



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 02:49 pm BST

PDB ID : 2Q3S  
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At5g06450  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-30  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

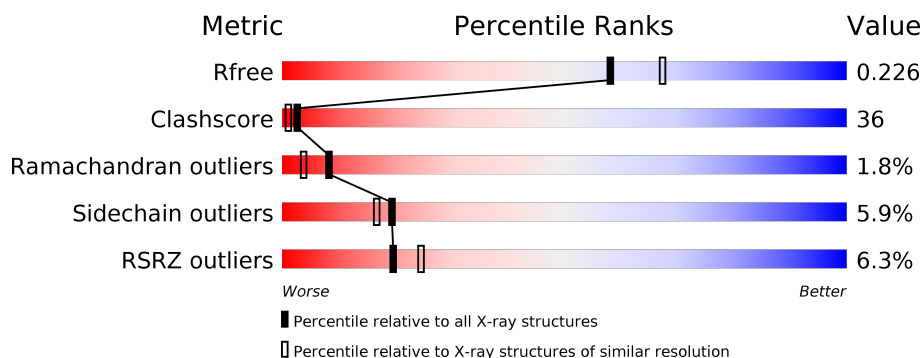
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	1-A	206	<div> <div>9%</div> <div>53%</div> <div>40%</div> <div>• •</div> </div>
1	1-B	206	<div> <div>6%</div> <div>46%</div> <div>44%</div> <div>7%</div> <div>•</div> </div>
1	1-C	206	<div> <div>5%</div> <div>50%</div> <div>42%</div> <div>5%</div> <div>•</div> </div>
1	1-D	206	<div> <div>4%</div> <div>49%</div> <div>45%</div> <div>• •</div> </div>
1	1-E	206	<div> <div>6%</div> <div>53%</div> <div>39%</div> <div>• •</div> </div>
1	1-F	206	<div> <div>5%</div> <div>53%</div> <div>40%</div> <div>• • •</div> </div>

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Mol	Chain	Length	Quality of chain
1	2-A	206	
1	2-B	206	
1	2-C	206	
1	2-D	206	
1	2-E	206	
1	2-F	206	
1	3-A	206	
1	3-B	206	
1	3-C	206	
1	3-D	206	
1	3-E	206	
1	3-F	206	
1	4-A	206	
1	4-B	206	
1	4-C	206	
1	4-D	206	
1	4-E	206	
1	4-F	206	
1	5-A	206	
1	5-B	206	
1	5-C	206	
1	5-D	206	
1	5-E	206	
1	5-F	206	
1	6-A	206	

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Mol	Chain	Length	Quality of chain
1	6-B	206	
1	6-C	206	
1	6-D	206	
1	6-E	206	
1	6-F	206	
1	7-A	206	
1	7-B	206	
1	7-C	206	
1	7-D	206	
1	7-E	206	
1	7-F	206	
1	8-A	206	
1	8-B	206	
1	8-C	206	
1	8-D	206	
1	8-E	206	
1	8-F	206	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 81528 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 Protein At5g06450.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	2-A	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	3-A	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	4-A	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	5-A	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	6-A	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	7-A	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	8-A	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	1-B	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	2-B	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	3-B	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	4-B	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	5-B	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	6-B	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	7-B	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	8-B	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-C	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	2-C	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	3-C	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	4-C	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	5-C	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	6-C	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	7-C	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	8-C	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	1-D	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	2-D	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	3-D	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	4-D	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	5-D	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	6-D	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	7-D	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	8-D	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	1-E	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	2-E	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	3-E	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	4-E	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0
1	5-E	200	Total 1591	C 1020	N 266	O 303	S 1	Se 1	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	6-E	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	7-E	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	8-E	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	1-F	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	2-F	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	3-F	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	4-F	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	5-F	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	6-F	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	7-F	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	8-F	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9FNG3
A	11	MSE	MET	MODIFIED RESIDUE	UNP Q9FNG3
B	1	SER	-	EXPRESSION TAG	UNP Q9FNG3
B	11	MSE	MET	MODIFIED RESIDUE	UNP Q9FNG3
C	1	SER	-	EXPRESSION TAG	UNP Q9FNG3
C	11	MSE	MET	MODIFIED RESIDUE	UNP Q9FNG3
D	1	SER	-	EXPRESSION TAG	UNP Q9FNG3
D	11	MSE	MET	MODIFIED RESIDUE	UNP Q9FNG3
E	1	SER	-	EXPRESSION TAG	UNP Q9FNG3
E	11	MSE	MET	MODIFIED RESIDUE	UNP Q9FNG3
F	1	SER	-	EXPRESSION TAG	UNP Q9FNG3
F	11	MSE	MET	MODIFIED RESIDUE	UNP Q9FNG3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	121	Total O 121 121	0	0
2	2-A	120	Total O 120 120	0	0
2	3-A	117	Total O 117 117	0	0
2	4-A	118	Total O 118 118	0	0
2	5-A	118	Total O 118 118	0	0
2	6-A	117	Total O 117 117	0	0
2	7-A	120	Total O 120 120	0	0
2	8-A	117	Total O 117 117	0	0
2	1-B	115	Total O 115 115	0	0
2	2-B	118	Total O 118 118	0	0
2	3-B	120	Total O 120 120	0	0
2	4-B	125	Total O 125 125	0	0
2	5-B	118	Total O 118 118	0	0
2	6-B	117	Total O 117 117	0	0
2	7-B	120	Total O 120 120	0	0
2	8-B	123	Total O 123 123	0	0
2	1-C	103	Total O 103 103	0	0
2	2-C	104	Total O 104 104	0	0
2	3-C	103	Total O 103 103	0	0
2	4-C	97	Total O 97 97	0	0
2	5-C	101	Total O 101 101	0	0
2	6-C	98	Total O 98 98	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-C	100	Total 100	O 100	0	0
2	8-C	101	Total 101	O 101	0	0
2	1-D	96	Total 96	O 96	0	0
2	2-D	96	Total 96	O 96	0	0
2	3-D	92	Total 92	O 92	0	0
2	4-D	97	Total 97	O 97	0	0
2	5-D	93	Total 93	O 93	0	0
2	6-D	99	Total 99	O 99	0	0
2	7-D	95	Total 95	O 95	0	0
2	8-D	97	Total 97	O 97	0	0
2	1-E	99	Total 99	O 99	0	0
2	2-E	97	Total 97	O 97	0	0
2	3-E	104	Total 104	O 104	0	0
2	4-E	97	Total 97	O 97	0	0
2	5-E	102	Total 102	O 102	0	0
2	6-E	104	Total 104	O 104	0	0
2	7-E	102	Total 102	O 102	0	0
2	8-E	98	Total 98	O 98	0	0
2	1-F	111	Total 111	O 111	0	0
2	2-F	110	Total 110	O 110	0	0
2	3-F	109	Total 109	O 109	0	0

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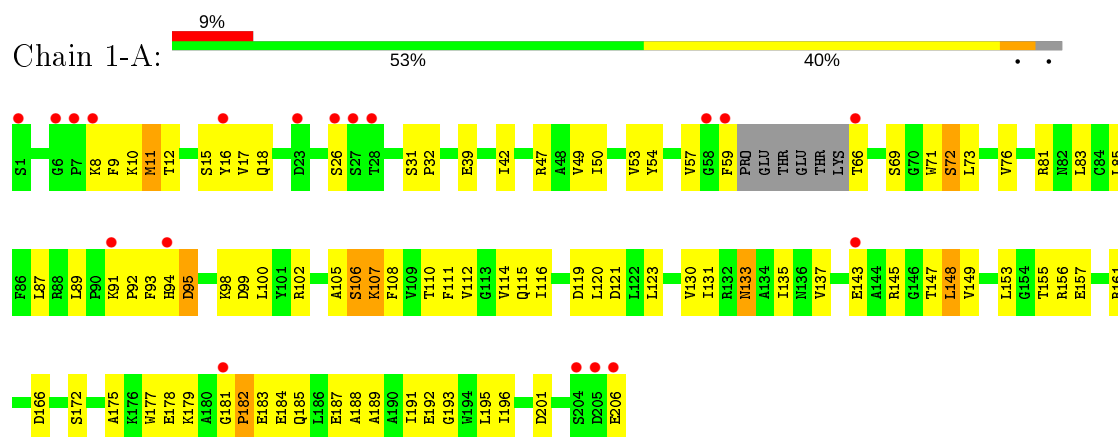
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	4-F	111	Total 111	O 111	0	0
2	5-F	113	Total 113	O 113	0	0
2	6-F	110	Total 110	O 110	0	0
2	7-F	108	Total 108	O 108	0	0
2	8-F	109	Total 109	O 109	0	0

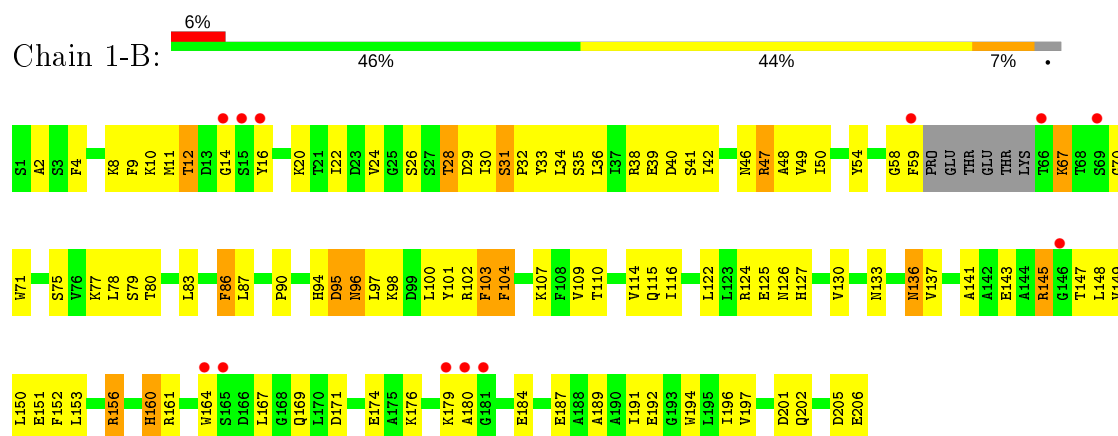
### 3 Residue-property plots [i](#)

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.

