



# Full wwPDB NMR Structure Validation Report i

May 29, 2020 – 11:27 am BST

PDB ID : 6U4N  
Title : Solution structure of paxillin LIM4 in complex with kindlin-2 F0  
Authors : Zhu, L.; Qin, J.  
Deposited on : 2019-08-26

This is a Full wwPDB NMR 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

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

with specific help available everywhere you see the i symbol.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

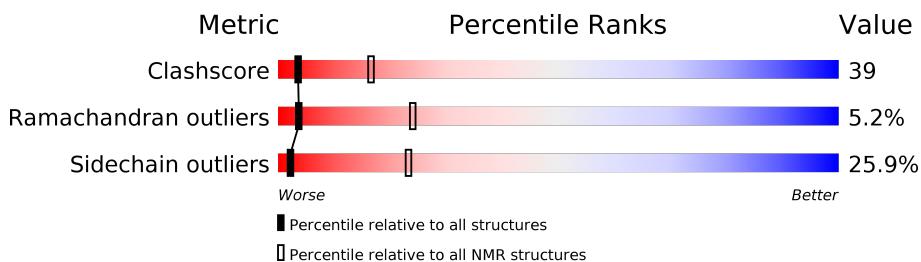
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbit	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	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*

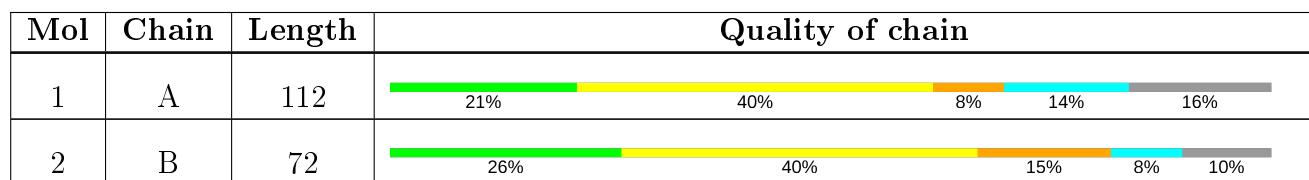
The overall completeness of chemical shifts assignment is 73%.

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  $\leq 5\%$



## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 12 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:16-A:93, B:547-B:605 (137)	0.51	12

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 4 clusters and 1 single-model cluster was found.

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

### 3 Entry composition [\(i\)](#)

There are 3 unique types of molecules in this entry. The entry contains 2573 atoms, of which 1279 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fermitin family homolog 2.

Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1532	494	765	132	137	4	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q96AC1
A	-5	ALA	-	expression tag	UNP Q96AC1
A	-4	MET	-	expression tag	UNP Q96AC1
A	-3	ASP	-	expression tag	UNP Q96AC1
A	-2	PRO	-	expression tag	UNP Q96AC1
A	-1	GLU	-	expression tag	UNP Q96AC1
A	0	PHE	-	expression tag	UNP Q96AC1

- Molecule 2 is a protein called Paxillin.

Mol	Chain	Residues	Atoms						Trace
2	B	65	Total	C	H	N	O	S	0
			1039	333	514	95	88	9	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	534	GLY	-	expression tag	UNP P49023
B	535	ALA	-	expression tag	UNP P49023
B	536	MET	-	expression tag	UNP P49023
B	537	ASP	-	expression tag	UNP P49023
B	538	PRO	-	expression tag	UNP P49023
B	539	GLU	-	expression tag	UNP P49023
B	540	PHE	-	expression tag	UNP P49023

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

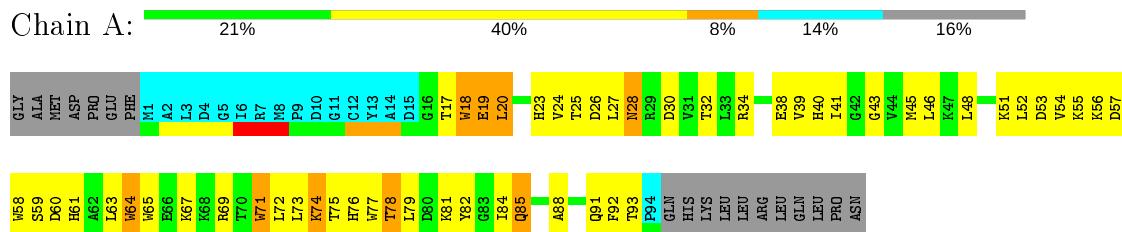
Mol	Chain	Residues	Atoms						
3	B	2	Total	Zn					
			2	2					

## 4 Residue-property plots [\(i\)](#)

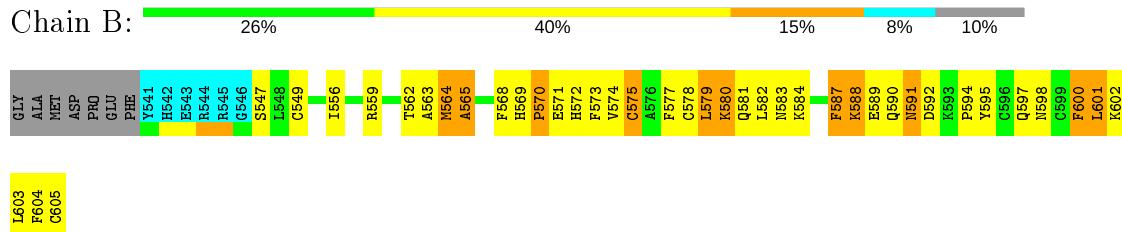
### 4.1 Average score per residue in the NMR ensemble

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: Fermitin family homolog 2



- Molecule 2: Paxillin

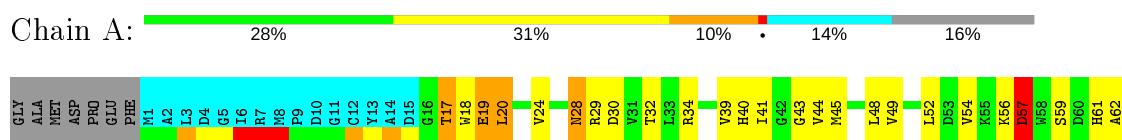


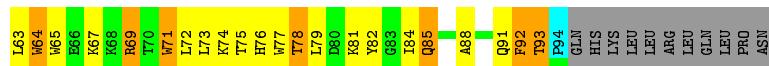
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

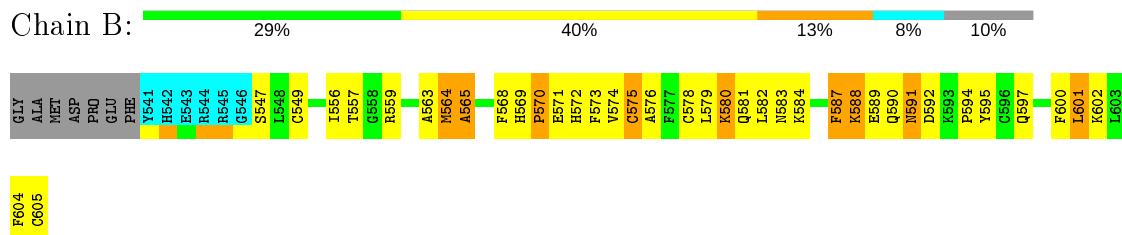
#### 4.2.1 Score per residue for model 1

- Molecule 1: Fermitin family homolog 2





- Molecule 2: Paxillin





L603  
F604  
C605

#### 4.2.4 Score per residue for model 4

- Molecule 1: Fermitin family homolog 2

Chain A: 26% 29% 14% 14% 16%



S559  
I600  
H601  
L602  
W603  
E604  
P605  
Y541  
H542  
B543  
R544  
R545  
G546  
S547  
K548  
K602

I603  
F604  
C605

- Molecule 2: Paxillin

Chain B: 31% 36% 15% 8% 10%



H61  
A62  
L63  
W64  
W65  
E66  
P67  
Y541  
H542  
B543  
R544  
R545  
G546  
S547  
K548  
K602

#### 4.2.5 Score per residue for model 5

- Molecule 1: Fermitin family homolog 2

Chain A: 21% 34% 14% 14% 16%



H61  
A62  
L63  
W64  
W65  
E66  
P67  
Y541  
H542  
B543  
R544  
R545  
G546  
S547  
K548  
K602

- Molecule 2: Paxillin

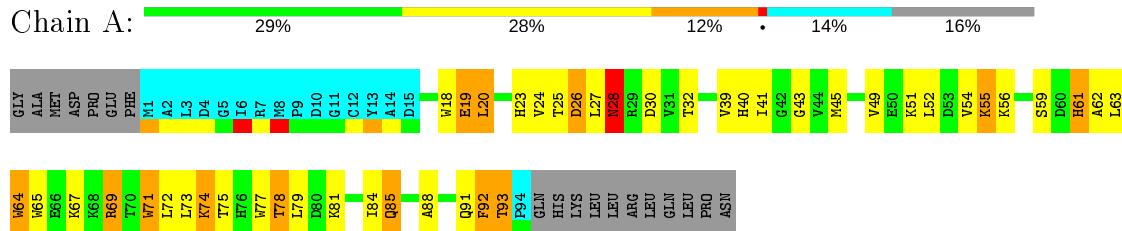
Chain B: 28% 36% 18% 8% 10%



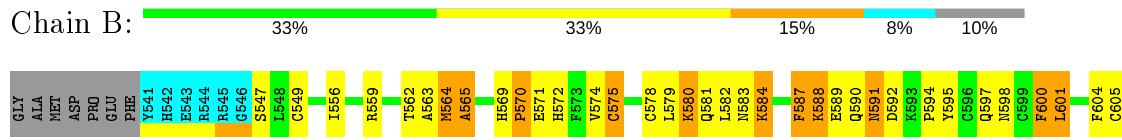
L603  
F604  
C605

#### 4.2.6 Score per residue for model 6

- Molecule 1: Fermitin family homolog 2

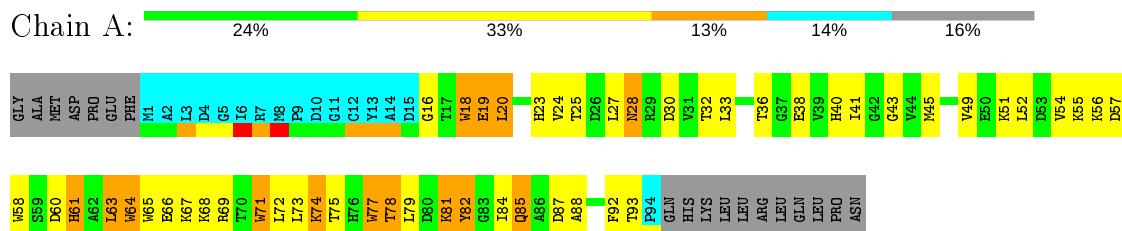


- Molecule 2: Paxillin

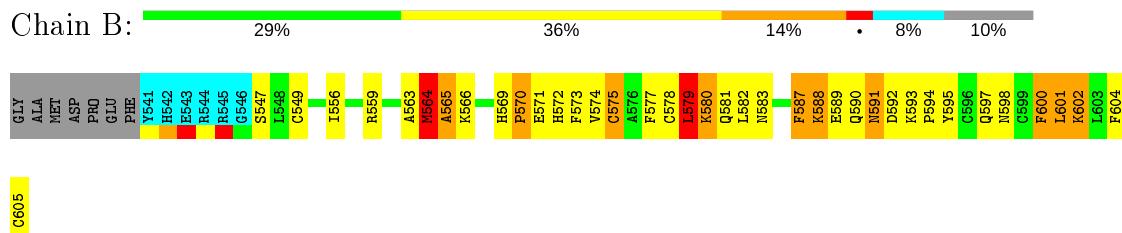


#### 4.2.7 Score per residue for model 7

- Molecule 1: Fermitin family homolog 2

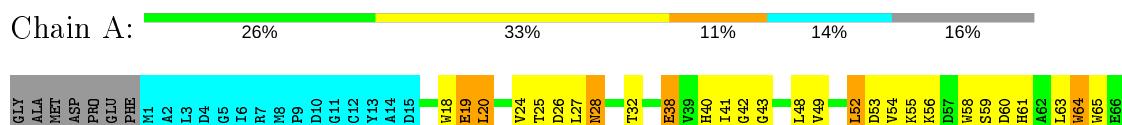


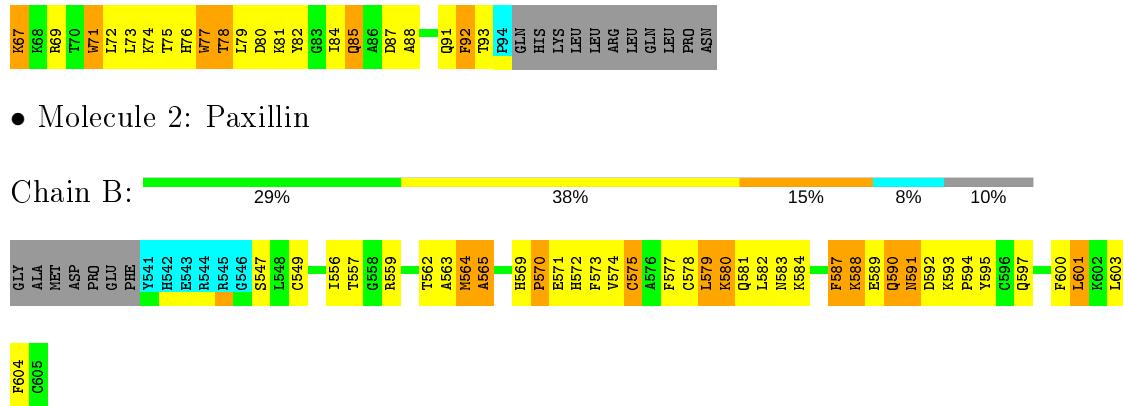
- Molecule 2: Paxillin



#### 4.2.8 Score per residue for model 8

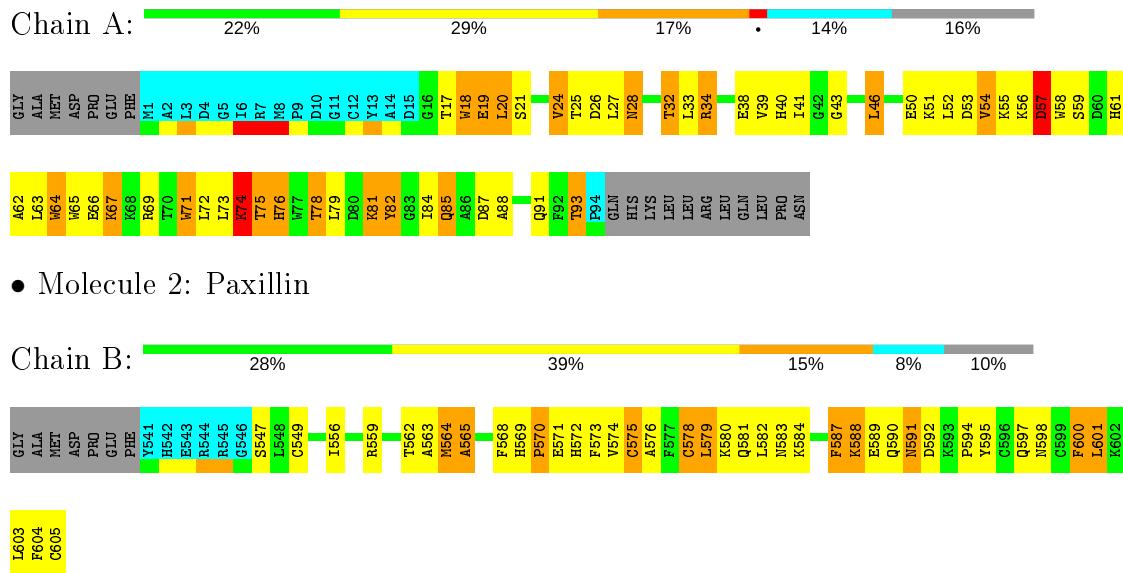
- Molecule 1: Fermitin family homolog 2





#### 4.2.9 Score per residue for model 9

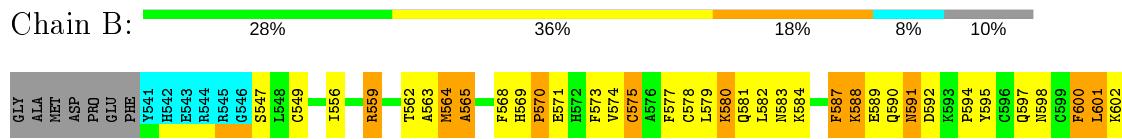
- Molecule 1: Fermitin family homolog 2



#### 4.2.10 Score per residue for model 10

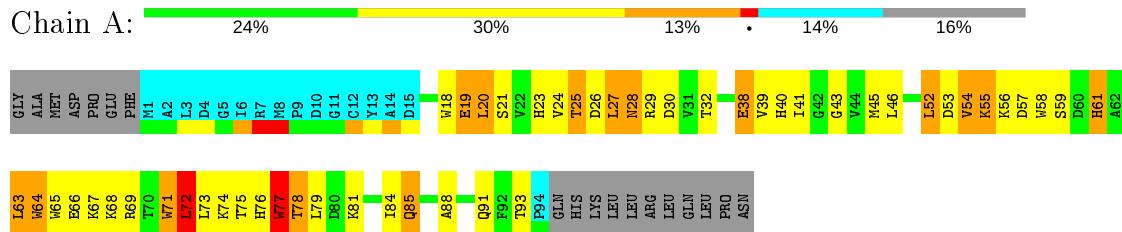
- Molecule 1: Fermitin family homolog 2



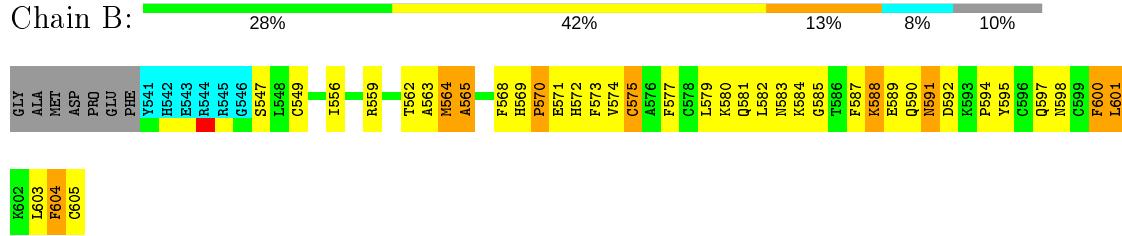


#### 4.2.11 Score per residue for model 11

- Molecule 1: Fermitin family homolog 2

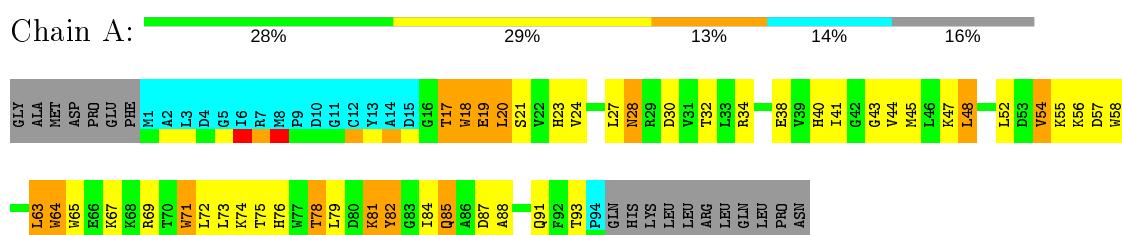


- Molecule 2: Paxillin

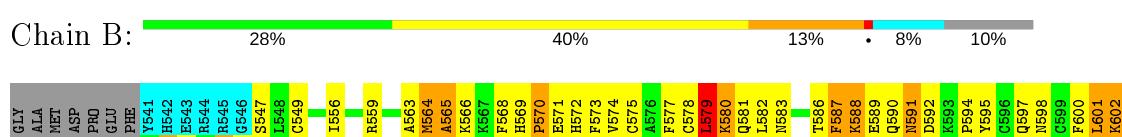


#### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Fermitin family homolog 2



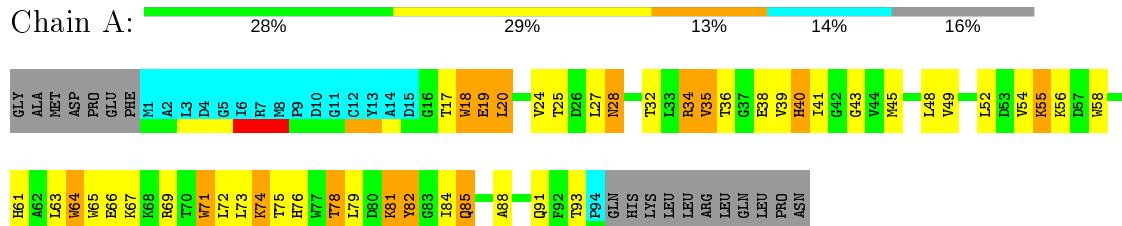
- Molecule 2: Paxillin



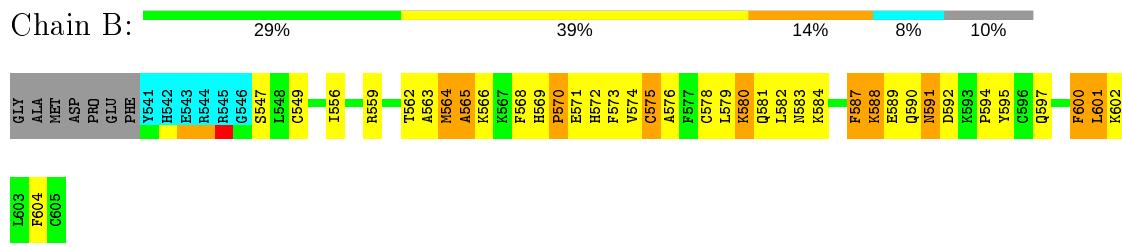


#### 4.2.13 Score per residue for model 13

- Molecule 1: Fermitin family homolog 2

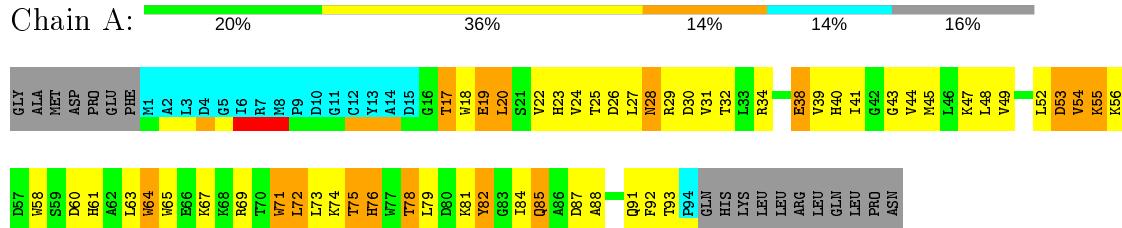


- Molecule 2: Paxillin

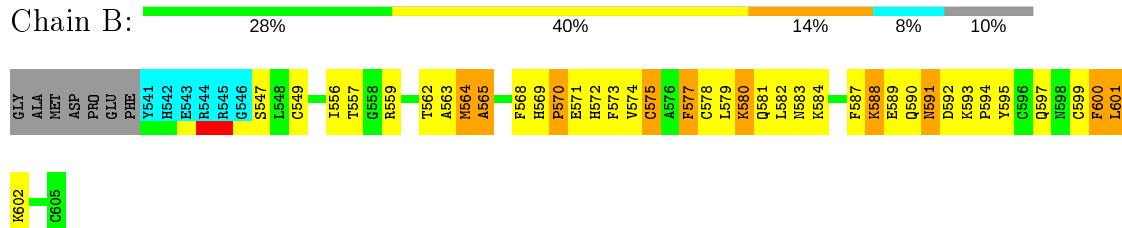


#### 4.2.14 Score per residue for model 14

- Molecule 1: Fermitin family homolog 2

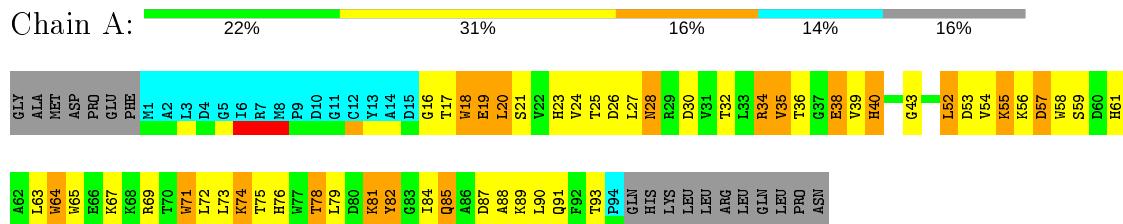


- Molecule 2: Paxillin

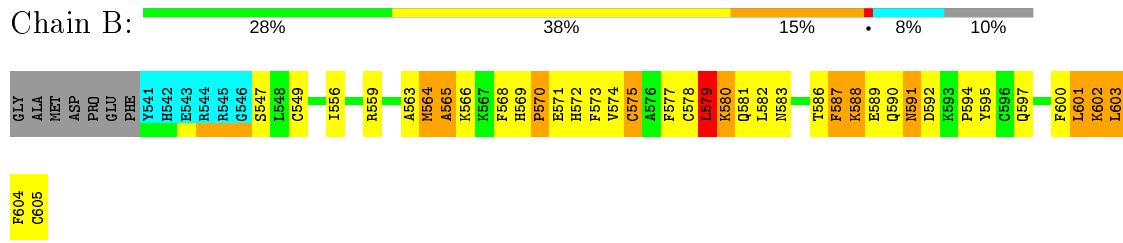


#### 4.2.15 Score per residue for model 15

- Molecule 1: Fermitin family homolog 2

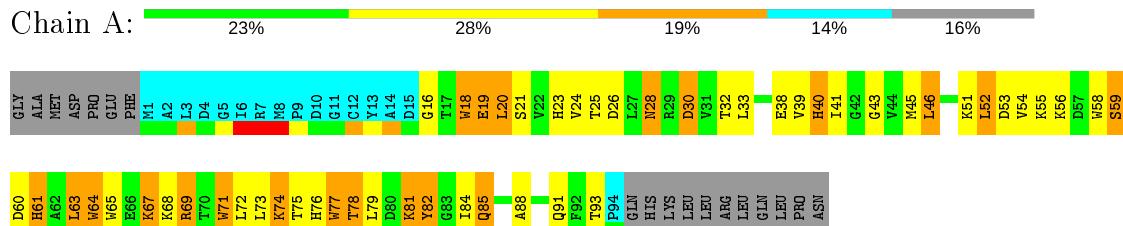


- Molecule 2: Paxillin



#### 4.2.16 Score per residue for model 16

- Molecule 1: Fermitin family homolog 2

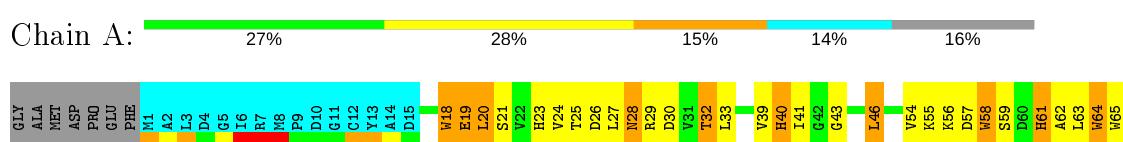


- Molecule 2: Paxillin



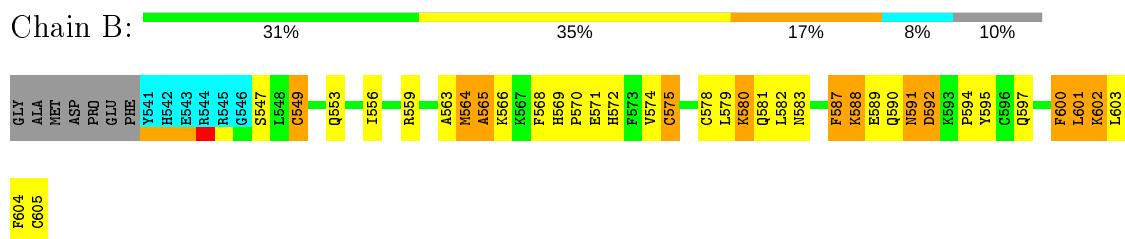
#### 4.2.17 Score per residue for model 17

- Molecule 1: Fermitin family homolog 2



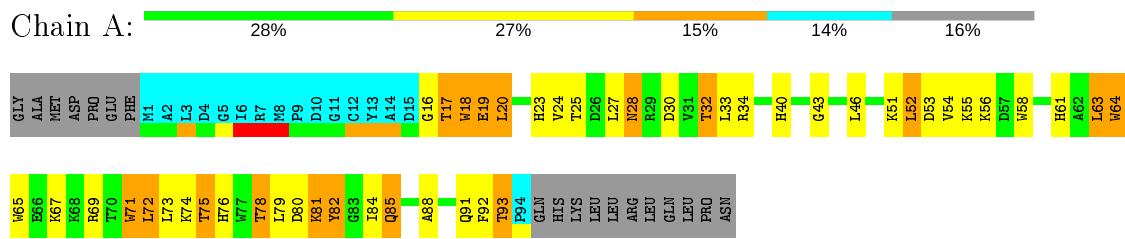


- Molecule 2: Paxillin

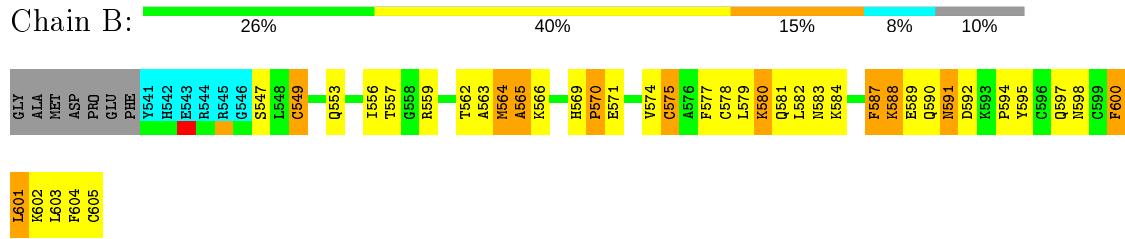


#### 4.2.18 Score per residue for model 18

- Molecule 1: Fermitin family homolog 2

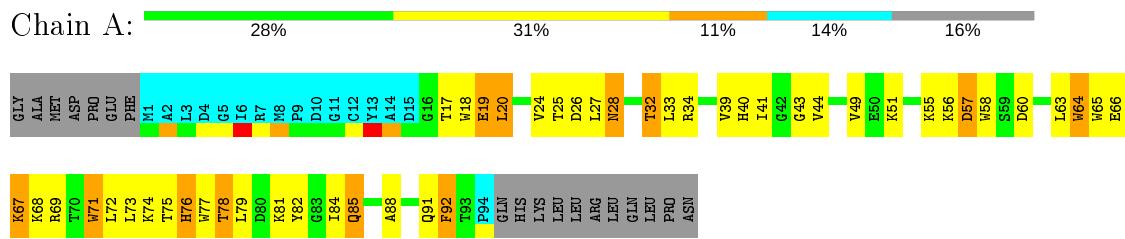


- Molecule 2: Paxillin

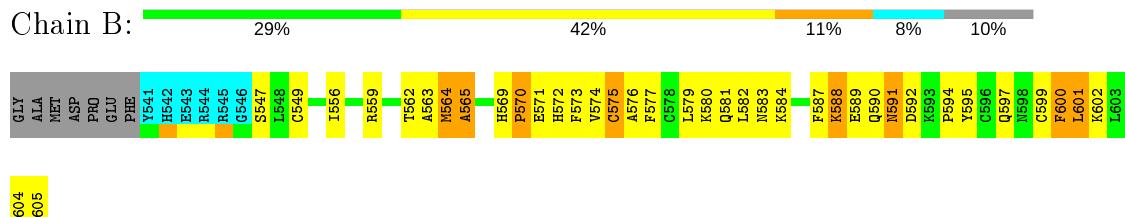


#### 4.2.19 Score per residue for model 19

- Molecule 1: Fermitin family homolog 2

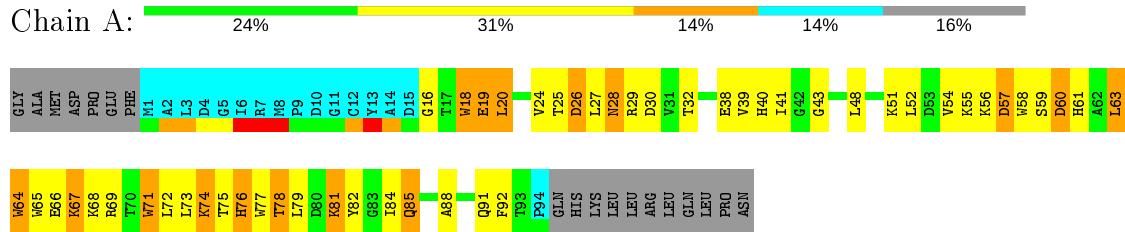


- Molecule 2: Paxillin

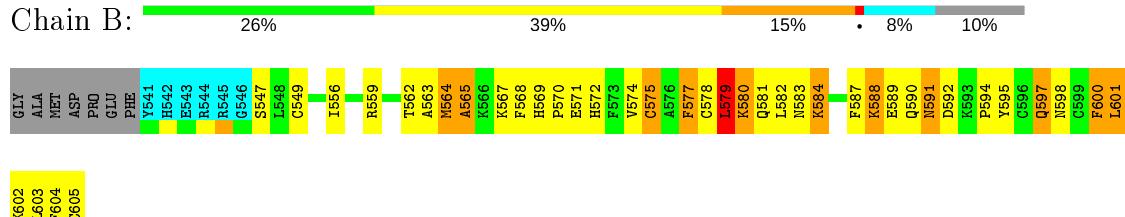


#### 4.2.20 Score per residue for model 20

- Molecule 1: Fermitin family homolog 2



- Molecule 2: Paxillin



## 5 Refinement protocol and experimental data overview i

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
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	1649
Number of shifts mapped to atoms	1649
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	73%

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

## 6 Model quality i

### 6.1 Standard geometry i

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 i

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	650	656	656	47±6
2	B	468	463	465	43±5
All	All	22400	22380	22420	1770

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:B:579:LEU:H	2:B:579:LEU:HD22	0.88	1.25	9	3
2:B:579:LEU:H	2:B:579:LEU:HD13	0.85	1.31	7	1
2:B:571:GLU:O	2:B:574:VAL:HG13	0.85	1.72	3	20
2:B:579:LEU:HD22	2:B:579:LEU:N	0.80	1.92	3	2
2:B:579:LEU:N	2:B:579:LEU:HD22	0.79	1.92	9	3
1:A:89:LYS:O	1:A:90:LEU:HD23	0.78	1.77	15	1
1:A:63:LEU:HD22	1:A:63:LEU:H	0.78	1.39	10	5
2:B:601:LEU:HD23	2:B:602:LYS:H	0.78	1.36	20	1
1:A:63:LEU:HD22	1:A:63:LEU:N	0.77	1.95	19	11
1:A:63:LEU:N	1:A:63:LEU:HD22	0.77	1.95	13	7
2:B:601:LEU:HD23	2:B:602:LYS:N	0.76	1.96	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:579:LEU:HD13	2:B:579:LEU:H	0.71	1.46	20	3
2:B:591:ASN:N	2:B:591:ASN:ND2	0.71	2.39	7	13
2:B:591:ASN:ND2	2:B:591:ASN:N	0.67	2.40	1	7
1:A:58:TRP:CZ3	1:A:92:PHE:CZ	0.65	2.85	5	1
1:A:58:TRP:CH2	1:A:92:PHE:CE1	0.64	2.86	5	1
2:B:590:GLN:NE2	2:B:600:PHE:CE2	0.64	2.66	8	1
1:A:20:LEU:HD11	1:A:88:ALA:O	0.64	1.92	15	1
1:A:61:HIS:CD2	1:A:92:PHE:CE1	0.64	2.85	1	1
2:B:601:LEU:C	2:B:601:LEU:HD12	0.64	2.12	17	11
2:B:600:PHE:CD2	2:B:601:LEU:N	0.64	2.65	5	10
2:B:562:THR:H	2:B:584:LYS:HZ1	0.64	1.32	6	4
2:B:601:LEU:HD12	2:B:601:LEU:C	0.64	2.13	14	8
1:A:54:VAL:HG22	1:A:54:VAL:O	0.64	1.93	12	1
2:B:562:THR:H	2:B:584:LYS:NZ	0.64	1.90	11	8
2:B:563:ALA:C	2:B:565:ALA:H	0.63	1.97	20	20
1:A:79:LEU:N	1:A:79:LEU:HD23	0.63	2.08	7	2
1:A:58:TRP:O	1:A:61:HIS:CG	0.63	2.52	16	1
1:A:76:HIS:CD2	1:A:76:HIS:H	0.63	2.09	19	1
2:B:590:GLN:NE2	2:B:604:PHE:CD1	0.63	2.66	16	7
1:A:49:VAL:O	1:A:53:ASP:N	0.63	2.32	14	2
1:A:64:TRP:CD1	1:A:91:GLN:NE2	0.62	2.67	11	14
1:A:61:HIS:O	1:A:61:HIS:ND1	0.62	2.32	16	1
1:A:58:TRP:O	1:A:61:HIS:ND1	0.62	2.32	14	6
2:B:600:PHE:CD1	2:B:601:LEU:N	0.62	2.68	13	8
1:A:46:LEU:HD12	2:B:603:LEU:HD13	0.62	1.69	3	5
2:B:569:HIS:O	2:B:571:GLU:N	0.61	2.33	4	20
1:A:49:VAL:HG22	1:A:58:TRP:CD2	0.61	2.30	8	3
2:B:579:LEU:N	2:B:579:LEU:CD2	0.61	2.63	12	3
1:A:79:LEU:HD23	1:A:79:LEU:N	0.61	2.10	12	3
2:B:570:PRO:O	2:B:581:GLN:NE2	0.60	2.34	16	20
1:A:58:TRP:CZ3	1:A:92:PHE:CE1	0.60	2.89	5	1
1:A:61:HIS:N	1:A:61:HIS:ND1	0.60	2.49	11	2
1:A:56:LYS:NZ	1:A:58:TRP:CH2	0.60	2.68	16	2
1:A:63:LEU:N	1:A:63:LEU:CD2	0.60	2.65	16	9
2:B:601:LEU:HD12	2:B:601:LEU:O	0.60	1.97	18	11
2:B:594:PRO:O	2:B:595:TYR:CD1	0.60	2.55	7	1
1:A:61:HIS:CG	1:A:92:PHE:CE2	0.60	2.90	6	3
1:A:48:LEU:HD21	1:A:92:PHE:CD2	0.59	2.33	1	1
2:B:577:PHE:CD2	2:B:599:CYS:SG	0.59	2.95	14	2
1:A:78:THR:H	1:A:81:LYS:CG	0.59	2.11	1	10
1:A:54:VAL:HG22	1:A:55:LYS:H	0.59	1.57	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:THR:HG21	2:B:602:LYS:O	0.59	1.97	12	8
1:A:49:VAL:HG22	1:A:58:TRP:CE3	0.59	2.33	8	3
1:A:63:LEU:HD12	1:A:92:PHE:CD2	0.58	2.33	10	1
2:B:578:CYS:O	2:B:580:LYS:N	0.58	2.36	20	16
2:B:587:PHE:O	2:B:587:PHE:CG	0.58	2.57	9	9
1:A:39:VAL:O	1:A:78:THR:HG22	0.58	1.98	15	15
1:A:24:VAL:O	1:A:28:ASN:N	0.58	2.37	20	20
2:B:590:GLN:CG	2:B:591:ASN:ND2	0.58	2.67	16	16
1:A:64:TRP:NE1	1:A:91:GLN:NE2	0.58	2.51	3	10
1:A:54:VAL:O	1:A:56:LYS:N	0.58	2.37	12	17
1:A:17:THR:OG1	1:A:34:ARG:NE	0.57	2.37	1	5
1:A:79:LEU:HD12	1:A:79:LEU:N	0.57	2.13	3	9
1:A:48:LEU:HD23	1:A:61:HIS:NE2	0.57	2.14	1	1
1:A:63:LEU:CD2	1:A:63:LEU:N	0.57	2.67	8	9
2:B:587:PHE:CG	2:B:587:PHE:O	0.57	2.57	14	11
2:B:587:PHE:CD2	2:B:587:PHE:O	0.57	2.58	2	6
2:B:587:PHE:CD1	2:B:587:PHE:O	0.57	2.58	12	3
1:A:55:LYS:NZ	2:B:576:ALA:CB	0.57	2.68	19	1
2:B:579:LEU:CD1	2:B:579:LEU:H	0.57	2.10	12	3
1:A:92:PHE:O	1:A:92:PHE:CD1	0.56	2.58	6	1
1:A:74:LYS:NZ	1:A:82:TYR:CZ	0.56	2.72	10	1
2:B:564:MET:O	2:B:565:ALA:CB	0.56	2.54	16	20
2:B:601:LEU:O	2:B:601:LEU:HD12	0.56	2.01	8	8
2:B:594:PRO:O	2:B:595:TYR:CG	0.56	2.58	8	20
2:B:590:GLN:NE2	2:B:600:PHE:CD2	0.56	2.73	8	1
2:B:578:CYS:O	2:B:578:CYS:SG	0.56	2.64	16	10
1:A:71:TRP:CD1	1:A:71:TRP:N	0.56	2.74	11	7
1:A:71:TRP:N	1:A:71:TRP:CD1	0.56	2.74	1	5
1:A:54:VAL:HG22	1:A:55:LYS:N	0.56	2.14	14	1
2:B:547:SER:O	2:B:556:ILE:N	0.56	2.39	20	20
1:A:63:LEU:HD12	1:A:63:LEU:O	0.56	2.01	11	1
1:A:65:TRP:O	1:A:69:ARG:N	0.56	2.39	12	20
2:B:579:LEU:H	2:B:579:LEU:CD2	0.55	2.08	9	2
1:A:52:LEU:HD21	1:A:56:LYS:NZ	0.55	2.17	20	1
1:A:71:TRP:O	1:A:73:LEU:N	0.55	2.39	5	20
1:A:16:GLY:O	1:A:18:TRP:CE2	0.55	2.59	15	8
1:A:40:HIS:CD2	1:A:40:HIS:H	0.55	2.17	4	1
1:A:54:VAL:O	1:A:54:VAL:HG23	0.55	2.00	9	1
1:A:84:ILE:O	1:A:85:GLN:NE2	0.55	2.40	4	20
2:B:587:PHE:O	2:B:587:PHE:CD1	0.55	2.59	16	4
1:A:19:GLU:H	1:A:19:GLU:CD	0.55	2.05	10	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:O	1:A:28:ASN:CB	0.55	2.55	6	12
1:A:33:LEU:N	1:A:33:LEU:HD22	0.55	2.17	19	1
2:B:578:CYS:SG	2:B:578:CYS:O	0.55	2.65	17	6
1:A:63:LEU:H	1:A:63:LEU:HD22	0.55	1.62	12	3
2:B:590:GLN:NE2	2:B:604:PHE:CG	0.55	2.75	9	4
1:A:61:HIS:CD2	1:A:92:PHE:CE2	0.55	2.95	20	2
1:A:26:ASP:CB	1:A:61:HIS:NE2	0.55	2.70	9	1
2:B:562:THR:N	2:B:584:LYS:HZ1	0.54	1.99	6	3
2:B:591:ASN:N	2:B:591:ASN:HD22	0.54	2.00	19	3
2:B:569:HIS:ND1	2:B:572:HIS:CE1	0.54	2.75	20	15
1:A:79:LEU:N	1:A:79:LEU:HD12	0.54	2.17	14	5
1:A:59:SER:O	1:A:61:HIS:N	0.54	2.41	20	3
1:A:79:LEU:O	1:A:82:TYR:N	0.54	2.40	12	8
1:A:79:LEU:CD1	1:A:79:LEU:N	0.54	2.70	13	6
1:A:28:ASN:ND2	1:A:28:ASN:O	0.54	2.40	16	10
1:A:79:LEU:N	1:A:79:LEU:CD1	0.54	2.70	5	8
1:A:25:THR:O	1:A:27:LEU:N	0.54	2.41	6	9
1:A:79:LEU:HD23	1:A:79:LEU:H	0.54	1.61	8	1
1:A:29:ARG:NH1	1:A:52:LEU:HD22	0.54	2.18	14	1
1:A:58:TRP:CZ3	1:A:92:PHE:CE2	0.54	2.96	14	1
1:A:74:LYS:NZ	1:A:82:TYR:OH	0.54	2.41	5	1
1:A:56:LYS:O	1:A:58:TRP:CD1	0.54	2.61	11	6
1:A:23:HIS:CE1	1:A:30:ASP:OD2	0.54	2.61	10	4
1:A:61:HIS:O	1:A:61:HIS:CG	0.54	2.60	10	1
1:A:51:LYS:CB	1:A:51:LYS:NZ	0.54	2.70	3	4
1:A:57:ASP:O	1:A:61:HIS:CD2	0.54	2.61	5	2
1:A:23:HIS:CE1	1:A:30:ASP:OD1	0.53	2.61	5	1
1:A:53:ASP:O	1:A:54:VAL:O	0.53	2.25	14	2
1:A:44:VAL:CG1	1:A:45:MET:N	0.53	2.71	10	1
1:A:17:THR:OG1	1:A:18:TRP:N	0.53	2.41	13	1
1:A:40:HIS:N	1:A:40:HIS:ND1	0.53	2.56	16	1
1:A:40:HIS:O	1:A:43:GLY:N	0.53	2.41	8	19
1:A:79:LEU:CD2	1:A:79:LEU:H	0.53	2.16	8	1
1:A:28:ASN:O	1:A:28:ASN:ND2	0.53	2.41	6	10
1:A:64:TRP:NE1	1:A:91:GLN:OE1	0.53	2.41	14	6
2:B:562:THR:H	2:B:584:LYS:HZ2	0.53	1.45	5	1
2:B:588:LYS:O	2:B:595:TYR:N	0.53	2.42	2	20
2:B:587:PHE:O	2:B:587:PHE:CD2	0.53	2.60	3	2
1:A:64:TRP:CD1	1:A:64:TRP:C	0.53	2.82	7	11
1:A:17:THR:CG2	1:A:34:ARG:HE	0.53	2.16	15	2
2:B:588:LYS:N	2:B:595:TYR:O	0.53	2.41	20	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:HIS:CD2	1:A:30:ASP:OD2	0.53	2.62	18	7
2:B:562:THR:H	2:B:584:LYS:CE	0.53	2.16	13	2
1:A:18:TRP:N	1:A:18:TRP:CD1	0.53	2.75	17	3
2:B:590:GLN:C	2:B:591:ASN:ND2	0.53	2.62	12	20
1:A:54:VAL:O	1:A:58:TRP:CZ2	0.53	2.62	3	2
1:A:56:LYS:O	1:A:58:TRP:N	0.53	2.41	9	2
1:A:74:LYS:O	1:A:76:HIS:N	0.53	2.42	13	8
2:B:563:ALA:O	2:B:565:ALA:N	0.53	2.42	18	20
2:B:583:ASN:O	2:B:587:PHE:N	0.53	2.42	5	17
1:A:23:HIS:CG	1:A:30:ASP:OD2	0.53	2.62	15	3
1:A:57:ASP:O	1:A:61:HIS:CE1	0.53	2.62	4	2
1:A:79:LEU:N	1:A:79:LEU:CD2	0.53	2.72	7	3
1:A:20:LEU:CD1	1:A:88:ALA:O	0.52	2.57	4	19
1:A:26:ASP:N	1:A:26:ASP:OD2	0.52	2.42	16	2
1:A:55:LYS:HZ2	2:B:579:LEU:HD12	0.52	1.64	15	1
1:A:92:PHE:CD1	1:A:92:PHE:C	0.52	2.82	19	2
2:B:591:ASN:HD22	2:B:591:ASN:N	0.52	2.01	15	3
1:A:58:TRP:O	1:A:61:HIS:N	0.52	2.43	11	7
1:A:57:ASP:OD2	1:A:57:ASP:N	0.52	2.42	1	2
1:A:19:GLU:CD	1:A:19:GLU:H	0.52	2.06	3	9
1:A:23:HIS:NE2	1:A:30:ASP:OD2	0.52	2.42	4	4
1:A:76:HIS:O	1:A:77:TRP:CG	0.52	2.62	19	1
1:A:23:HIS:CD2	1:A:30:ASP:OD1	0.52	2.62	5	4
2:B:593:LYS:O	2:B:595:TYR:CE1	0.52	2.62	8	1
1:A:76:HIS:CE1	2:B:605:CYS:O	0.52	2.63	16	1
2:B:571:GLU:O	2:B:573:PHE:N	0.52	2.43	3	7
1:A:34:ARG:O	1:A:35:VAL:HG13	0.52	2.05	4	3
1:A:18:TRP:CD1	1:A:18:TRP:N	0.52	2.78	10	1
1:A:76:HIS:CD2	1:A:76:HIS:N	0.52	2.77	19	1
2:B:593:LYS:O	2:B:595:TYR:CD1	0.52	2.62	8	4
1:A:79:LEU:CD2	1:A:79:LEU:N	0.52	2.72	12	2
2:B:604:PHE:O	2:B:605:CYS:SG	0.52	2.68	17	8
1:A:49:VAL:O	1:A:52:LEU:N	0.51	2.43	2	3
1:A:25:THR:OG1	1:A:26:ASP:N	0.51	2.44	20	4
2:B:567:LYS:O	2:B:568:PHE:CD1	0.51	2.64	20	1
1:A:76:HIS:N	1:A:76:HIS:ND1	0.51	2.58	14	1
1:A:62:ALA:N	1:A:93:THR:O	0.51	2.44	6	2
1:A:61:HIS:CD2	1:A:62:ALA:N	0.51	2.79	17	1
2:B:579:LEU:CD2	2:B:579:LEU:H	0.51	2.06	3	3
1:A:87:ASP:OD2	1:A:88:ALA:N	0.51	2.42	15	1
1:A:89:LYS:C	1:A:90:LEU:HD23	0.51	2.26	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:VAL:HG13	1:A:92:PHE:CD2	0.51	2.41	1	1
1:A:17:THR:OG1	1:A:34:ARG:CD	0.51	2.59	12	4
1:A:53:ASP:O	1:A:54:VAL:C	0.51	2.50	5	1
1:A:20:LEU:HD21	1:A:84:ILE:HG22	0.51	1.82	16	1
1:A:78:THR:O	1:A:81:LYS:N	0.50	2.42	7	3
1:A:54:VAL:O	1:A:54:VAL:CG2	0.50	2.59	12	2
2:B:601:LEU:O	2:B:605:CYS:SG	0.50	2.69	3	1
1:A:61:HIS:CG	1:A:92:PHE:CD2	0.50	2.99	6	1
1:A:48:LEU:HD13	1:A:92:PHE:CZ	0.50	2.42	10	1
1:A:64:TRP:C	1:A:64:TRP:CD1	0.50	2.85	2	9
1:A:25:THR:C	1:A:27:LEU:N	0.50	2.64	2	5
2:B:575:CYS:HB2	2:B:582:LEU:HD13	0.50	1.83	16	19
2:B:579:LEU:H	2:B:579:LEU:CD1	0.50	2.09	7	1
1:A:56:LYS:CB	1:A:56:LYS:NZ	0.50	2.75	3	2
1:A:67:LYS:N	1:A:67:LYS:CD	0.50	2.75	17	5
1:A:23:HIS:NE2	1:A:30:ASP:OD1	0.50	2.45	14	1
2:B:601:LEU:CD2	2:B:602:LYS:N	0.50	2.72	20	1
1:A:57:ASP:OD1	1:A:57:ASP:N	0.50	2.45	2	2
1:A:52:LEU:O	1:A:53:ASP:CB	0.50	2.60	4	9
1:A:64:TRP:NE1	1:A:91:GLN:CD	0.50	2.65	5	14
1:A:74:LYS:C	1:A:76:HIS:N	0.49	2.65	15	10
1:A:32:THR:C	1:A:33:LEU:HD22	0.49	2.27	19	5
1:A:24:VAL:HG13	1:A:92:PHE:CD1	0.49	2.42	6	2
2:B:600:PHE:CE2	2:B:604:PHE:CD1	0.49	3.00	8	1
1:A:67:LYS:CD	1:A:67:LYS:N	0.49	2.75	19	2
1:A:92:PHE:C	1:A:92:PHE:CD1	0.49	2.83	17	3
1:A:22:VAL:CG1	1:A:23:HIS:N	0.49	2.75	10	1
1:A:64:TRP:CD1	1:A:64:TRP:O	0.49	2.65	11	1
2:B:591:ASN:O	2:B:592:ASP:CB	0.49	2.60	12	20
2:B:569:HIS:C	2:B:571:GLU:N	0.49	2.66	17	19
1:A:46:LEU:HD12	2:B:603:LEU:CD1	0.49	2.38	16	2
2:B:576:ALA:O	2:B:595:TYR:CE1	0.49	2.66	3	4
1:A:59:SER:C	1:A:61:HIS:N	0.49	2.65	6	4
2:B:556:ILE:CG2	2:B:559:ARG:O	0.49	2.61	19	20
2:B:590:GLN:NE2	2:B:604:PHE:CD2	0.49	2.81	10	3
2:B:579:LEU:H	2:B:579:LEU:HD12	0.49	1.67	4	1
2:B:595:TYR:CD1	2:B:600:PHE:CD1	0.49	3.01	8	1
1:A:33:LEU:N	1:A:33:LEU:CD2	0.49	2.75	19	1
1:A:51:LYS:NZ	1:A:51:LYS:CB	0.49	2.76	6	4
1:A:76:HIS:CD2	1:A:77:TRP:CE3	0.49	3.01	8	1
2:B:563:ALA:C	2:B:565:ALA:N	0.49	2.67	6	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:564:MET:O	2:B:565:ALA:HB3	0.49	2.08	7	18
1:A:61:HIS:HD1	1:A:62:ALA:N	0.48	2.06	1	1
1:A:64:TRP:CD1	1:A:91:GLN:CD	0.48	2.86	14	5
1:A:79:LEU:H	1:A:79:LEU:CD1	0.48	2.21	2	2
1:A:25:THR:C	1:A:27:LEU:H	0.48	2.12	2	12
1:A:76:HIS:O	1:A:77:TRP:CE3	0.48	2.66	11	1
1:A:17:THR:HG23	1:A:17:THR:O	0.48	2.09	9	2
1:A:19:GLU:CD	1:A:19:GLU:N	0.48	2.67	18	10
2:B:601:LEU:C	2:B:601:LEU:CD1	0.48	2.82	16	8
1:A:40:HIS:CD2	1:A:40:HIS:N	0.48	2.82	4	1
1:A:59:SER:C	1:A:61:HIS:H	0.48	2.11	6	4
1:A:61:HIS:CB	1:A:92:PHE:CE2	0.48	2.97	6	1
1:A:45:MET:O	1:A:49:VAL:CG2	0.48	2.62	7	1
1:A:92:PHE:C	1:A:92:PHE:CD2	0.48	2.87	8	1
1:A:48:LEU:HD13	1:A:92:PHE:CE1	0.48	2.44	10	1
1:A:19:GLU:N	1:A:19:GLU:CD	0.47	2.67	12	9
1:A:61:HIS:C	1:A:61:HIS:ND1	0.47	2.68	16	2
1:A:92:PHE:CD2	1:A:92:PHE:C	0.47	2.84	5	1
1:A:84:ILE:HG22	1:A:85:GLN:N	0.47	2.25	15	10
2:B:595:TYR:CE1	2:B:600:PHE:CD1	0.47	3.03	8	1
1:A:54:VAL:C	1:A:56:LYS:H	0.47	2.10	2	14
1:A:55:LYS:NZ	2:B:576:ALA:HB2	0.47	2.24	19	1
2:B:571:GLU:C	2:B:573:PHE:N	0.47	2.66	3	15
2:B:562:THR:O	2:B:584:LYS:CE	0.47	2.63	18	2
2:B:601:LEU:CD1	2:B:601:LEU:C	0.47	2.81	17	7
1:A:66:GLU:C	1:A:68:LYS:N	0.47	2.68	7	4
1:A:55:LYS:CD	2:B:579:LEU:HD11	0.47	2.39	11	1
1:A:41:ILE:C	1:A:43:GLY:N	0.47	2.67	20	16
1:A:64:TRP:HE1	1:A:91:GLN:CD	0.47	2.13	8	5
1:A:61:HIS:CD2	1:A:61:HIS:C	0.47	2.87	14	1
1:A:61:HIS:CB	1:A:92:PHE:CZ	0.47	2.97	3	2
1:A:65:TRP:HB2	1:A:72:LEU:HD21	0.47	1.86	11	2
1:A:55:LYS:NZ	2:B:579:LEU:HD12	0.47	2.23	15	1
1:A:81:LYS:HD3	1:A:82:TYR:N	0.47	2.24	7	8
1:A:64:TRP:CZ2	1:A:91:GLN:NE2	0.47	2.81	19	1
1:A:65:TRP:NE1	1:A:67:LYS:CG	0.47	2.78	12	13
1:A:58:TRP:O	1:A:61:HIS:O	0.46	2.33	13	2
1:A:61:HIS:ND1	1:A:92:PHE:CE2	0.46	2.83	3	1
2:B:575:CYS:CB	2:B:596:CYS:SG	0.46	3.02	3	1
1:A:55:LYS:O	1:A:55:LYS:CG	0.46	2.63	17	2
1:A:56:LYS:CG	1:A:57:ASP:N	0.46	2.77	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:TRP:HE1	1:A:37:GLY:N	0.46	2.09	3	1
1:A:54:VAL:C	1:A:56:LYS:N	0.46	2.68	12	2
1:A:25:THR:O	1:A:26:ASP:CB	0.46	2.63	11	5
1:A:23:HIS:CD2	1:A:30:ASP:CG	0.46	2.89	4	1
1:A:17:THR:CG2	1:A:17:THR:O	0.46	2.64	9	1
2:B:579:LEU:HD22	2:B:579:LEU:H	0.46	1.65	15	1
2:B:579:LEU:HD13	2:B:579:LEU:N	0.46	2.22	20	1
2:B:593:LYS:O	2:B:595:TYR:CE2	0.46	2.68	7	1
1:A:65:TRP:HE1	1:A:67:LYS:CG	0.46	2.24	6	13
2:B:603:LEU:HD23	2:B:603:LEU:N	0.46	2.26	10	1
1:A:16:GLY:O	1:A:18:TRP:CD2	0.46	2.68	5	3
2:B:547:SER:H	2:B:556:ILE:H	0.46	1.53	5	2
2:B:590:GLN:OE1	2:B:600:PHE:CD2	0.46	2.68	12	1
2:B:569:HIS:C	2:B:571:GLU:H	0.46	2.13	18	19
2:B:593:LYS:O	2:B:595:TYR:CD2	0.46	2.69	7	1
2:B:579:LEU:CD2	2:B:579:LEU:N	0.45	2.64	3	1
2:B:601:LEU:O	2:B:605:CYS:N	0.45	2.49	20	4
1:A:61:HIS:C	1:A:61:HIS:CD2	0.45	2.87	7	1
1:A:63:LEU:H	1:A:63:LEU:CD2	0.45	2.18	10	2
1:A:45:MET:SD	1:A:61:HIS:CE1	0.45	3.09	16	1
1:A:23:HIS:ND1	1:A:30:ASP:OD2	0.45	2.49	3	1
2:B:582:LEU:O	2:B:583:ASN:OD1	0.45	2.34	11	20
1:A:61:HIS:ND1	1:A:62:ALA:N	0.45	2.65	6	1
1:A:23:HIS:CG	1:A:30:ASP:OD1	0.45	2.70	7	1
1:A:34:ARG:CD	1:A:34:ARG:C	0.45	2.85	13	1
2:B:564:MET:CE	2:B:566:LYS:NZ	0.45	2.80	17	1
2:B:589:GLU:CG	2:B:590:GLN:N	0.45	2.79	8	20
1:A:74:LYS:C	1:A:76:HIS:H	0.45	2.15	9	7
2:B:590:GLN:OE1	2:B:600:PHE:CE2	0.45	2.70	12	1
2:B:583:ASN:O	2:B:586:THR:N	0.45	2.47	3	3
2:B:604:PHE:C	2:B:605:CYS:SG	0.45	2.95	3	3
1:A:46:LEU:HD23	1:A:46:LEU:C	0.45	2.32	4	1
1:A:78:THR:O	1:A:79:LEU:C	0.45	2.55	7	3
2:B:579:LEU:N	2:B:579:LEU:HD13	0.45	2.22	12	2
1:A:54:VAL:O	1:A:58:TRP:NE1	0.45	2.50	20	1
2:B:604:PHE:O	2:B:605:CYS:C	0.45	2.55	5	3
1:A:22:VAL:HG21	1:A:92:PHE:CE2	0.45	2.46	10	1
1:A:45:MET:O	1:A:49:VAL:HG23	0.45	2.12	7	2
2:B:549:CYS:O	2:B:553:GLN:N	0.45	2.46	17	2
1:A:55:LYS:HZ2	2:B:576:ALA:CB	0.45	2.25	19	1
1:A:74:LYS:CB	1:A:81:LYS:NZ	0.44	2.80	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:571:GLU:C	2:B:573:PHE:H	0.44	2.16	4	5
2:B:559:ARG:O	2:B:570:PRO:CG	0.44	2.66	1	20
2:B:575:CYS:O	2:B:578:CYS:O	0.44	2.35	9	2
1:A:41:ILE:HD13	1:A:72:LEU:HB3	0.44	1.88	4	1
1:A:79:LEU:CD1	1:A:79:LEU:H	0.44	2.25	10	1
1:A:76:HIS:O	1:A:77:TRP:CB	0.44	2.65	11	1
1:A:54:VAL:O	1:A:58:TRP:CE2	0.44	2.71	20	1
2:B:590:GLN:HG2	2:B:591:ASN:ND2	0.44	2.28	2	1
1:A:40:HIS:CD2	1:A:43:GLY:N	0.44	2.85	6	1
1:A:18:TRP:CZ3	1:A:85:GLN:HA	0.44	2.47	17	2
1:A:62:ALA:O	1:A:93:THR:O	0.44	2.36	1	1
1:A:35:VAL:HB	1:A:39:VAL:HG11	0.44	1.89	4	1
1:A:41:ILE:HD12	1:A:74:LYS:O	0.44	2.13	5	1
2:B:605:CYS:O	2:B:605:CYS:SG	0.44	2.76	10	1
2:B:575:CYS:CB	2:B:582:LEU:HD13	0.44	2.43	16	11
2:B:600:PHE:O	2:B:603:LEU:N	0.44	2.45	8	1
2:B:590:GLN:C	2:B:591:ASN:CG	0.43	2.76	7	15
1:A:60:ASP:OD1	1:A:60:ASP:O	0.43	2.36	16	1
1:A:29:ARG:O	1:A:30:ASP:OD1	0.43	2.36	10	3
1:A:60:ASP:OD2	1:A:60:ASP:O	0.43	2.36	19	3
1:A:19:GLU:OE2	1:A:19:GLU:O	0.43	2.36	6	1
2:B:601:LEU:O	2:B:605:CYS:OXT	0.43	2.37	7	3
1:A:61:HIS:CD2	1:A:61:HIS:O	0.43	2.72	14	1
1:A:66:GLU:OE2	1:A:91:GLN:OE1	0.43	2.37	13	1
1:A:26:ASP:OD1	1:A:26:ASP:O	0.43	2.36	15	1
1:A:57:ASP:N	1:A:57:ASP:OD1	0.43	2.50	5	1
2:B:557:THR:OG1	2:B:557:THR:O	0.43	2.37	4	4
1:A:50:GLU:O	1:A:53:ASP:OD1	0.43	2.36	9	1
1:A:38:GLU:C	1:A:78:THR:HG21	0.43	2.33	12	5
2:B:591:ASN:O	2:B:592:ASP:OD2	0.43	2.37	12	1
1:A:29:ARG:O	1:A:30:ASP:OD2	0.43	2.36	1	1
1:A:54:VAL:CG2	1:A:55:LYS:N	0.43	2.82	14	1
1:A:87:ASP:OD1	1:A:88:ALA:N	0.43	2.52	2	1
1:A:34:ARG:O	1:A:35:VAL:CG1	0.42	2.67	13	3
1:A:52:LEU:C	1:A:54:VAL:H	0.42	2.17	5	1
1:A:61:HIS:CD2	1:A:61:HIS:N	0.42	2.86	5	2
1:A:75:THR:O	1:A:76:HIS:O	0.42	2.36	5	1
1:A:58:TRP:O	1:A:59:SER:C	0.42	2.57	11	3
2:B:598:ASN:HA	2:B:601:LEU:HD22	0.42	1.91	20	1
1:A:36:THR:O	1:A:39:VAL:HG12	0.42	2.14	4	1
1:A:71:TRP:CD1	1:A:73:LEU:CD2	0.42	3.02	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:GLY:H	1:A:75:THR:HG23	0.42	1.74	8	2
1:A:76:HIS:ND1	1:A:76:HIS:N	0.42	2.67	18	2
2:B:594:PRO:O	2:B:595:TYR:CD2	0.42	2.72	8	1
1:A:36:THR:O	1:A:38:GLU:N	0.42	2.52	15	1
2:B:601:LEU:O	2:B:605:CYS:O	0.42	2.36	6	1
1:A:19:GLU:CG	1:A:34:ARG:CZ	0.42	2.97	9	1
1:A:63:LEU:HA	1:A:91:GLN:O	0.42	2.14	18	2
1:A:76:HIS:CE1	2:B:605:CYS:HG	0.42	2.33	5	1
1:A:66:GLU:OE1	1:A:91:GLN:OE1	0.42	2.37	2	2
1:A:44:VAL:HG12	1:A:45:MET:N	0.42	2.29	10	1
1:A:78:THR:N	1:A:81:LYS:CG	0.42	2.83	1	2
1:A:47:LYS:O	1:A:48:LEU:C	0.42	2.58	14	3
1:A:75:THR:O	2:B:605:CYS:O	0.42	2.38	4	1
1:A:36:THR:OG1	1:A:38:GLU:CG	0.42	2.68	7	1
1:A:38:GLU:OE2	1:A:38:GLU:O	0.42	2.37	8	2
1:A:25:THR:OG1	1:A:93:THR:CB	0.42	2.68	11	1
1:A:53:ASP:O	1:A:54:VAL:CG1	0.42	2.68	14	1
1:A:87:ASP:OD2	1:A:87:ASP:O	0.42	2.38	5	1
2:B:579:LEU:HD12	2:B:579:LEU:H	0.42	1.75	8	1
1:A:59:SER:N	2:B:577:PHE:O	0.42	2.50	20	1
1:A:60:ASP:CG	1:A:60:ASP:O	0.42	2.58	14	1
1:A:61:HIS:HD1	1:A:61:HIS:C	0.41	2.18	1	1
2:B:590:GLN:CD	2:B:591:ASN:HD21	0.41	2.18	2	1
2:B:590:GLN:CG	2:B:591:ASN:HD21	0.41	2.28	2	1
2:B:567:LYS:O	2:B:568:PHE:CD2	0.41	2.74	3	2
1:A:46:LEU:HD21	2:B:595:TYR:OH	0.41	2.15	3	1
1:A:84:ILE:CG2	1:A:85:GLN:N	0.41	2.83	15	2
1:A:74:LYS:O	1:A:75:THR:C	0.41	2.57	6	2
1:A:22:VAL:N	1:A:31:VAL:O	0.41	2.53	14	1
2:B:572:HIS:CD2	2:B:572:HIS:N	0.41	2.85	7	1
2:B:578:CYS:C	2:B:580:LYS:H	0.41	2.19	20	2
1:A:56:LYS:NZ	1:A:58:TRP:CZ3	0.41	2.88	14	1
1:A:22:VAL:HG12	1:A:23:HIS:N	0.41	2.31	10	1
1:A:33:LEU:HD11	1:A:51:LYS:HZ3	0.41	1.75	16	1
1:A:33:LEU:CD1	1:A:51:LYS:NZ	0.41	2.83	5	2
1:A:40:HIS:CD2	1:A:43:GLY:CA	0.41	3.04	6	1
1:A:64:TRP:O	1:A:64:TRP:CD1	0.41	2.74	10	1
1:A:64:TRP:CH2	1:A:91:GLN:NE2	0.41	2.88	20	1
1:A:34:ARG:CD	1:A:35:VAL:N	0.41	2.84	4	1
2:B:603:LEU:N	2:B:603:LEU:HD23	0.41	2.30	5	2
2:B:557:THR:O	2:B:557:THR:OG1	0.41	2.37	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:TRP:CZ3	1:A:85:GLN:CA	0.41	3.03	9	1
1:A:68:LYS:C	1:A:69:ARG:HH21	0.41	2.19	16	1
2:B:604:PHE:O	2:B:605:CYS:O	0.41	2.38	19	1
1:A:59:SER:O	1:A:60:ASP:C	0.41	2.59	20	1
2:B:590:GLN:O	2:B:592:ASP:N	0.41	2.54	12	2
2:B:562:THR:N	2:B:584:LYS:NZ	0.41	2.68	5	1
2:B:583:ASN:C	2:B:585:GLY:N	0.41	2.74	11	1
1:A:61:HIS:O	1:A:92:PHE:CZ	0.41	2.73	18	1
1:A:41:ILE:O	1:A:44:VAL:N	0.41	2.50	14	3
1:A:73:LEU:C	1:A:75:THR:H	0.41	2.19	9	1
1:A:27:LEU:HD12	1:A:29:ARG:HD2	0.41	1.93	11	1
1:A:53:ASP:O	1:A:58:TRP:NE1	0.41	2.48	14	1
1:A:53:ASP:O	1:A:54:VAL:HG12	0.41	2.15	14	1
2:B:572:HIS:N	2:B:572:HIS:CD2	0.41	2.89	9	2
2:B:590:GLN:OE1	2:B:604:PHE:CD1	0.40	2.74	7	1
1:A:44:VAL:O	1:A:45:MET:C	0.40	2.59	12	1
1:A:64:TRP:CE2	1:A:91:GLN:NE2	0.40	2.89	19	1
1:A:76:HIS:O	1:A:77:TRP:CD2	0.40	2.74	11	1
1:A:63:LEU:O	1:A:72:LEU:N	0.40	2.51	14	1
2:B:575:CYS:N	2:B:582:LEU:HB2	0.40	2.31	5	1
1:A:79:LEU:HG	1:A:80:ASP:N	0.40	2.31	8	2
2:B:595:TYR:CE1	2:B:600:PHE:CE1	0.40	3.10	8	1
1:A:58:TRP:O	1:A:61:HIS:CB	0.40	2.68	16	1
2:B:564:MET:CE	2:B:566:LYS:HZ1	0.40	2.29	17	1
2:B:597:GLN:HE21	2:B:597:GLN:HA	0.40	1.77	20	1
1:A:34:ARG:C	1:A:34:ARG:CD	0.40	2.90	15	1

## 6.3 Torsion angles (i)

### 6.3.1 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 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	78/112 (70%)	61±2 (78±3%)	14±3 (18±3%)	3±1 (4±2%)	4 29
2	B	58/72 (81%)	41±1 (70±2%)	14±1 (24±2%)	4±0 (6±1%)	3 19
All	All	2720/3680 (74%)	2028 (75%)	550 (20%)	142 (5%)	4 24

All 18 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	72	LEU	20
2	B	564	MET	20
2	B	565	ALA	20
2	B	570	PRO	17
1	A	55	LYS	16
2	B	579	LEU	16
1	A	77	TRP	6
1	A	54	VAL	5
1	A	75	THR	4
1	A	57	ASP	4
1	A	35	VAL	3
1	A	76	HIS	3
1	A	26	ASP	2
1	A	53	ASP	2
1	A	74	LYS	1
1	A	60	ASP	1
1	A	28	ASN	1
2	B	572	HIS	1

### 6.3.2 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 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	70/98 (71%)	51±3 (72±4%)	19±3 (28±4%)	2 20
2	B	53/63 (84%)	41±2 (77±4%)	12±2 (23±4%)	3 27
All	All	2460/3220 (76%)	1824 (74%)	636 (26%)	2 23

All 71 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)
2	B	601	LEU	20
1	A	19	GLU	20
1	A	20	LEU	20
1	A	32	THR	20

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Mol	Chain	Res	Type	Models (Total)
2	B	591	ASN	20
1	A	18	TRP	20
1	A	64	TRP	20
1	A	78	THR	20
1	A	71	TRP	20
2	B	549	CYS	20
1	A	28	ASN	20
2	B	580	LYS	20
2	B	597	GLN	20
2	B	588	LYS	20
2	B	575	CYS	20
1	A	85	GLN	20
1	A	93	THR	17
2	B	587	PHE	16
1	A	74	LYS	16
2	B	600	PHE	15
2	B	568	PHE	13
1	A	82	TYR	13
1	A	52	LEU	11
2	B	577	PHE	11
1	A	57	ASP	10
1	A	81	LYS	10
2	B	598	ASN	10
1	A	25	THR	8
1	A	38	GLU	8
1	A	61	HIS	7
2	B	602	LYS	7
2	B	603	LEU	7
1	A	40	HIS	7
1	A	63	LEU	7
1	A	67	LYS	7
2	B	566	LYS	7
2	B	579	LEU	7
1	A	21	SER	6
1	A	77	TRP	6
1	A	45	MET	6
1	A	87	ASP	6
1	A	92	PHE	6
1	A	48	LEU	6
1	A	55	LYS	5
1	A	46	LEU	5
1	A	75	THR	5

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Mol	Chain	Res	Type	Models (Total)
1	A	17	THR	5
1	A	69	ARG	4
1	A	34	ARG	4
1	A	76	HIS	4
2	B	604	PHE	4
2	B	584	LYS	3
1	A	26	ASP	3
1	A	30	ASP	3
2	B	590	GLN	3
1	A	59	SER	2
2	B	578	CYS	2
2	B	605	CYS	1
2	B	559	ARG	1
1	A	54	VAL	1
1	A	44	VAL	1
2	B	564	MET	1
1	A	41	ILE	1
1	A	39	VAL	1
1	A	58	TRP	1
1	A	27	LEU	1
1	A	24	VAL	1
1	A	36	THR	1
2	B	592	ASP	1
1	A	29	ARG	1
1	A	72	LEU	1

### 6.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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 73% for the well-defined parts and 73% 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	1649
Number of shifts mapped to atoms	1649
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

#### 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
$^{13}\text{C}_\alpha$	165	$0.15 \pm 0.17$	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	154	$0.33 \pm 0.11$	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	135	$0.32 \pm 0.35$	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 73%, i.e. 1281 atoms were assigned a chemical shift out of a possible 1757. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	495/679 (73%)	247/271 (91%)	137/274 (50%)	111/134 (83%)
Sidechain	774/887 (87%)	480/521 (92%)	284/327 (87%)	10/39 (26%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	12/191 (6%)	7/103 (7%)	0/78 (0%)	5/10 (50%)
Overall	1281/1757 (73%)	734/895 (82%)	421/679 (62%)	126/183 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1471 atoms were assigned a chemical shift out of a possible 2027. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	579/785 (74%)	289/313 (92%)	159/318 (50%)	131/154 (85%)
Sidechain	880/1028 (86%)	548/606 (90%)	322/374 (86%)	10/48 (21%)
Aromatic	12/214 (6%)	7/115 (6%)	0/88 (0%)	5/11 (45%)
Overall	1471/2027 (73%)	844/1034 (82%)	481/780 (62%)	146/213 (69%)

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

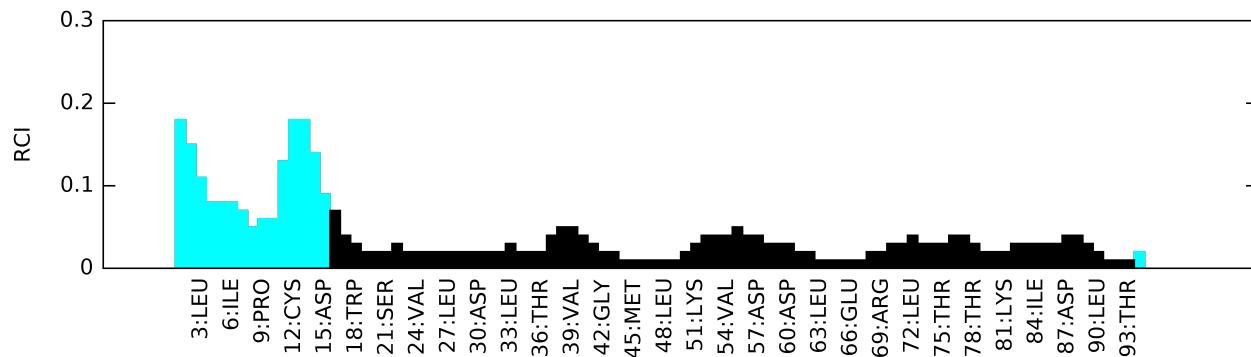
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	74	LYS	HD3	0.10	2.75 – 0.45	-6.5
1	A	35	VAL	HG21	-0.91	2.20 – -0.60	-6.1
1	A	35	VAL	HG22	-0.91	2.20 – -0.60	-6.1
1	A	35	VAL	HG23	-0.91	2.20 – -0.60	-6.1
1	A	68	LYS	HB3	0.12	3.10 – 0.40	-6.0
1	A	41	ILE	CG2	9.30	24.63 – 10.43	-5.8
1	A	61	HIS	HB3	0.83	5.00 – 1.10	-5.7
1	A	68	LYS	HG2	-0.10	2.67 – 0.07	-5.7
2	B	603	LEU	HB3	-0.48	3.34 – -0.26	-5.6
1	A	68	LYS	HG3	-0.15	2.76 – -0.04	-5.4
1	A	74	LYS	HB3	0.29	3.10 – 0.40	-5.4
1	A	81	LYS	HD3	0.37	2.75 – 0.45	-5.3

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

The images below report *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 A:



Random coil index (RCI) for chain B:

