



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:35 pm BST

PDB ID : 2LXP  
Title : NMR structure of two domains in ubiquitin ligase gp78, RING and G2BR, bound to its conjugating enzyme Ube2g  
Authors : Das, R.; Linag, Y.; Mariano, J.; Li, J.; Huang, T.; King, A.; Weissman, A.; Ji, X.; Byrd, R.  
Deposited on : 2012-08-30

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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/NMRValidationReportHelp>

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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

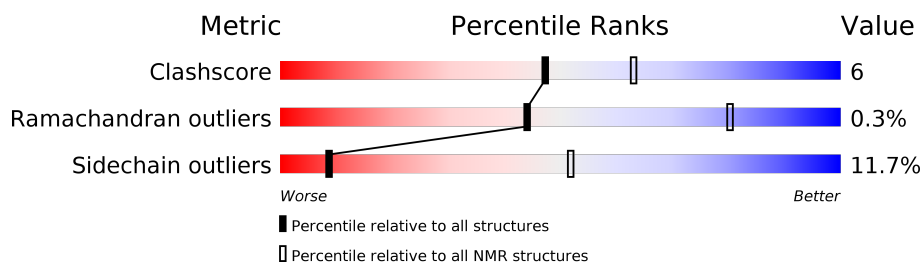
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 4%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	164	 79% 14% .. 5%
2	B	27	 52% 48%
3	C	58	 83% 17%

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:96, A:108-A:165, B:574-B:600, C:327-C:384 (238)	0.28	14

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	4, 6, 7, 8, 15, 17, 18
2	5, 14, 16, 20
3	1, 9, 11
4	2, 10
5	13, 19
Single-model clusters	3; 12

### 3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3795 atoms, of which 1880 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-conjugating enzyme E2 G2.

Mol	Chain	Residues	Atoms						Trace
1	A	156	Total	C	H	N	O	S	0
			2444	793	1213	200	228	10	

- Molecule 2 is a protein called E3 ubiquitin-protein ligase AMFR.

Mol	Chain	Residues	Atoms						Trace
2	B	27	Total	C	H	N	O	S	0
			483	142	248	50	42	1	

- Molecule 3 is a protein called E3 ubiquitin-protein ligase AMFR.

Mol	Chain	Residues	Atoms						Trace
3	C	58	Total	C	H	N	O	S	0
			866	272	419	80	87	8	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

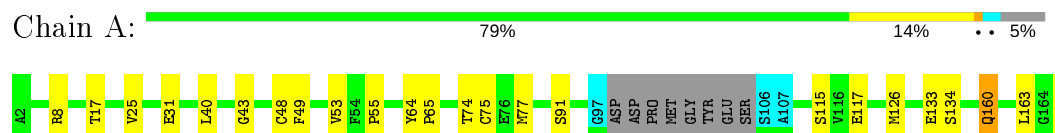
Mol	Chain	Residues	Atoms	
4	C	2	Total	Zn
			2	2

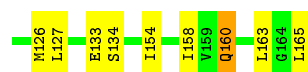
## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

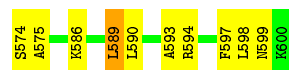
These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

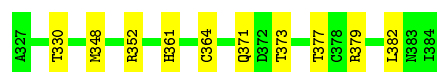
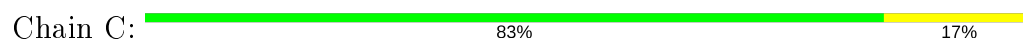




- Molecule 2: E3 ubiquitin-protein ligase AMFR

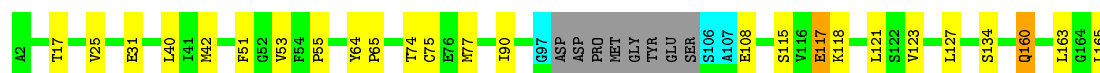
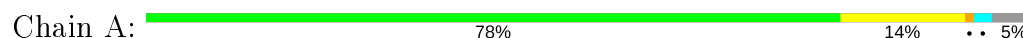


- Molecule 3: E3 ubiquitin-protein ligase AMFR



#### 4.2.2 Score per residue for model 2

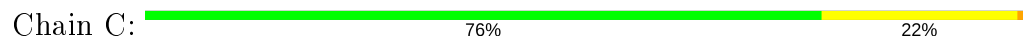
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

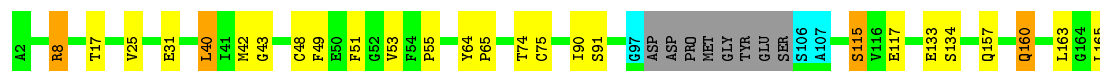
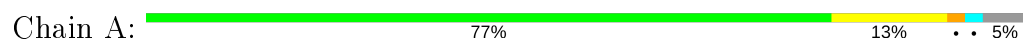


- Molecule 3: E3 ubiquitin-protein ligase AMFR



#### 4.2.3 Score per residue for model 3

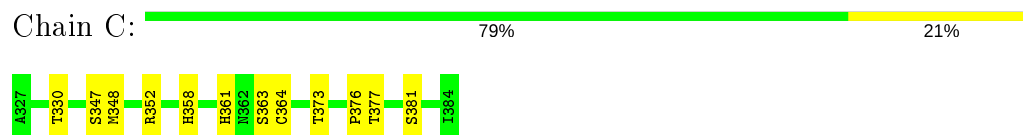
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

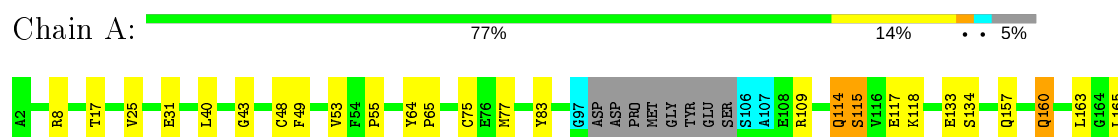


- Molecule 3: E3 ubiquitin-protein ligase AMFR

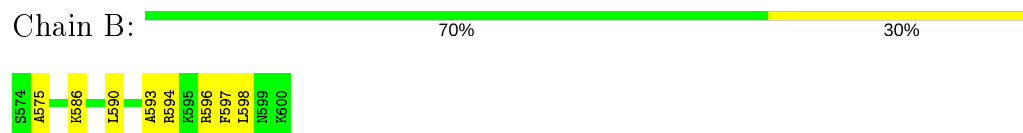


#### 4.2.4 Score per residue for model 4

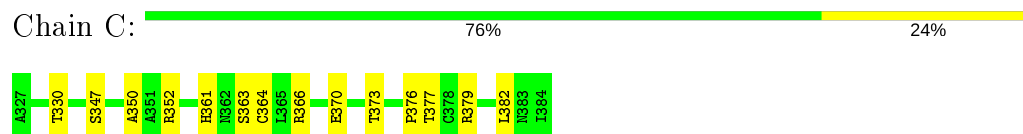
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

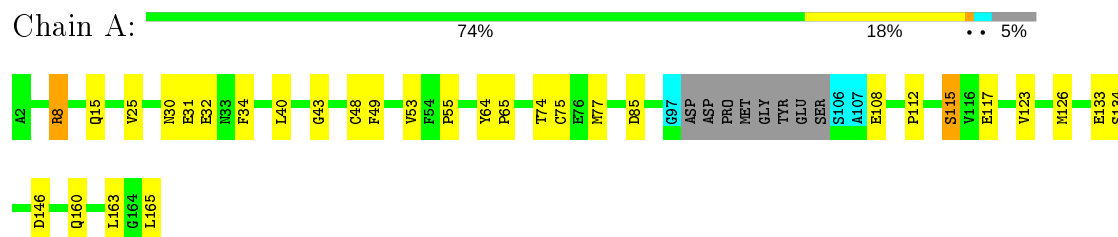


- Molecule 3: E3 ubiquitin-protein ligase AMFR



#### 4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2




- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B:  63% 37%




- Molecule 3: E3 ubiquitin-protein ligase AMFR

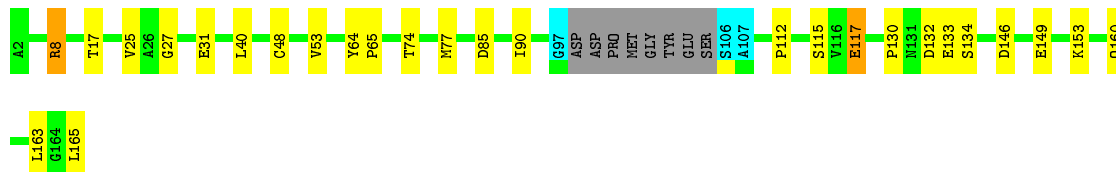
Chain C:  76% 24%



#### 4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

Chain A:  77% 15% 5%




- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B:  56% 44%




- Molecule 3: E3 ubiquitin-protein ligase AMFR

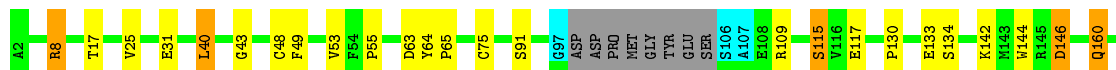
Chain C:  78% 22%



#### 4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

Chain A:  77% 13% 5%





L165

- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B:  67% 30% .

