



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 05:22 am GMT

PDB ID : 4NQK  
Title : Structure of an Ubiquitin complex  
Authors : Peisley, A.; Wu, B.; Hur, S.  
Deposited on : 2013-11-25  
Resolution : 3.70 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 : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

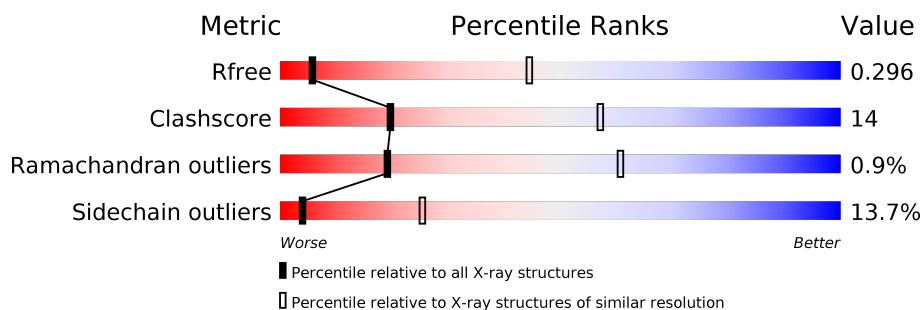
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1413 (3.90-3.50)
Clashscore	122126	1524 (3.90-3.50)
Ramachandran outliers	120053	1470 (3.90-3.50)
Sidechain outliers	120020	1467 (3.90-3.50)

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. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	203	
1	B	203	
1	C	203	
1	D	203	
2	E	79	
2	F	79	
2	G	79	

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Mol	Chain	Length	Quality of chain
2	H	79	<div><div></div><div>71%19%5%5%</div></div>
2	I	79	<div><div></div><div>57%22%8%•10%</div></div>
2	J	79	<div><div></div><div>72%18%•8%</div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19139 atoms, of which 9584 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	188	Total	C	H	N	O	S	0	0	0
			3041	990	1510	245	287	9			
1	B	188	Total	C	H	N	O	S	0	0	0
			3034	989	1505	243	288	9			
1	C	188	Total	C	H	N	O	S	0	0	0
			3000	981	1487	242	281	9			
1	D	188	Total	C	H	N	O	S	0	0	0
			3081	998	1535	248	291	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP O95786
A	-1	PRO	-	EXPRESSION TAG	UNP O95786
A	0	GLY	-	EXPRESSION TAG	UNP O95786
B	-2	GLY	-	EXPRESSION TAG	UNP O95786
B	-1	PRO	-	EXPRESSION TAG	UNP O95786
B	0	GLY	-	EXPRESSION TAG	UNP O95786
C	-2	GLY	-	EXPRESSION TAG	UNP O95786
C	-1	PRO	-	EXPRESSION TAG	UNP O95786
C	0	GLY	-	EXPRESSION TAG	UNP O95786
D	-2	GLY	-	EXPRESSION TAG	UNP O95786
D	-1	PRO	-	EXPRESSION TAG	UNP O95786
D	0	GLY	-	EXPRESSION TAG	UNP O95786

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	72	Total	C	H	N	O	S	0	0	0
			1169	362	595	98	113	1			
2	F	73	Total	C	H	N	O	S	0	0	0
			1171	365	595	96	114	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	71	Total	C	H	N	O	S	0	0	0
			1128	352	570	93	112	1			
2	H	75	Total	C	H	N	O	S	0	0	0
			1202	373	611	101	116	1			
2	I	71	Total	C	H	N	O	S	0	0	0
			1125	352	570	92	110	1			
2	J	73	Total	C	H	N	O	S	0	0	0
			1188	368	606	99	114	1			

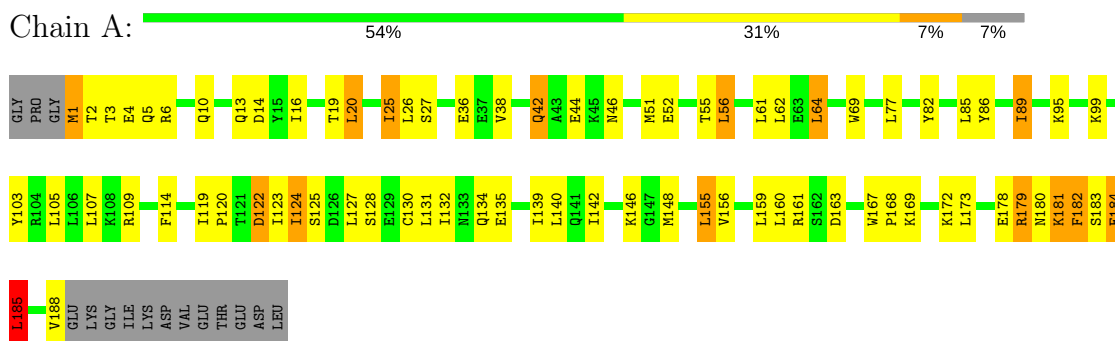
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP P0CG48
E	-1	PRO	-	EXPRESSION TAG	UNP P0CG48
F	-2	GLY	-	EXPRESSION TAG	UNP P0CG48
F	-1	PRO	-	EXPRESSION TAG	UNP P0CG48
G	-2	GLY	-	EXPRESSION TAG	UNP P0CG48
G	-1	PRO	-	EXPRESSION TAG	UNP P0CG48
H	-2	GLY	-	EXPRESSION TAG	UNP P0CG48
H	-1	PRO	-	EXPRESSION TAG	UNP P0CG48
I	-2	GLY	-	EXPRESSION TAG	UNP P0CG48
I	-1	PRO	-	EXPRESSION TAG	UNP P0CG48
J	-2	GLY	-	EXPRESSION TAG	UNP P0CG48
J	-1	PRO	-	EXPRESSION TAG	UNP P0CG48

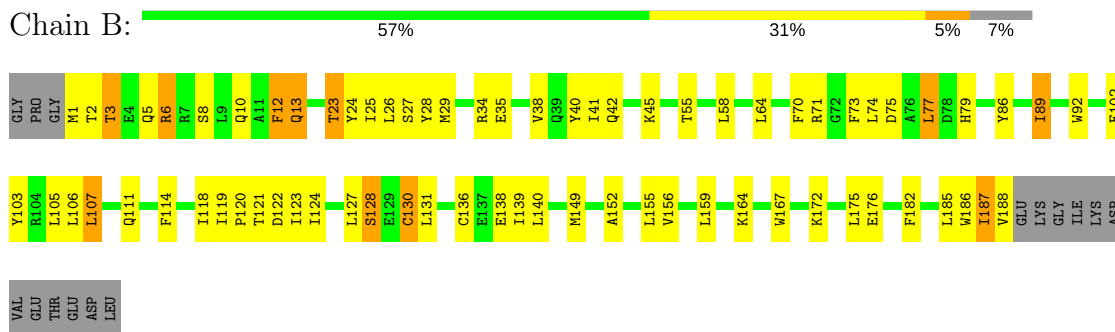
### 3 Residue-property plots

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

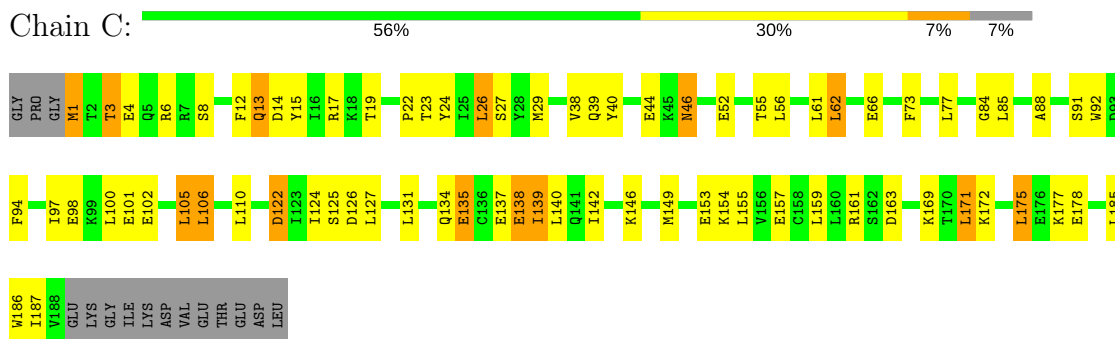
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



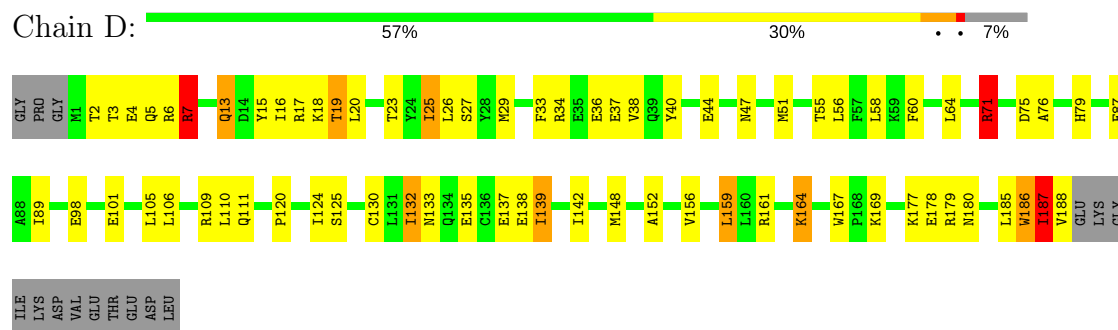
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



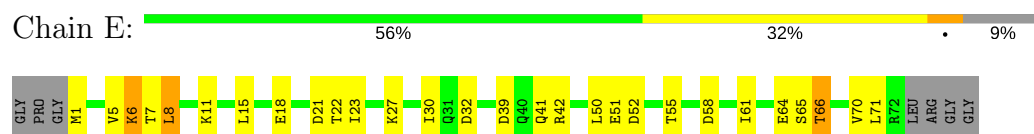
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



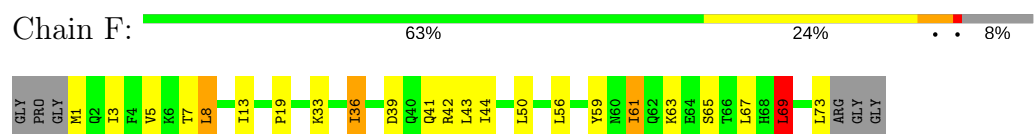
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



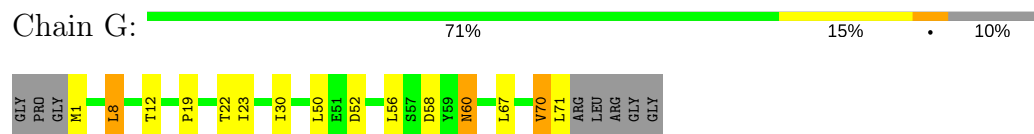
• Molecule 2: Ubiquitin



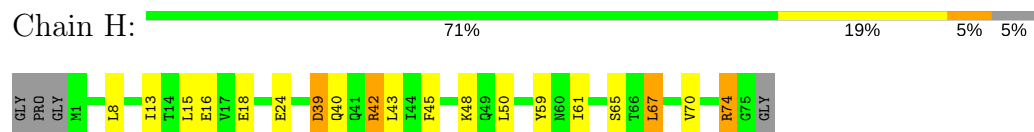
• Molecule 2: Ubiquitin



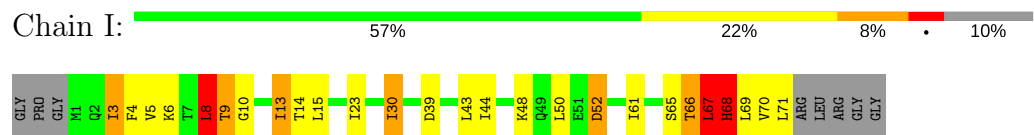
• Molecule 2: Ubiquitin



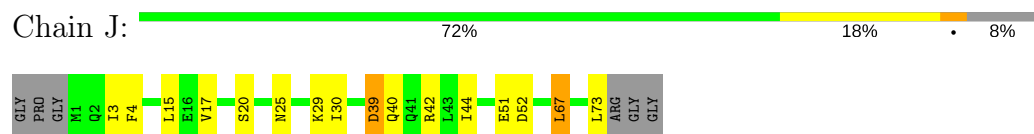
• Molecule 2: Ubiquitin



• Molecule 2: Ubiquitin



• Molecule 2: Ubiquitin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.54Å 101.85Å 88.15Å 90.00° 106.88° 90.00°	Depositor
Resolution (Å)	46.00 – 3.70 46.11 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.00-3.70) 98.3 (46.11-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.222 , 0.285 0.233 , 0.296	Depositor DCC
$R_{free}$ test set	903 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 62.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	19139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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

### 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	0.46	0/1563	0.83	1/2110 (0.0%)
1	B	0.46	0/1561	0.79	1/2108 (0.0%)
1	C	0.39	0/1545	0.75	2/2088 (0.1%)
1	D	0.42	0/1578	0.81	5/2128 (0.2%)
2	E	0.33	0/580	0.65	0/781
2	F	0.31	0/582	0.64	1/785 (0.1%)
2	G	0.35	0/564	0.66	0/761
2	H	0.32	0/597	0.65	0/804
2	I	0.65	0/561	0.99	4/757 (0.5%)
2	J	0.35	0/588	0.65	0/792
All	All	0.42	0/9719	0.77	14/13114 (0.1%)

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	D	0	1
2	I	0	3
All	All	0	6

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	71	ARG	NE-CZ-NH1	8.41	124.51	120.30
2	I	67	LEU	N-CA-C	-7.84	89.83	111.00
1	D	71	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	185	LEU	CA-CB-CG	6.31	129.81	115.30
1	C	26	LEU	CA-CB-CG	6.04	129.19	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	ARG	Peptide
1	B	13	GLN	Peptide
1	D	186	TRP	Peptide
2	I	3	ILE	Peptide
2	I	66	THR	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	1531	1510	1510	49	0
1	B	1529	1505	1505	50	0
1	C	1513	1487	1487	53	0
1	D	1546	1535	1535	44	0
2	E	574	595	599	18	0
2	F	576	595	599	13	0
2	G	558	570	574	5	0
2	H	591	611	615	11	0
2	I	555	570	574	28	0
2	J	582	606	610	8	0
All	All	9555	9584	9608	262	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 14.

The worst 5 of 262 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)
2:I:5:VAL:HG13	2:I:69:LEU:HB3	1.45	0.98
1:A:135:GLU:OE1	1:A:161:ARG:NH1	2.17	0.77
1:B:107:LEU:HD23	1:B:156:VAL:HG13	1.69	0.74
1:C:154:LYS:NZ	1:C:157:GLU:OE2	2.19	0.74
2:I:5:VAL:HG13	2:I:69:LEU:CB	2.17	0.74

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	186/203 (92%)	172 (92%)	11 (6%)	3 (2%)	11	50
1	B	186/203 (92%)	171 (92%)	14 (8%)	1 (0%)	31	71
1	C	186/203 (92%)	170 (91%)	13 (7%)	3 (2%)	11	50
1	D	186/203 (92%)	176 (95%)	8 (4%)	2 (1%)	16	58
2	E	70/79 (89%)	69 (99%)	1 (1%)	0	100	100
2	F	71/79 (90%)	69 (97%)	2 (3%)	0	100	100
2	G	69/79 (87%)	68 (99%)	1 (1%)	0	100	100
2	H	73/79 (92%)	71 (97%)	2 (3%)	0	100	100
2	I	69/79 (87%)	65 (94%)	3 (4%)	1 (1%)	12	52
2	J	71/79 (90%)	69 (97%)	2 (3%)	0	100	100
All	All	1167/1286 (91%)	1100 (94%)	57 (5%)	10 (1%)	19	61

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	187	ILE
1	C	66	GLU
1	C	139	ILE
1	D	139	ILE
1	A	180	ASN

### 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	162/182 (89%)	137 (85%)	25 (15%)	3	20
1	B	162/182 (89%)	142 (88%)	20 (12%)	5	29
1	C	158/182 (87%)	135 (85%)	23 (15%)	3	23
1	D	166/182 (91%)	142 (86%)	24 (14%)	3	23
2	E	66/69 (96%)	58 (88%)	8 (12%)	5	29
2	F	66/69 (96%)	57 (86%)	9 (14%)	4	26
2	G	64/69 (93%)	55 (86%)	9 (14%)	4	24
2	H	67/69 (97%)	58 (87%)	9 (13%)	4	26
2	I	63/69 (91%)	54 (86%)	9 (14%)	3	24
2	J	67/69 (97%)	60 (90%)	7 (10%)	8	36
All	All	1041/1142 (91%)	898 (86%)	143 (14%)	4	25

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	171	LEU
1	D	71	ARG
2	I	52	ASP
1	C	185	LEU
1	D	17	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	A	42	GLN
1	A	46	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no 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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.