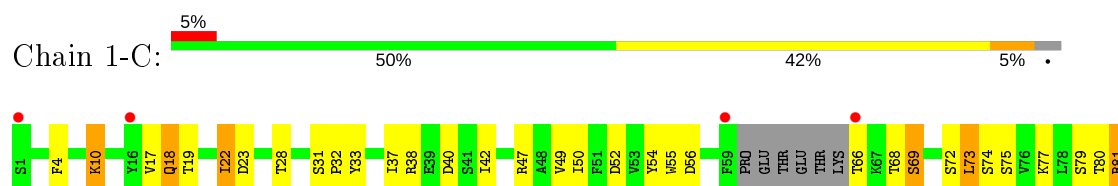
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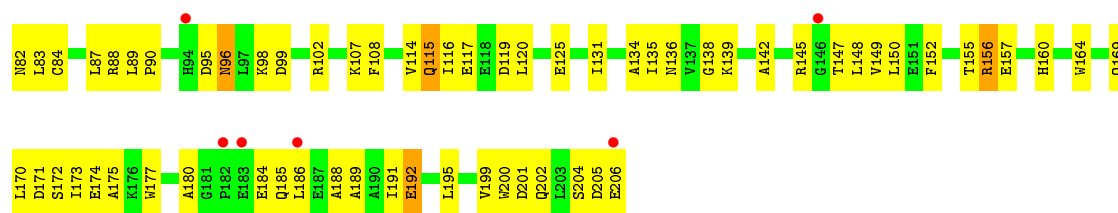


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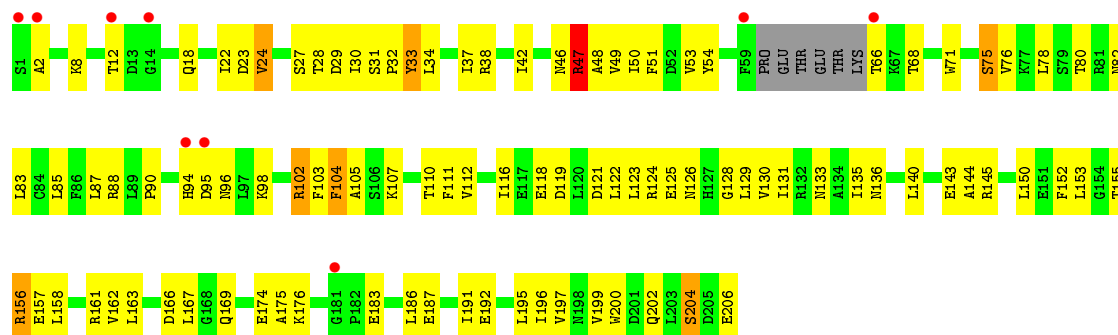


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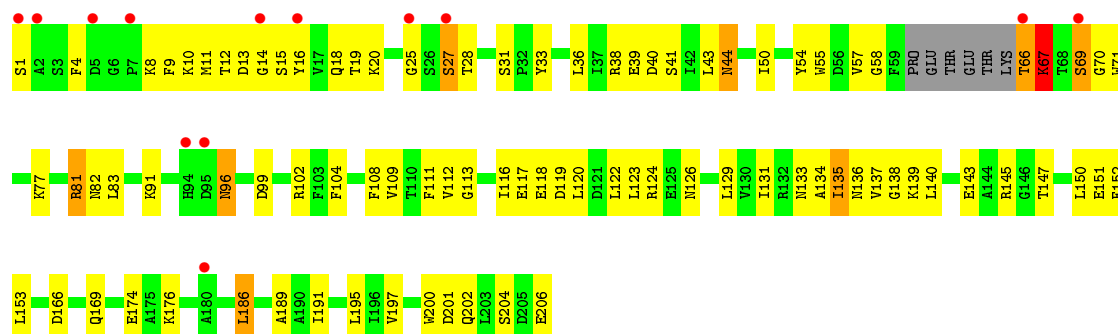




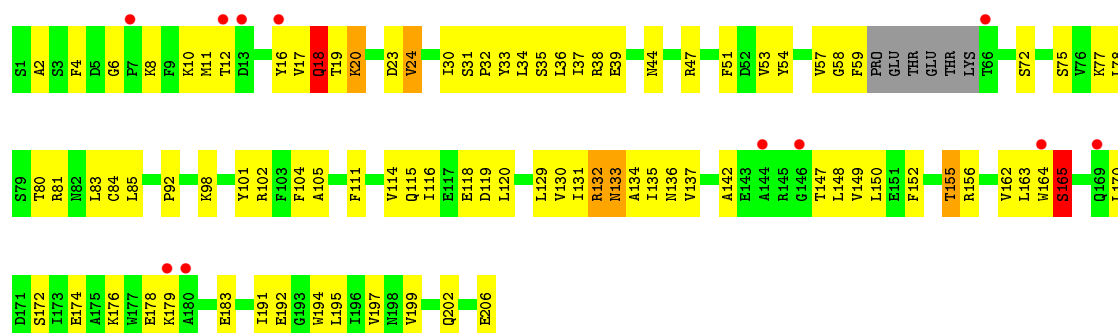
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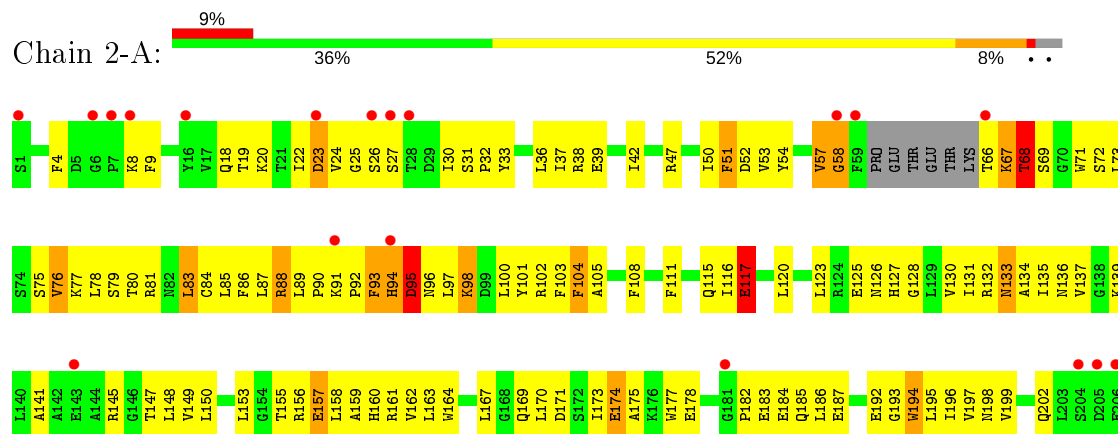
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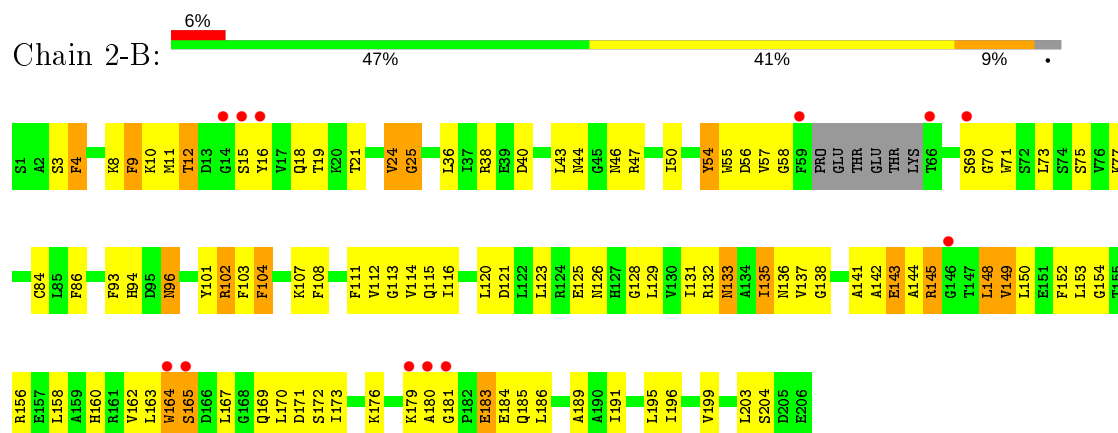
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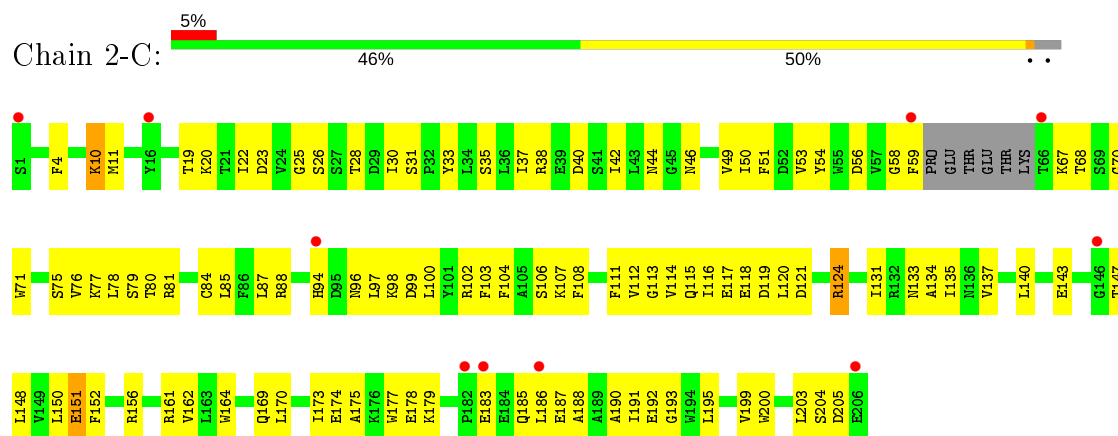
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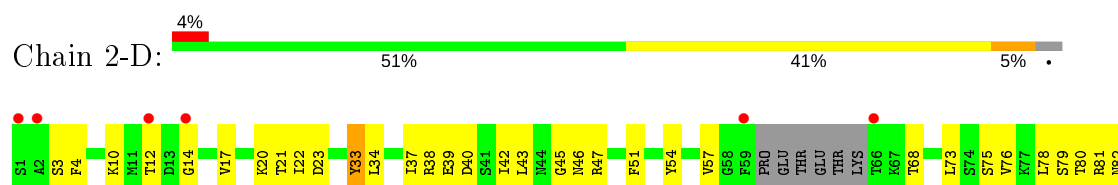
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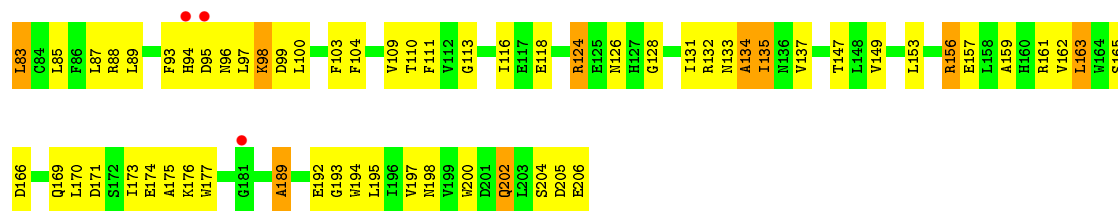


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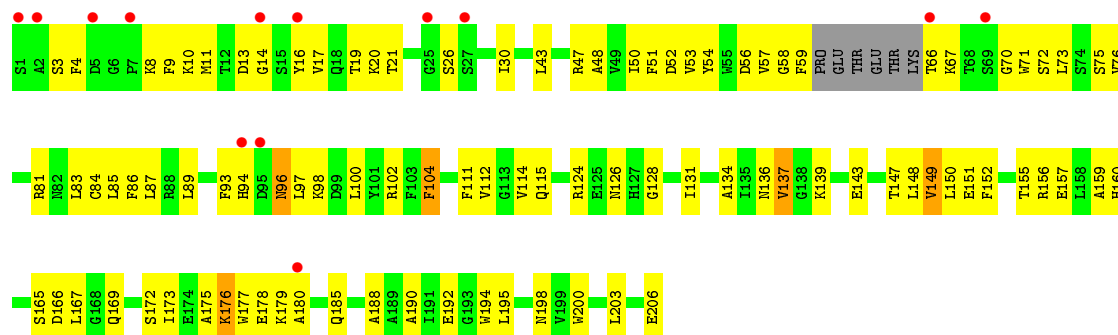


