



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:37 am BST

PDB ID : 6IQK  
Title : crystal structure of Arabidopsis thaliana Profilin 3  
Authors : Qiao, Z.; Gao, Y.  
Deposited on : 2018-11-08  
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

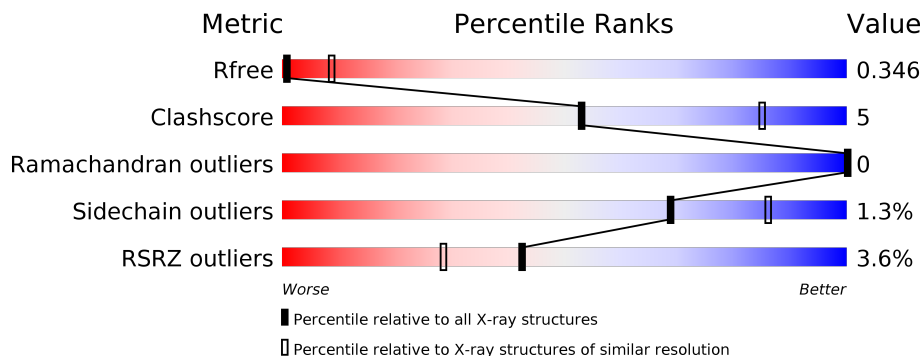
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

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



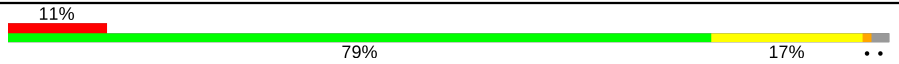


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	140	
1	B	140	
1	C	140	
1	D	140	
1	E	140	
1	F	140	

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Mol	Chain	Length	Quality of chain
1	G	140	 11% 79% 17% ..
1	H	140	 80% 19% ..
1	I	140	 4% 76% 21% .
1	J	140	 18% 87% 12% .
2	K	264	 96% .

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11558 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 Profilin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	137	1020	644	171	199	6	0	0	0
1	B	138	1024	648	171	199	6	0	0	0
1	C	137	1020	644	171	199	6	0	0	0
1	D	138	1024	648	171	199	6	0	0	0
1	E	137	1020	644	171	199	6	0	0	0
1	F	139	1033	654	173	200	6	0	0	0
1	I	136	1011	638	169	198	6	0	0	0
1	J	139	1033	654	173	200	6	0	0	0
1	G	137	1020	644	171	199	6	0	0	0
1	H	139	1033	654	173	200	6	0	0	0

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	LYS	-	expression tag	UNP Q9FE63
A	30	VAL	-	expression tag	UNP Q9FE63
A	31	LYS	-	expression tag	UNP Q9FE63
A	32	LYS	-	expression tag	UNP Q9FE63
A	33	ALA	-	expression tag	UNP Q9FE63
A	34	ALA	-	expression tag	UNP Q9FE63
A	35	ALA	-	expression tag	UNP Q9FE63
A	36	THR	-	expression tag	UNP Q9FE63
A	37	ASN	-	expression tag	UNP Q9FE63

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Chain	Residue	Modelled	Actual	Comment	Reference
A	136	GLN	LEU	conflict	UNP Q9FE63
A	154	LEU	MET	conflict	UNP Q9FE63
B	29	LYS	-	expression tag	UNP Q9FE63
B	30	VAL	-	expression tag	UNP Q9FE63
B	31	LYS	-	expression tag	UNP Q9FE63
B	32	LYS	-	expression tag	UNP Q9FE63
B	33	ALA	-	expression tag	UNP Q9FE63
B	34	ALA	-	expression tag	UNP Q9FE63
B	35	ALA	-	expression tag	UNP Q9FE63
B	36	THR	-	expression tag	UNP Q9FE63
B	37	ASN	-	expression tag	UNP Q9FE63
B	136	GLN	LEU	conflict	UNP Q9FE63
B	154	LEU	MET	conflict	UNP Q9FE63
C	29	LYS	-	expression tag	UNP Q9FE63
C	30	VAL	-	expression tag	UNP Q9FE63
C	31	LYS	-	expression tag	UNP Q9FE63
C	32	LYS	-	expression tag	UNP Q9FE63
C	33	ALA	-	expression tag	UNP Q9FE63
C	34	ALA	-	expression tag	UNP Q9FE63
C	35	ALA	-	expression tag	UNP Q9FE63
C	36	THR	-	expression tag	UNP Q9FE63
C	37	ASN	-	expression tag	UNP Q9FE63
C	136	GLN	LEU	conflict	UNP Q9FE63
C	154	LEU	MET	conflict	UNP Q9FE63
D	29	LYS	-	expression tag	UNP Q9FE63
D	30	VAL	-	expression tag	UNP Q9FE63
D	31	LYS	-	expression tag	UNP Q9FE63
D	32	LYS	-	expression tag	UNP Q9FE63
D	33	ALA	-	expression tag	UNP Q9FE63
D	34	ALA	-	expression tag	UNP Q9FE63
D	35	ALA	-	expression tag	UNP Q9FE63
D	36	THR	-	expression tag	UNP Q9FE63
D	37	ASN	-	expression tag	UNP Q9FE63
D	136	GLN	LEU	conflict	UNP Q9FE63
D	154	LEU	MET	conflict	UNP Q9FE63
E	29	LYS	-	expression tag	UNP Q9FE63
E	30	VAL	-	expression tag	UNP Q9FE63
E	31	LYS	-	expression tag	UNP Q9FE63
E	32	LYS	-	expression tag	UNP Q9FE63
E	33	ALA	-	expression tag	UNP Q9FE63
E	34	ALA	-	expression tag	UNP Q9FE63
E	35	ALA	-	expression tag	UNP Q9FE63

