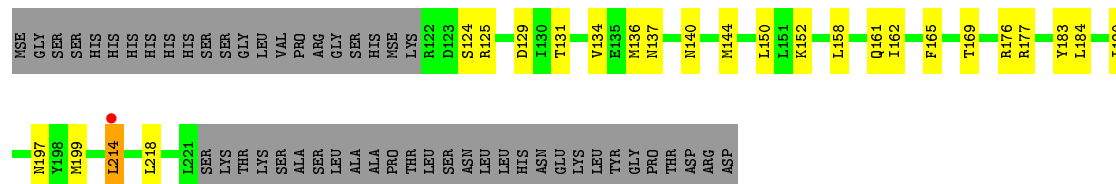
- Molecule 1: DBF4



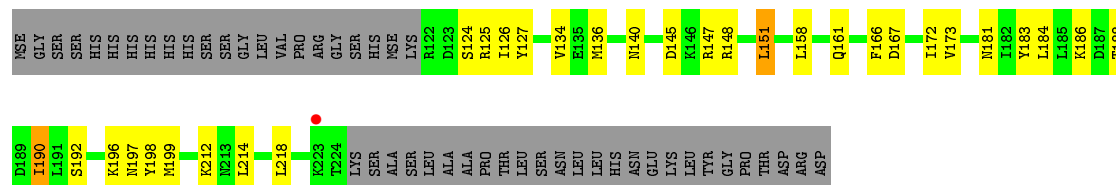
- Molecule 1: DBF4



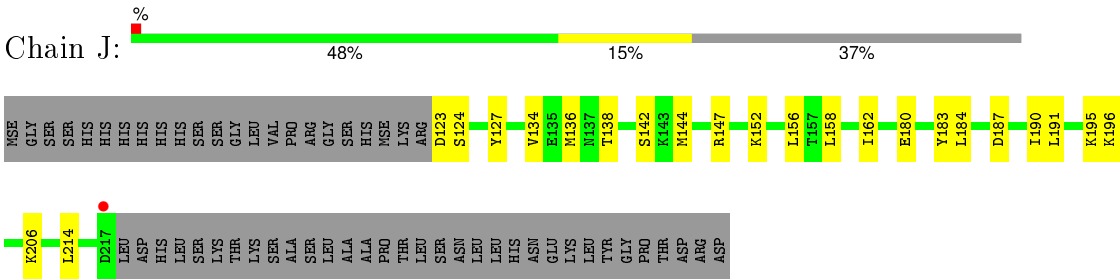
- Molecule 1: DBF4



- Molecule 1: DBF4



- Molecule 1: DBF4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.22Å 79.36Å 127.42Å 90.00° 110.74° 90.00°	Depositor
Resolution (Å)	35.52 – 2.70 35.52 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (35.52-2.70) 92.9 (35.52-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_159)	Depositor
R, $R_{free}$	0.205 , 0.244 0.201 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	43.5	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.9	EDS
Estimated twinning fraction	0.488 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 65124 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/867	0.62	0/1157
1	B	0.47	0/788	0.62	0/1052
1	C	0.44	0/843	0.62	0/1128
1	D	0.47	0/880	0.63	0/1176
1	E	0.49	0/812	0.61	0/1085
1	F	0.48	0/867	0.62	0/1157
1	G	0.47	0/788	0.63	0/1052
1	H	0.43	0/843	0.62	0/1128
1	I	0.48	0/880	0.63	0/1176
1	J	0.49	0/812	0.61	0/1085
All	All	0.47	0/8380	0.62	0/11196

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	855	0	875	19	0
1	B	780	0	799	25	0
1	C	834	0	847	22	0
1	D	868	0	889	26	0
1	E	801	0	818	19	0
1	F	855	0	875	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	780	0	799	24	0
1	H	834	0	847	21	0
1	I	868	0	889	29	0
1	J	801	0	818	20	0
2	A	20	0	0	1	0
2	B	10	0	0	1	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
2	E	14	0	0	0	0
2	F	13	0	0	0	0
2	G	3	0	0	0	0
2	H	2	0	0	0	0
2	I	8	0	0	0	0
2	J	14	0	0	0	0
All	All	8369	0	8456	196	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 12.

