wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2026 – 11:21 AM UTC

PDB ID	:	3OQ0 / pdb_00003oq0
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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

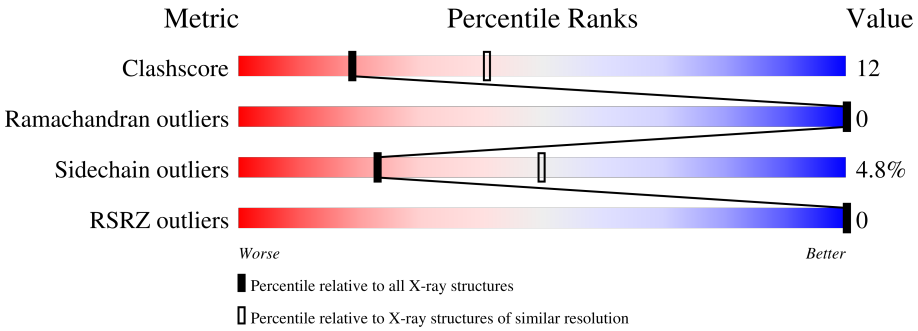
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of 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 <=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	54% 12% • 33%
1	B	151	44% 18% 38%
1	C	151	48% 17% • 34%
1	D	151	50% 16% • 32%
1	E	151	48% 13% • 37%
1	F	151	54% 11% • 33%

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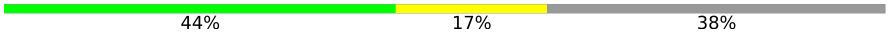
Mol	Chain	Length	Quality of chain
1	G	151	
1	H	151	
1	I	151	
1	J	151	

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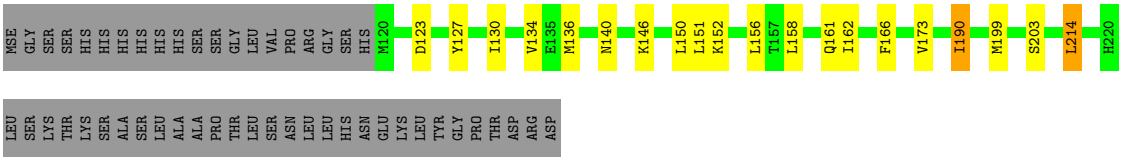
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	8	Total O 8 8	0	0
2	J	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

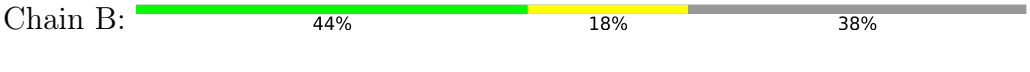
- Molecule 1: DBF4

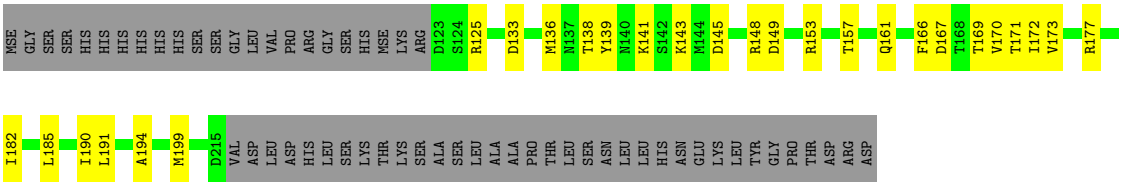
Chain A:



- Molecule 1: DBF4

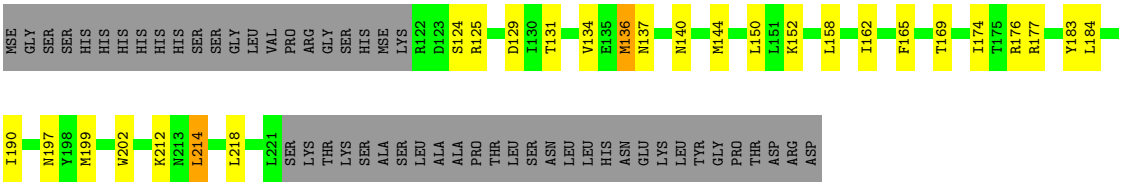
Chain B:





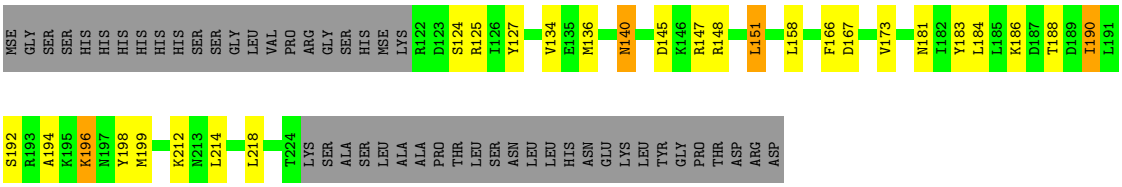
- Molecule 1: DBF4

Chain C:



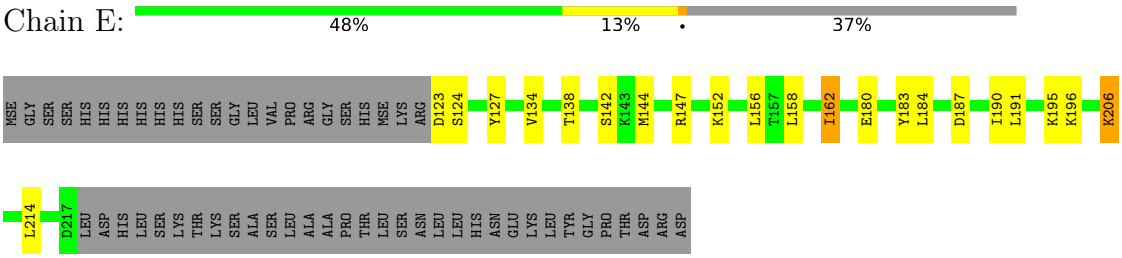
- Molecule 1: DBF4

Chain D:



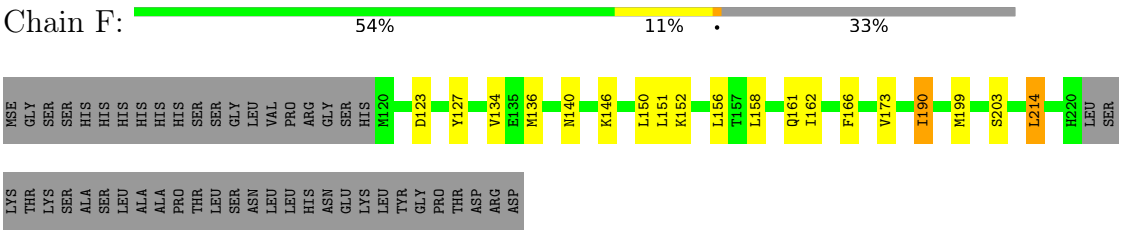
• Molecule 1: DBF4

Chain E:



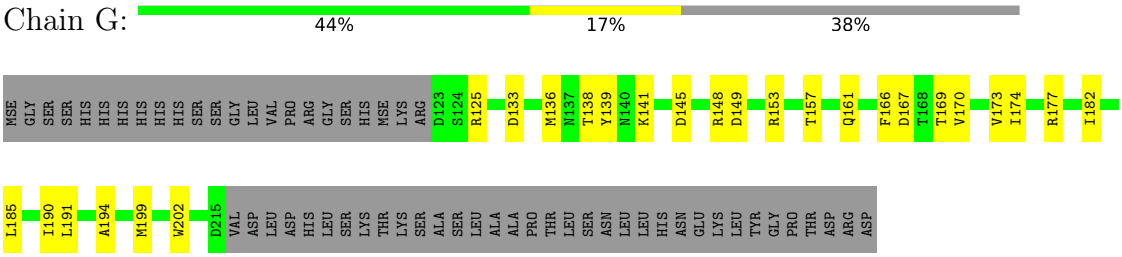
• Molecule 1: DBF4

Chain F:



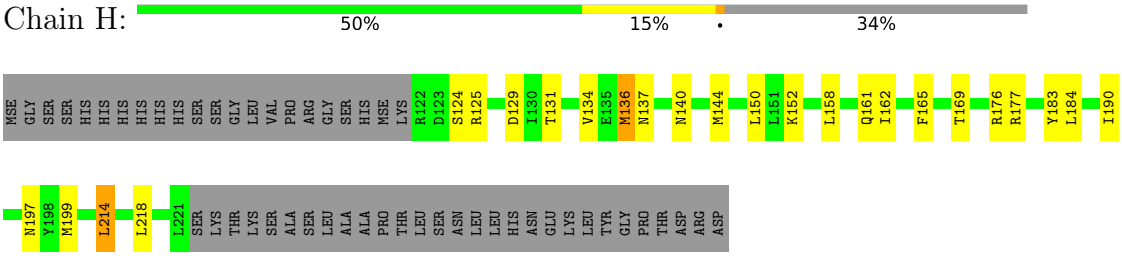
• Molecule 1: DBF4

Chain G:



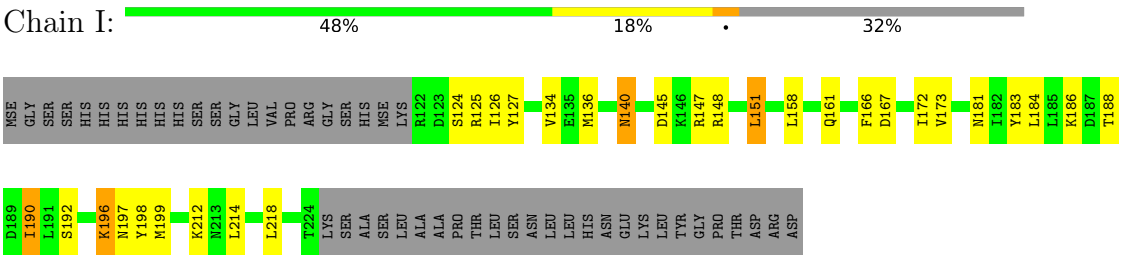
• Molecule 1: DBF4

Chain H:



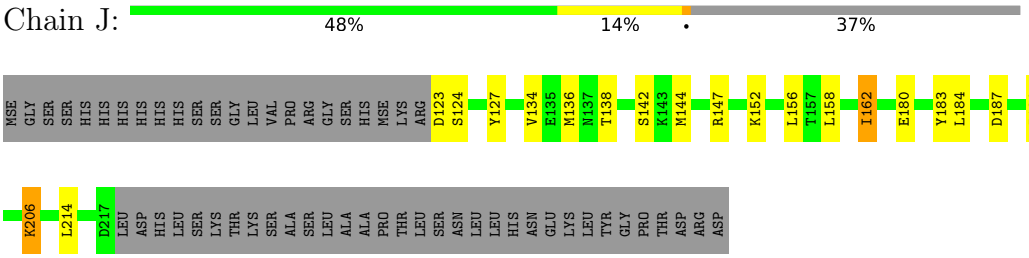
• Molecule 1: DBF4

Chain I:



• Molecule 1: DBF4

Chain J:


48%
14%
37%
MSE GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MSE LYS ARG D123 S124 Y127 V134 E135 M136 N137 T138 S142 K143 M144 R147 K152 L156 T157 L158 I162 E180 Y183 L184 D187 I190 L191 K195 K196
K206 L214 D217 LEU ASP HIS LEU SER LYS THR LYS SER ALA SER LEU ALA ALA PRO THR LEU SER ASN LEU LEU HIS ASN GLU LYS LEU TYR GLY PRO THR ASP ARG ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.22Å 79.36Å 127.42Å 90.00° 110.74° 90.00°	Depositor
Resolution (Å)	35.52 – 2.70 35.52 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (35.52-2.70) 95.9 (35.52-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_159)	Depositor
R, R_{free}	0.205 , 0.244 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8369	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.60	0/867	0.85	0/1157
1	B	0.55	0/788	0.84	0/1052
1	C	0.55	0/843	0.90	1/1128 (0.1%)
1	D	0.57	0/880	0.86	0/1176
1	E	0.57	0/812	0.89	0/1085
1	F	0.58	0/867	0.84	0/1157
1	G	0.54	0/788	0.85	0/1052
1	H	0.54	0/843	0.90	1/1128 (0.1%)
1	I	0.57	0/880	0.86	0/1176
1	J	0.57	0/812	0.90	0/1085
All	All	0.56	0/8380	0.87	2/11196 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	136	MSE	N-CA-C	5.95	117.89	108.79
1	C	136	MSE	N-CA-C	5.75	117.58	108.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	855	0	875	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	780	0	799	28	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	18	0
1	G	780	0	799	26	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	199	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.

The worst 5 of 199 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

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 (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	96/133 (72%)	89 (93%)	7 (7%)	13	32
1	B	87/133 (65%)	87 (100%)	0	100	100
1	C	93/133 (70%)	90 (97%)	3 (3%)	34	64
1	D	98/133 (74%)	92 (94%)	6 (6%)	17	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	90/133 (68%)	84 (93%)	6 (7%)	15 36
1	F	96/133 (72%)	89 (93%)	7 (7%)	13 32
1	G	87/133 (65%)	87 (100%)	0	100 100
1	H	93/133 (70%)	90 (97%)	3 (3%)	34 64
1	I	98/133 (74%)	92 (94%)	6 (6%)	17 40
1	J	90/133 (68%)	84 (93%)	6 (7%)	15 36
All	All	928/1330 (70%)	884 (95%)	44 (5%)	23 51

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	214	LEU
1	I	190	ILE
1	H	124	SER
1	I	124	SER
1	I	196	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	197	ASN
1	I	181	ASN
1	J	181	ASN
1	I	197	ASN
1	D	197	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	97/151 (64%)	-1.49	0	100	100	26, 49, 104, 137	1 (1%)
1	B	90/151 (59%)	-1.43	0	100	100	40, 56, 85, 124	0
1	C	97/151 (64%)	-1.33	0	100	100	41, 62, 95, 148	0
1	D	100/151 (66%)	-1.44	0	100	100	32, 53, 94, 121	1 (1%)
1	E	92/151 (60%)	-1.43	0	100	100	26, 50, 90, 150	1 (1%)
1	F	97/151 (64%)	-1.53	0	100	100	26, 48, 105, 137	1 (1%)
1	G	90/151 (59%)	-1.45	0	100	100	40, 56, 85, 124	0
1	H	97/151 (64%)	-1.31	0	100	100	41, 62, 95, 148	0
1	I	100/151 (66%)	-1.47	0	100	100	32, 53, 94, 121	1 (1%)
1	J	92/151 (60%)	-1.48	0	100	100	26, 50, 91, 150	1 (1%)
All	All	952/1510 (63%)	-1.44	0	100	100	26, 54, 95, 150	6 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.