



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

PDB ID : 2Q40  
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At2g17340  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 1.70 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

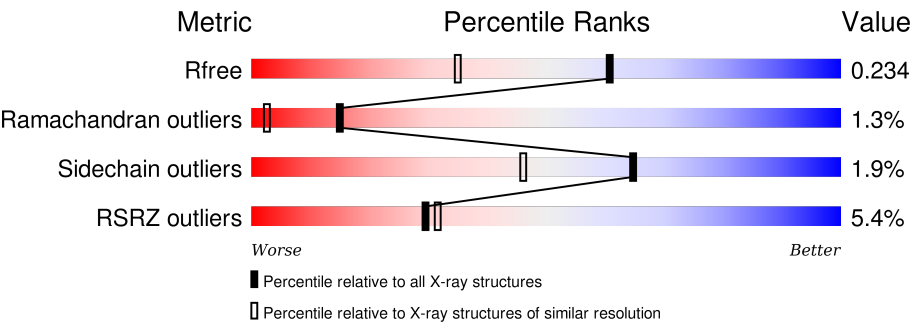
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3190 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	367	
1	10-A	367	
1	11-A	367	
1	12-A	367	
1	13-A	367	
1	14-A	367	
1	15-A	367	

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Mol	Chain	Length	Quality of chain
1	16-A	367	
1	2-A	367	
1	3-A	367	
1	4-A	367	
1	5-A	367	
1	6-A	367	
1	7-A	367	
1	8-A	367	
1	9-A	367	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	1-A	401	-	-	-	X
2	MG	10-A	401	-	-	-	X
2	MG	11-A	401	-	-	-	X
2	MG	12-A	401	-	-	-	X
2	MG	13-A	401	-	-	-	X
2	MG	14-A	401	-	-	-	X
2	MG	15-A	401	-	-	-	X
2	MG	2-A	401	-	-	-	X
2	MG	3-A	401	-	-	-	X
2	MG	4-A	401	-	-	-	X
2	MG	5-A	401	-	-	-	X
2	MG	7-A	401	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 48880 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 At2g17340.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	2-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	3-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	4-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	5-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	6-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	7-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	8-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	9-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	10-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	11-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	12-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	13-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	14-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	15-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			
1	16-A	343	Total	C	N	O	S	0	0	0
			2696	1723	456	506	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q949P3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	3-A	2	Total Mg 2 2	0	0
2	11-A	2	Total Mg 2 2	0	0
2	16-A	2	Total Mg 2 2	0	0
2	4-A	2	Total Mg 2 2	0	0
2	12-A	2	Total Mg 2 2	0	0
2	5-A	2	Total Mg 2 2	0	0
2	13-A	2	Total Mg 2 2	0	0
2	8-A	2	Total Mg 2 2	0	0
2	1-A	2	Total Mg 2 2	0	0
2	6-A	2	Total Mg 2 2	0	0
2	14-A	2	Total Mg 2 2	0	0
2	2-A	2	Total Mg 2 2	0	0
2	10-A	2	Total Mg 2 2	0	0
2	9-A	2	Total Mg 2 2	0	0
2	7-A	2	Total Mg 2 2	0	0
2	15-A	2	Total Mg 2 2	0	0

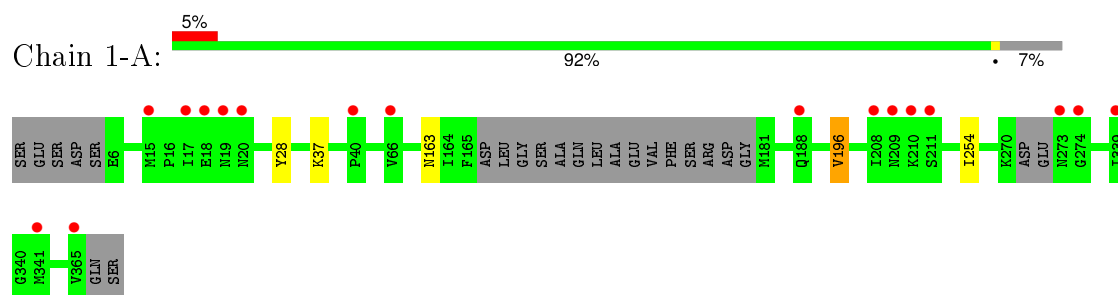
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	357	Total 357	O 357	0	0
3	2-A	357	Total 357	O 357	0	0
3	3-A	357	Total 357	O 357	0	0
3	4-A	357	Total 357	O 357	0	0
3	5-A	357	Total 357	O 357	0	0
3	6-A	357	Total 357	O 357	0	0
3	7-A	357	Total 357	O 357	0	0
3	8-A	357	Total 357	O 357	0	0
3	9-A	357	Total 357	O 357	0	0
3	10-A	357	Total 357	O 357	0	0
3	11-A	357	Total 357	O 357	0	0
3	12-A	357	Total 357	O 357	0	0
3	13-A	357	Total 357	O 357	0	0
3	14-A	357	Total 357	O 357	0	0
3	15-A	357	Total 357	O 357	0	0
3	16-A	357	Total 357	O 357	0	0

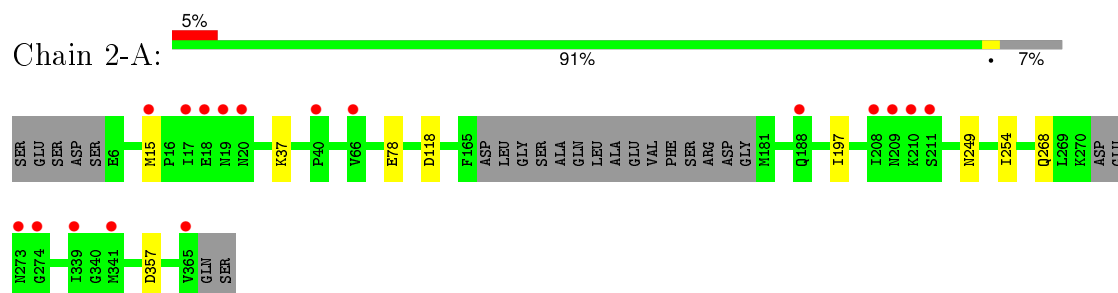
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

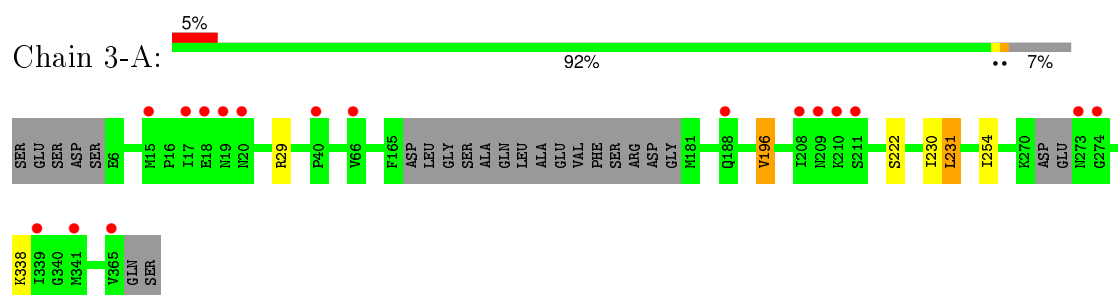
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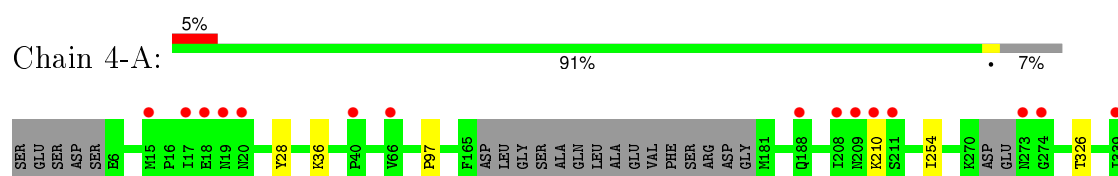
#### • Molecule 1: Protein At2g17340

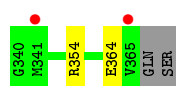


#### • Molecule 1: Protein At2g17340

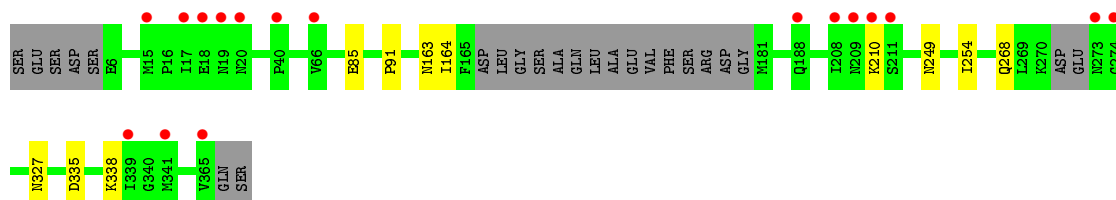
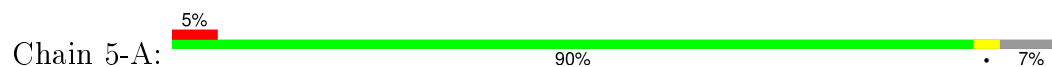


#### • Molecule 1: Protein At2g17340

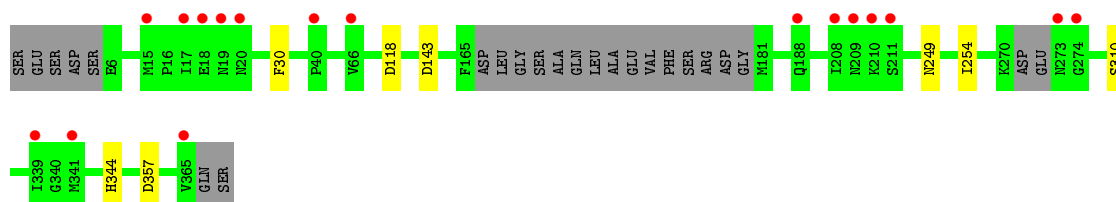




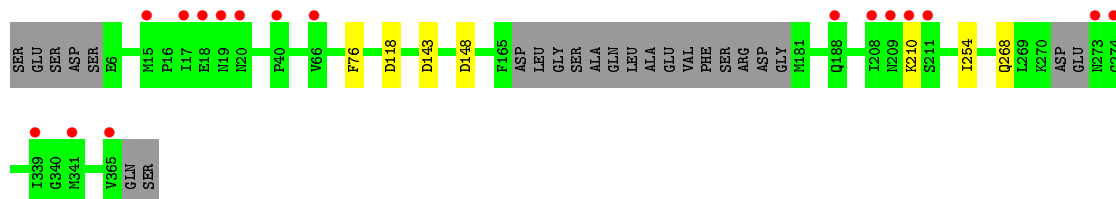
- Molecule 1: Protein At2g17340



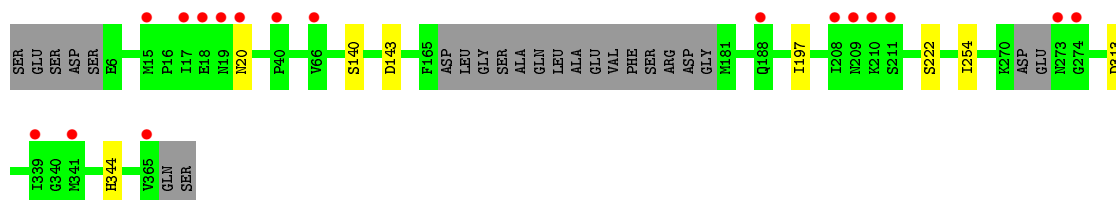
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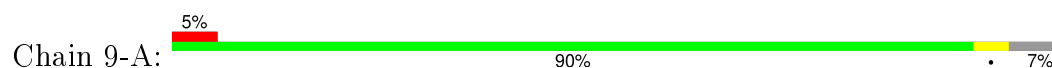
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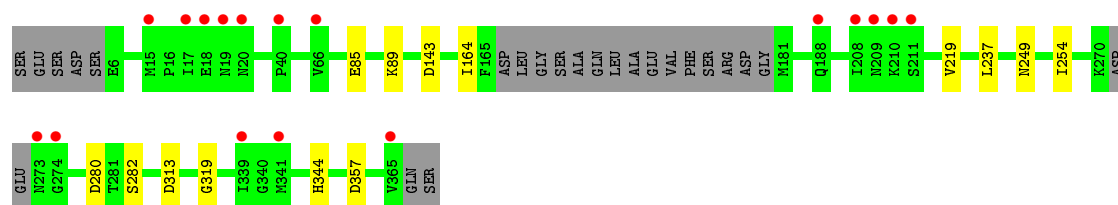
- Molecule 1: Protein At2g17340



- Molecule 1: Protein At2g17340

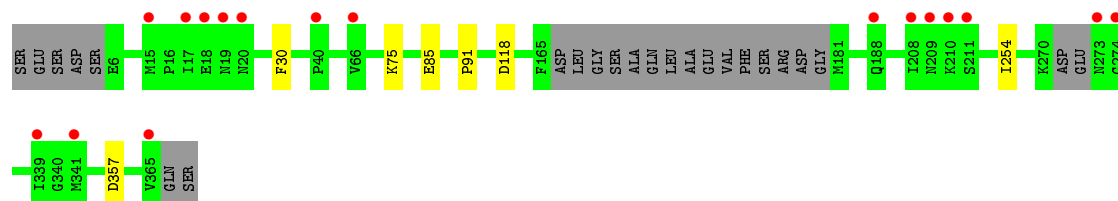






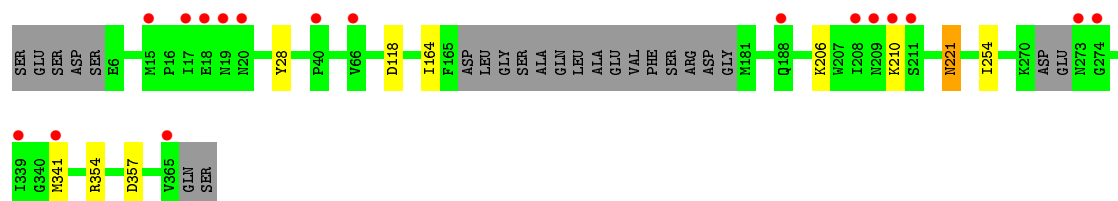
- Molecule 1: Protein At2g17340

Chain 10-A: 92% 5% 7%



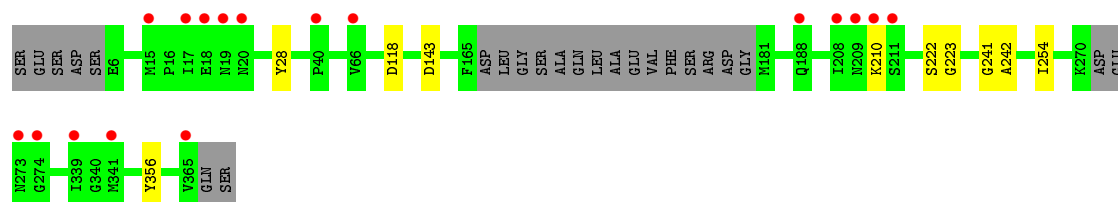
- Molecule 1: Protein At2g17340

Chain 11-A: 91% 5% 7%



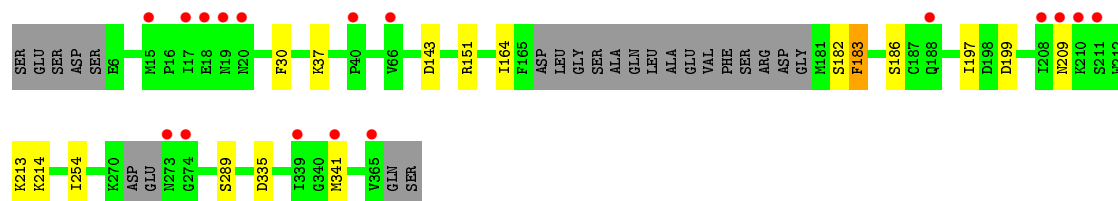
- Molecule 1: Protein At2g17340

Chain 12-A: 91% 5% 7%

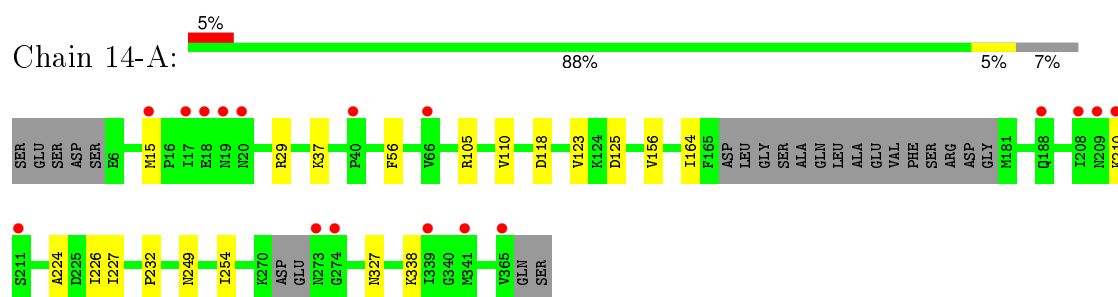


- Molecule 1: Protein At2g17340

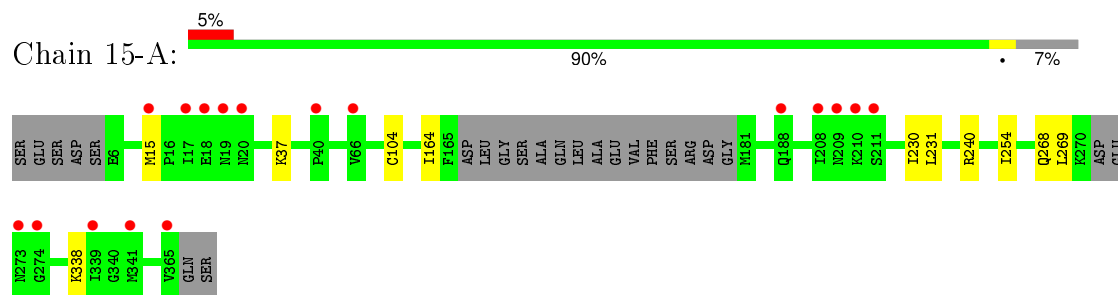
Chain 13-A: 89% 5% 7%



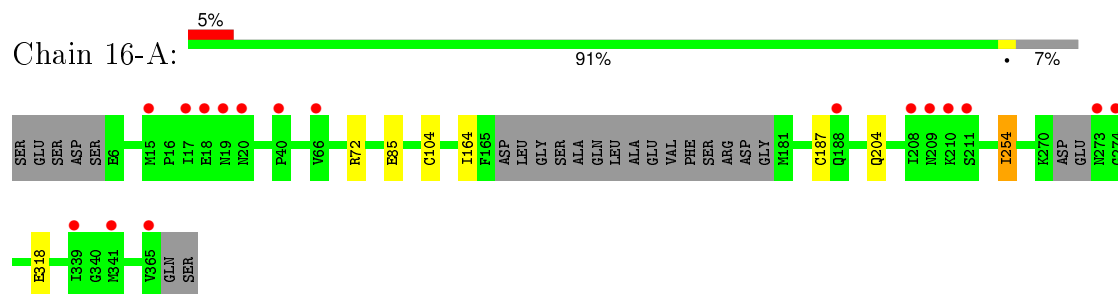
- Molecule 1: Protein At2g17340



• Molecule 1: Protein At2g17340



• Molecule 1: Protein At2g17340



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.17Å 43.28Å 52.64Å 74.57° 74.60° 84.04°	Depositor
Resolution (Å)	34.91 – 1.70 34.91 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (34.91-1.70) 89.3 (34.91-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.39 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.165 , 0.221 0.175 , 0.234	Depositor DCC
$R_{free}$ test set	1764 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35346 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	48880	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0/2747	0.60	0/3717
1	2-A	0.40	0/2747	0.60	0/3717
1	3-A	0.41	0/2747	0.61	0/3717
1	4-A	0.40	0/2747	0.60	0/3717
1	5-A	0.40	0/2747	0.61	0/3717
1	6-A	0.40	0/2747	0.61	0/3717
1	7-A	0.39	0/2747	0.60	0/3717
1	8-A	0.40	0/2747	0.59	0/3717
1	9-A	0.40	0/2747	0.61	0/3717
1	10-A	0.40	0/2747	0.61	0/3717