S574 A575 D576 E577 K586 L589 L590 F597 L598 K599 K600

- Molecule 3: E3 ubiquitin-protein ligase AMFR

Chain C:  78% 21% .

A327 T330 P331 E332 S347 K348 Q349 R352 H361 N362 S363 C364 T373 T377 C378 R379 L382 N383 I384

#### 4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

Chain A:  76% 16% 5% . .

A2 V25 L40 Q43 D46 T47 C48 F49 F51 G52 V53 P54 P55 Y64 P65 T74 C75 E76 M77 Y83 P84 I90 S91 Q97 ASP PRO MET GLY TYR GLU SER S106 A107 E108 R109 S115 V116 E117 V123 M126 E133 S134 D146


Q160 L163 G164 L165

- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B:  41% 52% 7%

S574 A575 D576 E577 Q579 V583 Q584 R585 K586 D587 E588 L589 L590 A593 R594 K595 R596 F597 L598 N599 K600

- Molecule 3: E3 ubiquitin-protein ligase AMFR

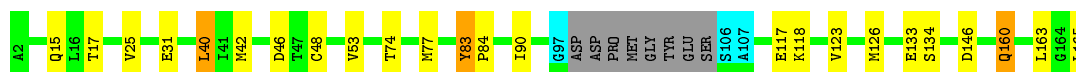
Chain C:  81% 19%

A327 T330 S347 R352 R361 N362 S363 C364 L369 E370 T373 P376 T377 I384

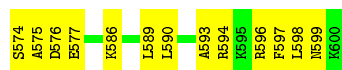
#### 4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

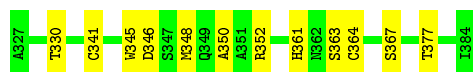
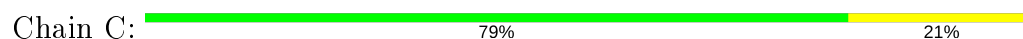
Chain A:  79% 13% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

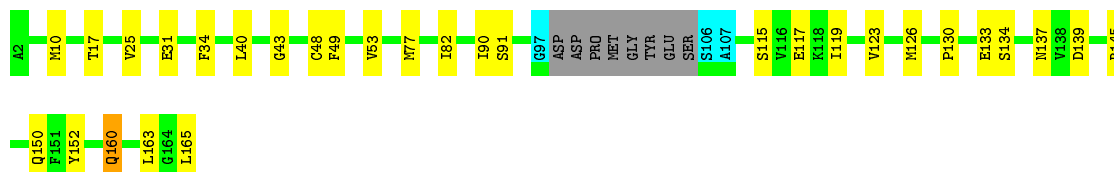


- Molecule 3: E3 ubiquitin-protein ligase AMFR



#### 4.2.10 Score per residue for model 10

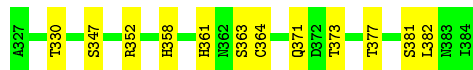
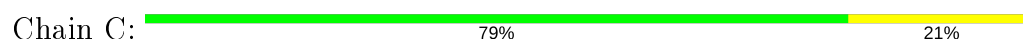
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR



- Molecule 3: E3 ubiquitin-protein ligase AMFR



#### 4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

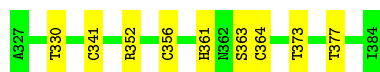
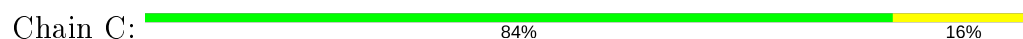




- Molecule 2: E3 ubiquitin-protein ligase AMFR

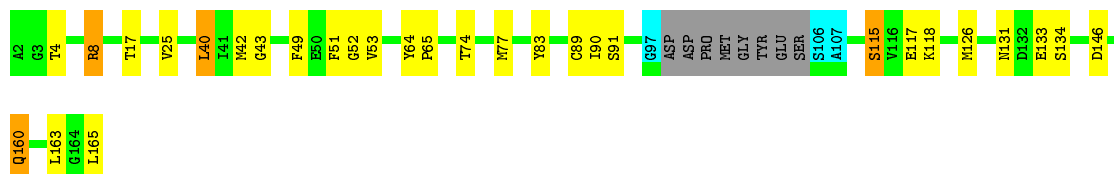


- Molecule 3: E3 ubiquitin-protein ligase AMFR

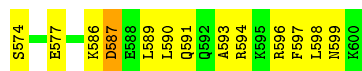


#### 4.2.12 Score per residue for model 12

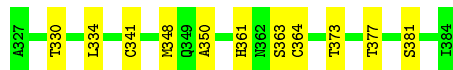
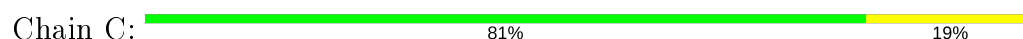
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR



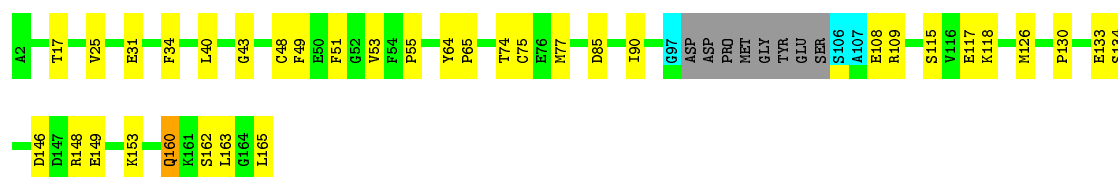
- Molecule 3: E3 ubiquitin-protein ligase AMFR



#### 4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

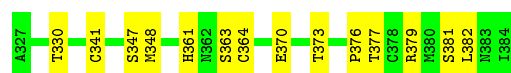




- Molecule 2: E3 ubiquitin-protein ligase AMFR

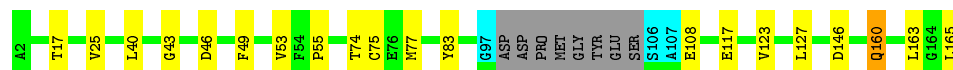
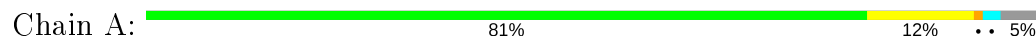


- Molecule 3: E3 ubiquitin-protein ligase AMFR



#### 4.2.14 Score per residue for model 14 (medoid)

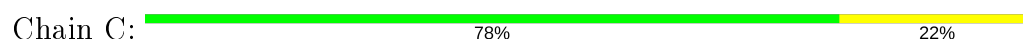
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR



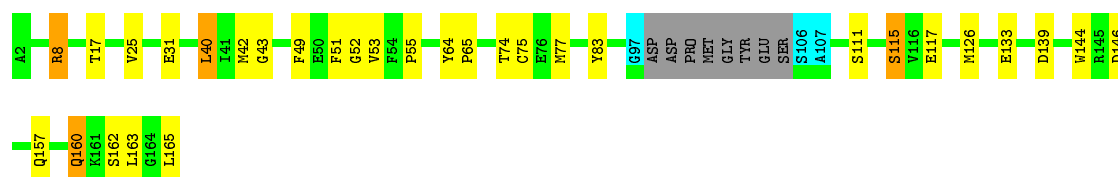
- Molecule 3: E3 ubiquitin-protein ligase AMFR



#### 4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

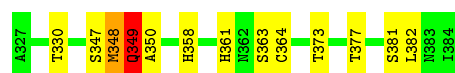




- Molecule 2: E3 ubiquitin-protein ligase AMFR

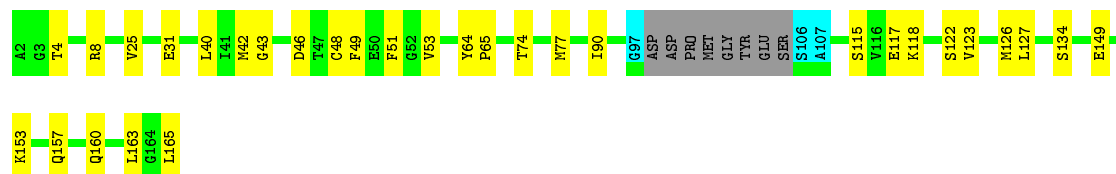


- Molecule 3: E3 ubiquitin-protein ligase AMFR



#### 4.2.16 Score per residue for model 16

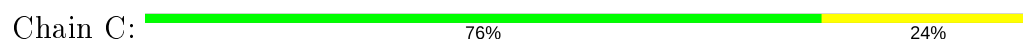
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