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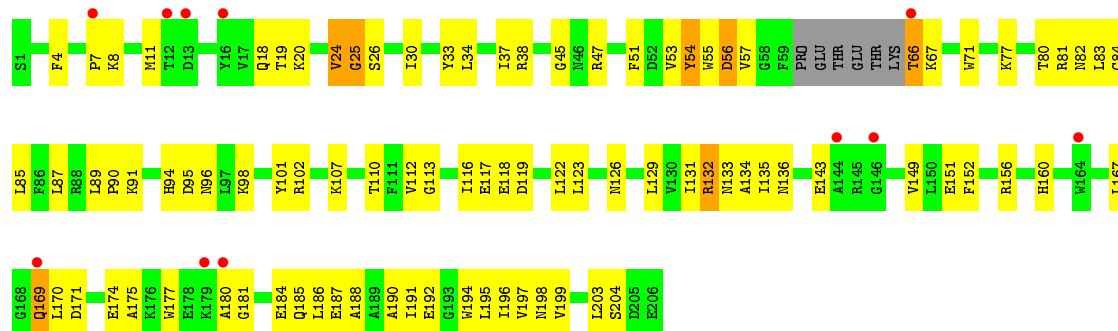




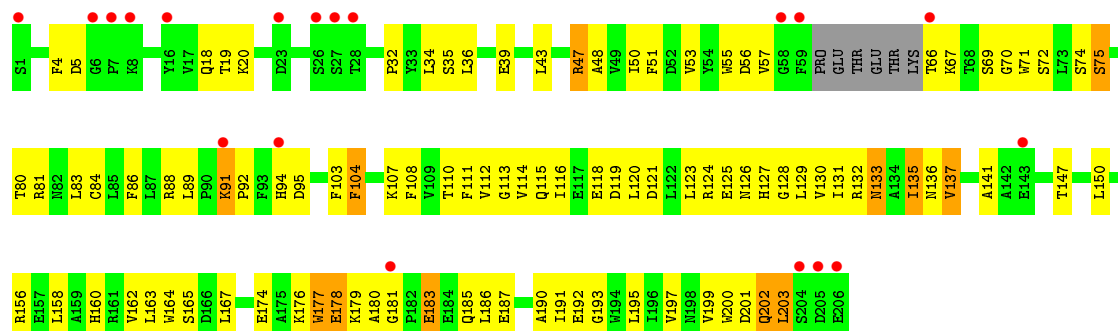
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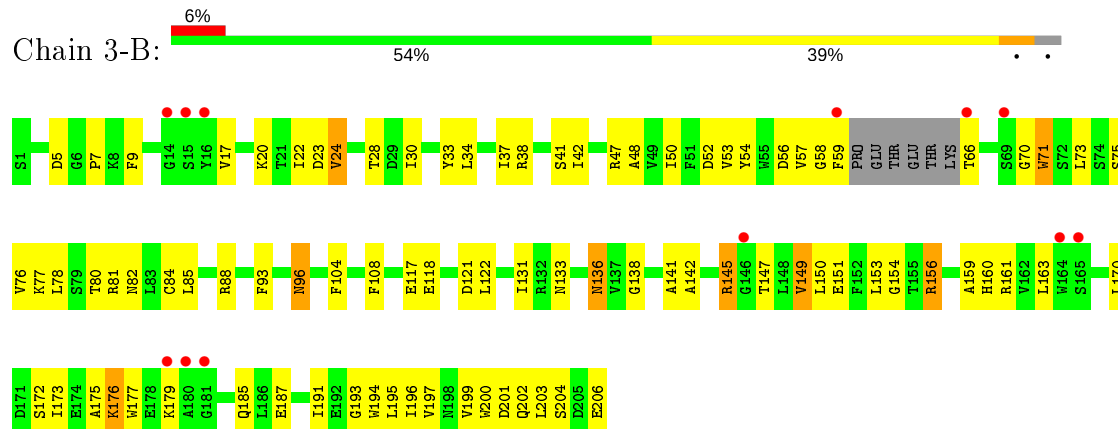
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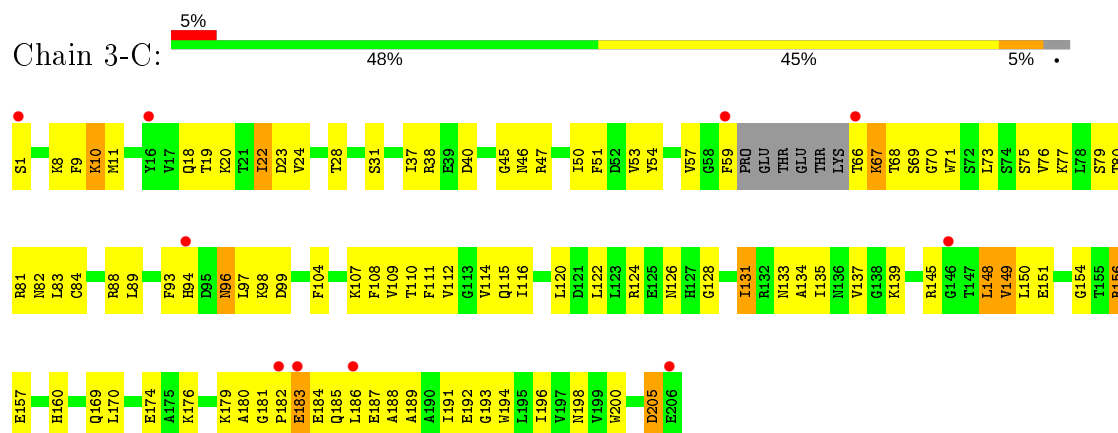
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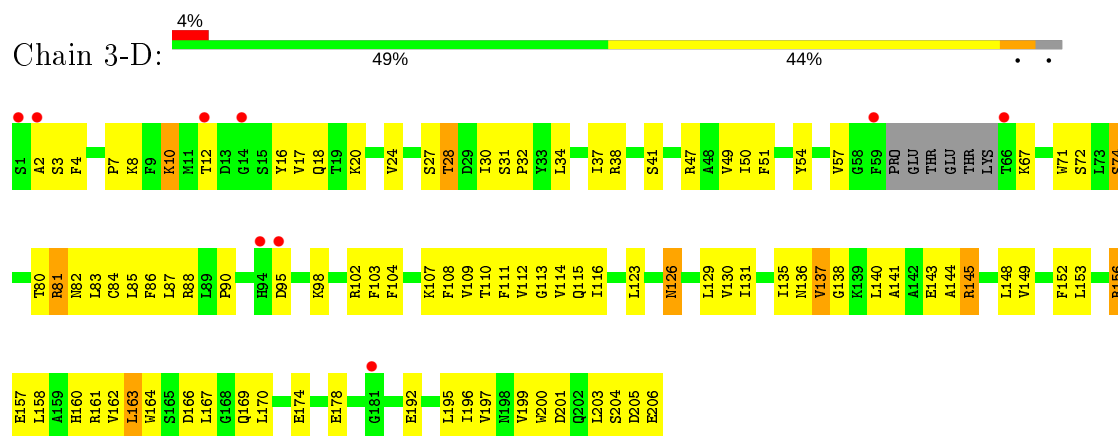
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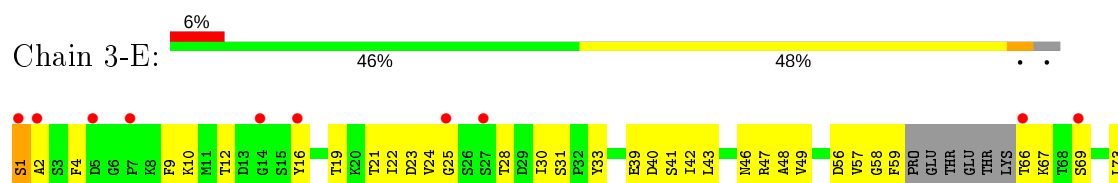
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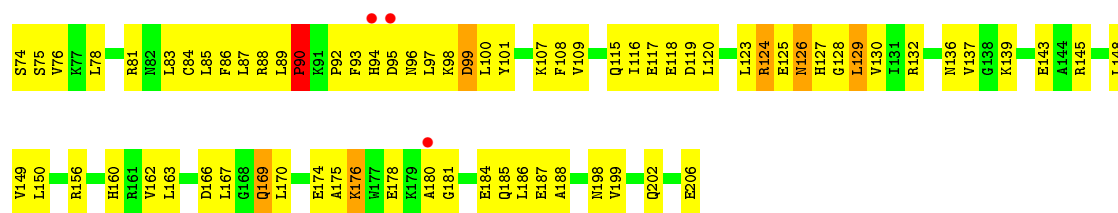


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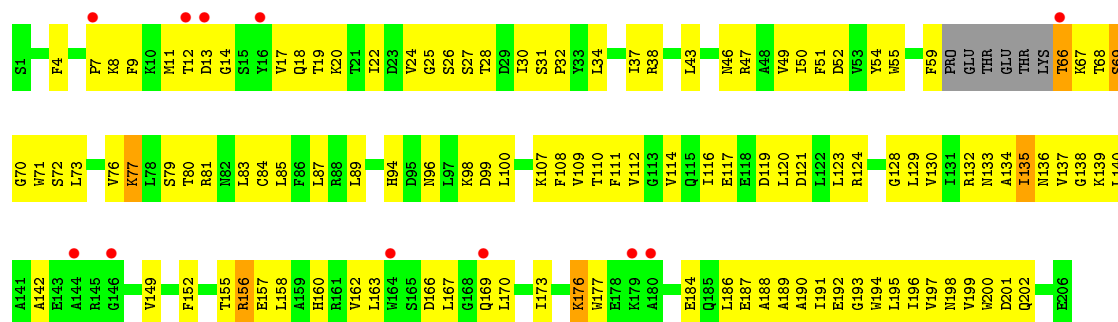
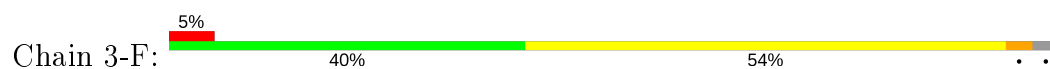


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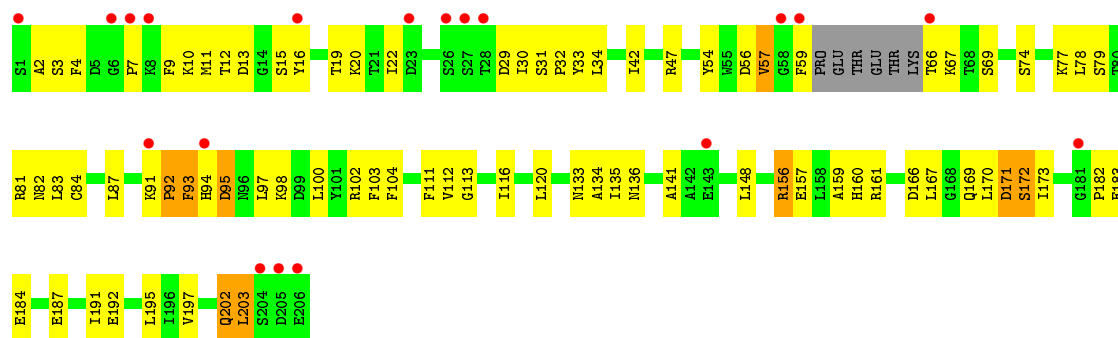




