



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:06 AM UTC

PDB ID : 2Q4E / pdb_00002q4e
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At4g09670
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 : 2.49 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
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

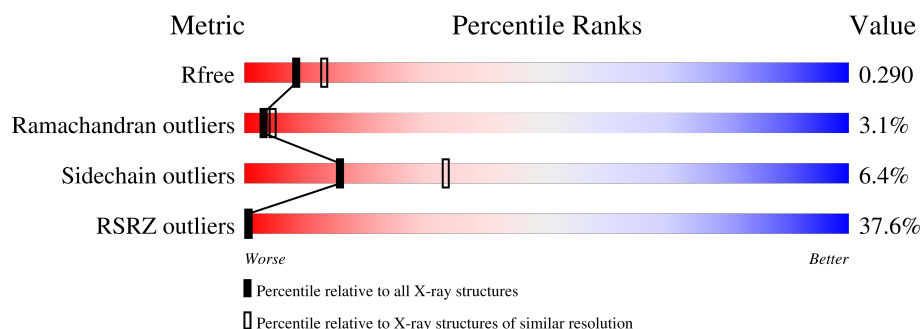
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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.



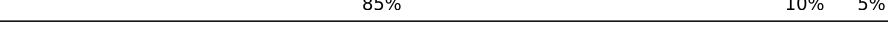
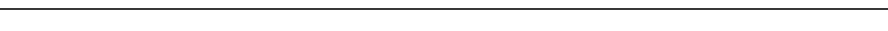
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	362	40% 87% 7% 5%
1	1-B	362	31% 90% 7% .
1	10-A	362	87% 7% 5%
1	10-B	362	89% 7% .
1	11-A	362	86% 8% 5%
1	11-B	362	88% 8% .
1	12-A	362	84% 10% 5%

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Mol	Chain	Length	Quality of chain
1	12-B	362	 90% 6% .
1	13-A	362	 85% 9% . 5%
1	13-B	362	 89% 7% .
1	14-A	362	 85% 9% 5%
1	14-B	362	 89% 8% .
1	15-A	362	 83% 11% 5%
1	15-B	362	 88% 9% .
1	16-A	362	 85% 9% . 5%
1	16-B	362	 88% 8% .
1	2-A	362	 88% 7% 5%
1	2-B	362	 90% 7% .
1	3-A	362	 85% 9% 5%
1	3-B	362	 90% 7% .
1	4-A	362	 85% 10% 5%
1	4-B	362	 91% 6% .
1	5-A	362	 87% 8% 5%
1	5-B	362	 89% 8% .
1	6-A	362	 88% 6% . 5%
1	6-B	362	 90% 7% .
1	7-A	362	 86% 9% 5%
1	7-B	362	 89% 7% .
1	8-A	362	 86% 8% . 5%
1	8-B	362	 90% 6% .
1	9-A	362	 88% 6% 5%
1	9-B	362	 91% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 87408 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 Probable oxidoreductase At4g09670.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	2-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	3-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	4-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	5-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	6-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	7-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	8-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	9-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	10-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	11-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	12-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	13-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	14-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	15-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	16-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	2-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	3-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	4-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	5-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	6-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	7-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	8-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	9-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	10-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	11-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	12-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	13-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	14-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	15-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0
1	16-B	350	Total 2692	C 1712	N 453	O 515	S 6	Se 6	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9SZ83
A	12	MSE	MET	modified residue	UNP Q9SZ83
A	106	MSE	MET	modified residue	UNP Q9SZ83
A	126	MSE	MET	modified residue	UNP Q9SZ83
A	130	MSE	MET	modified residue	UNP Q9SZ83
A	249	MSE	MET	modified residue	UNP Q9SZ83
A	310	MSE	MET	modified residue	UNP Q9SZ83

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP Q9SZ83
B	12	MSE	MET	modified residue	UNP Q9SZ83
B	106	MSE	MET	modified residue	UNP Q9SZ83
B	126	MSE	MET	modified residue	UNP Q9SZ83
B	130	MSE	MET	modified residue	UNP Q9SZ83
B	249	MSE	MET	modified residue	UNP Q9SZ83
B	310	MSE	MET	modified residue	UNP Q9SZ83

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	60	Total O 60 60	0	0
2	2-A	58	Total O 58 58	0	0
2	3-A	62	Total O 62 62	0	0
2	4-A	60	Total O 60 60	0	0
2	5-A	59	Total O 59 59	0	0
2	6-A	60	Total O 60 60	0	0
2	7-A	61	Total O 61 61	0	0
2	8-A	56	Total O 56 56	0	0
2	9-A	60	Total O 60 60	0	0
2	10-A	59	Total O 59 59	0	0
2	11-A	60	Total O 60 60	0	0
2	12-A	61	Total O 61 61	0	0
2	13-A	62	Total O 62 62	0	0
2	14-A	59	Total O 59 59	0	0
2	15-A	59	Total O 59 59	0	0
2	16-A	60	Total O 60 60	0	0

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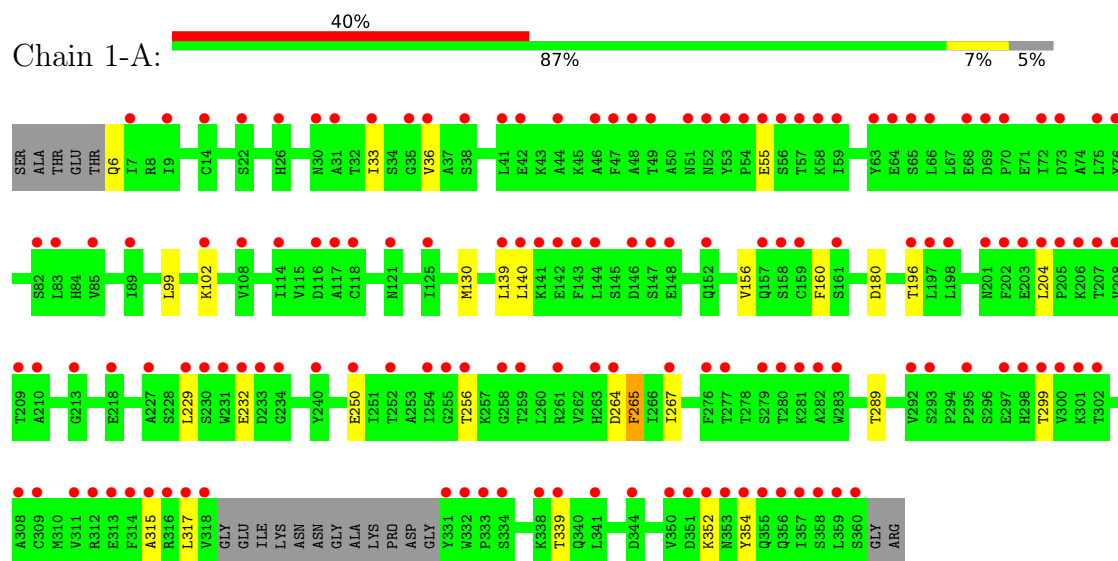
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-B	63	Total O 63 63	0	0
2	2-B	65	Total O 65 65	0	0
2	3-B	61	Total O 61 61	0	0
2	4-B	63	Total O 63 63	0	0
2	5-B	64	Total O 64 64	0	0
2	6-B	63	Total O 63 63	0	0
2	7-B	62	Total O 62 62	0	0
2	8-B	67	Total O 67 67	0	0
2	9-B	63	Total O 63 63	0	0
2	10-B	64	Total O 64 64	0	0
2	11-B	63	Total O 63 63	0	0
2	12-B	62	Total O 62 62	0	0
2	13-B	61	Total O 61 61	0	0
2	14-B	64	Total O 64 64	0	0
2	15-B	64	Total O 64 64	0	0
2	16-B	63	Total O 63 63	0	0

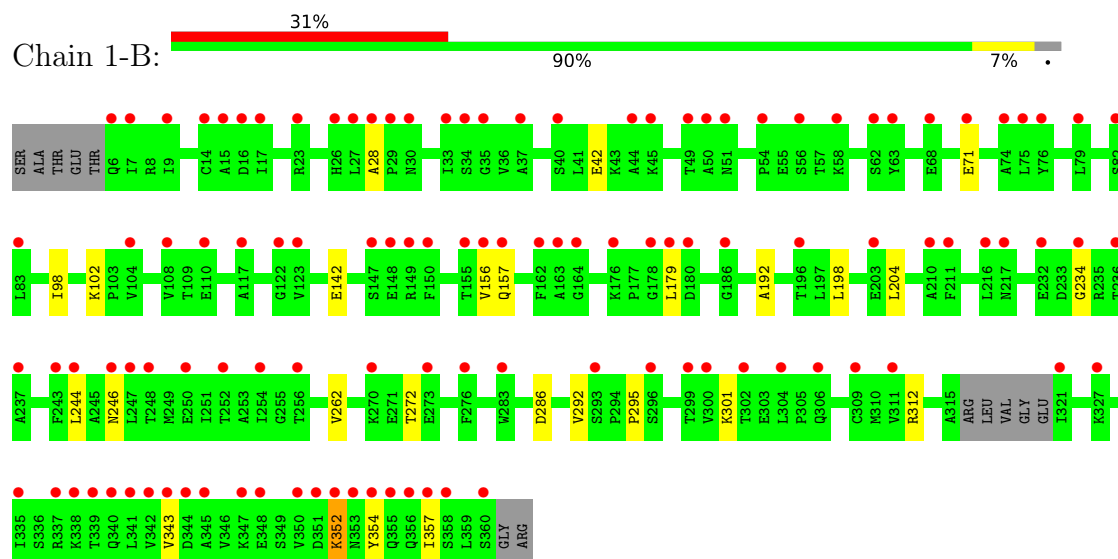
3 Residue-property plots [i](#)

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: Probable oxidoreductase At4g09670

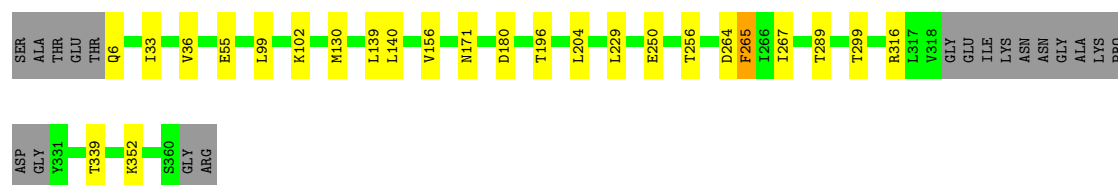


• Molecule 1: Probable oxidoreductase At4g09670



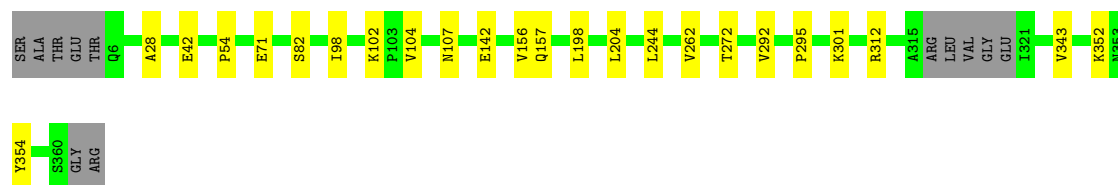
• Molecule 1: Probable oxidoreductase At4g09670

Chain 2-A: 



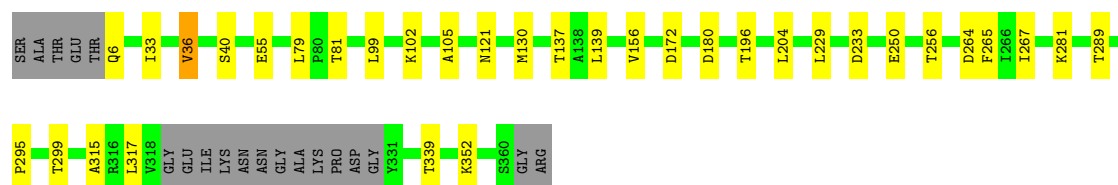
- Molecule 1: Probable oxidoreductase At4g09670

Chain 2-B: 



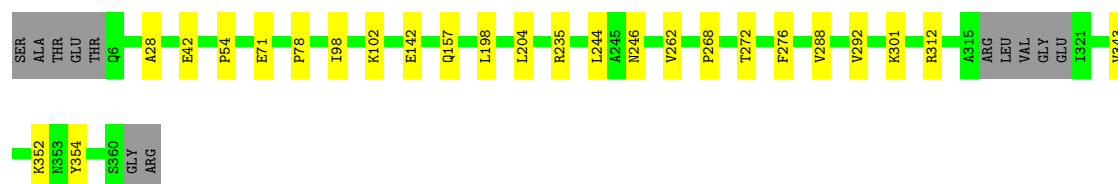
- Molecule 1: Probable oxidoreductase At4g09670

Chain 3-A: 



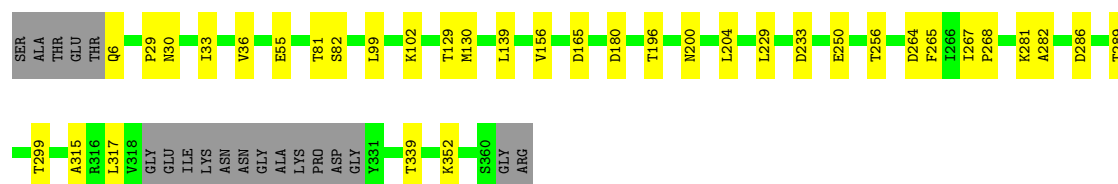
- Molecule 1: Probable oxidoreductase At4g09670

Chain 3-B: 



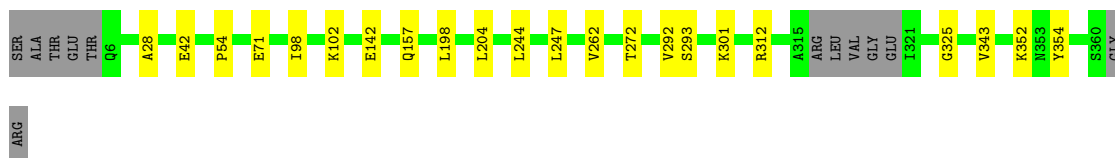
- Molecule 1: Probable oxidoreductase At4g09670

Chain 4-A: 



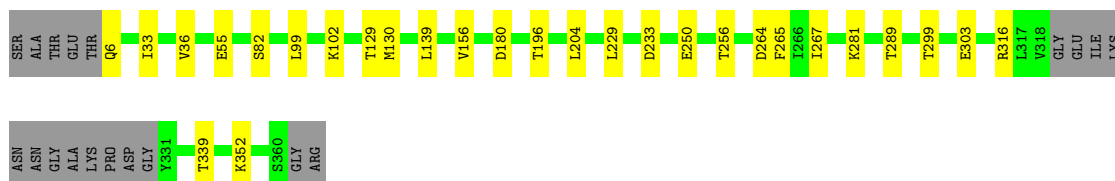
- Molecule 1: Probable oxidoreductase At4g09670

Chain 4-B:  91% 6% .



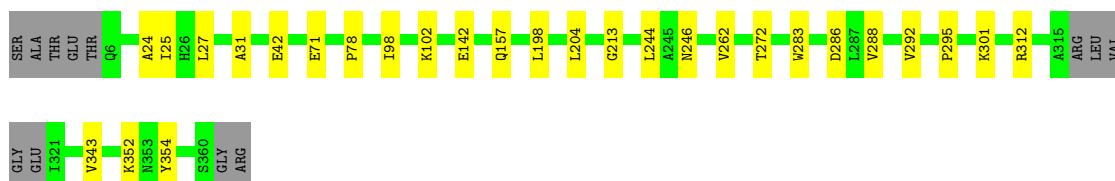
- Molecule 1: Probable oxidoreductase At4g09670

Chain 5-A:  87% 8% 5%



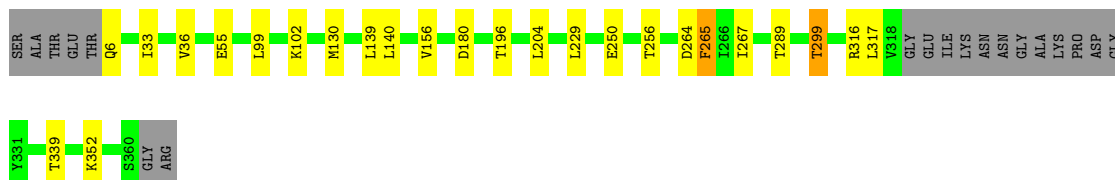
- Molecule 1: Probable oxidoreductase At4g09670

Chain 5-B:  89% 8% .



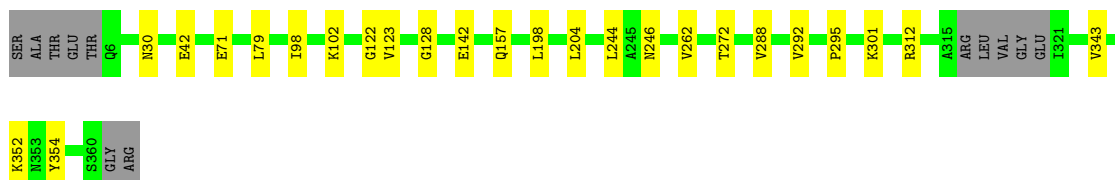
- Molecule 1: Probable oxidoreductase At4g09670

Chain 6-A:  88% 6% 5%



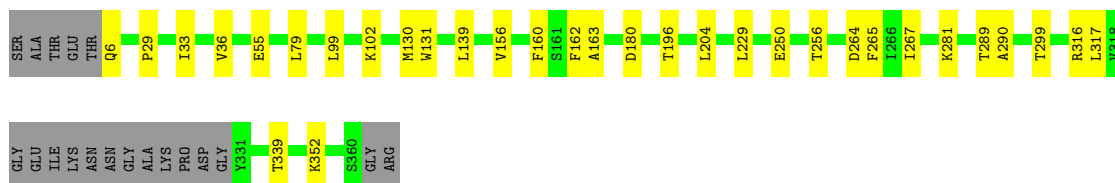
- Molecule 1: Probable oxidoreductase At4g09670

Chain 6-B:  90% 7% .



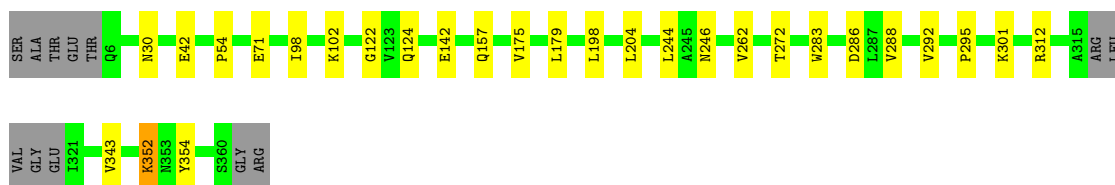
- Molecule 1: Probable oxidoreductase At4g09670

Chain 7-A:  86% 9% 5%



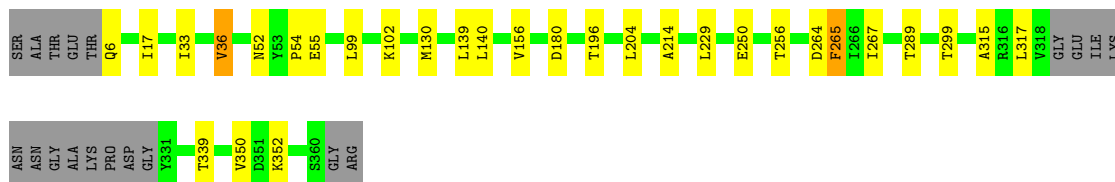
- Molecule 1: Probable oxidoreductase At4g09670

Chain 7-B:  89% 7% 4%



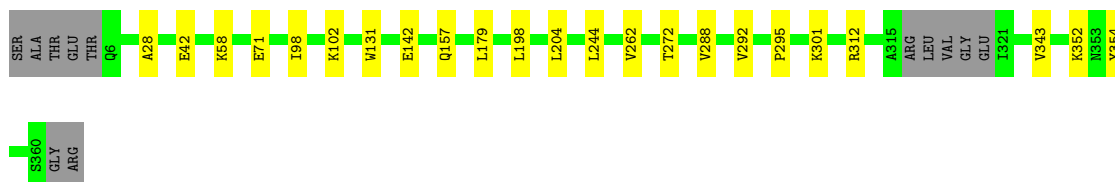
- Molecule 1: Probable oxidoreductase At4g09670