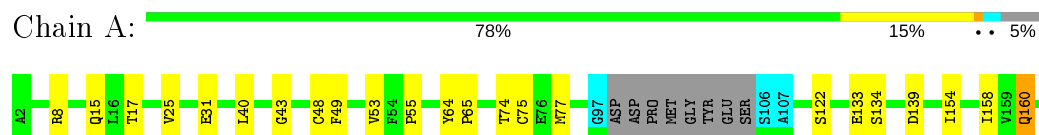


- Molecule 3: E3 ubiquitin-protein ligase AMFR



## 4.2.17 Score per residue for model 17

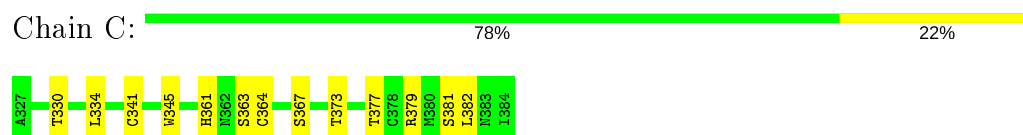
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

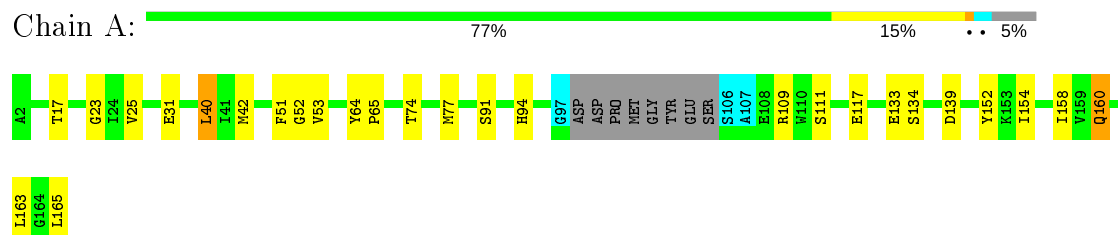


- Molecule 3: E3 ubiquitin-protein ligase AMFR



## 4.2.18 Score per residue for model 18

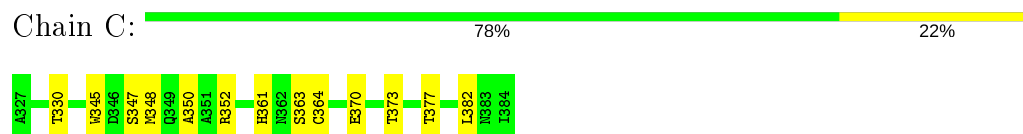
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

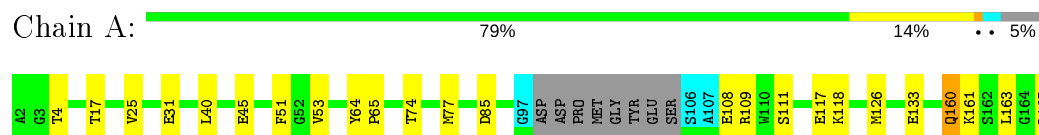


- Molecule 3: E3 ubiquitin-protein ligase AMFR



### 4.2.19 Score per residue for model 19

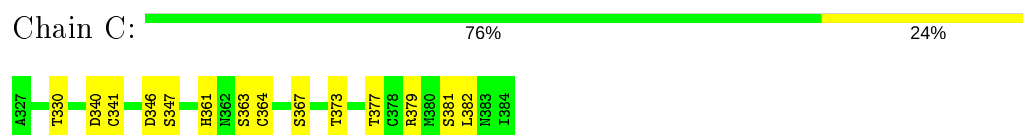
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

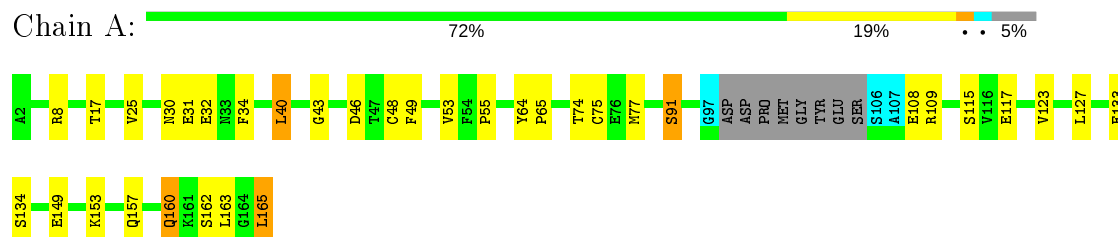


- Molecule 3: E3 ubiquitin-protein ligase AMFR

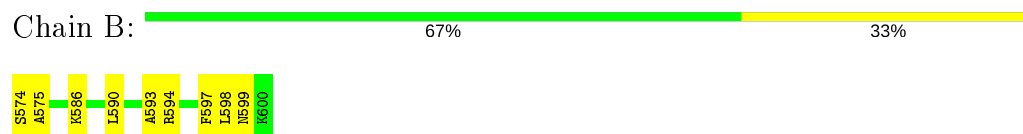


### 4.2.20 Score per residue for model 20

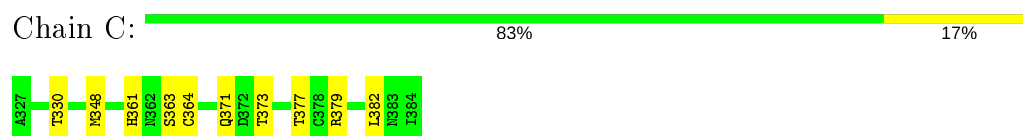
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR



- Molecule 3: E3 ubiquitin-protein ligase AMFR



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *Lowest Haddock Scores*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	structure solution	
CNS	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	110
Number of shifts mapped to atoms	110
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

No validations of the models with respect to experimental NMR restraints is performed at this time.



## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1216	1200	1197	20±3
2	B	235	248	247	16±2
3	C	447	419	416	3±3
All	All	38000	37340	37200	479

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 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:348:MET:CE	3:C:349:GLN:HB2	1.06	1.80	15	1
1:A:53:VAL:HG21	2:B:590:LEU:HA	1.03	1.28	2	20
3:C:348:MET:CE	3:C:349:GLN:CB	1.02	2.37	15	1
3:C:348:MET:HE3	3:C:349:GLN:HB2	1.02	1.28	15	1
3:C:348:MET:HE2	3:C:349:GLN:N	0.97	1.75	15	1
3:C:348:MET:HE2	3:C:349:GLN:CA	0.91	1.94	15	1
3:C:348:MET:CE	3:C:349:GLN:N	0.90	2.34	15	1
3:C:348:MET:HE2	3:C:350:ALA:N	0.82	1.90	15	1
3:C:348:MET:CE	3:C:350:ALA:H	0.79	1.91	15	1
3:C:348:MET:CE	3:C:349:GLN:CA	0.76	2.63	15	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:574:SER:N	2:B:577:GLU:HB2	0.71	2.00	15	13
1:A:25:VAL:HG23	2:B:589:LEU:HD22	0.69	1.61	9	6
1:A:165:LEU:HD21	2:B:594:ARG:HD3	0.69	1.64	20	15
3:C:361:HIS:HB2	3:C:364:CYS:SG	0.68	2.28	14	20
1:A:163:LEU:HD22	2:B:594:ARG:HG3	0.68	1.65	2	18
3:C:348:MET:HE2	3:C:350:ALA:H	0.67	1.43	15	1
1:A:42:MET:HB2	2:B:589:LEU:HD11	0.67	1.65	12	9
1:A:40:LEU:HD12	2:B:586:LYS:HG2	0.65	1.68	4	17
1:A:163:LEU:HD21	2:B:593:ALA:HB3	0.64	1.68	10	18
3:C:348:MET:HE2	3:C:349:GLN:H	0.62	1.55	15	1
1:A:31:GLU:HG3	2:B:575:ALA:O	0.62	1.94	2	15
1:A:165:LEU:HD13	2:B:598:LEU:HD21	0.62	1.72	12	20
1:A:25:VAL:HG11	2:B:586:LYS:HG3	0.61	1.71	17	20
1:A:163:LEU:HD22	2:B:594:ARG:CG	0.60	2.27	11	19
1:A:55:PRO:HD2	1:A:75:CYS:SG	0.60	2.36	20	13
3:C:348:MET:HE2	3:C:349:GLN:C	0.59	2.18	15	1
1:A:25:VAL:CG1	2:B:586:LYS:HG3	0.58	2.27	1	16
1:A:40:LEU:CG	2:B:586:LYS:HG2	0.58	2.28	1	16
1:A:40:LEU:HD11	2:B:586:LYS:HG2	0.58	1.74	12	3
1:A:51:PHE:CE1	2:B:596:ARG:HB3	0.57	2.34	8	7
1:A:40:LEU:CD1	2:B:586:LYS:HG2	0.57	2.29	4	17
1:A:108:GLU:OE2	3:C:379:ARG:NH2	0.57	2.30	2	1
1:A:163:LEU:HD21	2:B:593:ALA:CB	0.57	2.29	10	8
1:A:160:GLN:NE2	2:B:597:PHE:HZ	0.56	1.99	9	17
2:B:595:LYS:O	2:B:599:ASN:HB3	0.55	2.01	15	1
1:A:53:VAL:HB	2:B:590:LEU:HD13	0.54	1.79	7	10
1:A:23:GLY:HA2	2:B:589:LEU:CD1	0.54	2.33	18	2
1:A:64:TYR:CD1	1:A:65:PRO:HA	0.53	2.39	6	16
1:A:149:GLU:O	1:A:153:LYS:HG2	0.52	2.04	6	4
1:A:43:GLY:HA3	1:A:49:PHE:O	0.51	2.05	12	14
1:A:8:ARG:NH2	1:A:115:SER:HA	0.51	2.21	5	7
1:A:40:LEU:HD12	2:B:589:LEU:HD23	0.51	1.83	3	2
1:A:53:VAL:CB	2:B:590:LEU:HD13	0.50	2.36	7	6
3:C:341:CYS:HB2	3:C:361:HIS:CE1	0.50	2.41	17	9
1:A:91:SER:O	1:A:109:ARG:HA	0.50	2.06	20	4
1:A:115:SER:HB2	1:A:117:GLU:OE1	0.50	2.06	6	1
1:A:123:VAL:O	1:A:127:LEU:HG	0.49	2.07	16	6
3:C:348:MET:HE3	3:C:349:GLN:CB	0.48	2.12	15	1
1:A:108:GLU:HA	3:C:379:ARG:NH1	0.47	2.23	13	5
3:C:366:ARG:O	3:C:370:GLU:HG3	0.47	2.10	16	1
1:A:30:ASN:OD1	1:A:32:GLU:HG2	0.47	2.10	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:GLU:O	1:A:121:LEU:HG	0.46	2.10	2	1
1:A:42:MET:HA	1:A:52:GLY:O	0.46	2.11	15	4
1:A:83:TYR:HE2	1:A:89:CYS:HG	0.45	1.54	12	1
1:A:40:LEU:HD12	2:B:586:LYS:CG	0.45	2.39	4	11
1:A:130:PRO:HD2	1:A:144:TRP:CH2	0.45	2.46	7	1
1:A:157:GLN:HA	1:A:160:GLN:OE1	0.45	2.12	20	2
1:A:94:HIS:O	1:A:109:ARG:HG2	0.45	2.12	18	1
1:A:82:ILE:O	1:A:137:ASN:HB2	0.45	2.12	10	1
1:A:31:GLU:OE2	2:B:578:ARG:HB2	0.45	2.12	16	1
1:A:83:TYR:CD1	1:A:84:PRO:HD2	0.44	2.48	9	1
2:B:587:ASP:O	2:B:591:GLN:HG2	0.44	2.13	12	1
2:B:596:ARG:HA	2:B:599:ASN:ND2	0.44	2.27	13	2
1:A:25:VAL:HB	1:A:40:LEU:HB2	0.44	1.88	20	1
1:A:123:VAL:O	1:A:126:MET:HG2	0.44	2.13	1	6
1:A:53:VAL:HG21	2:B:590:LEU:CA	0.44	2.33	3	1
3:C:350:ALA:O	3:C:361:HIS:HA	0.43	2.13	9	5
1:A:83:TYR:CD2	1:A:84:PRO:HD2	0.43	2.49	8	1
1:A:31:GLU:HG2	2:B:579:GLN:CG	0.43	2.44	16	1
3:C:348:MET:HE3	3:C:349:GLN:N	0.43	2.22	15	1
1:A:112:PRO:CB	3:C:343:ILE:HA	0.43	2.44	5	2
1:A:160:GLN:NE2	2:B:597:PHE:CZ	0.42	2.87	17	3
3:C:348:MET:CE	3:C:350:ALA:N	0.42	2.62	15	1
2:B:579:GLN:O	2:B:583:VAL:HG23	0.42	2.15	8	2
1:A:51:PHE:O	2:B:593:ALA:HB1	0.42	2.13	13	2
1:A:154:ILE:O	1:A:158:ILE:HG12	0.42	2.14	18	3
1:A:108:GLU:HB2	3:C:379:ARG:CZ	0.41	2.45	19	1
1:A:150:GLN:HA	1:A:150:GLN:OE1	0.41	2.15	10	1
3:C:358:HIS:CE1	3:C:377:THR:HB	0.41	2.51	2	1
3:C:366:ARG:O	3:C:370:GLU:HB2	0.41	2.16	4	1
1:A:40:LEU:HG	2:B:586:LYS:HG2	0.41	1.93	5	1
1:A:142:LYS:O	1:A:146:ASP:HB2	0.41	2.16	7	1
1:A:114:GLN:HA	1:A:114:GLN:HE21	0.41	1.74	4	1
1:A:27:GLY:HA3	2:B:582:LEU:HD21	0.40	1.92	6	1
1:A:119:ILE:O	1:A:123:VAL:HG23	0.40	2.16	10	1
1:A:83:TYR:HE2	1:A:89:CYS:SG	0.40	2.39	12	1
2:B:584:GLN:O	2:B:588:GLU:HG3	0.40	2.16	8	1
2:B:584:GLN:O	2:B:588:GLU:HG2	0.40	2.16	13	1