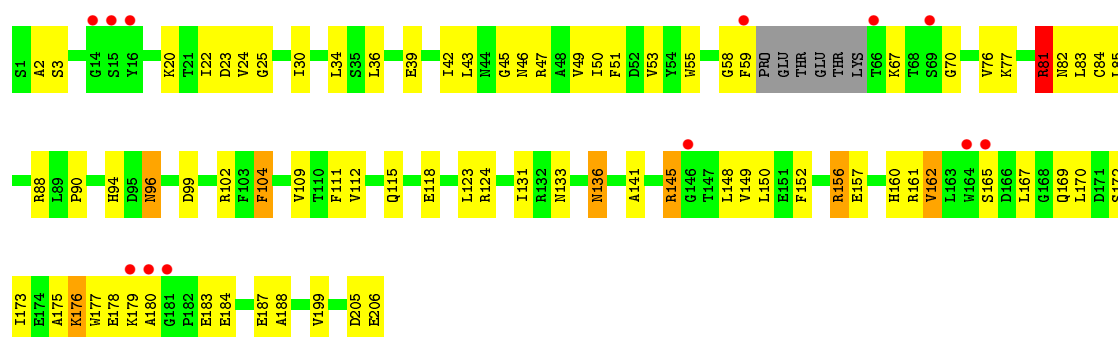
• Molecule 1: Protein At5g06450



• Molecule 1: Protein At5g06450

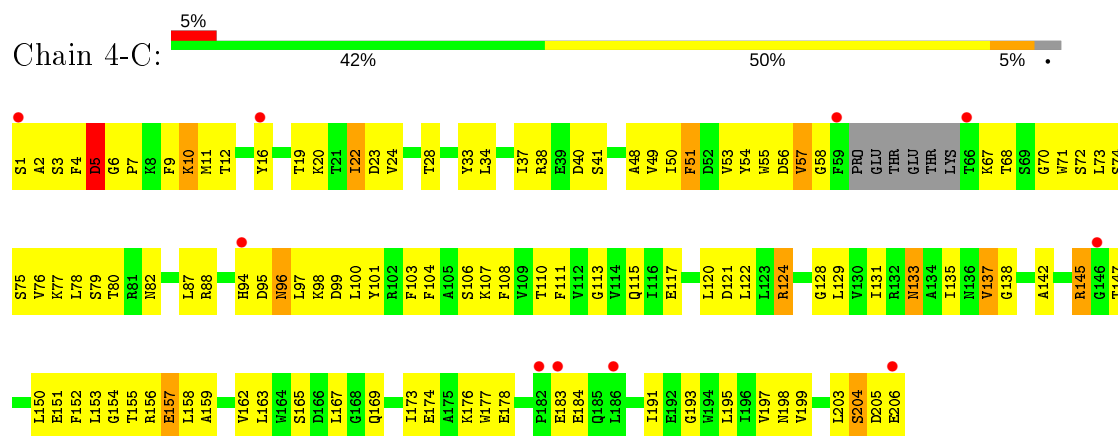


• Molecule 1: Protein At5g06450

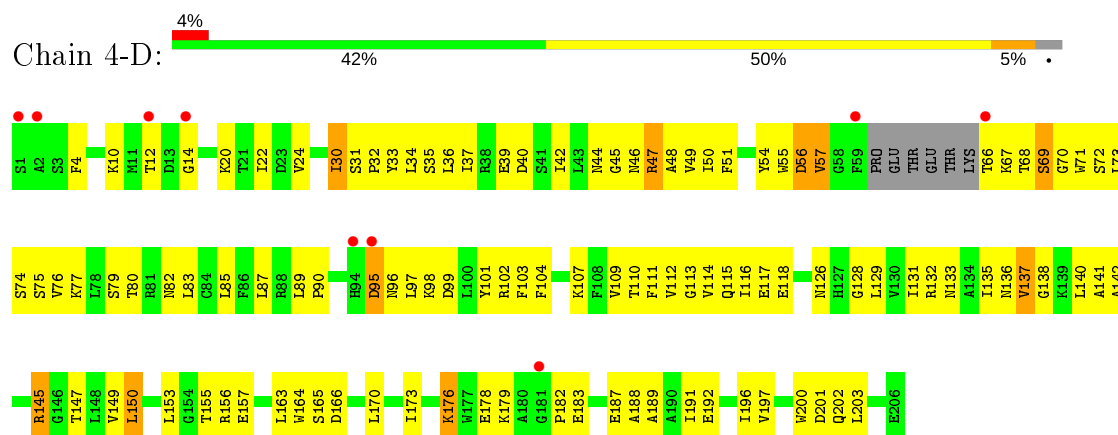




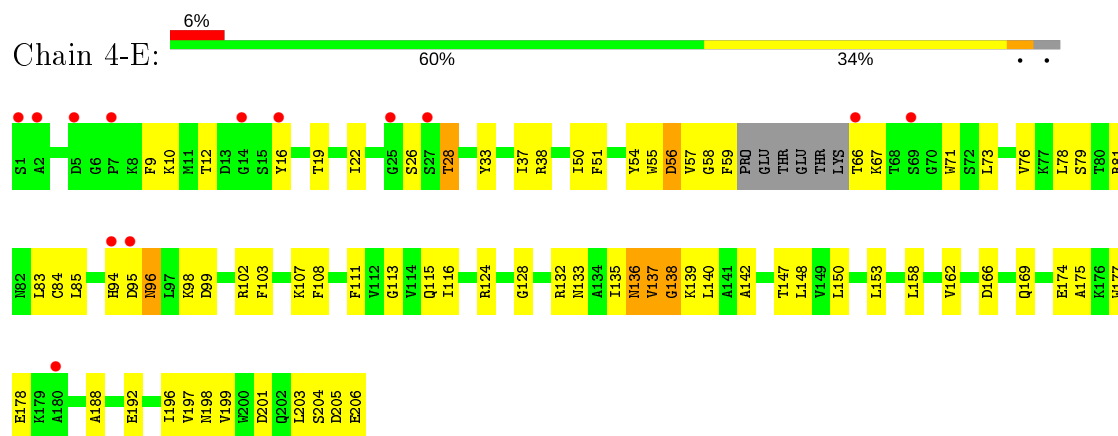
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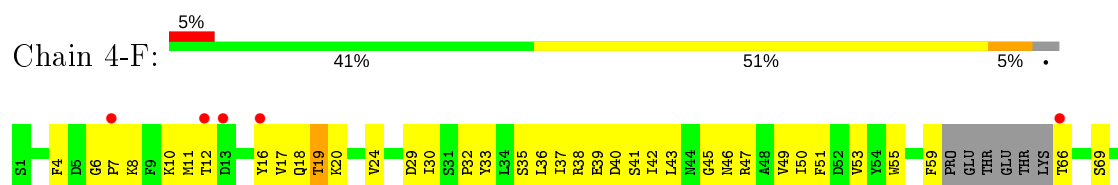
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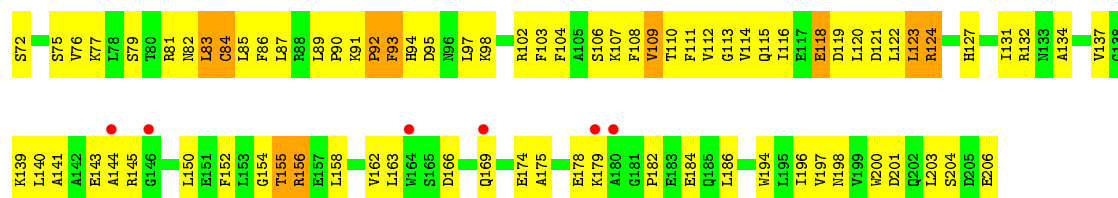


- Molecule 1: Protein At5g06450

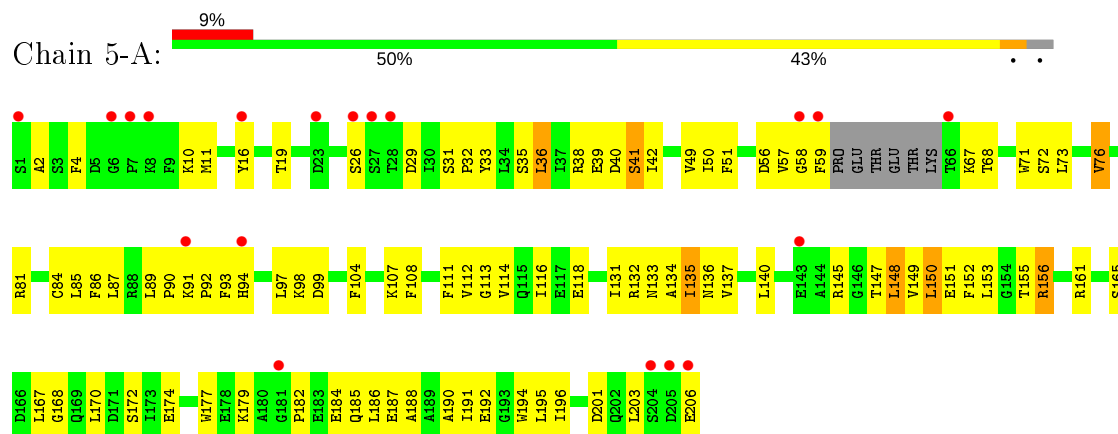


- Molecule 1: Protein At5g06450

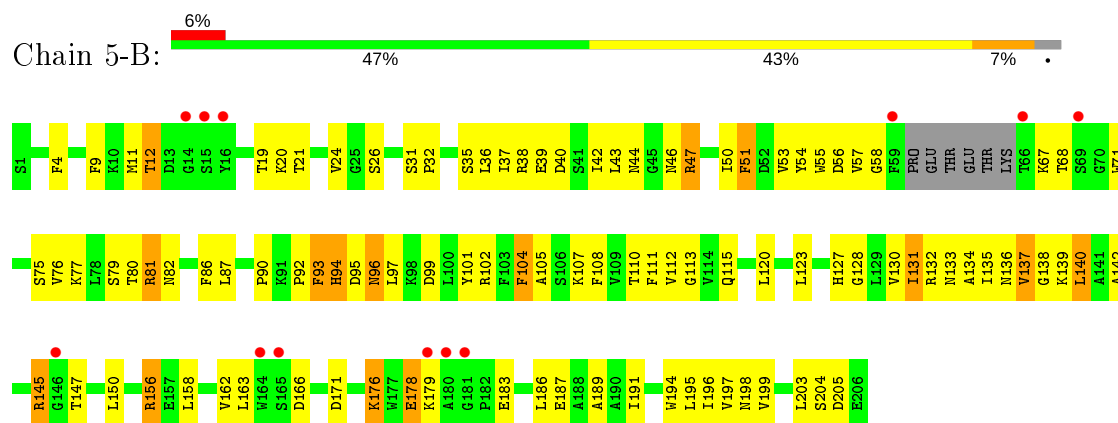




• Molecule 1: Protein At5g06450



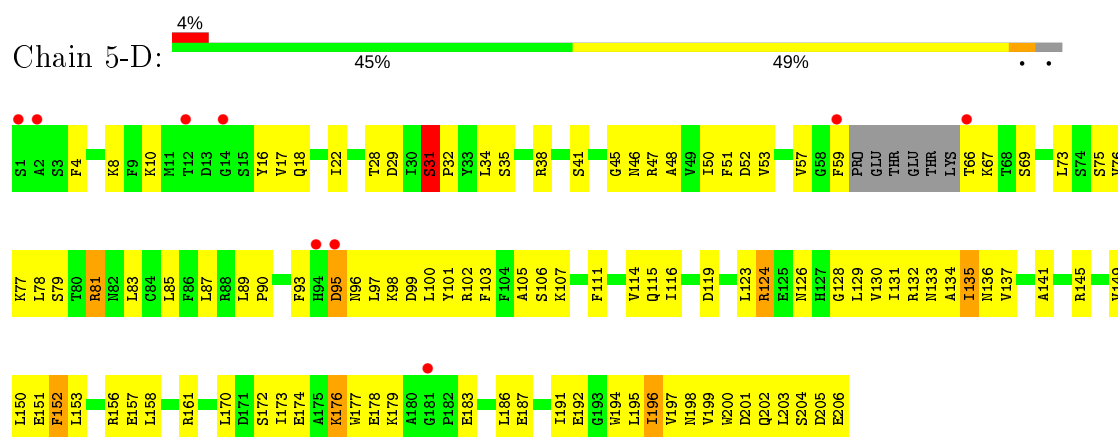
• Molecule 1: Protein At5g06450



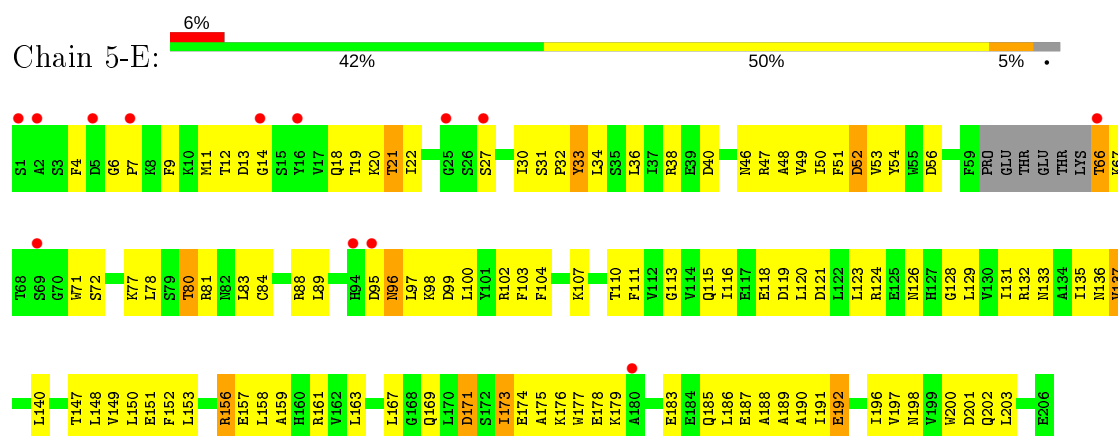
• Molecule 1: Protein At5g06450



• Molecule 1: Protein At5g06450



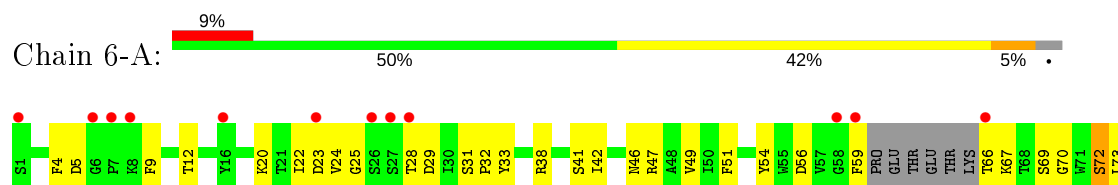
• Molecule 1: Protein At5g06450

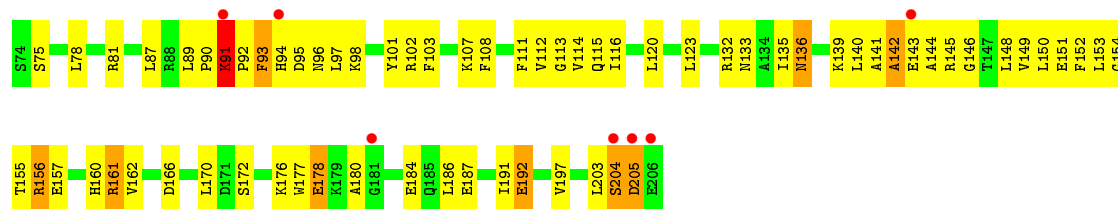


• Molecule 1: Protein At5g06450

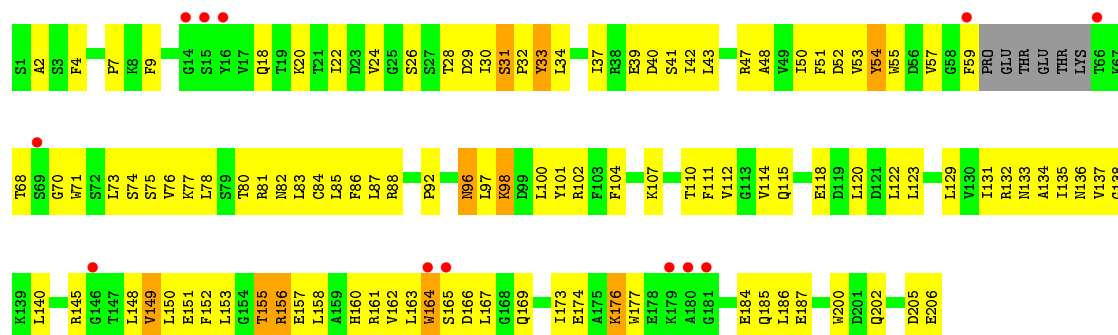


• Molecule 1: Protein At5g06450

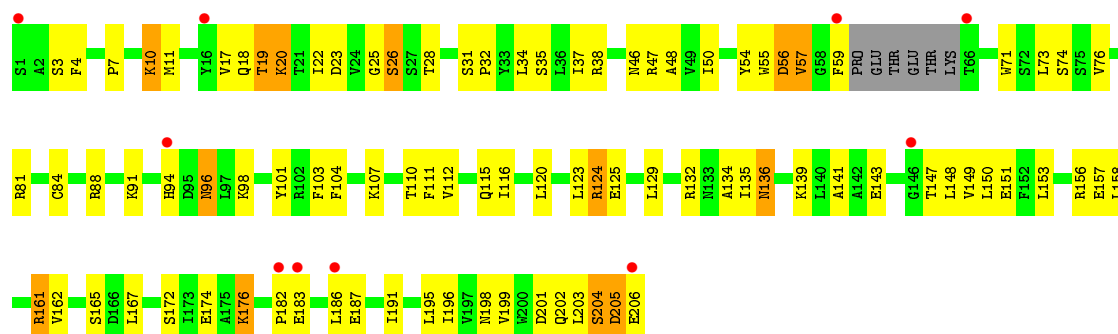




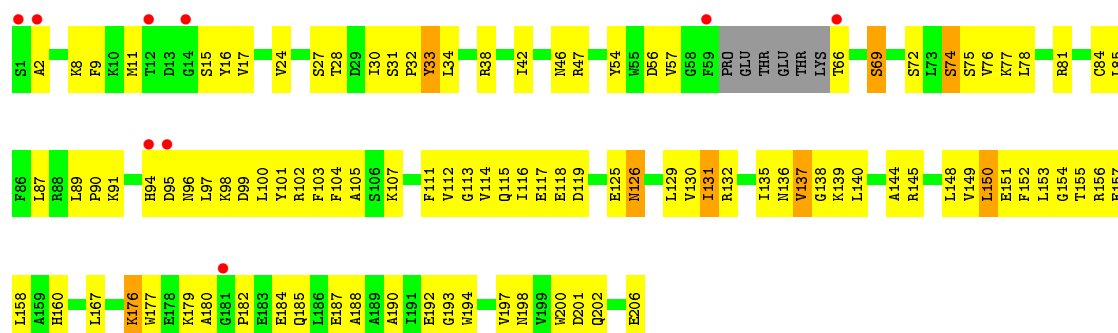
• Molecule 1: Protein At5g06450



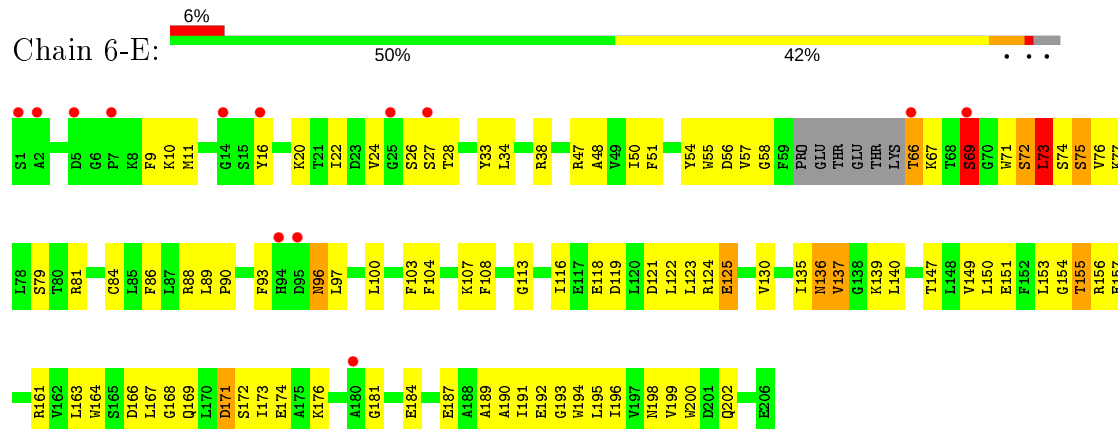
• Molecule 1: Protein At5g06450



• Molecule 1: Protein At5g06450



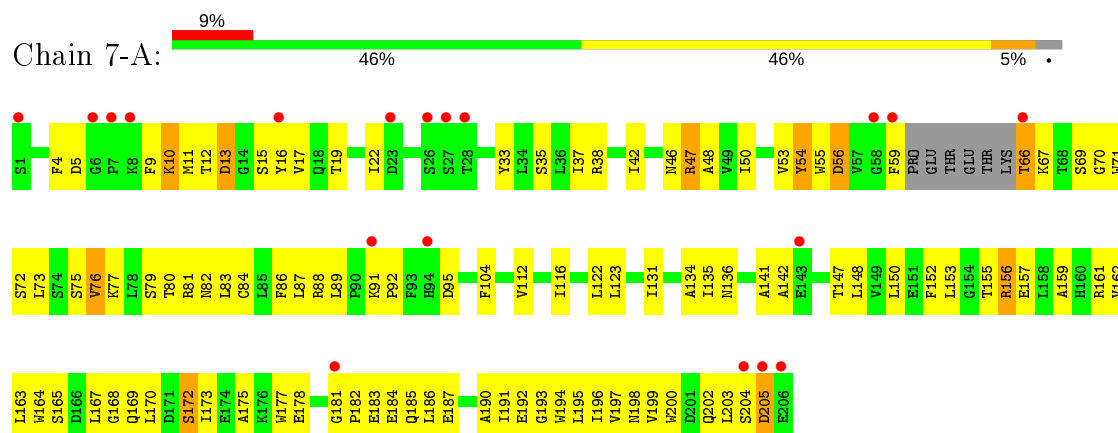
- Molecule 1: Protein At5g06450



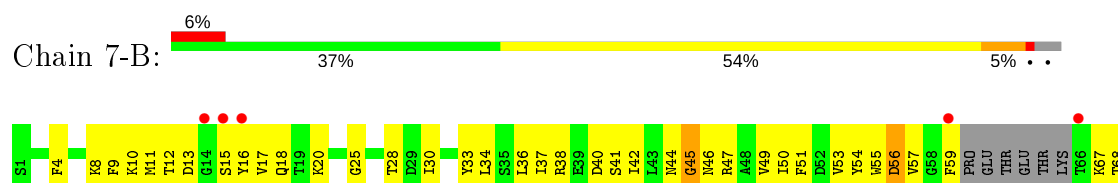
- Molecule 1: Protein At5g06450



- Molecule 1: Protein At5g06450



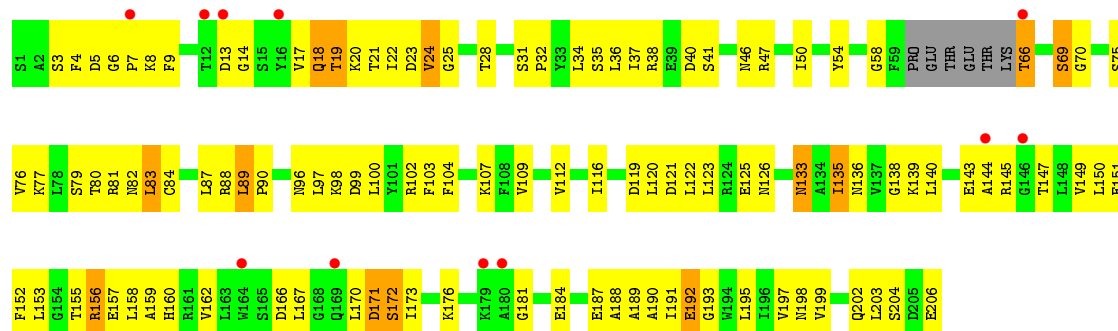
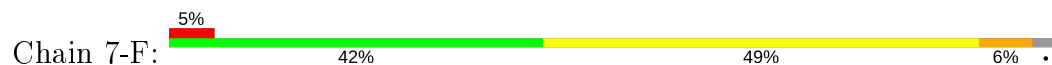
- Molecule 1: Protein At5g06450



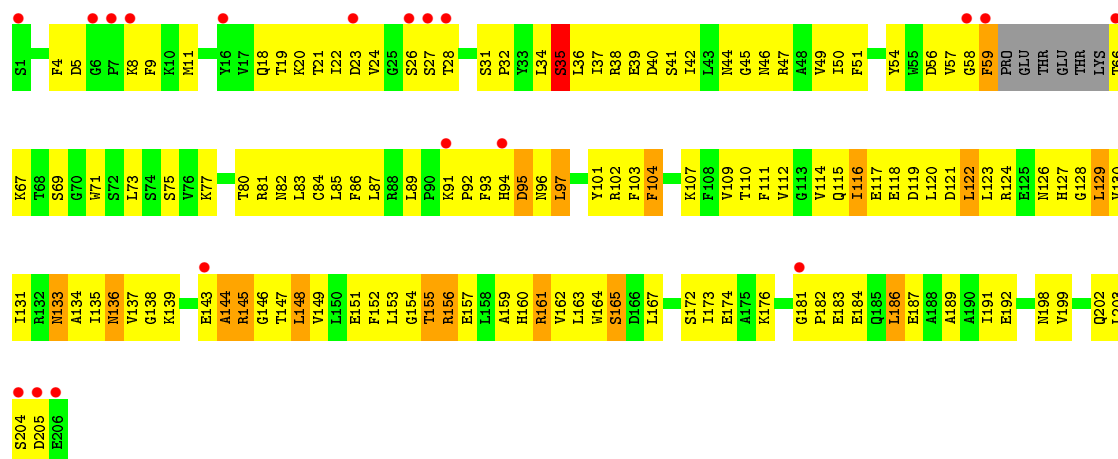




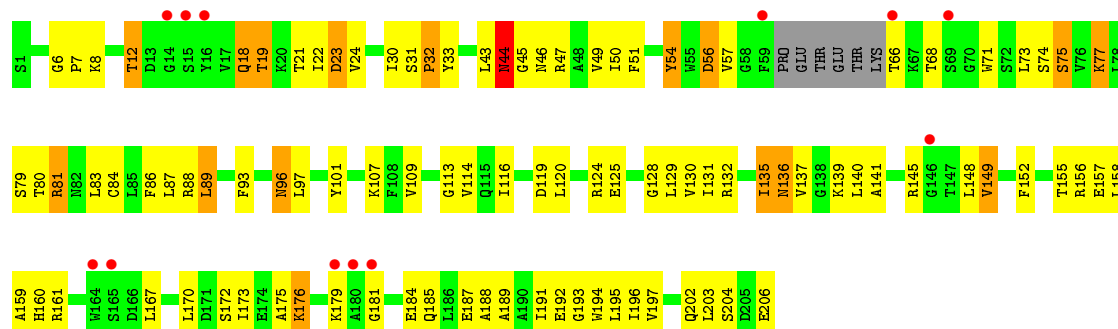
• Molecule 1: Protein At5g06450



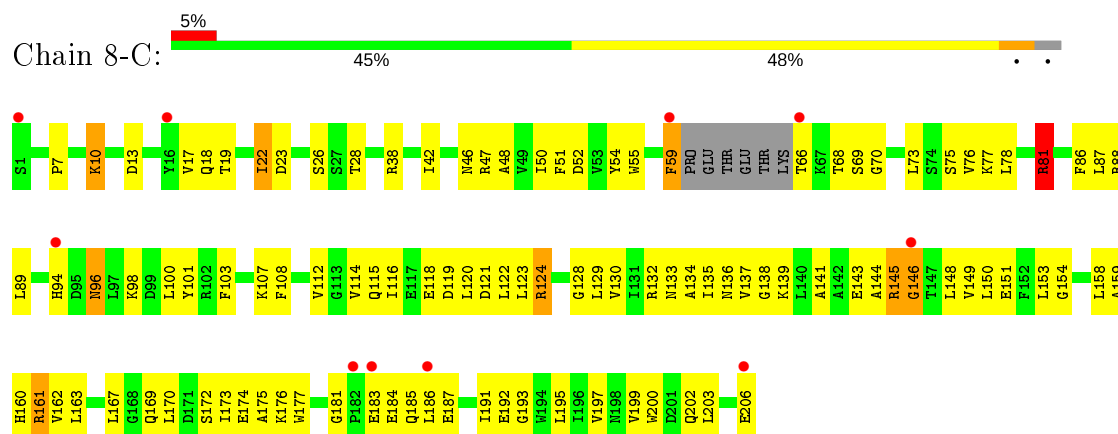
• Molecule 1: Protein At5g06450



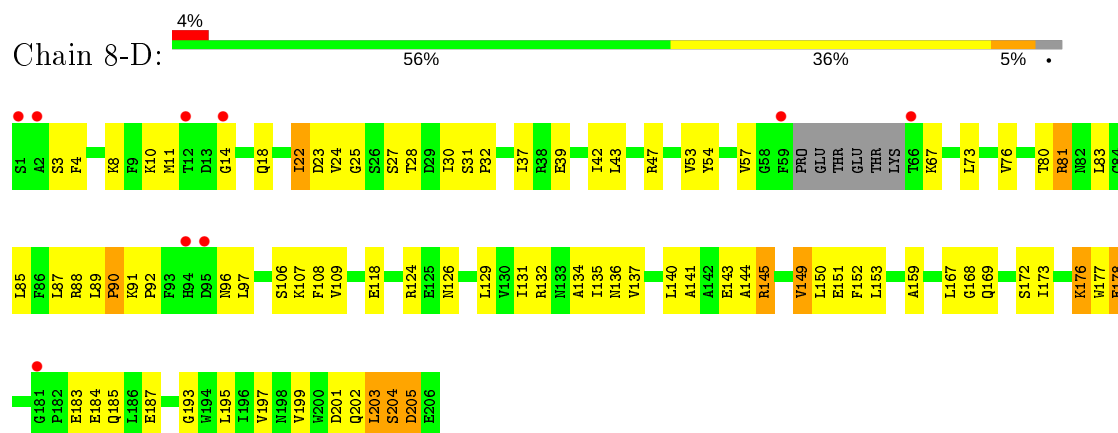
• Molecule 1: Protein At5g06450



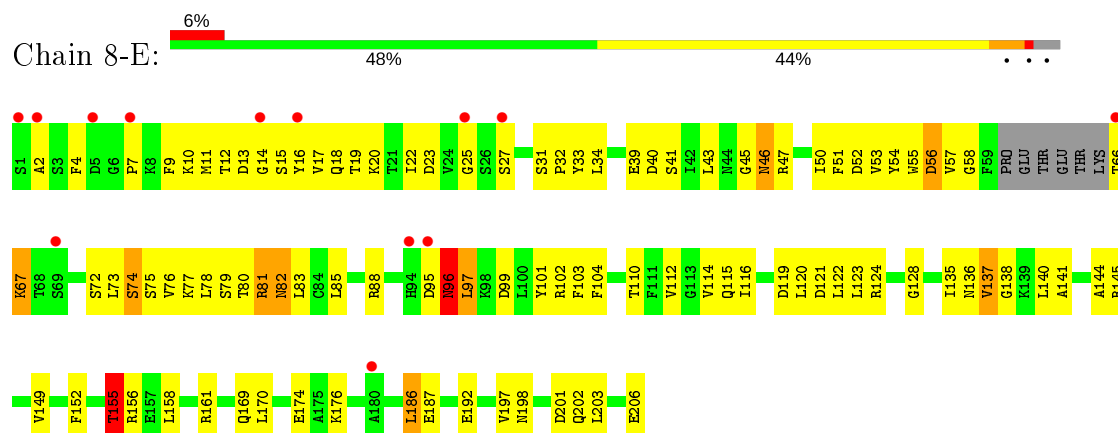
- Molecule 1: Protein At5g06450



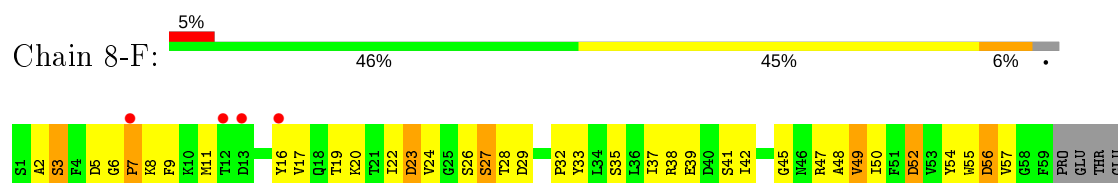
- Molecule 1: Protein At5g06450



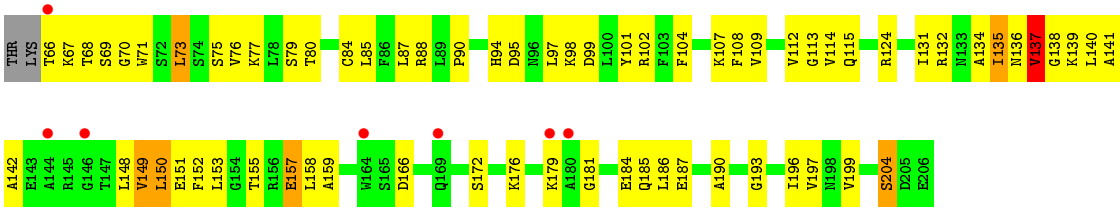
- Molecule 1: Protein At5g06450



- Molecule 1: Protein At5g06450







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.83Å 120.83Å 185.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.88 – 2.10 34.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.88-2.10) 100.0 (34.92-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.02 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.155 , 0.221 0.162 , 0.226	Depositor DCC
$R_{free}$ test set	4592 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	81528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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	1-A	0.86	0/1623	0.84	0/2196
1	1-B	0.86	0/1623	0.90	0/2196
1	1-C	0.88	2/1623 (0.1%)	0.87	3/2196 (0.1%)
1	1-D	0.82	0/1623	0.87	1/2196 (0.0%)
1	1-E	0.75	0/1623	0.82	2/2196 (0.1%)
1	1-F	0.81	0/1623	0.87	2/2196 (0.1%)
1	2-A	0.86	2/1623 (0.1%)	0.88	2/2196 (0.1%)
1	2-B	0.81	0/1623	0.87	1/2196 (0.0%)
1	2-C	0.84	0/1623	0.88	0/2196
1	2-D	0.78	0/1623	0.84	2/2196 (0.1%)
1	2-E	0.77	0/1623	0.81	1/2196 (0.0%)
1	2-F	0.80	0/1623	0.87	3/2196 (0.1%)
1	3-A	0.88	0/1623	0.87	0/2196
1	3-B	0.85	0/1623	0.83	1/2196 (0.0%)
1	3-C	0.83	1/1623 (0.1%)	0.85	1/2196 (0.0%)
1	3-D	0.82	0/1623	0.87	0/2196
1	3-E	0.75	0/1623	0.86	1/2196 (0.0%)
1	3-F	0.82	1/1623 (0.1%)	0.85	1/2196 (0.0%)
1	4-A	0.87	0/1623	0.82	0/2196
1	4-B	0.86	0/1623	0.86	2/2196 (0.1%)
1	4-C	0.83	0/1623	0.88	0/2196
1	4-D	0.81	0/1623	0.85	2/2196 (0.1%)
1	4-E	0.74	0/1623	0.78	0/2196
1	4-F	0.81	0/1623	0.87	1/2196 (0.0%)
1	5-A	0.97	1/1623 (0.1%)	0.94	2/2196 (0.1%)
1	5-B	0.93	1/1623 (0.1%)	0.95	2/2196 (0.1%)
1	5-C	0.91	1/1623 (0.1%)	0.90	1/2196 (0.0%)
1	5-D	0.86	0/1623	0.91	1/2196 (0.0%)
1	5-E	0.86	2/1623 (0.1%)	0.92	2/2196 (0.1%)
1	5-F	0.86	0/1623	0.90	2/2196 (0.1%)
1	6-A	0.95	2/1623 (0.1%)	0.90	1/2196 (0.0%)
1	6-B	0.96	2/1623 (0.1%)	0.95	1/2196 (0.0%)
1	6-C	0.90	1/1623 (0.1%)	0.89	2/2196 (0.1%)
1	6-D	0.89	0/1623	0.94	1/2196 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	6-E	0.83	0/1623	0.90	2/2196 (0.1%)
1	6-F	0.88	0/1623	0.90	2/2196 (0.1%)
1	7-A	0.95	0/1623	0.92	3/2196 (0.1%)
1	7-B	0.96	0/1623	1.04	6/2196 (0.3%)
1	7-C	0.92	1/1623 (0.1%)	0.94	3/2196 (0.1%)
1	7-D	0.86	0/1623	0.90	2/2196 (0.1%)
1	7-E	0.83	0/1623	0.89	0/2196
1	7-F	0.87	0/1623	0.92	2/2196 (0.1%)
1	8-A	0.94	0/1623	0.96	2/2196 (0.1%)
1	8-B	0.92	0/1623	0.96	1/2196 (0.0%)
1	8-C	0.93	0/1623	0.96	5/2196 (0.2%)
1	8-D	0.88	0/1623	0.90	2/2196 (0.1%)
1	8-E	0.82	0/1623	0.91	3/2196 (0.1%)
1	8-F	0.86	0/1623	0.94	2/2196 (0.1%)
All	All	0.86	17/77904 (0.0%)	0.89	76/105408 (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	1-D	0	1
1	2-C	0	1
1	2-D	0	1
1	5-D	0	1
1	5-E	0	1
1	6-B	0	2
1	6-D	0	1
1	8-B	0	1
1	8-E	0	1
All	All	0	10

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	134	ALA	CA-CB	6.64	1.66	1.52
1	5-E	192	GLU	CB-CG	6.39	1.64	1.52
1	3-C	84	CYS	CB-SG	6.38	1.93	1.82
1	6-A	178	GLU	CB-CG	6.14	1.63	1.52
1	1-C	192	GLU	CG-CD	6.04	1.61	1.51

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-B	102	ARG	NE-CZ-NH2	14.03	127.32	120.30
1	7-B	102	ARG	NE-CZ-NH1	-12.34	114.13	120.30
1	8-C	81	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	6-E	73	LEU	CA-CB-CG	7.62	132.84	115.30
1	8-C	81	ARG	NE-CZ-NH2	-7.44	116.58	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-D	33	TYR	Sidechain
1	2-C	33	TYR	Sidechain
1	2-D	33	TYR	Sidechain
1	5-D	152	PHE	Sidechain
1	5-E	33	TYR	Sidechain

## 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	1-A	1591	0	1575	115	0
1	1-B	1591	0	1575	122	0
1	1-C	1591	0	1575	120	0
1	1-D	1591	0	1575	125	0
1	1-E	1591	0	1575	96	0
1	1-F	1591	0	1575	101	0
1	2-A	1591	0	1575	171	0
1	2-B	1591	0	1575	123	0
1	2-C	1591	0	1575	132	0
1	2-D	1591	0	1575	123	0
1	2-E	1591	0	1575	110	0
1	2-F	1591	0	1575	116	0
1	3-A	1591	0	1575	119	0
1	3-B	1591	0	1575	97	0
1	3-C	1591	0	1575	115	0
1	3-D	1591	0	1575	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-E	1591	0	1575	123	0
1	3-F	1591	0	1575	144	0
1	4-A	1591	0	1575	92	0
1	4-B	1591	0	1575	95	0
1	4-C	1591	0	1575	165	0
1	4-D	1591	0	1575	137	0
1	4-E	1591	0	1575	99	0
1	4-F	1591	0	1575	157	0
1	5-A	1591	0	1575	111	0
1	5-B	1591	0	1575	104	0
1	5-C	1591	0	1575	131	0
1	5-D	1591	0	1575	105	0
1	5-E	1591	0	1575	159	0
1	5-F	1591	0	1575	116	0
1	6-A	1591	0	1575	114	0
1	6-B	1591	0	1575	118	0
1	6-C	1591	0	1575	114	0
1	6-D	1591	0	1575	128	0
1	6-E	1591	0	1575	92	0
1	6-F	1591	0	1575	95	0
1	7-A	1591	0	1575	123	0
1	7-B	1591	0	1575	170	0
1	7-C	1591	0	1575	134	0
1	7-D	1591	0	1575	142	0
1	7-E	1591	0	1575	134	0
1	7-F	1591	0	1575	155	0
1	8-A	1591	0	1575	187	0
1	8-B	1591	0	1575	130	0
1	8-C	1591	0	1575	123	0
1	8-D	1591	0	1575	86	0
1	8-E	1591	0	1575	136	0
1	8-F	1591	0	1575	138	0
2	1-A	121	0	0	22	0
2	1-B	115	0	0	12	0
2	1-C	103	0	0	19	0
2	1-D	96	0	0	12	0
2	1-E	99	0	0	11	0
2	1-F	111	0	0	17	0
2	2-A	120	0	0	28	0
2	2-B	118	0	0	15	0
2	2-C	104	0	0	17	0
2	2-D	96	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2-E	97	0	0	9	0
2	2-F	110	0	0	19	0
2	3-A	117	0	0	23	0
2	3-B	120	0	0	9	0
2	3-C	103	0	0	14	0
2	3-D	92	0	0	7	0
2	3-E	104	0	0	12	0
2	3-F	109	0	0	15	0
2	4-A	118	0	0	16	0
2	4-B	125	0	0	13	0
2	4-C	97	0	0	18	0
2	4-D	97	0	0	15	0
2	4-E	97	0	0	6	0
2	4-F	111	0	0	15	0
2	5-A	118	0	0	23	0
2	5-B	118	0	0	6	0
2	5-C	101	0	0	11	0
2	5-D	93	0	0	9	0
2	5-E	102	0	0	26	0
2	5-F	113	0	0	16	0
2	6-A	117	0	0	11	0
2	6-B	117	0	0	11	0
2	6-C	98	0	0	16	0
2	6-D	99	0	0	16	0
2	6-E	104	0	0	11	0
2	6-F	110	0	0	12	0
2	7-A	120	0	0	24	0
2	7-B	120	0	0	24	0
2	7-C	100	0	0	11	0
2	7-D	95	0	0	10	0
2	7-E	102	0	0	15	0
2	7-F	108	0	0	19	0
2	8-A	117	0	0	33	0
2	8-B	123	0	0	36	0
2	8-C	101	0	0	11	0
2	8-D	97	0	0	5	0
2	8-E	98	0	0	29	0
2	8-F	109	0	0	8	0
All	All	81528	0	75600	5480	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 36.

The worst 5 of 5480 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:A:192:GLU:OE1	2:A:316:HOH:O	1.57	1.21
1:D:106:SER:OG	2:D:244:HOH:O	1.54	1.21
1:B:81:ARG:HA	2:B:288:HOH:O	1.36	1.18
1:D:12:THR:HG23	2:D:264:HOH:O	1.44	1.18
1:C:157:GLU:HB2	2:C:214:HOH:O	1.41	1.17

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	1-A	196/206 (95%)	178 (91%)	14 (7%)	4 (2%)	7	3
1	1-B	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	10	5
1	1-C	196/206 (95%)	173 (88%)	21 (11%)	2 (1%)	15	11
1	1-D	196/206 (95%)	173 (88%)	21 (11%)	2 (1%)	15	11
1	1-E	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	10	5
1	1-F	196/206 (95%)	173 (88%)	17 (9%)	6 (3%)	4	1
1	2-A	196/206 (95%)	170 (87%)	20 (10%)	6 (3%)	4	1
1	2-B	196/206 (95%)	179 (91%)	10 (5%)	7 (4%)	3	1
1	2-C	196/206 (95%)	183 (93%)	13 (7%)	0	100	100
1	2-D	196/206 (95%)	171 (87%)	19 (10%)	6 (3%)	4	1
1	2-E	196/206 (95%)	174 (89%)	21 (11%)	1 (0%)	29	26
1	2-F	196/206 (95%)	183 (93%)	11 (6%)	2 (1%)	15	11
1	3-A	196/206 (95%)	182 (93%)	10 (5%)	4 (2%)	7	3
1	3-B	196/206 (95%)	185 (94%)	10 (5%)	1 (0%)	29	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-C	196/206 (95%)	181 (92%)	13 (7%)	2 (1%)	15	11
1	3-D	196/206 (95%)	169 (86%)	23 (12%)	4 (2%)	7	3
1	3-E	196/206 (95%)	172 (88%)	20 (10%)	4 (2%)	7	3
1	3-F	196/206 (95%)	177 (90%)	15 (8%)	4 (2%)	7	3
1	4-A	196/206 (95%)	180 (92%)	10 (5%)	6 (3%)	4	1
1	4-B	196/206 (95%)	176 (90%)	18 (9%)	2 (1%)	15	11
1	4-C	196/206 (95%)	171 (87%)	22 (11%)	3 (2%)	10	5
1	4-D	196/206 (95%)	173 (88%)	19 (10%)	4 (2%)	7	3
1	4-E	196/206 (95%)	184 (94%)	9 (5%)	3 (2%)	10	5
1	4-F	196/206 (95%)	172 (88%)	21 (11%)	3 (2%)	10	5
1	5-A	196/206 (95%)	181 (92%)	11 (6%)	4 (2%)	7	3
1	5-B	196/206 (95%)	174 (89%)	17 (9%)	5 (3%)	5	2
1	5-C	196/206 (95%)	188 (96%)	6 (3%)	2 (1%)	15	11
1	5-D	196/206 (95%)	175 (89%)	17 (9%)	4 (2%)	7	3
1	5-E	196/206 (95%)	171 (87%)	22 (11%)	3 (2%)	10	5
1	5-F	196/206 (95%)	181 (92%)	14 (7%)	1 (0%)	29	26
1	6-A	196/206 (95%)	168 (86%)	22 (11%)	6 (3%)	4	1
1	6-B	196/206 (95%)	176 (90%)	16 (8%)	4 (2%)	7	3
1	6-C	196/206 (95%)	178 (91%)	18 (9%)	0	100	100
1	6-D	196/206 (95%)	179 (91%)	14 (7%)	3 (2%)	10	5
1	6-E	196/206 (95%)	177 (90%)	15 (8%)	4 (2%)	7	3
1	6-F	196/206 (95%)	180 (92%)	13 (7%)	3 (2%)	10	5
1	7-A	196/206 (95%)	179 (91%)	13 (7%)	4 (2%)	7	3
1	7-B	196/206 (95%)	179 (91%)	15 (8%)	2 (1%)	15	11
1	7-C	196/206 (95%)	184 (94%)	9 (5%)	3 (2%)	10	5
1	7-D	196/206 (95%)	174 (89%)	17 (9%)	5 (3%)	5	2
1	7-E	196/206 (95%)	176 (90%)	17 (9%)	3 (2%)	10	5
1	7-F	196/206 (95%)	176 (90%)	19 (10%)	1 (0%)	29	26
1	8-A	196/206 (95%)	167 (85%)	17 (9%)	12 (6%)	1	0
1	8-B	196/206 (95%)	180 (92%)	15 (8%)	1 (0%)	29	26
1	8-C	196/206 (95%)	179 (91%)	15 (8%)	2 (1%)	15	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-D	196/206 (95%)	181 (92%)	10 (5%)	5 (3%)	5	2
1	8-E	196/206 (95%)	170 (87%)	20 (10%)	6 (3%)	4	1
1	8-F	196/206 (95%)	170 (87%)	20 (10%)	6 (3%)	4	1
All	All	9408/9888 (95%)	8478 (90%)	759 (8%)	171 (2%)	8	4

5 of 171 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	148	LEU
1	1-B	47	ARG
1	1-D	47	ARG
1	1-E	67	LYS
1	1-F	11	MSE

### 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	1-A	173/178 (97%)	168 (97%)	5 (3%)	42	46
1	1-B	173/178 (97%)	158 (91%)	15 (9%)	10	7
1	1-C	173/178 (97%)	165 (95%)	8 (5%)	27	26
1	1-D	173/178 (97%)	165 (95%)	8 (5%)	27	26
1	1-E	173/178 (97%)	162 (94%)	11 (6%)	17	14
1	1-F	173/178 (97%)	166 (96%)	7 (4%)	31	32
1	2-A	173/178 (97%)	157 (91%)	16 (9%)	9	6
1	2-B	173/178 (97%)	157 (91%)	16 (9%)	9	6
1	2-C	173/178 (97%)	165 (95%)	8 (5%)	27	26
1	2-D	173/178 (97%)	163 (94%)	10 (6%)	20	17
1	2-E	173/178 (97%)	165 (95%)	8 (5%)	27	26
1	2-F	173/178 (97%)	168 (97%)	5 (3%)	42	46
1	3-A	173/178 (97%)	162 (94%)	11 (6%)	17	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-B	173/178 (97%)	163 (94%)	10 (6%)	20	17
1	3-C	173/178 (97%)	164 (95%)	9 (5%)	23	21
1	3-D	173/178 (97%)	163 (94%)	10 (6%)	20	17
1	3-E	173/178 (97%)	167 (96%)	6 (4%)	36	38
1	3-F	173/178 (97%)	167 (96%)	6 (4%)	36	38
1	4-A	173/178 (97%)	165 (95%)	8 (5%)	27	26
1	4-B	173/178 (97%)	163 (94%)	10 (6%)	20	17
1	4-C	173/178 (97%)	160 (92%)	13 (8%)	13	10
1	4-D	173/178 (97%)	162 (94%)	11 (6%)	17	14
1	4-E	173/178 (97%)	167 (96%)	6 (4%)	36	38
1	4-F	173/178 (97%)	159 (92%)	14 (8%)	11	8
1	5-A	173/178 (97%)	168 (97%)	5 (3%)	42	46
1	5-B	173/178 (97%)	158 (91%)	15 (9%)	10	7
1	5-C	173/178 (97%)	160 (92%)	13 (8%)	13	10
1	5-D	173/178 (97%)	165 (95%)	8 (5%)	27	26
1	5-E	173/178 (97%)	166 (96%)	7 (4%)	31	32
1	5-F	173/178 (97%)	165 (95%)	8 (5%)	27	26
1	6-A	173/178 (97%)	166 (96%)	7 (4%)	31	32
1	6-B	173/178 (97%)	161 (93%)	12 (7%)	15	12
1	6-C	173/178 (97%)	158 (91%)	15 (9%)	10	7
1	6-D	173/178 (97%)	165 (95%)	8 (5%)	27	26
1	6-E	173/178 (97%)	159 (92%)	14 (8%)	11	8
1	6-F	173/178 (97%)	164 (95%)	9 (5%)	23	21
1	7-A	173/178 (97%)	161 (93%)	12 (7%)	15	12
1	7-B	173/178 (97%)	162 (94%)	11 (6%)	17	14
1	7-C	173/178 (97%)	161 (93%)	12 (7%)	15	12
1	7-D	173/178 (97%)	159 (92%)	14 (8%)	11	8
1	7-E	173/178 (97%)	165 (95%)	8 (5%)	27	26
1	7-F	173/178 (97%)	159 (92%)	14 (8%)	11	8
1	8-A	173/178 (97%)	162 (94%)	11 (6%)	17	14
1	8-B	173/178 (97%)	155 (90%)	18 (10%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-C	173/178 (97%)	163 (94%)	10 (6%)	20	17
1	8-D	173/178 (97%)	166 (96%)	7 (4%)	31	32
1	8-E	173/178 (97%)	161 (93%)	12 (7%)	15	12
1	8-F	173/178 (97%)	160 (92%)	13 (8%)	13	10
All	All	8304/8544 (97%)	7810 (94%)	494 (6%)	19	17

5 of 494 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4-F	92	PRO
1	5-E	96	ASN
1	8-C	81	ARG
1	4-F	182	PRO
1	5-B	178	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 191 such sidechains are listed below:

Mol	Chain	Res	Type
1	4-C	46	ASN
1	4-F	198	ASN
1	8-B	136	ASN
1	4-C	133	ASN
1	4-E	94	HIS

### 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	1-A	199/206 (96%)	0.21	19 (9%) 8 10	8, 20, 39, 73	199 (100%)
1	1-B	199/206 (96%)	0.32	12 (6%) 21 27	9, 19, 41, 64	199 (100%)
1	1-C	199/206 (96%)	0.19	10 (5%) 28 34	10, 20, 41, 67	199 (100%)
1	1-D	199/206 (96%)	0.15	9 (4%) 33 38	10, 23, 42, 58	199 (100%)
1	1-E	199/206 (96%)	0.31	13 (6%) 18 23	12, 25, 43, 63	199 (100%)
1	1-F	199/206 (96%)	0.17	11 (5%) 25 31	12, 23, 44, 57	199 (100%)
1	2-A	199/206 (96%)	0.21	19 (9%) 8 10	8, 20, 39, 73	199 (100%)
1	2-B	199/206 (96%)	0.32	12 (6%) 21 27	9, 19, 41, 64	199 (100%)
1	2-C	199/206 (96%)	0.19	10 (5%) 28 34	10, 20, 41, 67	199 (100%)
1	2-D	199/206 (96%)	0.15	9 (4%) 33 38	10, 23, 42, 58	199 (100%)
1	2-E	199/206 (96%)	0.31	13 (6%) 18 23	12, 25, 43, 63	199 (100%)
1	2-F	199/206 (96%)	0.17	11 (5%) 25 31	12, 23, 44, 57	199 (100%)
1	3-A	199/206 (96%)	0.21	19 (9%) 8 10	8, 20, 39, 73	199 (100%)
1	3-B	199/206 (96%)	0.32	12 (6%) 21 27	9, 19, 41, 64	199 (100%)
1	3-C	199/206 (96%)	0.19	10 (5%) 28 34	10, 20, 41, 67	199 (100%)
1	3-D	199/206 (96%)	0.15	9 (4%) 33 38	10, 23, 42, 58	199 (100%)
1	3-E	199/206 (96%)	0.31	13 (6%) 18 23	12, 25, 43, 63	199 (100%)
1	3-F	199/206 (96%)	0.17	11 (5%) 25 31	12, 23, 44, 57	199 (100%)
1	4-A	199/206 (96%)	0.21	19 (9%) 8 10	8, 20, 39, 73	199 (100%)
1	4-B	199/206 (96%)	0.32	12 (6%) 21 27	9, 19, 41, 64	199 (100%)
1	4-C	199/206 (96%)	0.19	10 (5%) 28 34	10, 20, 41, 67	199 (100%)
1	4-D	199/206 (96%)	0.15	9 (4%) 33 38	10, 23, 42, 58	199 (100%)
1	4-E	199/206 (96%)	0.31	13 (6%) 18 23	12, 25, 43, 63	199 (100%)
1	4-F	199/206 (96%)	0.17	11 (5%) 25 31	12, 23, 44, 57	199 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	5-A	199/206 (96%)	0.21	19 (9%) 8 10	8, 20, 39, 73	199 (100%)
1	5-B	199/206 (96%)	0.32	12 (6%) 21 27	9, 19, 41, 64	199 (100%)
1	5-C	199/206 (96%)	0.19	10 (5%) 28 34	10, 20, 41, 67	199 (100%)
1	5-D	199/206 (96%)	0.15	9 (4%) 33 38	10, 23, 42, 58	199 (100%)
1	5-E	199/206 (96%)	0.31	13 (6%) 18 23	12, 25, 43, 63	199 (100%)
1	5-F	199/206 (96%)	0.17	11 (5%) 25 31	12, 23, 44, 57	199 (100%)
1	6-A	199/206 (96%)	0.21	19 (9%) 8 10	8, 20, 39, 73	199 (100%)
1	6-B	199/206 (96%)	0.32	12 (6%) 21 27	9, 19, 41, 64	199 (100%)
1	6-C	199/206 (96%)	0.19	10 (5%) 28 34	10, 20, 41, 67	199 (100%)
1	6-D	199/206 (96%)	0.15	9 (4%) 33 38	10, 23, 42, 58	199 (100%)
1	6-E	199/206 (96%)	0.31	13 (6%) 18 23	12, 25, 43, 63	199 (100%)
1	6-F	199/206 (96%)	0.17	11 (5%) 25 31	12, 23, 44, 57	199 (100%)
1	7-A	199/206 (96%)	0.21	19 (9%) 8 10	8, 20, 39, 73	199 (100%)
1	7-B	199/206 (96%)	0.32	12 (6%) 21 27	9, 19, 41, 64	199 (100%)
1	7-C	199/206 (96%)	0.19	10 (5%) 28 34	10, 20, 41, 67	199 (100%)
1	7-D	199/206 (96%)	0.15	9 (4%) 33 38	10, 23, 42, 58	199 (100%)
1	7-E	199/206 (96%)	0.31	13 (6%) 18 23	12, 25, 43, 63	199 (100%)
1	7-F	199/206 (96%)	0.17	11 (5%) 25 31	12, 23, 44, 57	199 (100%)
1	8-A	199/206 (96%)	0.21	19 (9%) 8 10	8, 20, 39, 73	199 (100%)
1	8-B	199/206 (96%)	0.32	12 (6%) 21 27	9, 19, 41, 64	199 (100%)
1	8-C	199/206 (96%)	0.19	10 (5%) 28 34	10, 20, 41, 67	199 (100%)
1	8-D	199/206 (96%)	0.15	9 (4%) 33 38	10, 23, 42, 58	199 (100%)
1	8-E	199/206 (96%)	0.31	13 (6%) 18 23	12, 25, 43, 63	199 (100%)
1	8-F	199/206 (96%)	0.17	11 (5%) 25 31	12, 23, 44, 57	199 (100%)
All	All	9552/9888 (96%)	0.22	592 (6%) 20 25	8, 22, 42, 73	9552 (100%)

The worst 5 of 592 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-C	59	PHE	12.9
1	2-C	59	PHE	12.9
1	3-C	59	PHE	12.9
1	4-C	59	PHE	12.9
1	5-C	59	PHE	12.9

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.