



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 11:46 am BST

PDB ID : 4P4H  
Title : Caught-in-action signaling complex of RIG-I 2CARD domain and MAVS CARD domain  
Authors : Wu, B.; Hur, S.  
Deposited on : 2014-03-12  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

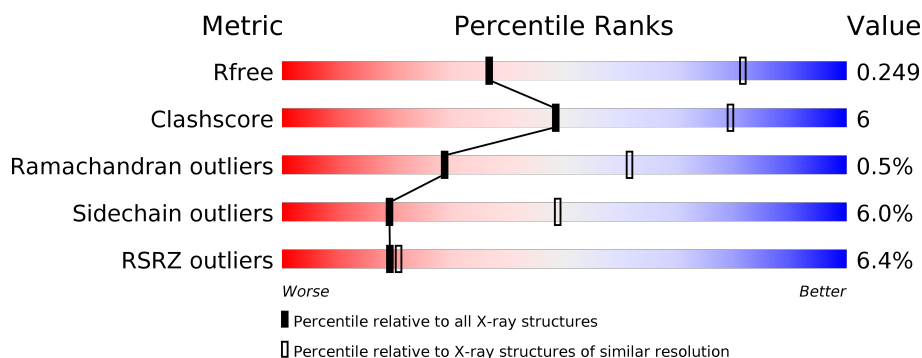
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	205	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>8%</div> </div> </div>
1	B	205	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>8%</div> </div> </div>
1	C	205	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>8%</div> </div> </div>
1	D	205	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>8%</div> </div> </div>
1	E	205	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>8%</div> </div> </div>
1	F	205	<div> <div></div> <div> <div></div> <div>72%</div> <div>18%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	205	
1	H	205	
2	I	108	
2	J	108	
2	K	108	
2	L	108	
2	M	108	
2	N	108	
2	O	108	
2	P	108	
3	S	79	
3	T	79	
3	U	79	
3	W	79	
3	X	79	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43332 atoms, of which 21621 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
			3112	1007	1550	255	291	9			
1	B	189	Total	C	H	N	O	S	0	0	0
			3127	1012	1556	256	294	9			
1	C	189	Total	C	H	N	O	S	0	0	0
			3127	1012	1556	256	294	9			
1	D	188	Total	C	H	N	O	S	0	0	0
			3112	1007	1550	255	291	9			
1	E	188	Total	C	H	N	O	S	0	0	0
			3073	1000	1524	250	290	9			
1	F	189	Total	C	H	N	O	S	0	0	0
			3085	1004	1530	250	292	9			
1	G	189	Total	C	H	N	O	S	0	0	0
			3111	1008	1548	256	290	9			
1	H	188	Total	C	H	N	O	S	0	0	0
			3112	1007	1550	255	291	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP O95786
A	-2	PRO	-	expression tag	UNP O95786
A	-1	GLY	-	expression tag	UNP O95786
A	0	ALA	-	expression tag	UNP O95786
A	52	ALA	GLU	engineered mutation	UNP O95786
B	-3	GLY	-	expression tag	UNP O95786
B	-2	PRO	-	expression tag	UNP O95786
B	-1	GLY	-	expression tag	UNP O95786
B	0	ALA	-	expression tag	UNP O95786
B	52	ALA	GLU	engineered mutation	UNP O95786
C	-3	GLY	-	expression tag	UNP O95786
C	-2	PRO	-	expression tag	UNP O95786
C	-1	GLY	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP 095786
C	52	ALA	GLU	engineered mutation	UNP 095786
D	-3	GLY	-	expression tag	UNP 095786
D	-2	PRO	-	expression tag	UNP 095786
D	-1	GLY	-	expression tag	UNP 095786
D	0	ALA	-	expression tag	UNP 095786
D	52	ALA	GLU	engineered mutation	UNP 095786
E	-3	GLY	-	expression tag	UNP 095786
E	-2	PRO	-	expression tag	UNP 095786
E	-1	GLY	-	expression tag	UNP 095786
E	0	ALA	-	expression tag	UNP 095786
E	52	ALA	GLU	engineered mutation	UNP 095786
F	-3	GLY	-	expression tag	UNP 095786
F	-2	PRO	-	expression tag	UNP 095786
F	-1	GLY	-	expression tag	UNP 095786
F	0	ALA	-	expression tag	UNP 095786
F	52	ALA	GLU	engineered mutation	UNP 095786
G	-3	GLY	-	expression tag	UNP 095786
G	-2	PRO	-	expression tag	UNP 095786
G	-1	GLY	-	expression tag	UNP 095786
G	0	ALA	-	expression tag	UNP 095786
G	52	ALA	GLU	engineered mutation	UNP 095786
H	-3	GLY	-	expression tag	UNP 095786
H	-2	PRO	-	expression tag	UNP 095786
H	-1	GLY	-	expression tag	UNP 095786
H	0	ALA	-	expression tag	UNP 095786
H	52	ALA	GLU	engineered mutation	UNP 095786