All (196) 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:F:136:MSE:HE2	1:F:140:ASN:HB3	1.42	1.01
1:A:136:MSE:HE2	1:A:140:ASN:HB3	1.43	1.00
1:H:136:MSE:HE2	1:H:140:ASN:HB3	1.49	0.93
1:C:136:MSE:HE2	1:C:140:ASN:HB3	1.50	0.92
1:A:161:GLN:HG2	1:B:136:MSE:HE2	1.56	0.86
1:I:127:TYR:HE2	1:I:190:ILE:HD12	1.40	0.85
1:F:161:GLN:HG2	1:G:136:MSE:HE2	1.59	0.83
1:D:127:TYR:HE2	1:D:190:ILE:HD12	1.42	0.83
1:B:166:PHE:HE1	1:B:199:MSE:HE1	1.42	0.82
1:G:166:PHE:HE1	1:G:199:MSE:HE1	1.42	0.82
1:B:170:VAL:HG12	1:B:199:MSE:HE3	1.62	0.81
1:G:170:VAL:HG12	1:G:199:MSE:HE3	1.63	0.80
1:I:125:ARG:NH2	1:J:134:VAL:HG21	1.98	0.78
1:D:125:ARG:NH2	1:E:134:VAL:HG21	2.00	0.76
1:I:125:ARG:HH22	1:J:134:VAL:HG21	1.51	0.75
1:H:144:MSE:HE3	1:H:176:ARG:HD2	1.69	0.74
1:C:144:MSE:HE3	1:C:176:ARG:HD2	1.70	0.73
1:B:170:VAL:CG1	1:B:199:MSE:HE3	2.18	0.73
1:I:166:PHE:HE1	1:I:199:MSE:HE1	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ARG:HH22	1:E:134:VAL:HG21	1.53	0.72
1:G:170:VAL:CG1	1:G:199:MSE:HE3	2.19	0.72
1:A:166:PHE:HE1	1:A:199:MSE:HE1	1.56	0.71
1:D:173:VAL:HG23	1:D:199:MSE:CE	2.21	0.70
1:B:161:GLN:HG2	1:C:136:MSE:HE3	1.75	0.69
1:G:161:GLN:HG2	1:H:136:MSE:HE3	1.75	0.69
1:D:166:PHE:HE1	1:D:199:MSE:HE1	1.57	0.68
1:H:158:LEU:HD11	1:H:214:LEU:HD23	1.73	0.68
1:I:173:VAL:HG23	1:I:199:MSE:CE	2.23	0.68
1:C:158:LEU:HD11	1:C:214:LEU:HD23	1.74	0.68
1:F:166:PHE:HE1	1:F:199:MSE:HE1	1.62	0.65
1:A:173:VAL:HG23	1:A:199:MSE:CE	2.27	0.64
1:F:173:VAL:HG23	1:F:199:MSE:CE	2.27	0.64
1:G:173:VAL:HG23	1:G:199:MSE:HE2	1.81	0.62
1:H:144:MSE:HE3	1:H:176:ARG:CD	2.29	0.62
1:B:173:VAL:HG23	1:B:199:MSE:HE2	1.81	0.62
1:C:165:PHE:HB3	1:D:181:ASN:ND2	2.14	0.62
1:B:125:ARG:NH2	1:C:134:VAL:HG21	2.16	0.60
1:G:125:ARG:NH2	1:H:134:VAL:HG21	2.16	0.60
1:C:144:MSE:HE3	1:C:176:ARG:CD	2.31	0.60
1:B:148:ARG:HG3	1:B:149:ASP:N	2.17	0.60
1:G:190:ILE:HG13	1:G:191:LEU:N	2.15	0.60
1:F:136:MSE:CE	1:F:140:ASN:HB3	2.25	0.60
1:I:158:LEU:HD13	1:I:214:LEU:HD23	1.84	0.59
1:E:144:MSE:HE1	1:E:147:ARG:HH11	1.66	0.59
1:J:127:TYR:HE2	1:J:190:ILE:HD12	1.67	0.59
1:D:158:LEU:HD13	1:D:214:LEU:HD23	1.84	0.59
1:J:144:MSE:HE1	1:J:147:ARG:HH11	1.67	0.59
1:J:127:TYR:CE2	1:J:190:ILE:HD12	2.38	0.58
1:A:136:MSE:CE	1:A:140:ASN:HB3	2.26	0.58
1:H:165:PHE:HB3	1:I:181:ASN:ND2	2.18	0.58
1:A:161:GLN:HG2	1:B:136:MSE:CE	2.31	0.58
1:G:148:ARG:HG3	1:G:149:ASP:N	2.19	0.58
1:G:145:ASP:HA	1:G:148:ARG:NH1	2.19	0.57
