



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 07:29 pm BST

PDB ID : 1CFF  
Title : NMR SOLUTION STRUCTURE OF A COMPLEX OF CALMODULIN  
WITH A BINDING PEPTIDE OF THE CA<sup>2+</sup>-PUMP  
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C.  
Deposited on : 1999-03-18

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 ⓘ 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

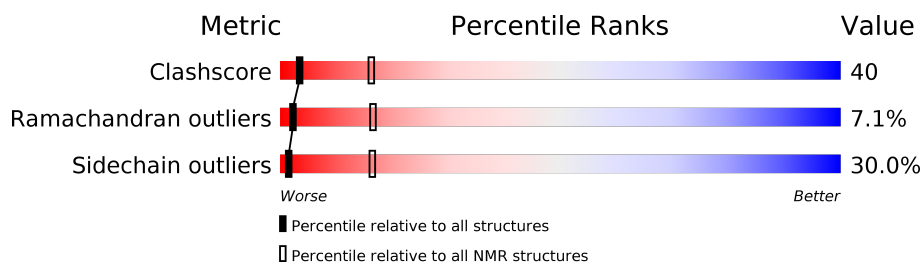
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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	148	
2	B	20	

## 2 Ensemble composition and analysis

This entry contains 26 models. Model 7 is the overall representative, medoid model (most similar to other models).

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:4-A:74 (71)	0.56	12
2	A:85-A:146, B:4-B:18 (77)	0.41	7

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	2, 4, 8, 9, 10, 11, 13, 14, 16, 17, 23, 26
2	5, 6, 7, 12, 22
3	18, 20, 21, 24, 25
4	1, 3, 15
Single-model clusters	19

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2638 atoms, of which 1291 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CALMODULIN.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2262	714	1096	188	255	9	

- Molecule 2 is a protein called CALCIUM PUMP.

Mol	Chain	Residues	Atoms					Trace
2	B	20	Total	C	H	N	O	0
			372	113	195	38	26	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	LYS	ARG	ENGINEERED MUTATION	UNP P62155

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

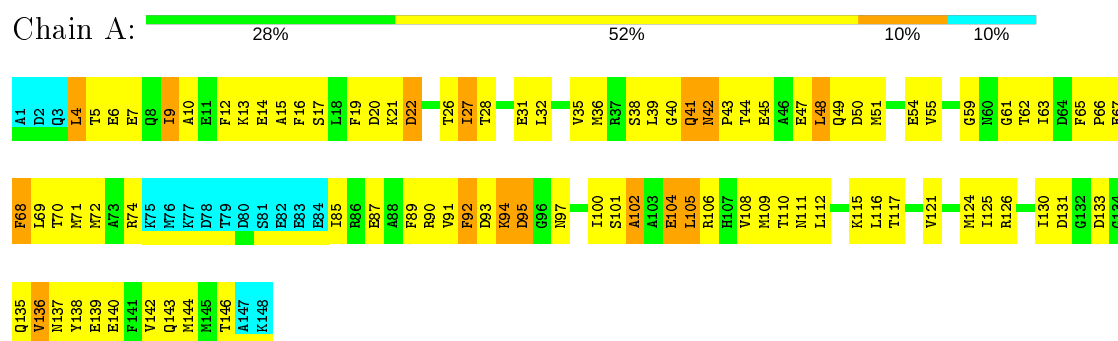
Mol	Chain	Residues	Atoms	
3	A	4	Total	Ca
			4	4

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

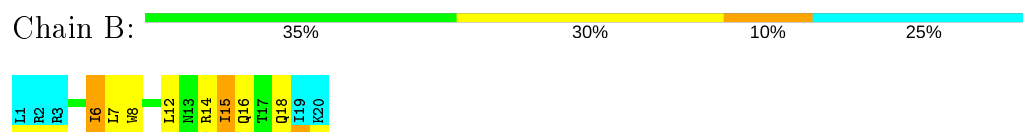
### 4.1 Average score per residue in the NMR ensemble

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: CALMODULIN



#### • Molecule 2: CALCIUM PUMP

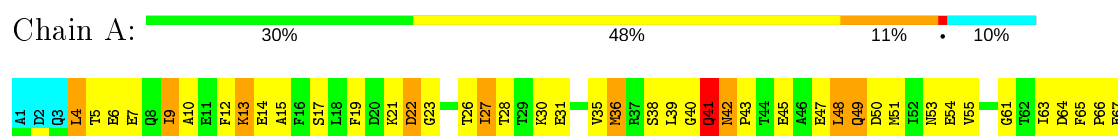


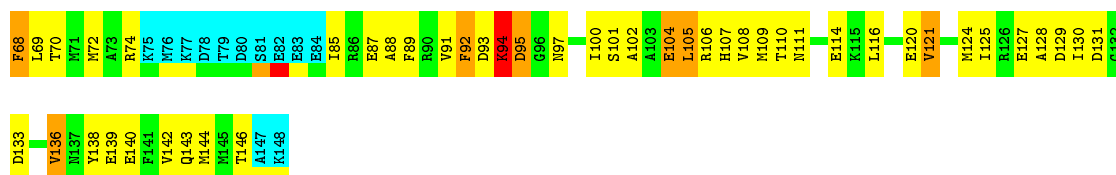
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

#### • Molecule 1: CALMODULIN





#### • Molecule 2: CALCIUM PUMP

Chain B: 45% 15% 15% 25%



### 4.2.2 Score per residue for model 2

#### • Molecule 1: CALMODULIN

Chain A: 30% 45% 13% 10%



#### • Molecule 2: CALCIUM PUMP

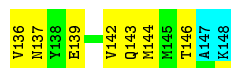
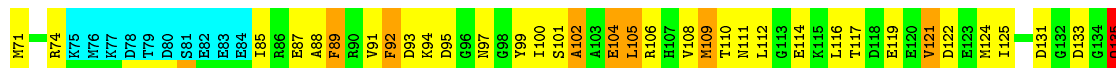
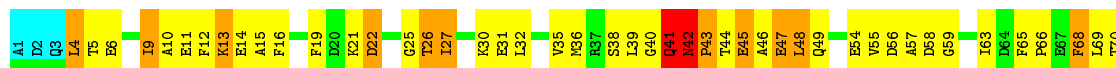
Chain B: 40% 25% 10% 25%



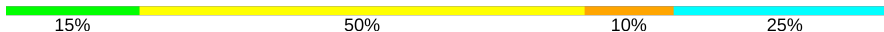
### 4.2.3 Score per residue for model 3

#### • Molecule 1: CALMODULIN

Chain A: 30% 45% 12% 10%



- Molecule 2: CALCIUM PUMP

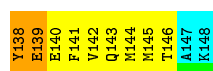
Chain B: 



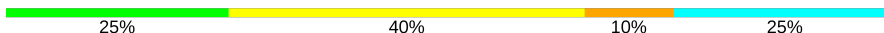
#### 4.2.4 Score per residue for model 4

- Molecule 1: CALMODULIN

Chain A: 



- Molecule 2: CALCIUM PUMP

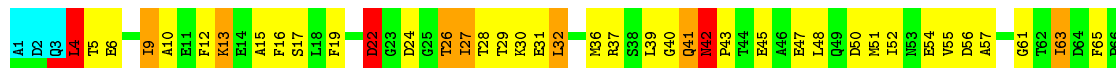
Chain B: 



#### 4.2.5 Score per residue for model 5

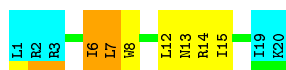
- Molecule 1: CALMODULIN

Chain A: 



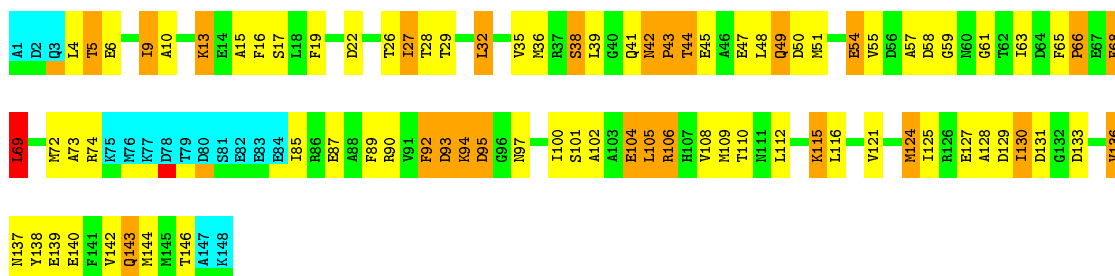
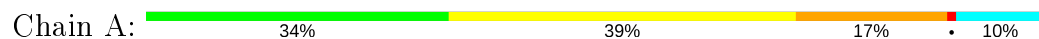
- Molecule 2: CALCIUM PUMP

Chain B: 

