



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2017 – 06:46 AM EST

PDB ID : 4DDG  
Title : Crystal structure of human OTUB1/UbcH5b Ub/Ub  
Authors : Juang, Y.C.; Sanches, M.; Sicheri, F.  
Deposited on : unknown  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

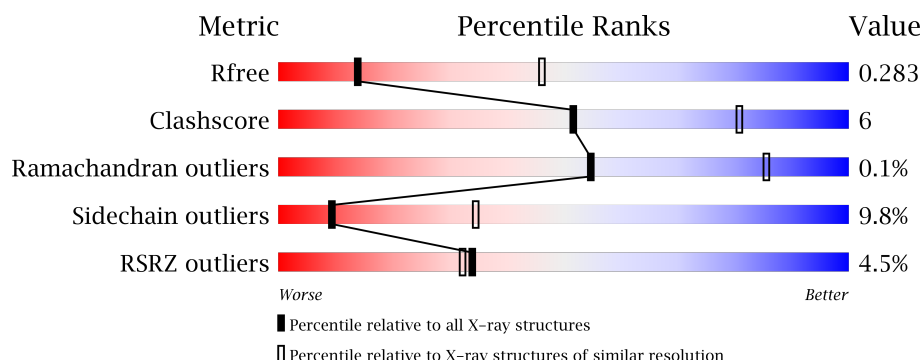
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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

Mol	Chain	Length	Quality of chain
1	A	399	<div> <div>12%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div> </div>
1	B	399	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
1	C	399	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	J	399	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
1	K	399	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	L	399	<div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div>
2	D	76	<div> <div>12%</div> <div></div> <div>70%</div> <div>29%</div> <div>.</div> </div>
2	E	76	<div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div>
2	F	76	<div> <div>18%</div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div>
2	G	76	<div> <div>7%</div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div>
2	H	76	<div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	I	76	<div> <div>4%</div> <div></div> <div>79%</div> <div>17%</div> <div>.</div> </div>
2	M	76	<div> <div></div> <div>72%</div> <div>26%</div> <div>.</div> </div>
2	N	76	<div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	O	76	<div> <div>17%</div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div>
2	P	76	<div> <div>4%</div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	Q	76	<div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	R	76	<div> <div>3%</div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26568 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 Ubiquitin-conjugating enzyme E2 D2, Ubiquitin thioesterase OTUB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3226	2055	542	616	13			
1	B	399	Total	C	N	O	S	0	0	0
			3226	2055	542	616	13			
1	C	399	Total	C	N	O	S	0	0	0
			3226	2055	542	616	13			
1	J	399	Total	C	N	O	S	0	0	0
			3226	2055	542	616	13			
1	K	399	Total	C	N	O	S	0	0	0
			3226	2055	542	616	13			
1	L	399	Total	C	N	O	S	0	0	0
			3226	2055	542	616	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P62837
A	0	ALA	-	EXPRESSION TAG	UNP P62837
A	85	SER	CYS	CONFLICT	UNP P62837
A	148	GLY	-	LINKER	UNP Q96FW1
A	149	GLY	-	LINKER	UNP Q96FW1
A	150	SER	-	LINKER	UNP Q96FW1
A	1091	SER	CYS	CONFLICT	UNP Q96FW1
B	-1	GLY	-	EXPRESSION TAG	UNP P62837
B	0	ALA	-	EXPRESSION TAG	UNP P62837
B	85	SER	CYS	CONFLICT	UNP P62837
B	148	GLY	-	LINKER	UNP Q96FW1
B	149	GLY	-	LINKER	UNP Q96FW1
B	150	SER	-	LINKER	UNP Q96FW1
B	1091	SER	CYS	CONFLICT	UNP Q96FW1
C	-1	GLY	-	EXPRESSION TAG	UNP P62837
C	0	ALA	-	EXPRESSION TAG	UNP P62837

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	85	SER	CYS	CONFLICT	UNP P62837
C	148	GLY	-	LINKER	UNP Q96FW1
C	149	GLY	-	LINKER	UNP Q96FW1
C	150	SER	-	LINKER	UNP Q96FW1
C	1091	SER	CYS	CONFLICT	UNP Q96FW1
J	-1	GLY	-	EXPRESSION TAG	UNP P62837
J	0	ALA	-	EXPRESSION TAG	UNP P62837
J	85	SER	CYS	CONFLICT	UNP P62837
J	148	GLY	-	LINKER	UNP Q96FW1
J	149	GLY	-	LINKER	UNP Q96FW1
J	150	SER	-	LINKER	UNP Q96FW1
J	1091	SER	CYS	CONFLICT	UNP Q96FW1
K	-1	GLY	-	EXPRESSION TAG	UNP P62837
K	0	ALA	-	EXPRESSION TAG	UNP P62837
K	85	SER	CYS	CONFLICT	UNP P62837
K	148	GLY	-	LINKER	UNP Q96FW1
K	149	GLY	-	LINKER	UNP Q96FW1
K	150	SER	-	LINKER	UNP Q96FW1
K	1091	SER	CYS	CONFLICT	UNP Q96FW1
L	-1	GLY	-	EXPRESSION TAG	UNP P62837
L	0	ALA	-	EXPRESSION TAG	UNP P62837
L	85	SER	CYS	CONFLICT	UNP P62837
L	148	GLY	-	LINKER	UNP Q96FW1
L	149	GLY	-	LINKER	UNP Q96FW1
L	150	SER	-	LINKER	UNP Q96FW1
L	1091	SER	CYS	CONFLICT	UNP Q96FW1

- Molecule 2 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	E	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	F	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	G	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	H	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	I	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

*Continued on next page...*

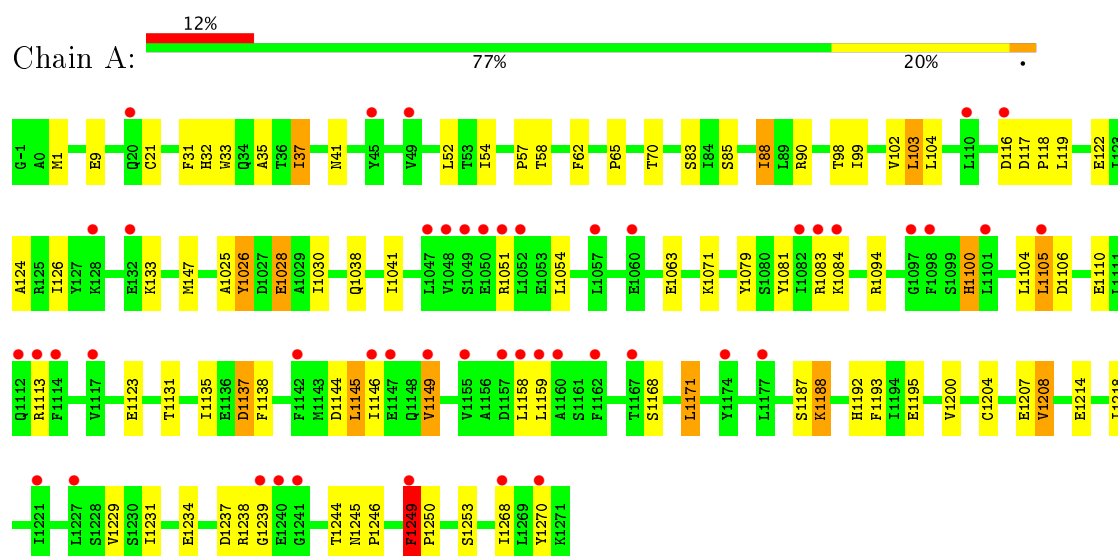
*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	76	Total 601	C 378	N 105	O 117	S 1	0	0	0
2	N	76	Total 601	C 378	N 105	O 117	S 1	0	0	0
2	O	76	Total 601	C 378	N 105	O 117	S 1	0	0	0
2	P	76	Total 601	C 378	N 105	O 117	S 1	0	0	0
2	Q	76	Total 601	C 378	N 105	O 117	S 1	0	0	0
2	R	76	Total 601	C 378	N 105	O 117	S 1	0	0	0

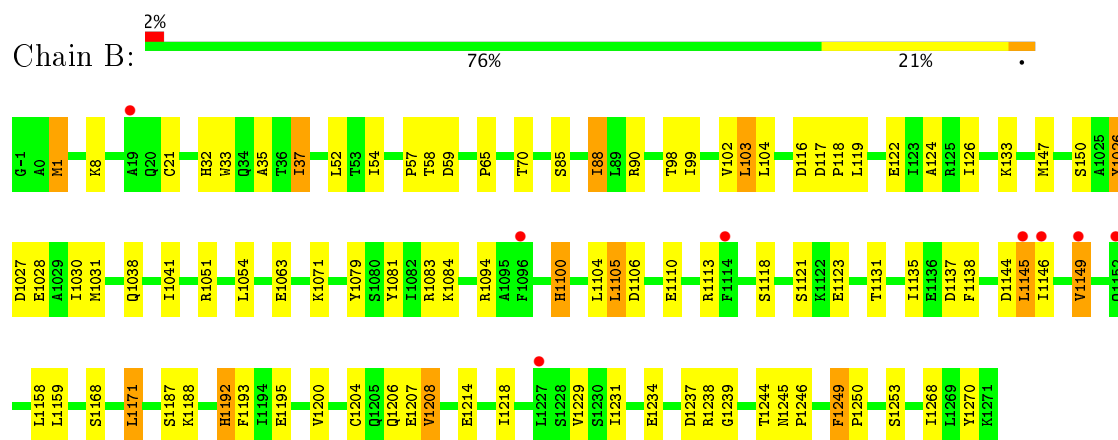
### 3 Residue-property plots

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.

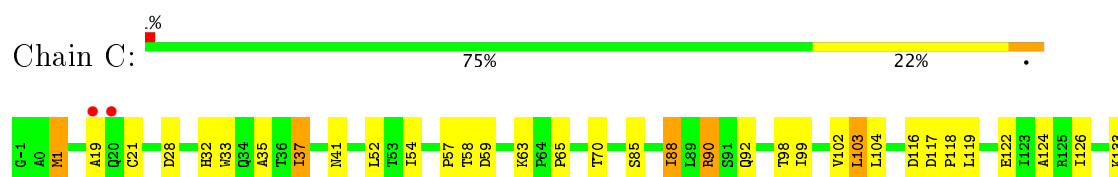
- Molecule 1: Ubiquitin-conjugating enzyme E2 D2, Ubiquitin thioesterase OTUB1

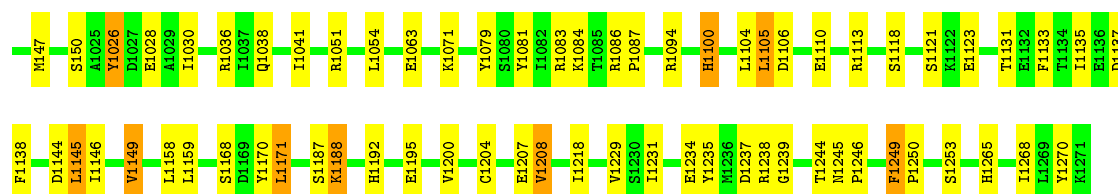


- Molecule 1: Ubiquitin-conjugating enzyme E2 D2, Ubiquitin thioesterase OTUB1

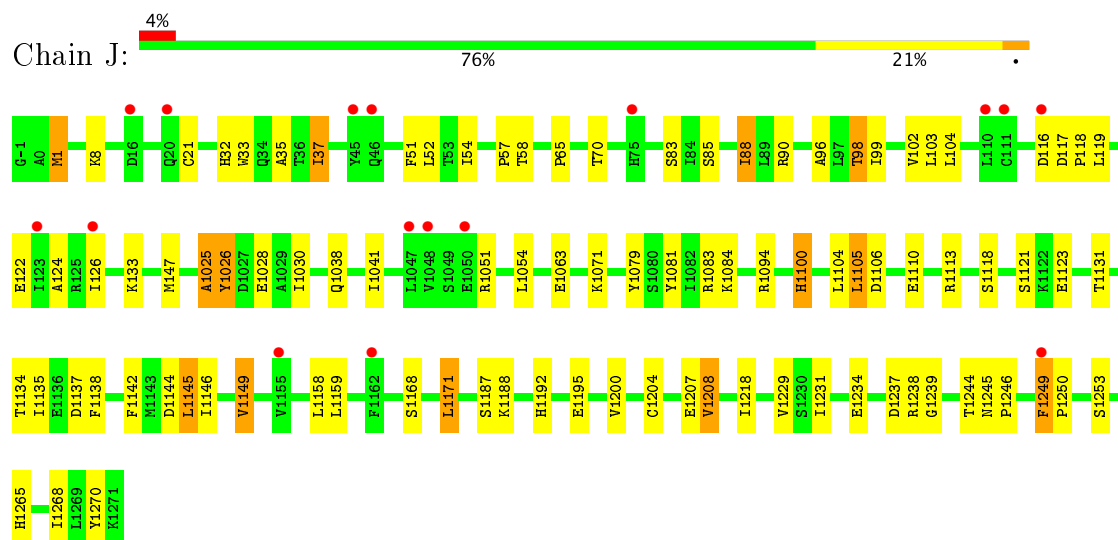


- Molecule 1: Ubiquitin-conjugating enzyme E2 D2, Ubiquitin thioesterase OTUB1

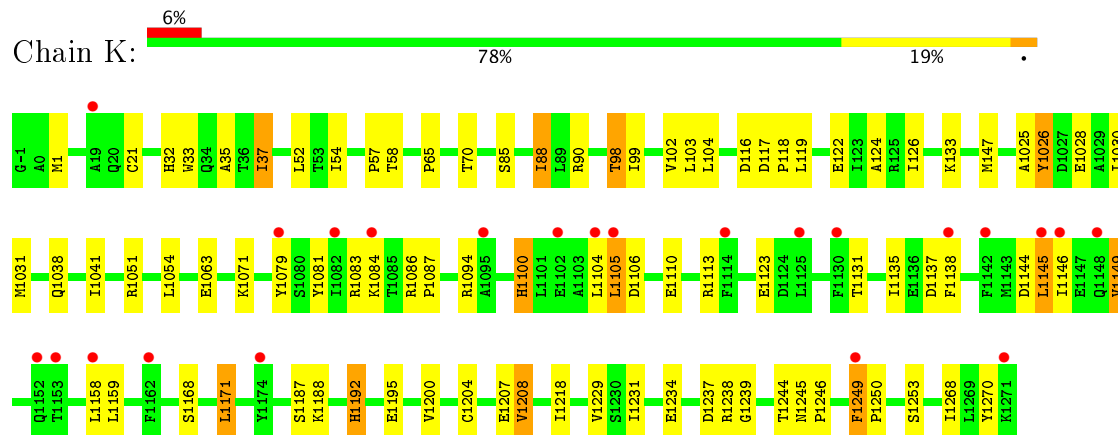




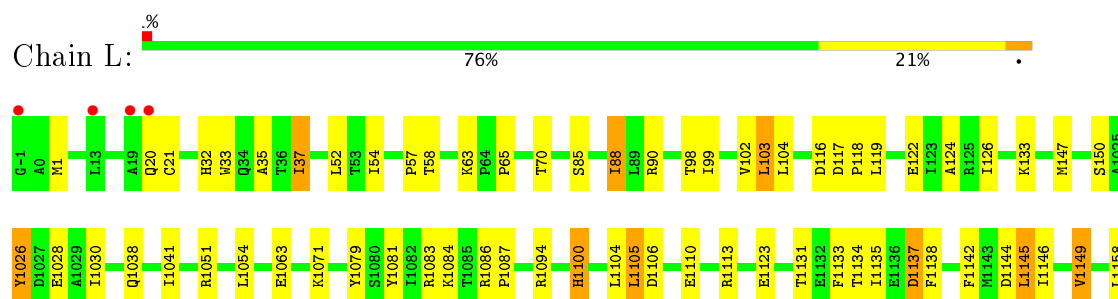
- Molecule 1: Ubiquitin-conjugating enzyme E2 D2, Ubiquitin thioesterase OTUB1



- Molecule 1: Ubiquitin-conjugating enzyme E2 D2, Ubiquitin thioesterase OTUB1



- Molecule 1: Ubiquitin-conjugating enzyme E2 D2, Ubiquitin thioesterase OTUB1



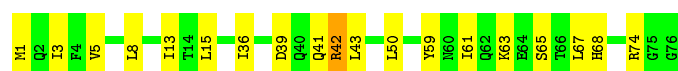




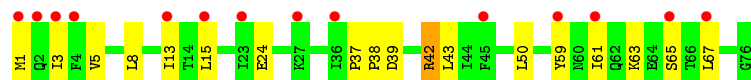
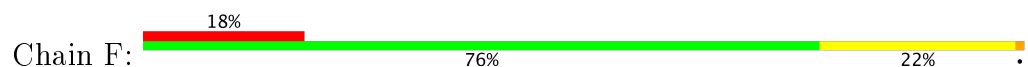
• Molecule 2: Polyubiquitin-C



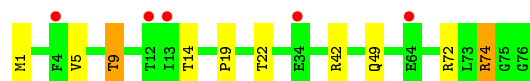
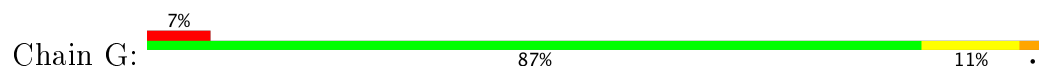
• Molecule 2: Polyubiquitin-C



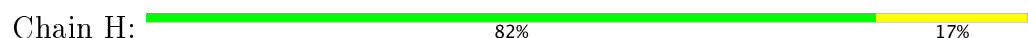
• Molecule 2: Polyubiquitin-C



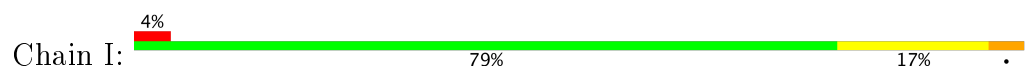
• Molecule 2: Polyubiquitin-C



• Molecule 2: Polyubiquitin-C



• Molecule 2: Polyubiquitin-C

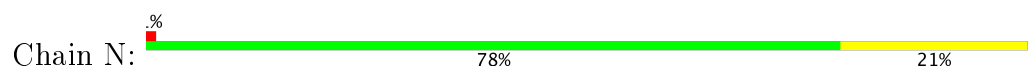


• Molecule 2: Polyubiquitin-C

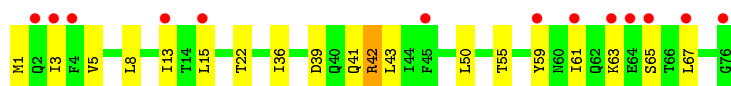
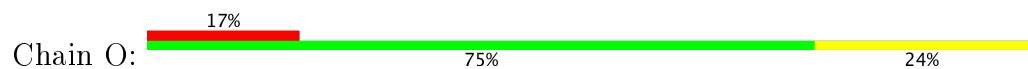




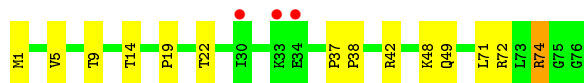
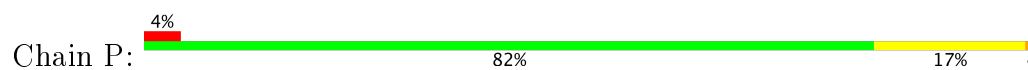
- Molecule 2: Polyubiquitin-C



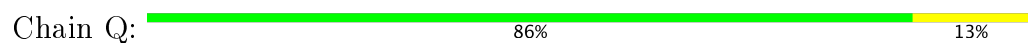
- Molecule 2: Polyubiquitin-C



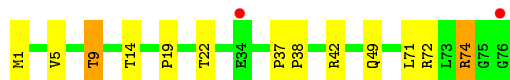
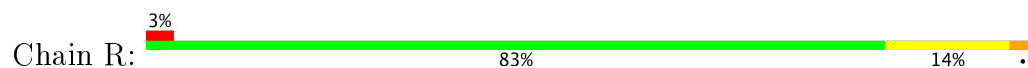
- Molecule 2: Polyubiquitin-C



- Molecule 2: Polyubiquitin-C



- Molecule 2: Polyubiquitin-C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.57Å 104.93Å 148.48Å 90.00° 104.19° 90.00°	Depositor
Resolution (Å)	49.12 – 3.30 49.29 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.12-3.30) 99.8 (49.29-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.233 , 0.280 0.234 , 0.283	Depositor DCC
$R_{free}$ test set	3055 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.7	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 103.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.37 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.3759e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 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	A	0.25	0/3306	0.48	0/4476
1	B	0.26	0/3306	0.49	0/4476
1	C	0.26	0/3306	0.49	0/4476
1	J	0.26	0/3306	0.48	0/4476
1	K	0.26	0/3306	0.48	0/4476
1	L	0.26	0/3306	0.48	0/4476
2	D	0.22	0/607	0.47	0/816
2	E	0.22	0/607	0.47	0/816
2	F	0.22	0/607	0.47	0/816
2	G	0.24	0/607	0.48	0/816
2	H	0.24	0/607	0.48	0/816
2	I	0.24	0/607	0.47	0/816
2	M	0.22	0/607	0.47	0/816
2	N	0.22	0/607	0.47	0/816
2	O	0.22	0/607	0.47	0/816
2	P	0.24	0/607	0.47	0/816
2	Q	0.24	0/607	0.48	0/816
2	R	0.24	0/607	0.47	0/816
All	All	0.25	0/27120	0.48	0/36648

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1249	PHE	Peptide
1	B	1249	PHE	Peptide
1	C	1249	PHE	Peptide
1	J	1249	PHE	Peptide
1	K	1249	PHE	Peptide
1	L	1249	PHE	Peptide

## 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	A	3226	0	3141	47	0
1	B	3226	0	3141	47	0
1	C	3226	0	3141	55	0
1	J	3226	0	3141	48	0
1	K	3226	0	3141	39	0
1	L	3226	0	3141	53	0
2	D	601	0	629	12	0
2	E	601	0	629	11	0
2	F	601	0	629	9	0
2	G	601	0	629	4	0
2	H	601	0	629	6	0
2	I	601	0	629	9	0
2	M	601	0	629	10	0
2	N	601	0	629	9	0
2	O	601	0	629	9	0
2	P	601	0	629	6	0
2	Q	601	0	629	5	0
2	R	601	0	629	6	0
All	All	26568	0	26394	339	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 6.

All (339) 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:L:85:SER:OG	2:Q:76:GLY:O	1.85	0.94
1:A:1188:LYS:NZ	2:N:31:GLN:OE1	2.05	0.89
1:C:85:SER:OG	2:H:76:GLY:O	1.93	0.86
1:L:1187:SER:HB2	1:L:1200:VAL:HG11	1.58	0.85
1:A:1187:SER:HB2	1:A:1200:VAL:HG11	1.59	0.84
1:C:1187:SER:HB2	1:C:1200:VAL:HG11	1.59	0.84
1:B:1187:SER:HB2	1:B:1200:VAL:HG11	1.59	0.84
1:J:1187:SER:HB2	1:J:1200:VAL:HG11	1.59	0.83
1:K:1187:SER:HB2	1:K:1200:VAL:HG11	1.59	0.83
1:C:1204:CYS:HA	1:C:1208:VAL:HG13	1.63	0.81
1:A:1204:CYS:HA	1:A:1208:VAL:HG13	1.63	0.81
1:B:1204:CYS:HA	1:B:1208:VAL:HG13	1.63	0.81
1:J:1204:CYS:HA	1:J:1208:VAL:HG13	1.63	0.81
1:K:1204:CYS:HA	1:K:1208:VAL:HG13	1.63	0.80
1:L:1204:CYS:HA	1:L:1208:VAL:HG13	1.63	0.80
1:B:1195:GLU:OE1	2:E:42:ARG:NH2	2.16	0.78
1:K:35:ALA:HB3	1:K:52:LEU:HB2	1.66	0.77
1:J:35:ALA:HB3	1:J:52:LEU:HB2	1.66	0.77
1:B:35:ALA:HB3	1:B:52:LEU:HB2	1.66	0.77
1:K:1195:GLU:OE1	2:N:42:ARG:NH2	2.17	0.77
1:A:31:PHE:CD1	1:C:28:ASP:HB2	2.18	0.77
1:C:35:ALA:HB3	1:C:52:LEU:HB2	1.66	0.77
1:L:35:ALA:HB3	1:L:52:LEU:HB2	1.66	0.76
1:A:35:ALA:HB3	1:A:52:LEU:HB2	1.66	0.76
1:C:1195:GLU:OE1	2:F:42:ARG:NH2	2.23	0.71
2:I:42:ARG:HD3	2:I:72:ARG:HH21	1.56	0.71
2:R:42:ARG:HD3	2:R:72:ARG:HH21	1.56	0.70
2:H:42:ARG:HD3	2:H:72:ARG:HH21	1.56	0.70
2:Q:42:ARG:HD3	2:Q:72:ARG:HH21	1.56	0.70
2:P:42:ARG:HD3	2:P:72:ARG:HH21	1.56	0.70
2:G:42:ARG:HD3	2:G:72:ARG:HH21	1.56	0.69
1:J:83:SER:OG	1:L:150:SER:HB2	1.94	0.66
1:J:1110:GLU:OE2	1:J:1113:ARG:NH2	2.30	0.65
1:K:1110:GLU:OE2	1:K:1113:ARG:NH2	2.30	0.65
1:C:1110:GLU:OE2	1:C:1113:ARG:NH2	2.30	0.64
1:C:41:ASN:ND2	2:I:11:LYS:HD2	2.12	0.64
1:B:1110:GLU:OE2	1:B:1113:ARG:NH2	2.30	0.64
1:L:1195:GLU:OE1	2:O:42:ARG:NH2	2.30	0.63
1:A:1110:GLU:OE2	1:A:1113:ARG:NH2	2.30	0.63
1:L:1110:GLU:OE2	1:L:1113:ARG:NH2	2.30	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:SER:OG	1:C:150:SER:HB2	1.99	0.62
1:B:1192:HIS:HB2	2:E:68:HIS:CE1	2.34	0.62
1:J:98:THR:HG22	1:L:1134:THR:HG21	1.81	0.61
1:L:1105:LEU:HD12	1:L:1149:VAL:HG23	1.83	0.60
1:A:1105:LEU:HD12	1:A:1149:VAL:HG23	1.83	0.60
1:K:1094:ARG:NH1	1:K:1168:SER:OG	2.36	0.59
1:B:1094:ARG:NH1	1:B:1168:SER:OG	2.36	0.59
1:J:1105:LEU:HD12	1:J:1149:VAL:HG23	1.83	0.59
1:L:1094:ARG:NH1	1:L:1168:SER:OG	2.36	0.59
1:C:1105:LEU:HD12	1:C:1149:VAL:HG23	1.83	0.59
1:B:1105:LEU:HD12	1:B:1149:VAL:HG23	1.83	0.59
1:J:1094:ARG:NH1	1:J:1168:SER:OG	2.35	0.59
1:C:1094:ARG:NH1	1:C:1168:SER:OG	2.35	0.59
1:A:1094:ARG:NH1	1:A:1168:SER:OG	2.35	0.59
1:K:1105:LEU:HD12	1:K:1149:VAL:HG23	1.83	0.58
1:A:1195:GLU:OE1	2:D:42:ARG:NH2	2.36	0.58
2:R:1:MET:HG2	2:R:19:PRO:HD3	1.86	0.57
2:I:1:MET:HG2	2:I:19:PRO:HD3	1.86	0.57
2:P:1:MET:HG2	2:P:19:PRO:HD3	1.86	0.57
2:H:1:MET:HG2	2:H:19:PRO:HD3	1.86	0.56
2:Q:1:MET:HG2	2:Q:19:PRO:HD3	1.86	0.56
1:L:1071:LYS:HE3	1:L:1244:THR:HG22	1.89	0.55
2:G:1:MET:HG2	2:G:19:PRO:HD3	1.86	0.55
1:B:1071:LYS:HE3	1:B:1244:THR:HG22	1.89	0.54
1:J:1071:LYS:HE3	1:J:1244:THR:HG22	1.89	0.54
1:K:1083:ARG:HB3	1:K:1268:ILE:HB	1.90	0.54
1:C:1071:LYS:HE3	1:C:1244:THR:HG22	1.89	0.54
1:C:1083:ARG:HB3	1:C:1268:ILE:HB	1.90	0.54
1:K:1071:LYS:HE3	1:K:1244:THR:HG22	1.89	0.54
1:L:1083:ARG:HB3	1:L:1268:ILE:HB	1.90	0.54
1:A:1071:LYS:HE3	1:A:1244:THR:HG22	1.88	0.53
1:B:1083:ARG:HB3	1:B:1268:ILE:HB	1.90	0.53
1:B:1031:MET:SD	1:C:63:LYS:HE3	2.48	0.53
1:B:1193:PHE:CG	2:E:8:LEU:HD13	2.43	0.53
1:J:1083:ARG:HB3	1:J:1268:ILE:HB	1.90	0.53
1:J:8:LYS:HE2	1:L:1137:ASP:OD1	2.06	0.53
2:N:61:ILE:HD13	2:N:67:LEU:HD11	1.91	0.53
1:A:1083:ARG:HB3	1:A:1268:ILE:HB	1.90	0.53
1:J:83:SER:CB	1:L:150:SER:HB2	2.39	0.53
1:J:1195:GLU:OE1	2:M:42:ARG:NH2	2.42	0.52
2:O:61:ILE:HD13	2:O:67:LEU:HD11	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:OD1	2:G:9:THR:HG21	2.08	0.52
2:D:61:ILE:HD13	2:D:67:LEU:HD11	1.91	0.52
2:E:61:ILE:HD13	2:E:67:LEU:HD11	1.91	0.52
1:A:1193:PHE:CE1	2:D:68:HIS:HB3	2.44	0.52
2:F:61:ILE:HD13	2:F:67:LEU:HD11	1.91	0.52
1:B:1193:PHE:CD1	2:E:8:LEU:HD13	2.44	0.51
1:L:20:GLN:HE21	2:R:9:THR:HG22	1.76	0.51
1:J:1250:PRO:HG2	1:J:1253:SER:OG	2.10	0.51
1:A:1250:PRO:HG2	1:A:1253:SER:OG	2.10	0.51
1:B:1250:PRO:HG2	1:B:1253:SER:OG	2.10	0.51
1:L:1250:PRO:HG2	1:L:1253:SER:OG	2.10	0.51
1:C:1250:PRO:HG2	1:C:1253:SER:OG	2.11	0.51
1:J:83:SER:OG	1:L:150:SER:CB	2.59	0.51
2:M:61:ILE:HD13	2:M:67:LEU:HD11	1.91	0.51
1:A:1025:ALA:O	1:A:1028:GLU:N	2.44	0.50
1:K:1250:PRO:HG2	1:K:1253:SER:OG	2.10	0.50
2:M:1:MET:HE1	2:M:63:LYS:HG3	1.93	0.50
2:N:3:ILE:HD11	2:N:65:SER:HB2	1.94	0.50
2:E:3:ILE:HD11	2:E:65:SER:HB2	1.94	0.49
2:D:3:ILE:HD11	2:D:65:SER:HB2	1.94	0.49
1:J:1237:ASP:CG	1:J:1238:ARG:H	2.16	0.49
2:M:3:ILE:HD11	2:M:65:SER:HB2	1.94	0.49
1:B:85:SER:HB2	1:B:119:LEU:HD22	1.94	0.49
1:C:85:SER:HB2	1:C:119:LEU:HD22	1.94	0.49
1:L:85:SER:HB2	1:L:119:LEU:HD22	1.94	0.49
1:C:1081:TYR:HB2	1:C:1270:TYR:HB2	1.95	0.48
1:A:85:SER:HB2	1:A:119:LEU:HD22	1.94	0.48
1:A:1081:TYR:HB2	1:A:1270:TYR:HB2	1.95	0.48
2:O:3:ILE:HD11	2:O:65:SER:HB2	1.94	0.48
1:A:1237:ASP:CG	1:A:1238:ARG:H	2.16	0.48
1:B:1237:ASP:CG	1:B:1238:ARG:H	2.16	0.48
1:C:1237:ASP:CG	1:C:1238:ARG:H	2.16	0.48
2:F:3:ILE:HD11	2:F:65:SER:HB2	1.94	0.48
1:J:85:SER:HB2	1:J:119:LEU:HD22	1.94	0.48
1:K:85:SER:HB2	1:K:119:LEU:HD22	1.94	0.48
1:K:1237:ASP:CG	1:K:1238:ARG:H	2.16	0.48
1:L:1081:TYR:HB2	1:L:1270:TYR:HB2	1.95	0.48
1:L:1237:ASP:CG	1:L:1238:ARG:H	2.16	0.48
1:B:1081:TYR:HB2	1:B:1270:TYR:HB2	1.95	0.47
1:K:1081:TYR:HB2	1:K:1270:TYR:HB2	1.95	0.47
1:J:1081:TYR:HB2	1:J:1270:TYR:HB2	1.95	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1:MET:N	1:J:1:MET:SD	2.79	0.47
1:C:1265:HIS:HB2	2:I:48:LYS:HD3	1.96	0.47
1:C:1218:ILE:HA	2:F:8:LEU:HD21	1.96	0.47
1:K:1245:ASN:HA	1:K:1246:PRO:HD3	1.78	0.47
1:J:1265:HIS:HB2	2:P:48:LYS:HD3	1.97	0.47
1:J:118:PRO:HB3	1:J:124:ALA:HB2	1.97	0.47
1:A:118:PRO:HB3	1:A:124:ALA:HB2	1.97	0.47
1:B:118:PRO:HB3	1:B:124:ALA:HB2	1.97	0.47
1:K:33:TRP:HB2	1:K:54:ILE:HB	1.97	0.47
1:B:88:ILE:HD11	1:B:102:VAL:HA	1.98	0.46
1:J:1079:TYR:CE1	1:J:1234:GLU:HG3	2.51	0.46
2:N:1:MET:HE1	2:N:63:LYS:HG3	1.98	0.46
1:C:88:ILE:HD11	1:C:102:VAL:HA	1.98	0.46
1:B:1100:HIS:NE2	1:B:1229:VAL:HB	2.30	0.46
1:B:33:TRP:HB2	1:B:54:ILE:HB	1.97	0.46
1:C:118:PRO:HB3	1:C:124:ALA:HB2	1.97	0.46
1:J:1100:HIS:NE2	1:J:1229:VAL:HB	2.30	0.46
1:K:1100:HIS:NE2	1:K:1229:VAL:HB	2.30	0.46
1:C:33:TRP:HB2	1:C:54:ILE:HB	1.97	0.46
2:O:1:MET:HE1	2:O:63:LYS:HG3	1.97	0.46
1:J:88:ILE:HD11	1:J:102:VAL:HA	1.98	0.46
1:K:118:PRO:HB3	1:K:124:ALA:HB2	1.97	0.46
1:L:118:PRO:HB3	1:L:124:ALA:HB2	1.97	0.46
1:K:1079:TYR:CE1	1:K:1234:GLU:HG3	2.51	0.46
1:L:1079:TYR:CE1	1:L:1234:GLU:HG3	2.51	0.46
1:A:88:ILE:HD11	1:A:102:VAL:HA	1.98	0.46
1:A:1079:TYR:CE1	1:A:1234:GLU:HG3	2.51	0.46
1:K:88:ILE:HD11	1:K:102:VAL:HA	1.98	0.46
1:L:88:ILE:HD11	1:L:102:VAL:HA	1.98	0.46
1:L:1083:ARG:NE	1:L:1270:TYR:OH	2.49	0.46
1:J:1118:SER:O	1:J:1121:SER:OG	2.33	0.46
1:A:1100:HIS:NE2	1:A:1229:VAL:HB	2.30	0.45
1:B:1079:TYR:CE1	1:B:1234:GLU:HG3	2.51	0.45
1:B:150:SER:O	1:B:1027:ASP:HB2	2.16	0.45
1:C:1100:HIS:NE2	1:C:1229:VAL:HB	2.30	0.45
1:C:1079:TYR:CE1	1:C:1234:GLU:HG3	2.51	0.45
1:J:33:TRP:HB2	1:J:54:ILE:HB	1.97	0.45
2:D:37:PRO:HA	2:D:38:PRO:HD3	1.86	0.45
1:L:1100:HIS:NE2	1:L:1229:VAL:HB	2.30	0.45
1:B:1218:ILE:HG13	1:B:1218:ILE:H	1.52	0.45
1:J:1134:THR:HG21	1:K:98:THR:HG22	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:ASP:OD1	1:B:8:LYS:HE2	2.16	0.45
1:A:1146:ILE:O	1:A:1149:VAL:HG12	2.17	0.45
1:L:33:TRP:HB2	1:L:54:ILE:HB	1.97	0.45
1:A:33:TRP:HB2	1:A:54:ILE:HB	1.97	0.45
1:B:1118:SER:O	1:B:1121:SER:OG	2.33	0.45
1:C:1245:ASN:HA	1:C:1246:PRO:HD3	1.78	0.45
1:C:19:ALA:HA	1:C:1036:ARG:CD	2.47	0.45
2:F:1:MET:HE1	2:F:63:LYS:HG3	1.99	0.45
1:L:1146:ILE:O	1:L:1149:VAL:HG12	2.17	0.45
1:C:1146:ILE:O	1:C:1149:VAL:HG12	2.17	0.44
1:A:1038:GLN:HA	1:A:1041:ILE:HB	1.99	0.44
1:B:1146:ILE:O	1:B:1149:VAL:HG12	2.17	0.44
1:J:1146:ILE:O	1:J:1149:VAL:HG12	2.17	0.44
1:L:1245:ASN:HA	1:L:1246:PRO:HD3	1.78	0.44
1:C:1235:TYR:OH	2:I:54:ARG:NH2	2.45	0.44
1:L:1038:GLN:HA	1:L:1041:ILE:HB	1.99	0.44
2:P:74:ARG:HE	2:P:74:ARG:HA	1.83	0.44
1:B:1026:TYR:O	1:B:1030:ILE:HG13	2.18	0.44
1:B:1083:ARG:NE	1:B:1270:TYR:OH	2.49	0.44
1:J:1026:TYR:HD1	1:J:1026:TYR:HA	1.69	0.44
1:A:1105:LEU:HA	1:A:1149:VAL:HG22	2.00	0.44
1:C:1026:TYR:O	1:C:1030:ILE:HG13	2.18	0.44
2:H:74:ARG:HA	2:H:74:ARG:HE	1.83	0.44
1:K:1083:ARG:NE	1:K:1270:TYR:OH	2.49	0.44
1:L:1026:TYR:O	1:L:1030:ILE:HG13	2.18	0.44
1:A:1135:ILE:HA	1:A:1138:PHE:HD2	1.83	0.44
1:B:1038:GLN:HA	1:B:1041:ILE:HB	1.99	0.44
1:B:1245:ASN:HA	1:B:1246:PRO:HD3	1.78	0.44
2:I:74:ARG:HE	2:I:74:ARG:HA	1.83	0.44
2:Q:74:ARG:HA	2:Q:74:ARG:HE	1.83	0.44
2:R:74:ARG:HE	2:R:74:ARG:HA	1.83	0.44
1:B:57:PRO:HD3	1:B:65:PRO:HA	2.00	0.44
2:D:50:LEU:HD22	2:D:59:TYR:CD2	2.53	0.44
1:A:1249:PHE:HB3	2:D:9:THR:HG22	2.00	0.44
1:K:1146:ILE:O	1:K:1149:VAL:HG12	2.17	0.44
1:K:57:PRO:HD3	1:K:65:PRO:HA	2.00	0.44
1:C:1083:ARG:NE	1:C:1270:TYR:OH	2.49	0.44
2:F:50:LEU:HD22	2:F:59:TYR:CD2	2.53	0.44
2:M:50:LEU:HD22	2:M:59:TYR:CD2	2.53	0.44
1:J:57:PRO:HD3	1:J:65:PRO:HA	2.00	0.43
1:J:96:ALA:HB2	1:L:1177:LEU:HD11	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1026:TYR:O	1:K:1030:ILE:HG13	2.18	0.43
2:N:50:LEU:HD22	2:N:59:TYR:CD2	2.53	0.43
1:B:1135:ILE:HA	1:B:1138:PHE:HD2	1.83	0.43
1:B:1105:LEU:HA	1:B:1149:VAL:HG22	2.00	0.43
1:C:1135:ILE:HA	1:C:1138:PHE:HD2	1.83	0.43
1:C:41:ASN:OD1	2:I:9:THR:HG21	2.18	0.43
1:J:1026:TYR:O	1:J:1030:ILE:HG13	2.18	0.43
1:K:1135:ILE:HA	1:K:1138:PHE:HD2	1.83	0.43
1:L:116:ASP:O	1:L:118:PRO:HD3	2.19	0.43
1:A:1245:ASN:HA	1:A:1246:PRO:HD3	1.78	0.43
1:B:116:ASP:O	1:B:118:PRO:HD3	2.19	0.43
2:E:50:LEU:HD22	2:E:59:TYR:CD2	2.53	0.43
1:K:116:ASP:O	1:K:118:PRO:HD3	2.19	0.43
1:A:1026:TYR:O	1:A:1030:ILE:HG13	2.18	0.43
1:C:1038:GLN:HA	1:C:1041:ILE:HB	1.99	0.43
1:C:116:ASP:O	1:C:118:PRO:HD3	2.19	0.43
1:C:59:ASP:OD1	1:C:59:ASP:N	2.47	0.43
1:L:1145:LEU:HD12	1:L:1145:LEU:HA	1.91	0.43
1:L:1188:LYS:H	1:L:1188:LYS:HG2	1.58	0.43
2:G:74:ARG:HE	2:G:74:ARG:HA	1.83	0.43
1:J:1105:LEU:HA	1:J:1149:VAL:HG22	2.00	0.43
1:A:116:ASP:O	1:A:118:PRO:HD3	2.19	0.43
1:K:1038:GLN:HA	1:K:1041:ILE:HB	1.99	0.43
2:O:50:LEU:HD22	2:O:59:TYR:CD2	2.53	0.43
1:L:1218:ILE:HA	2:O:8:LEU:HD21	2.01	0.43
2:F:37:PRO:HA	2:F:38:PRO:HD3	1.86	0.43
1:J:1245:ASN:HA	1:J:1246:PRO:HD3	1.78	0.43
1:B:1026:TYR:HA	1:B:1026:TYR:HD1	1.69	0.43
1:B:59:ASP:N	1:B:59:ASP:OD1	2.47	0.43
2:M:37:PRO:HA	2:M:38:PRO:HD3	1.86	0.43
2:O:5:VAL:HG13	2:O:13:ILE:HB	2.01	0.43
1:J:1135:ILE:HA	1:J:1138:PHE:HD2	1.83	0.43
1:K:1105:LEU:HA	1:K:1149:VAL:HG22	2.00	0.43
1:J:116:ASP:O	1:J:118:PRO:HD3	2.18	0.43
2:D:5:VAL:HG13	2:D:13:ILE:HB	2.01	0.42
1:J:1038:GLN:HA	1:J:1041:ILE:HB	1.99	0.42
1:L:1135:ILE:HA	1:L:1138:PHE:HD2	1.83	0.42
1:A:57:PRO:HD3	1:A:65:PRO:HA	2.00	0.42
1:C:1105:LEU:HA	1:C:1149:VAL:HG22	2.00	0.42
1:K:1218:ILE:HA	2:N:8:LEU:HD21	2.01	0.42
1:L:57:PRO:HD3	1:L:65:PRO:HA	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:GLU:HG2	2:D:75:GLY:O	2.19	0.42
1:B:1:MET:N	1:B:1:MET:SD	2.79	0.42
1:L:1105:LEU:HA	1:L:1149:VAL:HG22	2.00	0.42
1:A:1071:LYS:HD2	1:A:1239:GLY:H	1.85	0.42
1:C:57:PRO:HD3	1:C:65:PRO:HA	2.00	0.42
1:K:1031:MET:SD	1:L:63:LYS:HE3	2.59	0.42
2:N:5:VAL:HG13	2:N:13:ILE:HB	2.01	0.42
2:R:37:PRO:HA	2:R:38:PRO:HD3	1.91	0.42
1:J:1218:ILE:H	1:J:1218:ILE:HG13	1.52	0.42
1:J:1083:ARG:NE	1:J:1270:TYR:OH	2.49	0.42
1:A:122:GLU:O	1:A:126:ILE:HG12	2.20	0.42
1:A:1083:ARG:NE	1:A:1270:TYR:OH	2.49	0.42
1:B:1214:GLU:OE1	2:E:74:ARG:HD2	2.20	0.42
2:E:1:MET:HE1	2:E:63:LYS:HG3	2.02	0.42
2:F:5:VAL:HG13	2:F:13:ILE:HB	2.01	0.42
1:K:1086:ARG:HA	1:K:1087:PRO:HD3	1.88	0.42
1:L:85:SER:OG	2:Q:76:GLY:C	2.55	0.42
1:B:1071:LYS:HD2	1:B:1239:GLY:H	1.85	0.42
1:C:1071:LYS:HD2	1:C:1239:GLY:H	1.85	0.42
1:C:1188:LYS:HG2	1:C:1188:LYS:H	1.58	0.42
1:C:122:GLU:O	1:C:126:ILE:HG12	2.20	0.42
2:F:24:GLU:HG2	2:F:24:GLU:H	1.69	0.42
1:C:90:ARG:CZ	2:H:75:GLY:HA2	2.50	0.42
1:L:1083:ARG:HD2	1:L:1268:ILE:HD12	2.02	0.42
1:C:103:LEU:HD12	1:C:103:LEU:HA	1.83	0.42
1:C:1218:ILE:H	1:C:1218:ILE:HG13	1.52	0.42
1:K:1026:TYR:HA	1:K:1026:TYR:HD1	1.69	0.42
1:B:122:GLU:O	1:B:126:ILE:HG12	2.20	0.41
1:J:126:ILE:HD12	1:J:133:LYS:HE3	2.02	0.41
1:J:98:THR:HB	1:L:1133:PHE:HZ	1.84	0.41
1:B:103:LEU:HD12	1:B:103:LEU:HA	1.83	0.41
1:J:1083:ARG:HD2	1:J:1268:ILE:HD12	2.02	0.41
1:J:1145:LEU:HD23	1:J:1171:LEU:HD13	2.03	0.41
1:L:126:ILE:HD12	1:L:133:LYS:HE3	2.03	0.41
1:A:21:CYS:HB3	1:A:37:ILE:HB	2.03	0.41
1:J:1071:LYS:HD2	1:J:1239:GLY:H	1.85	0.41
2:M:5:VAL:HG13	2:M:13:ILE:HB	2.01	0.41
1:A:9:GLU:HG2	1:C:1133:PHE:HE2	1.86	0.41
1:C:1083:ARG:HD2	1:C:1268:ILE:HD12	2.02	0.41
1:K:1192:HIS:HB2	2:N:68:HIS:CE1	2.55	0.41
1:K:21:CYS:HB3	1:K:37:ILE:HB	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:LEU:HD23	1:A:1171:LEU:HD13	2.02	0.41
1:C:1:MET:N	1:C:1:MET:SD	2.79	0.41
1:L:1145:LEU:HD23	1:L:1171:LEU:HD13	2.03	0.41
1:L:122:GLU:O	1:L:126:ILE:HG12	2.20	0.41
2:O:22:THR:HA	2:O:55:THR:HA	2.03	0.41
1:C:126:ILE:HD12	1:C:133:LYS:HE3	2.02	0.41
1:C:21:CYS:HB3	1:C:37:ILE:HB	2.03	0.41
2:E:5:VAL:HG13	2:E:13:ILE:HB	2.01	0.41
1:J:51:PHE:HZ	1:J:1025:ALA:HA	1.84	0.41
1:K:122:GLU:O	1:K:126:ILE:HG12	2.20	0.41
1:C:1145:LEU:HD23	1:C:1171:LEU:HD13	2.02	0.41
2:M:24:GLU:H	2:M:24:GLU:HG2	1.69	0.41
2:O:36:ILE:O	2:O:41:GLN:NE2	2.54	0.41
1:A:103:LEU:HA	1:A:103:LEU:HD12	1.84	0.41
1:A:1218:ILE:H	1:A:1218:ILE:HG13	1.52	0.41
1:A:126:ILE:HD12	1:A:133:LYS:HE3	2.02	0.41
1:B:1206:GLN:HG2	1:C:92:GLN:CD	2.41	0.41
1:L:103:LEU:HD12	1:L:103:LEU:HA	1.83	0.41
2:M:22:THR:HA	2:M:55:THR:HA	2.03	0.41
1:A:62:PHE:HZ	1:C:1170:TYR:CD1	2.38	0.41
1:J:122:GLU:O	1:J:126:ILE:HG12	2.20	0.41
1:K:1071:LYS:HD2	1:K:1239:GLY:H	1.85	0.41
1:B:1083:ARG:HD2	1:B:1268:ILE:HD12	2.02	0.41
2:D:22:THR:HA	2:D:55:THR:HA	2.03	0.41
1:K:126:ILE:HD12	1:K:133:LYS:HE3	2.02	0.41
1:B:1145:LEU:HD23	1:B:1171:LEU:HD13	2.03	0.41
1:B:126:ILE:HD12	1:B:133:LYS:HE3	2.02	0.41
2:D:1:MET:HE1	2:D:63:LYS:HG3	2.02	0.41
1:L:1026:TYR:HA	1:L:1026:TYR:HD1	1.70	0.41
1:L:1071:LYS:HD2	1:L:1239:GLY:H	1.85	0.41
1:L:1086:ARG:HA	1:L:1087:PRO:HD3	1.88	0.41
1:B:21:CYS:HB3	1:B:37:ILE:HB	2.02	0.40
2:D:36:ILE:O	2:D:41:GLN:NE2	2.54	0.40
2:I:37:PRO:HA	2:I:38:PRO:HD3	1.91	0.40
1:J:21:CYS:HB3	1:J:37:ILE:HB	2.02	0.40
1:A:62:PHE:HZ	1:C:1170:TYR:HD1	1.68	0.40
2:I:5:VAL:HG13	2:I:13:ILE:HB	2.03	0.40
1:L:21:CYS:HB3	1:L:37:ILE:HB	2.02	0.40
1:C:1086:ARG:HA	1:C:1087:PRO:HD3	1.88	0.40
1:K:1083:ARG:HD2	1:K:1268:ILE:HD12	2.02	0.40
2:P:37:PRO:HA	2:P:38:PRO:HD3	1.91	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:ARG:HD2	1:A:1268:ILE:HD12	2.02	0.40
1:K:1145:LEU:HD23	1:K:1171:LEU:HD13	2.02	0.40
1:L:1183:LEU:HA	1:L:1183:LEU:HD23	1.96	0.40
2:P:71:LEU:H	2:P:71:LEU:HD12	1.87	0.40
1:C:1118:SER:O	1:C:1121:SER:OG	2.33	0.40
2:E:36:ILE:O	2:E:41:GLN:NE2	2.54	0.40
2:H:26:VAL:HG21	2:H:56:LEU:HD11	2.04	0.40
1:J:1142:PHE:O	1:J:1146:ILE:HG13	2.22	0.40
1:L:1142:PHE:O	1:L:1146:ILE:HG13	2.22	0.40
1:L:1218:ILE:HG13	1:L:1218:ILE:H	1.52	0.40
2:M:36:ILE:O	2:M:41:GLN:NE2	2.54	0.40
2:R:71:LEU:H	2:R:71:LEU:HD12	1.86	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	397/399 (100%)	380 (96%)	17 (4%)	0	100	100
1	B	397/399 (100%)	379 (96%)	18 (4%)	0	100	100
1	C	397/399 (100%)	381 (96%)	16 (4%)	0	100	100
1	J	397/399 (100%)	380 (96%)	16 (4%)	1 (0%)	44	76
1	K	397/399 (100%)	380 (96%)	16 (4%)	1 (0%)	44	76
1	L	397/399 (100%)	380 (96%)	17 (4%)	0	100	100
2	D	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	E	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	F	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	G	74/76 (97%)	73 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	I	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	M	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	N	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	O	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	P	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	Q	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	R	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
All	All	3270/3306 (99%)	3144 (96%)	124 (4%)	2 (0%)	55	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	1025	ALA
1	K	1025	ALA

### 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	354/354 (100%)	316 (89%)	38 (11%)	8	30
1	B	354/354 (100%)	316 (89%)	38 (11%)	8	30
1	C	354/354 (100%)	316 (89%)	38 (11%)	8	30
1	J	354/354 (100%)	316 (89%)	38 (11%)	8	30
1	K	354/354 (100%)	316 (89%)	38 (11%)	8	30
1	L	354/354 (100%)	316 (89%)	38 (11%)	8	30
2	D	68/68 (100%)	64 (94%)	4 (6%)	23	58
2	E	68/68 (100%)	64 (94%)	4 (6%)	23	58
2	F	68/68 (100%)	64 (94%)	4 (6%)	23	58
2	G	68/68 (100%)	62 (91%)	6 (9%)	12	40

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	68/68 (100%)	62 (91%)	6 (9%)	12	40
2	I	68/68 (100%)	62 (91%)	6 (9%)	12	40
2	M	68/68 (100%)	64 (94%)	4 (6%)	23	58
2	N	68/68 (100%)	64 (94%)	4 (6%)	23	58
2	O	68/68 (100%)	64 (94%)	4 (6%)	23	58
2	P	68/68 (100%)	62 (91%)	6 (9%)	12	40
2	Q	68/68 (100%)	62 (91%)	6 (9%)	12	40
2	R	68/68 (100%)	62 (91%)	6 (9%)	12	40
All	All	2940/2940 (100%)	2652 (90%)	288 (10%)	9	34

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	32	HIS
1	A	37	ILE
1	A	58	THR
1	A	70	THR
1	A	88	ILE
1	A	90	ARG
1	A	98	THR
1	A	99	ILE
1	A	103	LEU
1	A	104	LEU
1	A	117	ASP
1	A	147	MET
1	A	1026	TYR
1	A	1028	GLU
1	A	1051	ARG
1	A	1054	LEU
1	A	1063	GLU
1	A	1084	LYS
1	A	1100	HIS
1	A	1104	LEU
1	A	1105	LEU
1	A	1106	ASP
1	A	1123	GLU
1	A	1131	THR
1	A	1137	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1144	ASP
1	A	1145	LEU
1	A	1149	VAL
1	A	1158	LEU
1	A	1159	LEU
1	A	1171	LEU
1	A	1188	LYS
1	A	1192	HIS
1	A	1207	GLU
1	A	1208	VAL
1	A	1231	ILE
1	A	1249	PHE
1	B	1	MET
1	B	32	HIS
1	B	37	ILE
1	B	58	THR
1	B	70	THR
1	B	88	ILE
1	B	90	ARG
1	B	98	THR
1	B	99	ILE
1	B	103	LEU
1	B	104	LEU
1	B	117	ASP
1	B	147	MET
1	B	1026	TYR
1	B	1028	GLU
1	B	1051	ARG
1	B	1054	LEU
1	B	1063	GLU
1	B	1084	LYS
1	B	1100	HIS
1	B	1104	LEU
1	B	1105	LEU
1	B	1106	ASP
1	B	1123	GLU
1	B	1131	THR
1	B	1137	ASP
1	B	1144	ASP
1	B	1145	LEU
1	B	1149	VAL
1	B	1158	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1159	LEU
1	B	1171	LEU
1	B	1188	LYS
1	B	1192	HIS
1	B	1207	GLU
1	B	1208	VAL
1	B	1231	ILE
1	B	1249	PHE
1	C	1	MET
1	C	32	HIS
1	C	37	ILE
1	C	58	THR
1	C	70	THR
1	C	88	ILE
1	C	90	ARG
1	C	98	THR
1	C	99	ILE
1	C	103	LEU
1	C	104	LEU
1	C	117	ASP
1	C	147	MET
1	C	1026	TYR
1	C	1028	GLU
1	C	1051	ARG
1	C	1054	LEU
1	C	1063	GLU
1	C	1084	LYS
1	C	1100	HIS
1	C	1104	LEU
1	C	1105	LEU
1	C	1106	ASP
1	C	1123	GLU
1	C	1131	THR
1	C	1137	ASP
1	C	1144	ASP
1	C	1145	LEU
1	C	1149	VAL
1	C	1158	LEU
1	C	1159	LEU
1	C	1171	LEU
1	C	1188	LYS
1	C	1192	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1207	GLU
1	C	1208	VAL
1	C	1231	ILE
1	C	1249	PHE
2	D	15	LEU
2	D	39	ASP
2	D	42	ARG
2	D	43	LEU
2	E	15	LEU
2	E	39	ASP
2	E	42	ARG
2	E	43	LEU
2	F	15	LEU
2	F	39	ASP
2	F	42	ARG
2	F	43	LEU
2	G	5	VAL
2	G	9	THR
2	G	14	THR
2	G	22	THR
2	G	49	GLN
2	G	74	ARG
2	H	5	VAL
2	H	9	THR
2	H	14	THR
2	H	22	THR
2	H	49	GLN
2	H	74	ARG
2	I	5	VAL
2	I	9	THR
2	I	14	THR
2	I	22	THR
2	I	49	GLN
2	I	74	ARG
1	J	1	MET
1	J	32	HIS
1	J	37	ILE
1	J	58	THR
1	J	70	THR
1	J	88	ILE
1	J	90	ARG
1	J	98	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	99	ILE
1	J	103	LEU
1	J	104	LEU
1	J	117	ASP
1	J	147	MET
1	J	1026	TYR
1	J	1028	GLU
1	J	1051	ARG
1	J	1054	LEU
1	J	1063	GLU
1	J	1084	LYS
1	J	1100	HIS
1	J	1104	LEU
1	J	1105	LEU
1	J	1106	ASP
1	J	1123	GLU
1	J	1131	THR
1	J	1137	ASP
1	J	1144	ASP
1	J	1145	LEU
1	J	1149	VAL
1	J	1158	LEU
1	J	1159	LEU
1	J	1171	LEU
1	J	1188	LYS
1	J	1192	HIS
1	J	1207	GLU
1	J	1208	VAL
1	J	1231	ILE
1	J	1249	PHE
1	K	1	MET
1	K	32	HIS
1	K	37	ILE
1	K	58	THR
1	K	70	THR
1	K	88	ILE
1	K	90	ARG
1	K	98	THR
1	K	99	ILE
1	K	103	LEU
1	K	104	LEU
1	K	117	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	147	MET
1	K	1026	TYR
1	K	1028	GLU
1	K	1051	ARG
1	K	1054	LEU
1	K	1063	GLU
1	K	1084	LYS
1	K	1100	HIS
1	K	1104	LEU
1	K	1105	LEU
1	K	1106	ASP
1	K	1123	GLU
1	K	1131	THR
1	K	1137	ASP
1	K	1144	ASP
1	K	1145	LEU
1	K	1149	VAL
1	K	1158	LEU
1	K	1159	LEU
1	K	1171	LEU
1	K	1188	LYS
1	K	1192	HIS
1	K	1207	GLU
1	K	1208	VAL
1	K	1231	ILE
1	K	1249	PHE
1	L	1	MET
1	L	32	HIS
1	L	37	ILE
1	L	58	THR
1	L	70	THR
1	L	88	ILE
1	L	90	ARG
1	L	98	THR
1	L	99	ILE
1	L	103	LEU
1	L	104	LEU
1	L	117	ASP
1	L	147	MET
1	L	1026	TYR
1	L	1028	GLU
1	L	1051	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	1054	LEU
1	L	1063	GLU
1	L	1084	LYS
1	L	1100	HIS
1	L	1104	LEU
1	L	1105	LEU
1	L	1106	ASP
1	L	1123	GLU
1	L	1131	THR
1	L	1137	ASP
1	L	1144	ASP
1	L	1145	LEU
1	L	1149	VAL
1	L	1158	LEU
1	L	1159	LEU
1	L	1171	LEU
1	L	1188	LYS
1	L	1192	HIS
1	L	1207	GLU
1	L	1208	VAL
1	L	1231	ILE
1	L	1249	PHE
2	M	15	LEU
2	M	39	ASP
2	M	42	ARG
2	M	43	LEU
2	N	15	LEU
2	N	39	ASP
2	N	42	ARG
2	N	43	LEU
2	O	15	LEU
2	O	39	ASP
2	O	42	ARG
2	O	43	LEU
2	P	5	VAL
2	P	9	THR
2	P	14	THR
2	P	22	THR
2	P	49	GLN
2	P	74	ARG
2	Q	5	VAL
2	Q	9	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	Q	14	THR
2	Q	22	THR
2	Q	49	GLN
2	Q	74	ARG
2	R	5	VAL
2	R	9	THR
2	R	14	THR
2	R	22	THR
2	R	49	GLN
2	R	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	GLN
1	L	20	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 ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	399/399 (100%)	0.58	47 (11%) 5 4	79, 152, 233, 299	0
1	B	399/399 (100%)	0.01	8 (2%) 65 63	70, 131, 196, 273	0
1	C	399/399 (100%)	-0.03	2 (0%) 90 90	69, 126, 196, 247	0
1	J	399/399 (100%)	0.07	16 (4%) 39 36	82, 134, 195, 245	0
1	K	399/399 (100%)	0.14	23 (5%) 24 23	76, 135, 196, 276	0
1	L	399/399 (100%)	-0.00	4 (1%) 82 81	75, 130, 195, 243	0
2	D	76/76 (100%)	0.62	9 (11%) 5 4	127, 165, 215, 235	0
2	E	76/76 (100%)	-0.04	0 100 100	82, 154, 204, 220	0
2	F	76/76 (100%)	0.82	14 (18%) 1 1	90, 160, 197, 214	0
2	G	76/76 (100%)	0.36	5 (6%) 19 18	111, 151, 210, 226	0
2	H	76/76 (100%)	-0.13	0 100 100	79, 122, 175, 199	0
2	I	76/76 (100%)	0.03	3 (3%) 40 37	80, 125, 174, 196	0
2	M	76/76 (100%)	0.10	0 100 100	95, 155, 204, 219	0
2	N	76/76 (100%)	0.04	1 (1%) 77 75	107, 155, 201, 212	0
2	O	76/76 (100%)	0.72	13 (17%) 2 1	90, 154, 212, 226	0
2	P	76/76 (100%)	0.06	3 (3%) 40 37	90, 131, 175, 200	0
2	Q	76/76 (100%)	-0.10	0 100 100	87, 125, 175, 198	0
2	R	76/76 (100%)	0.10	2 (2%) 56 53	81, 124, 175, 203	0
All	All	3306/3306 (100%)	0.15	150 (4%) 34 32	69, 137, 204, 299	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1049	SER	7.9
1	A	1149	VAL	6.5
1	A	1050	GLU	5.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1162	PHE	5.7
1	K	1145	LEU	5.1
1	A	1159	LEU	5.1
1	L	20	GLN	4.9
1	C	19	ALA	4.5
2	D	8	LEU	4.4
1	A	1158	LEU	4.3
1	A	1048	VAL	4.3
2	D	34	GLU	4.3
1	A	1227	LEU	4.3
1	K	1249	PHE	4.2
1	A	1052	LEU	4.0
2	F	59	TYR	4.0
1	A	1160	ALA	3.8
1	A	1101	LEU	3.8
1	K	1146	ILE	3.8
1	C	20	GLN	3.7
1	A	1155	VAL	3.7
2	O	3	ILE	3.6
2	P	34	GLU	3.5
1	K	1102	GLU	3.5
1	J	110	LEU	3.4
2	R	76	GLY	3.4
1	J	1050	GLU	3.4
1	A	1241	GLY	3.3
2	F	2	GLN	3.3
2	O	45	PHE	3.3
1	A	1146	ILE	3.3
2	D	30	ILE	3.3
2	D	6	LYS	3.3
2	D	2	GLN	3.2
2	G	13	ILE	3.2
1	K	1148	GLN	3.2
1	J	1048	VAL	3.2
1	K	1174	TYR	3.2
1	K	1271	LYS	3.2
1	A	1147	GLU	3.2
1	A	1105	LEU	3.1
1	B	1152	GLN	3.1
2	G	34	GLU	3.1
1	A	1268	ILE	3.1
2	O	13	ILE	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	1145	LEU	3.1
2	P	33	LYS	3.1
1	K	1142	PHE	3.1
2	O	4	PHE	3.0
2	O	2	GLN	3.0
1	L	-1	GLY	3.0
2	N	71	LEU	3.0
1	A	1051	ARG	3.0
2	F	3	ILE	3.0
1	A	1157	ASP	2.9
1	J	45	TYR	2.9
2	O	64	GLU	2.9
1	K	1104	LEU	2.9
1	B	1114	PHE	2.9
2	F	1	MET	2.9
1	A	110	LEU	2.8
1	A	1097	GLY	2.8
1	B	1227	LEU	2.8
1	J	116	ASP	2.8
1	K	1152	GLN	2.8
2	F	4	PHE	2.8
2	D	3	ILE	2.8
2	F	23	ILE	2.8
1	A	1177	LEU	2.8
1	K	1114	PHE	2.8
1	A	1221	ILE	2.7
1	A	1114	PHE	2.7
1	A	45	TYR	2.7
1	K	19	ALA	2.7
1	A	1082	ILE	2.7
1	A	1270	TYR	2.6
2	I	76	GLY	2.6
1	A	1240	GLU	2.6
2	G	4	PHE	2.6
1	A	1060	GLU	2.6
1	K	1158	LEU	2.6
2	D	15	LEU	2.5
1	L	13	LEU	2.5
1	J	1249	PHE	2.5
2	O	63	LYS	2.5
1	K	1105	LEU	2.5
2	D	67	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	G	12	THR	2.5
1	A	116	ASP	2.5
1	K	1138	PHE	2.5
2	O	61	ILE	2.5
2	R	34	GLU	2.4
2	F	13	ILE	2.4
1	A	1083	ARG	2.4
1	K	1095	ALA	2.4
2	F	67	LEU	2.4
1	A	1174	TYR	2.4
2	F	45	PHE	2.4
1	J	1047	LEU	2.4
1	J	1155	VAL	2.4
1	A	1142	PHE	2.4
1	J	111	CYS	2.4
2	D	61	ILE	2.4
1	J	16	ASP	2.4
2	O	65	SER	2.4
1	A	132	GLU	2.4
1	A	49	VAL	2.3
1	A	1112	GLN	2.3
1	B	1096	PHE	2.3
2	F	36	ILE	2.3
1	L	19	ALA	2.3
2	I	15	LEU	2.3
2	F	27	LYS	2.3
1	A	1117	VAL	2.3
1	J	123	ILE	2.3
2	I	13	ILE	2.3
1	B	1149	VAL	2.3
2	F	65	SER	2.3
2	O	15	LEU	2.3
1	K	1079	TYR	2.3
1	A	1084	LYS	2.3
1	A	1167	THR	2.3
1	J	126	ILE	2.3
1	K	1130	PHE	2.2
1	A	20	GLN	2.2
1	A	1239	GLY	2.2
1	A	1047	LEU	2.2
1	A	1057	LEU	2.2
1	B	1146	ILE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	K	1082	ILE	2.2
1	J	1162	PHE	2.2
2	P	30	ILE	2.2
2	F	61	ILE	2.2
1	B	19	ALA	2.2
1	J	20	GLN	2.2
2	O	59	TYR	2.2
2	O	67	LEU	2.1
1	J	46	GLN	2.1
1	K	1153	THR	2.1
2	F	15	LEU	2.1
1	A	128	LYS	2.1
1	K	1162	PHE	2.1
1	A	1249	PHE	2.1
1	K	1084	LYS	2.1
1	J	75	HIS	2.1
1	A	1098	PHE	2.1
1	K	1125	LEU	2.0
2	O	76	GLY	2.0
2	G	64	GLU	2.0
1	A	1113	ARG	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.