1:J:158:LEU:HD13	1:J:214:LEU:HD23	1.85	0.57
1:B:145:ASP:HA	1:B:148:ARG:NH1	2.19	0.57
1:E:152:LYS:CG	1:E:162:ILE:HD12	2.34	0.57
1:E:144:MSE:HE3	1:E:147:ARG:HD2	1.86	0.57
1:J:152:LYS:CG	1:J:162:ILE:HD12	2.34	0.57
1:J:144:MSE:HE3	1:J:147:ARG:HD2	1.86	0.56
1:B:190:ILE:HG13	1:B:191:LEU:N	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PHE:CE1	1:B:199:MSE:HE1	2.30	0.56
1:G:166:PHE:CE1	1:G:199:MSE:HE1	2.31	0.56
1:D:198:TYR:CD1	1:F:158:LEU:HB3	2.41	0.56
1:F:161:GLN:HG2	1:G:136:MSE:CE	2.33	0.56
1:C:131:THR:HG22	1:C:177:ARG:HD3	1.88	0.55
1:H:131:THR:HG22	1:H:177:ARG:HD3	1.88	0.55
1:E:158:LEU:HD13	1:E:214:LEU:HD23	1.88	0.55
1:J:127:TYR:HE2	1:J:190:ILE:CD1	2.19	0.55
1:D:196:LYS:HE2	1:F:123:ASP:OD1	2.07	0.55
1:H:125:ARG:HH12	1:I:134:VAL:HG21	1.72	0.55
1:A:158:LEU:HB3	1:I:198:TYR:CD1	2.42	0.55
1:A:123:ASP:OD1	1:I:196:LYS:HE2	2.07	0.55
1:A:156:LEU:HG	1:A:162:ILE:HD12	1.89	0.54
1:E:127:TYR:HE2	1:E:190:ILE:CD1	2.20	0.54
1:E:127:TYR:CE2	1:E:190:ILE:HD12	2.43	0.54
1:D:198:TYR:HD1	1:F:158:LEU:HB3	1.73	0.54
1:G:173:VAL:HG23	1:G:199:MSE:CE	2.36	0.54
1:D:173:VAL:HG23	1:D:199:MSE:HE3	1.90	0.54
1:A:158:LEU:HB3	1:I:198:TYR:HD1	1.73	0.54
1:B:173:VAL:HG23	1:B:199:MSE:CE	2.37	0.53
1:E:127:TYR:HE2	1:E:190:ILE:HD12	1.73	0.53
1:F:156:LEU:HG	1:F:162:ILE:HD12	1.90	0.53
1:F:127:TYR:CE2	1:F:190:ILE:HD13	2.43	0.53
1:A:152:LYS:HG3	1:A:162:ILE:HD13	1.91	0.53
1:C:125:ARG:HH12	1:D:134:VAL:HG21	1.74	0.53
1:H:144:MSE:CE	1:H:176:ARG:HD2	2.37	0.53
1:I:173:VAL:HG23	1:I:199:MSE:HE3	1.91	0.52
1:F:152:LYS:HG3	1:F:162:ILE:HD13	1.92	0.52
1:G:153:ARG:O	1:G:157:THR:HG23	2.10	0.52
1:B:153:ARG:O	1:B:157:THR:HG23	2.10	0.52
1:J:152:LYS:HG2	1:J:162:ILE:HD12	1.91	0.51
1:H:129:ASP:OD1	1:H:190:ILE:HD11	2.11	0.51
1:E:152:LYS:HG2	1:E:162:ILE:HD12	1.92	0.51
1:H:152:LYS:HG3	1:H:162:ILE:HD12	1.92	0.51
1:B:177:ARG:NH2	1:B:191:LEU:HD12	2.25	0.50
1:H:150:LEU:HD21	1:H:218:LEU:HG	1.92	0.50
1:B:143:LYS:NZ	2:B:253:HOH:O	2.43	0.50
1:D:173:VAL:HG23	1:D:199:MSE:HE1	1.91	0.50
1:E:152:LYS:HG3	1:E:162:ILE:HD12	1.94	0.50
1:D:167:ASP:HB2	1:E:180[B]:GLU:OE1	2.12	0.50
1:A:127:TYR:CE2	1:A:190:ILE:HD13	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LEU:HD21	1:C:218:LEU:HG	1.93	0.49
1:C:144:MSE:CE	1:C:176:ARG:HD2	2.40	0.49
1:C:152:LYS:HG3	1:C:162:ILE:HD12	1.93	0.49
1:I:183:TYR:CE1	1:I:184:LEU:CD2	2.96	0.49
1:H:136:MSE:CE	1:H:140:ASN:HB3	2.32	0.49
1:D:183:TYR:CE1	1:D:184:LEU:CD2	2.97	0.48
1:J:152:LYS:HG3	1:J:162:ILE:HD12	1.95	0.48
1:G:177:ARG:NH2	1:G:191:LEU:HD12	2.28	0.48
1:C:129:ASP:OD1	1:C:190:ILE:HD11	2.14	0.48
1:G:125:ARG:NH1	1:G:169:THR:OG1	2.46	0.48
1:B:125:ARG:NH1	1:B:169:THR:OG1	2.46	0.48
1:I:167:ASP:HB2	1:J:180[B]:GLU:OE1	2.14	0.47
1:G:182:ILE:O	1:G:185:LEU:HB2	2.14	0.47
1:I:173:VAL:HG23	1:I:199:MSE:HE1	1.94	0.47
1:A:152:LYS:CG	1:A:162:ILE:HD13	2.43	0.47
1:E:195:LYS:HA	1:E:195:LYS:HD2	1.64	0.47
1:I:127:TYR:CE2	1:I:190:ILE:HD12	2.33	0.47
1:F:173:VAL:HG23	1:F:199:MSE:HE1	1.96	0.47
1:F:152:LYS:CG	1:F:162:ILE:HD13	2.44	0.47
1:B:182:ILE:O	1:B:185:LEU:HB2	2.15	0.47
1:E:206:LYS:HB2	1:E:206:LYS:HE3	1.47	0.46
1:G:194:ALA:HA	1:G:199:MSE:SE	2.65	0.46
1:J:206:LYS:HE3	1:J:206:LYS:HB2	1.47	0.46
1:G:167:ASP:OD1	1:G:169:THR:HG23	2.15	0.46
1:F:156:LEU:HA	1:F:156:LEU:HD23	1.81	0.46
1:C:197:ASN:HB2	1:C:199:MSE:HE3	1.96	0.46
1:I:212:LYS:HE3	1:I:218:LEU:HD12	1.96	0.46
1:I:147:ARG:O	1:I:151:LEU:HD22	2.15	0.46
1:E:156:LEU:CD2	1:E:162:ILE:HG13	2.46	0.46
1:F:214:LEU:HA	1:F:214:LEU:HD12	1.66	0.46
1:D:212:LYS:HE3	1:D:218:LEU:HD12	1.97	0.46
1:I:186:LYS:HB3	1:I:188:THR:HG22	1.99	0.46
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.81	0.45
1:J:195:LYS:HA	1:J:195:LYS:HD2	1.66	0.45
1:D:173:VAL:CG2	1:D:199:MSE:HE1	2.46	0.45
1:H:152:LYS:HG3	1:H:162:ILE:CD1	2.46	0.45
1:E:183:TYR:CE1	1:E:184:LEU:HG	2.51	0.45
1:D:147:ARG:O	1:D:151:LEU:HD22	2.16	0.45
1:D:127:TYR:CE2	1:D:190:ILE:HD12	2.34	0.45
1:J:183:TYR:CE1	1:J:184:LEU:HG	2.51	0.45
1:E:156:LEU:HD21	1:E:162:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HA	1:A:214:LEU:HD12	1.68	0.45
1:E:191:LEU:HD23	1:E:191:LEU:HA	1.80	0.45
1:C:152:LYS:HG3	1:C:162:ILE:CD1	2.47	0.44
1:J:191:LEU:HA	1:J:191:LEU:HD23	1.81	0.44
1:D:186:LYS:HB3	1:D:188:THR:HG22	2.00	0.44
1:B:161:GLN:HB3	1:C:134:VAL:CG1	2.48	0.44
1:J:156:LEU:CD2	1:J:162:ILE:HG13	2.48	0.44
1:H:197:ASN:HB2	1:H:199:MSE:HE3	1.99	0.44
1:G:141:LYS:HD3	1:G:141:LYS:O	2.17	0.44
1:B:141:LYS:HD3	1:B:141:LYS:O	2.18	0.44
1:G:161:GLN:HB3	1:H:134:VAL:CG1	2.48	0.44
1:H:183:TYR:CE2	1:H:184:LEU:HG	2.52	0.44
1:C:183:TYR:CE2	1:C:184:LEU:HG	2.52	0.43
1:A:173:VAL:HG23	1:A:199:MSE:HE1	1.99	0.43
1:E:187:ASP:OD1	1:E:196:LYS:HE2	2.18	0.43
1:F:173:VAL:HG23	1:F:199:MSE:HE2	2.01	0.43
1:J:156:LEU:HD21	1:J:162:ILE:HG13	1.98	0.43
1:A:173:VAL:HG23	1:A:199:MSE:HE2	2.01	0.43
1:D:173:VAL:CG2	1:D:199:MSE:CE	2.95	0.43
1:J:187:ASP:OD1	1:J:196:LYS:HE2	2.18	0.43
1:I:161:GLN:HB3	1:J:136:MSE:HE2	2.00	0.43
1:I:214:LEU:HA	1:I:214:LEU:HD12	1.82	0.43
1:B:177:ARG:CZ	1:B:191:LEU:HD12	2.48	0.43
1:C:136:MSE:CE	1:C:140:ASN:HB3	2.33	0.42
1:D:158:LEU:HA	1:D:158:LEU:HD23	1.87	0.42
1:D:214:LEU:HA	1:D:214:LEU:HD12	1.81	0.42
1:F:127:TYR:HE2	1:F:190:ILE:HD13	1.83	0.42
1:D:145:ASP:O	1:D:148:ARG:HB3	2.20	0.42
1:I:158:LEU:HA	1:I:158:LEU:HD23	1.89	0.42
1:G:145:ASP:CG	1:G:148:ARG:HH12	2.23	0.41
1:I:145:ASP:O	1:I:148:ARG:HB3	2.20	0.41
1:I:173:VAL:CG2	1:I:199:MSE:HE1	2.50	0.41
1:I:197:ASN:O	1:I:198:TYR:HB2	2.20	0.41
1:I:126:ILE:HG12	1:I:172:ILE:HB	2.02	0.41
1:G:174:ILE:HA	1:G:202:TRP:O	2.20	0.41
1:H:131:THR:O	1:H:177:ARG:HG3	2.19	0.41
1:A:130:ILE:HG12	2:A:57:HOH:O	2.20	0.41
1:I:136:MSE:HE2	1:I:140:ASN:HB3	2.03	0.41
1:D:136:MSE:HE2	1:D:140:ASN:HB3	2.03	0.41
1:B:167:ASP:OD1	1:B:169:THR:HG23	2.21	0.41
1:B:194:ALA:HA	1:B:199:MSE:SE	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LYS:HB2	1:C:212:LYS:HE3	1.92	0.41
1:H:137:ASN:HB3	1:H:140:ASN:HB2	2.01	0.41
1:B:145:ASP:CG	1:B:148:ARG:HH12	2.24	0.41
1:C:131:THR:O	1:C:177:ARG:HG3	2.20	0.41
1:C:137:ASN:HB3	1:C:140:ASN:HB2	2.01	0.41
1:H:161:GLN:HG2	1:I:136:MSE:HE3	2.03	0.40
1:B:138:THR:O	1:B:139:TYR:C	2.57	0.40
1:C:174:ILE:HA	1:C:202:TRP:O	2.22	0.40
1:D:194:ALA:CB	1:D:199:MSE:HE2	2.52	0.40
1:G:138:THR:O	1:G:139:TYR:C	2.59	0.40
1:I:183:TYR:CE1	1:I:184:LEU:HD21	2.56	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	100/151 (66%)	96 (96%)	4 (4%)	0	100	100
1	B	91/151 (60%)	90 (99%)	1 (1%)	0	100	100
1	C	98/151 (65%)	94 (96%)	4 (4%)	0	100	100
1	D	102/151 (68%)	99 (97%)	3 (3%)	0	100	100
1	E	94/151 (62%)	90 (96%)	4 (4%)	0	100	100
1	F	100/151 (66%)	96 (96%)	4 (4%)	0	100	100
1	G	91/151 (60%)	89 (98%)	2 (2%)	0	100	100
1	H	98/151 (65%)	94 (96%)	4 (4%)	0	100	100
1	I	102/151 (68%)	98 (96%)	4 (4%)	0	100	100
1	J	94/151 (62%)	90 (96%)	4 (4%)	0	100	100
All	All	970/1510 (64%)	936 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	96/133 (72%)	91 (95%)	5 (5%)	29	58
1	B	87/133 (65%)	86 (99%)	1 (1%)	80	94
1	C	93/133 (70%)	90 (97%)	3 (3%)	46	77
1	D	98/133 (74%)	94 (96%)	4 (4%)	37	69
1	E	90/133 (68%)	86 (96%)	4 (4%)	35	65
1	F	96/133 (72%)	91 (95%)	5 (5%)	29	58
1	G	87/133 (65%)	86 (99%)	1 (1%)	80	94
1	H	93/133 (70%)	90 (97%)	3 (3%)	46	77
1	I	98/133 (74%)	94 (96%)	4 (4%)	37	69
1	J	90/133 (68%)	86 (96%)	4 (4%)	35	65
All	All	928/1330 (70%)	894 (96%)	34 (4%)	41	72

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	LEU
1	A	151	LEU
1	A	190	ILE
1	A	203	SER
1	A	214	LEU
1	B	123	ASP
1	C	124	SER
1	C	169	THR
1	C	214	LEU
1	D	124	SER
1	D	151	LEU
1	D	190	ILE
1	D	192	SER
1	E	123	ASP

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Mol	Chain	Res	Type
1	E	124	SER
1	E	138	THR
1	E	142	SER
1	F	150	LEU
1	F	151	LEU
1	F	190	ILE
1	F	203	SER
1	F	214	LEU
1	G	123	ASP
1	H	124	SER
1	H	169	THR
1	H	214	LEU
1	I	124	SER
1	I	151	LEU
1	I	190	ILE
1	I	192	SER
1	J	123	ASP
1	J	124	SER
1	J	138	THR
1	J	142	SER

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

Mol	Chain	Res	Type
1	C	197	ASN

### 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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	97/151 (64%)	-0.13	1 (1%) 84 85	32, 49, 104, 137	0
1	B	90/151 (59%)	-0.12	1 (1%) 82 83	40, 56, 85, 124	0
1	C	97/151 (64%)	0.00	1 (1%) 84 85	41, 62, 95, 148	0
1	D	100/151 (66%)	-0.15	1 (1%) 84 85	39, 53, 94, 121	0
1	E	92/151 (60%)	-0.06	2 (2%) 65 66	34, 50, 90, 150	0
1	F	97/151 (64%)	-0.15	0 100 100	32, 48, 105, 137	0
1	G	90/151 (59%)	-0.12	1 (1%) 82 83	40, 56, 85, 124	0
1	H	97/151 (64%)	0.01	1 (1%) 84 85	41, 62, 95, 148	0
1	I	100/151 (66%)	-0.17	1 (1%) 84 85	39, 53, 94, 121	0
1	J	92/151 (60%)	-0.16	1 (1%) 82 83	34, 50, 91, 150	0
All	All	952/1510 (63%)	-0.11	10 (1%) 82 83	32, 54, 95, 150	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	ASP	3.5
1	D	223	LYS	2.9
1	G	215	ASP	2.8
1	I	223	LYS	2.8
1	A	220	HIS	2.3
1	E	216	VAL	2.3
1	E	217	ASP	2.2
1	J	217	ASP	2.2
1	C	212	LYS	2.2
1	H	214	LEU	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.