



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 07:12 PM UTC

PDB ID : 1CFF / pdb_00001cff
Title : NMR SOLUTION STRUCTURE OF A COMPLEX OF CALMODULIN
WITH A BINDING PEPTIDE OF THE CA²⁺-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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

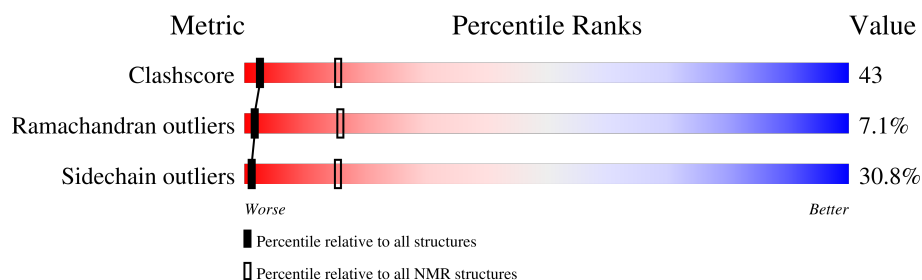
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 ≥ 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	27% 53% 9% 10%
2	B	20	30% 30% 15% 25%

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)	0.98	12
2	A:85-A:146, B:4-B:18 (77)	0.71	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 (CCD ID: CA) (formula: Ca).

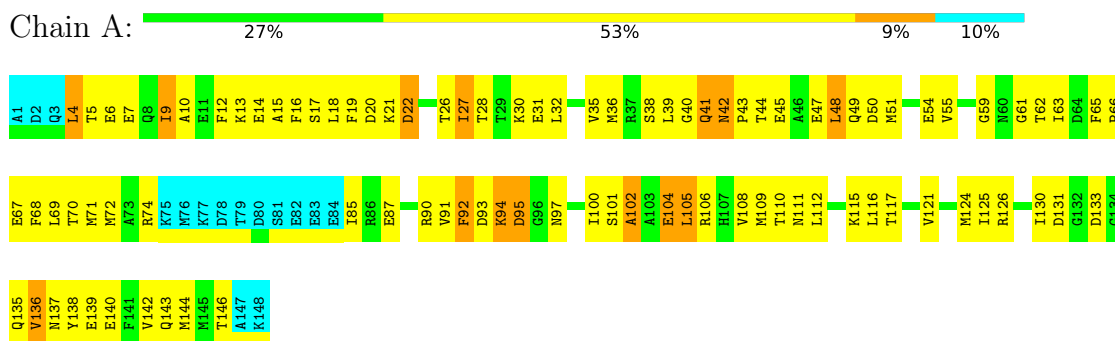
Mol	Chain	Residues	Atoms	
3	A	4	Total	Ca
			4	4

4 Residue-property plots

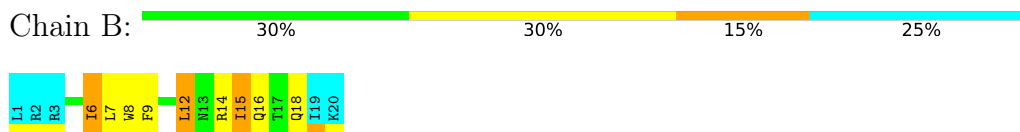
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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

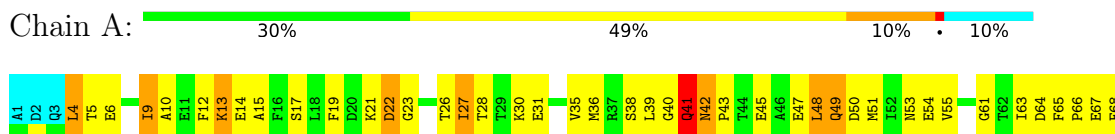


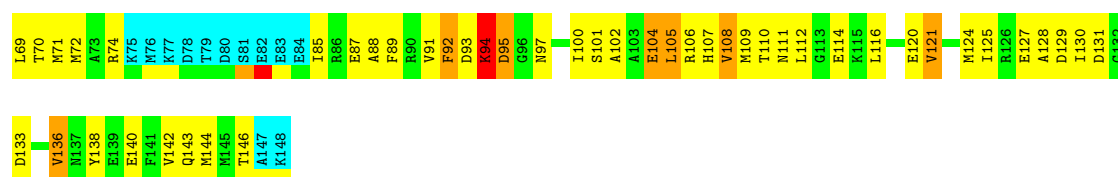
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

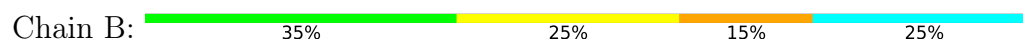
4.2.1 Score per residue for model 1

• Molecule 1: CALMODULIN





• Molecule 2: CALCIUM PUMP

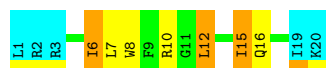


4.2.2 Score per residue for model 2

• Molecule 1: CALMODULIN

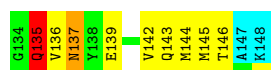
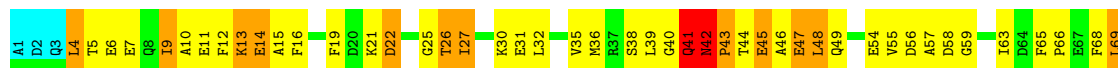


• Molecule 2: CALCIUM PUMP



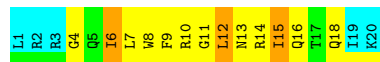
4.2.3 Score per residue for model 3

• Molecule 1: CALMODULIN



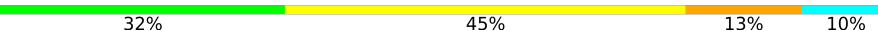
- Molecule 2: CALCIUM PUMP

Chain B: 



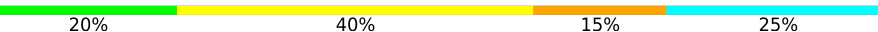
4.2.4 Score per residue for model 4

- Molecule 1: CALMODULIN

Chain A: 



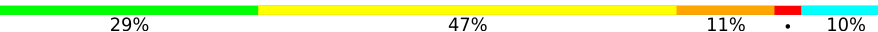
- Molecule 2: CALCIUM PUMP

Chain B: 



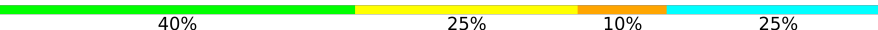
4.2.5 Score per residue for model 5

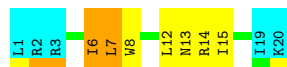
- Molecule 1: CALMODULIN

Chain A: 



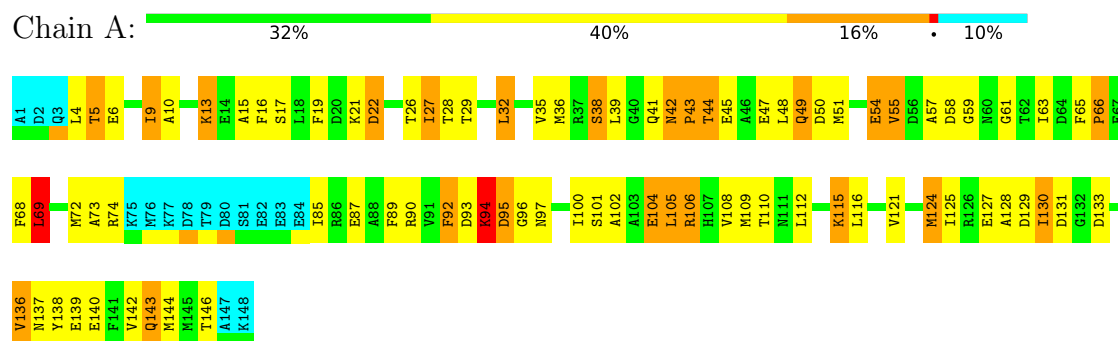
- Molecule 2: CALCIUM PUMP

Chain B: 

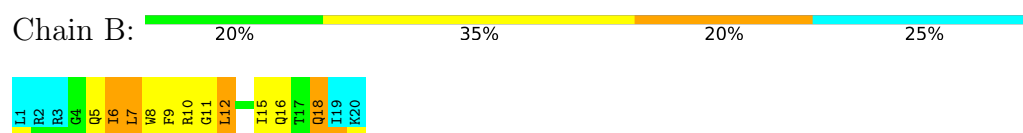


4.2.6 Score per residue for model 6

• Molecule 1: CALMODULIN

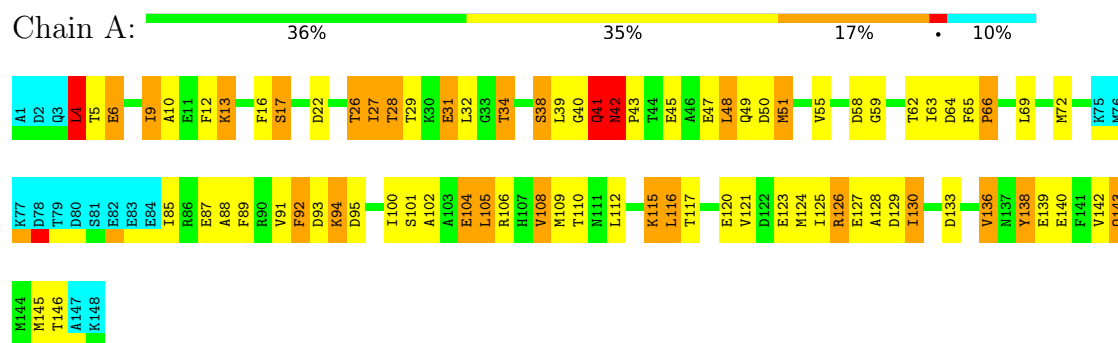


• Molecule 2: CALCIUM PUMP

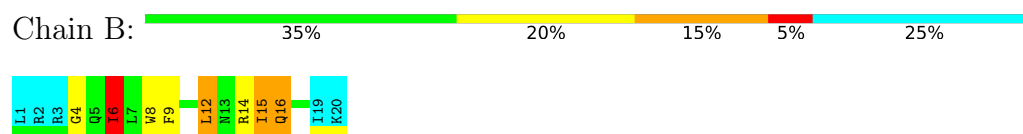


4.2.7 Score per residue for model 7 (medoid)

• Molecule 1: CALMODULIN



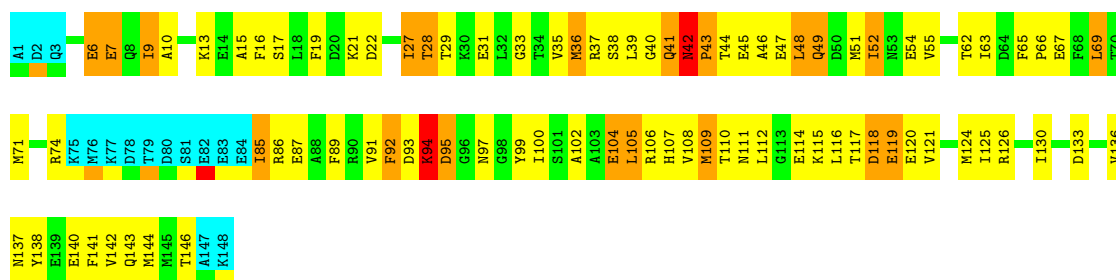
• Molecule 2: CALCIUM PUMP



4.2.8 Score per residue for model 8

• Molecule 1: CALMODULIN





• Molecule 2: CALCIUM PUMP

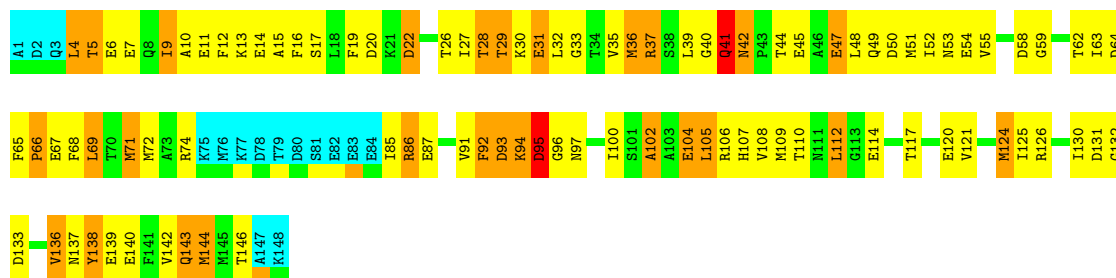
Chain B: 30% 30% 15% 25%



4.2.9 Score per residue for model 9

• Molecule 1: CALMODULIN

Chain A: 26% 45% 18% 10%



• Molecule 2: CALCIUM PUMP

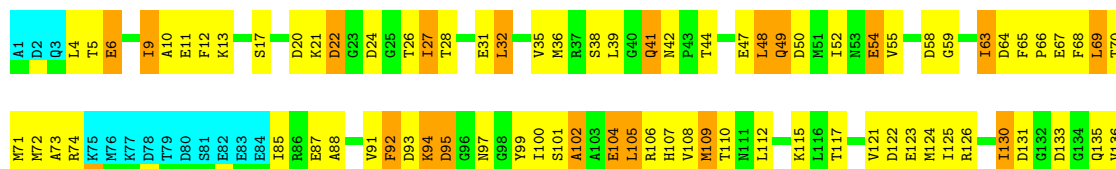
Chain B: 15% 30% 30% 25%



4.2.10 Score per residue for model 10

• Molecule 1: CALMODULIN

Chain A: 30% 46% 14% 10%





- Molecule 2: CALCIUM PUMP

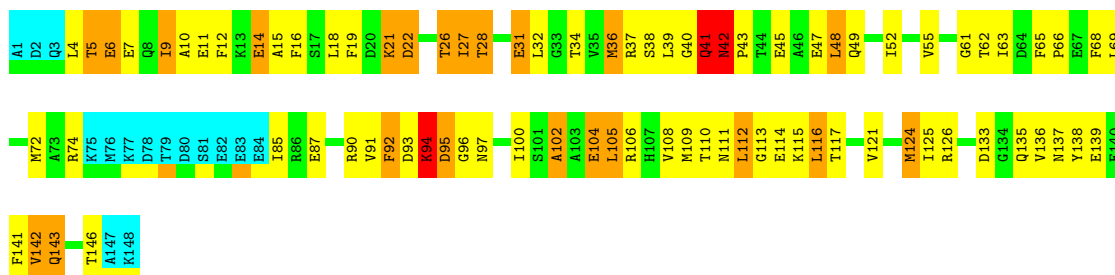
Chain B: 35% 20% 20% 25%



4.2.11 Score per residue for model 11

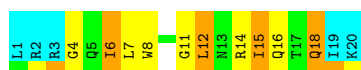
- Molecule 1: CALMODULIN

Chain A: 34% 39% 15% 10%



- Molecule 2: CALCIUM PUMP

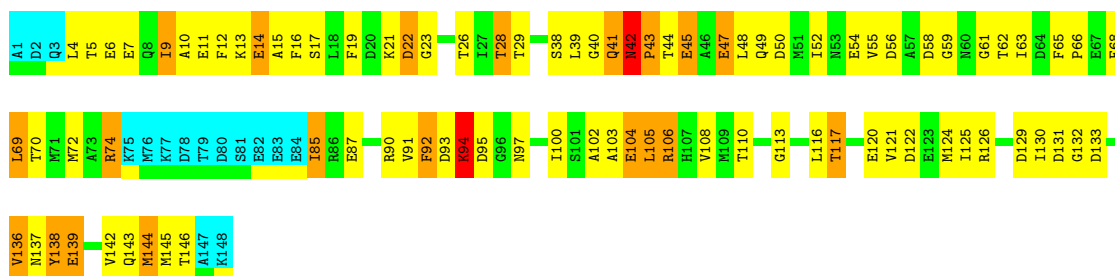
Chain B: 25% 30% 20% 25%



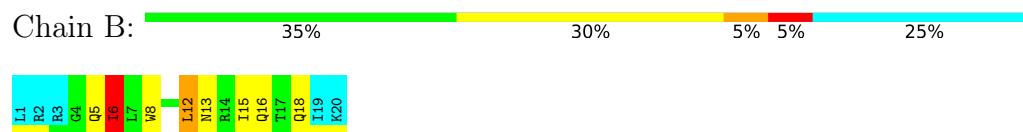
4.2.12 Score per residue for model 12

- Molecule 1: CALMODULIN

Chain A: 30% 45% 14% 10%

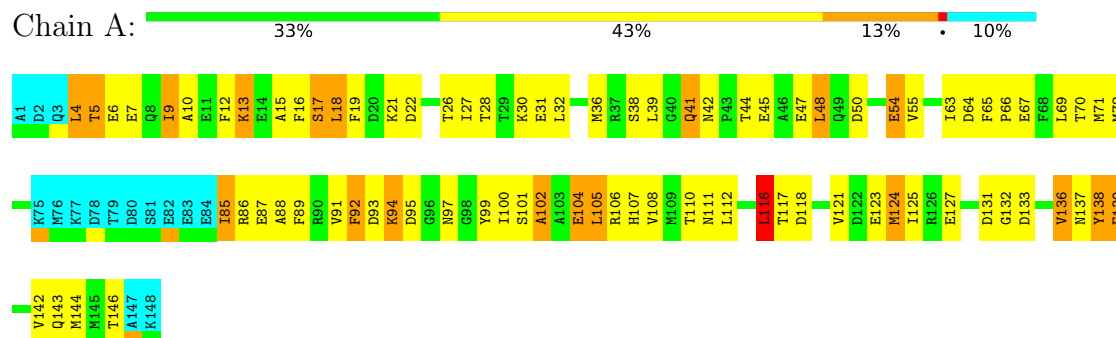


- Molecule 2: CALCIUM PUMP

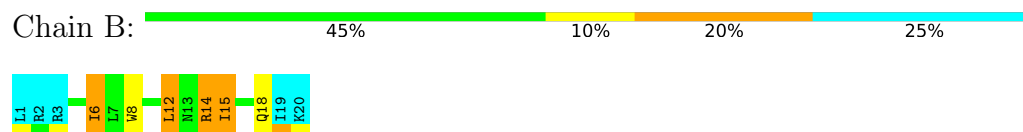


4.2.13 Score per residue for model 13

- Molecule 1: CALMODULIN

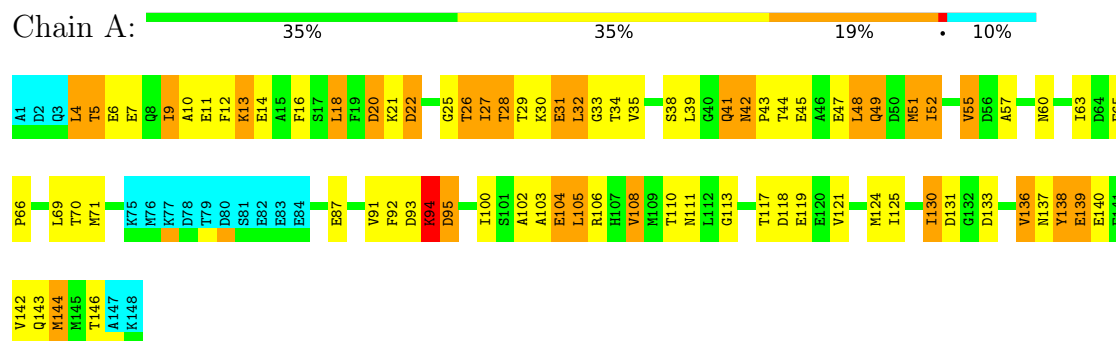


- Molecule 2: CALCIUM PUMP

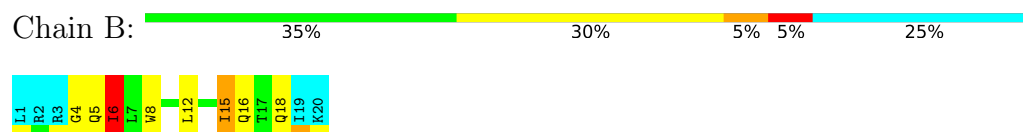


4.2.14 Score per residue for model 14

- Molecule 1: CALMODULIN

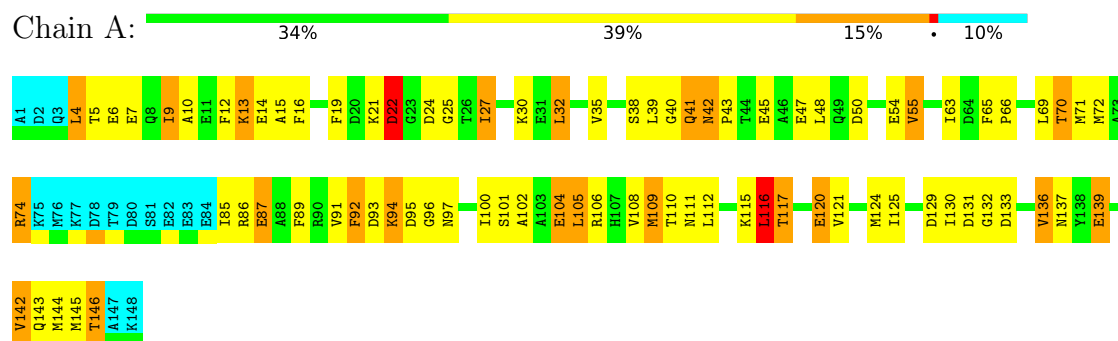


- Molecule 2: CALCIUM PUMP

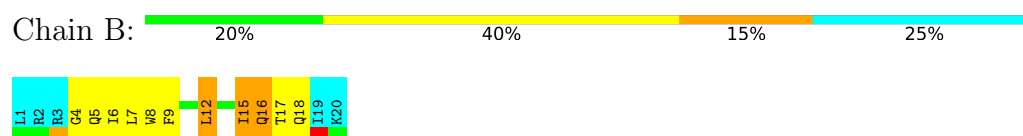


4.2.15 Score per residue for model 15

• Molecule 1: CALMODULIN

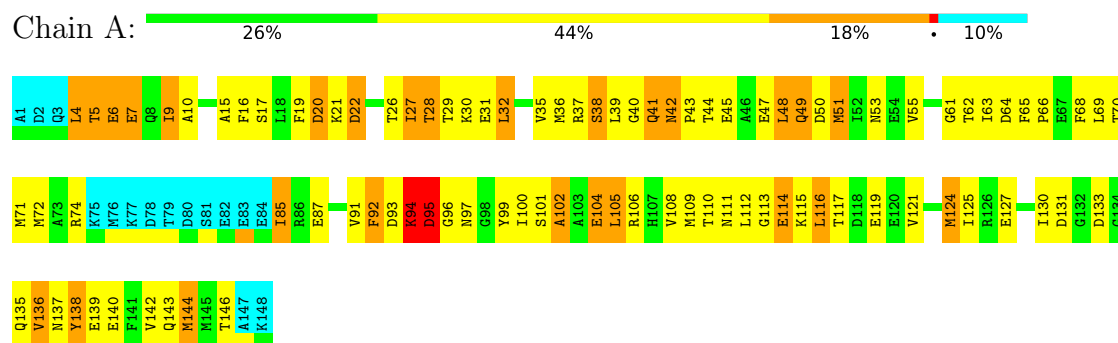


• Molecule 2: CALCIUM PUMP

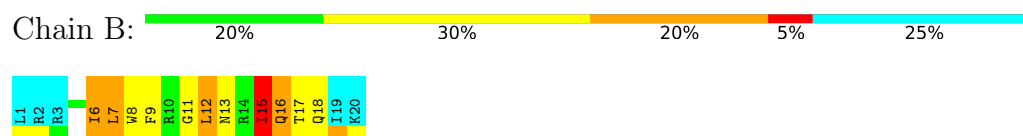


4.2.16 Score per residue for model 16

• Molecule 1: CALMODULIN



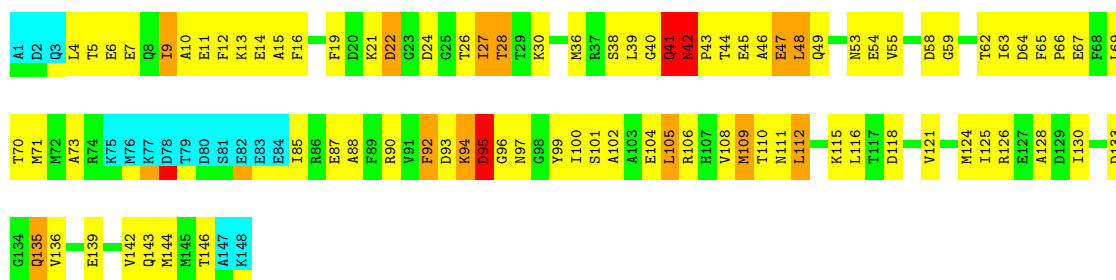
• Molecule 2: CALCIUM PUMP



4.2.17 Score per residue for model 17

• Molecule 1: CALMODULIN





• Molecule 2: CALCIUM PUMP

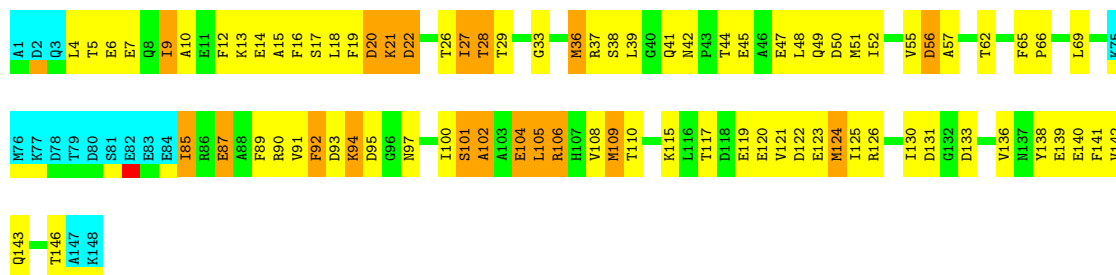
Chain B: 15% 45% 10% 5% 25%



4.2.18 Score per residue for model 18

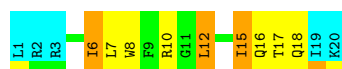
• Molecule 1: CALMODULIN

Chain A: 34% 43% 13% 10%



• Molecule 2: CALCIUM PUMP

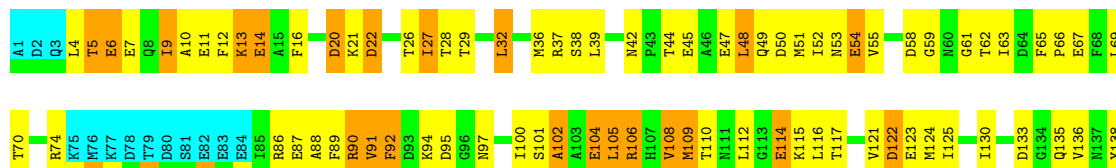
Chain B: 30% 30% 15% 25%

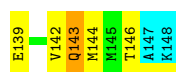


4.2.19 Score per residue for model 19

• Molecule 1: CALMODULIN

Chain A: 32% 42% 16% 10%



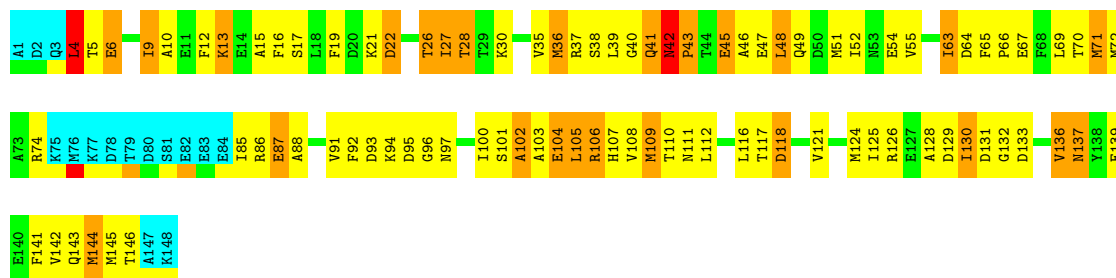


- Molecule 2: CALCIUM PUMP

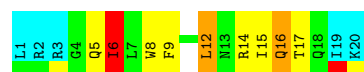
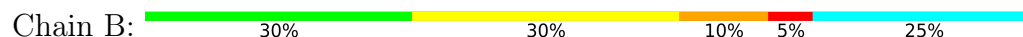


4.2.20 Score per residue for model 20

- Molecule 1: CALMODULIN

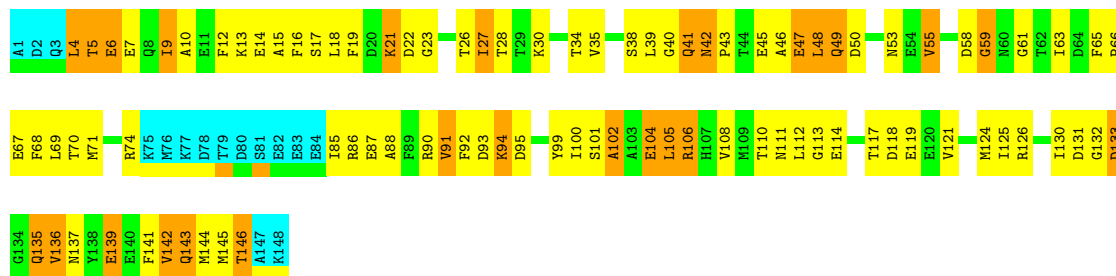


- Molecule 2: CALCIUM PUMP

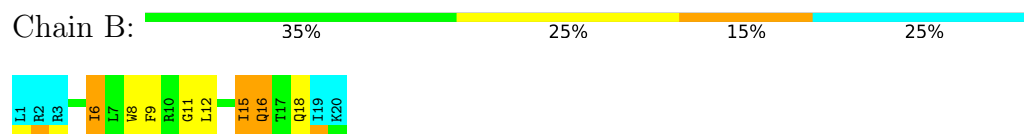


4.2.21 Score per residue for model 21

- Molecule 1: CALMODULIN

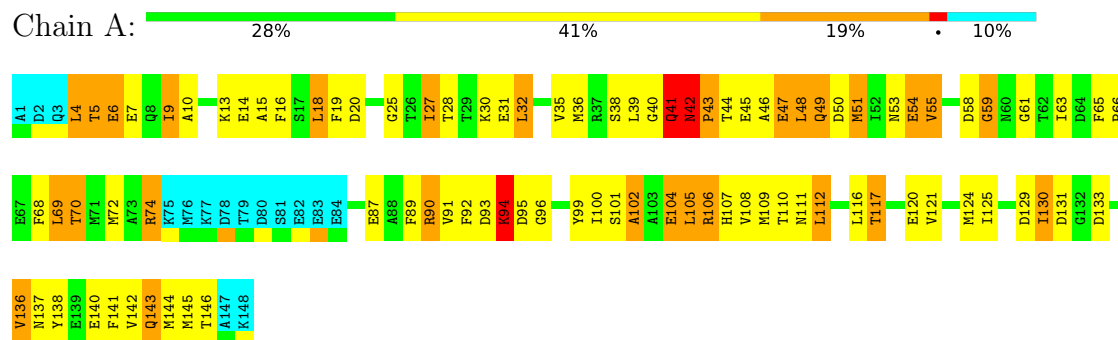


- Molecule 2: CALCIUM PUMP

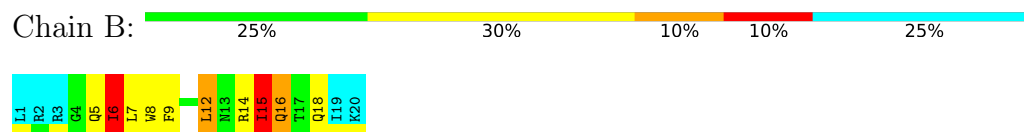


4.2.22 Score per residue for model 22

- Molecule 1: CALMODULIN

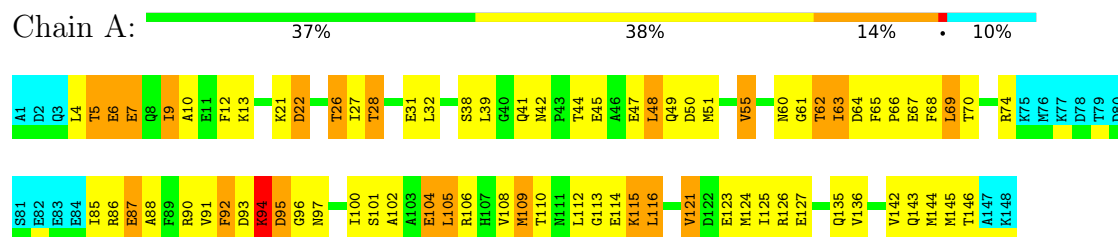


- Molecule 2: CALCIUM PUMP

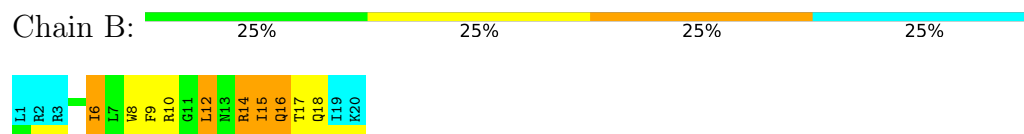


4.2.23 Score per residue for model 23

- Molecule 1: CALMODULIN

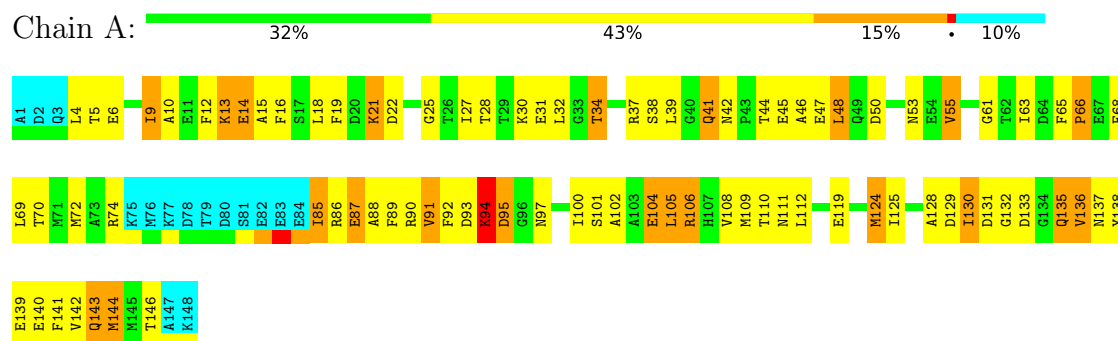


- Molecule 2: CALCIUM PUMP

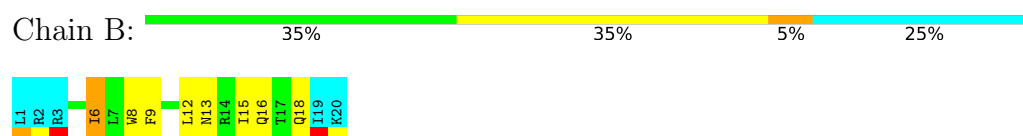


4.2.24 Score per residue for model 24

• Molecule 1: CALMODULIN

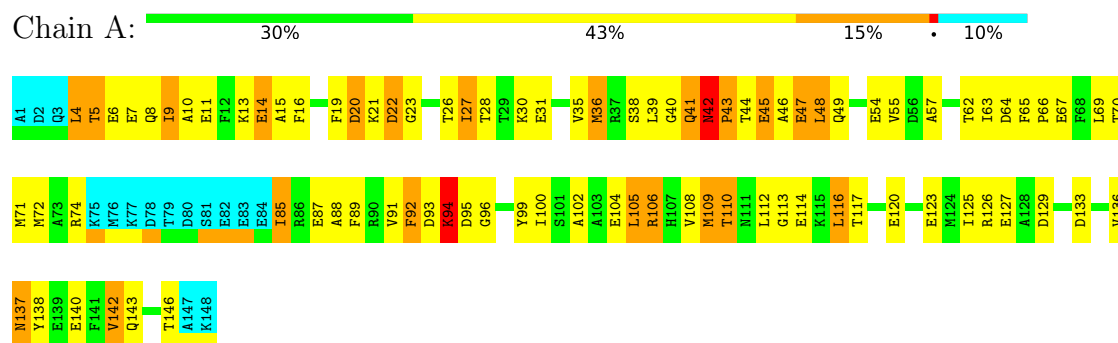


• Molecule 2: CALCIUM PUMP

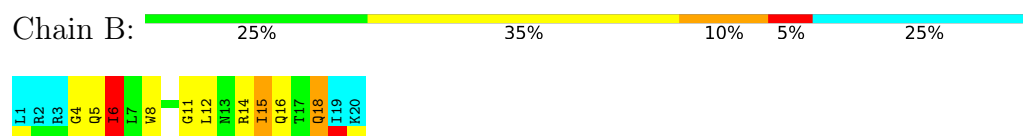


4.2.25 Score per residue for model 25

• Molecule 1: CALMODULIN



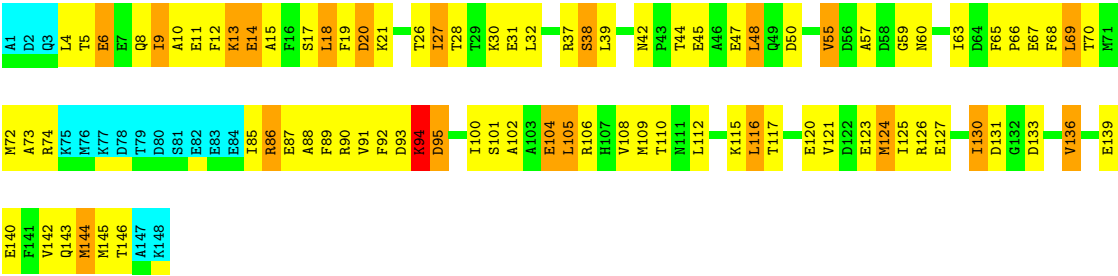
• Molecule 2: CALCIUM PUMP



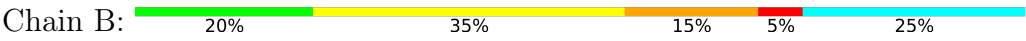
4.2.26 Score per residue for model 26

• 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.

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	91±8
2	B	129	132	132	15±5
All	All	30680	29068	29068	2540

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 43.

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:32:LEU:HD21	1:A:51:MET:HE3	0.96	1.37	14	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:PHE:CE2	2:B:12:LEU:HD21	0.86	2.05	7	15
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
1:A:38:SER:C	1:A:39:LEU:HD22	0.82	2.00	23	15
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:HD22	2:B:12:LEU:O	0.82	1.73	9	2
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
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:144:MET:HE2	2:B:9:PHE:CZ	0.78	2.14	16	3
1:A:91:VAL:O	1:A:108:VAL:HG11	0.78	1.79	4	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:GLU:O	1:A:10:ALA:HB2	0.73	1.82	7	23
1:A:92:PHE:CD2	2:B:12:LEU:HD13	0.73	2.17	20	1
1:A:145:MET:HE3	2:B:9:PHE:CD2	0.73	2.18	7	2
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:124:MET:HE1	2:B:8:TRP:HB3	0.72	1.60	11	7
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:18:LEU:C	1:A:18:LEU:HD13	0.71	2.09	4	2
1:A:9:ILE:HG23	1:A:65:PHE:CZ	0.71	2.21	22	3
1:A:112:LEU:HD21	2:B:11:GLY:C	0.71	2.10	11	6
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:109:MET:HE3	2:B:8:TRP:HA	0.70	1.61	19	8
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
2:B:12:LEU:HD13	2:B:12:LEU:C	0.70	2.12	3	2
1:A:124:MET:HE1	2:B:8:TRP:CD1	0.70	2.21	18	3
1:A:145:MET:HE1	2:B:9:PHE:CD1	0.69	2.21	21	1
1:A:38:SER:C	1:A:39:LEU:HD12	0.69	2.12	15	7
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:124:MET:HE1	2:B:8:TRP:CG	0.68	2.24	18	8
1:A:100:ILE:HG23	1:A:104:GLU:HG2	0.68	1.64	3	6
1:A:144:MET:HE3	2:B:9:PHE:CE1	0.67	2.24	10	2
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:HD13	1:A:4:LEU:N	0.66	2.05	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	17
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
1:A:63:ILE:HG21	1:A:68:PHE:CD2	0.65	2.27	12	10
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
1:A:109:MET:HB3	1:A:116:LEU:HD12	0.64	1.70	19	3
1:A:142:VAL:O	1:A:146:THR:HG22	0.64	1.93	25	1
1:A:124:MET:HE3	2:B:4:GLY:HA2	0.64	1.69	11	2
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	2
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:4:LEU:C	1:A:4:LEU:HD22	0.61	2.21	25	3
1:A:32:LEU:CD2	1:A:51:MET:HE3	0.61	2.21	14	1
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
2:B:7:LEU:HD13	2:B:7:LEU:C	0.60	2.21	18	10
1:A:136:VAL:O	1:A:136:VAL:HG13	0.60	1.95	4	9
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:9:ILE:CG1	1:A:69:LEU:HD13	0.60	2.25	26	11
1:A:39:LEU:HD22	1:A:39:LEU:N	0.60	2.11	1	15
1:A:85:ILE:O	1:A:85:ILE:HG22	0.60	1.96	12	3
1:A:4:LEU:HD23	1:A:9:ILE:HG13	0.60	1.73	25	1
1:A:39:LEU:HD12	1:A:39:LEU:N	0.60	2.12	15	7
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:B:12:LEU:HD22	2:B:12:LEU:C	0.60	2.21	3	2
1:A:55:VAL:HG12	1:A:55:VAL:O	0.60	1.96	4	1
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:20:ASP:OD1	1:A:27:ILE:HD13	0.59	1.97	25	1
1:A:105:LEU:CG	1:A:125:ILE:HD11	0.59	2.27	23	13
1:A:124:MET:HE3	2:B:8:TRP:CD1	0.59	2.32	17	3
1:A:112:LEU:HD11	2:B:15:ILE:HG12	0.59	1.73	9	2
1:A:69:LEU:C	1:A:69:LEU:HD12	0.59	2.20	12	5
2:B:6:ILE:O	2:B:6:ILE:HG23	0.59	1.98	21	6
1:A:144:MET:HE3	2:B:9:PHE:CZ	0.59	2.33	24	4
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:27:ILE:HD13	1:A:27:ILE:N	0.59	2.13	5	12
1:A:92:PHE:CE2	2:B:8:TRP:CE3	0.59	2.91	1	6
1:A:14:GLU:O	1:A:18:LEU:HD23	0.59	1.98	22	2
1:A:92:PHE:CE2	2:B:8:TRP:CZ3	0.58	2.91	14	4
1:A:106:ARG:HG3	1:A:121:VAL:HG11	0.58	1.74	2	2
1:A:4:LEU:CG	1:A:69:LEU:HD21	0.58	2.28	21	5
1:A:144:MET:HE2	2:B:9:PHE:CE1	0.58	2.33	6	1
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:32:LEU:O	1:A:32:LEU:HD13	0.58	1.98	26	4
1:A:112:LEU:HD21	2:B:11:GLY:CA	0.58	2.27	6	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	2
2:B:7:LEU:C	2:B:7:LEU:HD12	0.57	2.23	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:MET:O	1:A:51:MET:HE2	0.57	1.99	16	3
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:35:VAL:HA	1:A:39:LEU:HD23	0.56	1.77	22	6
1:A:55:VAL:HG22	1:A:55:VAL:O	0.56	2.00	17	9
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
2:B:15:ILE:C	2:B:15:ILE:HD12	0.56	2.26	20	1
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
1:A:124:MET:HE3	2:B:8:TRP:CG	0.56	2.36	17	1
1:A:4:LEU:HD13	1:A:4:LEU:H	0.56	1.60	25	2
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:5:THR:O	1:A:9:ILE:CG2	0.55	2.54	23	23
1:A:92:PHE:CZ	2:B:12:LEU:CD2	0.55	2.90	1	2
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
1:A:105:LEU:CD2	2:B:8:TRP:CZ3	0.55	2.90	3	2
1:A:35:VAL:HG13	1:A:39:LEU:HD23	0.55	1.77	3	1
1:A:130:ILE:HD11	1:A:144:MET:CG	0.55	2.31	26	1
1:A:101:SER:HG	1:A:135:GLN:CD	0.55	2.09	4	1
1:A:26:THR:C	1:A:27:ILE:HD13	0.55	2.27	5	1
1:A:104:GLU:O	1:A:108:VAL:HG23	0.55	2.01	21	6
1:A:9:ILE:HG13	1:A:69:LEU:HD22	0.55	1.79	10	2
2:B:5:GLN:O	2:B:6:ILE:HG22	0.54	2.02	17	4
1:A:124:MET:HE1	2:B:8:TRP:CB	0.54	2.30	11	1
1:A:4:LEU:HD23	1:A:9:ILE:HG12	0.54	1.79	22	1
1:A:106:ARG:HA	1:A:121:VAL:HG11	0.54	1.78	22	1
1:A:92:PHE:CZ	2:B:12:LEU:HD11	0.54	2.37	24	1
1:A:124:MET:HE2	2:B:4:GLY:HA2	0.54	1.79	7	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:63:ILE:N	1:A:63:ILE:HD13	0.54	2.17	23	2
1:A:117:THR:O	1:A:118:ASP:CB	0.54	2.56	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:9:ILE:HD12	1:A:65:PHE:CZ	0.54	2.38	18	5
1:A:92:PHE:HB3	1:A:100:ILE:HD11	0.54	1.79	25	6
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: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
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
1:A:18:LEU:C	1:A:18:LEU:CD1	0.53	2.81	4	2
1:A:145:MET:HE3	2:B:9:PHE:CG	0.53	2.38	7	1
1:A:13:LYS:CG	1:A:65:PHE:CE1	0.53	2.91	6	5
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: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
1:A:136:VAL:HG13	1:A:136:VAL:O	0.52	2.04	23	1
2:B:7:LEU:HD12	2:B:7:LEU:O	0.52	2.05	5	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ILE:HG23	1:A:10:ALA:N	0.51	2.20	24	17
2:B:6:ILE:O	2:B:6:ILE:CG2	0.51	2.58	22	17
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:32:LEU:HD13	1:A:32:LEU:C	0.51	2.30	26	1
1:A:55:VAL:CG1	1:A:63:ILE:CD1	0.51	2.89	7	9
1:A:144:MET:HE2	2:B:9:PHE:CE2	0.51	2.41	4	2
1:A:55:VAL:O	1:A:55:VAL:HG12	0.51	2.06	12	4
1:A:142:VAL:CG2	1:A:146:THR:OG1	0.51	2.59	11	1
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:109:MET:HE1	1:A:112:LEU:HD23	0.50	1.81	6	1
1:A:106:ARG:CD	1:A:106:ARG:C	0.50	2.84	18	2
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:109:MET:CG	1:A:116:LEU:HD12	0.50	2.36	7	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:CD1	2:B:6:ILE:N	0.49	2.75	22	1
1:A:5:THR:O	1:A:9:ILE:HG22	0.49	2.07	9	14
1:A:9:ILE:CG2	1:A:10:ALA:N	0.49	2.76	20	17
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:144:MET:HE3	2:B:5:GLN:HG3	0.49	1.83	9	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:VAL:CG2	1:A:109:MET:N	0.49	2.75	19	5
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:4:LEU:C	1:A:4:LEU:HD12	0.49	2.32	12	2
1:A:39:LEU:N	1:A:39:LEU:CD2	0.49	2.75	18	10
1:A:61:GLY:O	1:A:62:THR:HG23	0.49	2.08	16	2
1:A:65:PHE:N	1:A:66:PRO:CD	0.49	2.76	23	9
1:A:35:VAL:HG13	1:A:39:LEU:HD22	0.49	1.84	15	1
1:A:15:ALA:O	1:A:19:PHE:N	0.48	2.43	2	12
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:40:GLY:O	1:A:41:GLN:C	0.48	2.56	3	10
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
1:A:48:LEU:HD23	1:A:48:LEU:N	0.48	2.23	15	5
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:65:PHE:N	1:A:66:PRO:HD2	0.48	2.24	14	16
1:A:142:VAL:HG23	1:A:143:GLN:N	0.48	2.24	1	16
1:A:55:VAL:HG13	1:A:71:MET:HG3	0.48	1.85	4	1
1:A:106:ARG:HG2	1:A:107:HIS:N	0.48	2.23	5	1
1:A:116:LEU:HD23	1:A:116:LEU:N	0.48	2.23	11	1
2:B:7:LEU:HD22	2:B:7:LEU:C	0.48	2.33	6	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: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: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:116:LEU:CD1	1:A:124:MET:HE3	0.47	2.39	16	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:4:LEU:HD23	1:A:4:LEU:C	0.47	2.35	9	1
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:N	1:A:63:ILE:CD1	0.47	2.78	5	2
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
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
1:A:145:MET:HE1	2:B:12:LEU:HD23	0.47	1.86	10	1
1:A:48:LEU:O	1:A:52:ILE:HG12	0.47	2.10	14	1
1:A:89:PHE:C	1:A:89:PHE:CD1	0.47	2.93	3	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:144:MET:HE3	2:B:9:PHE:CE2	0.46	2.45	24	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	2
1:A:13:LYS:HG2	1:A:65:PHE:CD1	0.46	2.45	15	2
1:A:39:LEU:N	1:A:39:LEU:CD1	0.46	2.79	15	1
1:A:145:MET:CG	2:B:9:PHE:CE2	0.46	2.97	22	1
1:A:4:LEU:C	1:A:4:LEU:CD2	0.46	2.88	25	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: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
1:A:142:VAL:O	1:A:146:THR:N	0.46	2.49	7	23
2:B:6:ILE:HG22	2:B:10:ARG:HD2	0.46	1.88	1	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:PHE:O	1:A:69:LEU:CB	0.46	2.64	6	10
1:A:15:ALA:O	1:A:19:PHE:CB	0.46	2.64	24	6
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: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
2:B:12:LEU:C	2:B:12:LEU:CD1	0.45	2.83	9	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: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
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:40:GLY:O	1:A:42:ASN:N	0.45	2.50	17	8
1:A:100:ILE:N	1:A:135:GLN:OE1	0.45	2.50	3	1
1:A:102:ALA:O	1:A:121:VAL:HG21	0.45	2.12	19	1
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:124:MET:CE	2:B:8:TRP:CG	0.45	2.99	2	3
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
2:B:15:ILE:O	2:B:16:GLN:C	0.45	2.59	22	18
1:A:46:ALA:O	1:A:49:GLN:N	0.45	2.50	8	7
2:B:7:LEU:HD13	2:B:7:LEU:O	0.45	2.12	4	1
1:A:142:VAL:C	1:A:146:THR:HG1	0.45	2.18	18	5
1:A:4:LEU:HD23	1:A:5:THR:O	0.45	2.12	17	2
1:A:116:LEU:CD1	1:A:116:LEU:O	0.45	2.64	15	2
1:A:4:LEU:C	1:A:4:LEU:HD13	0.45	2.37	24	1
1:A:4:LEU:O	1:A:5:THR:O	0.45	2.34	25	1
1:A:4:LEU:HD12	1:A:4:LEU:C	0.45	2.36	4	2
1:A:85:ILE:O	1:A:88:ALA:N	0.45	2.50	26	2
1:A:135:GLN:NE2	1:A:136:VAL:HG12	0.45	2.26	23	1
1:A:22:ASP:OD1	1:A:23:GLY:N	0.45	2.50	12	6
1:A:144:MET:HE1	2:B:9:PHE:CE1	0.45	2.47	3	1
1:A:4:LEU:CD2	1:A:4:LEU:O	0.45	2.65	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:THR:OG1	1:A:120:GLU:CG	0.45	2.65	25	1
1:A:93:ASP:O	1:A:95:ASP:CG	0.45	2.59	9	6
1:A:131:ASP:OD1	1:A:132:GLY:N	0.45	2.49	24	9
1:A:38:SER:C	1:A:39:LEU:HD13	0.45	2.37	2	2
1:A:136:VAL:O	1:A:136:VAL:CG1	0.45	2.65	3	7
1:A:105:LEU:O	1:A:109:MET:N	0.45	2.46	24	6
1:A:112:LEU:HD11	2:B:15:ILE:HG13	0.45	1.89	11	3
1:A:122:ASP:O	1:A:126:ARG:CD	0.45	2.64	12	2
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:144:MET:HE2	2:B:9:PHE:CD1	0.44	2.47	6	1
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
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	2
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:14:GLU:O	1:A:18:LEU:CD2	0.44	2.65	22	1
1:A:106:ARG:HB2	1:A:121:VAL:HG11	0.44	1.88	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: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:94:LYS:CD	1:A:94:LYS:C	0.44	2.91	15	1
1:A:10:ALA:O	1:A:13:LYS:CB	0.44	2.66	9	9
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:64:ASP:C	1:A:66:PRO:CD	0.43	2.91	2	3
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:124:MET:HE1	2:B:8:TRP:CD2	0.43	2.48	7	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	1
1:A:54:GLU:OE1	1:A:54:GLU:CA	0.43	2.65	6	1
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: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
1:A:61:GLY:O	1:A:62:THR:CG2	0.43	2.67	16	3
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:93:ASP:O	1:A:94:LYS:C	0.43	2.62	22	11
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: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
1:A:112:LEU:HD21	2:B:12:LEU:HA	0.43	1.88	9	1
1:A:9:ILE:HG13	1:A:69:LEU:CD2	0.43	2.43	10	1
1:A:52:ILE:HD13	1:A:63:ILE:CD1	0.43	2.44	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: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:18:LEU:O	1:A:21:LYS:N	0.43	2.50	21	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:TYR:O	1:A:141:PHE:N	0.43	2.51	11	3
1:A:103:ALA:O	1:A:106:ARG:HG2	0.43	2.13	14	1
1:A:54:GLU:OE1	1:A:54:GLU:N	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:4:LEU:O	1:A:4:LEU:CD2	0.43	2.66	22	1
1:A:101:SER:N	1:A:135:GLN:CD	0.43	2.76	24	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:28:THR:N	1:A:31:GLU:OE2	0.43	2.51	9	2
1:A:120:GLU:O	1:A:124:MET:CB	0.43	2.66	9	1
1:A:60:ASN:OD1	1:A:60:ASN:N	0.43	2.52	14	3
1:A:16:PHE:CD1	1:A:16:PHE:C	0.43	2.97	20	1
1:A:5:THR:O	1:A:9:ILE:CD1	0.43	2.67	22	1
1:A:58:ASP:OD1	1:A:59:GLY:N	0.43	2.52	19	9
2:B:6:ILE:O	2:B:10:ARG:CG	0.43	2.67	18	2
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:20:ASP:OD1	1:A:22:ASP:CB	0.43	2.67	18	2
1:A:122:ASP:OD1	1:A:123:GLU:N	0.43	2.52	18	1
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:94:LYS:CB	1:A:104:GLU:HG2	0.42	2.44	15	5
1:A:128:ALA:O	1:A:130:ILE:N	0.42	2.51	1	6
1:A:141:PHE:HA	1:A:144:MET:HE2	0.42	1.89	21	2
1:A:12:PHE:CE2	1:A:69:LEU:HA	0.42	2.49	11	2
1:A:94:LYS:HB2	1:A:104:GLU:CB	0.42	2.44	11	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:95:ASP:CG	1:A:96:GLY:N	0.42	2.77	23	2
1:A:74:ARG:CG	1:A:74:ARG:O	0.42	2.67	24	3
1:A:10:ALA:O	1:A:14:GLU:N	0.42	2.51	22	4
2:B:8:TRP:CD1	2:B:9:PHE:CD1	0.42	3.07	15	1
1:A:116:LEU:N	1:A:116:LEU:HD22	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:61:GLY:C	1:A:62:THR:CG2	0.42	2.92	5	1
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
1:A:4:LEU:CD2	1:A:69:LEU:CD2	0.42	2.96	7	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:18:LEU:C	1:A:20:ASP:N	0.42	2.77	26	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:22:ASP:OD1	1:A:22:ASP:C	0.42	2.63	6	3
1:A:69:LEU:O	1:A:73:ALA:N	0.42	2.52	17	2
1:A:144:MET:HG2	2:B:9:PHE:CZ	0.42	2.49	6	1
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:4:LEU:CD2	1:A:4:LEU:C	0.42	2.92	22	1
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:122:ASP:CG	1:A:123:GLU:N	0.42	2.77	19	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:16:PHE:CE2	1:A:27:ILE:HG12	0.42	2.50	15	1
1:A:137:ASN:ND2	1:A:139:GLU:HG2	0.42	2.30	15	4
2:B:5:GLN:HB2	2:B:9:PHE:CE2	0.42	2.49	15	1
1:A:67:GLU:CG	1:A:68:PHE:N	0.42	2.82	26	2
1:A:108:VAL:O	1:A:112:LEU:N	0.42	2.51	26	2
1:A:69:LEU:HD12	1:A:69:LEU:C	0.42	2.39	23	1
1:A:46:ALA:O	1:A:50:ASP:N	0.42	2.52	2	2
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
2:B:15:ILE:C	2:B:15:ILE:CD1	0.42	2.92	20	1
1:A:39:LEU:HB2	1:A:41:GLN:CG	0.42	2.45	14	5
1:A:28:THR:HG23	1:A:62:THR:HB	0.42	1.91	8	2
1:A:137:ASN:O	1:A:140:GLU:CG	0.42	2.68	8	1
1:A:131:ASP:N	1:A:131:ASP:OD1	0.42	2.53	10	1
1:A:137:ASN:CG	1:A:139:GLU:CG	0.42	2.92	13	1
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
2:B:7:LEU:C	2:B:7:LEU:CD1	0.42	2.93	5	3
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
2:B:12:LEU:C	2:B:12:LEU:CD2	0.42	2.92	9	1
1:A:87:GLU:O	1:A:91:VAL:CG2	0.42	2.66	10	2
1:A:105:LEU:CB	1:A:121:VAL:HG23	0.42	2.42	10	1
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:131:ASP:OD1	1:A:131:ASP:N	0.41	2.53	3	4
1:A:95:ASP:N	1:A:95:ASP:OD1	0.41	2.52	12	2
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:137:ASN:O	1:A:138:TYR:C	0.41	2.63	11	5
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:GLY:O	1:A:62:THR:HG22	0.41	2.15	23	1
1:A:109:MET:HG3	1:A:116:LEU:HD23	0.41	1.92	1	1
1:A:109:MET:CG	1:A:116:LEU:HD23	0.41	2.46	1	1
1:A:55:VAL:O	1:A:67:GLU:CG	0.41	2.68	2	1
1:A:93:ASP:O	1:A:95:ASP:OD1	0.41	2.38	8	4
1:A:99:TYR:CE1	1:A:137:ASN:HA	0.41	2.49	5	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:64:ASP:CG	1:A:66:PRO:CD	0.41	2.94	2	1
1:A:112:LEU:HD11	2:B:15:ILE:HG23	0.41	1.92	6	1
1:A:116:LEU:O	1:A:116:LEU:HD13	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: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:58:ASP:O	1:A:59:GLY:C	0.41	2.63	6	3
1:A:94:LYS:O	1:A:95:ASP:HB3	0.41	2.15	6	2
2:B:7:LEU:C	2:B:7:LEU:HD23	0.41	2.40	11	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
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:13:LYS:HG3	1:A:65:PHE:CE1	0.41	2.51	18	2
1:A:85:ILE:CD1	1:A:146:THR:HG22	0.41	2.46	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:101:SER:O	1:A:102:ALA:C	0.41	2.63	5	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:ASP:OD1	1:A:119:GLU:N	0.41	2.54	8	1
1:A:85:ILE:O	1:A:86:ARG:C	0.41	2.64	26	1
1:A:51:MET:HE2	1:A:55:VAL:CG2	0.41	2.46	1	1
1:A:35:VAL:HG13	1:A:39:LEU:CD2	0.41	2.44	3	1
1:A:102:ALA:O	1:A:105:LEU:N	0.41	2.54	11	1
1:A:112:LEU:CD2	2:B:11:GLY:C	0.41	2.89	11	2
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:93:ASP:C	1:A:104:GLU:OE1	0.41	2.64	18	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
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:64:ASP:CG	1:A:66:PRO:HD2	0.40	2.42	2	1
1:A:105:LEU:O	1:A:109:MET:HB2	0.40	2.16	7	2
1:A:55:VAL:O	1:A:55:VAL:CG1	0.40	2.67	4	1
1:A:94:LYS:HB2	1:A:104:GLU:HG2	0.40	1.93	5	1
1:A:9:ILE:HG12	1:A:65:PHE:CE1	0.40	2.51	9	1
1:A:20:ASP:O	1:A:20:ASP:OD1	0.40	2.39	9	1
1:A:20:ASP:OD1	1:A:31:GLU:CD	0.40	2.65	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:141:PHE:CE1	1:A:145:MET:HE3	0.40	2.51	10	1
1:A:138:TYR:O	1:A:142:VAL:CG1	0.40	2.63	11	1
1:A:42:ASN:O	1:A:43:PRO:C	0.40	2.65	12	1
1:A:106:ARG:NH2	1:A:118:ASP:OD2	0.40	2.55	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:N	1:A:4:LEU:HD13	0.40	2.31	3	1
1:A:112:LEU:HD22	2:B:11:GLY:O	0.40	2.16	3	1
1:A:120:GLU:CG	1:A:121:VAL:N	0.40	2.84	7	1
2:B:15:ILE:C	2:B:17:THR:N	0.40	2.80	9	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:4:LEU:HD21	1:A:9:ILE:HG13	0.40	1.92	21	1
1:A:6:GLU:HA	1:A:9:ILE:CG2	0.40	2.47	21	2
1:A:27:ILE:N	1:A:27:ILE:HD13	0.40	2.31	2	1
1:A:40:GLY:O	1:A:43:PRO:CD	0.40	2.70	3	1
1:A:105:LEU:HD13	1:A:124:MET:HE3	0.40	1.93	6	1
1:A:20:ASP:OD2	1:A:24:ASP:N	0.40	2.53	10	1
1:A:48:LEU:N	1:A:48:LEU:HD12	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
2:B:15:ILE:O	2:B:18:GLN:C	0.40	2.65	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	17
2	B	15/20 (75%)	10±1 (66±7%)	3±1 (22±6%)	2±1 (12±5%)	1	6
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	94	LYS	26
1	A	102	ALA	26
2	B	6	ILE	24

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Mol	Chain	Res	Type	Models (Total)
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	61	GLY	9
1	A	129	ASP	9
1	A	113	GLY	9
1	A	4	LEU	8
1	A	95	ASP	8
1	A	117	THR	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
2	B	16	GLN	4
1	A	59	GLY	4
1	A	56	ASP	3
1	A	86	ARG	3
1	A	118	ASP	2
2	B	4	GLY	2
1	A	69	LEU	1
1	A	5	THR	1
2	B	5	GLN	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%)	77±4 (69±3%)	36±4 (31±3%)	1	14
2	B	13/18 (72%)	10±1 (75±11%)	3±1 (25±11%)	2	24
All	All	3276/3744 (88%)	2266 (69%)	1010 (31%)	1	15

All 101 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	9	ILE	26
1	A	42	ASN	26
1	A	105	LEU	26
1	A	27	ILE	25
1	A	104	GLU	24
1	A	133	ASP	24
1	A	28	THR	23
1	A	21	LYS	22
1	A	26	THR	22
1	A	48	LEU	20
2	B	12	LEU	19
1	A	7	GLU	19
1	A	70	THR	18
1	A	92	PHE	18
1	A	97	ASN	18
1	A	72	MET	17
1	A	74	ARG	17
1	A	139	GLU	17
1	A	30	LYS	16
1	A	136	VAL	16
1	A	32	LEU	16
1	A	13	LYS	15
1	A	41	GLN	15
1	A	94	LYS	15
1	A	144	MET	15
1	A	22	ASP	15
1	A	31	GLU	14
1	A	49	GLN	14
1	A	71	MET	14
1	A	111	ASN	14
1	A	124	MET	14
1	A	17	SER	13
1	A	54	GLU	13
1	A	90	ARG	13
2	B	14	ARG	13
1	A	126	ARG	12
1	A	36	MET	12
1	A	143	GLN	12
1	A	109	MET	11
1	A	6	GLU	11
1	A	4	LEU	10
1	A	14	GLU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	95	ASP	10
1	A	127	GLU	10
1	A	87	GLU	10
1	A	115	LYS	10
1	A	106	ARG	10
1	A	5	THR	10
2	B	6	ILE	10
1	A	112	LEU	10
1	A	53	ASN	9
1	A	69	LEU	9
1	A	37	ARG	9
1	A	47	GLU	8
1	A	114	GLU	8
1	A	119	GLU	8
1	A	55	VAL	8
2	B	16	GLN	8
2	B	17	THR	7
1	A	101	SER	7
2	B	13	ASN	7
1	A	20	ASP	7
1	A	108	VAL	6
1	A	18	LEU	6
1	A	38	SER	6
1	A	45	GLU	6
1	A	145	MET	6
2	B	7	LEU	6
2	B	18	GLN	6
1	A	85	ILE	6
1	A	86	ARG	6
2	B	15	ILE	5
1	A	51	MET	5
1	A	91	VAL	5
1	A	137	ASN	4
1	A	63	ILE	4
1	A	116	LEU	4
1	A	142	VAL	4
1	A	123	GLU	4
1	A	120	GLU	3
1	A	121	VAL	3
1	A	131	ASP	3
1	A	135	GLN	3
2	B	5	GLN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	34	THR	3
1	A	11	GLU	3
1	A	44	THR	2
1	A	67	GLU	2
1	A	52	ILE	2
1	A	56	ASP	2
1	A	146	THR	2
1	A	8	GLN	2
2	B	10	ARG	1
1	A	138	TYR	1
1	A	29	THR	1
1	A	93	ASP	1
1	A	58	ASP	1
1	A	122	ASP	1
1	A	130	ILE	1
1	A	62	THR	1
1	A	110	THR	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided