



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 08:30 PM UTC

PDB ID : 2Q40 / pdb_00002q40
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

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
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

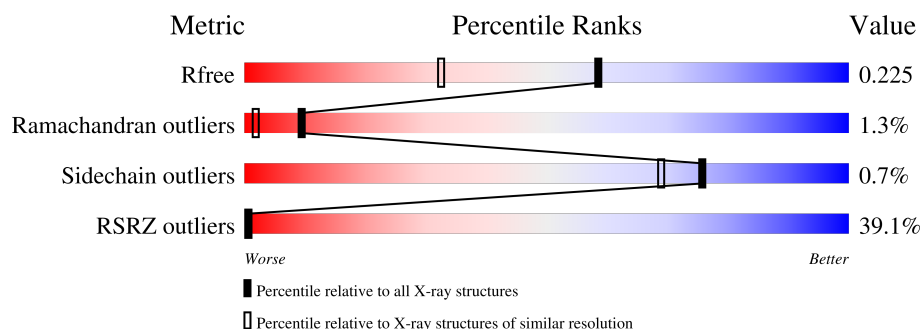
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5551 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	367	37% 92% 7%
1	10-A	367	92% 7%
1	11-A	367	92% 7%
1	12-A	367	91% 7%
1	13-A	367	91% 7%
1	14-A	367	90% 7%
1	15-A	367	92% 7%

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Mol	Chain	Length	Quality of chain
1	16-A	367	 93% • 7%
1	2-A	367	 92% • 7%
1	3-A	367	 92% • 7%
1	4-A	367	 92% • 7%
1	5-A	367	 92% • 7%
1	6-A	367	 92% • 7%
1	7-A	367	 92% • 7%
1	8-A	367	 92% • 7%
1	9-A	367	 92% • 7%

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 (CCD ID: MG) (formula: Mg).

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

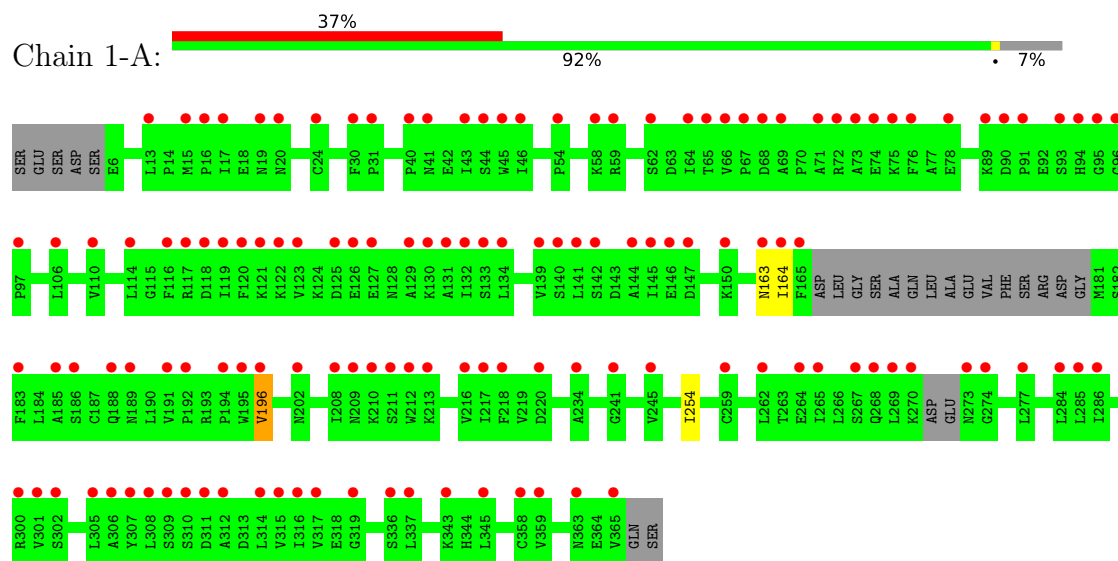
- Molecule 3 is water.

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

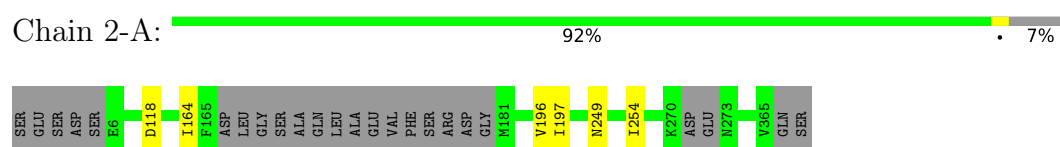
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

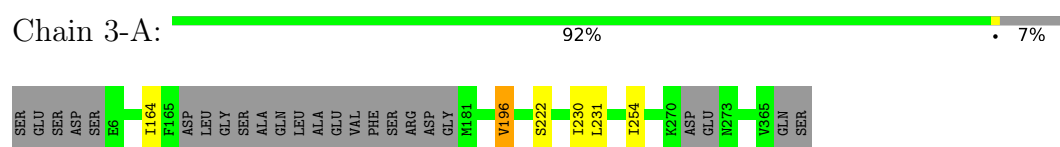
• Molecule 1: Protein At2g17340



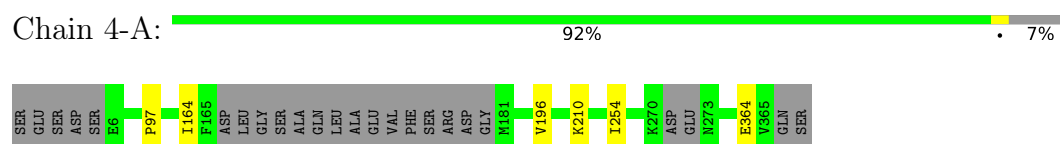
• Molecule 1: Protein At2g17340



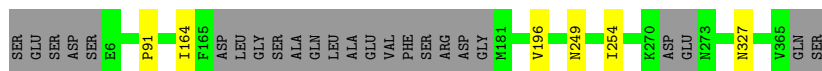
• Molecule 1: Protein At2g17340



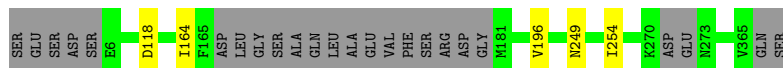
• Molecule 1: Protein At2g17340



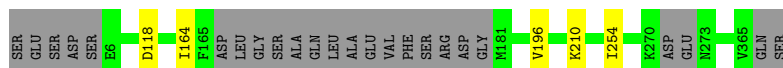
• Molecule 1: Protein At2g17340

Chain 5-A:  92% • 7%

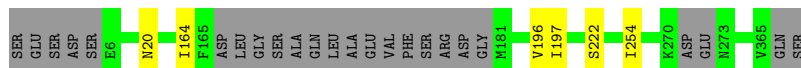
• Molecule 1: Protein At2g17340

Chain 6-A:  92% • 7%

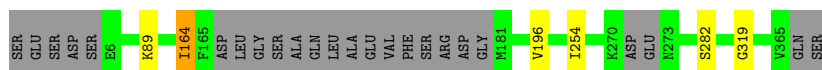
• Molecule 1: Protein At2g17340

Chain 7-A:  92% • 7%

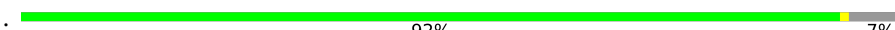
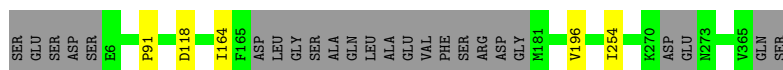
• Molecule 1: Protein At2g17340

Chain 8-A:  92% • 7%

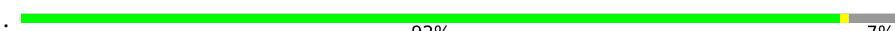
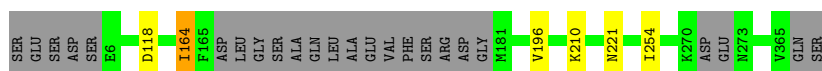
• Molecule 1: Protein At2g17340

Chain 9-A:  92% • 7%

• Molecule 1: Protein At2g17340

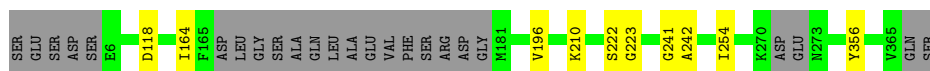
Chain 10-A:  92% • 7%

• Molecule 1: Protein At2g17340

Chain 11-A:  92% • 7%

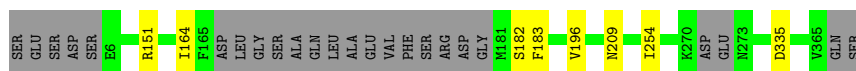
• Molecule 1: Protein At2g17340

Chain 12-A:  91% 7%



• Molecule 1: Protein At2g17340

Chain 13-A:  91% 7%



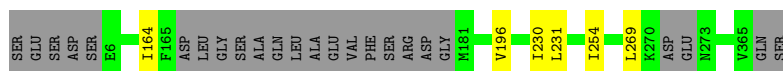
• Molecule 1: Protein At2g17340

Chain 14-A:  90% 7%



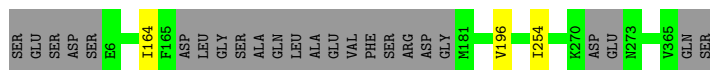
• Molecule 1: Protein At2g17340

Chain 15-A:  92% 7%



• Molecule 1: Protein At2g17340

Chain 16-A:  93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 97.1 (34.91-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.39 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.165 , 0.221 0.167 , 0.225	Depositor DCC
R_{free} test set	1773 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	48880	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	0.19	0/2747	0.34	0/3717
1	2-A	0.19	0/2747	0.34	0/3717
1	3-A	0.19	0/2747	0.34	0/3717
1	4-A	0.19	0/2747	0.34	0/3717
1	5-A	0.19	0/2747	0.34	0/3717
1	6-A	0.19	0/2747	0.34	0/3717
1	7-A	0.19	0/2747	0.34	0/3717
1	8-A	0.19	0/2747	0.34	0/3717
1	9-A	0.19	0/2747	0.34	0/3717
1	10-A	0.19	0/2747	0.34	0/3717
1	11-A	0.19	0/2747	0.34	0/3717
1	12-A	0.19	0/2747	0.34	0/3717
1	13-A	0.19	0/2747	0.34	0/3717
1	14-A	0.19	0/2747	0.34	0/3717
1	15-A	0.19	0/2747	0.34	0/3717
1	16-A	0.19	0/2747	0.34	0/3717
All	All	0.19	0/43952	0.34	0/59472

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

5.3.1 Protein backbone

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%)	14	4
1	2-A	337/367 (92%)	310 (92%)	23 (7%)	4 (1%)	10	2
1	3-A	337/367 (92%)	314 (93%)	18 (5%)	5 (2%)	8	1
1	4-A	337/367 (92%)	310 (92%)	23 (7%)	4 (1%)	10	2
1	5-A	337/367 (92%)	315 (94%)	18 (5%)	4 (1%)	10	2
1	6-A	337/367 (92%)	317 (94%)	17 (5%)	3 (1%)	14	4
1	7-A	337/367 (92%)	316 (94%)	18 (5%)	3 (1%)	14	4
1	8-A	337/367 (92%)	310 (92%)	23 (7%)	4 (1%)	10	2
1	9-A	337/367 (92%)	308 (91%)	24 (7%)	5 (2%)	8	1
1	10-A	337/367 (92%)	315 (94%)	19 (6%)	3 (1%)	14	4
1	11-A	337/367 (92%)	311 (92%)	21 (6%)	5 (2%)	8	1
1	12-A	337/367 (92%)	308 (91%)	21 (6%)	8 (2%)	4	1
1	13-A	337/367 (92%)	302 (90%)	29 (9%)	6 (2%)	6	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	14-A	337/367 (92%)	300 (89%)	27 (8%)	10 (3%)	3	0
1	15-A	337/367 (92%)	307 (91%)	26 (8%)	4 (1%)	10	2
1	16-A	337/367 (92%)	309 (92%)	27 (8%)	1 (0%)	36	22
All	All	5392/5872 (92%)	4969 (92%)	351 (6%)	72 (1%)	9	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
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

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Mol	Chain	Res	Type
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
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%)	295 (99%)	2 (1%)	76	69
1	2-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	3-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	4-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	5-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	6-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	7-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	8-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	9-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	10-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	11-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	12-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	13-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	14-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	15-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
1	16-A	297/317 (94%)	295 (99%)	2 (1%)	76	69
All	All	4752/5072 (94%)	4720 (99%)	32 (1%)	76	69

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	164	ILE
1	1-A	196	VAL
1	2-A	164	ILE
1	2-A	196	VAL
1	3-A	164	ILE
1	3-A	196	VAL
1	4-A	164	ILE
1	4-A	196	VAL

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Mol	Chain	Res	Type
1	5-A	164	ILE
1	5-A	196	VAL
1	6-A	164	ILE
1	6-A	196	VAL
1	7-A	164	ILE
1	7-A	196	VAL
1	8-A	164	ILE
1	8-A	196	VAL
1	9-A	164	ILE
1	9-A	196	VAL
1	10-A	164	ILE
1	10-A	196	VAL
1	11-A	164	ILE
1	11-A	196	VAL
1	12-A	164	ILE
1	12-A	196	VAL
1	13-A	164	ILE
1	13-A	196	VAL
1	14-A	164	ILE
1	14-A	196	VAL
1	15-A	164	ILE
1	15-A	196	VAL
1	16-A	164	ILE
1	16-A	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	19	ASN
1	1-A	47	ASN
1	1-A	188	GLN
1	1-A	268	GLN
1	1-A	275	GLN
1	1-A	291	ASN
1	1-A	363	ASN
1	2-A	19	ASN
1	2-A	109	GLN
1	2-A	268	GLN
1	2-A	275	GLN
1	2-A	363	ASN
1	3-A	268	GLN
1	3-A	275	GLN

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Mol	Chain	Res	Type
1	3-A	291	ASN
1	4-A	12	GLN
1	4-A	19	ASN
1	4-A	41	ASN
1	4-A	137	GLN
1	4-A	154	ASN
1	4-A	204	GLN
1	4-A	221	ASN
1	4-A	268	GLN
1	4-A	275	GLN
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	275	GLN
1	5-A	363	ASN
1	6-A	163	ASN
1	6-A	188	GLN
1	6-A	268	GLN
1	6-A	363	ASN
1	7-A	109	GLN
1	7-A	204	GLN
1	7-A	268	GLN
1	7-A	363	ASN
1	8-A	268	GLN
1	8-A	275	GLN
1	8-A	363	ASN
1	9-A	12	GLN
1	9-A	19	ASN
1	9-A	188	GLN
1	9-A	243	GLN
1	9-A	268	GLN
1	9-A	363	ASN
1	10-A	19	ASN
1	10-A	41	ASN
1	10-A	109	GLN
1	10-A	154	ASN
1	10-A	204	GLN
1	10-A	268	GLN
1	10-A	363	ASN
1	11-A	12	GLN

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Mol	Chain	Res	Type
1	11-A	19	ASN
1	11-A	188	GLN
1	11-A	221	ASN
1	11-A	268	GLN
1	11-A	363	ASN
1	12-A	19	ASN
1	12-A	41	ASN
1	12-A	188	GLN
1	12-A	268	GLN
1	12-A	275	GLN
1	13-A	12	GLN
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	13-A	363	ASN
1	14-A	12	GLN
1	14-A	19	ASN
1	14-A	209	ASN
1	14-A	268	GLN
1	15-A	19	ASN
1	15-A	128	ASN
1	15-A	188	GLN
1	15-A	189	ASN
1	15-A	249	ASN
1	15-A	344	HIS
1	16-A	19	ASN
1	16-A	20	ASN
1	16-A	154	ASN
1	16-A	189	ASN
1	16-A	243	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	343/367 (93%)	1.97	134 (39%) 1 0	0, 1, 2, 3	343 (100%)
1	2-A	0/367	-	-	-	-
1	3-A	0/367	-	-	-	-
1	4-A	0/367	-	-	-	-
1	5-A	0/367	-	-	-	-
1	6-A	0/367	-	-	-	-
1	7-A	0/367	-	-	-	-
1	8-A	0/367	-	-	-	-
1	9-A	0/367	-	-	-	-
1	10-A	0/367	-	-	-	-
1	11-A	0/367	-	-	-	-
1	12-A	0/367	-	-	-	-
1	13-A	0/367	-	-	-	-
1	14-A	0/367	-	-	-	-
1	15-A	0/367	-	-	-	-
1	16-A	0/367	-	-	-	-
All	All	343/5872 (5%)	1.97	134 (39%) 1 0	0, 1, 2, 3	343 (100%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	163	ASN	7.9
1	1-A	120	PHE	7.3
1	1-A	317	VAL	6.4
1	1-A	165	PHE	6.4
1	1-A	129	ALA	6.0
1	1-A	133	SER	6.0
1	1-A	319	GLY	5.9
1	1-A	307	TYR	5.6
1	1-A	359	VAL	5.5
1	1-A	146	GLU	5.3
1	1-A	164	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	97	PRO	4.9
1	1-A	67	PRO	4.8
1	1-A	17	ILE	4.8
1	1-A	141	LEU	4.7
1	1-A	315	VAL	4.6
1	1-A	301	VAL	4.6
1	1-A	123	VAL	4.5
1	1-A	365	VAL	4.5
1	1-A	274	GLY	4.4
1	1-A	192	PRO	4.4
1	1-A	188	GLN	4.4
1	1-A	185	ALA	4.4
1	1-A	132	ILE	4.4
1	1-A	316	ILE	4.4
1	1-A	268	GLN	4.3
1	1-A	270	LYS	4.3
1	1-A	305	LEU	4.0
1	1-A	64	ILE	3.9
1	1-A	20	ASN	3.9
1	1-A	45	TRP	3.9
1	1-A	145	ILE	3.9
1	1-A	310	SER	3.8
1	1-A	286	ILE	3.8
1	1-A	216	VAL	3.8
1	1-A	119	ILE	3.7
1	1-A	68	ASP	3.7
1	1-A	314	LEU	3.7
1	1-A	116	PHE	3.7
1	1-A	147	ASP	3.7
1	1-A	122	LYS	3.6
1	1-A	89	LYS	3.6
1	1-A	117	ARG	3.6
1	1-A	54	PRO	3.5
1	1-A	209	ASN	3.5
1	1-A	241	GLY	3.5
1	1-A	277	LEU	3.5
1	1-A	269	LEU	3.4
1	1-A	308	LEU	3.3
1	1-A	196	VAL	3.3
1	1-A	202	ASN	3.3
1	1-A	114	LEU	3.3
1	1-A	144	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	46	ILE	3.2
1	1-A	24	CYS	3.2
1	1-A	211	SER	3.2
1	1-A	30	PHE	3.2
1	1-A	125	ASP	3.2
1	1-A	150	LYS	3.1
1	1-A	59	ARG	3.0
1	1-A	218	PHE	3.0
1	1-A	189	ASN	3.0
1	1-A	210	LYS	3.0
1	1-A	191	VAL	3.0
1	1-A	267	SER	3.0
1	1-A	71	ALA	3.0
1	1-A	106	LEU	3.0
1	1-A	208	ILE	2.9
1	1-A	142	SER	2.8
1	1-A	194	PRO	2.8
1	1-A	309	SER	2.8
1	1-A	93	SER	2.8
1	1-A	140	SER	2.8
1	1-A	336	SER	2.8
1	1-A	91	PRO	2.8
1	1-A	363	ASN	2.8
1	1-A	44	SER	2.8
1	1-A	78	GLU	2.7
1	1-A	212	TRP	2.7
1	1-A	15	MET	2.7
1	1-A	31	PRO	2.7
1	1-A	96	GLY	2.7
1	1-A	58	LYS	2.7
1	1-A	130	LYS	2.6
1	1-A	118	ASP	2.6
1	1-A	41	ASN	2.6
1	1-A	358	CYS	2.6
1	1-A	74	GLU	2.6
1	1-A	43	ILE	2.6
1	1-A	311	ASP	2.5
1	1-A	13	LEU	2.5
1	1-A	273	ASN	2.5
1	1-A	259	CYS	2.5
1	1-A	121	LYS	2.5
1	1-A	127	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	195	TRP	2.5
1	1-A	126	GLU	2.5
1	1-A	90	ASP	2.4
1	1-A	76	PHE	2.4
1	1-A	306	ALA	2.4
1	1-A	69	ALA	2.4
1	1-A	234	ALA	2.4
1	1-A	265	ILE	2.4
1	1-A	95	GLY	2.4
1	1-A	94	HIS	2.4
1	1-A	19	ASN	2.3
1	1-A	312	ALA	2.3
1	1-A	285	LEU	2.3
1	1-A	337	LEU	2.3
1	1-A	302	SER	2.3
1	1-A	16	PRO	2.3
1	1-A	62	SER	2.3
1	1-A	66	VAL	2.3
1	1-A	343	LYS	2.2
1	1-A	217	ILE	2.2
1	1-A	139	VAL	2.2
1	1-A	73	ALA	2.2
1	1-A	75	LYS	2.2
1	1-A	345	LEU	2.2
1	1-A	183	PHE	2.2
1	1-A	284	LEU	2.1
1	1-A	220	ASP	2.1
1	1-A	131	ALA	2.1
1	1-A	40	PRO	2.1
1	1-A	72	ARG	2.1
1	1-A	300	ARG	2.1
1	1-A	110	VAL	2.1
1	1-A	186	SER	2.1
1	1-A	262	LEU	2.1
1	1-A	65	THR	2.1
1	1-A	213	LYS	2.1
1	1-A	245	VAL	2.0
1	1-A	134	LEU	2.0
1	1-A	264	GLU	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	1-A	401	1/1	0.91	0.10	43,43,43,43	1
2	MG	2-A	400	1/1	-	-	16,16,16,16	1
2	MG	3-A	400	1/1	-	-	10,10,10,10	1
2	MG	4-A	400	1/1	-	-	19,19,19,19	1
2	MG	5-A	400	1/1	-	-	16,16,16,16	1
2	MG	6-A	400	1/1	-	-	16,16,16,16	1
2	MG	7-A	400	1/1	-	-	18,18,18,18	1
2	MG	8-A	400	1/1	-	-	11,11,11,11	1
2	MG	9-A	400	1/1	-	-	12,12,12,12	1
2	MG	10-A	400	1/1	-	-	18,18,18,18	1
2	MG	11-A	400	1/1	-	-	11,11,11,11	1
2	MG	12-A	400	1/1	-	-	10,10,10,10	1
2	MG	13-A	400	1/1	-	-	10,10,10,10	1
2	MG	14-A	400	1/1	-	-	6,6,6,6	1
2	MG	15-A	400	1/1	-	-	7,7,7,7	1
2	MG	16-A	400	1/1	-	-	7,7,7,7	1
2	MG	1-A	400	1/1	0.92	0.07	10,10,10,10	1
2	MG	2-A	401	1/1	-	-	43,43,43,43	1
2	MG	3-A	401	1/1	-	-	43,43,43,43	1
2	MG	4-A	401	1/1	-	-	43,43,43,43	1
2	MG	5-A	401	1/1	-	-	43,43,43,43	1
2	MG	6-A	401	1/1	-	-	43,43,43,43	1
2	MG	7-A	401	1/1	-	-	43,43,43,43	1
2	MG	8-A	401	1/1	-	-	43,43,43,43	1
2	MG	9-A	401	1/1	-	-	43,43,43,43	1
2	MG	10-A	401	1/1	-	-	43,43,43,43	1
2	MG	11-A	401	1/1	-	-	43,43,43,43	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	12-A	401	1/1	-	-	43,43,43,43	1
2	MG	13-A	401	1/1	-	-	42,42,42,42	1
2	MG	14-A	401	1/1	-	-	42,42,42,42	1
2	MG	15-A	401	1/1	-	-	42,42,42,42	1
2	MG	16-A	401	1/1	-	-	42,42,42,42	1

6.5 Other polymers [i](#)

There are no such residues in this entry.