## 6.3 Torsion angles

### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	151/164 (92%)	143±2 (95±1%)	8±2 (5±1%)	0±1 (0±0%)	50	82
2	B	25/27 (93%)	21±0 (82±2%)	4±0 (18±2%)	0±0 (0±0%)	100	100
3	C	56/58 (97%)	47±2 (83±4%)	9±2 (16±4%)	1±1 (1±1%)	21	69
All	All	4640/4980 (93%)	4200 (91%)	425 (9%)	15 (0%)	44	80

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	C	376	PRO	8
1	A	130	PRO	3
3	C	349	GLN	2
1	A	132	ASP	1
1	A	148	ARG	1

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	134/142 (94%)	121±2 (90±2%)	13±2 (10±2%)	11	56
2	B	25/25 (100%)	22±1 (90±4%)	3±1 (10±4%)	10	55
3	C	51/51 (100%)	42±1 (83±3%)	9±1 (17±3%)	5	40
All	All	4200/4360 (96%)	3709 (88%)	491 (12%)	9	52

All 74 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	C	330	THR	20
3	C	377	THR	20
1	A	160	GLN	20
1	A	117	GLU	19
1	A	77	MET	18
3	C	363	SER	18
1	A	133	GLU	17
1	A	74	THR	17
1	A	134	SER	17
3	C	373	THR	17
1	A	17	THR	17
3	C	382	LEU	15
1	A	48	CYS	14
2	B	576	ASP	13
1	A	115	SER	13
3	C	352	ARG	12
3	C	381	SER	12
2	B	599	ASN	11
3	C	348	MET	11
1	A	90	ILE	10
3	C	347	SER	10
1	A	146	ASP	9
1	A	8	ARG	9
1	A	118	LYS	8
3	C	345	TRP	7
1	A	40	LEU	7
2	B	574	SER	7
2	B	587	ASP	6
1	A	46	ASP	6
1	A	91	SER	6
1	A	85	ASP	5
1	A	126	MET	5
1	A	34	PHE	5
1	A	83	TYR	5
1	A	139	ASP	4
3	C	370	GLU	4
3	C	371	GLN	4
2	B	596	ARG	4
3	C	358	HIS	4
1	A	4	THR	4
1	A	109	ARG	3
2	B	600	LYS	3
3	C	367	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	111	SER	3
1	A	122	SER	3
1	A	15	GLN	3
1	A	157	GLN	3
3	C	379	ARG	3
1	A	162	SER	3
2	B	592	GLN	2
3	C	349	GLN	2
3	C	346	ASP	2
3	C	334	LEU	2
2	B	595	LYS	2
1	A	152	TYR	2
1	A	45	GLU	2
2	B	589	LEU	2
3	C	340	ASP	2
3	C	356	CYS	1
1	A	63	ASP	1
2	B	577	GLU	1
3	C	332	GLU	1
1	A	165	LEU	1
2	B	581	MET	1
1	A	145	ARG	1
1	A	131	ASN	1
1	A	62	LEU	1
1	A	144	TRP	1
3	C	366	ARG	1
3	C	369	LEU	1
1	A	114	GLN	1
1	A	161	LYS	1
1	A	38	GLU	1
1	A	10	MET	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 4% for the well-defined parts and 4% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	110
Number of shifts mapped to atoms	110
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	55	$0.45 \pm 0.28$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 109 atoms were assigned a chemical shift out of a possible 2988. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	109/1156 (9%)	54/459 (12%)	0/476 (0%)	55/221 (25%)
Sidechain	0/1613 (0%)	0/956 (0%)	0/581 (0%)	0/76 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/219 (0%)	0/117 (0%)	0/93 (0%)	0/9 (0%)
Overall	109/2988 (4%)	54/1532 (4%)	0/1150 (0%)	55/306 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 109 atoms were assigned a chemical shift out of a possible 3008. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	109/1171 (9%)	54/465 (12%)	0/482 (0%)	55/224 (25%)
Sidechain	0/1618 (0%)	0/959 (0%)	0/583 (0%)	0/76 (0%)
Aromatic	0/219 (0%)	0/117 (0%)	0/93 (0%)	0/9 (0%)
Overall	109/3008 (4%)	54/1541 (4%)	0/1158 (0%)	55/309 (18%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain C:

