



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:02 AM UTC

PDB ID : 2Q3S / pdb_00002q3s
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

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

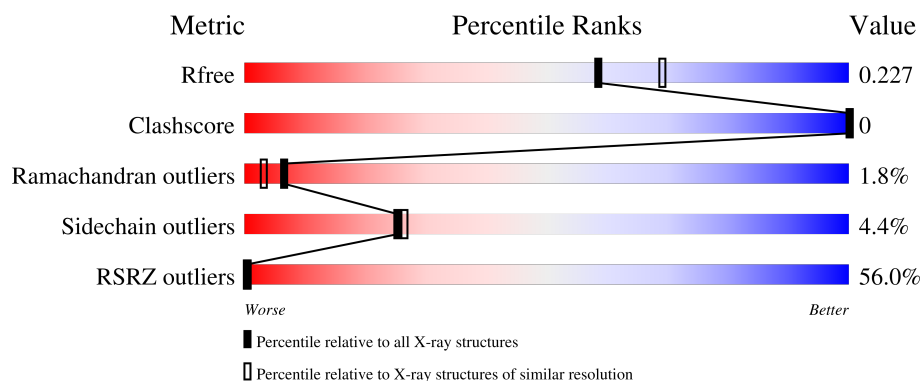
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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 $\leq 5\%$. 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	48% 93%
1	1-B	206	51% 91% 6%
1	1-C	206	63% 92% 5%
1	1-D	206	66% 93%
1	1-E	206	48% 90% 6%

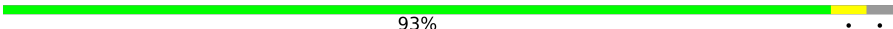
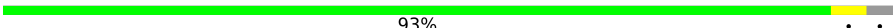
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Mol	Chain	Length	Quality of chain
1	1-F	206	50% 93% ...
1	2-A	206	92% 5% .
1	2-B	206	89% 7% ..
1	2-C	206	93% . .
1	2-D	206	91% 6% .
1	2-E	206	91% 6% .
1	2-F	206	93% . .
1	3-A	206	93% . .
1	3-B	206	92% 5% .
1	3-C	206	92% 5% .
1	3-D	206	92% 5% .
1	3-E	206	89% 8% .
1	3-F	206	93% . .
1	4-A	206	92% 5% .
1	4-B	206	91% 5% .
1	4-C	206	92% 5% .
1	4-D	206	92% 5% .
1	4-E	206	90% 6% .
1	4-F	206	93% . .
1	5-A	206	93% . .
1	5-B	206	90% 6% .
1	5-C	206	93% . .
1	5-D	206	92% 5% .
1	5-E	206	89% 8% .
1	5-F	206	94% . .

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Mol	Chain	Length	Quality of chain
1	6-A	206	 92% 5% .
1	6-B	206	 90% 6% .
1	6-C	206	 93% . .
1	6-D	206	 92% 5% .
1	6-E	206	 90% 7% .
1	6-F	206	 93% . .
1	7-A	206	 93% . .
1	7-B	206	 92% . . .
1	7-C	206	 92% 5% .
1	7-D	206	 92% 5% .
1	7-E	206	 90% 6% .
1	7-F	206	 94% . .
1	8-A	206	 89% 8% .
1	8-B	206	 91% 5% .
1	8-C	206	 92% 5% .
1	8-D	206	 92% . .
1	8-E	206	 89% 7% . .
1	8-F	206	 92% 5% .

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	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	2-C	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	3-C	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	4-C	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	5-C	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	6-C	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	7-C	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	8-C	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	1-D	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	2-D	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	3-D	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	4-D	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	5-D	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	6-D	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	7-D	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	8-D	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	1-E	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	2-E	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	3-E	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	4-E	200	Total	C	N	O	S	Se	0	0	0
			1591	1020	266	303	1	1			
1	5-E	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	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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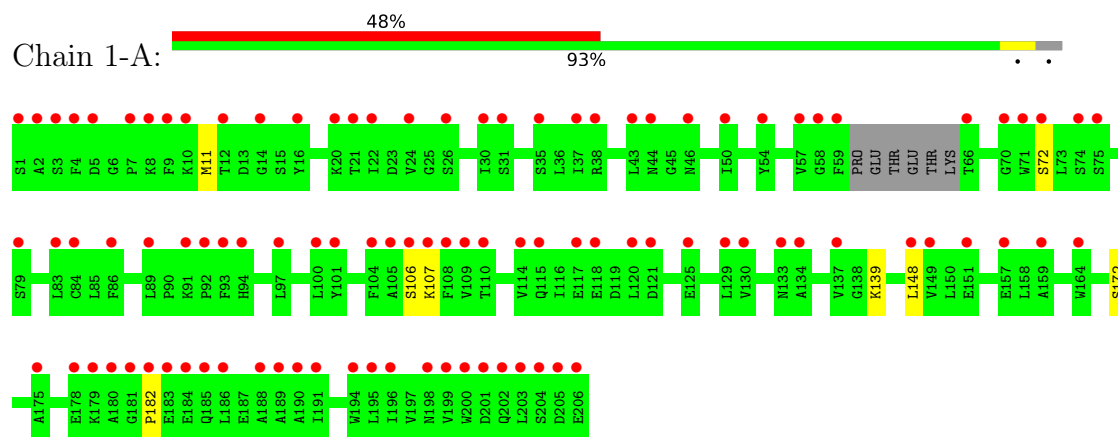
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	4-F	111	Total 111	O 111	0	0
2	5-F	113	Total 113	O 113	0	0
2	6-F	110	Total 110	O 110	0	0
2	7-F	108	Total 108	O 108	0	0
2	8-F	109	Total 109	O 109	0	0

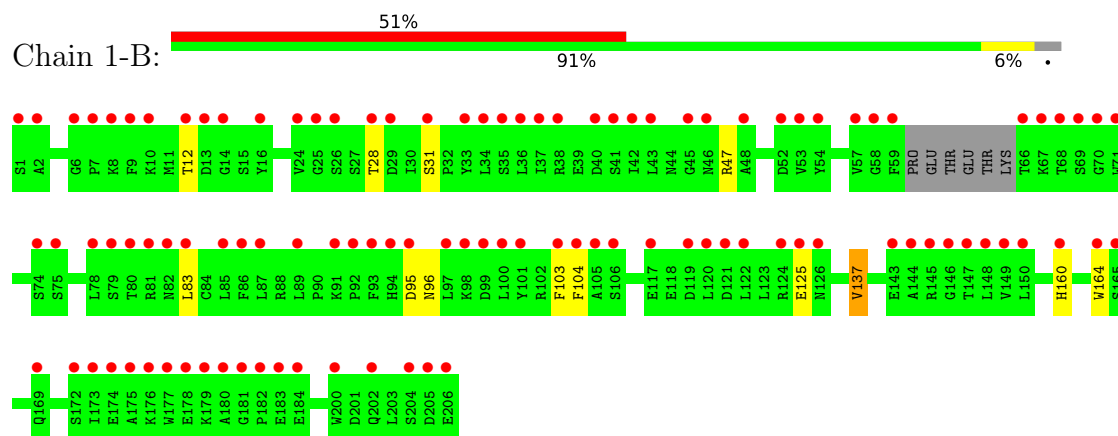
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

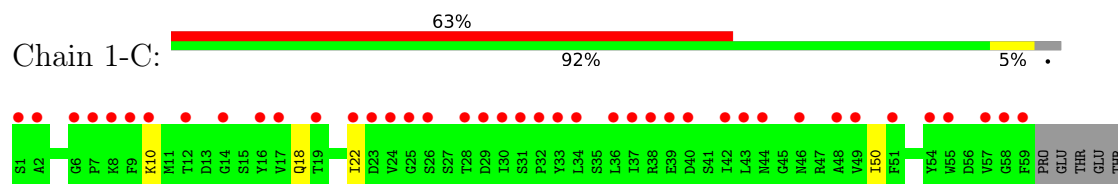
• Molecule 1: Protein At5g06450

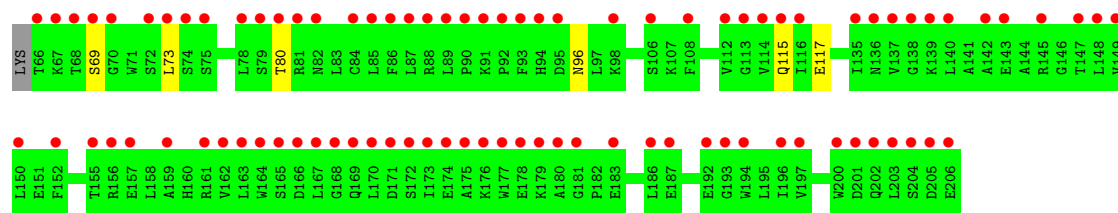


• Molecule 1: Protein At5g06450



• Molecule 1: Protein At5g06450





● Molecule 1: Protein At5g06450



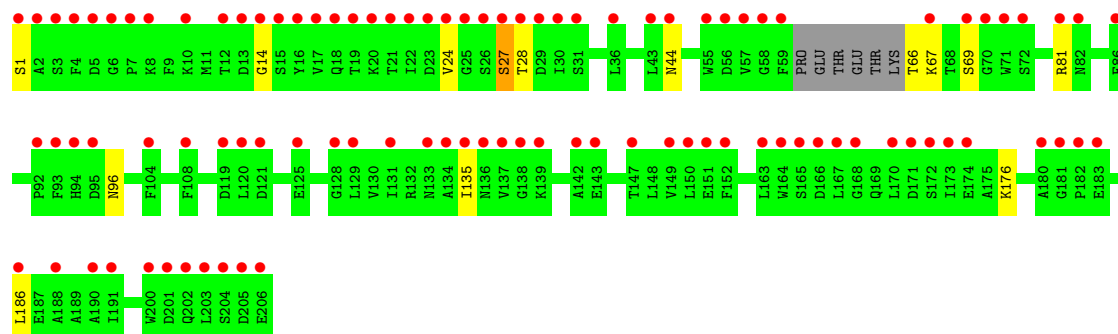
Chain 1-D:



● Molecule 1: Protein At5g06450



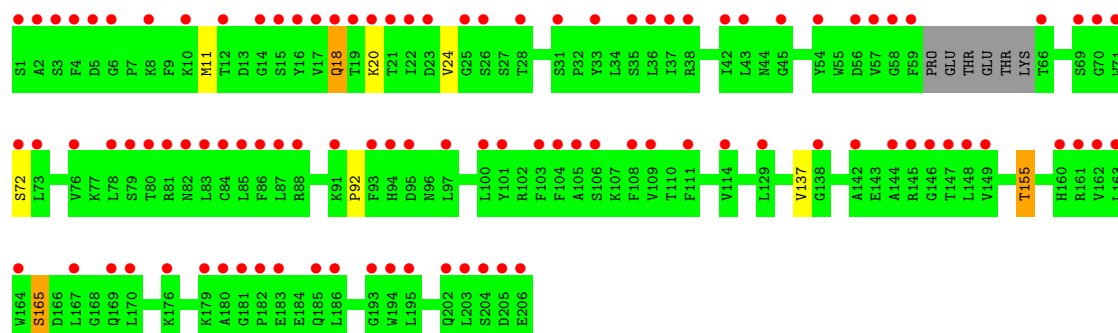
Chain 1-E:



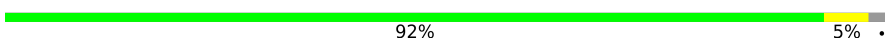
● Molecule 1: Protein At5g06450



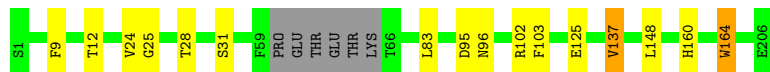
Chain 1-F:



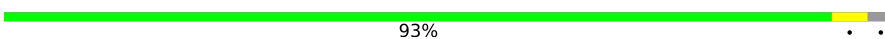
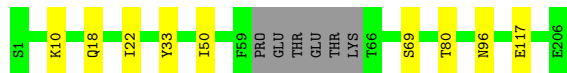
• Molecule 1: Protein At5g06450

Chain 2-A:  92% 5% .

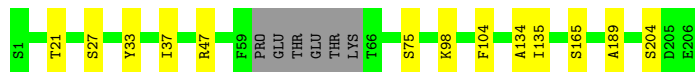
• Molecule 1: Protein At5g06450

Chain 2-B:  89% 7% . .

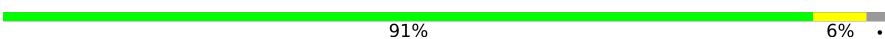
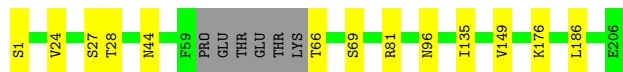
• Molecule 1: Protein At5g06450

Chain 2-C:  93% . .

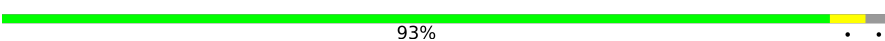
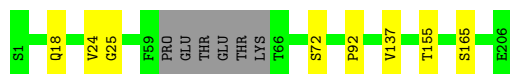
• Molecule 1: Protein At5g06450

Chain 2-D:  91% 6% .

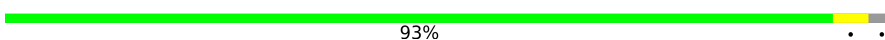
• Molecule 1: Protein At5g06450

Chain 2-E:  91% 6% .

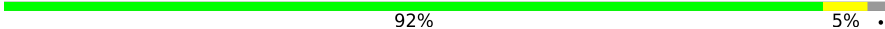
• Molecule 1: Protein At5g06450

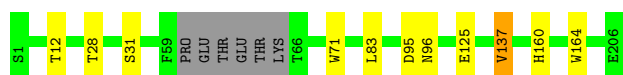
Chain 2-F:  93% . .

• Molecule 1: Protein At5g06450

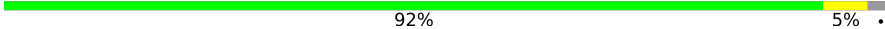
Chain 3-A:  93% . .

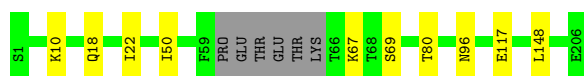
• Molecule 1: Protein At5g06450

Chain 3-B:  92% 5% .

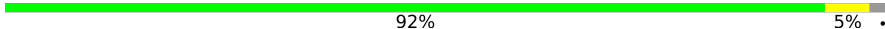


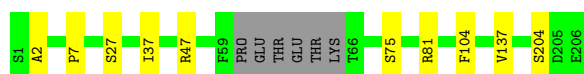
- Molecule 1: Protein At5g06450

Chain 3-C:  92% 5% .



- Molecule 1: Protein At5g06450

Chain 3-D:  92% 5% .

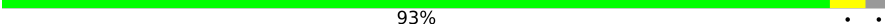


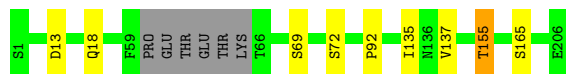
- Molecule 1: Protein At5g06450

Chain 3-E:  89% 8% .



- Molecule 1: Protein At5g06450

Chain 3-F:  93% . .



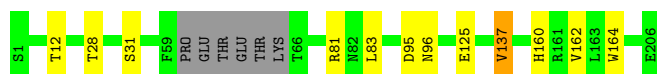
- Molecule 1: Protein At5g06450

Chain 4-A:  92% 5% .

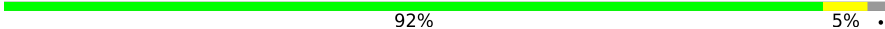


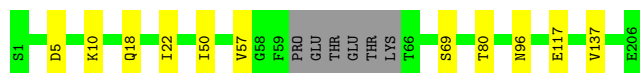
- Molecule 1: Protein At5g06450

Chain 4-B:  91% 5% .

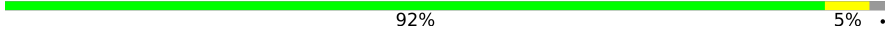


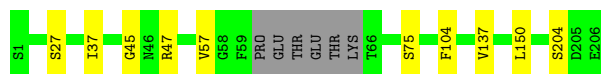
- Molecule 1: Protein At5g06450

Chain 4-C:  92% 5% .



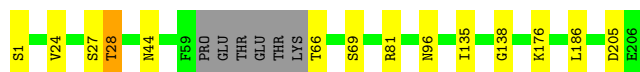
• Molecule 1: Protein At5g06450

Chain 4-D:  92% 5% .



• Molecule 1: Protein At5g06450

Chain 4-E:  90% 6% .



• Molecule 1: Protein At5g06450

Chain 4-F:  93% . .



• Molecule 1: Protein At5g06450

Chain 5-A:  93% . .



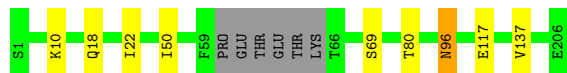
• Molecule 1: Protein At5g06450

Chain 5-B:  90% 6% .



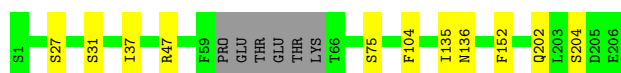
• Molecule 1: Protein At5g06450

Chain 5-C:  93% . .



• Molecule 1: Protein At5g06450

Chain 5-D:  92% 5% .



• Molecule 1: Protein At5g06450

Chain 5-E:  89% 8% .



• Molecule 1: Protein At5g06450

Chain 5-F:  94% . .



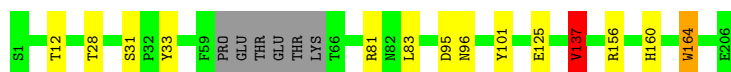
• Molecule 1: Protein At5g06450

Chain 6-A:  92% 5% .

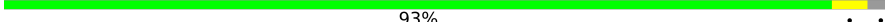


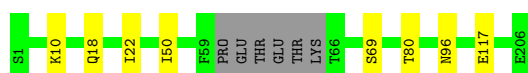
• Molecule 1: Protein At5g06450

Chain 6-B:  90% 6% .



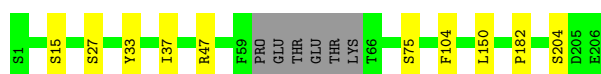
• Molecule 1: Protein At5g06450

Chain 6-C:  93% . .



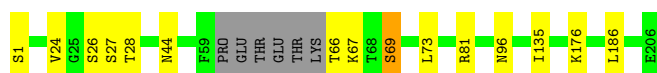
• Molecule 1: Protein At5g06450

Chain 6-D:  92% 5% .



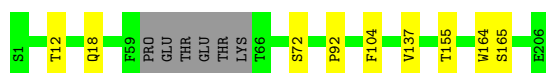
• Molecule 1: Protein At5g06450

Chain 6-E:  90% 7% .



• Molecule 1: Protein At5g06450

Chain 6-F:  93% . .



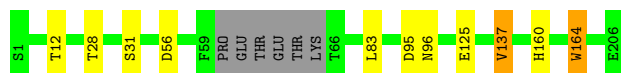
• Molecule 1: Protein At5g06450

Chain 7-A:  93% . .



• Molecule 1: Protein At5g06450

Chain 7-B:  92% . . .



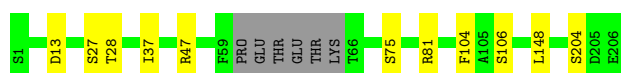
• Molecule 1: Protein At5g06450

Chain 7-C:  92% 5% .



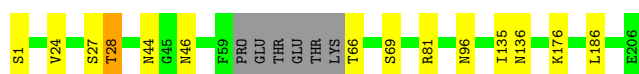
• Molecule 1: Protein At5g06450

Chain 7-D:  92% 5% .

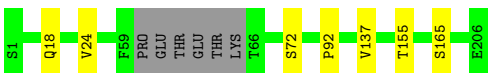


• Molecule 1: Protein At5g06450

Chain 7-E:  90% 6% .



• Molecule 1: Protein At5g06450

Chain 7-F:  94% 

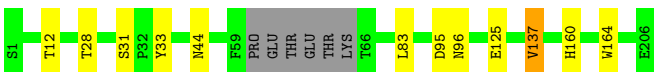


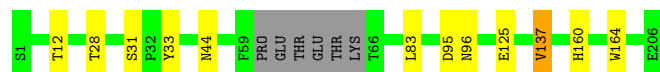
• Molecule 1: Protein At5g06450

Chain 8-A:  89% 

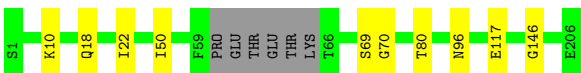


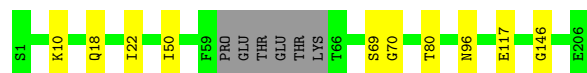
• Molecule 1: Protein At5g06450

Chain 8-B:  91% 



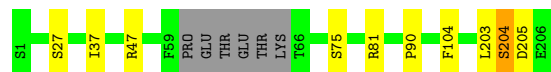
• Molecule 1: Protein At5g06450

Chain 8-C:  92% 



• Molecule 1: Protein At5g06450

Chain 8-D:  92% 

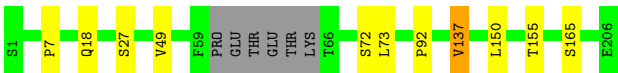


• Molecule 1: Protein At5g06450

Chain 8-E:  89% 



• Molecule 1: Protein At5g06450

Chain 8-F:  92% 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.83Å 120.83Å 185.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.88 – 2.10 34.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.88-2.10) 99.9 (34.88-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.02 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.155 , 0.221 0.162 , 0.227	Depositor DCC
R_{free} test set	4592 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	81528	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.41	0/1623	0.38	0/2196
1	1-B	0.42	0/1623	0.44	1/2196 (0.0%)
1	1-C	0.39	0/1623	0.44	0/2196
1	1-D	0.39	0/1623	0.43	0/2196
1	1-E	0.38	0/1623	0.43	0/2196
1	1-F	0.39	0/1623	0.39	0/2196
1	2-A	0.41	0/1623	0.38	0/2196
1	2-B	0.42	0/1623	0.44	1/2196 (0.0%)
1	2-C	0.39	0/1623	0.44	0/2196
1	2-D	0.39	0/1623	0.43	0/2196
1	2-E	0.38	0/1623	0.43	0/2196
1	2-F	0.39	0/1623	0.39	0/2196
1	3-A	0.41	0/1623	0.38	0/2196
1	3-B	0.42	0/1623	0.44	1/2196 (0.0%)
1	3-C	0.39	0/1623	0.44	0/2196
1	3-D	0.39	0/1623	0.43	0/2196
1	3-E	0.38	0/1623	0.43	0/2196
1	3-F	0.39	0/1623	0.39	0/2196
1	4-A	0.41	0/1623	0.38	0/2196
1	4-B	0.42	0/1623	0.44	1/2196 (0.0%)
1	4-C	0.39	0/1623	0.44	0/2196
1	4-D	0.39	0/1623	0.43	0/2196
1	4-E	0.38	0/1623	0.43	0/2196
1	4-F	0.39	0/1623	0.39	0/2196
1	5-A	0.41	0/1623	0.38	0/2196
1	5-B	0.42	0/1623	0.44	1/2196 (0.0%)
1	5-C	0.39	0/1623	0.44	0/2196
1	5-D	0.39	0/1623	0.43	0/2196
1	5-E	0.38	0/1623	0.43	0/2196
1	5-F	0.39	0/1623	0.39	0/2196
1	6-A	0.41	0/1623	0.38	0/2196
1	6-B	0.42	0/1623	0.44	1/2196 (0.0%)
1	6-C	0.39	0/1623	0.44	0/2196
1	6-D	0.39	0/1623	0.43	0/2196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	6-E	0.38	0/1623	0.43	0/2196
1	6-F	0.39	0/1623	0.39	0/2196
1	7-A	0.41	0/1623	0.38	0/2196
1	7-B	0.42	0/1623	0.44	1/2196 (0.0%)
1	7-C	0.39	0/1623	0.44	0/2196
1	7-D	0.39	0/1623	0.43	0/2196
1	7-E	0.38	0/1623	0.43	0/2196
1	7-F	0.39	0/1623	0.39	0/2196
1	8-A	0.41	0/1623	0.38	0/2196
1	8-B	0.42	0/1623	0.44	1/2196 (0.0%)
1	8-C	0.39	0/1623	0.44	0/2196
1	8-D	0.39	0/1623	0.43	0/2196
1	8-E	0.38	0/1623	0.43	0/2196
1	8-F	0.39	0/1623	0.39	0/2196
All	All	0.40	0/77904	0.42	8/105408 (0.0%)

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

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-B	137	VAL	N-CA-C	5.08	119.90	109.34
1	2-B	137	VAL	N-CA-C	5.08	119.90	109.34
1	3-B	137	VAL	N-CA-C	5.08	119.90	109.34
1	4-B	137	VAL	N-CA-C	5.08	119.90	109.34
1	5-B	137	VAL	N-CA-C	5.08	119.90	109.34

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	0	0
1	1-B	1591	0	1575	0	0
1	1-C	1591	0	1575	0	0
1	1-D	1591	0	1575	0	0
1	1-E	1591	0	1575	0	0
1	1-F	1591	0	1575	0	0
1	2-A	1591	0	1575	0	0
1	2-B	1591	0	1575	0	0
1	2-C	1591	0	1575	0	0
1	2-D	1591	0	1575	0	0
1	2-E	1591	0	1575	0	0
1	2-F	1591	0	1575	0	0
1	3-A	1591	0	1575	0	0
1	3-B	1591	0	1575	0	0
1	3-C	1591	0	1575	0	0
1	3-D	1591	0	1575	0	0
1	3-E	1591	0	1575	0	0
1	3-F	1591	0	1575	0	0
1	4-A	1591	0	1575	0	0
1	4-B	1591	0	1575	0	0
1	4-C	1591	0	1575	0	0
1	4-D	1591	0	1575	0	0
1	4-E	1591	0	1575	0	0
1	4-F	1591	0	1575	0	0
1	5-A	1591	0	1575	0	0
1	5-B	1591	0	1575	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5-C	1591	0	1575	0	0
1	5-D	1591	0	1575	0	0
1	5-E	1591	0	1575	0	0
1	5-F	1591	0	1575	0	0
1	6-A	1591	0	1575	0	0
1	6-B	1591	0	1575	0	0
1	6-C	1591	0	1575	0	0
1	6-D	1591	0	1575	0	0
1	6-E	1591	0	1575	0	0
1	6-F	1591	0	1575	0	0
1	7-A	1591	0	1575	0	0
1	7-B	1591	0	1575	0	0
1	7-C	1591	0	1575	0	0
1	7-D	1591	0	1575	0	0
1	7-E	1591	0	1575	0	0
1	7-F	1591	0	1575	0	0
1	8-A	1591	0	1575	0	0
1	8-B	1591	0	1575	0	0
1	8-C	1591	0	1575	0	0
1	8-D	1591	0	1575	0	0
1	8-E	1591	0	1575	0	0
1	8-F	1591	0	1575	0	0
2	1-A	121	0	0	0	0
2	1-B	115	0	0	0	0
2	1-C	103	0	0	0	0
2	1-D	96	0	0	0	0
2	1-E	99	0	0	0	0
2	1-F	111	0	0	0	0
2	2-A	120	0	0	0	0
2	2-B	118	0	0	0	0
2	2-C	104	0	0	0	0
2	2-D	96	0	0	0	0
2	2-E	97	0	0	0	0
2	2-F	110	0	0	0	0
2	3-A	117	0	0	0	0
2	3-B	120	0	0	0	0
2	3-C	103	0	0	0	0
2	3-D	92	0	0	0	0
2	3-E	104	0	0	0	0
2	3-F	109	0	0	0	0
2	4-A	118	0	0	0	0
2	4-B	125	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4-C	97	0	0	0	0
2	4-D	97	0	0	0	0
2	4-E	97	0	0	0	0
2	4-F	111	0	0	0	0
2	5-A	118	0	0	0	0
2	5-B	118	0	0	0	0
2	5-C	101	0	0	0	0
2	5-D	93	0	0	0	0
2	5-E	102	0	0	0	0
2	5-F	113	0	0	0	0
2	6-A	117	0	0	0	0
2	6-B	117	0	0	0	0
2	6-C	98	0	0	0	0
2	6-D	99	0	0	0	0
2	6-E	104	0	0	0	0
2	6-F	110	0	0	0	0
2	7-A	120	0	0	0	0
2	7-B	120	0	0	0	0
2	7-C	100	0	0	0	0
2	7-D	95	0	0	0	0
2	7-E	102	0	0	0	0
2	7-F	108	0	0	0	0
2	8-A	117	0	0	0	0
2	8-B	123	0	0	0	0
2	8-C	101	0	0	0	0
2	8-D	97	0	0	0	0
2	8-E	98	0	0	0	0
2	8-F	109	0	0	0	0
All	All	81528	0	75600	0	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 0.

There are no clashes within the asymmetric unit.

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%)	6	2
1	1-B	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	8	4
1	1-C	196/206 (95%)	173 (88%)	21 (11%)	2 (1%)	12	9
1	1-D	196/206 (95%)	173 (88%)	21 (11%)	2 (1%)	12	9
1	1-E	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	8	4
1	1-F	196/206 (95%)	173 (88%)	17 (9%)	6 (3%)	3	1
1	2-A	196/206 (95%)	170 (87%)	20 (10%)	6 (3%)	3	1
1	2-B	196/206 (95%)	179 (91%)	10 (5%)	7 (4%)	2	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%)	3	1
1	2-E	196/206 (95%)	174 (89%)	21 (11%)	1 (0%)	24	22
1	2-F	196/206 (95%)	183 (93%)	11 (6%)	2 (1%)	12	9
1	3-A	196/206 (95%)	182 (93%)	10 (5%)	4 (2%)	6	2
1	3-B	196/206 (95%)	185 (94%)	10 (5%)	1 (0%)	24	22
1	3-C	196/206 (95%)	181 (92%)	13 (7%)	2 (1%)	12	9
1	3-D	196/206 (95%)	169 (86%)	23 (12%)	4 (2%)	6	2
1	3-E	196/206 (95%)	172 (88%)	20 (10%)	4 (2%)	6	2
1	3-F	196/206 (95%)	177 (90%)	15 (8%)	4 (2%)	6	2
1	4-A	196/206 (95%)	180 (92%)	10 (5%)	6 (3%)	3	1
1	4-B	196/206 (95%)	176 (90%)	18 (9%)	2 (1%)	12	9
1	4-C	196/206 (95%)	171 (87%)	22 (11%)	3 (2%)	8	4
1	4-D	196/206 (95%)	173 (88%)	19 (10%)	4 (2%)	6	2
1	4-E	196/206 (95%)	184 (94%)	9 (5%)	3 (2%)	8	4
1	4-F	196/206 (95%)	172 (88%)	21 (11%)	3 (2%)	8	4
1	5-A	196/206 (95%)	181 (92%)	11 (6%)	4 (2%)	6	2
1	5-B	196/206 (95%)	174 (89%)	17 (9%)	5 (3%)	4	1
1	5-C	196/206 (95%)	188 (96%)	6 (3%)	2 (1%)	12	9
1	5-D	196/206 (95%)	175 (89%)	17 (9%)	4 (2%)	6	2
1	5-E	196/206 (95%)	171 (87%)	22 (11%)	3 (2%)	8	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-F	196/206 (95%)	181 (92%)	14 (7%)	1 (0%)	24	22
1	6-A	196/206 (95%)	168 (86%)	22 (11%)	6 (3%)	3	1
1	6-B	196/206 (95%)	176 (90%)	16 (8%)	4 (2%)	6	2
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%)	8	4
1	6-E	196/206 (95%)	177 (90%)	15 (8%)	4 (2%)	6	2
1	6-F	196/206 (95%)	180 (92%)	13 (7%)	3 (2%)	8	4
1	7-A	196/206 (95%)	179 (91%)	13 (7%)	4 (2%)	6	2
1	7-B	196/206 (95%)	179 (91%)	15 (8%)	2 (1%)	12	9
1	7-C	196/206 (95%)	184 (94%)	9 (5%)	3 (2%)	8	4
1	7-D	196/206 (95%)	174 (89%)	17 (9%)	5 (3%)	4	1
1	7-E	196/206 (95%)	176 (90%)	17 (9%)	3 (2%)	8	4
1	7-F	196/206 (95%)	176 (90%)	19 (10%)	1 (0%)	24	22
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%)	24	22
1	8-C	196/206 (95%)	179 (91%)	15 (8%)	2 (1%)	12	9
1	8-D	196/206 (95%)	181 (92%)	10 (5%)	5 (3%)	4	1
1	8-E	196/206 (95%)	170 (87%)	20 (10%)	6 (3%)	3	1
1	8-F	196/206 (95%)	170 (87%)	20 (10%)	6 (3%)	3	1
All	All	9408/9888 (95%)	8478 (90%)	759 (8%)	171 (2%)	6	3

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%)	169 (98%)	4 (2%)	44	51
1	1-B	173/178 (97%)	163 (94%)	10 (6%)	18	16
1	1-C	173/178 (97%)	165 (95%)	8 (5%)	24	25
1	1-D	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	1-E	173/178 (97%)	161 (93%)	12 (7%)	14	12
1	1-F	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	2-A	173/178 (97%)	169 (98%)	4 (2%)	44	51
1	2-B	173/178 (97%)	163 (94%)	10 (6%)	18	16
1	2-C	173/178 (97%)	165 (95%)	8 (5%)	24	25
1	2-D	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	2-E	173/178 (97%)	161 (93%)	12 (7%)	14	12
1	2-F	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	3-A	173/178 (97%)	169 (98%)	4 (2%)	44	51
1	3-B	173/178 (97%)	163 (94%)	10 (6%)	18	16
1	3-C	173/178 (97%)	165 (95%)	8 (5%)	24	25
1	3-D	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	3-E	173/178 (97%)	161 (93%)	12 (7%)	14	12
1	3-F	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	4-A	173/178 (97%)	169 (98%)	4 (2%)	44	51
1	4-B	173/178 (97%)	163 (94%)	10 (6%)	18	16
1	4-C	173/178 (97%)	165 (95%)	8 (5%)	24	25
1	4-D	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	4-E	173/178 (97%)	161 (93%)	12 (7%)	14	12
1	4-F	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	5-A	173/178 (97%)	169 (98%)	4 (2%)	44	51
1	5-B	173/178 (97%)	163 (94%)	10 (6%)	18	16
1	5-C	173/178 (97%)	165 (95%)	8 (5%)	24	25
1	5-D	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	5-E	173/178 (97%)	161 (93%)	12 (7%)	14	12
1	5-F	173/178 (97%)	167 (96%)	6 (4%)	32	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-A	173/178 (97%)	169 (98%)	4 (2%)	44	51
1	6-B	173/178 (97%)	163 (94%)	10 (6%)	18	16
1	6-C	173/178 (97%)	165 (95%)	8 (5%)	24	25
1	6-D	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	6-E	173/178 (97%)	161 (93%)	12 (7%)	14	12
1	6-F	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	7-A	173/178 (97%)	169 (98%)	4 (2%)	44	51
1	7-B	173/178 (97%)	163 (94%)	10 (6%)	18	16
1	7-C	173/178 (97%)	165 (95%)	8 (5%)	24	25
1	7-D	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	7-E	173/178 (97%)	161 (93%)	12 (7%)	14	12
1	7-F	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	8-A	173/178 (97%)	169 (98%)	4 (2%)	44	51
1	8-B	173/178 (97%)	163 (94%)	10 (6%)	18	16
1	8-C	173/178 (97%)	165 (95%)	8 (5%)	24	25
1	8-D	173/178 (97%)	167 (96%)	6 (4%)	32	35
1	8-E	173/178 (97%)	161 (93%)	12 (7%)	14	12
1	8-F	173/178 (97%)	167 (96%)	6 (4%)	32	35
All	All	8304/8544 (97%)	7936 (96%)	368 (4%)	25	26

5 of 368 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6-A	107	LYS
1	7-B	125	GLU
1	6-B	95	ASP
1	6-E	27	SER
1	7-D	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 217 such sidechains are listed below:

Mol	Chain	Res	Type
1	5-A	133	ASN
1	6-B	202	GLN
1	8-B	46	ASN

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Mol	Chain	Res	Type
1	5-B	160	HIS
1	5-E	96	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	1-A	199/206 (96%)	2.19	99 (49%) 0 0	1, 2, 5, 9	199 (100%)
1	1-B	199/206 (96%)	2.27	106 (53%) 0 0	1, 2, 5, 8	199 (100%)
1	1-C	199/206 (96%)	2.74	129 (64%) 0 0	1, 3, 5, 8	199 (100%)
1	1-D	199/206 (96%)	2.81	135 (67%) 0 0	1, 3, 5, 7	199 (100%)
1	1-E	199/206 (96%)	2.28	98 (49%) 0 0	1, 3, 5, 8	199 (100%)
1	1-F	199/206 (96%)	2.31	102 (51%) 0 0	2, 3, 5, 7	199 (100%)
1	2-A	0/206	-	-	-	-
1	2-B	0/206	-	-	-	-
1	2-C	0/206	-	-	-	-
1	2-D	0/206	-	-	-	-
1	2-E	0/206	-	-	-	-
1	2-F	0/206	-	-	-	-
1	3-A	0/206	-	-	-	-
1	3-B	0/206	-	-	-	-
1	3-C	0/206	-	-	-	-
1	3-D	0/206	-	-	-	-
1	3-E	0/206	-	-	-	-
1	3-F	0/206	-	-	-	-
1	4-A	0/206	-	-	-	-
1	4-B	0/206	-	-	-	-
1	4-C	0/206	-	-	-	-
1	4-D	0/206	-	-	-	-
1	4-E	0/206	-	-	-	-
1	4-F	0/206	-	-	-	-
1	5-A	0/206	-	-	-	-
1	5-B	0/206	-	-	-	-
1	5-C	0/206	-	-	-	-
1	5-D	0/206	-	-	-	-
1	5-E	0/206	-	-	-	-
1	5-F	0/206	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	6-A	0/206	-	-	-	-
1	6-B	0/206	-	-	-	-
1	6-C	0/206	-	-	-	-
1	6-D	0/206	-	-	-	-
1	6-E	0/206	-	-	-	-
1	6-F	0/206	-	-	-	-
1	7-A	0/206	-	-	-	-
1	7-B	0/206	-	-	-	-
1	7-C	0/206	-	-	-	-
1	7-D	0/206	-	-	-	-
1	7-E	0/206	-	-	-	-
1	7-F	0/206	-	-	-	-
1	8-A	0/206	-	-	-	-
1	8-B	0/206	-	-	-	-
1	8-C	0/206	-	-	-	-
1	8-D	0/206	-	-	-	-
1	8-E	0/206	-	-	-	-
1	8-F	0/206	-	-	-	-
All	All	1194/9888 (12%)	2.43	669 (56%) 0 0	1, 3, 5, 9	1194 (100%)

The worst 5 of 669 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-F	59	PHE	8.9
1	1-C	114	VAL	8.3
1	1-E	27	SER	8.2
1	1-F	164	TRP	7.9
1	1-D	49	VAL	7.9

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.