



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 06:08 PM EDT

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 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

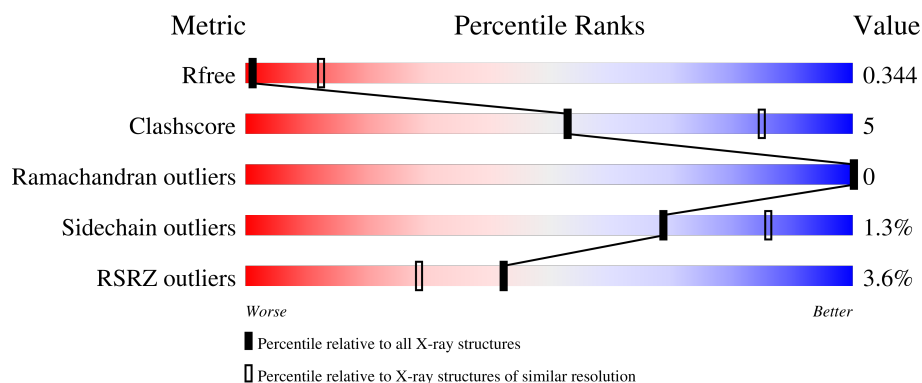
1 Overall quality at a glance

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 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	A	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 81%, yellow 81%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 81% 16% </div> </div>
1	B	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 88%, yellow 88%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 88% 11% </div> </div>
1	C	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 0%, green 90%, yellow 90%, yellow 98%, green 98%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 90% 8% </div> </div>
1	D	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 0%, green 91%, yellow 91%, yellow 98%, green 98%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 91% 7% </div> </div>
1	E	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 0%, green 84%, yellow 84%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 84% 13% </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	140	<div><div></div><div>86%14%</div><div></div></div>
1	G	140	<div><div>11%</div><div></div><div>79%17%</div><div></div></div>
1	H	140	<div><div></div><div>80%19%</div><div></div></div>
1	I	140	<div><div>4%</div><div></div><div>76%21%</div><div></div></div>
1	J	140	<div><div>18%</div><div></div><div>87%12%</div><div></div></div>
2	K	264	<div><div></div><div>96%</div><div></div></div>

2 Entry composition

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

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

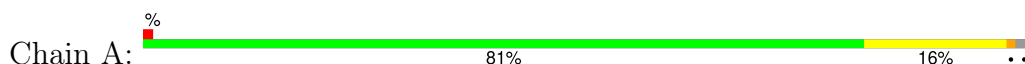
- Molecule 2 is a protein called AtPRF3.

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

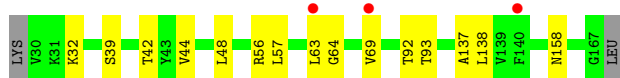
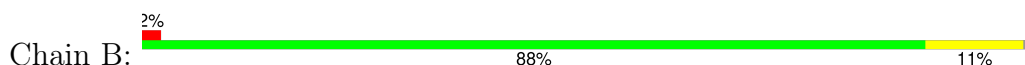
3 Residue-property plots [i](#)

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.

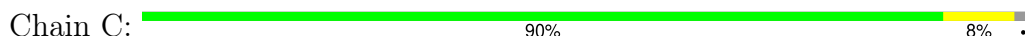
- Molecule 1: Profilin-5



- Molecule 1: Profilin-5



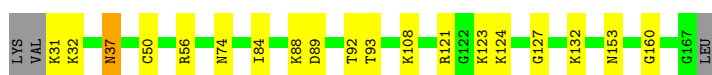
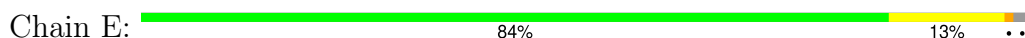
- Molecule 1: Profilin-5



- Molecule 1: Profilin-5



- Molecule 1: Profilin-5

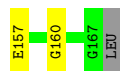
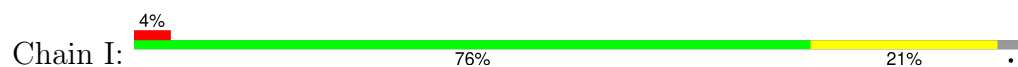


- Molecule 1: Profilin-5

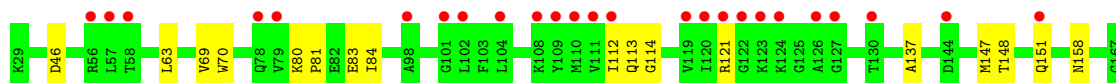
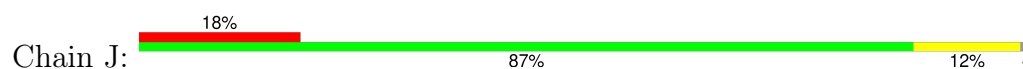