1	11-A	0.40	0/2747	0.60	0/3717
1	12-A	0.41	0/2747	0.62	0/3717
1	13-A	0.46	0/2747	0.70	1/3717 (0.0%)
1	14-A	0.45	0/2747	0.69	0/3717
1	15-A	0.44	0/2747	0.69	0/3717
1	16-A	0.47	1/2747 (0.0%)	0.69	1/3717 (0.0%)
All	All	0.42	1/43952 (0.0%)	0.63	2/59472 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	187	CYS	CB-SG	-5.10	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	104	CYS	CA-CB-SG	6.33	125.40	114.00
1	13-A	197	ILE	N-CA-C	-5.13	97.14	111.00

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	1-A	2696	0	2720	0	0
1	2-A	2696	0	2720	0	0
1	3-A	2696	0	2720	0	0
1	4-A	2696	0	2720	0	0
1	5-A	2696	0	2720	0	0
1	6-A	2696	0	2720	0	0
1	7-A	2696	0	2720	0	0
1	8-A	2696	0	2720	0	0
1	9-A	2696	0	2720	0	0
1	10-A	2696	0	2720	0	0
1	11-A	2696	0	2720	0	0
1	12-A	2696	0	2720	0	0
1	13-A	2696	0	2720	0	0
1	14-A	2696	0	2720	0	0
1	15-A	2696	0	2720	0	0
1	16-A	2696	0	2720	0	0
2	1-A	2	0	0	0	0
2	2-A	2	0	0	0	0
2	3-A	2	0	0	0	0
2	4-A	2	0	0	0	0
2	5-A	2	0	0	0	0
2	6-A	2	0	0	0	0
2	7-A	2	0	0	0	0
2	8-A	2	0	0	0	0
2	9-A	2	0	0	0	0
2	10-A	2	0	0	0	0
2	11-A	2	0	0	0	0
2	12-A	2	0	0	0	0
2	13-A	2	0	0	0	0
2	14-A	2	0	0	0	0
2	15-A	2	0	0	0	0
2	16-A	2	0	0	0	0
3	1-A	357	0	0	0	0
3	2-A	357	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3-A	357	0	0	0	0
3	4-A	357	0	0	0	0
3	5-A	357	0	0	0	0
3	6-A	357	0	0	0	0
3	7-A	357	0	0	0	0
3	8-A	357	0	0	0	0
3	9-A	357	0	0	0	0
3	10-A	357	0	0	0	0
3	11-A	357	0	0	0	0
3	12-A	357	0	0	0	0
3	13-A	357	0	0	0	0
3	14-A	357	0	0	0	0
3	15-A	357	0	0	0	0
3	16-A	357	0	0	0	0
All	All	48880	0	43520	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

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	337/367 (92%)	317 (94%)	17 (5%)	3 (1%)	21	5
1	2-A	337/367 (92%)	310 (92%)	23 (7%)	4 (1%)	16	3
1	3-A	337/367 (92%)	314 (93%)	18 (5%)	5 (2%)	13	2
1	4-A	337/367 (92%)	310 (92%)	23 (7%)	4 (1%)	16	3
1	5-A	337/367 (92%)	315 (94%)	18 (5%)	4 (1%)	16	3
1	6-A	337/367 (92%)	317 (94%)	17 (5%)	3 (1%)	21	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7-A	337/367 (92%)	316 (94%)	18 (5%)	3 (1%)	21	5
1	8-A	337/367 (92%)	310 (92%)	23 (7%)	4 (1%)	16	3
1	9-A	337/367 (92%)	308 (91%)	24 (7%)	5 (2%)	13	2
1	10-A	337/367 (92%)	315 (94%)	19 (6%)	3 (1%)	21	5
1	11-A	337/367 (92%)	311 (92%)	21 (6%)	5 (2%)	13	2
1	12-A	337/367 (92%)	308 (91%)	21 (6%)	8 (2%)	7	1
1	13-A	337/367 (92%)	302 (90%)	29 (9%)	6 (2%)	11	1
1	14-A	337/367 (92%)	300 (89%)	27 (8%)	10 (3%)	5	1
1	15-A	337/367 (92%)	307 (91%)	26 (8%)	4 (1%)	16	3
1	16-A	337/367 (92%)	309 (92%)	27 (8%)	1 (0%)	46	26
All	All	5392/5872 (92%)	4969 (92%)	351 (6%)	72 (1%)	15	2

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	4-A	210	LYS
1	4-A	364	GLU
1	6-A	118	ASP
1	8-A	20	ASN
1	9-A	89	LYS
1	9-A	319	GLY
1	11-A	210	LYS
1	11-A	221	ASN
1	12-A	222	SER
1	12-A	241	GLY
1	13-A	209	ASN
1	14-A	118	ASP
1	15-A	230	ILE
1	1-A	254	ILE
1	2-A	249	ASN
1	3-A	254	ILE
1	5-A	327	ASN
1	6-A	249	ASN
1	8-A	222	SER
1	9-A	164	ILE
1	12-A	223	GLY
1	12-A	242	ALA
1	13-A	151	ARG

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Mol	Chain	Res	Type
1	13-A	183	PHE
1	13-A	335	ASP
1	14-A	226	ILE
1	16-A	254	ILE
1	1-A	163	ASN
1	2-A	254	ILE
1	3-A	222	SER
1	3-A	230	ILE
1	5-A	249	ASN
1	5-A	254	ILE
1	10-A	118	ASP
1	11-A	118	ASP
1	12-A	118	ASP
1	12-A	210	LYS
1	12-A	254	ILE
1	13-A	254	ILE
1	14-A	210	LYS
1	14-A	254	ILE
1	15-A	231	LEU
1	15-A	254	ILE
1	2-A	118	ASP
1	3-A	231	LEU
1	4-A	97	PRO
1	4-A	254	ILE
1	6-A	254	ILE
1	7-A	118	ASP
1	8-A	254	ILE
1	10-A	254	ILE
1	11-A	254	ILE
1	14-A	156	VAL
1	14-A	224	ALA
1	15-A	269	LEU
1	7-A	210	LYS
1	7-A	254	ILE
1	8-A	197	ILE
1	9-A	254	ILE
1	9-A	282	SER
1	14-A	327	ASN
1	10-A	91	PRO
1	11-A	164	ILE
1	12-A	356	TYR
1	13-A	182	SER

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Mol	Chain	Res	Type
1	14-A	227	ILE
1	1-A	196	VAL
1	3-A	196	VAL
1	14-A	232	PRO
1	2-A	197	ILE
1	14-A	110	VAL
1	5-A	91	PRO

### 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	297/317 (94%)	294 (99%)	3 (1%)	82	72
1	2-A	297/317 (94%)	292 (98%)	5 (2%)	68	51
1	3-A	297/317 (94%)	293 (99%)	4 (1%)	76	62
1	4-A	297/317 (94%)	293 (99%)	4 (1%)	76	62
1	5-A	297/317 (94%)	290 (98%)	7 (2%)	57	36
1	6-A	297/317 (94%)	292 (98%)	5 (2%)	68	51
1	7-A	297/317 (94%)	293 (99%)	4 (1%)	76	62
1	8-A	297/317 (94%)	293 (99%)	4 (1%)	76	62
1	9-A	297/317 (94%)	288 (97%)	9 (3%)	48	26
1	10-A	297/317 (94%)	293 (99%)	4 (1%)	76	62
1	11-A	297/317 (94%)	291 (98%)	6 (2%)	63	44
1	12-A	297/317 (94%)	295 (99%)	2 (1%)	88	82
1	13-A	297/317 (94%)	286 (96%)	11 (4%)	41	18
1	14-A	297/317 (94%)	287 (97%)	10 (3%)	44	21
1	15-A	297/317 (94%)	290 (98%)	7 (2%)	57	36
1	16-A	297/317 (94%)	291 (98%)	6 (2%)	63	44
All	All	4752/5072 (94%)	4661 (98%)	91 (2%)	65	46

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	28	TYR
1	1-A	37	LYS
1	1-A	196	VAL
1	2-A	15	MET
1	2-A	37	LYS
1	2-A	78	GLU
1	2-A	268	GLN
1	2-A	357	ASP
1	3-A	29	ARG
1	3-A	196	VAL
1	3-A	231	LEU
1	3-A	338	LYS
1	4-A	28	TYR
1	4-A	36	LYS
1	4-A	326	THR
1	4-A	354	ARG
1	5-A	85	GLU
1	5-A	163	ASN
1	5-A	164	ILE
1	5-A	210	LYS
1	5-A	268	GLN
1	5-A	335	ASP
1	5-A	338	LYS
1	6-A	30	PHE
1	6-A	143	ASP
1	6-A	310	SER
1	6-A	344	HIS
1	6-A	357	ASP
1	7-A	76	PHE
1	7-A	143	ASP
1	7-A	148	ASP
1	7-A	268	GLN
1	8-A	140	SER
1	8-A	143	ASP
1	8-A	313	ASP
1	8-A	344	HIS
1	9-A	85	GLU
1	9-A	143	ASP
1	9-A	219	VAL
1	9-A	237	LEU
1	9-A	249	ASN
1	9-A	280	ASP
1	9-A	313	ASP

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Mol	Chain	Res	Type
1	9-A	344	HIS
1	9-A	357	ASP
1	10-A	30	PHE
1	10-A	75	LYS
1	10-A	85	GLU
1	10-A	357	ASP
1	11-A	28	TYR
1	11-A	206	LYS
1	11-A	221	ASN
1	11-A	341	MET
1	11-A	354	ARG
1	11-A	357	ASP
1	12-A	28	TYR
1	12-A	143	ASP
1	13-A	30	PHE
1	13-A	37	LYS
1	13-A	143	ASP
1	13-A	164	ILE
1	13-A	183	PHE
1	13-A	186	SER
1	13-A	199	ASP
1	13-A	213	LYS
1	13-A	214	LYS
1	13-A	289	SER
1	13-A	341	MET
1	14-A	15	MET
1	14-A	29	ARG
1	14-A	37	LYS
1	14-A	56	PHE
1	14-A	105	ARG
1	14-A	123	VAL
1	14-A	125	ASP
1	14-A	164	ILE
1	14-A	249	ASN
1	14-A	338	LYS
1	15-A	15	MET
1	15-A	37	LYS
1	15-A	104	CYS
1	15-A	164	ILE
1	15-A	240	ARG
1	15-A	268	GLN
1	15-A	338	LYS

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Mol	Chain	Res	Type
1	16-A	72	ARG
1	16-A	85	GLU
1	16-A	164	ILE
1	16-A	204	GLN
1	16-A	254	ILE
1	16-A	318	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	19	ASN
1	1-A	188	GLN
1	1-A	268	GLN
1	1-A	363	ASN
1	2-A	51	ASN
1	2-A	268	GLN
1	2-A	344	HIS
1	2-A	363	ASN
1	3-A	41	ASN
1	3-A	268	GLN
1	4-A	19	ASN
1	4-A	204	GLN
1	4-A	221	ASN
1	4-A	268	GLN
1	4-A	344	HIS
1	4-A	363	ASN
1	5-A	19	ASN
1	5-A	188	GLN
1	5-A	204	GLN
1	5-A	268	GLN
1	5-A	363	ASN
1	6-A	188	GLN
1	6-A	268	GLN
1	6-A	363	ASN
1	7-A	12	GLN
1	7-A	19	ASN
1	7-A	189	ASN
1	7-A	204	GLN
1	7-A	268	GLN
1	7-A	344	HIS
1	7-A	363	ASN
1	8-A	20	ASN

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Mol	Chain	Res	Type
1	8-A	268	GLN
1	8-A	275	GLN
1	8-A	363	ASN
1	9-A	19	ASN
1	9-A	188	GLN
1	9-A	268	GLN
1	9-A	363	ASN
1	10-A	19	ASN
1	10-A	41	ASN
1	10-A	154	ASN
1	10-A	268	GLN
1	10-A	363	ASN
1	11-A	19	ASN
1	11-A	51	ASN
1	11-A	188	GLN
1	11-A	221	ASN
1	11-A	255	ASN
1	11-A	268	GLN
1	11-A	363	ASN
1	12-A	12	GLN
1	12-A	41	ASN
1	12-A	188	GLN
1	12-A	268	GLN
1	12-A	344	HIS
1	12-A	363	ASN
1	13-A	19	ASN
1	13-A	20	ASN
1	13-A	163	ASN
1	13-A	204	GLN
1	13-A	344	HIS
1	14-A	12	GLN
1	14-A	19	ASN
1	14-A	41	ASN
1	14-A	209	ASN
1	14-A	268	GLN
1	14-A	344	HIS
1	14-A	363	ASN
1	15-A	19	ASN
1	15-A	188	GLN
1	15-A	189	ASN
1	15-A	204	GLN
1	15-A	344	HIS

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Mol	Chain	Res	Type
1	15-A	363	ASN
1	16-A	19	ASN
1	16-A	20	ASN
1	16-A	154	ASN
1	16-A	189	ASN
1	16-A	268	GLN
1	16-A	363	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 ⓘ

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	2-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	3-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	4-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	5-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	6-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	7-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	8-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	9-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	10-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	11-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	12-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	13-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	14-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	15-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
1	16-A	343/367 (93%)	0.29	17 (4%) 32 35	6, 17, 32, 45	343 (100%)
All	All	5488/5872 (93%)	0.29	272 (4%) 29 35	6, 17, 32, 45	5488 (100%)

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	20	ASN	5.8
1	2-A	20	ASN	5.8
1	3-A	20	ASN	5.8
1	4-A	20	ASN	5.8
1	5-A	20	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	6-A	20	ASN	5.8
1	7-A	20	ASN	5.8
1	8-A	20	ASN	5.8
1	9-A	20	ASN	5.8
1	10-A	20	ASN	5.8
1	11-A	20	ASN	5.8
1	12-A	20	ASN	5.8
1	13-A	20	ASN	5.8
1	14-A	20	ASN	5.8
1	15-A	20	ASN	5.8
1	16-A	20	ASN	5.8
1	1-A	365	VAL	4.4
1	2-A	365	VAL	4.4
1	3-A	365	VAL	4.4
1	4-A	365	VAL	4.4
1	5-A	365	VAL	4.4
1	6-A	365	VAL	4.4
1	7-A	365	VAL	4.4
1	8-A	365	VAL	4.4
1	9-A	365	VAL	4.4
1	10-A	365	VAL	4.4
1	11-A	365	VAL	4.4
1	12-A	365	VAL	4.4
1	13-A	365	VAL	4.4
1	14-A	365	VAL	4.4
1	15-A	365	VAL	4.4
1	16-A	365	VAL	4.4
1	1-A	15	MET	4.0
1	2-A	15	MET	4.0
1	3-A	15	MET	4.0
1	4-A	15	MET	4.0
1	5-A	15	MET	4.0
1	6-A	15	MET	4.0
1	7-A	15	MET	4.0
1	8-A	15	MET	4.0
1	9-A	15	MET	4.0
1	10-A	15	MET	4.0
1	11-A	15	MET	4.0
1	12-A	15	MET	4.0
1	13-A	15	MET	4.0
1	14-A	15	MET	4.0
1	15-A	15	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	16-A	15	MET	4.0
1	1-A	209	ASN	4.0
1	2-A	209	ASN	4.0
1	3-A	209	ASN	4.0
1	4-A	209	ASN	4.0
1	5-A	209	ASN	4.0
1	6-A	209	ASN	4.0
1	7-A	209	ASN	4.0
1	8-A	209	ASN	4.0
1	9-A	209	ASN	4.0
1	10-A	209	ASN	4.0
1	11-A	209	ASN	4.0
1	12-A	209	ASN	4.0
1	13-A	209	ASN	4.0
1	14-A	209	ASN	4.0
1	15-A	209	ASN	4.0
1	16-A	209	ASN	4.0
1	1-A	17	ILE	3.5
1	2-A	17	ILE	3.5
1	3-A	17	ILE	3.5
1	4-A	17	ILE	3.5
1	5-A	17	ILE	3.5
1	6-A	17	ILE	3.5
1	7-A	17	ILE	3.5
1	8-A	17	ILE	3.5
1	9-A	17	ILE	3.5
1	10-A	17	ILE	3.5
1	11-A	17	ILE	3.5
1	12-A	17	ILE	3.5
1	13-A	17	ILE	3.5
1	14-A	17	ILE	3.5
1	15-A	17	ILE	3.5
1	16-A	17	ILE	3.5
1	1-A	274	GLY	3.2
1	2-A	274	GLY	3.2
1	3-A	274	GLY	3.2
1	4-A	274	GLY	3.2
1	5-A	274	GLY	3.2
1	6-A	274	GLY	3.2
1	7-A	274	GLY	3.2
1	8-A	274	GLY	3.2
1	9-A	274	GLY	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	10-A	274	GLY	3.2
1	11-A	274	GLY	3.2
1	12-A	274	GLY	3.2
1	13-A	274	GLY	3.2
1	14-A	274	GLY	3.2
1	15-A	274	GLY	3.2
1	16-A	274	GLY	3.2
1	1-A	40	PRO	3.1
1	2-A	40	PRO	3.1
1	3-A	40	PRO	3.1
1	4-A	40	PRO	3.1
1	5-A	40	PRO	3.1
1	6-A	40	PRO	3.1
1	7-A	40	PRO	3.1
1	8-A	40	PRO	3.1
1	9-A	40	PRO	3.1
1	10-A	40	PRO	3.1
1	11-A	40	PRO	3.1
1	12-A	40	PRO	3.1
1	13-A	40	PRO	3.1
1	14-A	40	PRO	3.1
1	15-A	40	PRO	3.1
1	16-A	40	PRO	3.1
1	1-A	208	ILE	3.1
1	2-A	208	ILE	3.1
1	3-A	208	ILE	3.1
1	4-A	208	ILE	3.1
1	5-A	208	ILE	3.1
1	6-A	208	ILE	3.1
1	7-A	208	ILE	3.1
1	8-A	208	ILE	3.1
1	9-A	208	ILE	3.1
1	10-A	208	ILE	3.1
1	11-A	208	ILE	3.1
1	12-A	208	ILE	3.1
1	13-A	208	ILE	3.1
1	14-A	208	ILE	3.1
1	15-A	208	ILE	3.1
1	16-A	208	ILE	3.1
1	1-A	210	LYS	3.0
1	2-A	210	LYS	3.0
1	3-A	210	LYS	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	4-A	210	LYS	3.0
1	5-A	210	LYS	3.0
1	6-A	210	LYS	3.0
1	7-A	210	LYS	3.0
1	8-A	210	LYS	3.0
1	9-A	210	LYS	3.0
1	10-A	210	LYS	3.0
1	11-A	210	LYS	3.0
1	12-A	210	LYS	3.0
1	13-A	210	LYS	3.0
1	14-A	210	LYS	3.0
1	15-A	210	LYS	3.0
1	16-A	210	LYS	3.0
1	1-A	19	ASN	2.9
1	2-A	19	ASN	2.9
1	3-A	19	ASN	2.9
1	4-A	19	ASN	2.9
1	5-A	19	ASN	2.9
1	6-A	19	ASN	2.9
1	7-A	19	ASN	2.9
1	8-A	19	ASN	2.9
1	9-A	19	ASN	2.9
1	10-A	19	ASN	2.9
1	11-A	19	ASN	2.9
1	12-A	19	ASN	2.9
1	13-A	19	ASN	2.9
1	14-A	19	ASN	2.9
1	15-A	19	ASN	2.9
1	16-A	19	ASN	2.9
1	1-A	273	ASN	2.5
1	2-A	273	ASN	2.5
1	3-A	273	ASN	2.5
1	4-A	273	ASN	2.5
1	5-A	273	ASN	2.5
1	6-A	273	ASN	2.5
1	7-A	273	ASN	2.5
1	8-A	273	ASN	2.5
1	9-A	273	ASN	2.5
1	10-A	273	ASN	2.5
1	11-A	273	ASN	2.5
1	12-A	273	ASN	2.5
1	13-A	273	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	14-A	273	ASN	2.5
1	15-A	273	ASN	2.5
1	16-A	273	ASN	2.5
1	1-A	66	VAL	2.4
1	2-A	66	VAL	2.4
1	3-A	66	VAL	2.4
1	4-A	66	VAL	2.4
1	5-A	66	VAL	2.4
1	6-A	66	VAL	2.4
1	7-A	66	VAL	2.4
1	8-A	66	VAL	2.4
1	9-A	66	VAL	2.4
1	10-A	66	VAL	2.4
1	11-A	66	VAL	2.4
1	12-A	66	VAL	2.4
1	13-A	66	VAL	2.4
1	14-A	66	VAL	2.4
1	15-A	66	VAL	2.4
1	16-A	66	VAL	2.4
1	1-A	339	ILE	2.2
1	2-A	339	ILE	2.2
1	3-A	339	ILE	2.2
1	4-A	339	ILE	2.2
1	5-A	339	ILE	2.2
1	6-A	339	ILE	2.2
1	7-A	339	ILE	2.2
1	8-A	339	ILE	2.2
1	9-A	339	ILE	2.2
1	10-A	339	ILE	2.2
1	11-A	339	ILE	2.2
1	12-A	339	ILE	2.2
1	13-A	339	ILE	2.2
1	14-A	339	ILE	2.2
1	15-A	339	ILE	2.2
1	16-A	339	ILE	2.2
1	1-A	188	GLN	2.2
1	2-A	188	GLN	2.2
1	3-A	188	GLN	2.2
1	4-A	188	GLN	2.2
1	5-A	188	GLN	2.2
1	6-A	188	GLN	2.2
1	7-A	188	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	8-A	188	GLN	2.2
1	9-A	188	GLN	2.2
1	10-A	188	GLN	2.2
1	11-A	188	GLN	2.2
1	12-A	188	GLN	2.2
1	13-A	188	GLN	2.2
1	14-A	188	GLN	2.2
1	15-A	188	GLN	2.2
1	16-A	188	GLN	2.2
1	1-A	341	MET	2.1
1	2-A	341	MET	2.1
1	3-A	341	MET	2.1
1	4-A	341	MET	2.1
1	5-A	341	MET	2.1
1	6-A	341	MET	2.1
1	7-A	341	MET	2.1
1	8-A	341	MET	2.1
1	9-A	341	MET	2.1
1	10-A	341	MET	2.1
1	11-A	341	MET	2.1
1	12-A	341	MET	2.1
1	13-A	341	MET	2.1
1	14-A	341	MET	2.1
1	15-A	341	MET	2.1
1	16-A	341	MET	2.1
1	1-A	18	GLU	2.1
1	2-A	18	GLU	2.1
1	3-A	18	GLU	2.1
1	4-A	18	GLU	2.1
1	5-A	18	GLU	2.1
1	6-A	18	GLU	2.1
1	7-A	18	GLU	2.1
1	8-A	18	GLU	2.1
1	9-A	18	GLU	2.1
1	10-A	18	GLU	2.1
1	11-A	18	GLU	2.1
1	12-A	18	GLU	2.1
1	13-A	18	GLU	2.1
1	14-A	18	GLU	2.1
1	15-A	18	GLU	2.1
1	16-A	18	GLU	2.1
1	1-A	211	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	2-A	211	SER	2.0
1	3-A	211	SER	2.0
1	4-A	211	SER	2.0
1	5-A	211	SER	2.0
1	6-A	211	SER	2.0
1	7-A	211	SER	2.0
1	8-A	211	SER	2.0
1	9-A	211	SER	2.0
1	10-A	211	SER	2.0
1	11-A	211	SER	2.0
1	12-A	211	SER	2.0
1	13-A	211	SER	2.0
1	14-A	211	SER	2.0
1	15-A	211	SER	2.0
1	16-A	211	SER	2.0

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	7-A	401	1/1	0.93	0.14	2.78	43,43,43,43	1
2	MG	10-A	401	1/1	0.93	0.14	2.78	43,43,43,43	1
2	MG	3-A	401	1/1	0.93	0.14	2.78	43,43,43,43	1
2	MG	11-A	401	1/1	0.93	0.14	2.78	43,43,43,43	1
2	MG	14-A	401	1/1	0.93	0.14	2.78	42,42,42,42	1
2	MG	2-A	401	1/1	0.93	0.14	2.78	43,43,43,43	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	5-A	401	1/1	0.93	0.14	2.78	43,43,43,43	1
2	MG	1-A	401	1/1	0.93	0.14	2.78	43,43,43,43	1
2	MG	13-A	401	1/1	0.93	0.14	2.73	42,42,42,42	1
2	MG	4-A	401	1/1	0.93	0.14	2.65	43,43,43,43	1
2	MG	12-A	401	1/1	0.93	0.14	2.65	43,43,43,43	1
2	MG	15-A	401	1/1	0.93	0.14	2.65	42,42,42,42	1
2	MG	16-A	401	1/1	0.93	0.14	1.93	42,42,42,42	1
2	MG	9-A	401	1/1	0.93	0.14	1.88	43,43,43,43	1
2	MG	6-A	401	1/1	0.93	0.14	1.88	43,43,43,43	1
2	MG	8-A	401	1/1	0.93	0.14	1.71	43,43,43,43	1
2	MG	16-A	400	1/1	0.99	0.04	-1.80	7,7,7,7	1
2	MG	3-A	400	1/1	0.99	0.04	-1.80	10,10,10,10	1
2	MG	15-A	400	1/1	0.99	0.04	-1.80	7,7,7,7	1
2	MG	12-A	400	1/1	0.99	0.04	-1.94	10,10,10,10	1
2	MG	1-A	400	1/1	0.99	0.04	-1.94	10,10,10,10	1
2	MG	13-A	400	1/1	0.99	0.04	-	10,10,10,10	1
2	MG	11-A	400	1/1	0.99	0.04	-	11,11,11,11	1
2	MG	6-A	400	1/1	0.99	0.04	-	16,16,16,16	1
2	MG	9-A	400	1/1	0.99	0.04	-	12,12,12,12	1
2	MG	8-A	400	1/1	0.99	0.04	-	11,11,11,11	1
2	MG	14-A	400	1/1	0.99	0.04	-	6,6,6,6	1
2	MG	7-A	400	1/1	0.99	0.04	-	18,18,18,18	1
2	MG	5-A	400	1/1	0.99	0.04	-	16,16,16,16	1
2	MG	2-A	400	1/1	0.99	0.04	-	16,16,16,16	1
2	MG	4-A	400	1/1	0.99	0.04	-	19,19,19,19	1
2	MG	10-A	400	1/1	0.99	0.04	-	18,18,18,18	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.