- Molecule 2 is a protein called Mitochondrial antiviral-signaling protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	J	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	K	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	L	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	N	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	O	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	M	97	Total	C	H	N	O	S	0	0	0
			1581	511	785	139	140	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	GLY	-	expression tag	UNP Q7Z434
I	-7	SER	-	expression tag	UNP Q7Z434
I	-6	GLY	-	expression tag	UNP Q7Z434
I	-5	THR	-	expression tag	UNP Q7Z434
I	-4	GLY	-	expression tag	UNP Q7Z434
I	-3	SER	-	expression tag	UNP Q7Z434
I	-2	THR	-	expression tag	UNP Q7Z434
I	-1	GLY	-	expression tag	UNP Q7Z434
I	0	SER	-	expression tag	UNP Q7Z434
I	23	LYS	ASP	engineered mutation	UNP Q7Z434
I	26	LYS	GLU	engineered mutation	UNP Q7Z434
I	80	LYS	GLU	engineered mutation	UNP Q7Z434
J	-8	GLY	-	expression tag	UNP Q7Z434
J	-7	SER	-	expression tag	UNP Q7Z434
J	-6	GLY	-	expression tag	UNP Q7Z434
J	-5	THR	-	expression tag	UNP Q7Z434
J	-4	GLY	-	expression tag	UNP Q7Z434
J	-3	SER	-	expression tag	UNP Q7Z434
J	-2	THR	-	expression tag	UNP Q7Z434
J	-1	GLY	-	expression tag	UNP Q7Z434
J	0	SER	-	expression tag	UNP Q7Z434
J	23	LYS	ASP	engineered mutation	UNP Q7Z434
J	26	LYS	GLU	engineered mutation	UNP Q7Z434
J	80	LYS	GLU	engineered mutation	UNP Q7Z434
K	-8	GLY	-	expression tag	UNP Q7Z434
K	-7	SER	-	expression tag	UNP Q7Z434
K	-6	GLY	-	expression tag	UNP Q7Z434
K	-5	THR	-	expression tag	UNP Q7Z434
K	-4	GLY	-	expression tag	UNP Q7Z434
K	-3	SER	-	expression tag	UNP Q7Z434
K	-2	THR	-	expression tag	UNP Q7Z434
K	-1	GLY	-	expression tag	UNP Q7Z434
K	0	SER	-	expression tag	UNP Q7Z434
K	23	LYS	ASP	engineered mutation	UNP Q7Z434

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Chain	Residue	Modelled	Actual	Comment	Reference
K	26	LYS	GLU	engineered mutation	UNP Q7Z434
K	80	LYS	GLU	engineered mutation	UNP Q7Z434
L	-8	GLY	-	expression tag	UNP Q7Z434
L	-7	SER	-	expression tag	UNP Q7Z434
L	-6	GLY	-	expression tag	UNP Q7Z434
L	-5	THR	-	expression tag	UNP Q7Z434
L	-4	GLY	-	expression tag	UNP Q7Z434
L	-3	SER	-	expression tag	UNP Q7Z434
L	-2	THR	-	expression tag	UNP Q7Z434
L	-1	GLY	-	expression tag	UNP Q7Z434
L	0	SER	-	expression tag	UNP Q7Z434
L	23	LYS	ASP	engineered mutation	UNP Q7Z434
L	26	LYS	GLU	engineered mutation	UNP Q7Z434
L	80	LYS	GLU	engineered mutation	UNP Q7Z434
N	-8	GLY	-	expression tag	UNP Q7Z434
N	-7	SER	-	expression tag	UNP Q7Z434
N	-6	GLY	-	expression tag	UNP Q7Z434
N	-5	THR	-	expression tag	UNP Q7Z434
N	-4	GLY	-	expression tag	UNP Q7Z434
N	-3	SER	-	expression tag	UNP Q7Z434
N	-2	THR	-	expression tag	UNP Q7Z434
N	-1	GLY	-	expression tag	UNP Q7Z434
N	0	SER	-	expression tag	UNP Q7Z434
N	23	LYS	ASP	engineered mutation	UNP Q7Z434
N	26	LYS	GLU	engineered mutation	UNP Q7Z434
N	80	LYS	GLU	engineered mutation	UNP Q7Z434
O	-8	GLY	-	expression tag	UNP Q7Z434
O	-7	SER	-	expression tag	UNP Q7Z434
O	-6	GLY	-	expression tag	UNP Q7Z434
O	-5	THR	-	expression tag	UNP Q7Z434
O	-4	GLY	-	expression tag	UNP Q7Z434
O	-3	SER	-	expression tag	UNP Q7Z434
O	-2	THR	-	expression tag	UNP Q7Z434
O	-1	GLY	-	expression tag	UNP Q7Z434
O	0	SER	-	expression tag	UNP Q7Z434
O	23	LYS	ASP	engineered mutation	UNP Q7Z434
O	26	LYS	GLU	engineered mutation	UNP Q7Z434
O	80	LYS	GLU	engineered mutation	UNP Q7Z434
P	-8	GLY	-	expression tag	UNP Q7Z434
P	-7	SER	-	expression tag	UNP Q7Z434
P	-6	GLY	-	expression tag	UNP Q7Z434
P	-5	THR	-	expression tag	UNP Q7Z434

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-4	GLY	-	expression tag	UNP Q7Z434
P	-3	SER	-	expression tag	UNP Q7Z434
P	-2	THR	-	expression tag	UNP Q7Z434
P	-1	GLY	-	expression tag	UNP Q7Z434
P	0	SER	-	expression tag	UNP Q7Z434
P	23	LYS	ASP	engineered mutation	UNP Q7Z434
P	26	LYS	GLU	engineered mutation	UNP Q7Z434
P	80	LYS	GLU	engineered mutation	UNP Q7Z434
M	-8	GLY	-	expression tag	UNP Q7Z434
M	-7	SER	-	expression tag	UNP Q7Z434
M	-6	GLY	-	expression tag	UNP Q7Z434
M	-5	THR	-	expression tag	UNP Q7Z434
M	-4	GLY	-	expression tag	UNP Q7Z434
M	-3	SER	-	expression tag	UNP Q7Z434
M	-2	THR	-	expression tag	UNP Q7Z434
M	-1	GLY	-	expression tag	UNP Q7Z434
M	0	SER	-	expression tag	UNP Q7Z434
M	23	LYS	ASP	engineered mutation	UNP Q7Z434
M	26	LYS	GLU	engineered mutation	UNP Q7Z434
M	80	LYS	GLU	engineered mutation	UNP Q7Z434

- Molecule 3 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	S	71	Total	C	H	N	O	S	0	0	0
			1146	356	583	94	112	1			
3	T	73	Total	C	H	N	O	S	0	0	0
			1189	368	607	99	114	1			
3	U	72	Total	C	H	N	O	S	0	0	0
			1140	356	574	96	113	1			
3	W	71	Total	C	H	N	O	S	0	0	0
			1126	352	571	92	110	1			
3	X	73	Total	C	H	N	O	S	0	0	0
			1189	368	607	99	114	1			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	GLY	-	expression tag	UNP P62987
S	-1	PRO	-	expression tag	UNP P62987
S	0	GLY	-	expression tag	UNP P62987
T	-2	GLY	-	expression tag	UNP P62987

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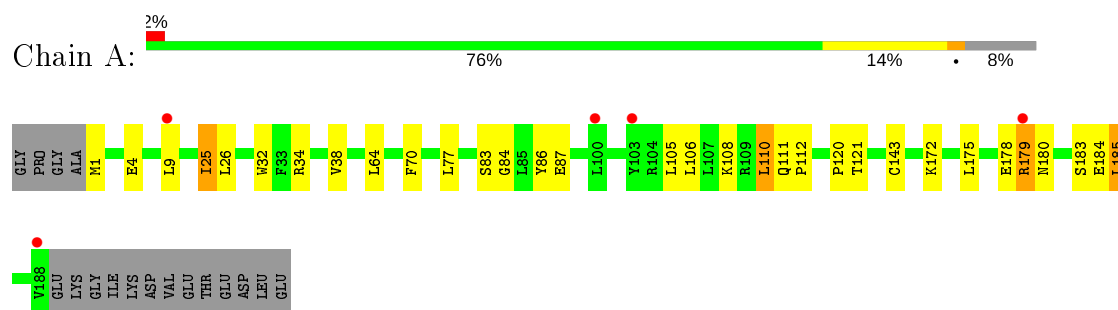
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Chain	Residue	Modelled	Actual	Comment	Reference
T	-1	PRO	-	expression tag	UNP P62987
T	0	GLY	-	expression tag	UNP P62987
U	-2	GLY	-	expression tag	UNP P62987
U	-1	PRO	-	expression tag	UNP P62987
U	0	GLY	-	expression tag	UNP P62987
W	-2	GLY	-	expression tag	UNP P62987
W	-1	PRO	-	expression tag	UNP P62987
W	0	GLY	-	expression tag	UNP P62987
X	-2	GLY	-	expression tag	UNP P62987
X	-1	PRO	-	expression tag	UNP P62987
X	0	GLY	-	expression tag	UNP P62987