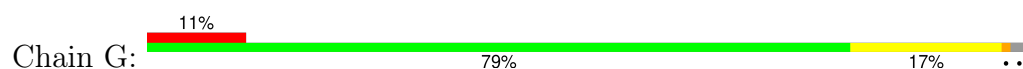
• Molecule 1: Profilin-5



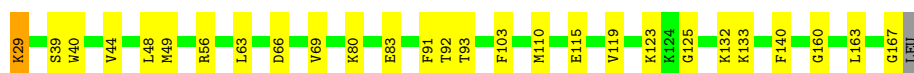
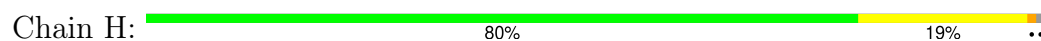
• Molecule 1: Profilin-5



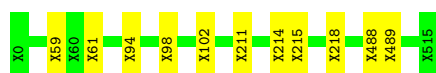
• Molecule 1: Profilin-5



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.309 , 0.346 0.310 , 0.344	Depositor DCC
R_{free} test set	4828 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 105.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11558	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage'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.*

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 [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.

All (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
1:J:148:THR:O	1:J:151:GLN:NE2	2.28	0.67
1:I:57:LEU:HA	1:I:147:MET:HE1	1.78	0.66
1:B:39:SER:OG	1:B:42:THR:OG1	2.12	0.65
1:I:91:PHE:O	1:I:117:ASN:ND2	2.28	0.65
1:D:135:THR:HG21	1:D:167:GLY:HA2	1.79	0.64
2:K:59:UNK:C	2:K:61:UNK:H	2.10	0.63
1:G:51:ASP:HB2	1:G:56:ARG:HE	1.64	0.62
1:B:63:LEU:HG	1:B:69:VAL:HA	1.84	0.60
1:D:113:GLN:HG3	1:H:66:ASP:OD2	2.02	0.60
1:F:135:THR:HG21	1:F:167:GLY:HA2	1.82	0.59
1:A:91:PHE:O	1:A:117:ASN:ND2	2.33	0.59
1:G:82:GLU:HA	1:G:85:GLN:HG2	1.83	0.59
1:J:112:ILE:HG12	1:J:113:GLN:H	1.67	0.59
1:B:64:GLY:HA2	1:B:137:ALA:HA	1.85	0.58
1:F:44:VAL:HG22	1:F:48:LEU:HD12	1.86	0.58
1:A:63:LEU:O	1:A:138:LEU:N	2.34	0.58
2:K:214:UNK:O	2:K:218:UNK:N	2.37	0.58
1:C:132:LYS:HG2	1:C:160:GLY:HA3	1.85	0.57
2:K:211:UNK:O	2:K:215:UNK:N	2.37	0.57
1:B:44:VAL:HG22	1:B:48:LEU:HD12	1.88	0.56
1:H:49:MET:O	1:H:56:ARG:NH1	2.39	0.56
1:H:80:LYS:HB2	1:H:83:GLU:HG2	1.89	0.55
1:G:98:ALA:HA	1:G:111:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:HG3	1:A:45:ASP:OD2	2.07	0.55
1:E:37:ASN:O	1:E:37:ASN:ND2	2.39	0.55
1:H:132:LYS:HG2	1:H:160:GLY:HA3	1.88	0.55
1:D:99:PRO:O	1:H:39:SER:OG	2.24	0.54
1:G:37:ASN:N	1:G:37:ASN:OD1	2.39	0.54
1:H:83:GLU:OE2	1:H:103:PHE:HB2	2.07	0.54
1:B:63:LEU:O	1:B:138:LEU:N	2.41	0.54
1:I:143:TYR:HB3	1:I:152:CYS:HB2	1.89	0.54
1:G:63:LEU:HD23	1:G:69:VAL:HA	1.89	0.53
1:H:115:GLU:HB2	1:H:119:VAL:HB	1.91	0.53
1:J:114:GLY:HA2	1:J:121:ARG:NH1	2.24	0.53
2:K:98:UNK:O	2:K:102:UNK:N	2.42	0.52
1:I:132:LYS:HG2	1:I:160:GLY:HA3	1.91	0.52
1:F:126:ALA:HB1	1:F:145:GLU:HB3	1.92	0.52
1:H:63:LEU:HD12	1:H:140:PHE:CE1	2.46	0.51
2:K:94:UNK:O	2:K:98:UNK:N	2.42	0.51
1:J:80:LYS:HB2	1:J:83:GLU:HG3	1.93	0.51
1:J:147:MET:HE3	1:J:151:GLN:HE22	1.75	0.51
1:D:99:PRO:HA	1:H:40:TRP:HB2	1.93	0.51
1:A:49:MET:O	1:A:56:ARG:NH2	2.44	0.50
1:E:121:ARG:NE	1:E:153:ASN:HD21	2.10	0.50
1:A:89:ASP:O	1:A:93:THR:OG1	2.28	0.49
1:C:92:THR:HG22	1:C:93:THR:HG23	1.94	0.49
1:I:44:VAL:HG22	1:I:48:LEU:HD12	1.95	0.49
1:H:63:LEU:HD23	1:H:69:VAL:HA	1.95	0.49