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Chain	Residue	Modelled	Actual	Comment	Reference
E	36	THR	-	expression tag	UNP Q9FE63
E	37	ASN	-	expression tag	UNP Q9FE63
E	136	GLN	LEU	conflict	UNP Q9FE63
E	154	LEU	MET	conflict	UNP Q9FE63
F	29	LYS	-	expression tag	UNP Q9FE63
F	30	VAL	-	expression tag	UNP Q9FE63
F	31	LYS	-	expression tag	UNP Q9FE63
F	32	LYS	-	expression tag	UNP Q9FE63
F	33	ALA	-	expression tag	UNP Q9FE63
F	34	ALA	-	expression tag	UNP Q9FE63
F	35	ALA	-	expression tag	UNP Q9FE63
F	36	THR	-	expression tag	UNP Q9FE63
F	37	ASN	-	expression tag	UNP Q9FE63
F	136	GLN	LEU	conflict	UNP Q9FE63
F	154	LEU	MET	conflict	UNP Q9FE63
I	29	LYS	-	expression tag	UNP Q9FE63
I	30	VAL	-	expression tag	UNP Q9FE63
I	31	LYS	-	expression tag	UNP Q9FE63
I	32	LYS	-	expression tag	UNP Q9FE63
I	33	ALA	-	expression tag	UNP Q9FE63
I	34	ALA	-	expression tag	UNP Q9FE63
I	35	ALA	-	expression tag	UNP Q9FE63
I	36	THR	-	expression tag	UNP Q9FE63
I	37	ASN	-	expression tag	UNP Q9FE63
I	136	GLN	LEU	conflict	UNP Q9FE63
I	154	LEU	MET	conflict	UNP Q9FE63
J	29	LYS	-	expression tag	UNP Q9FE63
J	30	VAL	-	expression tag	UNP Q9FE63
J	31	LYS	-	expression tag	UNP Q9FE63
J	32	LYS	-	expression tag	UNP Q9FE63
J	33	ALA	-	expression tag	UNP Q9FE63
J	34	ALA	-	expression tag	UNP Q9FE63
J	35	ALA	-	expression tag	UNP Q9FE63
J	36	THR	-	expression tag	UNP Q9FE63
J	37	ASN	-	expression tag	UNP Q9FE63
J	136	GLN	LEU	conflict	UNP Q9FE63
J	154	LEU	MET	conflict	UNP Q9FE63
G	29	LYS	-	expression tag	UNP Q9FE63
G	30	VAL	-	expression tag	UNP Q9FE63
G	31	LYS	-	expression tag	UNP Q9FE63
G	32	LYS	-	expression tag	UNP Q9FE63
G	33	ALA	-	expression tag	UNP Q9FE63

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Chain	Residue	Modelled	Actual	Comment	Reference
G	34	ALA	-	expression tag	UNP Q9FE63
G	35	ALA	-	expression tag	UNP Q9FE63
G	36	THR	-	expression tag	UNP Q9FE63
G	37	ASN	-	expression tag	UNP Q9FE63
G	136	GLN	LEU	conflict	UNP Q9FE63
G	154	LEU	MET	conflict	UNP Q9FE63
H	29	LYS	-	expression tag	UNP Q9FE63
H	30	VAL	-	expression tag	UNP Q9FE63
H	31	LYS	-	expression tag	UNP Q9FE63
H	32	LYS	-	expression tag	UNP Q9FE63
H	33	ALA	-	expression tag	UNP Q9FE63
H	34	ALA	-	expression tag	UNP Q9FE63
H	35	ALA	-	expression tag	UNP Q9FE63
H	36	THR	-	expression tag	UNP Q9FE63
H	37	ASN	-	expression tag	UNP Q9FE63
H	136	GLN	LEU	conflict	UNP Q9FE63
H	154	LEU	MET	conflict	UNP Q9FE63

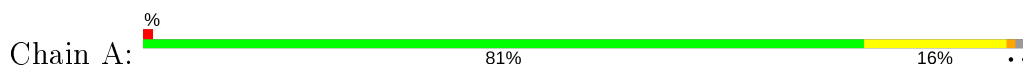
- Molecule 2 is a protein called AtPRF3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
2	K	264	1320	792	264	264	0	0	0

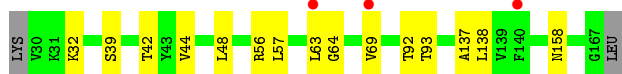
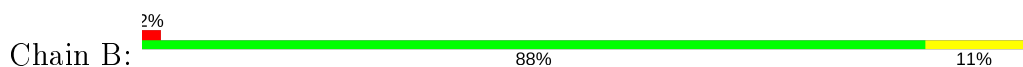
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Profilin-5



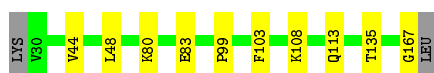
- Molecule 1: Profilin-5



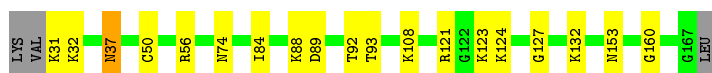
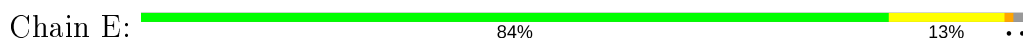
- Molecule 1: Profilin-5



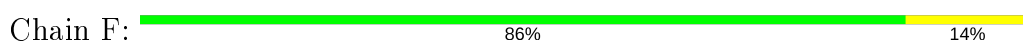
- Molecule 1: Profilin-5



- Molecule 1: Profilin-5



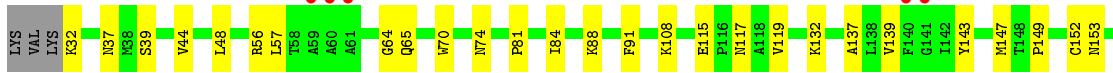
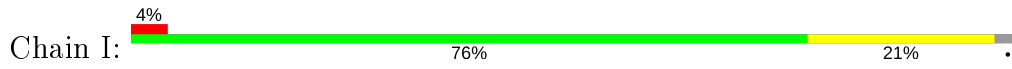
- Molecule 1: Profilin-5



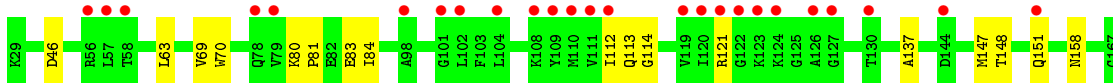
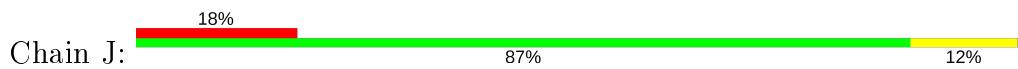




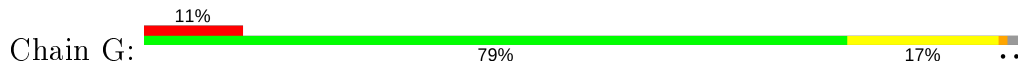
- Molecule 1: Profilin-5



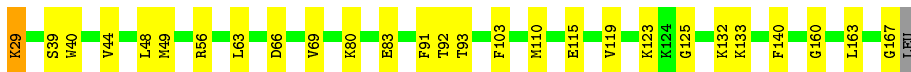
- Molecule 1: Profilin-5



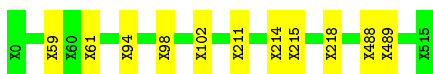
- Molecule 1: Profilin-5



- Molecule 1: Profilin-5



- Molecule 2: AtPRF3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.90Å 153.37Å 196.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.60 49.24 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.24-3.60) 100.0 (49.24-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.309 , 0.346 0.309 , 0.346	Depositor DCC
$R_{free}$ test set	4828 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	114.5	Xtrriage
Anisotropy	0.522	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 105.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	11558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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	A	0.25	0/1039	0.43	0/1410
1	B	0.25	0/1043	0.45	0/1416
1	C	0.26	0/1039	0.43	0/1410
1	D	0.26	0/1043	0.45	0/1416
1	E	0.25	0/1039	0.44	0/1410
1	F	0.25	0/1052	0.44	0/1427
1	G	0.25	0/1039	0.44	0/1410
1	H	0.26	0/1052	0.45	0/1427
1	I	0.25	0/1030	0.44	0/1399
1	J	0.25	0/1052	0.44	0/1427
All	All	0.25	0/10428	0.44	0/14152

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 [i](#)

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	A	1020	0	1008	12	0
1	B	1024	0	1013	8	0
1	C	1020	0	1008	5	0
1	D	1024	0	1013	7	0
1	E	1020	0	1008	12	0
1	F	1033	0	1026	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1020	0	1008	17	0
1	H	1033	0	1026	17	0
1	I	1011	0	995	20	0
1	J	1033	0	1026	12	0
2	K	1320	0	353	6	0
All	All	11558	0	10484	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 119 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:LYS:NZ	1:J:46:ASP:OD2	2.17	0.76
1:G:91:PHE:O	1:G:117:ASN:ND2	2.19	0.75
1:E:50:CYS:SG	1:F:31:LYS:NZ	2.60	0.74
1:A:37:ASN:O	1:A:37:ASN:ND2	2.20	0.73
1:G:80:LYS:HB3	1:G:82:GLU:OE2	1.92	0.69

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	A	135/140 (96%)	130 (96%)	5 (4%)	0	100	100
1	B	136/140 (97%)	127 (93%)	9 (7%)	0	100	100
1	C	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
1	D	136/140 (97%)	129 (95%)	7 (5%)	0	100	100
1	E	135/140 (96%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	137/140 (98%)	131 (96%)	6 (4%)	0	100	100
1	G	135/140 (96%)	128 (95%)	7 (5%)	0	100	100
1	H	137/140 (98%)	131 (96%)	6 (4%)	0	100	100
1	I	134/140 (96%)	129 (96%)	5 (4%)	0	100	100
1	J	137/140 (98%)	129 (94%)	8 (6%)	0	100	100
All	All	1357/1400 (97%)	1291 (95%)	66 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	A	107/111 (96%)	103 (96%)	4 (4%)	34	66
1	B	107/111 (96%)	106 (99%)	1 (1%)	78	90
1	C	107/111 (96%)	106 (99%)	1 (1%)	78	90
1	D	107/111 (96%)	107 (100%)	0	100	100
1	E	107/111 (96%)	104 (97%)	3 (3%)	43	72
1	F	108/111 (97%)	108 (100%)	0	100	100
1	G	107/111 (96%)	104 (97%)	3 (3%)	43	72
1	H	108/111 (97%)	107 (99%)	1 (1%)	78	90
1	I	106/111 (96%)	105 (99%)	1 (1%)	78	90
1	J	108/111 (97%)	108 (100%)	0	100	100
All	All	1072/1110 (97%)	1058 (99%)	14 (1%)	69	86

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	37	ASN
1	E	56	ARG

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Mol	Chain	Res	Type
1	G	91	PHE
1	C	38	MET
1	G	38	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	151	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	K	27

The worst 5 of 27 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	87:UNK	C	94:UNK	N	104.00
1	K	24:UNK	C	32:UNK	N	82.70
1	K	180:UNK	C	185:UNK	N	75.31
1	K	188:UNK	C	209:UNK	N	75.18
1	K	36:UNK	C	40:UNK	N	70.73

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	A	137/140 (97%)	0.04	1 (0%) 87 78	104, 130, 146, 152	0
1	B	138/140 (98%)	0.08	3 (2%) 62 45	83, 111, 138, 164	0
1	C	137/140 (97%)	-0.16	0 100 100	70, 98, 120, 132	0
1	D	138/140 (98%)	-0.15	0 100 100	75, 94, 115, 138	0
1	E	137/140 (97%)	-0.23	0 100 100	90, 109, 128, 136	0
1	F	139/140 (99%)	-0.11	0 100 100	76, 96, 116, 161	0
1	G	137/140 (97%)	0.57	15 (10%) 5 3	98, 151, 183, 192	0
1	H	139/140 (99%)	-0.11	0 100 100	77, 100, 137, 169	0
1	I	136/140 (97%)	0.24	5 (3%) 41 27	93, 122, 145, 152	0
1	J	139/140 (99%)	0.92	25 (17%) 1 0	107, 176, 209, 220	0
2	K	0/264	-	-	-	-
All	All	1377/1664 (82%)	0.11	49 (3%) 42 28	70, 113, 184, 220	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	122	GLY	6.3
1	J	120	ILE	5.8
1	G	122	GLY	5.5
1	J	111	VAL	5.5
1	J	121	ARG	5.0

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.