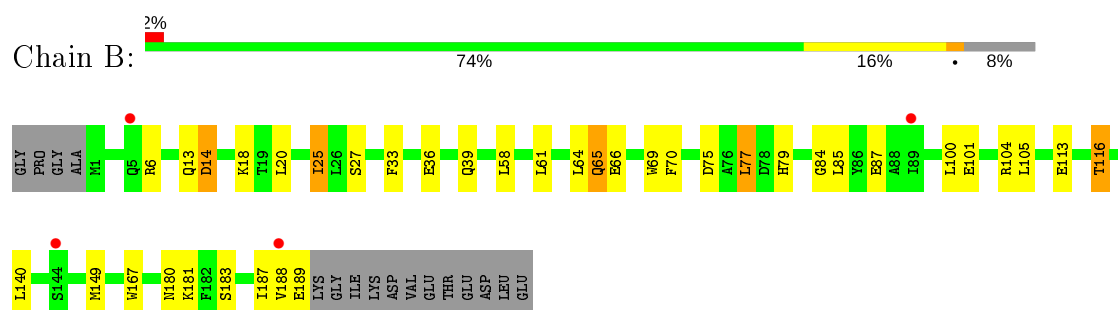
### 3 Residue-property plots [i](#)

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

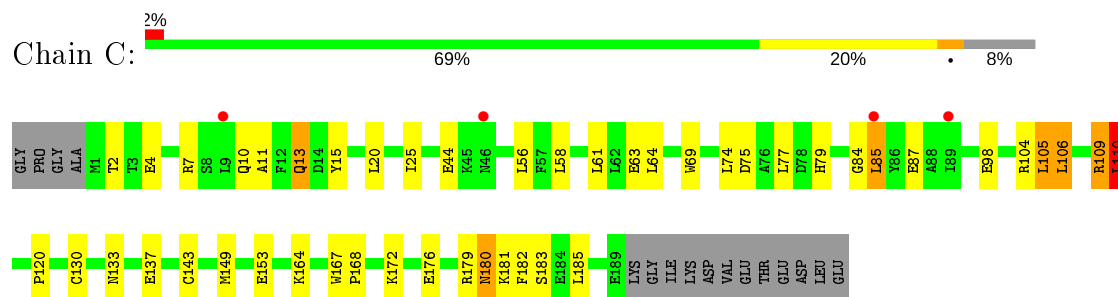
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



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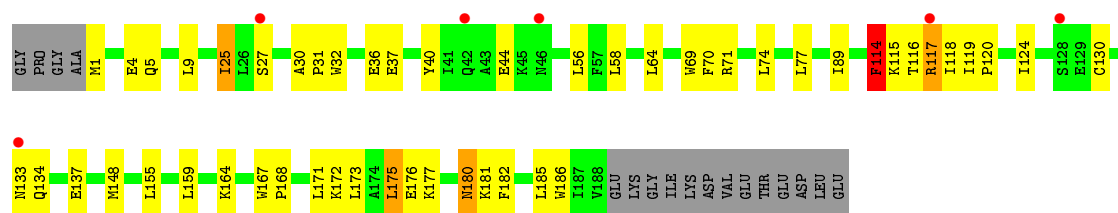


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

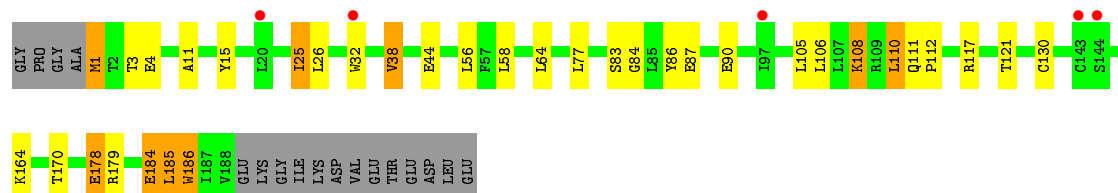
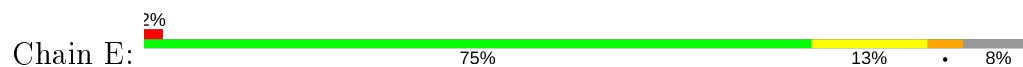


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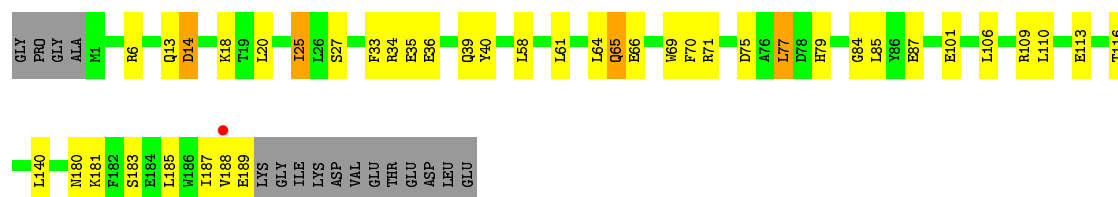




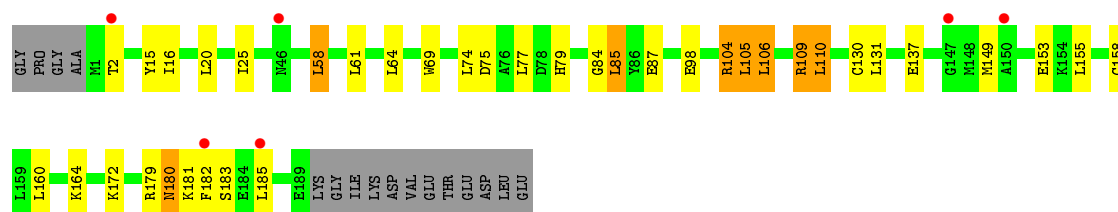
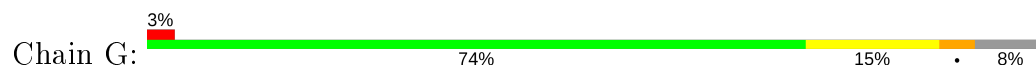
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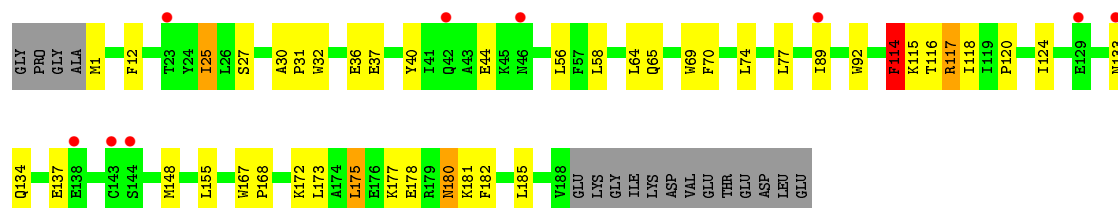
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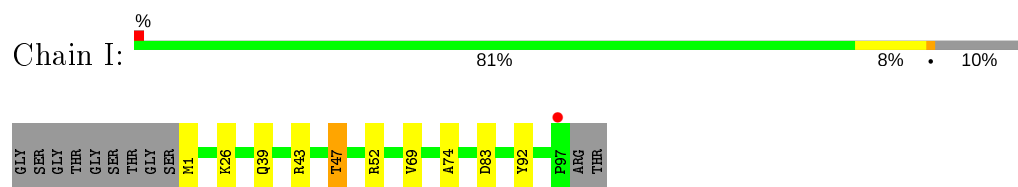
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



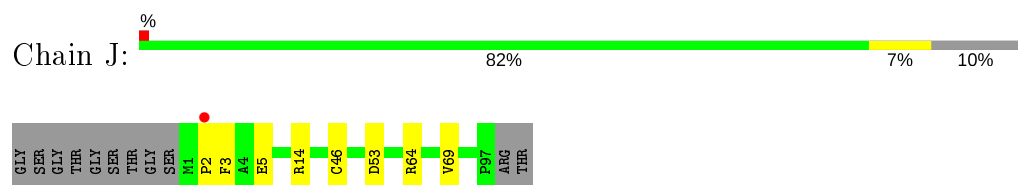
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



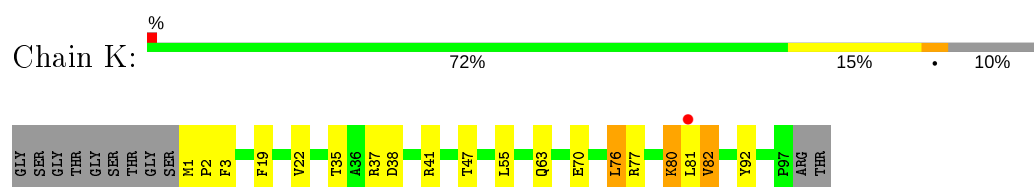
## • Molecule 2: Mitochondrial antiviral-signaling protein



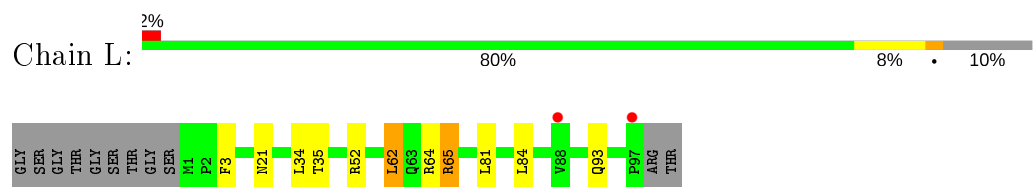
## • Molecule 2: Mitochondrial antiviral-signaling protein



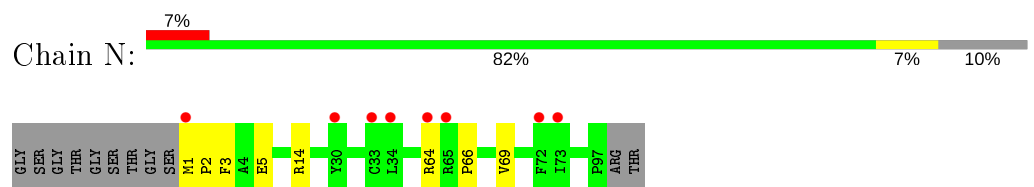
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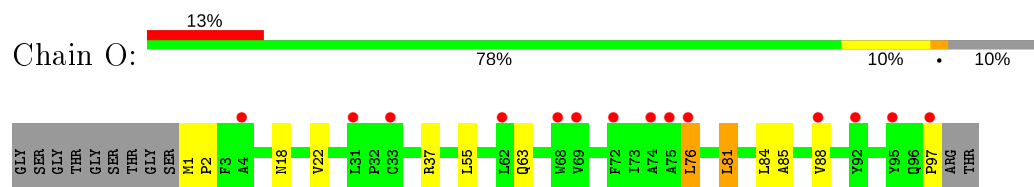
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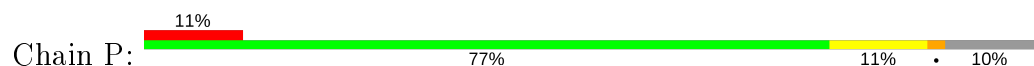
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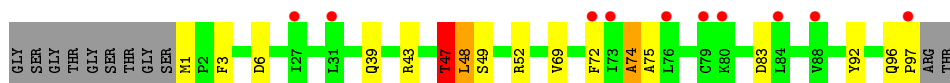
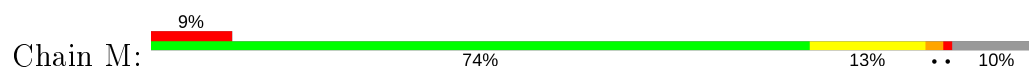


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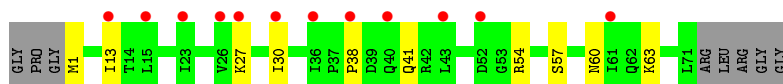
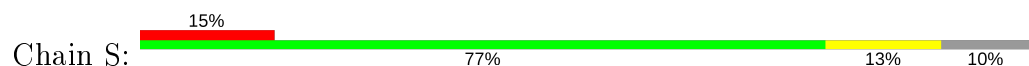




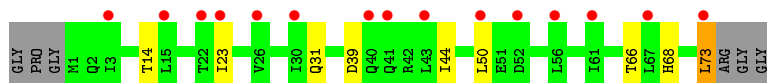
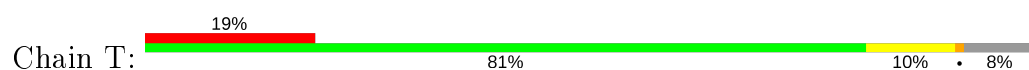
- Molecule 2: Mitochondrial antiviral-signaling protein



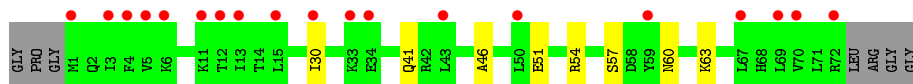
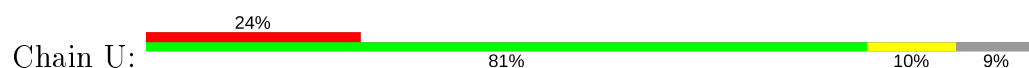
- Molecule 3: Ubiquitin-60S ribosomal protein L40



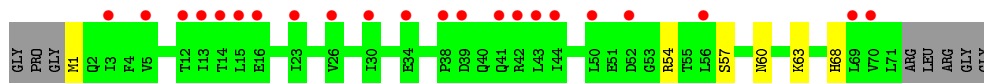
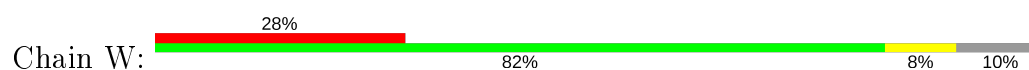
- Molecule 3: Ubiquitin-60S ribosomal protein L40



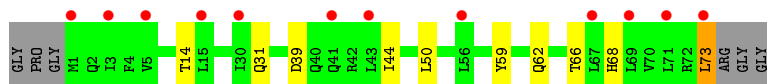
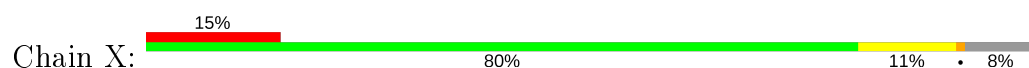
- Molecule 3: Ubiquitin-60S ribosomal protein L40



- Molecule 3: Ubiquitin-60S ribosomal protein L40



- Molecule 3: Ubiquitin-60S ribosomal protein L40



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.81Å 117.33Å 257.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 3.40 48.18 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.80-3.40) 99.2 (48.18-3.39)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.191 , 0.240 0.202 , 0.249	Depositor DCC
$R_{free}$ test set	2361 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 67.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	43332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 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	0.59	0/1594	0.68	1/2146 (0.0%)
1	B	0.54	0/1603	0.64	0/2158
1	C	0.59	0/1603	0.70	1/2158 (0.0%)
1	D	0.69	0/1594	0.71	0/2146
1	E	0.52	0/1581	0.73	4/2131 (0.2%)
1	F	0.49	0/1587	0.60	0/2139
1	G	0.62	0/1595	0.68	0/2148
1	H	0.59	0/1594	0.67	0/2146
2	I	0.57	0/816	0.66	0/1108
2	J	0.60	1/816 (0.1%)	0.61	0/1108
2	K	0.62	0/816	0.66	0/1108
2	L	0.43	0/816	0.53	0/1108
2	M	0.42	0/816	0.71	3/1108 (0.3%)
2	N	0.41	0/816	0.57	0/1108
2	O	0.40	0/816	0.55	0/1108
2	P	0.36	0/816	0.53	0/1108
3	S	0.47	0/569	0.54	0/767
3	T	0.41	0/588	0.56	0/792
3	U	0.36	0/572	0.51	0/773
3	W	0.36	0/561	0.51	0/757
3	X	0.44	0/588	0.54	0/792
All	All	0.54	1/22157 (0.0%)	0.64	9/29917 (0.0%)

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	2
1	C	0	1
1	D	0	1
1	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	H	0	1
2	I	0	2
2	M	0	2
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	46	CYS	CB-SG	-5.95	1.72	1.81

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	GLU	C-N-CA	8.81	143.74	121.70
2	M	74	ALA	C-N-CA	7.34	140.06	121.70
1	A	172	LYS	CD-CE-NZ	6.93	127.64	111.70
1	E	184	GLU	CA-C-N	6.76	132.08	117.20
1	E	184	GLU	O-C-N	-6.55	112.21	122.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	GLU	Mainchain,Peptide
1	C	180	ASN	Mainchain
1	D	114	PHE	Mainchain
1	E	178	GLU	Mainchain
1	E	184	GLU	Mainchain

## 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	1562	1550	1571	20	0
1	B	1571	1556	1577	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1571	1556	1577	30	0
1	D	1562	1550	1571	27	0
1	E	1549	1524	1545	28	0
1	F	1555	1530	1551	26	0
1	G	1563	1548	1569	24	0
1	H	1562	1550	1571	23	0
2	I	796	790	793	4	0
2	J	796	790	793	5	0
2	K	796	790	793	13	0
2	L	796	790	793	5	0
2	M	796	785	793	12	0
2	N	796	790	793	5	0
2	O	796	790	793	7	0
2	P	796	790	793	7	0
3	S	563	583	586	10	0
3	T	582	607	610	5	0
3	U	566	574	577	9	0
3	W	555	571	574	4	0
3	X	582	607	610	6	0
All	All	21711	21621	21833	260	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.

The worst 5 of 260 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:G:106:LEU:HD12	1:G:110:LEU:HD11	1.40	1.03
1:C:106:LEU:HD12	1:C:110:LEU:HD11	1.42	1.02
1:C:180:ASN:O	1:C:182:PHE:N	2.02	0.91
1:A:175:LEU:O	1:A:180:ASN:ND2	2.12	0.81
1:F:18:LYS:NZ	1:F:101:GLU:OE1	2.15	0.78

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	186/205 (91%)	180 (97%)	5 (3%)	1 (0%)	29	61
1	B	187/205 (91%)	182 (97%)	5 (3%)	0	100	100
1	C	187/205 (91%)	184 (98%)	2 (1%)	1 (0%)	29	61
1	D	186/205 (91%)	176 (95%)	8 (4%)	2 (1%)	14	44
1	E	186/205 (91%)	179 (96%)	6 (3%)	1 (0%)	29	61
1	F	187/205 (91%)	182 (97%)	5 (3%)	0	100	100
1	G	187/205 (91%)	184 (98%)	2 (1%)	1 (0%)	29	61
1	H	186/205 (91%)	177 (95%)	7 (4%)	2 (1%)	14	44
2	I	95/108 (88%)	90 (95%)	4 (4%)	1 (1%)	14	44
2	J	95/108 (88%)	93 (98%)	2 (2%)	0	100	100
2	K	95/108 (88%)	91 (96%)	3 (3%)	1 (1%)	14	44
2	L	95/108 (88%)	93 (98%)	2 (2%)	0	100	100
2	M	95/108 (88%)	88 (93%)	5 (5%)	2 (2%)	7	30
2	N	95/108 (88%)	93 (98%)	2 (2%)	0	100	100
2	O	95/108 (88%)	93 (98%)	2 (2%)	0	100	100
2	P	95/108 (88%)	94 (99%)	1 (1%)	0	100	100
3	S	69/79 (87%)	68 (99%)	1 (1%)	0	100	100
3	T	71/79 (90%)	70 (99%)	1 (1%)	0	100	100
3	U	70/79 (89%)	68 (97%)	2 (3%)	0	100	100
3	W	69/79 (87%)	68 (99%)	1 (1%)	0	100	100
3	X	71/79 (90%)	70 (99%)	1 (1%)	0	100	100
All	All	2602/2899 (90%)	2523 (97%)	67 (3%)	12 (0%)	29	61

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	181	LYS
1	D	115	LYS
2	K	82	VAL
2	M	48	LEU
1	E	186	TRP

### 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	169/182 (93%)	160 (95%)	9 (5%)	22	52
1	B	170/182 (93%)	160 (94%)	10 (6%)	19	49
1	C	170/182 (93%)	157 (92%)	13 (8%)	13	41
1	D	169/182 (93%)	154 (91%)	15 (9%)	9	33
1	E	166/182 (91%)	156 (94%)	10 (6%)	19	49
1	F	167/182 (92%)	155 (93%)	12 (7%)	14	43
1	G	168/182 (92%)	156 (93%)	12 (7%)	14	44
1	H	169/182 (93%)	154 (91%)	15 (9%)	9	33
2	I	87/94 (93%)	85 (98%)	2 (2%)	50	74
2	J	87/94 (93%)	85 (98%)	2 (2%)	50	74
2	K	87/94 (93%)	82 (94%)	5 (6%)	20	50
2	L	87/94 (93%)	81 (93%)	6 (7%)	15	45
2	M	87/94 (93%)	84 (97%)	3 (3%)	37	65
2	N	87/94 (93%)	84 (97%)	3 (3%)	37	65
2	O	87/94 (93%)	83 (95%)	4 (5%)	27	57
2	P	87/94 (93%)	81 (93%)	6 (7%)	15	45
3	S	65/69 (94%)	62 (95%)	3 (5%)	27	57
3	T	67/69 (97%)	63 (94%)	4 (6%)	19	49
3	U	64/69 (93%)	62 (97%)	2 (3%)	40	68
3	W	63/69 (91%)	61 (97%)	2 (3%)	39	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	X	67/69 (97%)	63 (94%)	4 (6%)	19	49
All	All	2370/2553 (93%)	2228 (94%)	142 (6%)	19	49

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	77	LEU
1	G	179	ARG
3	U	57	SER
1	F	113	GLU
1	G	104	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	79	HIS
3	S	41	GLN
3	U	41	GLN
3	X	60	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	188/205 (91%)	0.29	5 (2%) 54 53	59, 90, 139, 156	0
1	B	189/205 (92%)	0.32	4 (2%) 63 62	57, 93, 147, 180	0
1	C	189/205 (92%)	0.26	4 (2%) 63 62	57, 90, 156, 243	0
1	D	188/205 (91%)	0.38	6 (3%) 47 46	55, 83, 122, 155	0
1	E	188/205 (91%)	0.34	5 (2%) 54 53	71, 108, 153, 196	0
1	F	189/205 (92%)	0.33	1 (0%) 91 90	69, 113, 159, 194	0
1	G	189/205 (92%)	0.29	6 (3%) 47 46	56, 88, 134, 168	0
1	H	188/205 (91%)	0.41	9 (4%) 30 31	60, 95, 138, 182	0
2	I	97/108 (89%)	0.10	1 (1%) 82 81	54, 80, 135, 187	0
2	J	97/108 (89%)	0.17	1 (1%) 82 81	54, 82, 139, 152	0
2	K	97/108 (89%)	0.08	1 (1%) 82 81	55, 79, 113, 223	0
2	L	97/108 (89%)	0.08	2 (2%) 63 62	76, 107, 151, 169	0
2	M	97/108 (89%)	0.43	10 (10%) 6 8	94, 145, 199, 219	0
2	N	97/108 (89%)	0.57	8 (8%) 11 13	109, 151, 198, 216	0
2	O	97/108 (89%)	0.83	14 (14%) 2 3	104, 158, 196, 240	0
2	P	97/108 (89%)	0.66	12 (12%) 4 5	121, 154, 185, 217	0
3	S	71/79 (89%)	0.80	12 (16%) 1 2	70, 112, 154, 189	0
3	T	73/79 (92%)	1.48	15 (20%) 1 1	94, 143, 182, 201	1 (1%)
3	U	72/79 (91%)	1.07	19 (26%) 0 0	123, 181, 218, 231	0
3	W	71/79 (89%)	1.57	22 (30%) 0 0	108, 150, 177, 208	0
3	X	73/79 (92%)	1.07	12 (16%) 1 2	82, 116, 157, 183	0
All	All	2644/2899 (91%)	0.46	169 (6%) 19 20	54, 104, 178, 243	1 (0%)

The worst 5 of 169 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	33	CYS	5.7
3	W	43	LEU	5.5
2	O	72	PHE	5.3
2	O	76	LEU	5.1
3	U	5	VAL	5.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.