1:J:63:LEU:HD22	1:J:69:VAL:HG22	1.95	0.48
1:B:92:THR:HG22	1:B:93:THR:HG23	1.95	0.48
1:F:80:LYS:HB2	1:F:83:GLU:HG3	1.96	0.48
1:E:108:LYS:HZ3	1:I:39:SER:H	1.62	0.48
1:A:64:GLY:HA2	1:A:137:ALA:HA	1.95	0.47
1:F:39:SER:O	1:F:42:THR:OG1	2.32	0.47
1:E:132:LYS:HG2	1:E:160:GLY:HA3	1.96	0.47
1:H:44:VAL:HG22	1:H:48:LEU:HD12	1.96	0.47
1:I:37:ASN:N	1:I:37:ASN:OD1	2.48	0.46
1:A:90:ASP:OD1	1:A:95:GLY:N	2.49	0.46
1:J:70:TRP:CZ3	1:J:137:ALA:HB2	2.51	0.46
1:H:92:THR:HG22	1:H:93:THR:HG23	1.97	0.46
1:D:44:VAL:HG22	1:D:48:LEU:HD12	1.98	0.45
1:G:121:ARG:CZ	1:G:153:ASN:HD21	2.29	0.45
1:H:29:LYS:N	1:H:29:LYS:HD3	2.31	0.45
1:I:65:GLN:O	1:I:88:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:TRP:CZ3	1:I:137:ALA:HB2	2.51	0.45
1:J:114:GLY:HA2	1:J:121:ARG:HH11	1.81	0.45
1:G:63:LEU:O	1:G:138:LEU:N	2.38	0.45
1:F:30:VAL:HG23	1:F:31:LYS:H	1.82	0.45
1:G:63:LEU:HD12	1:G:140:PHE:CE1	2.52	0.45
1:I:81:PRO:HA	1:I:84:ILE:HD12	1.99	0.45
1:I:115:GLU:HB3	1:I:119:VAL:HB	1.98	0.45
1:A:44:VAL:HG22	1:A:48:LEU:HD12	1.98	0.45
1:F:63:LEU:HD22	1:F:69:VAL:HA	1.98	0.45
1:G:91:PHE:HB2	1:G:133:LYS:NZ	2.31	0.45
1:E:123:LYS:HD3	1:E:127:GLY:O	2.17	0.45
1:F:57:LEU:HD23	1:F:147:MET:SD	2.58	0.44
1:D:80:LYS:HB2	1:D:83:GLU:HG3	1.99	0.44
1:D:103:PHE:CE2	1:D:108:LYS:HB3	2.52	0.43
1:C:91:PHE:O	1:C:117:ASN:ND2	2.39	0.43
1:G:51:ASP:HA	1:G:56:ARG:HG2	2.00	0.43
1:G:143:TYR:OH	1:G:149:PRO:HG3	2.18	0.43
1:C:49:MET:O	1:C:56:ARG:NH1	2.51	0.43
1:I:108:LYS:HB3	1:I:108:LYS:HE2	1.68	0.43
1:F:92:THR:HG22	1:F:93:THR:HG23	2.00	0.43
1:F:35:ALA:CB	1:H:125:GLY:HA2	2.48	0.43
1:I:143:TYR:CZ	1:I:149:PRO:HG3	2.53	0.43
1:H:110:MET:O	1:H:123:LYS:N	2.50	0.43
2:K:488:UNK:HA	2:K:489:UNK:HA	1.53	0.43
1:C:63:LEU:HG	1:C:69:VAL:HA	2.00	0.42
1:I:44:VAL:HA	1:I:48:LEU:HB2	2.01	0.42
1:G:70:TRP:CZ3	1:G:137:ALA:HB2	2.54	0.42
1:J:112:ILE:HG12	1:J:113:GLN:N	2.32	0.42
1:I:32:LYS:HB2	1:J:158:ASN:OD1	2.19	0.42
1:E:31:LYS:HB3	1:E:32:LYS:H	1.75	0.42
1:I:74:ASN:OD1	1:I:74:ASN:N	2.51	0.42
1:E:84:ILE:HG23	1:E:88:LYS:NZ	2.35	0.41
1:I:153:ASN:HB3	1:I:157:GLU:OE2	2.20	0.41
1:A:91:PHE:CE1	1:A:120:ILE:HG13	2.54	0.41
1:G:44:VAL:HG22	1:G:48:LEU:HD12	2.02	0.41
1:G:64:GLY:HA2	1:G:137:ALA:HA	2.01	0.41
1:J:81:PRO:HA	1:J:84:ILE:HG12	2.02	0.41
1:H:163:LEU:O	1:H:167:GLY:N	2.32	0.41
1:A:63:LEU:HG	1:A:69:VAL:HA	2.01	0.41
1:E:121:ARG:HE	1:E:153:ASN:HD21	1.69	0.41
1:I:64:GLY:HA2	1:I:137:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:HG2	1:B:57:LEU:N	2.36	0.41
1:E:89:ASP:HA	1:E:92:THR:HB	2.03	0.41
1:I:132:LYS:HB3	1:I:139:VAL:HB	2.02	0.41
1:G:120:ILE:HG13	1:G:133:LYS:NZ	2.36	0.41
1:H:91:PHE:CG	1:H:133:LYS:HD2	2.55	0.41
1:B:32:LYS:HA	1:B:32:LYS:HD3	1.96	0.41
1:E:92:THR:HG22	1:E:93:THR:HG23	2.02	0.41
1:A:132:LYS:HG2	1:A:160:GLY:HA3	2.03	0.40
1:I:147:MET:HE3	1:I:147:MET:HB3	1.88	0.40