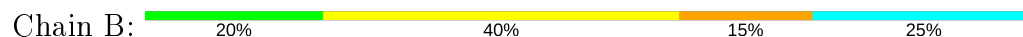


#### 4.2.6 Score per residue for model 6

- Molecule 1: CALMODULIN

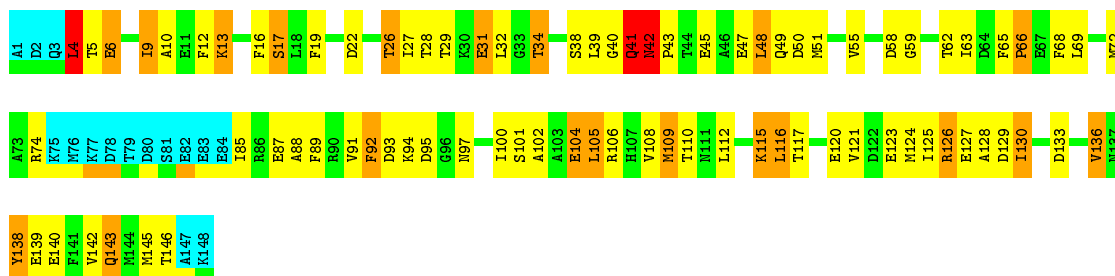


- Molecule 2: CALCIUM PUMP

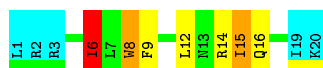


#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: CALMODULIN



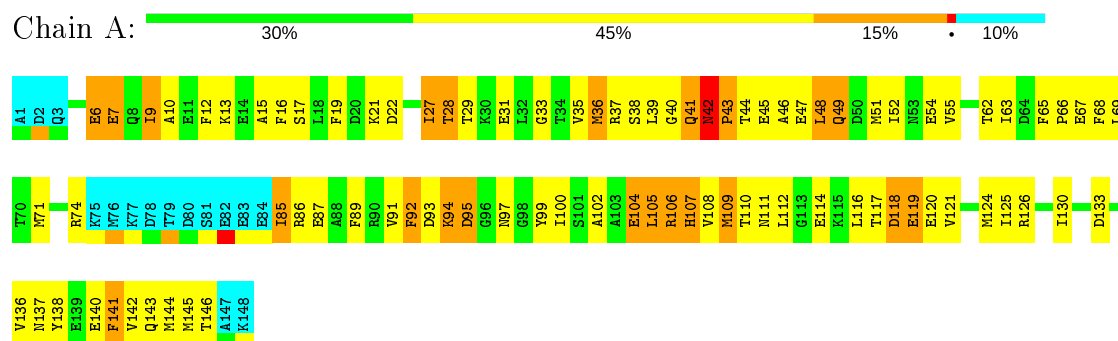
- Molecule 2: CALCIUM PUMP



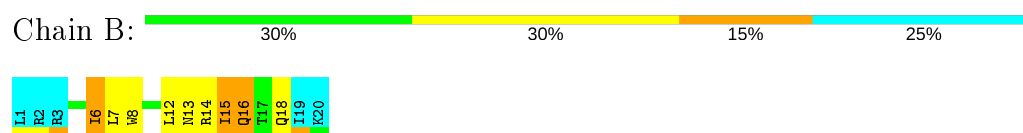


## 4.2.8 Score per residue for model 8

### • Molecule 1: CALMODULIN

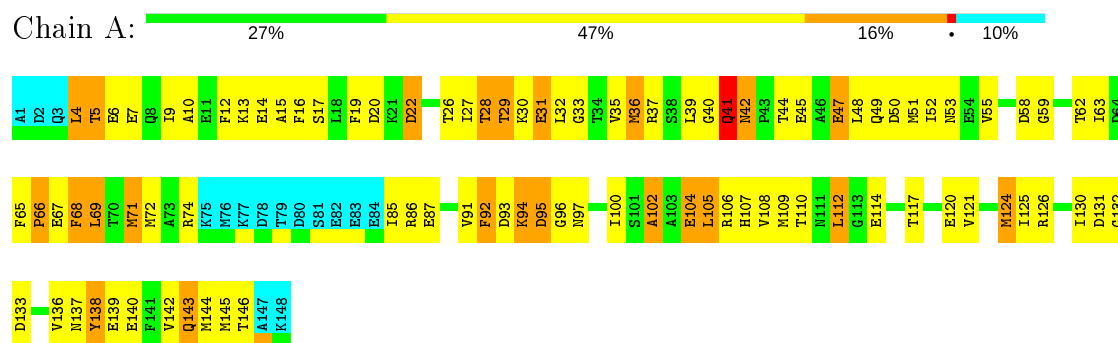


### • Molecule 2: CALCIUM PUMP

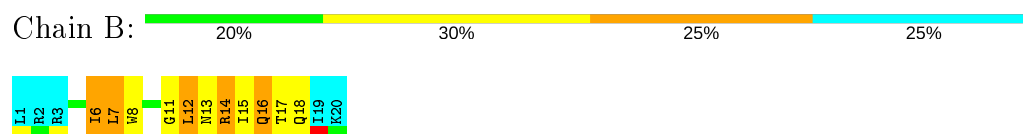


## 4.2.9 Score per residue for model 9

### • Molecule 1: CALMODULIN



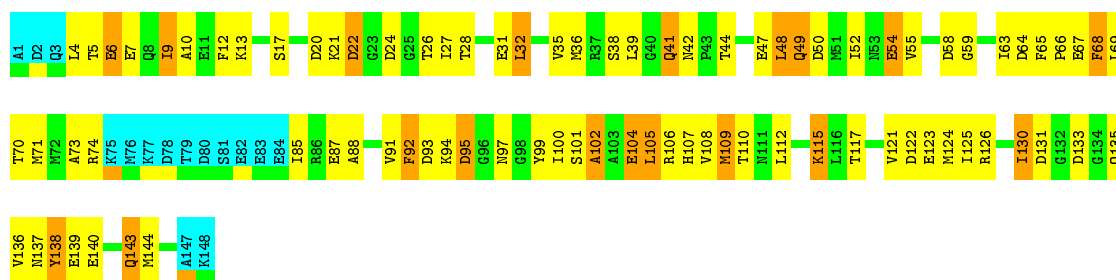
### • Molecule 2: CALCIUM PUMP



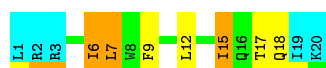
## 4.2.10 Score per residue for model 10

### • Molecule 1: CALMODULIN



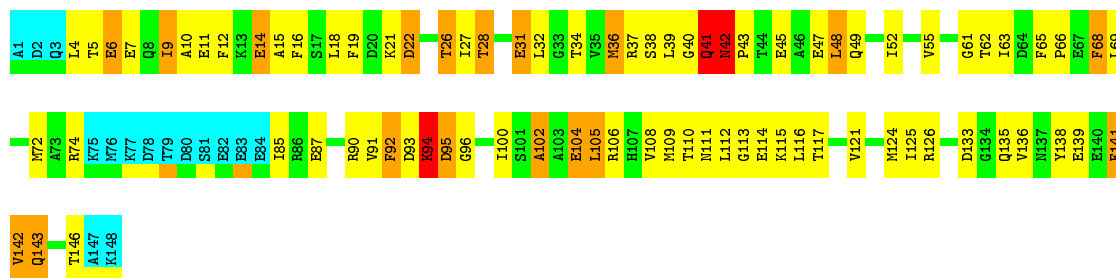


• Molecule 2: CALCIUM PUMP

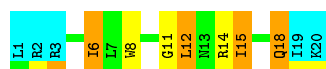


#### 4.2.11 Score per residue for model 11

• Molecule 1: CALMODULIN

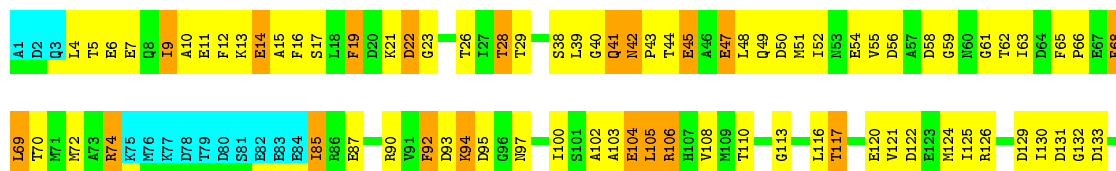


• Molecule 2: CALCIUM PUMP



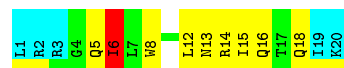
#### 4.2.12 Score per residue for model 12

• Molecule 1: CALMODULIN



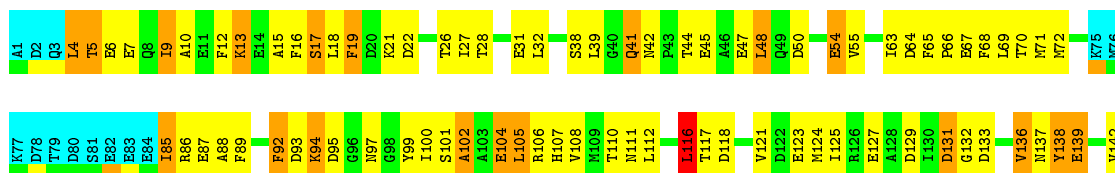


### • Molecule 2: CALCIUM PUMP

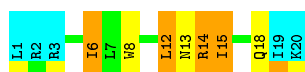


## 4.2.13 Score per residue for model 13

### • Molecule 1: CALMODULIN

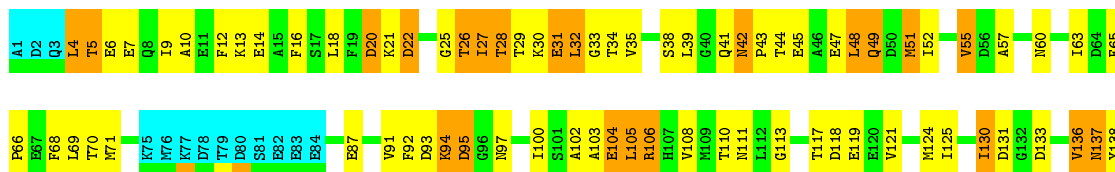


### • Molecule 2: CALCIUM PUMP

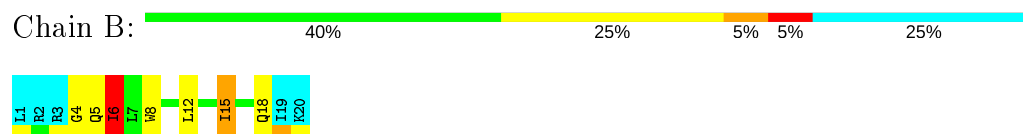


## 4.2.14 Score per residue for model 14

### • Molecule 1: CALMODULIN

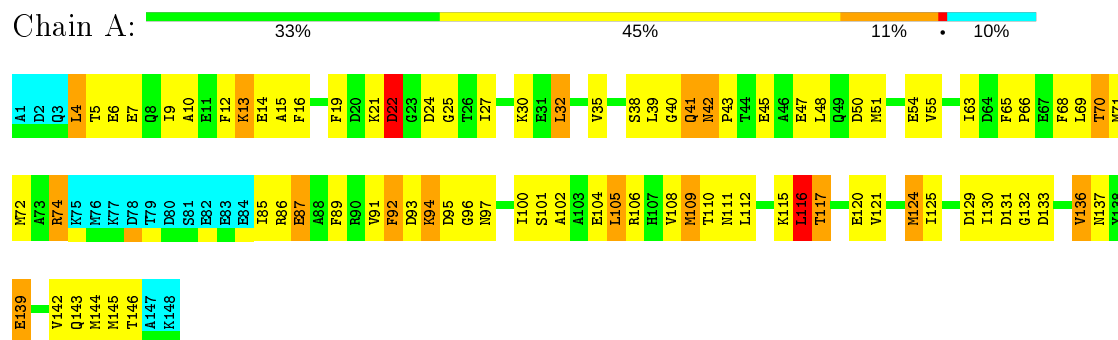


### • Molecule 2: CALCIUM PUMP

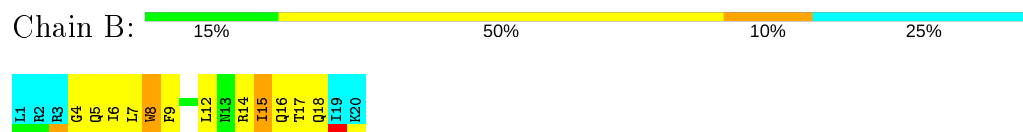


#### 4.2.15 Score per residue for model 15

- Molecule 1: CALMODULIN

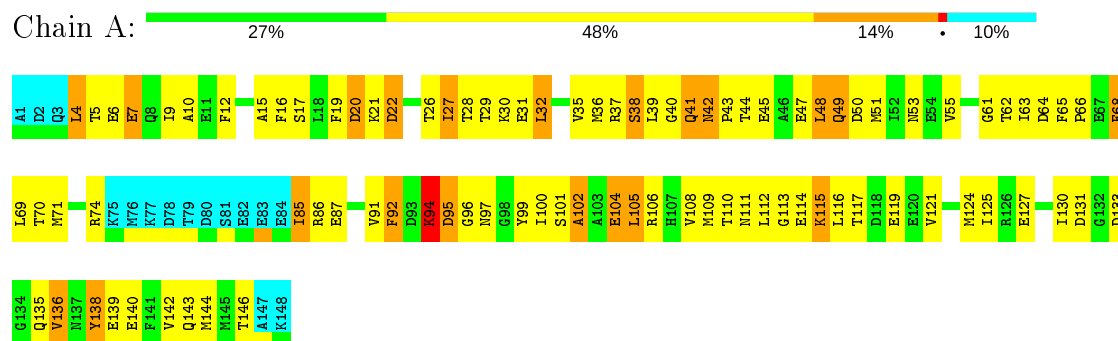


- Molecule 2: CALCIUM PUMP

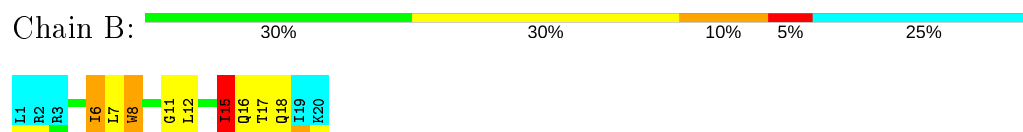


#### 4.2.16 Score per residue for model 16

- Molecule 1: CALMODULIN

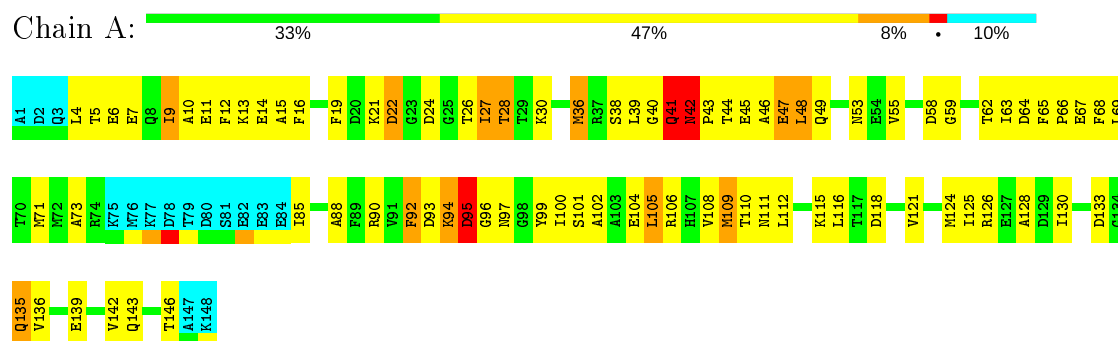


- Molecule 2: CALCIUM PUMP

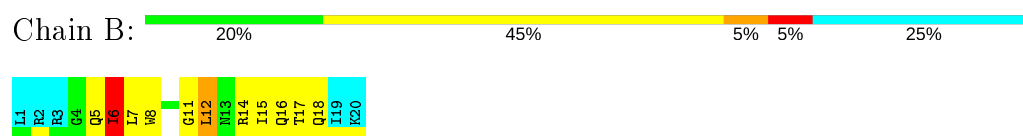


#### 4.2.17 Score per residue for model 17

- Molecule 1: CALMODULIN

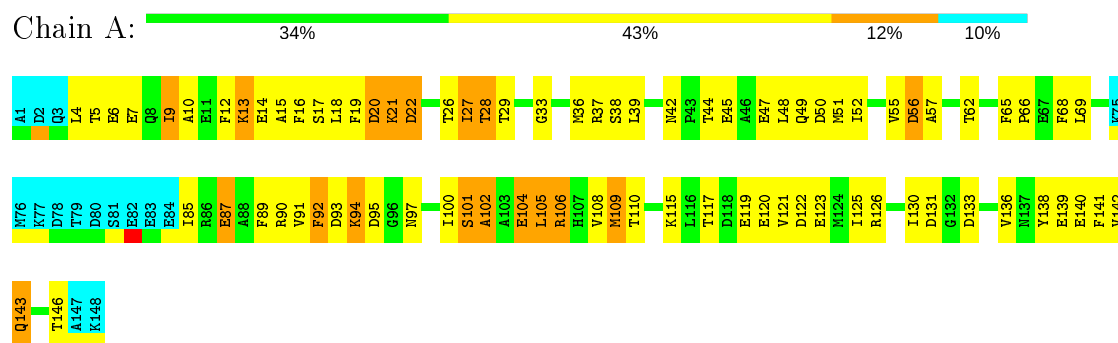


- Molecule 2: CALCIUM PUMP

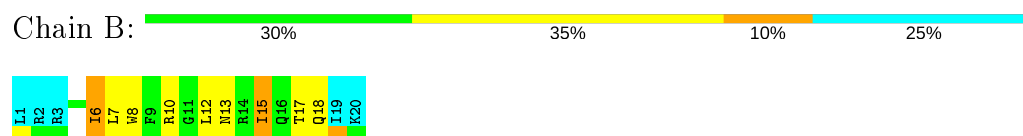


#### 4.2.18 Score per residue for model 18

- Molecule 1: CALMODULIN



- Molecule 2: CALCIUM PUMP

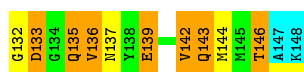


#### 4.2.19 Score per residue for model 19

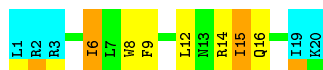
- Molecule 1: CALMODULIN





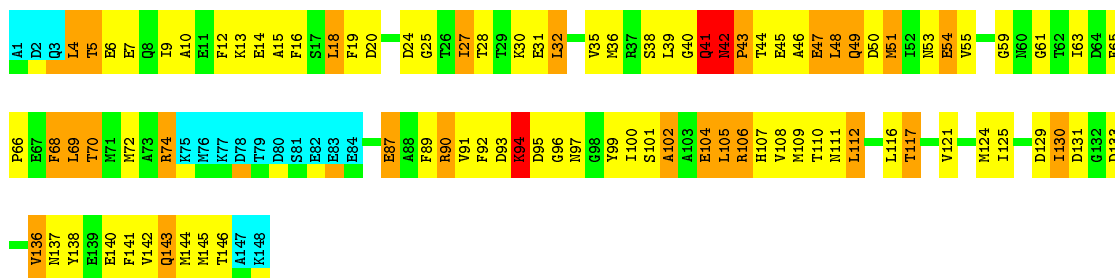


• Molecule 2: CALCIUM PUMP

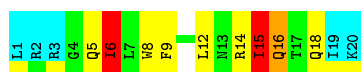
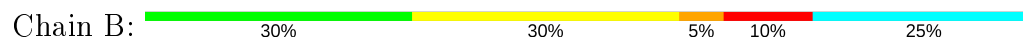


#### 4.2.22 Score per residue for model 22

• Molecule 1: CALMODULIN

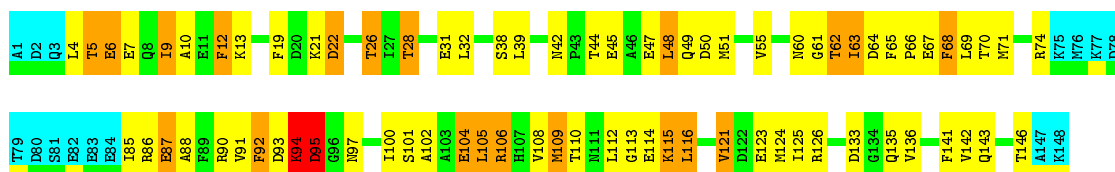


• Molecule 2: CALCIUM PUMP

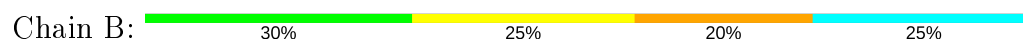


#### 4.2.23 Score per residue for model 23

• Molecule 1: CALMODULIN



• Molecule 2: CALCIUM PUMP

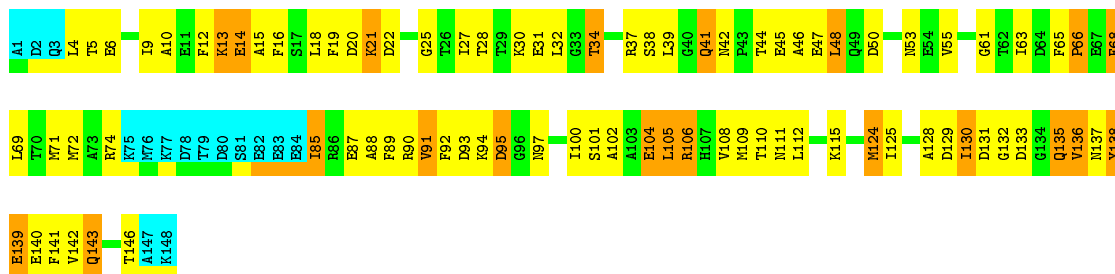




#### 4.2.24 Score per residue for model 24

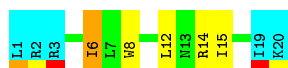
- Molecule 1: CALMODULIN

Chain A: 32% 43% 14% 10%



- Molecule 2: CALCIUM PUMP

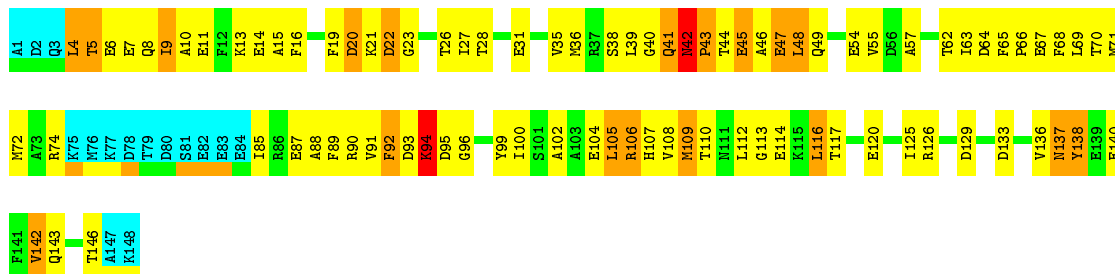
Chain B: 50% 20% 5% 25%



#### 4.2.25 Score per residue for model 25

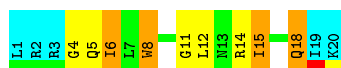
- Molecule 1: CALMODULIN

Chain A: 30% 46% 12% 10%



- Molecule 2: CALCIUM PUMP

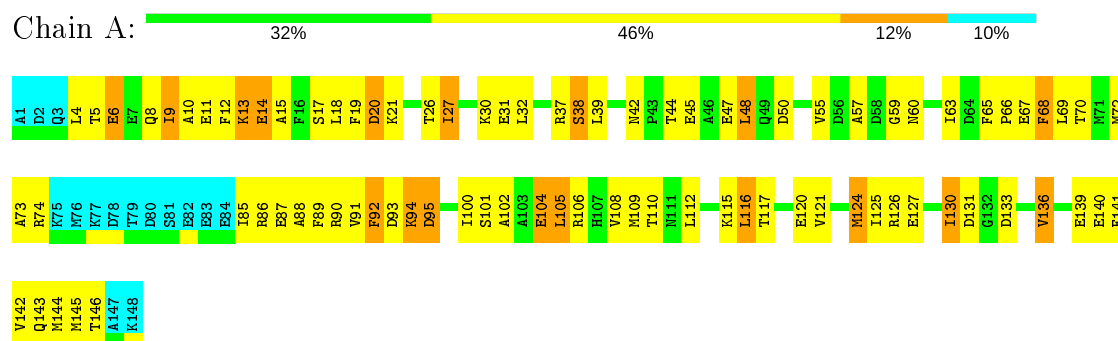
Chain B: 30% 25% 20% 25%



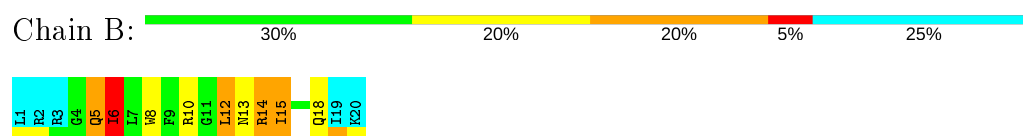


## 4.2.26 Score per residue for model 26

### • Molecule 1: CALMODULIN



### • Molecule 2: CALCIUM PUMP



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 200 calculated structures, 26 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
XPLOR	structure solution	

No chemical shift data was provided. 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:  
CA

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	1047	986	986	87±8
2	B	129	132	132	12±4
All	All	30680	29068	29068	2395

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD21	1:A:9:ILE:HD12	1.02	1.27	17	5
1:A:100:ILE:HG21	1:A:105:LEU:HD23	0.99	1.30	23	22
1:A:9:ILE:HD11	1:A:69:LEU:HD22	0.98	1.31	13	17
1:A:4:LEU:HD11	1:A:9:ILE:HD12	0.94	1.38	19	6
1:A:92:PHE:CD1	1:A:100:ILE:HD11	0.94	1.97	19	1
1:A:4:LEU:HD11	1:A:69:LEU:HD21	0.91	1.40	7	2
1:A:110:THR:HG23	1:A:114:GLU:CG	0.89	1.96	25	1
1:A:105:LEU:CD1	1:A:125:ILE:HD11	0.88	1.99	10	22
1:A:105:LEU:HD11	1:A:125:ILE:HD11	0.88	1.46	4	22
1:A:100:ILE:HG21	1:A:105:LEU:CD2	0.87	1.99	13	26
1:A:92:PHE:CE2	2:B:12:LEU:HD21	0.86	2.05	7	15

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*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD23	1:A:49:GLN:N	0.86	1.86	11	4
1:A:45:GLU:O	1:A:48:LEU:HD22	0.85	1.70	11	2
1:A:100:ILE:CG2	1:A:105:LEU:HD23	0.84	2.03	23	22
1:A:116:LEU:HD22	1:A:121:VAL:HG23	0.83	1.49	15	1
2:B:12:LEU:HD13	2:B:13:ASN:N	0.82	1.89	3	2
1:A:105:LEU:HD21	2:B:8:TRP:CZ3	0.82	2.08	5	25
2:B:12:LEU:HD13	2:B:15:ILE:HD12	0.82	1.51	25	9
1:A:92:PHE:CZ	2:B:12:LEU:HD23	0.82	2.09	11	2
2:B:12:LEU:O	2:B:12:LEU:HD22	0.82	1.73	9	1
1:A:9:ILE:CD1	1:A:69:LEU:HD22	0.82	2.04	11	19
1:A:4:LEU:HD22	1:A:69:LEU:HD21	0.81	1.52	5	3
1:A:44:THR:O	1:A:48:LEU:HD22	0.81	1.75	10	2
1:A:92:PHE:CD2	2:B:12:LEU:HD23	0.81	2.11	17	2
1:A:48:LEU:HD12	1:A:49:GLN:N	0.80	1.90	6	5
1:A:100:ILE:HG23	1:A:104:GLU:CG	0.80	2.06	16	15
1:A:92:PHE:CE2	2:B:12:LEU:HD13	0.79	2.13	20	1
2:B:12:LEU:HD22	2:B:12:LEU:O	0.79	1.76	3	1
1:A:4:LEU:HD13	1:A:4:LEU:O	0.79	1.78	1	1
1:A:4:LEU:CD1	1:A:69:LEU:HD21	0.79	2.08	7	1
1:A:91:VAL:O	1:A:108:VAL:HG11	0.78	1.79	4	4
1:A:38:SER:C	1:A:39:LEU:HD22	0.78	2.00	23	15
1:A:4:LEU:HD11	1:A:69:LEU:CD2	0.77	2.08	17	1
1:A:100:ILE:HG23	1:A:104:GLU:HG3	0.77	1.54	11	15
1:A:9:ILE:CD1	1:A:69:LEU:HD13	0.77	2.10	24	9
1:A:28:THR:HG23	1:A:62:THR:OG1	0.77	1.80	23	1
1:A:92:PHE:CD2	2:B:12:LEU:HD21	0.77	2.15	5	6
1:A:130:ILE:HD11	1:A:144:MET:HG3	0.77	1.57	14	2
1:A:138:TYR:O	1:A:142:VAL:HG12	0.76	1.80	11	1
1:A:16:PHE:CD1	1:A:27:ILE:HD11	0.76	2.15	21	11
1:A:92:PHE:CE2	2:B:12:LEU:HD23	0.76	2.15	26	5
1:A:4:LEU:HG	1:A:69:LEU:HD21	0.76	1.55	21	6
1:A:87:GLU:O	1:A:91:VAL:HG23	0.76	1.80	25	21
1:A:117:THR:HG23	1:A:120:GLU:OE2	0.75	1.82	18	4
1:A:110:THR:HG23	1:A:114:GLU:HG2	0.75	1.56	25	1
1:A:88:ALA:CB	2:B:12:LEU:HD21	0.74	2.12	3	1
1:A:4:LEU:HD22	1:A:69:LEU:CD2	0.74	2.12	4	4
1:A:9:ILE:HD13	1:A:65:PHE:CE2	0.74	2.17	17	16
1:A:130:ILE:HD13	1:A:140:GLU:HB3	0.74	1.58	10	10
1:A:4:LEU:HD21	1:A:9:ILE:CD1	0.74	2.12	17	3
1:A:116:LEU:O	1:A:117:THR:HG23	0.74	1.83	25	1
1:A:6:GLU:O	1:A:10:ALA:HB2	0.73	1.82	7	23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:PHE:CD2	2:B:12:LEU:HD13	0.73	2.17	20	1
1:A:55:VAL:HG22	1:A:67:GLU:HG3	0.73	1.59	5	7
1:A:142:VAL:HG23	1:A:146:THR:OG1	0.73	1.83	11	1
1:A:4:LEU:HD13	1:A:9:ILE:HD12	0.73	1.58	12	4
1:A:88:ALA:HB1	2:B:12:LEU:HG	0.72	1.60	7	4
1:A:100:ILE:O	1:A:125:ILE:HG21	0.72	1.84	10	3
1:A:88:ALA:HB1	2:B:12:LEU:HD11	0.72	1.60	20	1
1:A:5:THR:O	1:A:9:ILE:HD13	0.71	1.85	16	2
1:A:9:ILE:HG23	1:A:65:PHE:CZ	0.71	2.21	22	3
1:A:110:THR:HG23	1:A:115:LYS:HA	0.71	1.61	19	3
1:A:45:GLU:O	1:A:48:LEU:HD11	0.70	1.86	21	11
1:A:28:THR:HG23	1:A:62:THR:HG22	0.70	1.64	25	5
1:A:9:ILE:HD13	1:A:65:PHE:CZ	0.70	2.21	13	21
1:A:125:ILE:HG23	1:A:136:VAL:CG2	0.69	2.17	24	7
1:A:31:GLU:O	1:A:34:THR:HG22	0.69	1.87	11	3
1:A:104:GLU:O	1:A:108:VAL:HG22	0.69	1.87	14	6
1:A:26:THR:HG22	1:A:63:ILE:O	0.69	1.87	11	5
1:A:28:THR:HG23	1:A:62:THR:CG2	0.69	2.18	9	7
1:A:117:THR:HG23	1:A:120:GLU:OE1	0.69	1.88	8	1
1:A:92:PHE:CZ	2:B:12:LEU:HD21	0.69	2.23	14	3
1:A:101:SER:O	1:A:125:ILE:HG21	0.69	1.88	24	3
1:A:100:ILE:HG23	1:A:104:GLU:HB2	0.69	1.62	25	5
1:A:55:VAL:CG1	1:A:63:ILE:HD12	0.68	2.19	2	10
1:A:138:TYR:O	1:A:142:VAL:HG22	0.68	1.87	25	6
1:A:106:ARG:N	1:A:121:VAL:HG21	0.68	2.04	6	1
1:A:100:ILE:HG23	1:A:104:GLU:HG2	0.68	1.64	3	6
1:A:18:LEU:HD13	1:A:18:LEU:C	0.67	2.09	4	1
1:A:117:THR:O	1:A:121:VAL:HG12	0.67	1.89	2	11
2:B:7:LEU:HD22	2:B:7:LEU:O	0.67	1.90	6	1
1:A:4:LEU:N	1:A:4:LEU:HD13	0.66	2.05	16	3
1:A:112:LEU:HD21	2:B:11:GLY:C	0.66	2.10	11	4
1:A:55:VAL:HG11	1:A:63:ILE:HD12	0.66	1.66	11	5
1:A:104:GLU:O	1:A:108:VAL:HG13	0.66	1.91	22	5
1:A:130:ILE:HD13	1:A:140:GLU:HB2	0.66	1.67	14	3
1:A:48:LEU:HD23	1:A:49:GLN:H	0.66	1.50	11	4
2:B:6:ILE:HG22	2:B:6:ILE:O	0.65	1.91	5	11
1:A:9:ILE:HD11	1:A:69:LEU:HD13	0.65	1.68	1	11
1:A:38:SER:O	1:A:39:LEU:HD13	0.65	1.92	16	5
2:B:12:LEU:HD13	2:B:12:LEU:C	0.65	2.11	9	1
1:A:63:ILE:HG21	1:A:68:PHE:CD2	0.65	2.27	12	10
1:A:38:SER:C	1:A:39:LEU:HD12	0.65	2.12	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ASP:OD2	1:A:27:ILE:HD13	0.65	1.91	14	1
1:A:4:LEU:CD2	1:A:9:ILE:HD12	0.65	2.23	15	5
2:B:12:LEU:C	2:B:12:LEU:HD13	0.65	2.12	3	1
1:A:109:MET:HB3	1:A:116:LEU:HD12	0.64	1.70	19	3
2:B:6:ILE:O	2:B:6:ILE:HG22	0.64	1.92	16	6
1:A:18:LEU:C	1:A:18:LEU:HD13	0.64	2.12	13	1
1:A:142:VAL:O	1:A:146:THR:HG22	0.64	1.93	25	1
1:A:4:LEU:CD1	1:A:9:ILE:HD12	0.63	2.24	11	7
1:A:116:LEU:HD13	1:A:121:VAL:HB	0.63	1.71	20	2
1:A:92:PHE:HE2	2:B:12:LEU:HD21	0.63	1.52	2	2
1:A:112:LEU:HD21	2:B:11:GLY:O	0.63	1.94	19	2
1:A:124:MET:HE2	2:B:8:TRP:CD1	0.63	2.29	26	2
1:A:4:LEU:HD22	1:A:4:LEU:O	0.62	1.95	22	1
1:A:35:VAL:CG1	1:A:39:LEU:HD22	0.62	2.25	15	2
1:A:100:ILE:O	1:A:136:VAL:HG12	0.62	1.95	8	8
1:A:48:LEU:HD12	1:A:49:GLN:H	0.61	1.53	14	10
1:A:88:ALA:CB	2:B:12:LEU:HD12	0.61	2.25	25	1
1:A:125:ILE:HG23	1:A:136:VAL:HG21	0.61	1.72	20	5
1:A:105:LEU:HD12	1:A:121:VAL:CG2	0.61	2.26	20	2
1:A:105:LEU:HG	1:A:125:ILE:HD11	0.61	1.69	23	8
1:A:9:ILE:HG23	1:A:65:PHE:CE2	0.61	2.31	22	3
1:A:130:ILE:HD11	1:A:144:MET:SD	0.60	2.36	2	2
1:A:136:VAL:O	1:A:136:VAL:HG13	0.60	1.95	4	8
1:A:55:VAL:HG12	1:A:67:GLU:HG3	0.60	1.72	4	1
1:A:92:PHE:CE1	1:A:105:LEU:HD22	0.60	2.31	16	12
1:A:39:LEU:N	1:A:39:LEU:HD22	0.60	2.11	1	8
1:A:9:ILE:CG1	1:A:69:LEU:HD13	0.60	2.25	26	11
1:A:85:ILE:O	1:A:85:ILE:HG22	0.60	1.96	12	2
1:A:4:LEU:HD23	1:A:9:ILE:HG13	0.60	1.73	25	1
1:A:39:LEU:N	1:A:39:LEU:HD12	0.60	2.12	15	6
1:A:125:ILE:HD12	1:A:136:VAL:CG2	0.60	2.27	5	1
1:A:44:THR:O	1:A:48:LEU:HD11	0.60	1.96	13	3
2:B:8:TRP:O	2:B:12:LEU:HD22	0.60	1.97	2	2
1:A:88:ALA:HB1	2:B:12:LEU:HD21	0.60	1.73	3	1
2:B:15:ILE:HD12	2:B:16:GLN:N	0.60	2.12	3	3
1:A:9:ILE:CD1	1:A:65:PHE:CZ	0.60	2.85	13	23
1:A:55:VAL:HG12	1:A:55:VAL:O	0.60	1.96	4	2
1:A:16:PHE:CD2	1:A:27:ILE:HD11	0.60	2.31	20	1
2:B:12:LEU:CD1	2:B:15:ILE:HD12	0.59	2.26	11	6
1:A:39:LEU:HD22	1:A:39:LEU:N	0.59	2.12	21	7
1:A:20:ASP:OD1	1:A:27:ILE:HD13	0.59	1.97	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:CG	1:A:125:ILE:HD11	0.59	2.27	23	13
1:A:112:LEU:HD11	2:B:15:ILE:HG12	0.59	1.73	9	2
2:B:6:ILE:HG23	2:B:6:ILE:O	0.59	1.98	21	2
1:A:85:ILE:HG22	1:A:88:ALA:HB3	0.59	1.73	21	3
1:A:35:VAL:HG12	1:A:39:LEU:HD22	0.59	1.73	4	1
1:A:92:PHE:CE2	2:B:8:TRP:CE3	0.59	2.91	1	6
1:A:27:ILE:N	1:A:27:ILE:HD13	0.59	2.13	5	9
1:A:14:GLU:O	1:A:18:LEU:HD23	0.59	1.98	22	2
1:A:106:ARG:HG3	1:A:121:VAL:HG11	0.58	1.74	2	2
1:A:92:PHE:CE2	2:B:8:TRP:CZ3	0.58	2.91	14	4
1:A:4:LEU:CG	1:A:69:LEU:HD21	0.58	2.28	21	5
1:A:55:VAL:HG23	1:A:71:MET:CG	0.58	2.28	20	1
1:A:135:GLN:HE21	1:A:136:VAL:HG12	0.58	1.58	23	1
1:A:35:VAL:HG23	1:A:39:LEU:HD23	0.58	1.74	6	1
1:A:9:ILE:HG13	1:A:69:LEU:HD13	0.58	1.74	3	11
1:A:29:THR:HG22	1:A:52:ILE:HG13	0.58	1.76	9	4
1:A:112:LEU:HD21	2:B:11:GLY:CA	0.58	2.27	6	2
1:A:32:LEU:O	1:A:32:LEU:HD13	0.58	1.98	26	2
1:A:112:LEU:HD23	2:B:15:ILE:HG23	0.58	1.75	3	1
1:A:105:LEU:HD21	2:B:8:TRP:CE3	0.58	2.34	15	3
1:A:109:MET:HB3	1:A:116:LEU:HD21	0.58	1.74	15	1
1:A:62:THR:HG23	1:A:63:ILE:N	0.58	2.13	23	1
1:A:141:PHE:CE2	2:B:8:TRP:CH2	0.58	2.92	20	3
1:A:142:VAL:HA	1:A:146:THR:HG23	0.58	1.74	11	2
1:A:107:HIS:O	1:A:110:THR:HG22	0.58	1.98	20	3
1:A:106:ARG:CG	1:A:121:VAL:HG11	0.57	2.29	2	2
1:A:69:LEU:HD12	1:A:69:LEU:O	0.57	1.99	12	1
1:A:92:PHE:CE1	1:A:108:VAL:HG21	0.57	2.33	22	3
1:A:141:PHE:CE1	2:B:9:PHE:CE2	0.57	2.92	20	1
1:A:9:ILE:HD11	1:A:69:LEU:HD23	0.57	1.76	12	3
1:A:55:VAL:CG2	1:A:63:ILE:HD12	0.57	2.30	24	5
1:A:29:THR:HB	1:A:48:LEU:HD22	0.56	1.75	14	1
1:A:32:LEU:HD21	1:A:51:MET:CE	0.56	2.30	14	1
1:A:35:VAL:HA	1:A:39:LEU:HD23	0.56	1.77	22	6
1:A:55:VAL:O	1:A:55:VAL:HG22	0.56	2.00	17	6
1:A:4:LEU:HD21	1:A:69:LEU:CD2	0.56	2.30	7	1
1:A:100:ILE:H	1:A:136:VAL:HG13	0.56	1.59	23	2
1:A:105:LEU:HB3	1:A:121:VAL:HG23	0.56	1.78	10	6
1:A:112:LEU:HD21	2:B:12:LEU:N	0.56	2.16	11	2
2:B:7:LEU:C	2:B:7:LEU:HD13	0.56	2.21	18	8
1:A:4:LEU:HD13	1:A:4:LEU:H	0.56	1.60	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD22	1:A:4:LEU:C	0.56	2.21	25	1
1:A:100:ILE:HG22	1:A:100:ILE:O	0.56	2.01	5	1
1:A:52:ILE:HD13	1:A:63:ILE:HD11	0.56	1.77	19	3
1:A:92:PHE:CZ	2:B:8:TRP:CE3	0.56	2.94	9	3
1:A:35:VAL:HG23	1:A:39:LEU:CD2	0.56	2.31	6	1
1:A:109:MET:HG2	1:A:116:LEU:HD12	0.55	1.77	22	3
1:A:92:PHE:CZ	2:B:12:LEU:CD2	0.55	2.90	1	2
1:A:5:THR:O	1:A:9:ILE:CG2	0.55	2.54	23	23
1:A:4:LEU:HD12	1:A:5:THR:O	0.55	2.00	5	4
1:A:92:PHE:CE1	1:A:105:LEU:CD2	0.55	2.89	7	3
2:B:12:LEU:HD22	2:B:12:LEU:C	0.55	2.21	3	2
1:A:105:LEU:CD2	2:B:8:TRP:CZ3	0.55	2.90	3	2
1:A:4:LEU:C	1:A:4:LEU:HD22	0.55	2.22	3	2
1:A:35:VAL:HG13	1:A:39:LEU:HD23	0.55	1.77	3	1
2:B:6:ILE:O	2:B:6:ILE:HG23	0.55	2.01	12	4
1:A:130:ILE:HD11	1:A:144:MET:CG	0.55	2.31	26	1
1:A:104:GLU:O	1:A:108:VAL:HG23	0.55	2.01	21	6
1:A:55:VAL:HG22	1:A:55:VAL:O	0.55	2.02	13	3
1:A:9:ILE:HG13	1:A:69:LEU:HD22	0.55	1.79	10	2
1:A:69:LEU:HD12	1:A:69:LEU:C	0.54	2.20	12	2
2:B:5:GLN:O	2:B:6:ILE:HG22	0.54	2.02	17	4
1:A:106:ARG:HA	1:A:121:VAL:HG11	0.54	1.78	22	1
1:A:4:LEU:HD23	1:A:9:ILE:HG12	0.54	1.79	22	1
1:A:92:PHE:CZ	2:B:12:LEU:HD11	0.54	2.37	24	1
1:A:112:LEU:HD21	2:B:12:LEU:CA	0.54	2.32	9	1
1:A:92:PHE:CE2	2:B:12:LEU:CD2	0.54	2.90	6	10
1:A:124:MET:HE3	2:B:8:TRP:CD1	0.54	2.38	20	5
1:A:63:ILE:HD13	1:A:63:ILE:N	0.54	2.17	23	2
1:A:117:THR:O	1:A:118:ASP:CB	0.54	2.56	20	2
1:A:125:ILE:CG2	1:A:136:VAL:HG22	0.54	2.32	2	2
1:A:63:ILE:CG2	1:A:68:PHE:CG	0.54	2.91	21	4
1:A:92:PHE:HB3	1:A:100:ILE:HD11	0.54	1.79	25	6
1:A:9:ILE:HD12	1:A:65:PHE:CZ	0.54	2.38	18	5
1:A:16:PHE:O	1:A:27:ILE:HD11	0.53	2.03	6	3
1:A:92:PHE:CE2	2:B:12:LEU:CB	0.53	2.92	3	2
1:A:39:LEU:CD1	1:A:39:LEU:N	0.53	2.71	14	2
1:A:136:VAL:HG13	1:A:136:VAL:O	0.53	2.01	3	2
1:A:29:THR:HB	1:A:48:LEU:HD11	0.53	1.79	7	1
1:A:63:ILE:CG2	1:A:68:PHE:CD2	0.53	2.92	23	4
1:A:124:MET:CE	2:B:8:TRP:CD1	0.53	2.90	9	9
1:A:138:TYR:CE2	1:A:142:VAL:CG1	0.53	2.92	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:N	1:A:39:LEU:CD1	0.53	2.72	4	1
1:A:16:PHE:CZ	1:A:65:PHE:N	0.53	2.76	13	2
1:A:16:PHE:CE1	1:A:27:ILE:HD11	0.53	2.38	21	2
1:A:92:PHE:CD1	1:A:108:VAL:HG21	0.53	2.39	22	2
2:B:7:LEU:HD12	2:B:7:LEU:C	0.53	2.23	5	2
1:A:13:LYS:CG	1:A:65:PHE:CE1	0.53	2.91	6	5
1:A:27:ILE:HD13	1:A:27:ILE:N	0.53	2.18	7	4
1:A:87:GLU:O	1:A:91:VAL:HB	0.53	2.04	24	1
1:A:4:LEU:HD22	1:A:5:THR:O	0.53	2.03	1	3
1:A:13:LYS:CG	1:A:65:PHE:CD1	0.53	2.92	15	5
1:A:101:SER:O	1:A:102:ALA:HB2	0.53	2.04	21	9
1:A:29:THR:HB	1:A:48:LEU:HD13	0.53	1.79	14	2
1:A:141:PHE:CD1	2:B:9:PHE:CE2	0.53	2.97	20	1
1:A:92:PHE:O	1:A:104:GLU:CB	0.52	2.57	19	15
1:A:9:ILE:HD11	1:A:69:LEU:CD2	0.52	2.35	10	3
1:A:142:VAL:HG12	1:A:143:GLN:N	0.52	2.19	21	1
1:A:69:LEU:C	1:A:69:LEU:HD12	0.52	2.25	6	2
1:A:105:LEU:HD12	1:A:121:VAL:HG22	0.52	1.81	8	2
1:A:4:LEU:HD22	1:A:5:THR:N	0.52	2.19	18	2
1:A:100:ILE:HG21	1:A:105:LEU:HD21	0.52	1.79	4	7
1:A:100:ILE:O	1:A:136:VAL:HG23	0.52	2.05	9	12
1:A:101:SER:N	1:A:135:GLN:NE2	0.52	2.58	3	2
2:B:12:LEU:HD13	2:B:15:ILE:CD1	0.52	2.32	25	6
1:A:138:TYR:CE2	1:A:142:VAL:HG13	0.52	2.40	9	1
2:B:7:LEU:O	2:B:7:LEU:HD12	0.52	2.05	5	1
1:A:85:ILE:HD12	1:A:138:TYR:OH	0.52	2.04	9	1
1:A:92:PHE:CE1	1:A:108:VAL:CG2	0.52	2.93	17	1
1:A:13:LYS:HA	1:A:16:PHE:HB3	0.52	1.82	17	9
1:A:4:LEU:HD13	1:A:5:THR:O	0.51	2.04	14	1
1:A:125:ILE:HG23	1:A:136:VAL:HG22	0.51	1.83	12	6
1:A:27:ILE:CG2	1:A:32:LEU:HD23	0.51	2.35	15	1
2:B:15:ILE:HD12	2:B:15:ILE:C	0.51	2.26	20	1
1:A:9:ILE:HG23	1:A:10:ALA:N	0.51	2.20	24	17
2:B:6:ILE:CG2	2:B:6:ILE:O	0.51	2.58	22	12
1:A:85:ILE:HG22	1:A:85:ILE:O	0.51	2.05	8	1
1:A:9:ILE:CD1	1:A:69:LEU:CD2	0.51	2.89	12	4
1:A:93:ASP:O	1:A:95:ASP:N	0.51	2.43	1	23
1:A:106:ARG:CA	1:A:121:VAL:HG11	0.51	2.35	22	1
1:A:55:VAL:CG1	1:A:63:ILE:CD1	0.51	2.89	7	9
1:A:55:VAL:O	1:A:55:VAL:HG12	0.51	2.06	12	3
1:A:142:VAL:CG2	1:A:146:THR:OG1	0.51	2.59	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:THR:HB	1:A:62:THR:HG22	0.51	1.83	23	1
1:A:100:ILE:CG2	1:A:105:LEU:CD2	0.51	2.89	11	18
1:A:45:GLU:O	1:A:48:LEU:HD21	0.51	2.06	15	3
1:A:55:VAL:CG2	1:A:63:ILE:CD1	0.50	2.90	6	6
1:A:85:ILE:HD12	1:A:138:TYR:HH	0.50	1.66	9	1
1:A:9:ILE:CG1	1:A:69:LEU:HD22	0.50	2.36	10	2
2:B:15:ILE:O	2:B:18:GLN:N	0.50	2.44	22	11
1:A:106:ARG:O	1:A:110:THR:HG22	0.50	2.06	11	7
1:A:26:THR:C	1:A:27:ILE:HD13	0.50	2.27	5	1
1:A:109:MET:CG	1:A:116:LEU:HD12	0.50	2.36	7	1
1:A:124:MET:HE1	2:B:8:TRP:CD1	0.50	2.42	17	1
1:A:125:ILE:HD12	1:A:136:VAL:HG21	0.49	1.84	5	2
1:A:110:THR:HG23	1:A:114:GLU:HG3	0.49	1.83	25	1
1:A:32:LEU:O	1:A:35:VAL:HG12	0.49	2.07	14	3
1:A:103:ALA:O	1:A:106:ARG:HG3	0.49	2.07	20	2
1:A:35:VAL:CG2	1:A:39:LEU:HD22	0.49	2.37	14	1
1:A:35:VAL:HG13	1:A:39:LEU:HD13	0.49	1.84	25	2
2:B:6:ILE:N	2:B:6:ILE:CD1	0.49	2.75	22	1
1:A:9:ILE:CG2	1:A:10:ALA:N	0.49	2.76	20	17
1:A:5:THR:O	1:A:9:ILE:HG22	0.49	2.07	9	14
1:A:35:VAL:CG2	1:A:39:LEU:HD23	0.49	2.37	6	1
1:A:106:ARG:O	1:A:110:THR:CB	0.49	2.61	25	12
1:A:125:ILE:CG2	1:A:136:VAL:CG2	0.49	2.91	20	4
1:A:28:THR:CG2	1:A:62:THR:CG2	0.49	2.90	8	2
1:A:105:LEU:HB3	1:A:121:VAL:HG22	0.49	1.84	23	1
1:A:100:ILE:O	1:A:136:VAL:CG2	0.49	2.61	20	14
1:A:7:GLU:O	1:A:10:ALA:HB3	0.49	2.06	8	3
1:A:104:GLU:O	1:A:108:VAL:N	0.49	2.45	20	11
1:A:112:LEU:HD11	2:B:15:ILE:CG1	0.49	2.38	21	2
1:A:92:PHE:O	1:A:104:GLU:CG	0.49	2.61	2	22
1:A:108:VAL:CG2	1:A:109:MET:N	0.49	2.75	19	5
1:A:39:LEU:HD12	1:A:39:LEU:N	0.49	2.23	7	1
1:A:16:PHE:CE2	1:A:25:GLY:O	0.49	2.66	3	1
1:A:55:VAL:HG23	1:A:71:MET:HB2	0.49	1.84	9	2
1:A:65:PHE:N	1:A:66:PRO:CD	0.49	2.76	23	9
1:A:61:GLY:O	1:A:62:THR:HG23	0.49	2.08	16	2
1:A:39:LEU:CD2	1:A:39:LEU:N	0.49	2.75	18	7
1:A:106:ARG:HG2	1:A:107:HIS:N	0.49	2.23	5	1
1:A:35:VAL:HG13	1:A:39:LEU:HD22	0.49	1.84	15	1
2:B:7:LEU:HD13	2:B:7:LEU:C	0.49	2.28	19	1
1:A:15:ALA:O	1:A:19:PHE:N	0.48	2.43	2	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:PHE:CZ	1:A:25:GLY:O	0.48	2.66	24	4
1:A:109:MET:CE	1:A:112:LEU:HD23	0.48	2.38	6	1
1:A:69:LEU:O	1:A:73:ALA:HB2	0.48	2.09	26	1
1:A:114:GLU:CG	1:A:116:LEU:CD2	0.48	2.91	1	1
1:A:144:MET:CE	2:B:9:PHE:CZ	0.48	2.96	3	2
2:B:7:LEU:C	2:B:7:LEU:HD12	0.48	2.28	9	2
1:A:48:LEU:N	1:A:48:LEU:HD23	0.48	2.23	15	2
1:A:105:LEU:CB	1:A:121:VAL:CG2	0.48	2.91	19	5
1:A:55:VAL:HG21	1:A:63:ILE:HD12	0.48	1.85	26	2
1:A:88:ALA:HB1	2:B:12:LEU:HD12	0.48	1.84	25	1
1:A:142:VAL:HG23	1:A:143:GLN:N	0.48	2.24	1	16
1:A:65:PHE:N	1:A:66:PRO:HD2	0.48	2.24	14	16
1:A:55:VAL:HG13	1:A:71:MET:HG3	0.48	1.85	4	1
1:A:116:LEU:N	1:A:116:LEU:HD23	0.48	2.23	11	1
1:A:42:ASN:CB	1:A:43:PRO:CD	0.48	2.92	25	3
1:A:85:ILE:HG21	1:A:138:TYR:OH	0.48	2.09	13	2
1:A:45:GLU:O	1:A:48:LEU:CD2	0.48	2.62	5	7
1:A:36:MET:O	1:A:41:GLN:N	0.48	2.47	25	10
1:A:55:VAL:HG13	1:A:63:ILE:HD12	0.48	1.85	20	1
1:A:18:LEU:C	1:A:18:LEU:CD1	0.47	2.81	4	2
1:A:13:LYS:HG3	1:A:65:PHE:CD1	0.47	2.44	5	2
1:A:4:LEU:HD21	1:A:69:LEU:HD21	0.47	1.86	7	1
1:A:99:TYR:CB	1:A:135:GLN:NE2	0.47	2.77	16	3
1:A:4:LEU:HD11	1:A:9:ILE:HG13	0.47	1.84	21	1
1:A:63:ILE:CG2	1:A:68:PHE:CD1	0.47	2.97	4	2
1:A:6:GLU:O	1:A:10:ALA:CB	0.47	2.62	15	18
1:A:39:LEU:N	1:A:39:LEU:CD2	0.47	2.76	12	3
1:A:123:GLU:HA	1:A:126:ARG:HB2	0.47	1.85	7	2
1:A:51:MET:O	1:A:55:VAL:HG12	0.47	2.10	14	1
1:A:144:MET:CE	2:B:9:PHE:CE1	0.47	2.98	20	1
1:A:105:LEU:O	1:A:109:MET:CB	0.47	2.63	22	17
1:A:44:THR:OG1	1:A:47:GLU:CB	0.47	2.63	13	13
1:A:116:LEU:HD13	1:A:124:MET:SD	0.47	2.50	3	1
1:A:94:LYS:CB	1:A:104:GLU:CG	0.47	2.93	5	3
1:A:9:ILE:CD1	1:A:69:LEU:HD23	0.47	2.39	9	2
1:A:89:PHE:HA	1:A:92:PHE:CE1	0.47	2.45	19	1
1:A:55:VAL:HG23	1:A:71:MET:HG3	0.47	1.87	20	1
1:A:145:MET:HG3	2:B:9:PHE:CE2	0.47	2.45	22	1
1:A:63:ILE:CD1	1:A:63:ILE:N	0.47	2.78	5	1
1:A:102:ALA:HB1	1:A:121:VAL:HG13	0.47	1.86	19	2
1:A:27:ILE:HG22	1:A:32:LEU:HD23	0.47	1.86	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ARG:CZ	1:A:118:ASP:N	0.47	2.77	17	1
1:A:92:PHE:CE1	2:B:12:LEU:HD11	0.47	2.45	24	1
1:A:9:ILE:O	1:A:12:PHE:N	0.47	2.48	20	21
1:A:6:GLU:HA	1:A:9:ILE:HG22	0.47	1.87	7	3
2:B:12:LEU:HA	2:B:15:ILE:HD12	0.47	1.86	7	2
2:B:6:ILE:O	2:B:6:ILE:CG2	0.47	2.62	19	5
1:A:48:LEU:O	1:A:52:ILE:HG12	0.47	2.10	14	1
1:A:107:HIS:HA	1:A:110:THR:HG22	0.47	1.86	9	4
1:A:92:PHE:HB3	1:A:100:ILE:CD1	0.47	2.40	24	1
1:A:130:ILE:H	1:A:130:ILE:HD12	0.46	1.70	26	2
1:A:33:GLY:CA	1:A:48:LEU:HD23	0.46	2.40	14	1
1:A:28:THR:CG2	1:A:62:THR:HG22	0.46	2.39	12	4
2:B:4:GLY:O	2:B:8:TRP:CD1	0.46	2.69	15	1
1:A:47:GLU:O	1:A:50:ASP:N	0.46	2.49	15	17
1:A:4:LEU:N	1:A:4:LEU:CD1	0.46	2.78	3	1
1:A:32:LEU:C	1:A:32:LEU:HD13	0.46	2.30	26	1
1:A:13:LYS:HG2	1:A:65:PHE:CD1	0.46	2.45	15	2
1:A:145:MET:CG	2:B:9:PHE:CE2	0.46	2.97	22	1
2:B:15:ILE:O	2:B:17:THR:N	0.46	2.48	16	3
1:A:108:VAL:HG23	1:A:109:MET:N	0.46	2.25	26	2
1:A:69:LEU:O	1:A:69:LEU:HD12	0.46	2.11	23	1
1:A:114:GLU:CG	1:A:116:LEU:HD21	0.46	2.40	1	1
1:A:4:LEU:CD2	1:A:69:LEU:HD21	0.46	2.41	7	2
2:B:6:ILE:HG22	2:B:10:ARG:HD2	0.46	1.88	1	1
1:A:142:VAL:O	1:A:146:THR:N	0.46	2.49	7	23
1:A:11:GLU:O	1:A:14:GLU:CG	0.46	2.63	26	7
1:A:125:ILE:HG23	1:A:136:VAL:HB	0.46	1.88	23	2
1:A:99:TYR:CE1	1:A:137:ASN:HB3	0.46	2.46	3	3
1:A:65:PHE:O	1:A:69:LEU:CB	0.46	2.64	6	10
1:A:92:PHE:HD2	2:B:12:LEU:HD21	0.46	1.66	5	1
1:A:15:ALA:O	1:A:19:PHE:CB	0.46	2.64	24	6
1:A:15:ALA:O	1:A:19:PHE:HB2	0.46	2.11	2	17
1:A:35:VAL:O	1:A:39:LEU:CD2	0.46	2.64	2	1
1:A:137:ASN:ND2	1:A:139:GLU:CG	0.46	2.79	4	2
1:A:101:SER:CB	1:A:135:GLN:NE2	0.45	2.79	4	1
1:A:100:ILE:O	1:A:135:GLN:NE2	0.45	2.48	21	2
1:A:106:ARG:O	1:A:110:THR:CG2	0.45	2.65	2	10
1:A:100:ILE:HB	1:A:136:VAL:HG11	0.45	1.88	10	2
1:A:124:MET:HE1	2:B:8:TRP:CG	0.45	2.46	11	2
1:A:35:VAL:HG22	1:A:39:LEU:HD22	0.45	1.88	14	1
1:A:29:THR:HB	1:A:48:LEU:CD1	0.45	2.41	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ARG:C	1:A:106:ARG:CD	0.45	2.84	18	2
1:A:104:GLU:O	1:A:108:VAL:CG2	0.45	2.63	11	6
1:A:55:VAL:CG2	1:A:55:VAL:O	0.45	2.64	14	1
1:A:100:ILE:N	1:A:135:GLN:OE1	0.45	2.50	3	1
1:A:40:GLY:O	1:A:42:ASN:N	0.45	2.50	17	8
1:A:102:ALA:O	1:A:121:VAL:HG21	0.45	2.12	19	1
1:A:124:MET:CE	2:B:8:TRP:CG	0.45	2.99	2	3
1:A:45:GLU:O	1:A:48:LEU:CD1	0.45	2.64	3	13
1:A:94:LYS:CB	1:A:104:GLU:HB3	0.45	2.42	9	6
1:A:9:ILE:HG12	1:A:65:PHE:CZ	0.45	2.46	17	9
1:A:112:LEU:CD1	2:B:15:ILE:CG1	0.45	2.94	10	1
1:A:122:ASP:OD1	1:A:126:ARG:NE	0.45	2.50	12	1
1:A:116:LEU:HD22	1:A:121:VAL:CG2	0.45	2.33	15	1
1:A:142:VAL:HG13	1:A:146:THR:HG21	0.45	1.89	21	1
1:A:99:TYR:CE1	1:A:137:ASN:OD1	0.45	2.70	22	1
1:A:46:ALA:O	1:A:49:GLN:N	0.45	2.50	8	7
2:B:7:LEU:O	2:B:7:LEU:HD13	0.45	2.12	4	1
1:A:4:LEU:HD23	1:A:5:THR:O	0.45	2.12	17	2
1:A:4:LEU:C	1:A:4:LEU:HD12	0.45	2.32	12	2
1:A:116:LEU:CD1	1:A:116:LEU:O	0.45	2.64	15	2
1:A:4:LEU:O	1:A:5:THR:O	0.45	2.34	25	1
1:A:135:GLN:NE2	1:A:136:VAL:HG12	0.45	2.26	23	1
1:A:85:ILE:O	1:A:88:ALA:N	0.45	2.50	26	2
1:A:22:ASP:OD1	1:A:23:GLY:N	0.45	2.50	12	6
1:A:4:LEU:CD2	1:A:4:LEU:O	0.45	2.65	23	2
1:A:117:THR:OG1	1:A:120:GLU:CG	0.45	2.65	25	1
1:A:4:LEU:HD13	1:A:4:LEU:N	0.45	2.26	25	1
1:A:131:ASP:OD1	1:A:132:GLY:N	0.45	2.49	24	9
1:A:136:VAL:O	1:A:136:VAL:CG1	0.45	2.65	3	1
1:A:105:LEU:O	1:A:109:MET:N	0.45	2.46	24	6
1:A:122:ASP:O	1:A:126:ARG:CD	0.45	2.64	12	2
1:A:112:LEU:HD11	2:B:15:ILE:HG13	0.45	1.89	11	3
1:A:4:LEU:HD23	1:A:9:ILE:HD12	0.44	1.89	1	1
1:A:95:ASP:OD1	1:A:96:GLY:N	0.44	2.50	11	4
1:A:27:ILE:O	1:A:63:ILE:CG1	0.44	2.65	15	10
1:A:22:ASP:OD1	1:A:24:ASP:N	0.44	2.51	4	4
1:A:16:PHE:CE1	1:A:25:GLY:O	0.44	2.71	14	2
1:A:35:VAL:HA	1:A:39:LEU:HD13	0.44	1.88	15	1
1:A:112:LEU:CD2	2:B:15:ILE:HG12	0.44	2.42	20	1
1:A:54:GLU:CA	1:A:54:GLU:OE1	0.44	2.65	6	1
1:A:48:LEU:HD23	1:A:48:LEU:N	0.44	2.27	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:14:ARG:O	2:B:18:GLN:N	0.44	2.49	13	1
2:B:12:LEU:CD1	2:B:12:LEU:O	0.44	2.66	17	1
1:A:95:ASP:OD2	1:A:97:ASN:ND2	0.44	2.50	23	1
1:A:106:ARG:O	1:A:110:THR:HB	0.44	2.11	25	2
1:A:104:GLU:O	1:A:108:VAL:CB	0.44	2.65	20	4
1:A:64:ASP:N	1:A:67:GLU:OE1	0.44	2.50	17	3
1:A:92:PHE:CD1	1:A:100:ILE:CD1	0.44	2.88	19	1
1:A:106:ARG:HB2	1:A:121:VAL:HG11	0.44	1.88	22	1
1:A:14:GLU:O	1:A:18:LEU:CD2	0.44	2.65	22	1
1:A:102:ALA:O	1:A:106:ARG:N	0.44	2.50	5	3
1:A:32:LEU:HA	1:A:35:VAL:CG2	0.44	2.42	16	1
1:A:4:LEU:HD11	1:A:9:ILE:CG1	0.44	2.42	21	1
1:A:89:PHE:CE2	1:A:90:ARG:NE	0.44	2.85	22	1
1:A:55:VAL:O	1:A:57:ALA:N	0.44	2.49	5	7
1:A:85:ILE:O	1:A:89:PHE:CB	0.44	2.65	8	2
1:A:4:LEU:HD11	1:A:69:LEU:HG	0.44	1.88	9	1
1:A:138:TYR:CE1	1:A:141:PHE:CD2	0.44	3.05	24	1
1:A:44:THR:O	1:A:47:GLU:CG	0.44	2.66	22	4
1:A:38:SER:OG	1:A:39:LEU:HD22	0.44	2.13	19	1
2:B:12:LEU:O	2:B:12:LEU:CD1	0.44	2.66	26	1
2:B:12:LEU:O	2:B:12:LEU:HD12	0.44	2.13	26	1
1:A:85:ILE:CG2	1:A:138:TYR:OH	0.44	2.66	25	4
1:A:10:ALA:O	1:A:13:LYS:CB	0.44	2.66	9	9
1:A:40:GLY:O	1:A:41:GLN:C	0.44	2.56	3	8
1:A:37:ARG:O	1:A:41:GLN:CG	0.44	2.66	2	1
1:A:118:ASP:HA	1:A:121:VAL:HG12	0.44	1.89	21	3
1:A:117:THR:O	1:A:121:VAL:CG1	0.44	2.66	16	5
1:A:130:ILE:HG22	1:A:131:ASP:N	0.44	2.27	10	1
1:A:115:LYS:O	1:A:115:LYS:CG	0.44	2.65	16	5
1:A:35:VAL:O	1:A:39:LEU:HD23	0.43	2.13	2	1
1:A:105:LEU:HB3	1:A:121:VAL:CG2	0.43	2.43	6	4
1:A:42:ASN:N	1:A:43:PRO:HD2	0.43	2.28	14	3
1:A:144:MET:CG	2:B:9:PHE:CZ	0.43	3.01	6	1
1:A:64:ASP:N	1:A:67:GLU:OE2	0.43	2.51	10	1
1:A:95:ASP:OD1	1:A:95:ASP:N	0.43	2.50	19	2
1:A:67:GLU:O	1:A:71:MET:CB	0.43	2.67	8	1
1:A:70:THR:O	1:A:74:ARG:N	0.43	2.51	22	2
1:A:20:ASP:O	1:A:31:GLU:CG	0.43	2.65	16	1
1:A:4:LEU:O	1:A:4:LEU:HD22	0.43	2.13	16	1
1:A:38:SER:OG	1:A:39:LEU:CD2	0.43	2.66	19	1
1:A:35:VAL:CG1	1:A:39:LEU:HD23	0.43	2.44	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:GLY:O	1:A:62:THR:CG2	0.43	2.67	16	3
1:A:32:LEU:HD13	1:A:32:LEU:O	0.43	2.13	15	2
1:A:95:ASP:OD1	1:A:97:ASN:ND2	0.43	2.51	6	1
1:A:142:VAL:O	1:A:146:THR:OG1	0.43	2.34	11	1
1:A:137:ASN:O	1:A:139:GLU:N	0.43	2.51	13	3
1:A:16:PHE:CE2	1:A:27:ILE:HD11	0.43	2.48	20	1
1:A:137:ASN:ND2	1:A:139:GLU:HG3	0.43	2.28	4	1
1:A:13:LYS:HG3	1:A:65:PHE:CG	0.43	2.48	5	1
1:A:104:GLU:O	1:A:108:VAL:CG1	0.43	2.65	11	2
1:A:16:PHE:CE1	1:A:27:ILE:HG12	0.43	2.47	19	1
1:A:133:ASP:OD2	1:A:137:ASN:ND2	0.43	2.51	21	1
1:A:63:ILE:N	1:A:63:ILE:CD1	0.43	2.80	23	1
1:A:87:GLU:O	1:A:91:VAL:N	0.43	2.46	24	1
1:A:20:ASP:OD1	1:A:31:GLU:CB	0.43	2.67	26	1
1:A:88:ALA:HB1	2:B:12:LEU:CD1	0.43	2.44	1	1
1:A:13:LYS:CB	1:A:65:PHE:CE1	0.43	3.00	6	3
2:B:7:LEU:HD22	2:B:7:LEU:C	0.43	2.33	6	1
1:A:112:LEU:HD21	2:B:12:LEU:HA	0.43	1.88	9	1
1:A:52:ILE:HD13	1:A:63:ILE:CD1	0.43	2.44	10	1
1:A:9:ILE:HG13	1:A:69:LEU:CD2	0.43	2.43	10	1
1:A:88:ALA:HA	1:A:91:VAL:CG1	0.43	2.43	24	1
1:A:64:ASP:N	1:A:64:ASP:OD1	0.43	2.51	25	1
1:A:136:VAL:CG1	1:A:136:VAL:O	0.43	2.65	4	6
1:A:85:ILE:O	1:A:89:PHE:N	0.43	2.48	6	2
1:A:33:GLY:O	1:A:37:ARG:N	0.43	2.52	8	2
1:A:138:TYR:CD2	1:A:142:VAL:HG13	0.43	2.49	9	1
1:A:138:TYR:O	1:A:141:PHE:N	0.43	2.51	11	3
1:A:18:LEU:O	1:A:21:LYS:N	0.43	2.50	21	4
1:A:103:ALA:O	1:A:106:ARG:HG2	0.43	2.13	14	1
1:A:109:MET:HE1	1:A:112:LEU:HD23	0.43	1.91	16	1
1:A:54:GLU:N	1:A:54:GLU:OE1	0.43	2.52	19	1
1:A:137:ASN:N	1:A:140:GLU:OE2	0.43	2.50	25	1
1:A:124:MET:O	1:A:128:ALA:CB	0.43	2.67	1	1
1:A:50:ASP:O	1:A:54:GLU:CG	0.43	2.67	22	6
1:A:13:LYS:O	1:A:17:SER:N	0.43	2.52	26	5
1:A:65:PHE:CZ	1:A:69:LEU:HD22	0.43	2.49	8	1
1:A:32:LEU:O	1:A:35:VAL:CG2	0.43	2.67	16	1
1:A:69:LEU:O	1:A:73:ALA:CB	0.43	2.67	26	1
1:A:9:ILE:CD1	1:A:69:LEU:CD1	0.43	2.95	1	4
1:A:120:GLU:O	1:A:124:MET:CB	0.43	2.66	9	1
1:A:28:THR:N	1:A:31:GLU:OE2	0.43	2.51	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASN:OD1	1:A:60:ASN:N	0.43	2.52	14	1
1:A:5:THR:O	1:A:9:ILE:CD1	0.43	2.67	22	1
2:B:6:ILE:O	2:B:10:ARG:CG	0.43	2.67	18	2
1:A:58:ASP:OD1	1:A:59:GLY:N	0.43	2.52	19	9
1:A:112:LEU:CD2	2:B:11:GLY:CA	0.43	2.97	6	1
1:A:64:ASP:OD1	1:A:65:PHE:N	0.43	2.52	16	1
1:A:122:ASP:OD1	1:A:123:GLU:N	0.43	2.52	18	1
1:A:20:ASP:OD1	1:A:22:ASP:CB	0.43	2.67	18	2
1:A:86:ARG:O	1:A:90:ARG:CG	0.43	2.66	19	1
1:A:115:LYS:O	1:A:117:THR:N	0.43	2.52	4	1
1:A:137:ASN:OD1	1:A:138:TYR:N	0.43	2.52	10	4
1:A:29:THR:HB	1:A:48:LEU:CG	0.43	2.44	7	1
1:A:85:ILE:O	1:A:85:ILE:CG2	0.43	2.67	12	1
1:A:131:ASP:OD2	1:A:137:ASN:ND2	0.43	2.52	15	3
1:A:55:VAL:HG22	1:A:63:ILE:CD1	0.43	2.44	15	1
1:A:88:ALA:O	1:A:92:PHE:CD2	0.43	2.72	19	1
1:A:85:ILE:CG2	1:A:88:ALA:HB3	0.43	2.43	21	2
1:A:105:LEU:HD11	2:B:8:TRP:CE3	0.43	2.49	22	1
1:A:128:ALA:O	1:A:130:ILE:N	0.42	2.51	1	6
1:A:94:LYS:CB	1:A:104:GLU:HG2	0.42	2.44	15	5
1:A:94:LYS:HB2	1:A:104:GLU:CB	0.42	2.44	11	1
1:A:12:PHE:CE2	1:A:69:LEU:HA	0.42	2.49	11	2
1:A:44:THR:O	1:A:48:LEU:CD1	0.42	2.67	26	3
1:A:47:GLU:OE1	1:A:48:LEU:N	0.42	2.52	20	1
1:A:62:THR:CG2	1:A:63:ILE:N	0.42	2.80	23	1
1:A:121:VAL:CG1	1:A:122:ASP:N	0.42	2.82	3	1
1:A:74:ARG:CG	1:A:74:ARG:O	0.42	2.67	24	3
2:B:8:TRP:CD1	2:B:9:PHE:CD1	0.42	3.07	15	1
1:A:10:ALA:O	1:A:14:GLU:N	0.42	2.51	22	4
1:A:67:GLU:CG	1:A:68:PHE:N	0.42	2.82	21	2
1:A:116:LEU:HD22	1:A:116:LEU:N	0.42	2.29	1	1
1:A:13:LYS:HB2	1:A:65:PHE:CE1	0.42	2.49	18	6
1:A:39:LEU:O	1:A:41:GLN:CG	0.42	2.68	3	2
2:B:11:GLY:O	2:B:14:ARG:N	0.42	2.52	9	2
1:A:27:ILE:O	1:A:63:ILE:HG12	0.42	2.14	7	4
1:A:144:MET:HG3	2:B:9:PHE:CZ	0.42	2.50	10	2
1:A:104:GLU:O	1:A:108:VAL:HB	0.42	2.14	20	2
1:A:55:VAL:CG2	1:A:67:GLU:O	0.42	2.67	13	1
1:A:22:ASP:OD1	1:A:24:ASP:CB	0.42	2.67	17	1
1:A:28:THR:HA	1:A:52:ILE:HD12	0.42	1.90	18	2
1:A:44:THR:O	1:A:48:LEU:CG	0.42	2.66	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASN:N	1:A:60:ASN:OD1	0.42	2.53	23	2
1:A:4:LEU:CD2	1:A:69:LEU:CD2	0.42	2.96	7	1
1:A:4:LEU:C	1:A:4:LEU:HD23	0.42	2.35	9	1
1:A:44:THR:OG1	1:A:47:GLU:HB2	0.42	2.14	10	5
1:A:105:LEU:HB2	1:A:121:VAL:CG2	0.42	2.44	10	1
1:A:29:THR:O	1:A:48:LEU:HD12	0.42	2.14	19	1
1:A:93:ASP:O	1:A:96:GLY:N	0.42	2.52	22	1
1:A:36:MET:O	1:A:40:GLY:CA	0.42	2.67	2	1
1:A:137:ASN:ND2	1:A:140:GLU:OE1	0.42	2.52	4	1
1:A:137:ASN:N	1:A:140:GLU:OE1	0.42	2.52	9	3
1:A:144:MET:HG2	2:B:9:PHE:CZ	0.42	2.49	6	1
1:A:69:LEU:O	1:A:73:ALA:N	0.42	2.52	17	2
1:A:92:PHE:CZ	1:A:105:LEU:HD22	0.42	2.48	8	3
1:A:99:TYR:OH	1:A:137:ASN:ND2	0.42	2.52	8	1
1:A:28:THR:O	1:A:32:LEU:CB	0.42	2.68	9	1
1:A:100:ILE:O	1:A:136:VAL:CG1	0.42	2.68	11	3
1:A:27:ILE:N	1:A:27:ILE:CD1	0.42	2.80	21	1
1:A:131:ASP:OD1	1:A:131:ASP:N	0.42	2.52	22	2
1:A:28:THR:HG23	1:A:62:THR:CB	0.42	2.45	9	1
1:A:70:THR:O	1:A:74:ARG:CB	0.42	2.67	12	1
1:A:145:MET:HG2	2:B:9:PHE:CD2	0.42	2.49	22	1
1:A:4:LEU:CD2	1:A:5:THR:O	0.42	2.67	3	2
1:A:131:ASP:N	1:A:131:ASP:OD1	0.42	2.53	10	3
1:A:45:GLU:O	1:A:48:LEU:CG	0.42	2.67	4	2
1:A:47:GLU:O	1:A:51:MET:N	0.42	2.50	20	7
1:A:9:ILE:CG1	1:A:65:PHE:CZ	0.42	3.02	17	3
1:A:137:ASN:ND2	1:A:139:GLU:HG2	0.42	2.30	15	4
1:A:16:PHE:CE2	1:A:27:ILE:HG12	0.42	2.50	15	1
2:B:5:GLN:HB2	2:B:9:PHE:CE2	0.42	2.49	15	1
1:A:108:VAL:O	1:A:112:LEU:N	0.42	2.51	26	2
1:A:46:ALA:O	1:A:50:ASP:N	0.42	2.52	2	2
1:A:89:PHE:C	1:A:89:PHE:CD1	0.42	2.93	3	1
1:A:101:SER:O	1:A:103:ALA:N	0.42	2.53	5	1
1:A:128:ALA:O	1:A:130:ILE:CD1	0.42	2.67	5	2
1:A:63:ILE:HG21	1:A:68:PHE:CG	0.42	2.49	11	2
1:A:99:TYR:HB3	1:A:135:GLN:NE2	0.42	2.29	16	1
2:B:12:LEU:HD13	2:B:15:ILE:CG1	0.42	2.45	17	1
1:A:39:LEU:HB2	1:A:41:GLN:CG	0.42	2.45	14	5
1:A:137:ASN:O	1:A:140:GLU:CG	0.42	2.68	8	1
1:A:28:THR:HG23	1:A:62:THR:HB	0.42	1.91	8	2
1:A:115:LYS:CG	1:A:115:LYS:O	0.42	2.68	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:O	1:A:116:LEU:CD1	0.42	2.67	25	1
1:A:109:MET:HG3	1:A:116:LEU:CD2	0.42	2.45	1	1
1:A:6:GLU:O	1:A:10:ALA:N	0.42	2.53	16	2
1:A:44:THR:OG1	1:A:47:GLU:N	0.42	2.51	9	1
1:A:105:LEU:CB	1:A:121:VAL:HG23	0.42	2.42	10	1
1:A:87:GLU:O	1:A:91:VAL:CG2	0.42	2.66	10	2
1:A:101:SER:O	1:A:102:ALA:CB	0.42	2.68	21	2
1:A:9:ILE:O	1:A:12:PHE:CB	0.42	2.67	18	1
1:A:33:GLY:O	1:A:36:MET:N	0.42	2.53	18	1
1:A:4:LEU:HD11	1:A:9:ILE:CD1	0.42	2.26	19	1
2:B:6:ILE:O	2:B:10:ARG:CD	0.41	2.68	1	1
1:A:66:PRO:O	1:A:69:LEU:CB	0.41	2.68	9	1
1:A:100:ILE:CG2	1:A:105:LEU:HG	0.41	2.45	10	1
1:A:109:MET:CG	1:A:114:GLU:OE2	0.41	2.68	16	1
1:A:114:GLU:N	1:A:114:GLU:OE1	0.41	2.53	19	1
1:A:61:GLY:O	1:A:62:THR:HG22	0.41	2.15	23	1
1:A:109:MET:CG	1:A:116:LEU:HD23	0.41	2.46	1	1
1:A:109:MET:HG3	1:A:116:LEU:HD23	0.41	1.92	1	1
1:A:55:VAL:O	1:A:67:GLU:CG	0.41	2.68	2	1
1:A:99:TYR:CE1	1:A:137:ASN:HA	0.41	2.49	5	1
1:A:93:ASP:O	1:A:95:ASP:OD1	0.41	2.38	8	4
1:A:95:ASP:N	1:A:95:ASP:OD1	0.41	2.54	8	1
1:A:99:TYR:CD1	1:A:137:ASN:HA	0.41	2.51	13	3
1:A:50:ASP:O	1:A:54:GLU:CB	0.41	2.69	15	1
2:B:7:LEU:HD13	2:B:8:TRP:N	0.41	2.30	18	1
1:A:88:ALA:HA	1:A:91:VAL:HG12	0.41	1.93	24	1
1:A:112:LEU:HD11	2:B:15:ILE:HG23	0.41	1.92	6	1
1:A:116:LEU:HD13	1:A:116:LEU:O	0.41	2.15	15	1
1:A:105:LEU:CD1	1:A:121:VAL:CG2	0.41	2.98	20	1
1:A:142:VAL:CG1	1:A:143:GLN:N	0.41	2.83	21	1
1:A:4:LEU:CD2	1:A:4:LEU:C	0.41	2.88	25	1
1:A:4:LEU:HD23	1:A:9:ILE:CG1	0.41	2.43	25	1
2:B:5:GLN:O	2:B:6:ILE:HB	0.41	2.15	25	1
1:A:88:ALA:HB2	2:B:12:LEU:HD21	0.41	1.89	3	1
1:A:42:ASN:N	1:A:43:PRO:CD	0.41	2.83	6	1
1:A:94:LYS:O	1:A:95:ASP:HB3	0.41	2.15	6	2
1:A:4:LEU:CD1	1:A:4:LEU:N	0.41	2.83	22	1
1:A:5:THR:O	1:A:9:ILE:HB	0.41	2.15	22	1
1:A:85:ILE:O	1:A:87:GLU:N	0.41	2.53	26	1
2:B:10:ARG:O	2:B:14:ARG:N	0.41	2.54	3	3
1:A:94:LYS:HB2	1:A:104:GLU:CG	0.41	2.45	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:ALA:HB1	2:B:12:LEU:CG	0.41	2.40	7	1
1:A:106:ARG:CD	1:A:121:VAL:HG11	0.41	2.45	9	1
1:A:92:PHE:O	1:A:104:GLU:OE1	0.41	2.38	13	1
1:A:124:MET:HE3	2:B:8:TRP:CG	0.41	2.50	15	2
1:A:13:LYS:HG3	1:A:65:PHE:CE1	0.41	2.51	18	2
1:A:109:MET:HE3	2:B:8:TRP:HA	0.41	1.91	18	2
1:A:85:ILE:CD1	1:A:146:THR:HG22	0.41	2.46	16	1
2:B:7:LEU:HD12	2:B:7:LEU:O	0.41	2.15	16	1
1:A:29:THR:O	1:A:33:GLY:N	0.41	2.53	18	1
1:A:55:VAL:CG2	1:A:67:GLU:HG3	0.41	2.45	23	1
1:A:106:ARG:HG2	1:A:121:VAL:HG11	0.41	1.92	26	1
1:A:64:ASP:OD1	1:A:67:GLU:CG	0.41	2.68	23	4
1:A:105:LEU:CD1	1:A:124:MET:SD	0.41	3.09	6	1
1:A:32:LEU:O	1:A:35:VAL:CG1	0.41	2.69	14	1
1:A:125:ILE:O	1:A:129:ASP:N	0.41	2.52	25	1
1:A:100:ILE:HB	1:A:136:VAL:CG1	0.41	2.45	10	2
1:A:16:PHE:O	1:A:27:ILE:CD1	0.41	2.68	6	1
1:A:118:ASP:OD1	1:A:119:GLU:N	0.41	2.54	8	1
1:A:35:VAL:HG13	1:A:39:LEU:CD2	0.41	2.44	3	1
2:B:12:LEU:CD1	2:B:12:LEU:C	0.41	2.83	9	1
1:A:102:ALA:O	1:A:105:LEU:N	0.41	2.54	11	1
1:A:18:LEU:HD13	1:A:18:LEU:O	0.41	2.16	13	1
1:A:64:ASP:OD1	1:A:67:GLU:CB	0.41	2.68	13	2
1:A:34:THR:O	1:A:38:SER:CB	0.41	2.68	14	1
1:A:99:TYR:HB2	1:A:135:GLN:NE2	0.41	2.31	17	1
1:A:9:ILE:O	1:A:13:LYS:N	0.41	2.54	18	1
1:A:109:MET:HE2	1:A:114:GLU:HG3	0.41	1.92	21	1
1:A:109:MET:HB3	1:A:116:LEU:HD11	0.41	1.92	25	1
1:A:42:ASN:CB	1:A:43:PRO:HD3	0.41	2.46	8	3
1:A:55:VAL:HB	1:A:63:ILE:CD1	0.41	2.46	16	1
1:A:105:LEU:HB3	1:A:121:VAL:HG21	0.41	1.93	20	1
2:B:15:ILE:O	2:B:16:GLN:C	0.41	2.59	22	1
1:A:39:LEU:O	1:A:41:GLN:HG2	0.40	2.16	3	1
1:A:145:MET:HB2	2:B:9:PHE:CE2	0.40	2.51	7	1
1:A:55:VAL:CG1	1:A:63:ILE:CG1	0.40	2.99	10	1
1:A:69:LEU:CD1	1:A:73:ALA:HB2	0.40	2.46	10	1
1:A:10:ALA:O	1:A:13:LYS:N	0.40	2.54	21	1
1:A:142:VAL:CG2	1:A:143:GLN:N	0.40	2.84	1	1
1:A:105:LEU:O	1:A:109:MET:HB2	0.40	2.16	7	2
1:A:55:VAL:CG1	1:A:55:VAL:O	0.40	2.67	4	1
1:A:94:LYS:HB2	1:A:104:GLU:HG2	0.40	1.93	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ASP:OD1	1:A:20:ASP:O	0.40	2.39	9	1
1:A:9:ILE:HG12	1:A:65:PHE:CE1	0.40	2.51	9	1
1:A:51:MET:HG3	1:A:52:ILE:N	0.40	2.30	14	1
2:B:12:LEU:HD22	2:B:12:LEU:H	0.40	1.76	14	1
1:A:112:LEU:HD13	2:B:15:ILE:HD11	0.40	1.93	25	1
1:A:116:LEU:O	1:A:117:THR:CG2	0.40	2.64	25	1
1:A:136:VAL:HA	1:A:140:GLU:OE2	0.40	2.16	25	1
1:A:124:MET:HG3	1:A:125:ILE:N	0.40	2.32	1	1
1:A:55:VAL:O	1:A:55:VAL:CG2	0.40	2.70	7	1
1:A:35:VAL:O	1:A:39:LEU:HD13	0.40	2.16	9	1
1:A:138:TYR:O	1:A:142:VAL:CG1	0.40	2.63	11	1
1:A:106:ARG:NH2	1:A:118:ASP:OD2	0.40	2.55	13	1
1:A:48:LEU:N	1:A:48:LEU:CD2	0.40	2.85	19	1
1:A:35:VAL:O	1:A:39:LEU:N	0.40	2.52	22	1
1:A:4:LEU:C	1:A:4:LEU:HD13	0.40	2.37	24	1
1:A:112:LEU:HD22	2:B:11:GLY:O	0.40	2.16	3	1
1:A:4:LEU:HD12	1:A:4:LEU:C	0.40	2.36	4	1
1:A:120:GLU:CG	1:A:121:VAL:N	0.40	2.84	7	1
1:A:20:ASP:OD2	1:A:24:ASP:CB	0.40	2.69	10	1
1:A:92:PHE:CE1	2:B:8:TRP:CE3	0.40	3.10	20	1
1:A:6:GLU:HA	1:A:9:ILE:CG2	0.40	2.47	21	2
1:A:4:LEU:HD21	1:A:9:ILE:HG13	0.40	1.92	21	1
1:A:40:GLY:O	1:A:43:PRO:CD	0.40	2.70	3	1
1:A:20:ASP:OD2	1:A:24:ASP:N	0.40	2.53	10	1
1:A:48:LEU:HD12	1:A:48:LEU:N	0.40	2.32	13	1
1:A:29:THR:CG2	1:A:48:LEU:HD13	0.40	2.45	14	1
1:A:101:SER:HA	1:A:135:GLN:NE2	0.40	2.32	23	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	133/148 (90%)	102±3 (77±2%)	22±3 (17±2%)	9±3 (7±2%)	2	18
2	B	15/20 (75%)	10±1 (66±7%)	3±1 (22±6%)	2±1 (12±5%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3848/4368 (88%)	2915 (76%)	658 (17%)	275 (7%)	2 16

All 30 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	102	ALA	26
1	A	94	LYS	26
2	B	6	ILE	24
1	A	22	ASP	18
2	B	15	ILE	17
1	A	41	GLN	16
1	A	42	ASN	15
1	A	43	PRO	13
1	A	130	ILE	11
1	A	116	LEU	10
1	A	129	ASP	9
1	A	61	GLY	9
1	A	113	GLY	9
1	A	117	THR	8
1	A	4	LEU	8
1	A	95	ASP	8
1	A	138	TYR	7
1	A	85	ILE	6
1	A	66	PRO	5
1	A	135	GLN	5
1	A	96	GLY	4
1	A	59	GLY	4
2	B	16	GLN	4
1	A	56	ASP	3
1	A	86	ARG	3
2	B	4	GLY	2
1	A	118	ASP	2
2	B	5	GLN	1
1	A	69	LEU	1
1	A	5	THR	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	113/126 (90%)	78±3 (69±3%)	35±3 (31±3%)	1	15
2	B	13/18 (72%)	10±2 (76±12%)	3±2 (24±12%)	2	26
All	All	3276/3744 (88%)	2292 (70%)	984 (30%)	1	16

All 107 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)
1	A	105	LEU	26
1	A	42	ASN	26
1	A	68	PHE	26
1	A	133	ASP	25
1	A	104	GLU	23
1	A	26	THR	22
1	A	97	ASN	21
1	A	139	GLU	21
1	A	48	LEU	20
1	A	28	THR	20
1	A	27	ILE	19
1	A	9	ILE	19
1	A	92	PHE	19
1	A	21	LYS	19
2	B	14	ARG	18
1	A	74	ARG	18
1	A	7	GLU	17
1	A	22	ASP	16
1	A	32	LEU	16
1	A	70	THR	16
1	A	90	ARG	15
1	A	72	MET	15
1	A	31	GLU	14
1	A	124	MET	14
1	A	71	MET	14
1	A	111	ASN	14
1	A	136	VAL	14
1	A	13	LYS	14
1	A	143	GLN	13
1	A	30	LYS	13
1	A	94	LYS	13
1	A	17	SER	13
1	A	49	GLN	13

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Mol	Chain	Res	Type	Models (Total)
1	A	106	ARG	13
1	A	126	ARG	13
1	A	144	MET	13
1	A	109	MET	12
1	A	41	GLN	12
1	A	54	GLU	11
1	A	95	ASP	11
1	A	51	MET	10
1	A	36	MET	10
1	A	115	LYS	10
1	A	4	LEU	10
1	A	37	ARG	9
2	B	6	ILE	9
1	A	20	ASP	9
1	A	47	GLU	9
1	A	53	ASN	9
2	B	12	LEU	9
1	A	87	GLU	9
1	A	112	LEU	8
1	A	6	GLU	8
2	B	16	GLN	8
1	A	14	GLU	7
1	A	119	GLU	7
2	B	17	THR	7
1	A	127	GLU	7
1	A	5	THR	7
2	B	13	ASN	7
1	A	145	MET	7
1	A	114	GLU	7
1	A	101	SER	7
1	A	141	PHE	6
2	B	18	GLN	6
1	A	38	SER	6
1	A	86	ARG	6
1	A	45	GLU	6
2	B	8	TRP	6
1	A	19	PHE	5
1	A	138	TYR	4
1	A	69	LEU	4
1	A	85	ILE	4
2	B	7	LEU	4
1	A	12	PHE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	137	ASN	4
1	A	131	ASP	4
1	A	142	VAL	3
1	A	116	LEU	3
2	B	5	GLN	3
1	A	121	VAL	3
1	A	93	ASP	3
1	A	135	GLN	3
1	A	56	ASP	3
2	B	15	ILE	3
1	A	34	THR	3
1	A	67	GLU	2
1	A	8	GLN	2
1	A	123	GLU	2
1	A	63	ILE	2
1	A	107	HIS	2
1	A	18	LEU	2
2	B	10	ARG	1
1	A	62	THR	1
1	A	129	ASP	1
1	A	120	GLU	1
1	A	130	ILE	1
1	A	16	PHE	1
1	A	29	THR	1
1	A	89	PHE	1
1	A	146	THR	1
1	A	44	THR	1
1	A	58	ASP	1
1	A	91	VAL	1
1	A	24	ASP	1
1	A	122	ASP	1
1	A	55	VAL	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 4 ligands modelled in this entry, 4 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

No chemical shift data were provided