



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:08 pm BST

PDB ID : 6OOC  
Title : Structure of the pterocarpan synthase dirigent protein GePTS1  
Authors : Smith, C.A.  
Deposited on : 2019-04-23  
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

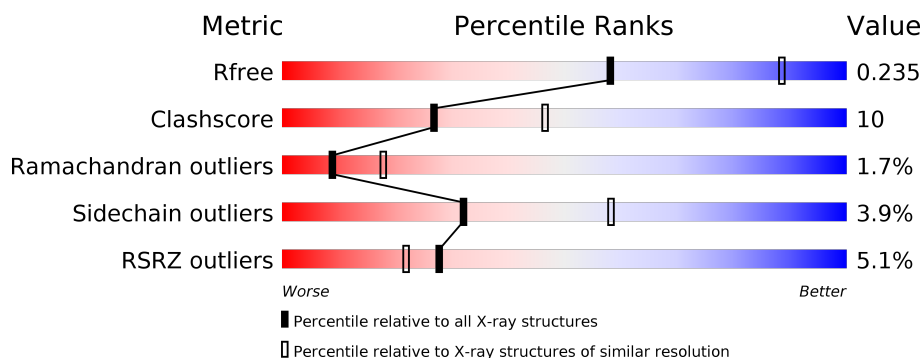
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	220	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>10%</div> <div>•</div> <div>27%</div> </div> </div>
1	B	220	<div> <div>5%</div> <div> <div></div> <div>59%</div> <div>17%</div> <div>•</div> <div>21%</div> </div> </div>
1	C	220	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>13%</div> <div>•</div> <div>25%</div> </div> </div>
1	D	220	<div> <div>6%</div> <div> <div></div> <div>56%</div> <div>18%</div> <div>•</div> <div>24%</div> </div> </div>
1	E	220	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>19%</div> <div>•</div> <div>24%</div> </div> </div>
1	F	220	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>17%</div> <div>•</div> <div>21%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7914 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 Dirigent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1248	807	195	235	11			
1	B	174	Total	C	N	O	S	0	0	0
			1344	862	217	254	11			
1	C	164	Total	C	N	O	S	0	0	0
			1268	816	202	239	11			
1	D	168	Total	C	N	O	S	0	0	0
			1296	834	206	245	11			
1	E	168	Total	C	N	O	S	0	0	0
			1298	835	206	246	11			
1	F	174	Total	C	N	O	S	0	1	0
			1359	872	218	258	11			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	LYS	-	expression tag	UNP A0A1V1FH01
A	190	GLY	-	expression tag	UNP A0A1V1FH01
A	191	GLU	-	expression tag	UNP A0A1V1FH01
A	192	LEU	-	expression tag	UNP A0A1V1FH01
A	193	ASN	-	expression tag	UNP A0A1V1FH01
A	194	SER	-	expression tag	UNP A0A1V1FH01
A	195	LYS	-	expression tag	UNP A0A1V1FH01
A	196	LEU	-	expression tag	UNP A0A1V1FH01
A	197	GLU	-	expression tag	UNP A0A1V1FH01
A	198	GLY	-	expression tag	UNP A0A1V1FH01
A	199	LYS	-	expression tag	UNP A0A1V1FH01
A	200	PRO	-	expression tag	UNP A0A1V1FH01
A	201	ILE	-	expression tag	UNP A0A1V1FH01
A	202	PRO	-	expression tag	UNP A0A1V1FH01
A	203	ASN	-	expression tag	UNP A0A1V1FH01
A	204	PRO	-	expression tag	UNP A0A1V1FH01
A	205	LEU	-	expression tag	UNP A0A1V1FH01

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Chain	Residue	Modelled	Actual	Comment	Reference
A	206	LEU	-	expression tag	UNP A0A1V1FH01
A	207	GLY	-	expression tag	UNP A0A1V1FH01
A	208	LEU	-	expression tag	UNP A0A1V1FH01
A	209	ASP	-	expression tag	UNP A0A1V1FH01
A	210	SER	-	expression tag	UNP A0A1V1FH01
A	211	THR	-	expression tag	UNP A0A1V1FH01
A	212	ARG	-	expression tag	UNP A0A1V1FH01
A	213	THR	-	expression tag	UNP A0A1V1FH01
A	214	GLY	-	expression tag	UNP A0A1V1FH01
A	215	HIS	-	expression tag	UNP A0A1V1FH01
A	216	HIS	-	expression tag	UNP A0A1V1FH01
A	217	HIS	-	expression tag	UNP A0A1V1FH01
A	218	HIS	-	expression tag	UNP A0A1V1FH01
A	219	HIS	-	expression tag	UNP A0A1V1FH01
A	220	HIS	-	expression tag	UNP A0A1V1FH01
B	189	LYS	-	expression tag	UNP A0A1V1FH01
B	190	GLY	-	expression tag	UNP A0A1V1FH01
B	191	GLU	-	expression tag	UNP A0A1V1FH01
B	192	LEU	-	expression tag	UNP A0A1V1FH01
B	193	ASN	-	expression tag	UNP A0A1V1FH01
B	194	SER	-	expression tag	UNP A0A1V1FH01
B	195	LYS	-	expression tag	UNP A0A1V1FH01
B	196	LEU	-	expression tag	UNP A0A1V1FH01
B	197	GLU	-	expression tag	UNP A0A1V1FH01
B	198	GLY	-	expression tag	UNP A0A1V1FH01
B	199	LYS	-	expression tag	UNP A0A1V1FH01
B	200	PRO	-	expression tag	UNP A0A1V1FH01
B	201	ILE	-	expression tag	UNP A0A1V1FH01
B	202	PRO	-	expression tag	UNP A0A1V1FH01
B	203	ASN	-	expression tag	UNP A0A1V1FH01
B	204	PRO	-	expression tag	UNP A0A1V1FH01
B	205	LEU	-	expression tag	UNP A0A1V1FH01
B	206	LEU	-	expression tag	UNP A0A1V1FH01
B	207	GLY	-	expression tag	UNP A0A1V1FH01
B	208	LEU	-	expression tag	UNP A0A1V1FH01
B	209	ASP	-	expression tag	UNP A0A1V1FH01
B	210	SER	-	expression tag	UNP A0A1V1FH01
B	211	THR	-	expression tag	UNP A0A1V1FH01
B	212	ARG	-	expression tag	UNP A0A1V1FH01
B	213	THR	-	expression tag	UNP A0A1V1FH01
B	214	GLY	-	expression tag	UNP A0A1V1FH01
B	215	HIS	-	expression tag	UNP A0A1V1FH01

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Chain	Residue	Modelled	Actual	Comment	Reference
B	216	HIS	-	expression tag	UNP A0A1V1FH01
B	217	HIS	-	expression tag	UNP A0A1V1FH01
B	218	HIS	-	expression tag	UNP A0A1V1FH01
B	219	HIS	-	expression tag	UNP A0A1V1FH01
B	220	HIS	-	expression tag	UNP A0A1V1FH01
C	189	LYS	-	expression tag	UNP A0A1V1FH01
C	190	GLY	-	expression tag	UNP A0A1V1FH01
C	191	GLU	-	expression tag	UNP A0A1V1FH01
C	192	LEU	-	expression tag	UNP A0A1V1FH01
C	193	ASN	-	expression tag	UNP A0A1V1FH01
C	194	SER	-	expression tag	UNP A0A1V1FH01
C	195	LYS	-	expression tag	UNP A0A1V1FH01
C	196	LEU	-	expression tag	UNP A0A1V1FH01
C	197	GLU	-	expression tag	UNP A0A1V1FH01
C	198	GLY	-	expression tag	UNP A0A1V1FH01
C	199	LYS	-	expression tag	UNP A0A1V1FH01
C	200	PRO	-	expression tag	UNP A0A1V1FH01
C	201	ILE	-	expression tag	UNP A0A1V1FH01
C	202	PRO	-	expression tag	UNP A0A1V1FH01
C	203	ASN	-	expression tag	UNP A0A1V1FH01
C	204	PRO	-	expression tag	UNP A0A1V1FH01
C	205	LEU	-	expression tag	UNP A0A1V1FH01
C	206	LEU	-	expression tag	UNP A0A1V1FH01
C	207	GLY	-	expression tag	UNP A0A1V1FH01
C	208	LEU	-	expression tag	UNP A0A1V1FH01
C	209	ASP	-	expression tag	UNP A0A1V1FH01
C	210	SER	-	expression tag	UNP A0A1V1FH01
C	211	THR	-	expression tag	UNP A0A1V1FH01
C	212	ARG	-	expression tag	UNP A0A1V1FH01
C	213	THR	-	expression tag	UNP A0A1V1FH01
C	214	GLY	-	expression tag	UNP A0A1V1FH01
C	215	HIS	-	expression tag	UNP A0A1V1FH01
C	216	HIS	-	expression tag	UNP A0A1V1FH01
C	217	HIS	-	expression tag	UNP A0A1V1FH01
C	218	HIS	-	expression tag	UNP A0A1V1FH01
C	219	HIS	-	expression tag	UNP A0A1V1FH01
C	220	HIS	-	expression tag	UNP A0A1V1FH01
D	189	LYS	-	expression tag	UNP A0A1V1FH01
D	190	GLY	-	expression tag	UNP A0A1V1FH01
D	191	GLU	-	expression tag	UNP A0A1V1FH01
D	192	LEU	-	expression tag	UNP A0A1V1FH01
D	193	ASN	-	expression tag	UNP A0A1V1FH01

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Chain	Residue	Modelled	Actual	Comment	Reference
D	194	SER	-	expression tag	UNP A0A1V1FH01
D	195	LYS	-	expression tag	UNP A0A1V1FH01
D	196	LEU	-	expression tag	UNP A0A1V1FH01
D	197	GLU	-	expression tag	UNP A0A1V1FH01
D	198	GLY	-	expression tag	UNP A0A1V1FH01
D	199	LYS	-	expression tag	UNP A0A1V1FH01
D	200	PRO	-	expression tag	UNP A0A1V1FH01
D	201	ILE	-	expression tag	UNP A0A1V1FH01
D	202	PRO	-	expression tag	UNP A0A1V1FH01
D	203	ASN	-	expression tag	UNP A0A1V1FH01
D	204	PRO	-	expression tag	UNP A0A1V1FH01
D	205	LEU	-	expression tag	UNP A0A1V1FH01
D	206	LEU	-	expression tag	UNP A0A1V1FH01
D	207	GLY	-	expression tag	UNP A0A1V1FH01
D	208	LEU	-	expression tag	UNP A0A1V1FH01
D	209	ASP	-	expression tag	UNP A0A1V1FH01
D	210	SER	-	expression tag	UNP A0A1V1FH01
D	211	THR	-	expression tag	UNP A0A1V1FH01
D	212	ARG	-	expression tag	UNP A0A1V1FH01
D	213	THR	-	expression tag	UNP A0A1V1FH01
D	214	GLY	-	expression tag	UNP A0A1V1FH01
D	215	HIS	-	expression tag	UNP A0A1V1FH01
D	216	HIS	-	expression tag	UNP A0A1V1FH01
D	217	HIS	-	expression tag	UNP A0A1V1FH01
D	218	HIS	-	expression tag	UNP A0A1V1FH01
D	219	HIS	-	expression tag	UNP A0A1V1FH01
D	220	HIS	-	expression tag	UNP A0A1V1FH01
E	189	LYS	-	expression tag	UNP A0A1V1FH01
E	190	GLY	-	expression tag	UNP A0A1V1FH01
E	191	GLU	-	expression tag	UNP A0A1V1FH01
E	192	LEU	-	expression tag	UNP A0A1V1FH01
E	193	ASN	-	expression tag	UNP A0A1V1FH01
E	194	SER	-	expression tag	UNP A0A1V1FH01
E	195	LYS	-	expression tag	UNP A0A1V1FH01
E	196	LEU	-	expression tag	UNP A0A1V1FH01
E	197	GLU	-	expression tag	UNP A0A1V1FH01
E	198	GLY	-	expression tag	UNP A0A1V1FH01
E	199	LYS	-	expression tag	UNP A0A1V1FH01
E	200	PRO	-	expression tag	UNP A0A1V1FH01
E	201	ILE	-	expression tag	UNP A0A1V1FH01
E	202	PRO	-	expression tag	UNP A0A1V1FH01
E	203	ASN	-	expression tag	UNP A0A1V1FH01

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Chain	Residue	Modelled	Actual	Comment	Reference
E	204	PRO	-	expression tag	UNP A0A1V1FH01
E	205	LEU	-	expression tag	UNP A0A1V1FH01
E	206	LEU	-	expression tag	UNP A0A1V1FH01
E	207	GLY	-	expression tag	UNP A0A1V1FH01
E	208	LEU	-	expression tag	UNP A0A1V1FH01
E	209	ASP	-	expression tag	UNP A0A1V1FH01
E	210	SER	-	expression tag	UNP A0A1V1FH01
E	211	THR	-	expression tag	UNP A0A1V1FH01
E	212	ARG	-	expression tag	UNP A0A1V1FH01
E	213	THR	-	expression tag	UNP A0A1V1FH01
E	214	GLY	-	expression tag	UNP A0A1V1FH01
E	215	HIS	-	expression tag	UNP A0A1V1FH01
E	216	HIS	-	expression tag	UNP A0A1V1FH01
E	217	HIS	-	expression tag	UNP A0A1V1FH01
E	218	HIS	-	expression tag	UNP A0A1V1FH01
E	219	HIS	-	expression tag	UNP A0A1V1FH01
E	220	HIS	-	expression tag	UNP A0A1V1FH01
F	189	LYS	-	expression tag	UNP A0A1V1FH01
F	190	GLY	-	expression tag	UNP A0A1V1FH01
F	191	GLU	-	expression tag	UNP A0A1V1FH01
F	192	LEU	-	expression tag	UNP A0A1V1FH01
F	193	ASN	-	expression tag	UNP A0A1V1FH01
F	194	SER	-	expression tag	UNP A0A1V1FH01
F	195	LYS	-	expression tag	UNP A0A1V1FH01
F	196	LEU	-	expression tag	UNP A0A1V1FH01
F	197	GLU	-	expression tag	UNP A0A1V1FH01
F	198	GLY	-	expression tag	UNP A0A1V1FH01
F	199	LYS	-	expression tag	UNP A0A1V1FH01
F	200	PRO	-	expression tag	UNP A0A1V1FH01
F	201	ILE	-	expression tag	UNP A0A1V1FH01
F	202	PRO	-	expression tag	UNP A0A1V1FH01
F	203	ASN	-	expression tag	UNP A0A1V1FH01
F	204	PRO	-	expression tag	UNP A0A1V1FH01
F	205	LEU	-	expression tag	UNP A0A1V1FH01
F	206	LEU	-	expression tag	UNP A0A1V1FH01
F	207	GLY	-	expression tag	UNP A0A1V1FH01
F	208	LEU	-	expression tag	UNP A0A1V1FH01
F	209	ASP	-	expression tag	UNP A0A1V1FH01
F	210	SER	-	expression tag	UNP A0A1V1FH01
F	211	THR	-	expression tag	UNP A0A1V1FH01
F	212	ARG	-	expression tag	UNP A0A1V1FH01
F	213	THR	-	expression tag	UNP A0A1V1FH01

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Chain	Residue	Modelled	Actual	Comment	Reference
F	214	GLY	-	expression tag	UNP A0A1V1FH01
F	215	HIS	-	expression tag	UNP A0A1V1FH01
F	216	HIS	-	expression tag	UNP A0A1V1FH01
F	217	HIS	-	expression tag	UNP A0A1V1FH01
F	218	HIS	-	expression tag	UNP A0A1V1FH01
F	219	HIS	-	expression tag	UNP A0A1V1FH01
F	220	HIS	-	expression tag	UNP A0A1V1FH01

- Molecule 2 is water.

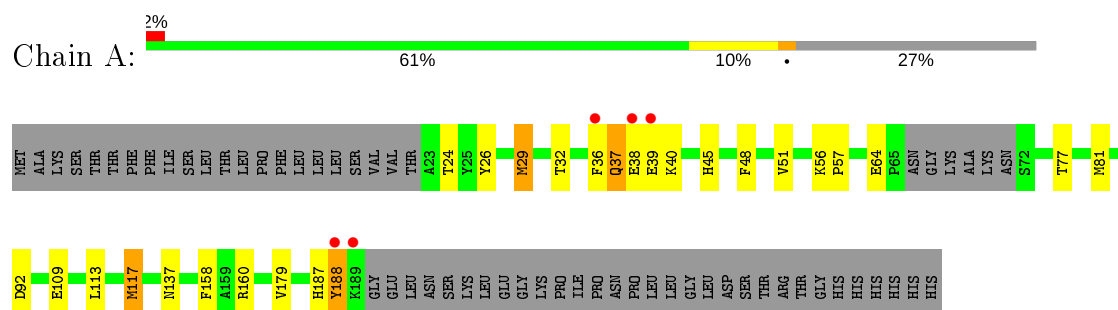
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	12	Total	O	0	0
			12	12		
2	C	20	Total	O	0	0
			20	20		
2	D	11	Total	O	0	0
			11	11		
2	E	13	Total	O	0	0
			13	13		
2	F	25	Total	O	0	0
			25	25		



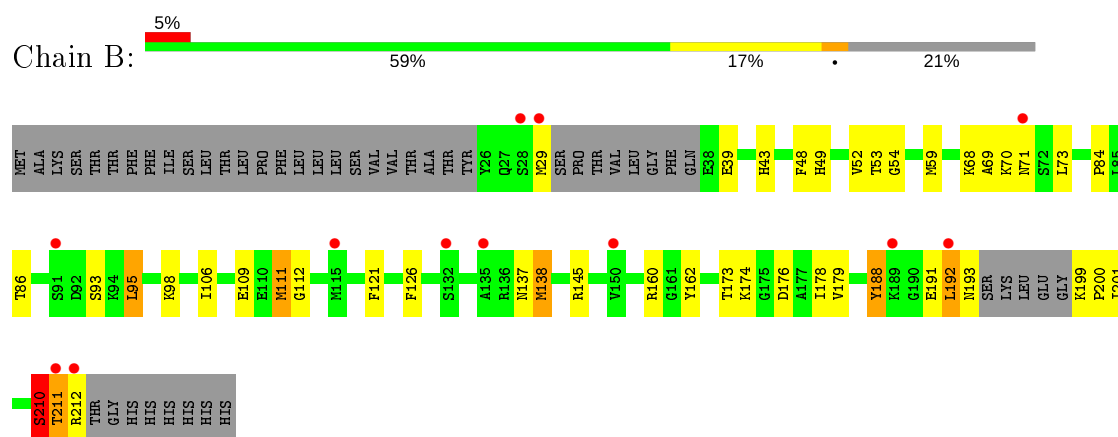
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

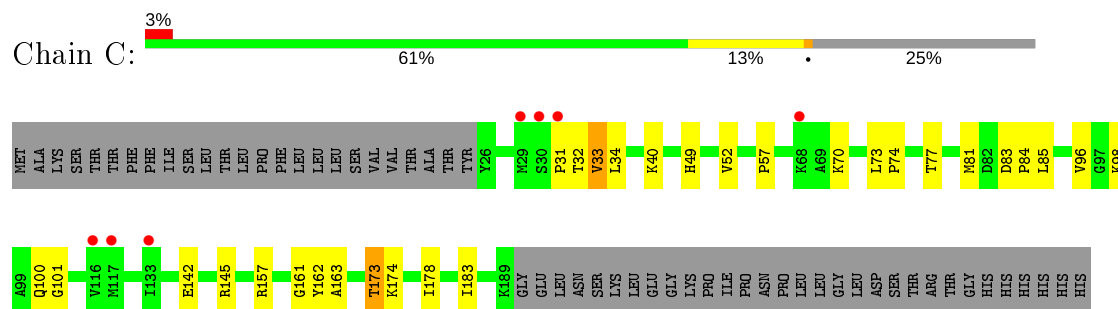
#### • Molecule 1: Dirigent protein



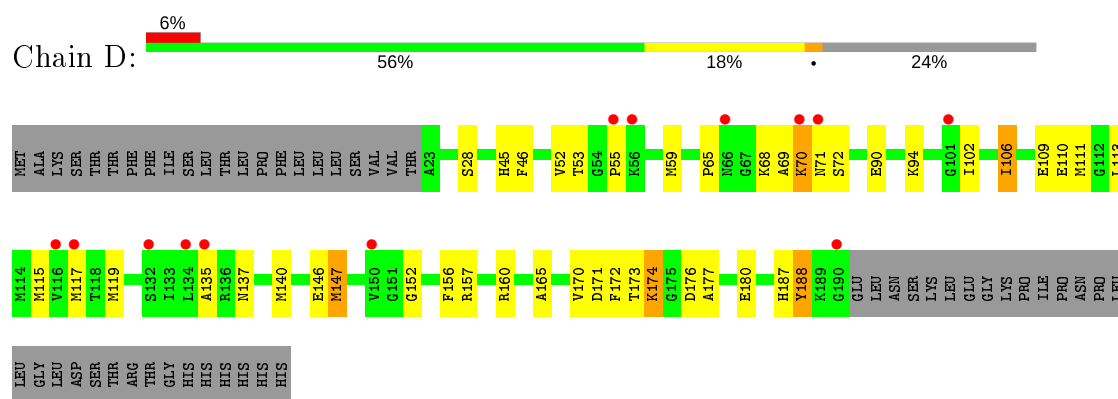
#### • Molecule 1: Dirigent protein



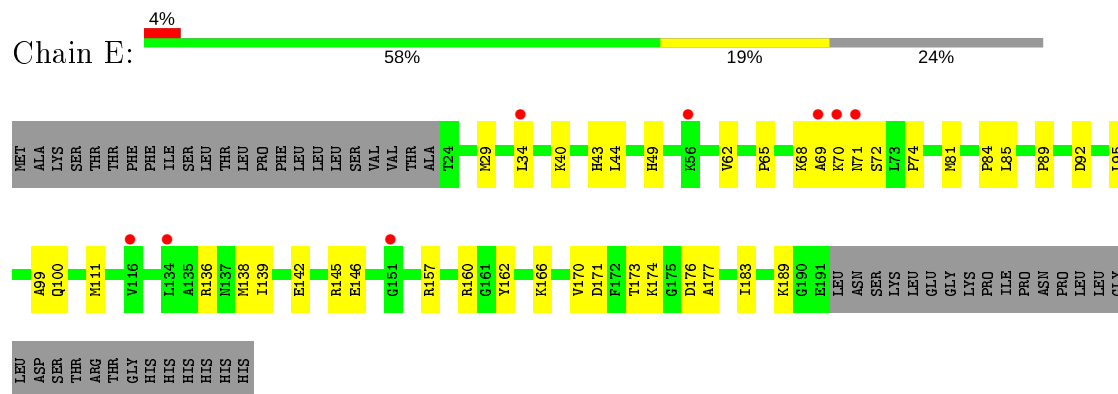
#### • Molecule 1: Dirigent protein



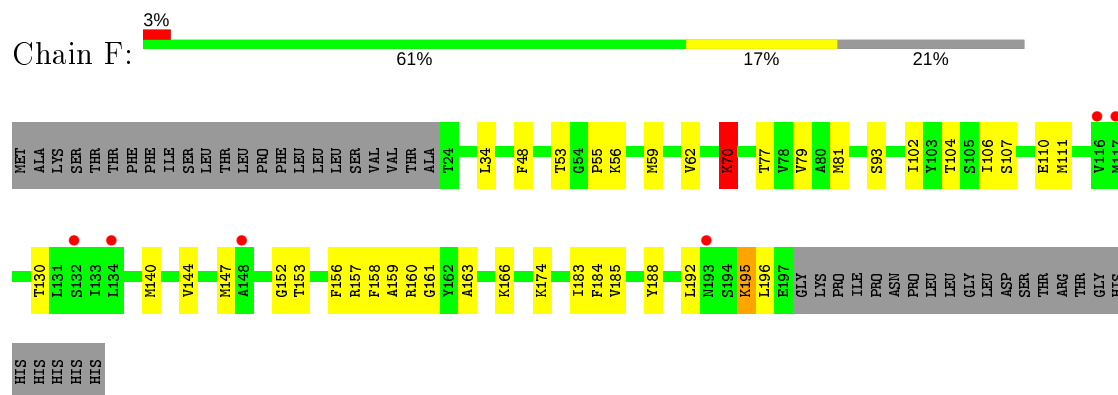
#### • Molecule 1: Dirigent protein



- Molecule 1: Dirigent protein



- Molecule 1: Dirigent protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.57Å 162.57Å 99.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.05 – 2.60 39.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.05-2.60) 99.8 (39.05-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.197 , 0.238 0.197 , 0.235	Depositor DCC
$R_{free}$ test set	2613 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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

### 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	0.49	0/1279	0.64	0/1728
1	B	0.46	0/1374	0.66	0/1852
1	C	0.56	0/1299	0.63	0/1753
1	D	0.52	0/1328	0.66	0/1793
1	E	0.51	0/1330	0.62	0/1795
1	F	0.50	0/1391	0.65	0/1876
All	All	0.51	0/8001	0.64	0/10797

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

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	1248	0	1209	22	0
1	B	1344	0	1319	39	0
1	C	1268	0	1238	25	0
1	D	1296	0	1262	34	0
1	E	1298	0	1258	25	0
1	F	1359	0	1327	32	0
2	A	20	0	0	0	0
2	B	12	0	0	0	0
2	C	20	0	0	0	0
2	D	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	13	0	0	1	0
2	F	25	0	0	1	0
All	All	7914	0	7613	157	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 10.

All (157) 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:B:73:LEU:H	1:B:111:MET:CE	1.48	1.27
1:A:32:THR:HG21	1:A:37:GLN:HG2	1.18	1.14
1:B:73:LEU:N	1:B:111:MET:HE2	1.67	1.08
1:D:71:ASN:HB3	1:D:172:PHE:O	1.54	1.08
1:B:73:LEU:H	1:B:111:MET:HE2	0.89	1.02
1:A:32:THR:HG21	1:A:37:GLN:CG	1.90	1.02
1:A:32:THR:CG2	1:A:37:GLN:HG2	1.92	0.99
1:D:71:ASN:CG	1:D:173:THR:HA	1.88	0.94
1:F:160[B]:ARG:HG3	1:F:160[B]:ARG:HH11	1.36	0.90
1:D:102:ILE:HD11	1:F:104:THR:HG21	1.57	0.85
1:B:73:LEU:HG	1:B:111:MET:HE1	1.57	0.85
1:B:73:LEU:N	1:B:111:MET:CE	2.33	0.85
1:D:71:ASN:ND2	1:D:173:THR:HA	1.95	0.81
1:B:52:VAL:H	1:B:176:ASP:HB3	1.47	0.79
1:B:106:ILE:HG13	1:C:100:GLN:HB3	1.64	0.79
1:D:140:MET:SD	1:D:172:PHE:CE2	2.78	0.77
1:A:40:LYS:HE2	1:B:29:MET:HG2	1.70	0.74
1:E:136:ARG:HG2	1:E:138:MET:HE3	1.68	0.74
1:E:111:MET:CE	1:E:139:ILE:HD11	2.20	0.70
1:E:111:MET:HE2	1:E:139:ILE:HD11	1.72	0.70
1:D:174:LYS:HE3	1:D:176:ASP:HB2	1.74	0.69
1:D:115:MET:HB3	1:D:117:MET:HE3	1.74	0.68
1:D:45:HIS:NE2	1:D:180:GLU:OE1	2.20	0.68
1:C:74:PRO:O	1:C:77:THR:HG22	1.93	0.67
1:B:73:LEU:H	1:B:111:MET:HE3	1.57	0.66
1:A:39:GLU:HA	1:A:188:TYR:HA	1.78	0.65
1:E:160:ARG:HD2	2:E:309:HOH:O	1.97	0.64
1:F:160[B]:ARG:CG	1:F:160[B]:ARG:HH11	2.11	0.64
1:A:40:LYS:N	1:A:187:HIS:O	2.27	0.63
1:B:73:LEU:HG	1:B:111:MET:CE	2.27	0.62
1:F:111:MET:HB3	1:F:140:MET:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:THR:HG21	1:A:37:GLN:CD	2.19	0.61
1:B:106:ILE:CG1	1:C:100:GLN:HB3	2.30	0.61
1:A:64:GLU:HG3	1:A:77:THR:HG23	1.83	0.60
1:D:52:VAL:HG13	1:D:53:THR:HG23	1.83	0.60
1:D:70:LYS:C	1:D:71:ASN:HD22	2.05	0.60
1:A:36:PHE:HB2	1:A:39:GLU:HB2	1.84	0.60
1:E:49:HIS:HB2	1:E:84:PRO:HG2	1.84	0.60
1:B:109:GLU:OE2	1:C:98:LYS:HE3	2.02	0.59
1:A:51:VAL:HG12	1:A:57:PRO:HA	1.85	0.58
1:C:173:THR:OG1	1:C:174:LYS:N	2.36	0.58
1:E:71:ASN:OD1	1:E:173:THR:HG22	2.03	0.58
1:C:85:LEU:O	1:C:96:VAL:HG12	2.03	0.58
1:C:40:LYS:HE3	1:D:28:SER:HB3	1.86	0.58
1:D:146:GLU:OE1	1:E:157:ARG:NH1	2.37	0.57
1:D:68:LYS:HG2	1:D:69:ALA:H	1.70	0.57
1:C:49:HIS:ND1	1:C:178:ILE:HD12	2.20	0.56
1:F:160[B]:ARG:NH1	2:F:301:HOH:O	2.39	0.56
1:B:68:LYS:NZ	1:B:69:ALA:H	2.04	0.56
1:E:85:LEU:HD21	1:E:99:ALA:HB2	1.87	0.56
1:D:152:GLY:HA3	1:D:156:PHE:O	2.06	0.56
1:D:140:MET:SD	1:D:172:PHE:HE2	2.29	0.55
1:F:107:SER:HB3	1:F:110:GLU:O	2.07	0.55
1:D:71:ASN:OD1	1:D:173:THR:HA	2.08	0.54
1:E:65:PRO:HG3	1:F:62:VAL:HA	1.88	0.54
1:B:121:PHE:HB2	1:B:126:PHE:O	2.08	0.54
1:D:46:PHE:HZ	1:D:119:MET:HE1	1.72	0.54
1:E:170:VAL:HG23	1:E:177:ALA:HB2	1.91	0.53
1:A:109:GLU:OE1	1:A:109:GLU:N	2.42	0.53
1:F:160[B]:ARG:HG3	1:F:160[B]:ARG:NH1	2.14	0.52
1:B:173:THR:OG1	1:B:174:LYS:HG3	2.10	0.52
1:C:73:LEU:HD22	1:C:77:THR:HG21	1.90	0.52
1:D:106:ILE:HG23	1:E:100:GLN:HB3	1.91	0.52
1:E:171:ASP:HB3	1:E:174:LYS:CG	2.39	0.52
1:F:104:THR:HG22	1:F:106:ILE:HG23	1.92	0.51
1:B:86:THR:HB	1:B:93:SER:HB3	1.91	0.51
1:B:106:ILE:HD11	1:C:101:GLY:CA	2.40	0.51
1:F:183:ILE:HG22	1:F:185:VAL:HG23	1.92	0.51
1:D:70:LYS:C	1:D:71:ASN:ND2	2.64	0.50
1:B:210:SER:O	1:B:211:THR:HB	2.10	0.50
1:D:71:ASN:N	1:D:71:ASN:ND2	2.59	0.50
1:A:45:HIS:CE1	1:B:201:ILE:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ALA:HB3	1:D:147:MET:HE1	1.93	0.50
1:D:71:ASN:CB	1:D:172:PHE:O	2.45	0.49
1:E:69:ALA:HB2	1:E:74:PRO:HG3	1.94	0.49
1:F:192:LEU:HD23	1:F:192:LEU:H	1.77	0.49
1:D:113:LEU:HB2	1:D:137:ASN:HB3	1.94	0.49
1:F:130:THR:OG1	1:F:153:THR:HB	2.13	0.49
1:F:160[B]:ARG:CG	1:F:160[B]:ARG:NH1	2.72	0.48
1:C:31:PRO:HB2	1:C:33:VAL:HG22	1.94	0.48
1:C:163:ALA:HB2	1:C:183:ILE:HD13	1.95	0.48
1:B:53:THR:HG22	1:B:54:GLY:N	2.28	0.48
1:B:173:THR:OG1	1:B:174:LYS:N	2.46	0.48
1:F:157:ARG:HG2	1:F:158:PHE:CD2	2.49	0.47
1:B:106:ILE:HD11	1:C:101:GLY:N	2.29	0.47
1:E:136:ARG:CG	1:E:138:MET:HE3	2.42	0.47
1:B:68:LYS:HZ3	1:B:69:ALA:H	1.61	0.47
1:D:106:ILE:HG23	1:D:106:ILE:O	2.14	0.47
1:F:144:VAL:HG22	1:F:166:LYS:HG2	1.96	0.47
1:A:81:MET:CE	1:A:117:MET:HE3	2.45	0.47
1:E:40:LYS:NZ	1:E:189:LYS:HD3	2.29	0.47
1:A:29:MET:HE1	1:C:162:TYR:HE1	1.79	0.46
1:F:34:LEU:HD22	1:F:188:TYR:CE2	2.51	0.46
1:A:29:MET:HE1	1:C:162:TYR:CE1	2.51	0.46
1:B:137:ASN:O	1:B:138:MET:HB2	2.16	0.46
1:B:191:GLU:HG3	1:B:192:LEU:H	1.81	0.46
1:C:73:LEU:HD23	1:C:73:LEU:HA	1.84	0.46
1:D:52:VAL:HA	1:D:59:MET:SD	2.56	0.46
1:F:158:PHE:HE2	1:F:195:LYS:NZ	2.14	0.45
1:E:162:TYR:OH	1:F:196:LEU:HD12	2.16	0.45
1:F:157:ARG:NH1	1:F:192:LEU:HB3	2.31	0.45
1:B:48:PHE:HB3	1:B:179:VAL:HB	1.99	0.45
1:E:166:LYS:HB3	1:E:166:LYS:HE3	1.63	0.45
1:B:73:LEU:CG	1:B:111:MET:HE1	2.36	0.45
1:F:161:GLY:HA3	1:F:184:PHE:O	2.17	0.45
1:E:146:GLU:HB3	1:F:153:THR:HG23	1.99	0.45
1:F:55:PRO:O	1:F:56:LYS:HD3	2.17	0.45
1:B:162:TYR:CD1	1:C:157:ARG:HD3	2.52	0.44
1:F:147:MET:HB2	1:F:163:ALA:HB3	1.98	0.44
1:E:171:ASP:HB3	1:E:174:LYS:HG3	1.98	0.44
1:D:90:GLU:CD	1:D:90:GLU:H	2.19	0.44
1:E:49:HIS:HE1	1:E:89:PRO:O	2.01	0.44
1:D:187:HIS:O	1:D:188:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:THR:HG21	1:F:174:LYS:HB3	2.00	0.44
1:A:81:MET:HE3	1:A:117:MET:HE3	2.01	0.43
1:D:170:VAL:HG23	1:D:177:ALA:HB2	2.00	0.43
1:D:165:ALA:HA	1:D:180:GLU:O	2.18	0.43
1:B:52:VAL:N	1:B:176:ASP:HB3	2.25	0.43
1:B:49:HIS:CE1	1:B:178:ILE:HD13	2.53	0.43
1:E:43:HIS:HA	1:E:183:ILE:O	2.19	0.43
1:F:48:PHE:HZ	1:F:81:MET:HE2	1.83	0.43
1:E:174:LYS:HE3	1:E:176:ASP:OD2	2.18	0.43
1:B:112:GLY:HA3	1:B:138:MET:CE	2.48	0.43
1:C:83:ASP:HA	1:C:84:PRO:HD3	1.93	0.43
1:B:71:ASN:HD22	1:B:71:ASN:N	2.16	0.43
1:D:135:ALA:HB3	1:D:147:MET:CE	2.48	0.43
1:B:160:ARG:HG3	1:B:160:ARG:HH11	1.84	0.43
1:D:65:PRO:HG3	1:E:62:VAL:HA	2.00	0.43
1:F:48:PHE:HZ	1:F:81:MET:CE	2.32	0.42
1:A:48:PHE:HB3	1:A:179:VAL:HB	2.01	0.42
1:B:199:LYS:N	1:B:200:PRO:HD2	2.34	0.42
1:B:39:GLU:HB2	1:B:188:TYR:CZ	2.53	0.42
1:C:49:HIS:HB2	1:C:84:PRO:HD2	2.01	0.42
1:F:152:GLY:HA3	1:F:156:PHE:O	2.19	0.42
1:B:162:TYR:CE1	1:C:157:ARG:HD3	2.54	0.42
1:F:156:PHE:O	1:F:159:ALA:HB2	2.20	0.42
1:A:39:GLU:HG2	1:A:187:HIS:C	2.40	0.42
1:C:32:THR:O	1:C:34:LEU:N	2.47	0.42
1:C:52:VAL:O	1:C:57:PRO:HB3	2.19	0.42
1:B:84:PRO:HB3	1:B:95:LEU:HD12	2.01	0.42
1:C:142:GLU:HB3	1:C:145:ARG:HG2	2.02	0.42
1:D:69:ALA:O	1:D:70:LYS:C	2.57	0.42
1:F:79:VAL:O	1:F:102:ILE:HA	2.20	0.41
1:A:24:THR:HG22	1:A:26:TYR:H	1.85	0.41
1:A:56:LYS:HD2	1:A:56:LYS:HA	1.84	0.41
1:A:113:LEU:HB2	1:A:137:ASN:HB3	2.03	0.41
1:E:142:GLU:HB2	1:E:145:ARG:HG2	2.03	0.41
1:F:77:THR:O	1:F:104:THR:HA	2.21	0.41
1:F:157:ARG:CZ	1:F:192:LEU:HB3	2.51	0.41
1:A:158:PHE:HE1	1:C:161:GLY:HA2	1.86	0.40
1:C:81:MET:O	1:C:100:GLN:HA	2.21	0.40
1:D:46:PHE:CZ	1:D:119:MET:HE1	2.54	0.40
1:D:157:ARG:HH11	1:D:157:ARG:HD2	1.73	0.40
1:F:70:LYS:HG3	1:F:70:LYS:H	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:O	1:B:145:ARG:HD2	2.22	0.40
1:B:192:LEU:HB2	1:B:193:ASN:H	1.55	0.40
1:E:111:MET:HE1	1:E:139:ILE:HD11	1.98	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	157/220 (71%)	150 (96%)	6 (4%)	1 (1%)	25	47
1	B	168/220 (76%)	148 (88%)	15 (9%)	5 (3%)	4	7
1	C	162/220 (74%)	147 (91%)	13 (8%)	2 (1%)	13	27
1	D	166/220 (76%)	153 (92%)	7 (4%)	6 (4%)	3	4
1	E	166/220 (76%)	158 (95%)	6 (4%)	2 (1%)	13	27
1	F	173/220 (79%)	162 (94%)	10 (6%)	1 (1%)	25	47
All	All	992/1320 (75%)	918 (92%)	57 (6%)	17 (2%)	9	18

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	LYS
1	D	70	LYS
1	D	109	GLU
1	E	70	LYS
1	F	70	LYS
1	B	192	LEU
1	B	210	SER
1	B	211	THR
1	C	33	VAL

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Mol	Chain	Res	Type
1	C	173	THR
1	D	72	SER
1	D	188	TYR
1	A	37	GLN
1	D	55	PRO
1	B	138	MET
1	D	110	GLU
1	E	34	LEU

### 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	134/187 (72%)	128 (96%)	6 (4%)	27	52
1	B	146/187 (78%)	138 (94%)	8 (6%)	21	43
1	C	137/187 (73%)	136 (99%)	1 (1%)	84	94
1	D	139/187 (74%)	132 (95%)	7 (5%)	24	47
1	E	139/187 (74%)	132 (95%)	7 (5%)	24	47
1	F	147/187 (79%)	143 (97%)	4 (3%)	44	71
All	All	842/1122 (75%)	809 (96%)	33 (4%)	32	58

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	38	GLU
1	A	92	ASP
1	A	117	MET
1	A	160	ARG
1	A	188	TYR
1	B	43	HIS
1	B	59	MET
1	B	95	LEU
1	B	98	LYS

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Mol	Chain	Res	Type
1	B	111	MET
1	B	188	TYR
1	B	210	SER
1	B	212	ARG
1	C	70	LYS
1	D	94	LYS
1	D	106	ILE
1	D	111	MET
1	D	147	MET
1	D	160	ARG
1	D	171	ASP
1	D	174	LYS
1	E	29	MET
1	E	44	LEU
1	E	68	LYS
1	E	72	SER
1	E	81	MET
1	E	92	ASP
1	E	95	LEU
1	F	59	MET
1	F	70	LYS
1	F	93	SER
1	F	195	LYS

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

Mol	Chain	Res	Type
1	B	71	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 [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<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	161/220 (73%)	-0.16	5 (3%)	49	42	47, 56, 82, 103	0
1	B	174/220 (79%)	0.18	12 (6%)	16	12	51, 73, 95, 102	0
1	C	164/220 (74%)	0.06	7 (4%)	35	28	47, 59, 89, 98	0
1	D	168/220 (76%)	0.09	13 (7%)	13	10	48, 69, 92, 102	0
1	E	168/220 (76%)	0.03	8 (4%)	30	24	51, 69, 91, 100	0
1	F	174/220 (79%)	-0.09	6 (3%)	45	38	47, 59, 84, 103	0
All	All	1009/1320 (76%)	0.02	51 (5%)	28	22	47, 65, 91, 103	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	34	LEU	4.8
1	F	134	LEU	4.3
1	C	29	MET	4.2
1	E	69	ALA	4.2
1	C	31	PRO	3.7
1	D	70	LYS	3.5
1	D	55	PRO	3.4
1	A	39	GLU	3.3
1	B	189	LYS	3.3
1	E	71	ASN	3.2
1	B	71	ASN	3.2
1	B	211	THR	3.1
1	E	70	LYS	3.0
1	F	116	VAL	3.0
1	A	38	GLU	2.9
1	E	134	LEU	2.9
1	D	116	VAL	2.9
1	A	188	TYR	2.9
1	F	193	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	56	LYS	2.8
1	E	56	LYS	2.7
1	E	116	VAL	2.6
1	D	190	GLY	2.6
1	D	71	ASN	2.5
1	C	116	VAL	2.5
1	B	135	ALA	2.5
1	F	132	SER	2.4
1	D	132	SER	2.4
1	C	133	ILE	2.4
1	B	212	ARG	2.4
1	C	30	SER	2.3
1	F	148	ALA	2.3
1	A	36	PHE	2.3
1	D	134	LEU	2.3
1	A	189	LYS	2.3
1	B	150	VAL	2.3
1	D	101	GLY	2.2
1	D	117	MET	2.2
1	B	192	LEU	2.2
1	B	29	MET	2.2
1	D	135	ALA	2.2
1	D	150	VAL	2.2
1	C	117	MET	2.2
1	F	117	MET	2.2
1	D	66	ASN	2.1
1	E	151	GLY	2.1
1	B	91	SER	2.1
1	B	115	MET	2.1
1	B	28	SER	2.1
1	C	68	LYS	2.0
1	B	132	SER	2.0

## 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 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.