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	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
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 ⓘ

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

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	32	LYS
1	A	37	ASN
1	A	39	SER
1	B	158	ASN
1	C	38	MET
1	E	37	ASN
1	E	56	ARG
1	E	74	ASN
1	I	56	ARG
1	G	38	MET
1	G	91	PHE
1	G	133	LYS
1	H	29	LYS

Sometimes 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 monosaccharides 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

All 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
1	K	304:UNK	C	337:UNK	N	62.22
1	K	502:UNK	C	512:UNK	N	37.39

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	63:UNK	C	78:UNK	N	36.14
1	K	113:UNK	C	127:UNK	N	33.77
1	K	255:UNK	C	275:UNK	N	28.47
1	K	280:UNK	C	296:UNK	N	27.98
1	K	459:UNK	C	466:UNK	N	26.33
1	K	44:UNK	C	47:UNK	N	26.30
1	K	410:UNK	C	418:UNK	N	23.76
1	K	444:UNK	C	454:UNK	N	23.61
1	K	373:UNK	C	383:UNK	N	21.01
1	K	346:UNK	C	367:UNK	N	19.90
1	K	471:UNK	C	479:UNK	N	18.62
1	K	137:UNK	C	164:UNK	N	17.56
1	K	247:UNK	C	249:UNK	N	16.60
1	K	423:UNK	C	431:UNK	N	15.39
1	K	391:UNK	C	398:UNK	N	14.45
1	K	231:UNK	C	233:UNK	N	10.29
1	K	238:UNK	C	243:UNK	N	9.07
1	K	402:UNK	C	404:UNK	N	8.72
1	K	18:UNK	C	22:UNK	N	8.64
1	K	8:UNK	C	10:UNK	N	4.22

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	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

All (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
1	G	121	ARG	4.6
1	G	102	LEU	4.3
1	J	110	MET	4.0
1	J	151	GLN	3.8
1	J	109	TYR	3.6
1	I	61	ALA	3.6
1	I	140	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	110	MET	3.4
1	J	123	LYS	3.4
1	I	59	ALA	3.2
1	J	108	LYS	3.2
1	J	78	GLN	3.1
1	J	102	LEU	3.1
1	G	112	ILE	3.1
1	J	144	ASP	2.9
1	G	140	PHE	2.8
1	G	109	TYR	2.7
1	J	119	VAL	2.7
1	J	79	VAL	2.6
1	G	104	LEU	2.5
1	J	126	ALA	2.5
1	G	130	THR	2.5
1	G	129	VAL	2.5
1	J	104	LEU	2.4
1	G	141	GLY	2.3
1	J	127	GLY	2.3
1	G	125	GLY	2.3
1	G	78	GLN	2.3
1	J	130	THR	2.3
1	I	60	ALA	2.3
1	B	140	PHE	2.3
1	J	57	LEU	2.3
1	J	98	ALA	2.2
1	G	120	ILE	2.2
1	B	69	VAL	2.2
1	J	112	ILE	2.2
1	J	124	LYS	2.2
1	B	63	LEU	2.1
1	J	101	GLY	2.1
1	J	56	ARG	2.1
1	J	58	THR	2.1
1	I	141	GLY	2.1
1	G	79	VAL	2.0
1	A	133	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.