Chain 8-A:  86% 8% 6%



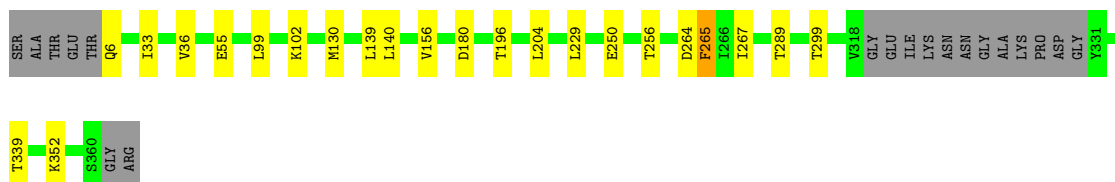
- Molecule 1: Probable oxidoreductase At4g09670

Chain 8-B:  90% 6% 4%



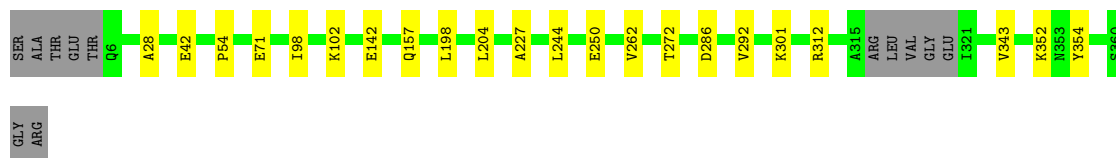
- Molecule 1: Probable oxidoreductase At4g09670

Chain 9-A:  88% 6% 6%



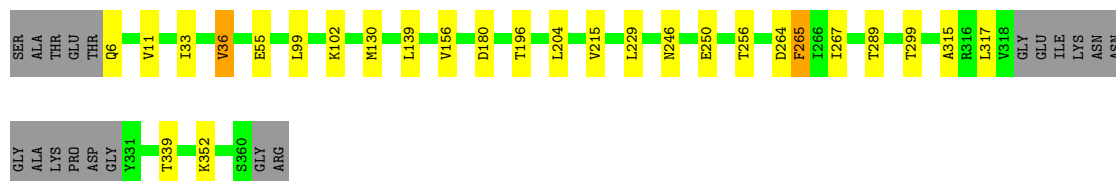
- Molecule 1: Probable oxidoreductase At4g09670

Chain 9-B:  91% 6% .



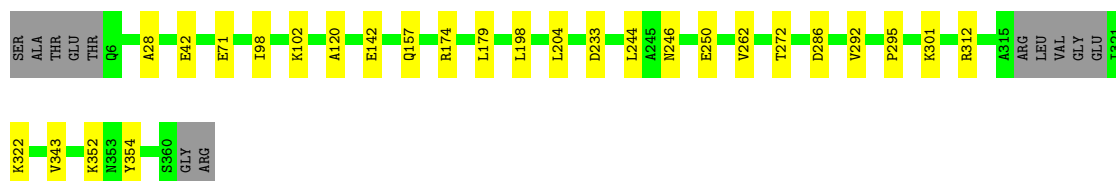
- Molecule 1: Probable oxidoreductase At4g09670

Chain 10-A:  87% 7% 5% .



- Molecule 1: Probable oxidoreductase At4g09670

Chain 10-B:  89% 7% .



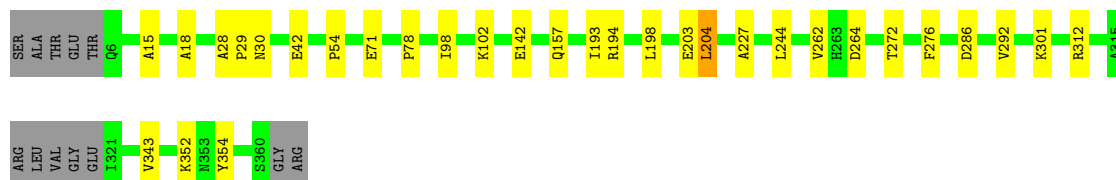
- Molecule 1: Probable oxidoreductase At4g09670

Chain 11-A:  86% 8% 5% .



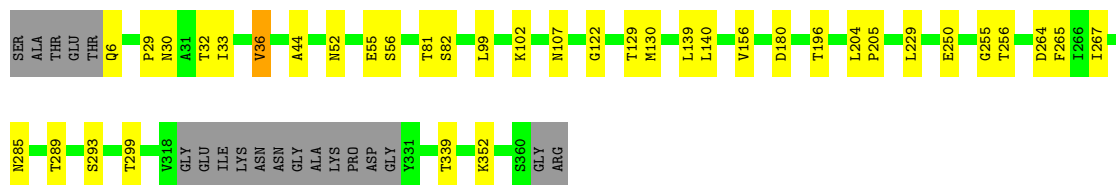
- Molecule 1: Probable oxidoreductase At4g09670

Chain 11-B:  88% 8% .



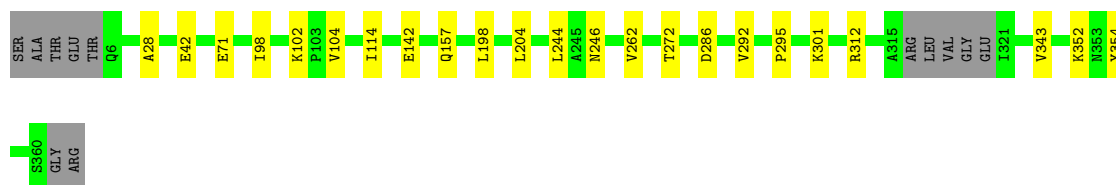
- Molecule 1: Probable oxidoreductase At4g09670

Chain 12-A:  84% 10% 5%



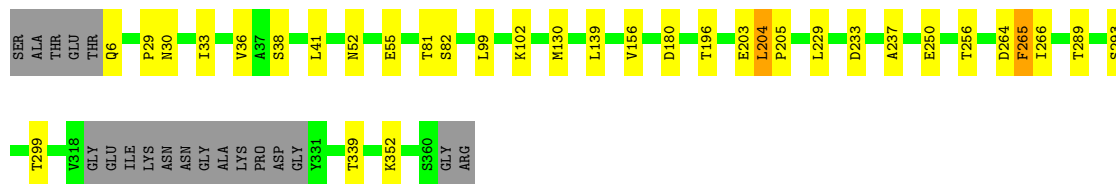
- Molecule 1: Probable oxidoreductase At4g09670

Chain 12-B:  90% 6% .



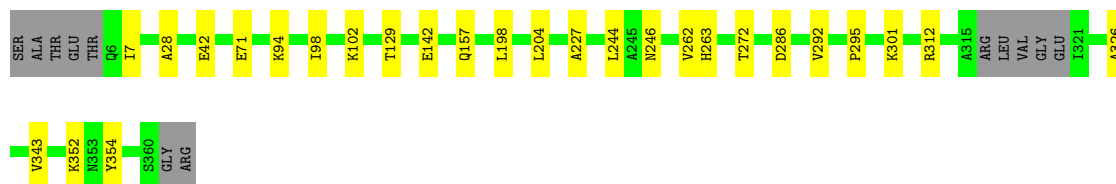
- Molecule 1: Probable oxidoreductase At4g09670

Chain 13-A:  85% 9% 5%



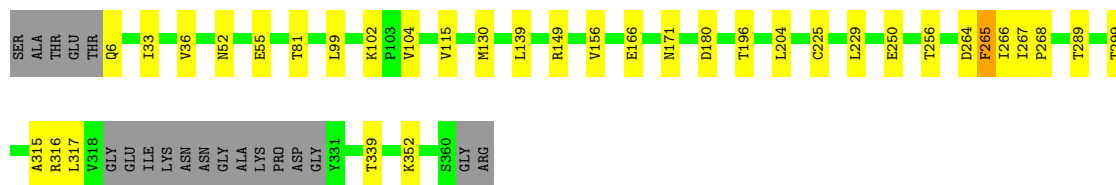
- Molecule 1: Probable oxidoreductase At4g09670

Chain 13-B:  89% 7% .



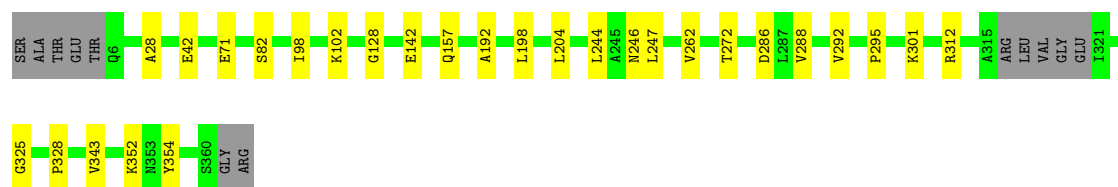
- Molecule 1: Probable oxidoreductase At4g09670

Chain 14-A:  85% 9% 5%



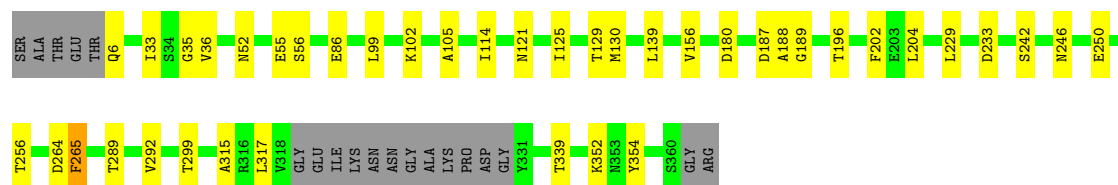
- Molecule 1: Probable oxidoreductase At4g09670

Chain 14-B:  89% 8% .



- Molecule 1: Probable oxidoreductase At4g09670

Chain 15-A:  83% 11% 5%



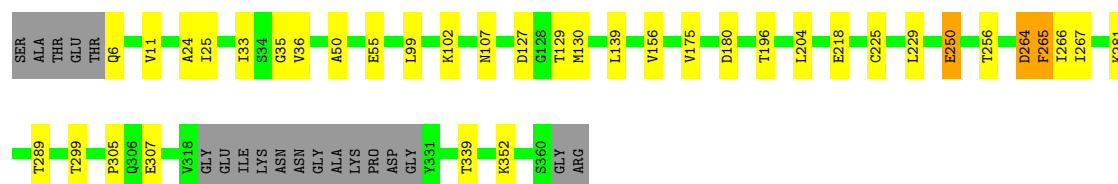
- Molecule 1: Probable oxidoreductase At4g09670

Chain 15-B:  88% 9% .



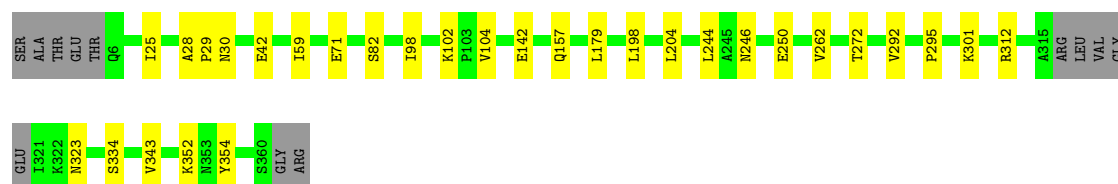
- Molecule 1: Probable oxidoreductase At4g09670

Chain 16-A:  85% 9% 5%



- Molecule 1: Probable oxidoreductase At4g09670

Chain 16-B:  88% 8% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.20Å 107.66Å 129.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 2.49 29.73 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.73-2.49) 98.4 (29.73-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.285 0.228 , 0.290	Depositor DCC
R_{free} test set	1472 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	87408	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.72% 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	0.18	0/2698	0.34	0/3656
1	1-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	2-A	0.18	0/2698	0.34	0/3656
1	2-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	3-A	0.18	0/2698	0.34	0/3656
1	3-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	4-A	0.18	0/2698	0.34	0/3656
1	4-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	5-A	0.18	0/2698	0.34	0/3656
1	5-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	6-A	0.18	0/2698	0.34	0/3656
1	6-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	7-A	0.18	0/2698	0.34	0/3656
1	7-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	8-A	0.18	0/2698	0.34	0/3656
1	8-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	9-A	0.18	0/2698	0.34	0/3656
1	9-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	10-A	0.18	0/2698	0.34	0/3656
1	10-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	11-A	0.18	0/2698	0.34	0/3656
1	11-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	12-A	0.18	0/2698	0.34	0/3656
1	12-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	13-A	0.18	0/2698	0.34	0/3656
1	13-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	14-A	0.18	0/2698	0.34	0/3656
1	14-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	15-A	0.18	0/2698	0.34	0/3656
1	15-B	0.19	0/2743	0.38	1/3716 (0.0%)
1	16-A	0.18	0/2698	0.34	0/3656
1	16-B	0.19	0/2743	0.38	1/3716 (0.0%)
All	All	0.18	0/87056	0.36	16/117952 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	1-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	2-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	3-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	4-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	5-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	6-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	7-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	8-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	9-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	10-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	11-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	12-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	13-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	14-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	15-B	98	ILE	N-CA-C	7.12	118.73	108.48
1	16-B	98	ILE	N-CA-C	7.12	118.73	108.48

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	2648	0	2642	0	0
1	1-B	2692	0	2680	0	0
1	2-A	2648	0	2642	0	0
1	2-B	2692	0	2680	0	0
1	3-A	2648	0	2642	0	0
1	3-B	2692	0	2680	0	0
1	4-A	2648	0	2642	0	0
1	4-B	2692	0	2680	0	0
1	5-A	2648	0	2642	0	0
1	5-B	2692	0	2680	0	0
1	6-A	2648	0	2642	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6-B	2692	0	2680	0	0
1	7-A	2648	0	2642	0	0
1	7-B	2692	0	2680	0	0
1	8-A	2648	0	2642	0	0
1	8-B	2692	0	2680	0	0
1	9-A	2648	0	2642	0	0
1	9-B	2692	0	2680	0	0
1	10-A	2648	0	2642	0	0
1	10-B	2692	0	2680	0	0
1	11-A	2648	0	2642	0	0
1	11-B	2692	0	2680	0	0
1	12-A	2648	0	2642	0	0
1	12-B	2692	0	2680	0	0
1	13-A	2648	0	2642	0	0
1	13-B	2692	0	2680	0	0
1	14-A	2648	0	2642	0	0
1	14-B	2692	0	2680	0	0
1	15-A	2648	0	2642	0	0
1	15-B	2692	0	2680	0	0
1	16-A	2648	0	2642	0	0
1	16-B	2692	0	2680	0	0
2	1-A	60	0	0	0	0
2	1-B	63	0	0	0	0
2	2-A	58	0	0	0	0
2	2-B	65	0	0	0	0
2	3-A	62	0	0	0	0
2	3-B	61	0	0	0	0
2	4-A	60	0	0	0	0
2	4-B	63	0	0	0	0
2	5-A	59	0	0	0	0
2	5-B	64	0	0	0	0
2	6-A	60	0	0	0	0
2	6-B	63	0	0	0	0
2	7-A	61	0	0	0	0
2	7-B	62	0	0	0	0
2	8-A	56	0	0	0	0
2	8-B	67	0	0	0	0
2	9-A	60	0	0	0	0
2	9-B	63	0	0	0	0
2	10-A	59	0	0	0	0
2	10-B	64	0	0	0	0
2	11-A	60	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	11-B	63	0	0	0	0
2	12-A	61	0	0	0	0
2	12-B	62	0	0	0	0
2	13-A	62	0	0	0	0
2	13-B	61	0	0	0	0
2	14-A	59	0	0	0	0
2	14-B	64	0	0	0	0
2	15-A	59	0	0	0	0
2	15-B	64	0	0	0	0
2	16-A	60	0	0	0	0
2	16-B	63	0	0	0	0
All	All	87408	0	85152	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	339/362 (94%)	294 (87%)	37 (11%)	8 (2%)	4	8
1	1-B	346/362 (96%)	300 (87%)	36 (10%)	10 (3%)	3	5
1	2-A	339/362 (94%)	300 (88%)	34 (10%)	5 (2%)	8	16
1	2-B	346/362 (96%)	307 (89%)	32 (9%)	7 (2%)	6	10
1	3-A	339/362 (94%)	276 (81%)	49 (14%)	14 (4%)	2	3
1	3-B	346/362 (96%)	286 (83%)	52 (15%)	8 (2%)	5	8
1	4-A	339/362 (94%)	287 (85%)	37 (11%)	15 (4%)	2	2
1	4-B	346/362 (96%)	315 (91%)	26 (8%)	5 (1%)	9	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-A	339/362 (94%)	295 (87%)	37 (11%)	7 (2%)	5	9
1	5-B	346/362 (96%)	298 (86%)	37 (11%)	11 (3%)	3	4
1	6-A	339/362 (94%)	298 (88%)	35 (10%)	6 (2%)	6	12
1	6-B	346/362 (96%)	309 (89%)	29 (8%)	8 (2%)	5	8
1	7-A	339/362 (94%)	291 (86%)	37 (11%)	11 (3%)	3	4
1	7-B	346/362 (96%)	294 (85%)	40 (12%)	12 (4%)	3	4
1	8-A	339/362 (94%)	280 (83%)	48 (14%)	11 (3%)	3	4
1	8-B	346/362 (96%)	303 (88%)	37 (11%)	6 (2%)	7	13
1	9-A	339/362 (94%)	299 (88%)	37 (11%)	3 (1%)	14	27
1	9-B	346/362 (96%)	309 (89%)	32 (9%)	5 (1%)	9	17
1	10-A	339/362 (94%)	294 (87%)	37 (11%)	8 (2%)	4	8
1	10-B	346/362 (96%)	296 (86%)	40 (12%)	10 (3%)	3	5
1	11-A	339/362 (94%)	284 (84%)	44 (13%)	11 (3%)	3	4
1	11-B	346/362 (96%)	288 (83%)	43 (12%)	15 (4%)	2	2
1	12-A	339/362 (94%)	272 (80%)	49 (14%)	18 (5%)	1	1
1	12-B	346/362 (96%)	294 (85%)	46 (13%)	6 (2%)	7	13
1	13-A	339/362 (94%)	281 (83%)	43 (13%)	15 (4%)	2	2
1	13-B	346/362 (96%)	309 (89%)	27 (8%)	10 (3%)	3	5
1	14-A	339/362 (94%)	288 (85%)	36 (11%)	15 (4%)	2	2
1	14-B	346/362 (96%)	302 (87%)	33 (10%)	11 (3%)	3	4
1	15-A	339/362 (94%)	265 (78%)	53 (16%)	21 (6%)	1	1
1	15-B	346/362 (96%)	282 (82%)	48 (14%)	16 (5%)	2	2
1	16-A	339/362 (94%)	270 (80%)	50 (15%)	19 (6%)	1	1
1	16-B	346/362 (96%)	291 (84%)	42 (12%)	13 (4%)	2	3
All	All	10960/11584 (95%)	9357 (85%)	1263 (12%)	340 (3%)	3	5

All (340) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	140	LEU
1	1-A	317	LEU
1	1-B	28	ALA
1	1-B	179	LEU
1	1-B	246	ASN

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Mol	Chain	Res	Type
1	2-B	28	ALA
1	2-B	104	VAL
1	3-A	81	THR
1	3-A	172	ASP
1	3-A	233	ASP
1	3-A	317	LEU
1	3-B	235	ARG
1	3-B	276	PHE
1	4-A	200	ASN
1	4-A	233	ASP
1	4-B	28	ALA
1	4-B	247	LEU
1	5-A	233	ASP
1	5-A	303	GLU
1	5-B	24	ALA
1	5-B	25	ILE
1	5-B	27	LEU
1	5-B	246	ASN
1	6-B	30	ASN
1	7-B	30	ASN
1	7-B	286	ASP
1	8-A	54	PRO
1	8-A	265	PHE
1	8-B	28	ALA
1	8-B	179	LEU
1	10-B	28	ALA
1	10-B	295	PRO
1	11-A	138	ALA
1	11-B	30	ASN
1	11-B	203	GLU
1	12-A	140	LEU
1	12-A	285	ASN
1	12-B	28	ALA
1	12-B	104	VAL
1	13-A	204	LEU
1	13-A	233	ASP
1	13-A	265	PHE
1	13-A	293	SER
1	13-B	7	ILE
1	13-B	28	ALA
1	13-B	263	HIS
1	13-B	286	ASP

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Mol	Chain	Res	Type
1	13-B	326	ALA
1	14-A	104	VAL
1	14-B	28	ALA
1	14-B	246	ASN
1	15-A	52	ASN
1	15-A	56	SER
1	15-A	233	ASP
1	15-A	354	TYR
1	15-B	28	ALA
1	15-B	30	ASN
1	15-B	202	PHE
1	15-B	303	GLU
1	15-B	334	SER
1	16-A	265	PHE
1	16-A	266	ILE
1	16-A	267	ILE
1	16-B	28	ALA
1	16-B	30	ASN
1	16-B	104	VAL
1	16-B	246	ASN
1	16-B	323	ASN
1	1-A	265	PHE
1	1-A	354	TYR
1	2-A	265	PHE
1	2-B	107	ASN
1	2-B	295	PRO
1	3-B	28	ALA
1	3-B	268	PRO
1	4-A	315	ALA
1	4-B	325	GLY
1	5-A	82	SER
1	5-A	281	LYS
1	5-A	316	ARG
1	5-B	286	ASP
1	6-A	140	LEU
1	6-A	265	PHE
1	6-B	128	GLY
1	6-B	246	ASN
1	6-B	295	PRO
1	7-A	162	PHE
1	7-A	281	LYS
1	7-B	179	LEU

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Mol	Chain	Res	Type
1	7-B	246	ASN
1	7-B	295	PRO
1	8-A	17	ILE
1	8-A	52	ASN
1	8-A	317	LEU
1	9-A	265	PHE
1	10-A	265	PHE
1	10-A	317	LEU
1	10-B	174	ARG
1	10-B	179	LEU
1	10-B	246	ASN
1	11-A	131	TRP
1	11-A	251	ILE
1	11-B	15	ALA
1	11-B	18	ALA
1	11-B	194	ARG
1	11-B	264	ASP
1	11-B	276	PHE
1	11-B	286	ASP
1	12-A	52	ASN
1	12-A	82	SER
1	12-B	246	ASN
1	12-B	286	ASP
1	12-B	295	PRO
1	13-A	41	LEU
1	13-A	82	SER
1	13-B	129	THR
1	13-B	227	ALA
1	13-B	246	ASN
1	14-A	166	GLU
1	14-A	265	PHE
1	14-A	316	ARG
1	14-B	128	GLY
1	14-B	192	ALA
1	14-B	247	LEU
1	14-B	286	ASP
1	14-B	325	GLY
1	15-A	114	ILE
1	15-A	265	PHE
1	15-B	129	THR
1	15-B	178	GLY
1	15-B	192	ALA

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Mol	Chain	Res	Type
1	15-B	235	ARG
1	15-B	264	ASP
1	15-B	299	THR
1	16-A	225	CYS
1	16-A	281	LYS
1	16-B	250	GLU
1	16-B	295	PRO
1	16-B	334	SER
1	1-A	232	GLU
1	1-A	315	ALA
1	1-B	352	LYS
1	2-A	140	LEU
1	2-A	171	ASN
1	2-B	82	SER
1	2-B	156	VAL
1	3-A	40	SER
1	3-A	281	LYS
1	3-A	295	PRO
1	4-A	30	ASN
1	4-A	82	SER
1	4-A	129	THR
1	4-A	165	ASP
1	4-A	281	LYS
1	4-A	282	ALA
1	4-A	317	LEU
1	5-A	129	THR
1	5-B	31	ALA
1	7-A	163	ALA
1	7-B	54	PRO
1	7-B	124	GLN
1	7-B	288	VAL
1	8-B	295	PRO
1	9-A	140	LEU
1	9-B	28	ALA
1	9-B	227	ALA
1	9-B	250	GLU
1	9-B	286	ASP
1	10-A	246	ASN
1	10-B	250	GLU
1	10-B	286	ASP
1	11-A	37	ALA
1	11-A	52	ASN

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Mol	Chain	Res	Type
1	11-B	78	PRO
1	11-B	227	ALA
1	12-A	30	ASN
1	12-A	44	ALA
1	12-A	56	SER
1	12-A	129	THR
1	12-A	293	SER
1	13-A	30	ASN
1	13-A	38	SER
1	13-A	81	THR
1	14-A	171	ASN
1	14-A	266	ILE
1	14-A	315	ALA
1	14-A	317	LEU
1	14-B	82	SER
1	14-B	295	PRO
1	15-A	105	ALA
1	15-A	121	ASN
1	15-A	129	THR
1	15-A	187	ASP
1	15-A	188	ALA
1	15-A	202	PHE
1	15-A	246	ASN
1	15-B	54	PRO
1	15-B	177	PRO
1	16-A	24	ALA
1	16-A	127	ASP
1	16-A	218	GLU
1	16-A	305	PRO
1	16-A	307	GLU
1	1-B	192	ALA
1	1-B	286	ASP
1	2-B	54	PRO
1	3-A	105	ALA
1	3-A	121	ASN
1	3-A	137	THR
1	3-A	267	ILE
1	3-A	315	ALA
1	3-B	54	PRO
1	4-A	81	THR
1	4-A	267	ILE
1	4-A	286	ASP

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Mol	Chain	Res	Type
1	4-B	293	SER
1	5-B	213	GLY
1	5-B	283	TRP
1	6-A	316	ARG
1	6-B	79	LEU
1	7-A	131	TRP
1	7-A	290	ALA
1	7-A	316	ARG
1	7-B	352	LYS
1	8-A	36	VAL
1	8-A	140	LEU
1	8-A	267	ILE
1	8-A	315	ALA
1	8-B	131	TRP
1	11-B	29	PRO
1	12-A	29	PRO
1	12-A	32	THR
1	12-A	107	ASN
1	12-A	205	PRO
1	13-A	29	PRO
1	13-A	52	ASN
1	13-A	203	GLU
1	13-A	266	ILE
1	13-B	94	LYS
1	14-A	52	ASN
1	14-A	81	THR
1	14-A	149	ARG
1	14-A	267	ILE
1	14-B	328	PRO
1	15-A	86	GLU
1	15-A	189	GLY
1	15-A	242	SER
1	15-A	315	ALA
1	15-B	306	GLN
1	16-A	107	ASN
1	16-A	250	GLU
1	16-B	82	SER
1	1-A	160	PHE
1	1-A	267	ILE
1	1-B	156	VAL
1	1-B	295	PRO
1	2-A	267	ILE

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Mol	Chain	Res	Type
1	2-A	316	ARG
1	3-A	36	VAL
1	3-B	246	ASN
1	5-A	267	ILE
1	5-B	288	VAL
1	5-B	295	PRO
1	6-A	267	ILE
1	6-A	317	LEU
1	7-A	29	PRO
1	7-A	79	LEU
1	7-A	267	ILE
1	7-B	283	TRP
1	8-A	214	ALA
1	8-B	58	LYS
1	9-A	267	ILE
1	9-B	54	PRO
1	10-A	267	ILE
1	10-A	315	ALA
1	10-B	120	ALA
1	10-B	233	ASP
1	10-B	322	LYS
1	11-A	79	LEU
1	11-A	267	ILE
1	11-B	28	ALA
1	11-B	54	PRO
1	11-B	193	ILE
1	12-A	81	THR
1	12-B	114	ILE
1	13-A	205	PRO
1	13-A	237	ALA
1	14-A	225	CYS
1	15-A	317	LEU
1	16-A	35	GLY
1	16-A	50	ALA
1	16-A	129	THR
1	16-A	175	VAL
1	16-A	264	ASP
1	16-B	59	ILE
1	16-B	179	LEU
1	3-A	79	LEU
1	6-A	299	THR
1	7-A	160	PHE

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Mol	Chain	Res	Type
1	7-A	317	LEU
1	8-B	288	VAL
1	11-A	281	LYS
1	12-A	122	GLY
1	15-A	292	VAL
1	15-B	213	GLY
1	10-A	11	VAL
1	10-A	215	VAL
1	11-A	36	VAL
1	12-A	36	VAL
1	12-A	267	ILE
1	16-B	25	ILE
1	4-A	268	PRO
1	4-B	54	PRO
1	6-B	122	GLY
1	7-B	122	GLY
1	11-B	204	LEU
1	12-A	255	GLY
1	14-B	288	VAL
1	15-A	35	GLY
1	15-A	125	ILE
1	1-B	234	GLY
1	1-B	357	ILE
1	6-B	123	VAL
1	6-B	288	VAL
1	7-B	175	VAL
1	10-A	36	VAL
1	13-B	295	PRO
1	16-A	11	VAL
1	3-B	78	PRO
1	3-B	288	VAL
1	4-A	29	PRO
1	11-A	61	GLY
1	14-A	115	VAL
1	16-A	25	ILE
1	5-B	78	PRO
1	8-A	350	VAL
1	11-A	29	PRO
1	14-A	268	PRO
1	15-B	29	PRO
1	16-B	29	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	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	1-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	2-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	2-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	3-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	3-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	4-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	4-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	5-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	5-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	6-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	6-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	7-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	7-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	8-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	8-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	9-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	9-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	10-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	10-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	11-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	11-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	12-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	12-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	13-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	13-B	290/293 (99%)	274 (94%)	16 (6%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	14-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	14-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	15-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	15-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
1	16-A	286/293 (98%)	265 (93%)	21 (7%)	13	27
1	16-B	290/293 (99%)	274 (94%)	16 (6%)	19	40
All	All	9216/9376 (98%)	8624 (94%)	592 (6%)	16	33

All (592) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	6	GLN
1	1-A	33	ILE
1	1-A	36	VAL
1	1-A	55	GLU
1	1-A	99	LEU
1	1-A	102	LYS
1	1-A	130	MSE
1	1-A	139	LEU
1	1-A	156	VAL
1	1-A	180	ASP
1	1-A	196	THR
1	1-A	204	LEU
1	1-A	229	LEU
1	1-A	250	GLU
1	1-A	256	THR
1	1-A	264	ASP
1	1-A	265	PHE
1	1-A	289	THR
1	1-A	299	THR
1	1-A	339	THR
1	1-A	352	LYS
1	1-B	42	GLU
1	1-B	71	GLU
1	1-B	102	LYS
1	1-B	142	GLU
1	1-B	157	GLN
1	1-B	198	LEU
1	1-B	204	LEU
1	1-B	244	LEU

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Mol	Chain	Res	Type
1	1-B	262	VAL
1	1-B	272	THR
1	1-B	292	VAL
1	1-B	301	LYS
1	1-B	312	ARG
1	1-B	343	VAL
1	1-B	352	LYS
1	1-B	354	TYR
1	2-A	6	GLN
1	2-A	33	ILE
1	2-A	36	VAL
1	2-A	55	GLU
1	2-A	99	LEU
1	2-A	102	LYS
1	2-A	130	MSE
1	2-A	139	LEU
1	2-A	156	VAL
1	2-A	180	ASP
1	2-A	196	THR
1	2-A	204	LEU
1	2-A	229	LEU
1	2-A	250	GLU
1	2-A	256	THR
1	2-A	264	ASP
1	2-A	265	PHE
1	2-A	289	THR
1	2-A	299	THR
1	2-A	339	THR
1	2-A	352	LYS
1	2-B	42	GLU
1	2-B	71	GLU
1	2-B	102	LYS
1	2-B	142	GLU
1	2-B	157	GLN
1	2-B	198	LEU
1	2-B	204	LEU
1	2-B	244	LEU
1	2-B	262	VAL
1	2-B	272	THR
1	2-B	292	VAL
1	2-B	301	LYS
1	2-B	312	ARG

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Mol	Chain	Res	Type
1	2-B	343	VAL
1	2-B	352	LYS
1	2-B	354	TYR
1	3-A	6	GLN
1	3-A	33	ILE
1	3-A	36	VAL
1	3-A	55	GLU
1	3-A	99	LEU
1	3-A	102	LYS
1	3-A	130	MSE
1	3-A	139	LEU
1	3-A	156	VAL
1	3-A	180	ASP
1	3-A	196	THR
1	3-A	204	LEU
1	3-A	229	LEU
1	3-A	250	GLU
1	3-A	256	THR
1	3-A	264	ASP
1	3-A	265	PHE
1	3-A	289	THR
1	3-A	299	THR
1	3-A	339	THR
1	3-A	352	LYS
1	3-B	42	GLU
1	3-B	71	GLU
1	3-B	102	LYS
1	3-B	142	GLU
1	3-B	157	GLN
1	3-B	198	LEU
1	3-B	204	LEU
1	3-B	244	LEU
1	3-B	262	VAL
1	3-B	272	THR
1	3-B	292	VAL
1	3-B	301	LYS
1	3-B	312	ARG
1	3-B	343	VAL
1	3-B	352	LYS
1	3-B	354	TYR
1	4-A	6	GLN
1	4-A	33	ILE

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Mol	Chain	Res	Type
1	4-A	36	VAL
1	4-A	55	GLU
1	4-A	99	LEU
1	4-A	102	LYS
1	4-A	130	MSE
1	4-A	139	LEU
1	4-A	156	VAL
1	4-A	180	ASP
1	4-A	196	THR
1	4-A	204	LEU
1	4-A	229	LEU
1	4-A	250	GLU
1	4-A	256	THR
1	4-A	264	ASP
1	4-A	265	PHE
1	4-A	289	THR
1	4-A	299	THR
1	4-A	339	THR
1	4-A	352	LYS
1	4-B	42	GLU
1	4-B	71	GLU
1	4-B	102	LYS
1	4-B	142	GLU
1	4-B	157	GLN
1	4-B	198	LEU
1	4-B	204	LEU
1	4-B	244	LEU
1	4-B	262	VAL
1	4-B	272	THR
1	4-B	292	VAL
1	4-B	301	LYS
1	4-B	312	ARG
1	4-B	343	VAL
1	4-B	352	LYS
1	4-B	354	TYR
1	5-A	6	GLN
1	5-A	33	ILE
1	5-A	36	VAL
1	5-A	55	GLU
1	5-A	99	LEU
1	5-A	102	LYS
1	5-A	130	MSE

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Mol	Chain	Res	Type
1	5-A	139	LEU
1	5-A	156	VAL
1	5-A	180	ASP
1	5-A	196	THR
1	5-A	204	LEU
1	5-A	229	LEU
1	5-A	250	GLU
1	5-A	256	THR
1	5-A	264	ASP
1	5-A	265	PHE
1	5-A	289	THR
1	5-A	299	THR
1	5-A	339	THR
1	5-A	352	LYS
1	5-B	42	GLU
1	5-B	71	GLU
1	5-B	102	LYS
1	5-B	142	GLU
1	5-B	157	GLN
1	5-B	198	LEU
1	5-B	204	LEU
1	5-B	244	LEU
1	5-B	262	VAL
1	5-B	272	THR
1	5-B	292	VAL
1	5-B	301	LYS
1	5-B	312	ARG
1	5-B	343	VAL
1	5-B	352	LYS
1	5-B	354	TYR
1	6-A	6	GLN
1	6-A	33	ILE
1	6-A	36	VAL
1	6-A	55	GLU
1	6-A	99	LEU
1	6-A	102	LYS
1	6-A	130	MSE
1	6-A	139	LEU
1	6-A	156	VAL
1	6-A	180	ASP
1	6-A	196	THR
1	6-A	204	LEU

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Mol	Chain	Res	Type
1	6-A	229	LEU
1	6-A	250	GLU
1	6-A	256	THR
1	6-A	264	ASP
1	6-A	265	PHE
1	6-A	289	THR
1	6-A	299	THR
1	6-A	339	THR
1	6-A	352	LYS
1	6-B	42	GLU
1	6-B	71	GLU
1	6-B	102	LYS
1	6-B	142	GLU
1	6-B	157	GLN
1	6-B	198	LEU
1	6-B	204	LEU
1	6-B	244	LEU
1	6-B	262	VAL
1	6-B	272	THR
1	6-B	292	VAL
1	6-B	301	LYS
1	6-B	312	ARG
1	6-B	343	VAL
1	6-B	352	LYS
1	6-B	354	TYR
1	7-A	6	GLN
1	7-A	33	ILE
1	7-A	36	VAL
1	7-A	55	GLU
1	7-A	99	LEU
1	7-A	102	LYS
1	7-A	130	MSE
1	7-A	139	LEU
1	7-A	156	VAL
1	7-A	180	ASP
1	7-A	196	THR
1	7-A	204	LEU
1	7-A	229	LEU
1	7-A	250	GLU
1	7-A	256	THR
1	7-A	264	ASP
1	7-A	265	PHE

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Mol	Chain	Res	Type
1	7-A	289	THR
1	7-A	299	THR
1	7-A	339	THR
1	7-A	352	LYS
1	7-B	42	GLU
1	7-B	71	GLU
1	7-B	102	LYS
1	7-B	142	GLU
1	7-B	157	GLN
1	7-B	198	LEU
1	7-B	204	LEU
1	7-B	244	LEU
1	7-B	262	VAL
1	7-B	272	THR
1	7-B	292	VAL
1	7-B	301	LYS
1	7-B	312	ARG
1	7-B	343	VAL
1	7-B	352	LYS
1	7-B	354	TYR
1	8-A	6	GLN
1	8-A	33	ILE
1	8-A	36	VAL
1	8-A	55	GLU
1	8-A	99	LEU
1	8-A	102	LYS
1	8-A	130	MSE
1	8-A	139	LEU
1	8-A	156	VAL
1	8-A	180	ASP
1	8-A	196	THR
1	8-A	204	LEU
1	8-A	229	LEU
1	8-A	250	GLU
1	8-A	256	THR
1	8-A	264	ASP
1	8-A	265	PHE
1	8-A	289	THR
1	8-A	299	THR
1	8-A	339	THR
1	8-A	352	LYS
1	8-B	42	GLU

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Mol	Chain	Res	Type
1	8-B	71	GLU
1	8-B	102	LYS
1	8-B	142	GLU
1	8-B	157	GLN
1	8-B	198	LEU
1	8-B	204	LEU
1	8-B	244	LEU
1	8-B	262	VAL
1	8-B	272	THR
1	8-B	292	VAL
1	8-B	301	LYS
1	8-B	312	ARG
1	8-B	343	VAL
1	8-B	352	LYS
1	8-B	354	TYR
1	9-A	6	GLN
1	9-A	33	ILE
1	9-A	36	VAL
1	9-A	55	GLU
1	9-A	99	LEU
1	9-A	102	LYS
1	9-A	130	MSE
1	9-A	139	LEU
1	9-A	156	VAL
1	9-A	180	ASP
1	9-A	196	THR
1	9-A	204	LEU
1	9-A	229	LEU
1	9-A	250	GLU
1	9-A	256	THR
1	9-A	264	ASP
1	9-A	265	PHE
1	9-A	289	THR
1	9-A	299	THR
1	9-A	339	THR
1	9-A	352	LYS
1	9-B	42	GLU
1	9-B	71	GLU
1	9-B	102	LYS
1	9-B	142	GLU
1	9-B	157	GLN
1	9-B	198	LEU

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Mol	Chain	Res	Type
1	9-B	204	LEU
1	9-B	244	LEU
1	9-B	262	VAL
1	9-B	272	THR
1	9-B	292	VAL
1	9-B	301	LYS
1	9-B	312	ARG
1	9-B	343	VAL
1	9-B	352	LYS
1	9-B	354	TYR
1	10-A	6	GLN
1	10-A	33	ILE
1	10-A	36	VAL
1	10-A	55	GLU
1	10-A	99	LEU
1	10-A	102	LYS
1	10-A	130	MSE
1	10-A	139	LEU
1	10-A	156	VAL
1	10-A	180	ASP
1	10-A	196	THR
1	10-A	204	LEU
1	10-A	229	LEU
1	10-A	250	GLU
1	10-A	256	THR
1	10-A	264	ASP
1	10-A	265	PHE
1	10-A	289	THR
1	10-A	299	THR
1	10-A	339	THR
1	10-A	352	LYS
1	10-B	42	GLU
1	10-B	71	GLU
1	10-B	102	LYS
1	10-B	142	GLU
1	10-B	157	GLN
1	10-B	198	LEU
1	10-B	204	LEU
1	10-B	244	LEU
1	10-B	262	VAL
1	10-B	272	THR
1	10-B	292	VAL

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Mol	Chain	Res	Type
1	10-B	301	LYS
1	10-B	312	ARG
1	10-B	343	VAL
1	10-B	352	LYS
1	10-B	354	TYR
1	11-A	6	GLN
1	11-A	33	ILE
1	11-A	36	VAL
1	11-A	55	GLU
1	11-A	99	LEU
1	11-A	102	LYS
1	11-A	130	MSE
1	11-A	139	LEU
1	11-A	156	VAL
1	11-A	180	ASP
1	11-A	196	THR
1	11-A	204	LEU
1	11-A	229	LEU
1	11-A	250	GLU
1	11-A	256	THR
1	11-A	264	ASP
1	11-A	265	PHE
1	11-A	289	THR
1	11-A	299	THR
1	11-A	339	THR
1	11-A	352	LYS
1	11-B	42	GLU
1	11-B	71	GLU
1	11-B	102	LYS
1	11-B	142	GLU
1	11-B	157	GLN
1	11-B	198	LEU
1	11-B	204	LEU
1	11-B	244	LEU
1	11-B	262	VAL
1	11-B	272	THR
1	11-B	292	VAL
1	11-B	301	LYS
1	11-B	312	ARG
1	11-B	343	VAL
1	11-B	352	LYS
1	11-B	354	TYR

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Mol	Chain	Res	Type
1	12-A	6	GLN
1	12-A	33	ILE
1	12-A	36	VAL
1	12-A	55	GLU
1	12-A	99	LEU
1	12-A	102	LYS
1	12-A	130	MSE
1	12-A	139	LEU
1	12-A	156	VAL
1	12-A	180	ASP
1	12-A	196	THR
1	12-A	204	LEU
1	12-A	229	LEU
1	12-A	250	GLU
1	12-A	256	THR
1	12-A	264	ASP
1	12-A	265	PHE
1	12-A	289	THR
1	12-A	299	THR
1	12-A	339	THR
1	12-A	352	LYS
1	12-B	42	GLU
1	12-B	71	GLU
1	12-B	102	LYS
1	12-B	142	GLU
1	12-B	157	GLN
1	12-B	198	LEU
1	12-B	204	LEU
1	12-B	244	LEU
1	12-B	262	VAL
1	12-B	272	THR
1	12-B	292	VAL
1	12-B	301	LYS
1	12-B	312	ARG
1	12-B	343	VAL
1	12-B	352	LYS
1	12-B	354	TYR
1	13-A	6	GLN
1	13-A	33	ILE
1	13-A	36	VAL
1	13-A	55	GLU
1	13-A	99	LEU

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Mol	Chain	Res	Type
1	13-A	102	LYS
1	13-A	130	MSE
1	13-A	139	LEU
1	13-A	156	VAL
1	13-A	180	ASP
1	13-A	196	THR
1	13-A	204	LEU
1	13-A	229	LEU
1	13-A	250	GLU
1	13-A	256	THR
1	13-A	264	ASP
1	13-A	265	PHE
1	13-A	289	THR
1	13-A	299	THR
1	13-A	339	THR
1	13-A	352	LYS
1	13-B	42	GLU
1	13-B	71	GLU
1	13-B	102	LYS
1	13-B	142	GLU
1	13-B	157	GLN
1	13-B	198	LEU
1	13-B	204	LEU
1	13-B	244	LEU
1	13-B	262	VAL
1	13-B	272	THR
1	13-B	292	VAL
1	13-B	301	LYS
1	13-B	312	ARG
1	13-B	343	VAL
1	13-B	352	LYS
1	13-B	354	TYR
1	14-A	6	GLN
1	14-A	33	ILE
1	14-A	36	VAL
1	14-A	55	GLU
1	14-A	99	LEU
1	14-A	102	LYS
1	14-A	130	MSE
1	14-A	139	LEU
1	14-A	156	VAL
1	14-A	180	ASP

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Mol	Chain	Res	Type
1	14-A	196	THR
1	14-A	204	LEU
1	14-A	229	LEU
1	14-A	250	GLU
1	14-A	256	THR
1	14-A	264	ASP
1	14-A	265	PHE
1	14-A	289	THR
1	14-A	299	THR
1	14-A	339	THR
1	14-A	352	LYS
1	14-B	42	GLU
1	14-B	71	GLU
1	14-B	102	LYS
1	14-B	142	GLU
1	14-B	157	GLN
1	14-B	198	LEU
1	14-B	204	LEU
1	14-B	244	LEU
1	14-B	262	VAL
1	14-B	272	THR
1	14-B	292	VAL
1	14-B	301	LYS
1	14-B	312	ARG
1	14-B	343	VAL
1	14-B	352	LYS
1	14-B	354	TYR
1	15-A	6	GLN
1	15-A	33	ILE
1	15-A	36	VAL
1	15-A	55	GLU
1	15-A	99	LEU
1	15-A	102	LYS
1	15-A	130	MSE
1	15-A	139	LEU
1	15-A	156	VAL
1	15-A	180	ASP
1	15-A	196	THR
1	15-A	204	LEU
1	15-A	229	LEU
1	15-A	250	GLU
1	15-A	256	THR

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Mol	Chain	Res	Type
1	15-A	264	ASP
1	15-A	265	PHE
1	15-A	289	THR
1	15-A	299	THR
1	15-A	339	THR
1	15-A	352	LYS
1	15-B	42	GLU
1	15-B	71	GLU
1	15-B	102	LYS
1	15-B	142	GLU
1	15-B	157	GLN
1	15-B	198	LEU
1	15-B	204	LEU
1	15-B	244	LEU
1	15-B	262	VAL
1	15-B	272	THR
1	15-B	292	VAL
1	15-B	301	LYS
1	15-B	312	ARG
1	15-B	343	VAL
1	15-B	352	LYS
1	15-B	354	TYR
1	16-A	6	GLN
1	16-A	33	ILE
1	16-A	36	VAL
1	16-A	55	GLU
1	16-A	99	LEU
1	16-A	102	LYS
1	16-A	130	MSE
1	16-A	139	LEU
1	16-A	156	VAL
1	16-A	180	ASP
1	16-A	196	THR
1	16-A	204	LEU
1	16-A	229	LEU
1	16-A	250	GLU
1	16-A	256	THR
1	16-A	264	ASP
1	16-A	265	PHE
1	16-A	289	THR
1	16-A	299	THR
1	16-A	339	THR

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Mol	Chain	Res	Type
1	16-A	352	LYS
1	16-B	42	GLU
1	16-B	71	GLU
1	16-B	102	LYS
1	16-B	142	GLU
1	16-B	157	GLN
1	16-B	198	LEU
1	16-B	204	LEU
1	16-B	244	LEU
1	16-B	262	VAL
1	16-B	272	THR
1	16-B	292	VAL
1	16-B	301	LYS
1	16-B	312	ARG
1	16-B	343	VAL
1	16-B	352	LYS
1	16-B	354	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	51	ASN
1	1-A	124	GLN
1	1-A	201	ASN
1	1-A	263	HIS
1	1-A	298	HIS
1	1-A	355	GLN
1	2-A	124	GLN
1	2-A	201	ASN
1	2-B	171	ASN
1	2-B	340	GLN
1	3-A	6	GLN
1	3-A	124	GLN
1	3-A	157	GLN
1	3-A	355	GLN
1	3-A	356	GLN
1	3-B	124	GLN
1	4-A	51	ASN
1	4-A	124	GLN
1	4-A	157	GLN
1	4-A	201	ASN
1	5-A	124	GLN

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Mol	Chain	Res	Type
1	5-A	152	GLN
1	5-A	200	ASN
1	5-A	201	ASN
1	5-A	355	GLN
1	5-B	26	HIS
1	5-B	60	HIS
1	5-B	340	GLN
1	6-A	51	ASN
1	6-A	124	GLN
1	6-A	200	ASN
1	6-A	201	ASN
1	6-A	263	HIS
1	6-A	298	HIS
1	6-A	340	GLN
1	6-B	124	GLN
1	6-B	157	GLN
1	6-B	246	ASN
1	6-B	340	GLN
1	6-B	355	GLN
1	6-B	356	GLN
1	7-A	121	ASN
1	7-A	124	GLN
1	7-A	157	GLN
1	7-A	201	ASN
1	7-A	340	GLN
1	7-A	356	GLN
1	7-B	26	HIS
1	7-B	30	ASN
1	7-B	52	ASN
1	7-B	124	GLN
1	8-A	6	GLN
1	8-A	124	GLN
1	8-A	157	GLN
1	8-A	201	ASN
1	8-A	246	ASN
1	8-A	340	GLN
1	8-A	355	GLN
1	8-A	356	GLN
1	8-B	52	ASN
1	8-B	107	ASN
1	8-B	121	ASN
1	8-B	157	GLN

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Mol	Chain	Res	Type
1	8-B	217	ASN
1	8-B	340	GLN
1	9-A	51	ASN
1	9-A	124	GLN
1	9-A	134	ASN
1	9-A	200	ASN
1	9-A	201	ASN
1	9-A	306	GLN
1	9-A	340	GLN
1	9-B	340	GLN
1	10-A	124	GLN
1	10-A	263	HIS
1	10-A	355	GLN
1	10-B	124	GLN
1	10-B	340	GLN
1	10-B	355	GLN
1	10-B	356	GLN
1	11-A	51	ASN
1	11-A	60	HIS
1	11-A	121	ASN
1	11-A	124	GLN
1	11-A	152	GLN
1	11-A	201	ASN
1	11-A	356	GLN
1	11-B	51	ASN
1	11-B	60	HIS
1	11-B	124	GLN
1	12-A	30	ASN
1	12-A	51	ASN
1	12-A	124	GLN
1	12-A	152	GLN
1	12-A	171	ASN
1	12-A	201	ASN
1	12-B	133	HIS
1	12-B	217	ASN
1	12-B	355	GLN
1	13-A	51	ASN
1	13-A	201	ASN
1	13-A	298	HIS
1	13-B	157	GLN
1	13-B	246	ASN
1	14-A	124	GLN

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Mol	Chain	Res	Type
1	14-A	134	ASN
1	14-A	201	ASN
1	14-A	263	HIS
1	14-A	355	GLN
1	14-B	124	GLN
1	14-B	133	HIS
1	14-B	263	HIS
1	14-B	324	ASN
1	15-A	51	ASN
1	15-A	107	ASN
1	15-A	121	ASN
1	15-A	124	GLN
1	15-A	340	GLN
1	15-A	356	GLN
1	15-B	124	GLN
1	15-B	134	ASN
1	15-B	157	GLN
1	15-B	263	HIS
1	15-B	298	HIS
1	15-B	306	GLN
1	15-B	353	ASN
1	16-A	51	ASN
1	16-A	124	GLN
1	16-A	152	GLN
1	16-A	201	ASN
1	16-A	356	GLN
1	16-B	6	GLN
1	16-B	26	HIS
1	16-B	134	ASN
1	16-B	157	GLN
1	16-B	171	ASN
1	16-B	306	GLN

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](#)

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	337/362 (93%)	2.01	143 (42%) 0 0	1, 2, 3, 5	337 (100%)
1	1-B	344/362 (95%)	1.82	113 (32%) 1 1	1, 2, 3, 3	344 (100%)
1	2-A	0/362	-	-	-	-
1	2-B	0/362	-	-	-	-
1	3-A	0/362	-	-	-	-
1	3-B	0/362	-	-	-	-
1	4-A	0/362	-	-	-	-
1	4-B	0/362	-	-	-	-
1	5-A	0/362	-	-	-	-
1	5-B	0/362	-	-	-	-
1	6-A	0/362	-	-	-	-
1	6-B	0/362	-	-	-	-
1	7-A	0/362	-	-	-	-
1	7-B	0/362	-	-	-	-
1	8-A	0/362	-	-	-	-
1	8-B	0/362	-	-	-	-
1	9-A	0/362	-	-	-	-
1	9-B	0/362	-	-	-	-
1	10-A	0/362	-	-	-	-
1	10-B	0/362	-	-	-	-
1	11-A	0/362	-	-	-	-
1	11-B	0/362	-	-	-	-
1	12-A	0/362	-	-	-	-
1	12-B	0/362	-	-	-	-
1	13-A	0/362	-	-	-	-
1	13-B	0/362	-	-	-	-
1	14-A	0/362	-	-	-	-
1	14-B	0/362	-	-	-	-
1	15-A	0/362	-	-	-	-
1	15-B	0/362	-	-	-	-
1	16-A	0/362	-	-	-	-
1	16-B	0/362	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	681/11584 (5%)	1.92	256 (37%) 1 0	1, 2, 3, 5	681 (100%)

