wwPDB X-ray Structure Validation Summary Report (i)

Sep 6, 2023 – 03:33 AM EDT

PDB ID	:	4DJM
Title	:	Crystal structure of the E. coli chaperone DraB
Authors	:	Dauter, Z.; Piatek, R.; Dauter, M.; Brzuszkiewicz, A.
Deposited on	:	2012-02-02
Resolution	:	2.52 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:

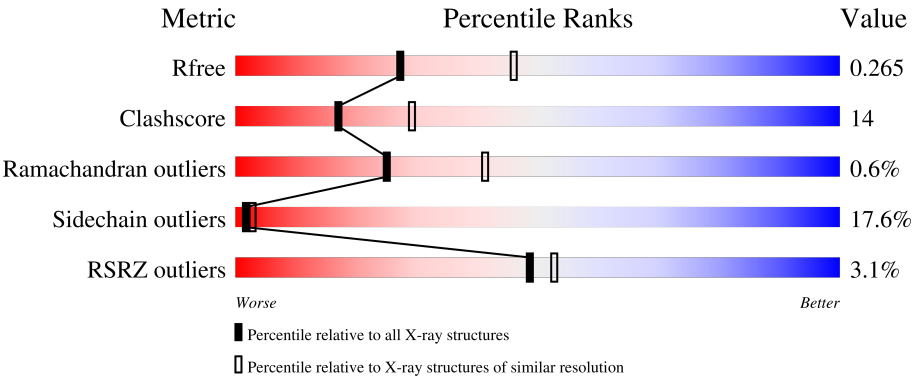
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.52 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 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	239	3% 55% 22% • • 18%
1	B	239	6% 56% 23% 6% 15%
1	C	239	4% 57% 19% 6% • 16%
1	D	239	56% 23% 6% 14%
1	E	239	5% 55% 22% 5% • 17%

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Mol	Chain	Length	Quality of chain
1	F	239	59% 21% 5% 15%
1	G	239	% 62% 15% 7% 16%
1	H	239	3% 56% 23% 5% 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12557 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 DraB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	Se	0	0	0
			1541	984	268	286	2	1			
1	B	203	Total	C	N	O	S	Se	0	0	0
			1581	1007	273	298	2	1			
1	C	200	Total	C	N	O	S	Se	0	0	0
			1552	989	269	291	2	1			
1	D	205	Total	C	N	O	S	Se	0	0	0
			1601	1019	279	300	2	1			
1	E	199	Total	C	N	O	S	Se	0	0	0
			1555	993	271	288	2	1			
1	F	203	Total	C	N	O	S	Se	0	0	0
			1587	1010	276	298	2	1			
1	G	200	Total	C	N	O	S	Se	0	0	0
			1561	995	272	291	2	1			
1	H	202	Total	C	N	O	S	Se	0	0	0
			1579	1006	275	295	2	1			

There are 232 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q7BG37
A	2	ALA	-	expression tag	UNP Q7BG37
A	3	MSE	-	expression tag	UNP Q7BG37
A	214	ALA	-	expression tag	UNP Q7BG37
A	215	SER	-	expression tag	UNP Q7BG37
A	216	GLY	-	expression tag	UNP Q7BG37
A	217	LYS	-	expression tag	UNP Q7BG37
A	218	VAL	-	expression tag	UNP Q7BG37
A	219	GLN	-	expression tag	UNP Q7BG37
A	220	TRP	-	expression tag	UNP Q7BG37
A	221	LYS	-	expression tag	UNP Q7BG37
A	222	VAL	-	expression tag	UNP Q7BG37
A	223	ILE	-	expression tag	UNP Q7BG37

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Chain	Residue	Modelled	Actual	Comment	Reference
A	224	THR	-	expression tag	UNP Q7BG37
A	225	ASP	-	expression tag	UNP Q7BG37
A	226	TYR	-	expression tag	UNP Q7BG37
A	227	GLY	-	expression tag	UNP Q7BG37
A	228	GLY	-	expression tag	UNP Q7BG37
A	229	THR	-	expression tag	UNP Q7BG37
A	230	SER	-	expression tag	UNP Q7BG37
A	231	LYS	-	expression tag	UNP Q7BG37
A	232	GLN	-	expression tag	UNP Q7BG37
A	233	PHE	-	expression tag	UNP Q7BG37
A	234	GLU	-	expression tag	UNP Q7BG37
A	235	ALA	-	expression tag	UNP Q7BG37
A	236	GLU	-	expression tag	UNP Q7BG37
A	237	LEU	-	expression tag	UNP Q7BG37
A	238	LYS	-	expression tag	UNP Q7BG37
A	239	GLY	-	expression tag	UNP Q7BG37
B	1	ALA	-	expression tag	UNP Q7BG37
B	2	ALA	-	expression tag	UNP Q7BG37
B	3	MSE	-	expression tag	UNP Q7BG37
B	214	ALA	-	expression tag	UNP Q7BG37
B	215	SER	-	expression tag	UNP Q7BG37
B	216	GLY	-	expression tag	UNP Q7BG37
B	217	LYS	-	expression tag	UNP Q7BG37
B	218	VAL	-	expression tag	UNP Q7BG37
B	219	GLN	-	expression tag	UNP Q7BG37
B	220	TRP	-	expression tag	UNP Q7BG37
B	221	LYS	-	expression tag	UNP Q7BG37
B	222	VAL	-	expression tag	UNP Q7BG37
B	223	ILE	-	expression tag	UNP Q7BG37
B	224	THR	-	expression tag	UNP Q7BG37
B	225	ASP	-	expression tag	UNP Q7BG37
B	226	TYR	-	expression tag	UNP Q7BG37
B	227	GLY	-	expression tag	UNP Q7BG37
B	228	GLY	-	expression tag	UNP Q7BG37
B	229	THR	-	expression tag	UNP Q7BG37
B	230	SER	-	expression tag	UNP Q7BG37
B	231	LYS	-	expression tag	UNP Q7BG37
B	232	GLN	-	expression tag	UNP Q7BG37
B	233	PHE	-	expression tag	UNP Q7BG37
B	234	GLU	-	expression tag	UNP Q7BG37
B	235	ALA	-	expression tag	UNP Q7BG37
B	236	GLU	-	expression tag	UNP Q7BG37

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Chain	Residue	Modelled	Actual	Comment	Reference
B	237	LEU	-	expression tag	UNP Q7BG37
B	238	LYS	-	expression tag	UNP Q7BG37
B	239	GLY	-	expression tag	UNP Q7BG37
C	1	ALA	-	expression tag	UNP Q7BG37
C	2	ALA	-	expression tag	UNP Q7BG37
C	3	MSE	-	expression tag	UNP Q7BG37
C	214	ALA	-	expression tag	UNP Q7BG37
C	215	SER	-	expression tag	UNP Q7BG37
C	216	GLY	-	expression tag	UNP Q7BG37
C	217	LYS	-	expression tag	UNP Q7BG37
C	218	VAL	-	expression tag	UNP Q7BG37
C	219	GLN	-	expression tag	UNP Q7BG37
C	220	TRP	-	expression tag	UNP Q7BG37
C	221	LYS	-	expression tag	UNP Q7BG37
C	222	VAL	-	expression tag	UNP Q7BG37
C	223	ILE	-	expression tag	UNP Q7BG37
C	224	THR	-	expression tag	UNP Q7BG37
C	225	ASP	-	expression tag	UNP Q7BG37
C	226	TYR	-	expression tag	UNP Q7BG37
C	227	GLY	-	expression tag	UNP Q7BG37
C	228	GLY	-	expression tag	UNP Q7BG37
C	229	THR	-	expression tag	UNP Q7BG37
C	230	SER	-	expression tag	UNP Q7BG37
C	231	LYS	-	expression tag	UNP Q7BG37
C	232	GLN	-	expression tag	UNP Q7BG37
C	233	PHE	-	expression tag	UNP Q7BG37
C	234	GLU	-	expression tag	UNP Q7BG37
C	235	ALA	-	expression tag	UNP Q7BG37
C	236	GLU	-	expression tag	UNP Q7BG37
C	237	LEU	-	expression tag	UNP Q7BG37
C	238	LYS	-	expression tag	UNP Q7BG37
C	239	GLY	-	expression tag	UNP Q7BG37
D	1	ALA	-	expression tag	UNP Q7BG37
D	2	ALA	-	expression tag	UNP Q7BG37
D	3	MSE	-	expression tag	UNP Q7BG37
D	214	ALA	-	expression tag	UNP Q7BG37
D	215	SER	-	expression tag	UNP Q7BG37
D	216	GLY	-	expression tag	UNP Q7BG37
D	217	LYS	-	expression tag	UNP Q7BG37
D	218	VAL	-	expression tag	UNP Q7BG37
D	219	GLN	-	expression tag	UNP Q7BG37
D	220	TRP	-	expression tag	UNP Q7BG37

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Chain	Residue	Modelled	Actual	Comment	Reference
D	221	LYS	-	expression tag	UNP Q7BG37
D	222	VAL	-	expression tag	UNP Q7BG37
D	223	ILE	-	expression tag	UNP Q7BG37
D	224	THR	-	expression tag	UNP Q7BG37
D	225	ASP	-	expression tag	UNP Q7BG37
D	226	TYR	-	expression tag	UNP Q7BG37
D	227	GLY	-	expression tag	UNP Q7BG37
D	228	GLY	-	expression tag	UNP Q7BG37
D	229	THR	-	expression tag	UNP Q7BG37
D	230	SER	-	expression tag	UNP Q7BG37
D	231	LYS	-	expression tag	UNP Q7BG37
D	232	GLN	-	expression tag	UNP Q7BG37
D	233	PHE	-	expression tag	UNP Q7BG37
D	234	GLU	-	expression tag	UNP Q7BG37
D	235	ALA	-	expression tag	UNP Q7BG37
D	236	GLU	-	expression tag	UNP Q7BG37
D	237	LEU	-	expression tag	UNP Q7BG37
D	238	LYS	-	expression tag	UNP Q7BG37
D	239	GLY	-	expression tag	UNP Q7BG37
E	1	ALA	-	expression tag	UNP Q7BG37
E	2	ALA	-	expression tag	UNP Q7BG37
E	3	MSE	-	expression tag	UNP Q7BG37
E	214	ALA	-	expression tag	UNP Q7BG37
E	215	SER	-	expression tag	UNP Q7BG37
E	216	GLY	-	expression tag	UNP Q7BG37
E	217	LYS	-	expression tag	UNP Q7BG37
E	218	VAL	-	expression tag	UNP Q7BG37
E	219	GLN	-	expression tag	UNP Q7BG37
E	220	TRP	-	expression tag	UNP Q7BG37
E	221	LYS	-	expression tag	UNP Q7BG37
E	222	VAL	-	expression tag	UNP Q7BG37
E	223	ILE	-	expression tag	UNP Q7BG37
E	224	THR	-	expression tag	UNP Q7BG37
E	225	ASP	-	expression tag	UNP Q7BG37
E	226	TYR	-	expression tag	UNP Q7BG37
E	227	GLY	-	expression tag	UNP Q7BG37
E	228	GLY	-	expression tag	UNP Q7BG37
E	229	THR	-	expression tag	UNP Q7BG37
E	230	SER	-	expression tag	UNP Q7BG37
E	231	LYS	-	expression tag	UNP Q7BG37
E	232	GLN	-	expression tag	UNP Q7BG37
E	233	PHE	-	expression tag	UNP Q7BG37

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Chain	Residue	Modelled	Actual	Comment	Reference
E	234	GLU	-	expression tag	UNP Q7BG37
E	235	ALA	-	expression tag	UNP Q7BG37
E	236	GLU	-	expression tag	UNP Q7BG37
E	237	LEU	-	expression tag	UNP Q7BG37
E	238	LYS	-	expression tag	UNP Q7BG37
E	239	GLY	-	expression tag	UNP Q7BG37
F	1	ALA	-	expression tag	UNP Q7BG37
F	2	ALA	-	expression tag	UNP Q7BG37
F	3	MSE	-	expression tag	UNP Q7BG37
F	214	ALA	-	expression tag	UNP Q7BG37
F	215	SER	-	expression tag	UNP Q7BG37
F	216	GLY	-	expression tag	UNP Q7BG37
F	217	LYS	-	expression tag	UNP Q7BG37
F	218	VAL	-	expression tag	UNP Q7BG37
F	219	GLN	-	expression tag	UNP Q7BG37
F	220	TRP	-	expression tag	UNP Q7BG37
F	221	LYS	-	expression tag	UNP Q7BG37
F	222	VAL	-	expression tag	UNP Q7BG37
F	223	ILE	-	expression tag	UNP Q7BG37
F	224	THR	-	expression tag	UNP Q7BG37
F	225	ASP	-	expression tag	UNP Q7BG37
F	226	TYR	-	expression tag	UNP Q7BG37
F	227	GLY	-	expression tag	UNP Q7BG37
F	228	GLY	-	expression tag	UNP Q7BG37
F	229	THR	-	expression tag	UNP Q7BG37
F	230	SER	-	expression tag	UNP Q7BG37
F	231	LYS	-	expression tag	UNP Q7BG37
F	232	GLN	-	expression tag	UNP Q7BG37
F	233	PHE	-	expression tag	UNP Q7BG37
F	234	GLU	-	expression tag	UNP Q7BG37
F	235	ALA	-	expression tag	UNP Q7BG37
F	236	GLU	-	expression tag	UNP Q7BG37
F	237	LEU	-	expression tag	UNP Q7BG37
F	238	LYS	-	expression tag	UNP Q7BG37
F	239	GLY	-	expression tag	UNP Q7BG37
G	1	ALA	-	expression tag	UNP Q7BG37
G	2	ALA	-	expression tag	UNP Q7BG37
G	3	MSE	-	expression tag	UNP Q7BG37
G	214	ALA	-	expression tag	UNP Q7BG37
G	215	SER	-	expression tag	UNP Q7BG37
G	216	GLY	-	expression tag	UNP Q7BG37
G	217	LYS	-	expression tag	UNP Q7BG37

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Chain	Residue	Modelled	Actual	Comment	Reference
G	218	VAL	-	expression tag	UNP Q7BG37
G	219	GLN	-	expression tag	UNP Q7BG37
G	220	TRP	-	expression tag	UNP Q7BG37
G	221	LYS	-	expression tag	UNP Q7BG37
G	222	VAL	-	expression tag	UNP Q7BG37
G	223	ILE	-	expression tag	UNP Q7BG37
G	224	THR	-	expression tag	UNP Q7BG37
G	225	ASP	-	expression tag	UNP Q7BG37
G	226	TYR	-	expression tag	UNP Q7BG37
G	227	GLY	-	expression tag	UNP Q7BG37
G	228	GLY	-	expression tag	UNP Q7BG37
G	229	THR	-	expression tag	UNP Q7BG37
G	230	SER	-	expression tag	UNP Q7BG37
G	231	LYS	-	expression tag	UNP Q7BG37
G	232	GLN	-	expression tag	UNP Q7BG37
G	233	PHE	-	expression tag	UNP Q7BG37
G	234	GLU	-	expression tag	UNP Q7BG37
G	235	ALA	-	expression tag	UNP Q7BG37
G	236	GLU	-	expression tag	UNP Q7BG37
G	237	LEU	-	expression tag	UNP Q7BG37
G	238	LYS	-	expression tag	UNP Q7BG37
G	239	GLY	-	expression tag	UNP Q7BG37
H	1	ALA	-	expression tag	UNP Q7BG37
H	2	ALA	-	expression tag	UNP Q7BG37
H	3	MSE	-	expression tag	UNP Q7BG37
H	214	ALA	-	expression tag	UNP Q7BG37
H	215	SER	-	expression tag	UNP Q7BG37
H	216	GLY	-	expression tag	UNP Q7BG37
H	217	LYS	-	expression tag	UNP Q7BG37
H	218	VAL	-	expression tag	UNP Q7BG37
H	219	GLN	-	expression tag	UNP Q7BG37
H	220	TRP	-	expression tag	UNP Q7BG37
H	221	LYS	-	expression tag	UNP Q7BG37
H	222	VAL	-	expression tag	UNP Q7BG37
H	223	ILE	-	expression tag	UNP Q7BG37
H	224	THR	-	expression tag	UNP Q7BG37
H	225	ASP	-	expression tag	UNP Q7BG37
H	226	TYR	-	expression tag	UNP Q7BG37
H	227	GLY	-	expression tag	UNP Q7BG37
H	228	GLY	-	expression tag	UNP Q7BG37
H	229	THR	-	expression tag	UNP Q7BG37
H	230	SER	-	expression tag	UNP Q7BG37

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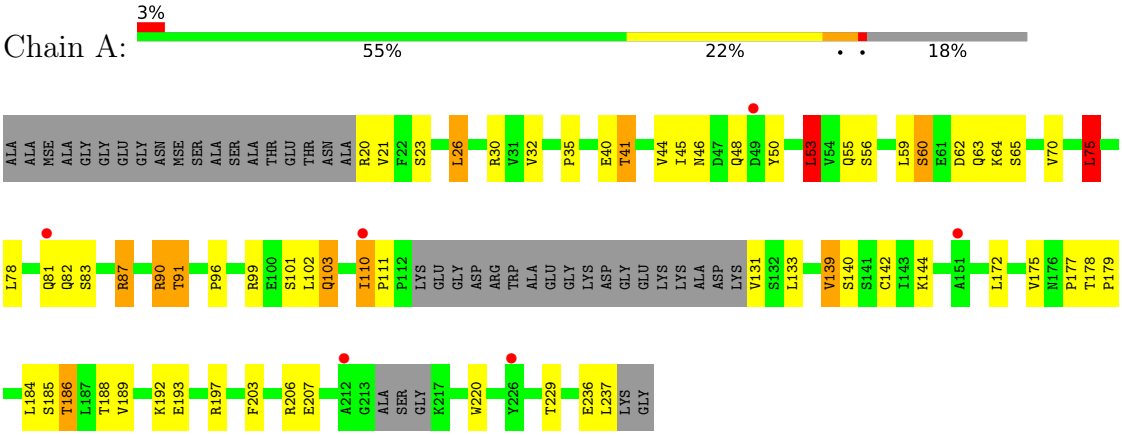
Chain	Residue	Modelled	Actual	Comment	Reference
H	231	LYS	-	expression tag	UNP Q7BG37
H	232	GLN	-	expression tag	UNP Q7BG37
H	233	PHE	-	expression tag	UNP Q7BG37
H	234	GLU	-	expression tag	UNP Q7BG37
H	235	ALA	-	expression tag	UNP Q7BG37
H	236	GLU	-	expression tag	UNP Q7BG37
H	237	LEU	-	expression tag	UNP Q7BG37
H	238	LYS	-	expression tag	UNP Q7BG37
H	239	GLY	-	expression tag	UNP Q7BG37

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.

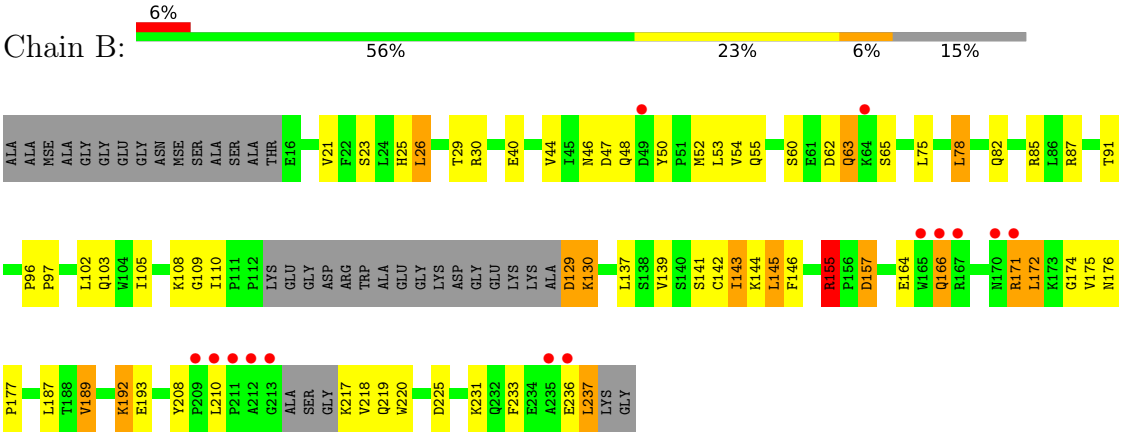
- Molecule 1: DraB

Chain A:



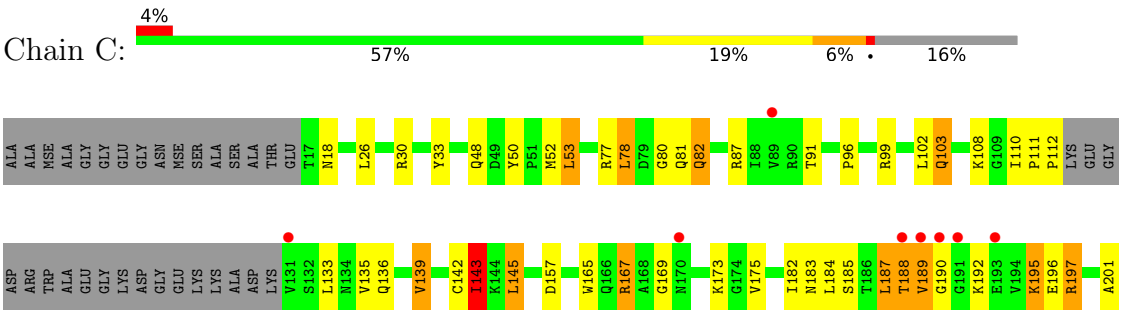
- Molecule 1: DraB

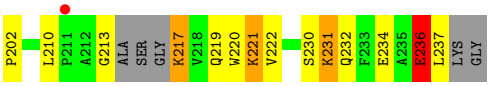
Chain B:



- Molecule 1: DraB

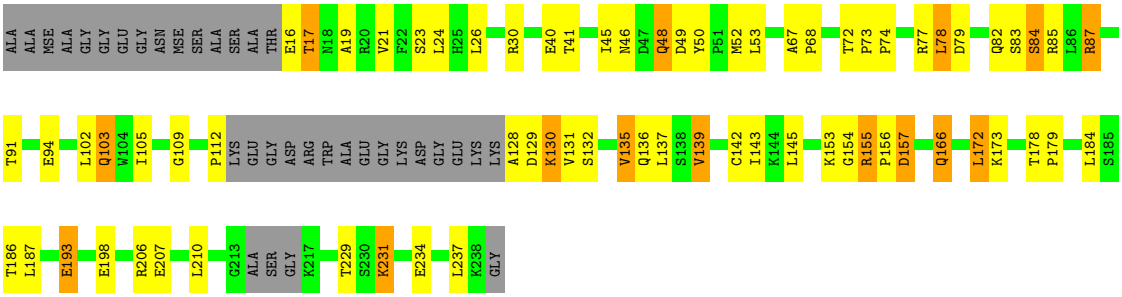
Chain C:





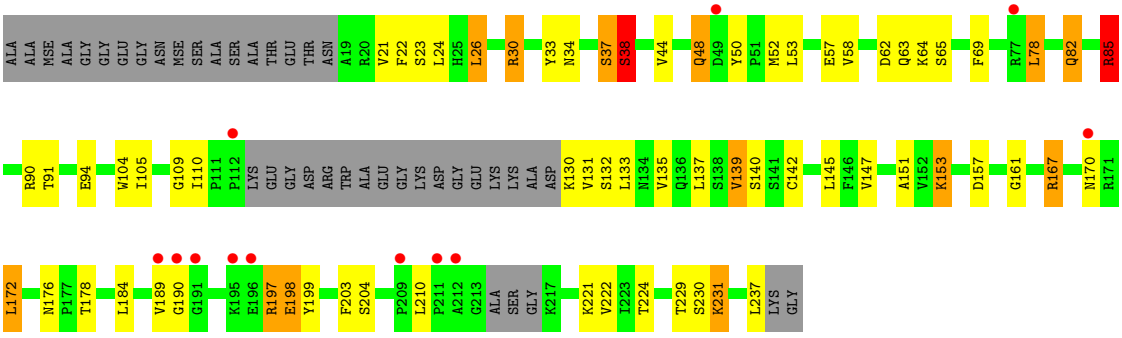
• Molecule 1: DraB

Chain D:



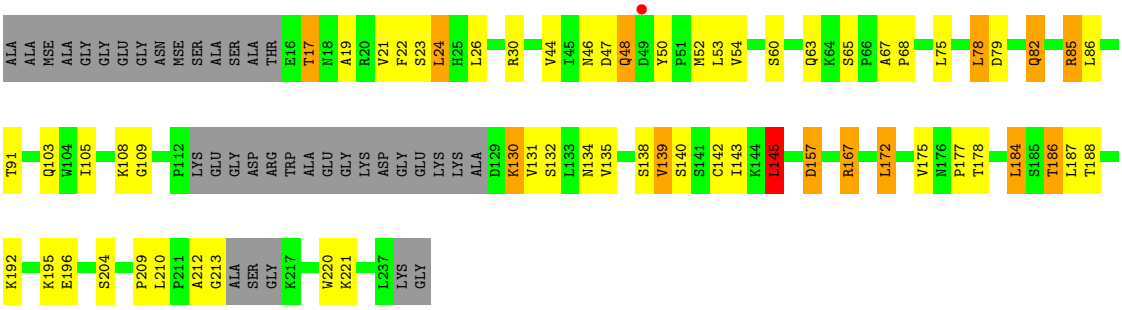
• Molecule 1: DraB

Chain E:



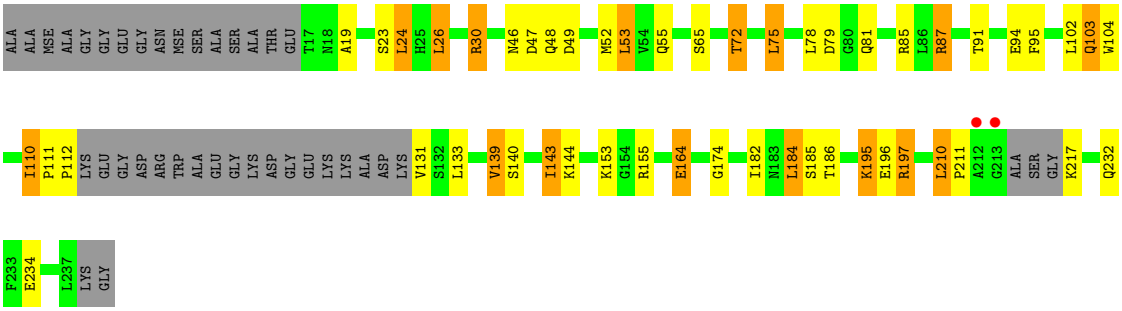
• Molecule 1: DraB

Chain F:



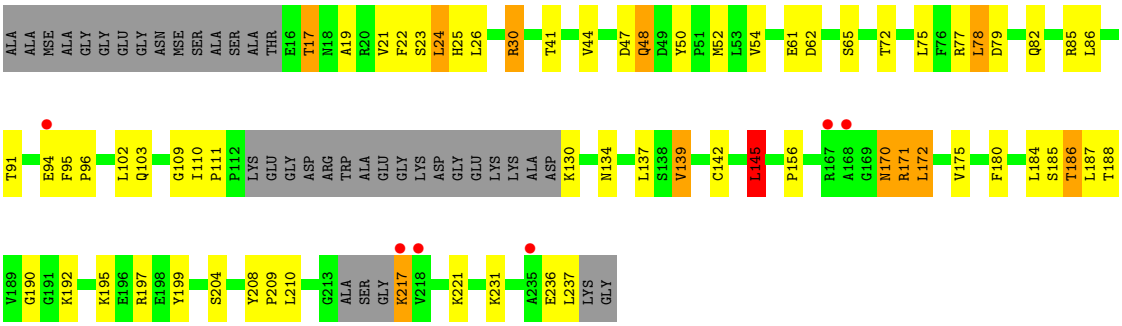
• Molecule 1: DraB

Chain G:



• Molecule 1: DraB

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.45Å 98.41Å 100.88Å 84.20° 89.80° 83.80°	Depositor
Resolution (Å)	30.00 – 2.52 29.99 – 2.52	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.52) 97.4 (29.99-2.52)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.269 0.207 , 0.265	Depositor DCC
R_{free} test set	1489 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12557	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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	1.00	1/1576 (0.1%)	1.01	3/2140 (0.1%)
1	B	1.05	1/1616 (0.1%)	1.02	4/2195 (0.2%)
1	C	1.07	2/1587 (0.1%)	1.01	4/2156 (0.2%)
1	D	1.08	1/1636 (0.1%)	1.04	1/2220 (0.0%)
1	E	1.02	2/1590 (0.1%)	1.04	3/2158 (0.1%)
1	F	1.17	1/1622 (0.1%)	1.13	9/2202 (0.4%)
1	G	1.09	2/1596 (0.1%)	1.03	0/2168
1	H	1.13	2/1614 (0.1%)	1.02	2/2191 (0.1%)
All	All	1.08	12/12837 (0.1%)	1.04	26/17430 (0.1%)

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	C	0	1
1	D	0	1
1	H	0	1
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	157	ASP	CB-CG	-7.42	1.36	1.51
1	D	40	GLU	CD-OE2	6.92	1.33	1.25
1	C	213	GLY	C-O	6.77	1.34	1.23
1	H	142	CYS	CB-SG	6.60	1.93	1.82
1	H	44	VAL	CB-CG1	-6.42	1.39	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	LEU	CA-CB-CG	8.47	134.78	115.30
1	A	75	LEU	CA-CB-CG	8.11	133.96	115.30
1	F	157	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	E	53	LEU	CA-CB-CG	6.97	131.34	115.30
1	B	155	ARG	NE-CZ-NH1	6.75	123.67	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	169	GLY	Peptide
1	D	156	PRO	Peptide
1	H	170	ASN	Peptide

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	1541	0	1553	42	0
1	B	1581	0	1583	49	0
1	C	1552	0	1552	55	0
1	D	1601	0	1612	52	0
1	E	1555	0	1571	47	0
1	F	1587	0	1594	47	0
1	G	1561	0	1571	33	0
1	H	1579	0	1590	50	0
All	All	12557	0	12626	353	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 14.

The worst 5 of 353 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:221:LYS:CE	1:C:221:LYS:HA	1.67	1.25
1:H:52:MSE:CE	1:H:109:GLY:HA3	1.69	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:MSE:HE1	1:F:109:GLY:HA3	1.21	1.15
1:D:52:MSE:HE1	1:D:109:GLY:HA3	1.26	1.14
1:C:167:ARG:HH11	1:C:167:ARG:HG2	1.04	1.13

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	191/239 (80%)	184 (96%)	5 (3%)	2 (1%)	15 27
1	B	197/239 (82%)	184 (93%)	12 (6%)	1 (0%)	29 47
1	C	194/239 (81%)	179 (92%)	13 (7%)	2 (1%)	15 27
1	D	199/239 (83%)	187 (94%)	11 (6%)	1 (0%)	29 47
1	E	193/239 (81%)	184 (95%)	6 (3%)	3 (2%)	9 16
1	F	197/239 (82%)	185 (94%)	11 (6%)	1 (0%)	29 47
1	G	194/239 (81%)	185 (95%)	9 (5%)	0	100 100
1	H	196/239 (82%)	186 (95%)	10 (5%)	0	100 100
All	All	1561/1912 (82%)	1474 (94%)	77 (5%)	10 (1%)	25 41

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	ASP
1	D	157	ASP
1	A	60	SER
1	A	197	ARG
1	C	189	VAL

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	173/195 (89%)	143 (83%)	30 (17%)	2	3
1	B	177/195 (91%)	146 (82%)	31 (18%)	2	3
1	C	173/195 (89%)	142 (82%)	31 (18%)	2	2
1	D	179/195 (92%)	143 (80%)	36 (20%)	1	2
1	E	174/195 (89%)	145 (83%)	29 (17%)	2	3
1	F	178/195 (91%)	147 (83%)	31 (17%)	2	3
1	G	175/195 (90%)	146 (83%)	29 (17%)	2	3
1	H	177/195 (91%)	146 (82%)	31 (18%)	2	3
All	All	1406/1560 (90%)	1158 (82%)	248 (18%)	2	3

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	153	LYS
1	H	30	ARG
1	E	140	SER
1	H	24	LEU
1	H	172	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	48	GLN
1	G	63	GLN
1	G	48	GLN
1	G	134	ASN
1	B	103	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 monosaccharides 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	196/239 (82%)	0.07	6 (3%) 49 53	29, 47, 74, 92	1 (0%)
1	B	202/239 (84%)	0.28	14 (6%) 16 17	23, 49, 88, 117	1 (0%)
1	C	199/239 (83%)	0.21	9 (4%) 33 36	24, 44, 94, 115	1 (0%)
1	D	204/239 (85%)	-0.13	0 100 100	22, 43, 63, 75	1 (0%)
1	E	198/239 (82%)	0.33	12 (6%) 21 22	32, 53, 87, 102	1 (0%)
1	F	202/239 (84%)	-0.14	1 (0%) 91 92	20, 38, 66, 86	1 (0%)
1	G	199/239 (83%)	-0.13	2 (1%) 82 84	23, 41, 63, 81	1 (0%)
1	H	201/239 (84%)	0.01	6 (2%) 50 54	20, 39, 78, 103	1 (0%)
All	All	1601/1912 (83%)	0.06	50 (3%) 49 53	20, 44, 80, 117	8 (0%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	189	VAL	7.9
1	C	190	GLY	5.3
1	C	170	ASN	4.6
1	E	190	GLY	4.5
1	C	189	VAL	4.5

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.