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	277	THR	8.4
1	1-A	357	ILE	6.9
1	1-A	317	LEU	6.9
1	1-B	28	ALA	6.7
1	1-B	353	ASN	6.5
1	1-B	354	TYR	6.4
1	1-B	335	ILE	6.2
1	1-B	273	GLU	6.2
1	1-B	49	THR	5.6
1	1-A	230	SER	5.5
1	1-B	341	LEU	5.5
1	1-A	318	VAL	5.4
1	1-B	234	GLY	5.4
1	1-A	72	ILE	5.4
1	1-B	344	ASP	5.3
1	1-A	352	LYS	5.2
1	1-A	315	ALA	5.2
1	1-B	179	LEU	5.2
1	1-B	355	GLN	5.1
1	1-B	58	LYS	5.0
1	1-B	178	GLY	5.0
1	1-A	312	ARG	5.0
1	1-A	209	THR	4.9
1	1-A	206	LYS	4.9
1	1-A	41	LEU	4.9
1	1-A	356	GLN	4.8
1	1-B	156	VAL	4.8
1	1-A	202	PHE	4.8
1	1-B	356	GLN	4.5
1	1-A	299	THR	4.4
1	1-B	147	SER	4.4
1	1-B	216	LEU	4.4
1	1-A	297	GLU	4.4
1	1-A	234	GLY	4.4
1	1-B	254	ILE	4.4
1	1-B	357	ILE	4.4
1	1-A	14	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	159	CYS	4.4
1	1-A	207	THR	4.3
1	1-A	353	ASN	4.3
1	1-A	233	ASP	4.3
1	1-B	232	GLU	4.3
1	1-B	29	PRO	4.2
1	1-B	299	THR	4.2
1	1-A	252	THR	4.2
1	1-A	36	VAL	4.2
1	1-A	229	LEU	4.2
1	1-A	44	ALA	4.2
1	1-B	163	ALA	4.2
1	1-A	57	THR	4.1
1	1-A	293	SER	4.1
1	1-A	51	ASN	4.0
1	1-A	359	LEU	4.0
1	1-A	47	PHE	4.0
1	1-B	26	HIS	4.0
1	1-B	250	GLU	4.0
1	1-A	316	ARG	4.0
1	1-A	264	ASP	3.9
1	1-B	236	THR	3.9
1	1-A	108	VAL	3.9
1	1-A	143	PHE	3.9
1	1-B	34	SER	3.9
1	1-A	198	LEU	3.9
1	1-B	155	THR	3.9
1	1-A	295	PRO	3.9
1	1-B	345	ALA	3.9
1	1-B	360	SER	3.9
1	1-A	341	LEU	3.8
1	1-A	203	GLU	3.7
1	1-A	73	ASP	3.7
1	1-A	358	SER	3.7
1	1-A	298	HIS	3.7
1	1-A	139	LEU	3.7
1	1-A	354	TYR	3.7
1	1-B	340	GLN	3.7
1	1-A	69	ASP	3.6
1	1-A	144	LEU	3.6
1	1-B	338	LYS	3.5
1	1-B	122	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	258	GLY	3.5
1	1-A	208	VAL	3.4
1	1-A	58	LYS	3.4
1	1-A	82	SER	3.4
1	1-A	360	SER	3.4
1	1-B	164	GLY	3.4
1	1-B	300	VAL	3.4
1	1-B	45	LYS	3.4
1	1-B	243	PHE	3.3
1	1-A	201	ASN	3.3
1	1-A	89	ILE	3.3
1	1-A	331	TYR	3.3
1	1-A	231	TRP	3.3
1	1-A	218	GLU	3.3
1	1-A	196	THR	3.3
1	1-A	308	ALA	3.3
1	1-A	142	GLU	3.2
1	1-A	301	LYS	3.2
1	1-B	237	ALA	3.2
1	1-B	351	ASP	3.2
1	1-B	203	GLU	3.2
1	1-B	321	ILE	3.2
1	1-B	337	ARG	3.2
1	1-A	83	LEU	3.2
1	1-A	204	LEU	3.2
1	1-A	250	GLU	3.2
1	1-A	152	GLN	3.2
1	1-B	211	PHE	3.1
1	1-A	279	SER	3.1
1	1-A	334	SER	3.1
1	1-A	52	ASN	3.1
1	1-A	53	TYR	3.0
1	1-A	282	ALA	3.0
1	1-B	50	ALA	3.0
1	1-B	71	GLU	3.0
1	1-A	205	PRO	3.0
1	1-A	114	ILE	3.0
1	1-A	344	ASP	3.0
1	1-A	33	ILE	3.0
1	1-A	148	GLU	3.0
1	1-A	31	ALA	3.0
1	1-A	227	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	1-B	30	ASN	3.0
1	1-A	210	ALA	2.9
1	1-B	247	LEU	2.9
1	1-B	62	SER	2.9
1	1-A	350	VAL	2.9
1	1-B	37	ALA	2.9
1	1-B	117	ALA	2.9
1	1-B	306	GLN	2.9
1	1-A	256	THR	2.9
1	1-A	232	GLU	2.9
1	1-B	348	GLU	2.9
1	1-B	6	GLN	2.9
1	1-A	355	GLN	2.8
1	1-A	283	TRP	2.8
1	1-A	311	VAL	2.8
1	1-B	27	LEU	2.8
1	1-B	63	TYR	2.8
1	1-A	292	VAL	2.8
1	1-A	49	THR	2.7
1	1-B	248	THR	2.7
1	1-B	276	PHE	2.7
1	1-A	261	ARG	2.7
1	1-A	314	PHE	2.7
1	1-B	51	ASN	2.7
1	1-B	246	ASN	2.7
1	1-A	63	TYR	2.7
1	1-A	259	THR	2.7
1	1-B	54	PRO	2.6
1	1-B	150	PHE	2.6
1	1-B	347	LYS	2.6
1	1-A	146	ASP	2.6
1	1-A	147	SER	2.6
1	1-A	240	TYR	2.6
1	1-B	210	ALA	2.6
1	1-B	311	VAL	2.6
1	1-B	343	VAL	2.6
1	1-B	74	ALA	2.6
1	1-B	256	THR	2.6
1	1-A	338	LYS	2.6
1	1-A	254	ILE	2.5
1	1-A	276	PHE	2.5
1	1-A	158	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	255	GLY	2.5
1	1-B	68	GLU	2.5
1	1-B	157	GLN	2.5
1	1-A	280	THR	2.5
1	1-B	40	SER	2.5
1	1-B	196	THR	2.5
1	1-B	23	ARG	2.5
1	1-B	149	ARG	2.5
1	1-B	186	GLY	2.5
1	1-A	281	LYS	2.5
1	1-A	313	GLU	2.5
1	1-A	118	CYS	2.4
1	1-A	117	ALA	2.4
1	1-A	125	ILE	2.4
1	1-A	140	LEU	2.4
1	1-A	197	LEU	2.4
1	1-B	75	LEU	2.4
1	1-A	121	ASN	2.4
1	1-A	300	VAL	2.4
1	1-A	68	GLU	2.4
1	1-B	56	SER	2.4
1	1-B	7	ILE	2.4
1	1-B	180	ASP	2.4
1	1-B	79	LEU	2.4
1	1-A	85	VAL	2.4
1	1-B	15	ALA	2.4
1	1-A	42	GLU	2.4
1	1-A	55	GLU	2.4
1	1-B	293	SER	2.4
1	1-A	102	LYS	2.4
1	1-A	70	PRO	2.3
1	1-A	302	THR	2.3
1	1-A	161	SER	2.3
1	1-B	17	ILE	2.3
1	1-B	16	ASP	2.3
1	1-B	83	LEU	2.3
1	1-A	54	PRO	2.3
1	1-A	9	ILE	2.3
1	1-B	9	ILE	2.3
1	1-A	351	ASP	2.3
1	1-A	309	CYS	2.3
1	1-B	14	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	213	GLY	2.3
1	1-B	296	SER	2.3
1	1-A	263	HIS	2.3
1	1-A	64	GLU	2.3
1	1-B	217	ASN	2.3
1	1-A	59	ILE	2.3
1	1-A	75	LEU	2.3
1	1-B	104	VAL	2.3
1	1-A	30	ASN	2.2
1	1-B	44	ALA	2.2
1	1-B	350	VAL	2.2
1	1-B	302	THR	2.2
1	1-B	176	LYS	2.2
1	1-B	270	LYS	2.2
1	1-A	7	ILE	2.2
1	1-B	358	SER	2.2
1	1-A	332	TRP	2.2
1	1-B	148	GLU	2.2
1	1-B	342	VAL	2.2
1	1-A	35	GLY	2.2
1	1-A	65	SER	2.2
1	1-B	123	VAL	2.2
1	1-B	309	CYS	2.2
1	1-B	33	ILE	2.2
1	1-A	26	HIS	2.1
1	1-A	157	GLN	2.1
1	1-A	339	THR	2.1
1	1-A	267	ILE	2.1
1	1-B	283	TRP	2.1
1	1-A	116	ASP	2.1
1	1-B	327	LYS	2.1
1	1-A	333	PRO	2.1
1	1-A	66	LEU	2.1
1	1-B	304	LEU	2.1
1	1-A	38	SER	2.1
1	1-A	48	ALA	2.1
1	1-B	244	LEU	2.1
1	1-B	339	THR	2.1
1	1-A	141	LYS	2.1
1	1-B	352	LYS	2.1
1	1-A	56	SER	2.1
1	1-A	46	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	1-B	252	THR	2.0
1	1-A	76	TYR	2.0
1	1-B	76	TYR	2.0
1	1-B	108	VAL	2.0
1	1-B	162	PHE	2.0
1	1-B	110	GLU	2.0
1	1-B	35	GLY	2.0
1	1-A	22	SER	2.0
1	1-B	82	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.