



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:36 PM BST

PDB ID : 1CFF
Title : NMR SOLUTION STRUCTURE OF A COMPLEX OF CALMODULIN
WITH A BINDING PEPTIDE OF THE CA²⁺-PUMP
Authors : Elshorst, B.; Hennig, M.; Foersterling, H.; Diener, A.; Maurer, M.; Schulte,
P.; Schwalbe, H.; Krebs, J.; Schmid, H.; Vorherr, T.; Carafoli, E.; Griesinger,
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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

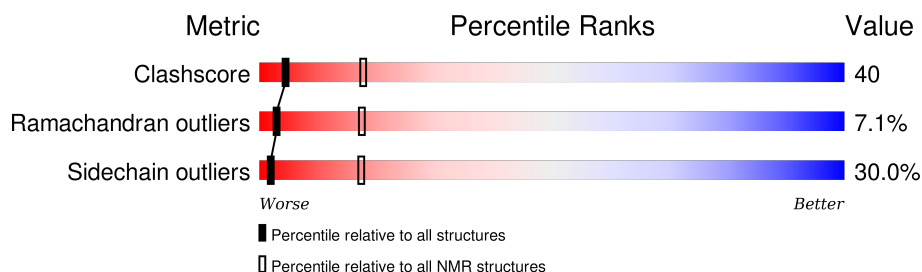
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	
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 [i](#)

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 PROTEIN (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 PROTEIN (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	MUTATION	UNP P62155

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

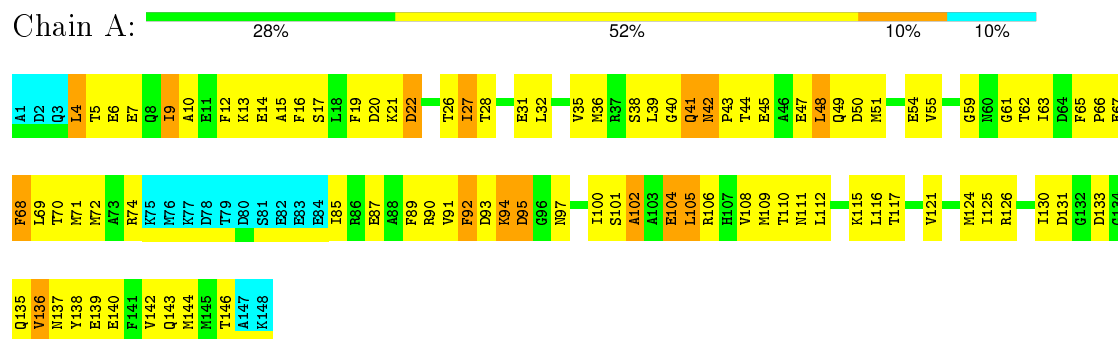
Mol	Chain	Residues	Atoms	
3	A	4	Total	Ca
			4	4

4 Residue-property plots

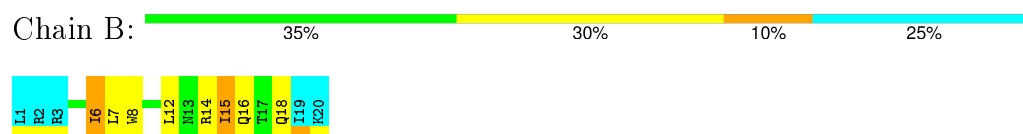
4.1 Average score per residue in the NMR ensemble

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: PROTEIN (CALMODULIN)



• Molecule 2: PROTEIN (CALCIUM PUMP)

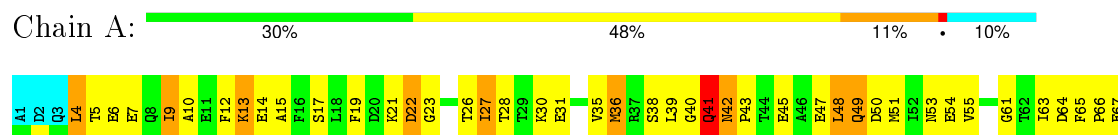


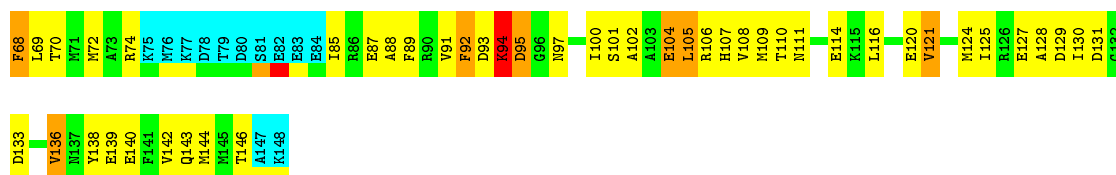
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PROTEIN (CALMODULIN)



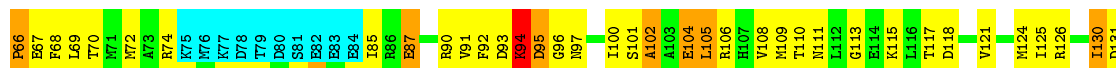
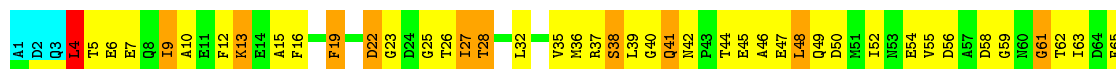


- Molecule 2: PROTEIN (CALCIUM PUMP)



4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (CALMODULIN)

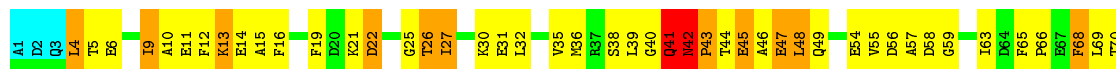


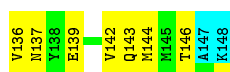
- Molecule 2: PROTEIN (CALCIUM PUMP)



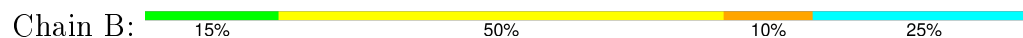
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (CALMODULIN)



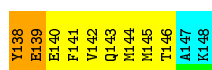
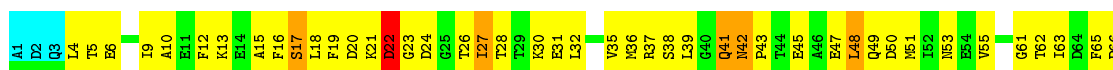


• Molecule 2: PROTEIN (CALCIUM PUMP)

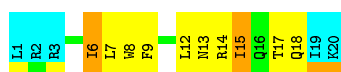


4.2.4 Score per residue for model 4

• Molecule 1: PROTEIN (CALMODULIN)

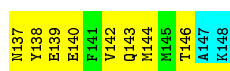
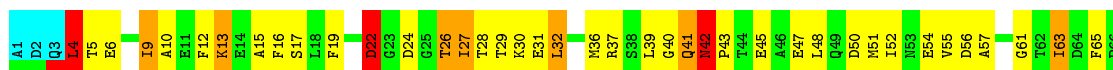


• Molecule 2: PROTEIN (CALCIUM PUMP)

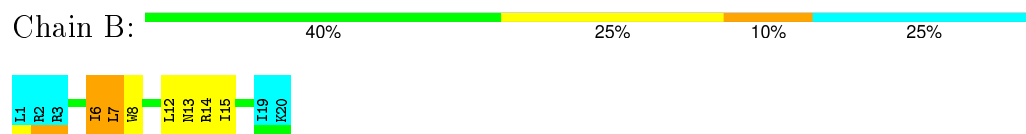


4.2.5 Score per residue for model 5

• Molecule 1: PROTEIN (CALMODULIN)

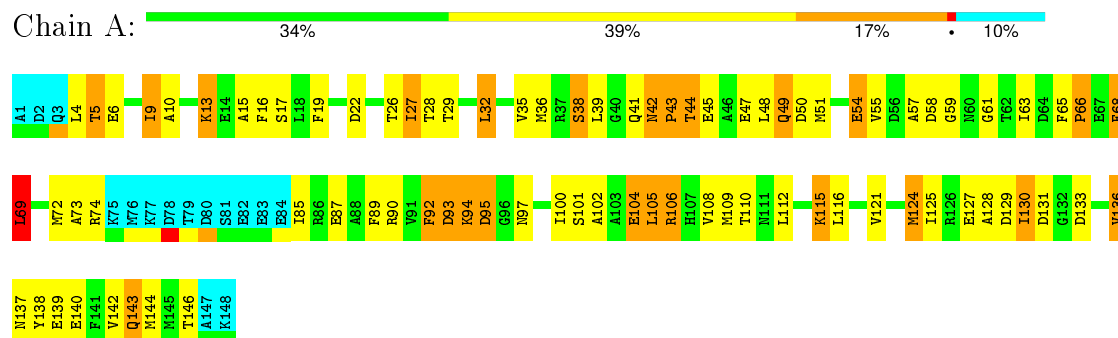


• Molecule 2: PROTEIN (CALCIUM PUMP)

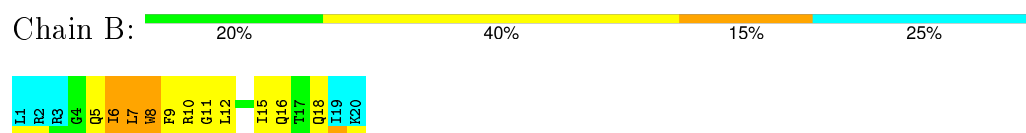


4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (CALMODULIN)

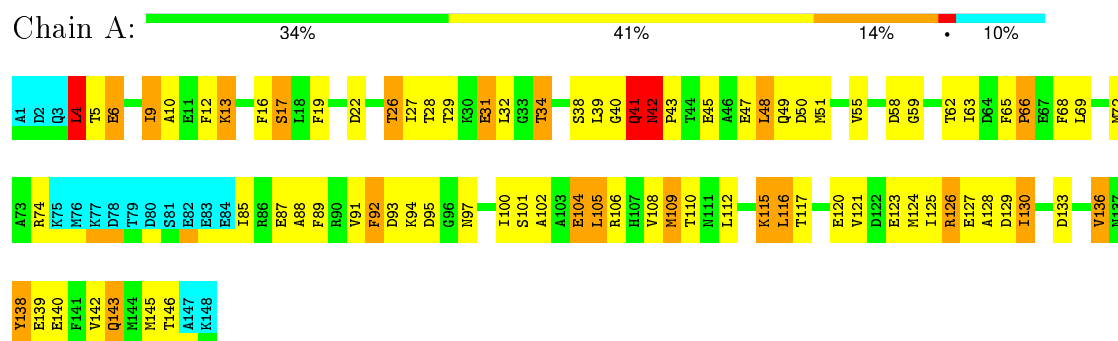


- Molecule 2: PROTEIN (CALCIUM PUMP)

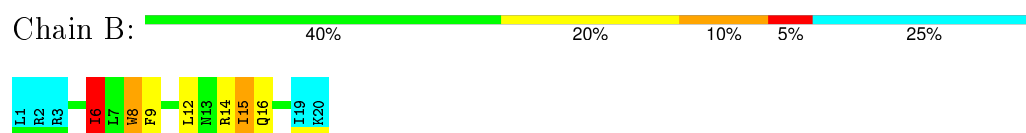


4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: PROTEIN (CALMODULIN)

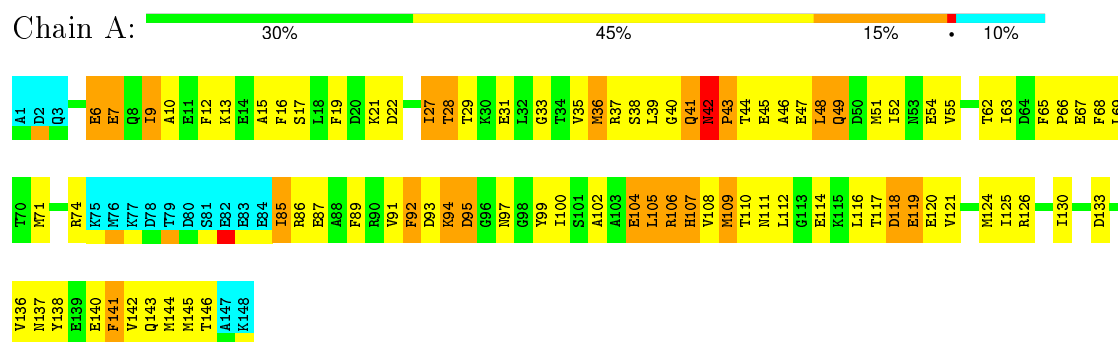


- Molecule 2: PROTEIN (CALCIUM PUMP)

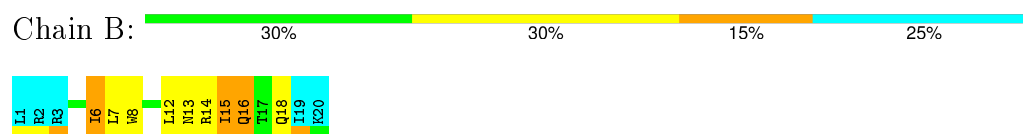


4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (CALMODULIN)

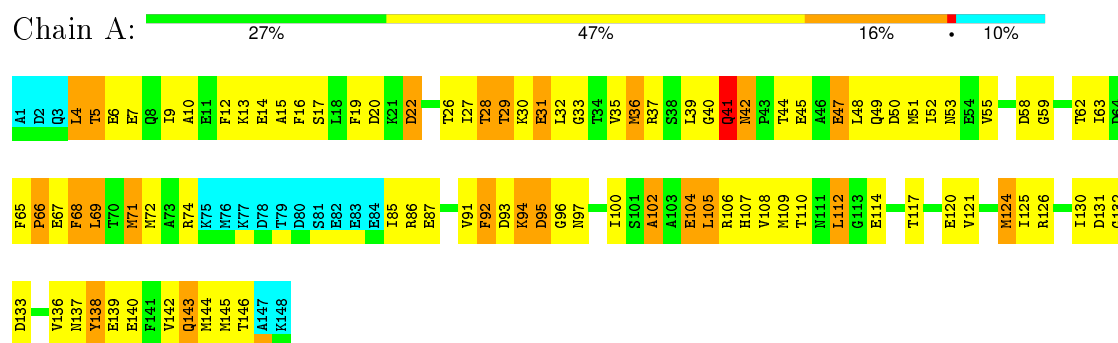


- Molecule 2: PROTEIN (CALCIUM PUMP)

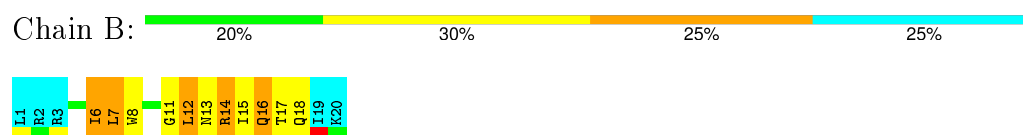


4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (CALMODULIN)

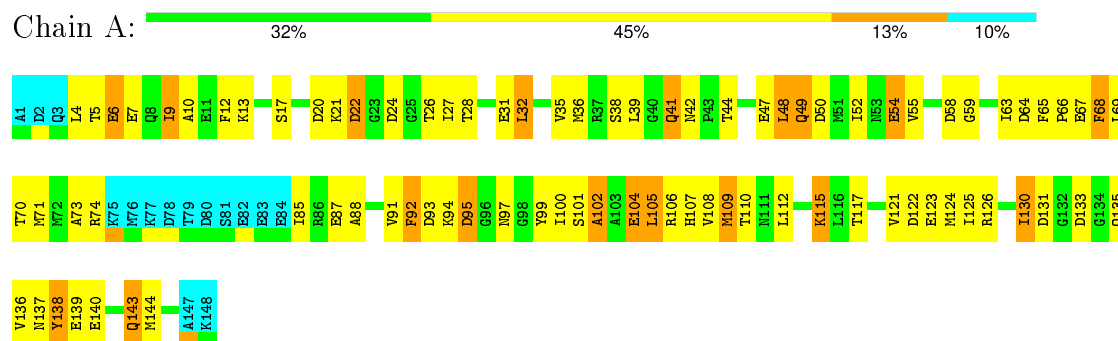


- Molecule 2: PROTEIN (CALCIUM PUMP)

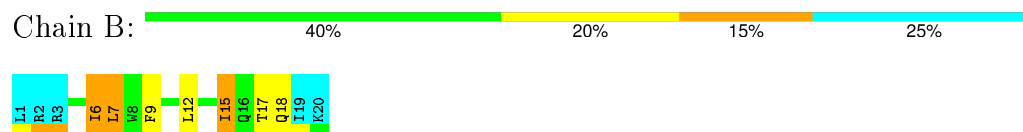


4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (CALMODULIN)

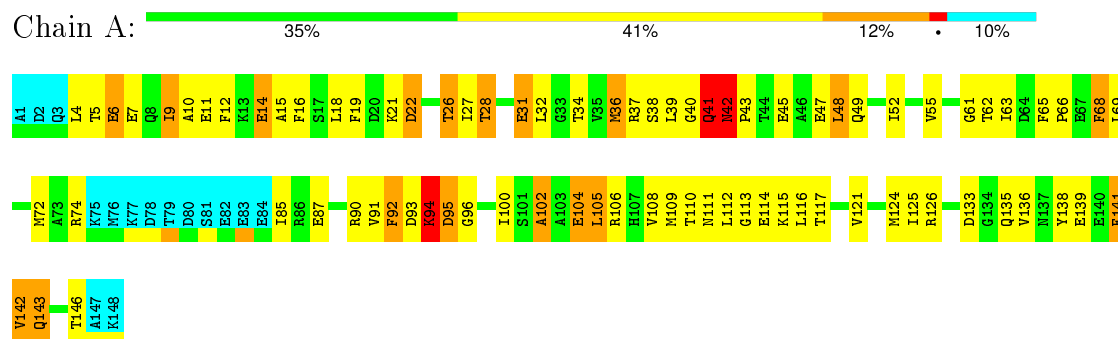


- Molecule 2: PROTEIN (CALCIUM PUMP)

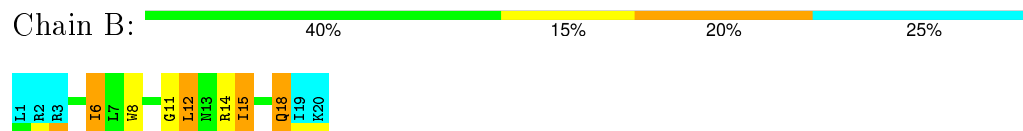


4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (CALMODULIN)

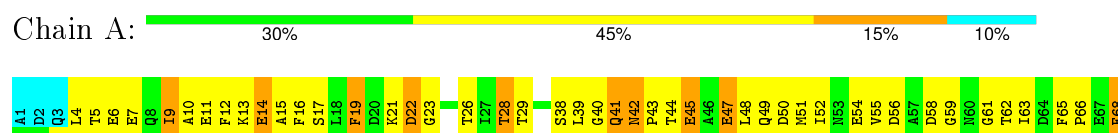


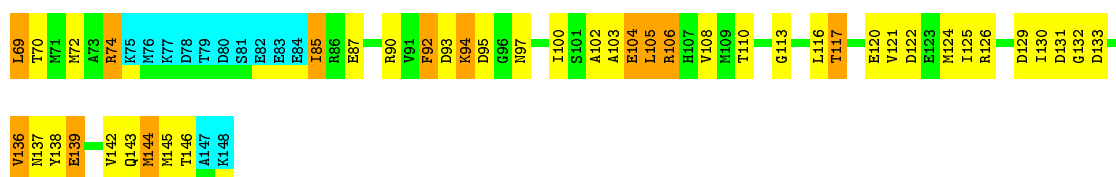
- Molecule 2: PROTEIN (CALCIUM PUMP)



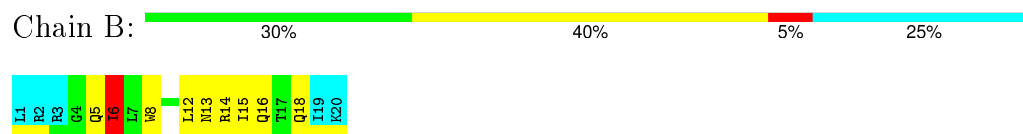
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (CALMODULIN)



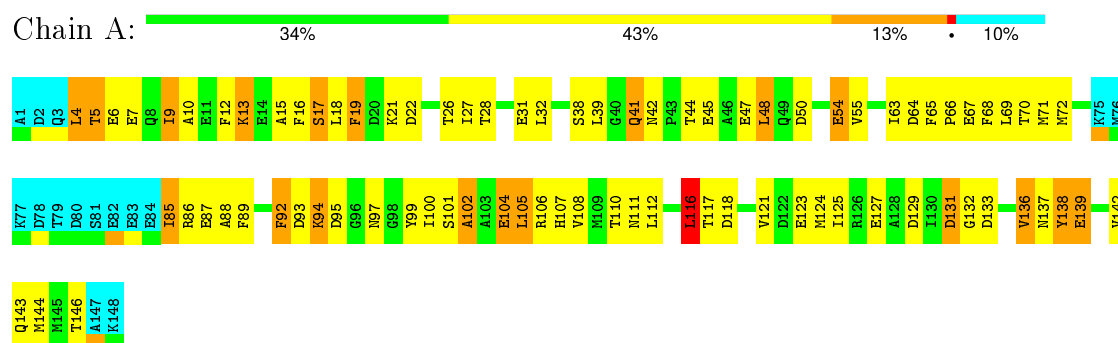


• Molecule 2: PROTEIN (CALCIUM PUMP)

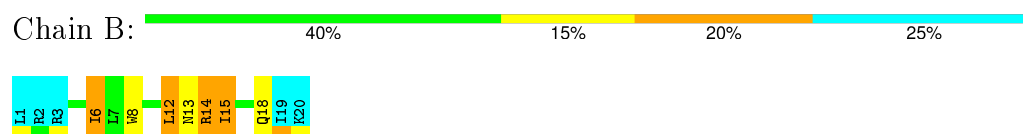


4.2.13 Score per residue for model 13

• Molecule 1: PROTEIN (CALMODULIN)

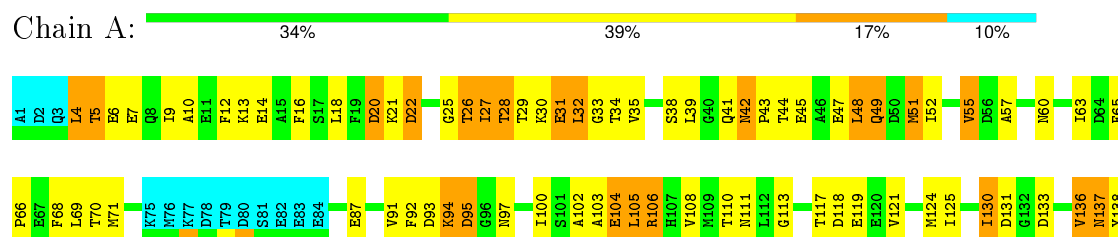


• Molecule 2: PROTEIN (CALCIUM PUMP)



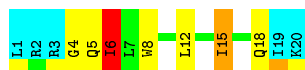
4.2.14 Score per residue for model 14

• Molecule 1: PROTEIN (CALMODULIN)



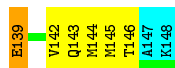
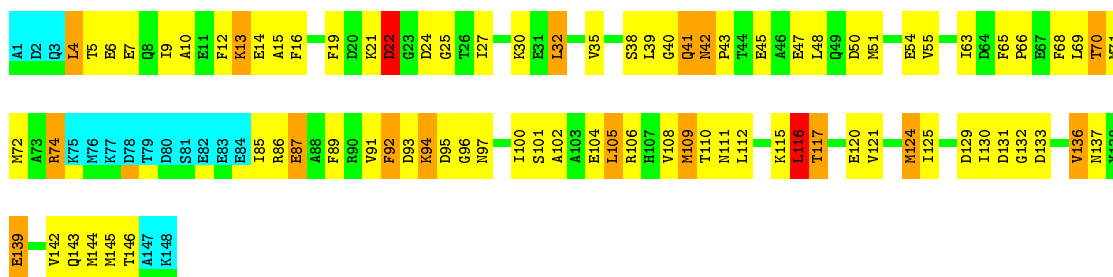


• Molecule 2: PROTEIN (CALCIUM PUMP)

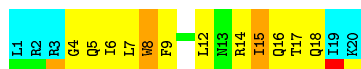
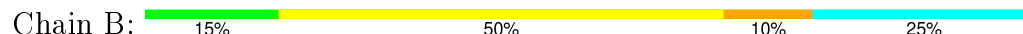


4.2.15 Score per residue for model 15

• Molecule 1: PROTEIN (CALMODULIN)

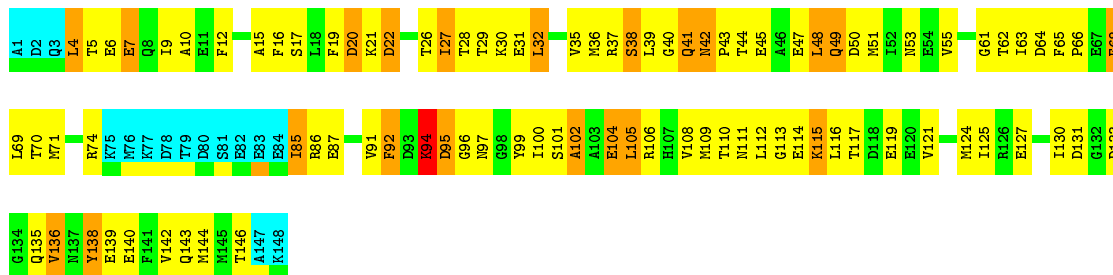


• Molecule 2: PROTEIN (CALCIUM PUMP)

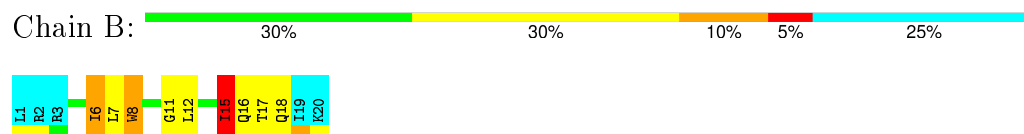


4.2.16 Score per residue for model 16

• Molecule 1: PROTEIN (CALMODULIN)

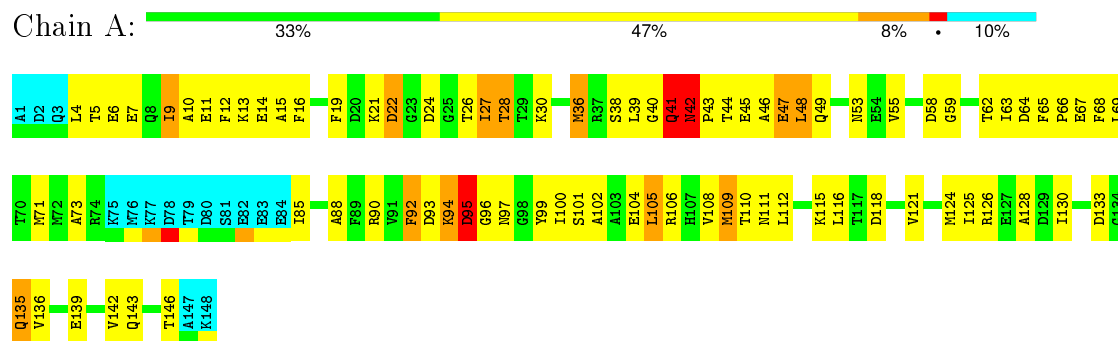


• Molecule 2: PROTEIN (CALCIUM PUMP)

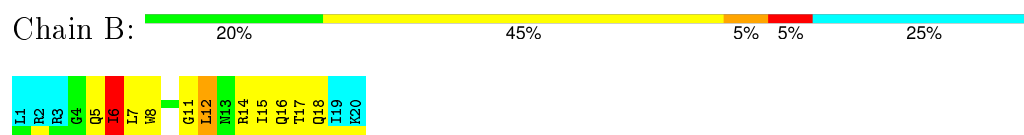


4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (CALMODULIN)

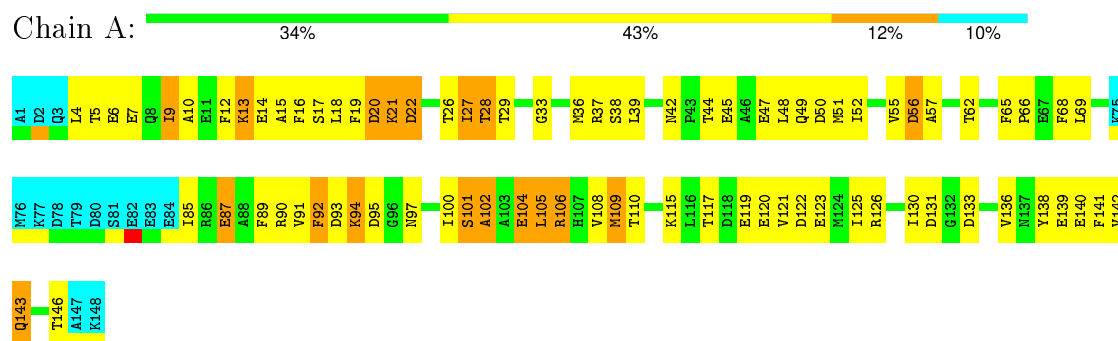


- Molecule 2: PROTEIN (CALCIUM PUMP)

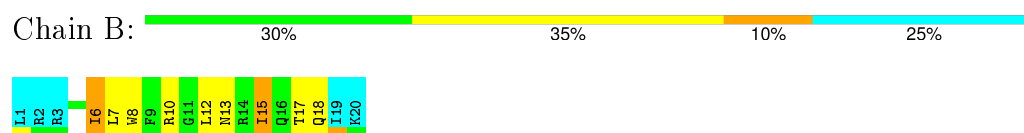


4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (CALMODULIN)

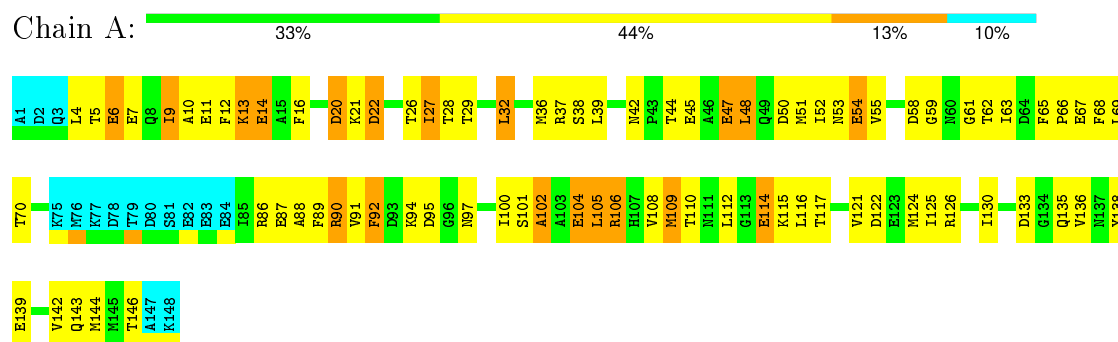


- Molecule 2: PROTEIN (CALCIUM PUMP)

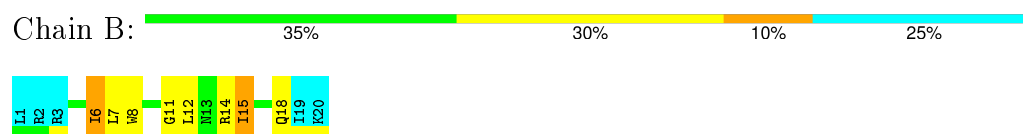


4.2.19 Score per residue for model 19

• Molecule 1: PROTEIN (CALMODULIN)

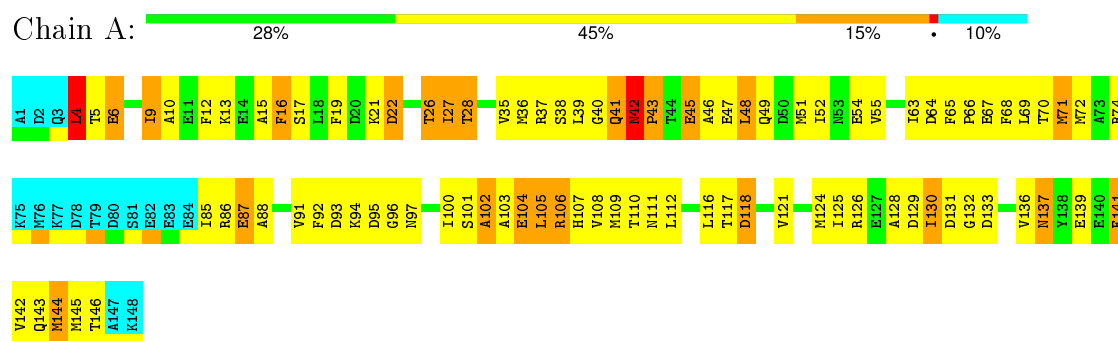


• Molecule 2: PROTEIN (CALCIUM PUMP)

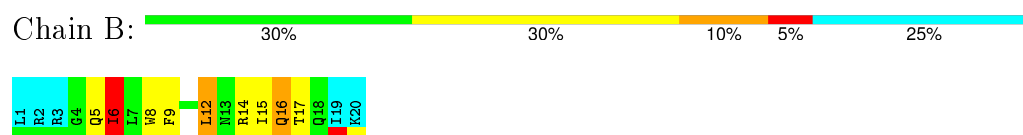


4.2.20 Score per residue for model 20

• Molecule 1: PROTEIN (CALMODULIN)

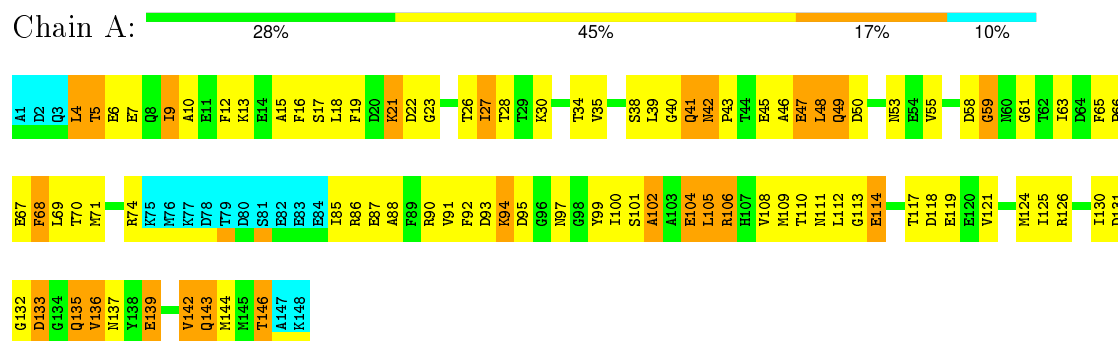


• Molecule 2: PROTEIN (CALCIUM PUMP)

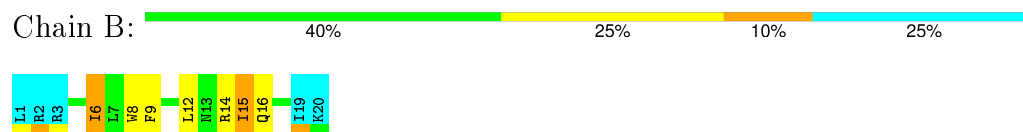


4.2.21 Score per residue for model 21

• Molecule 1: PROTEIN (CALMODULIN)

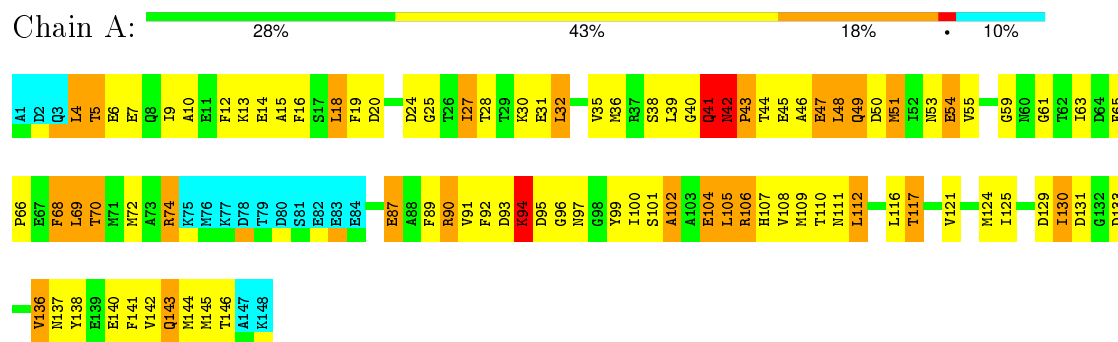


- Molecule 2: PROTEIN (CALCIUM PUMP)

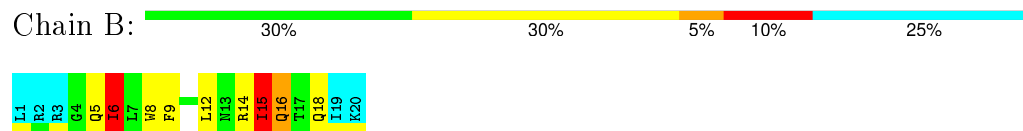


4.2.22 Score per residue for model 22

- Molecule 1: PROTEIN (CALMODULIN)

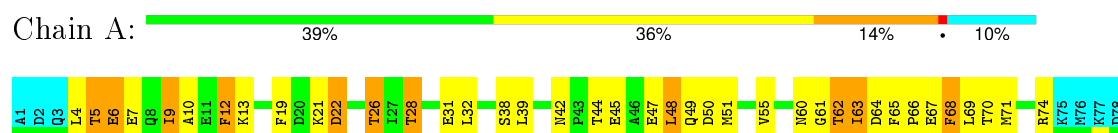


- Molecule 2: PROTEIN (CALCIUM PUMP)



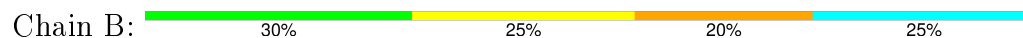
4.2.23 Score per residue for model 23

- Molecule 1: PROTEIN (CALMODULIN)





• Molecule 2: PROTEIN (CALCIUM PUMP)

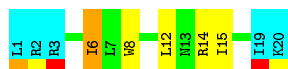


4.2.24 Score per residue for model 24

• Molecule 1: PROTEIN (CALMODULIN)

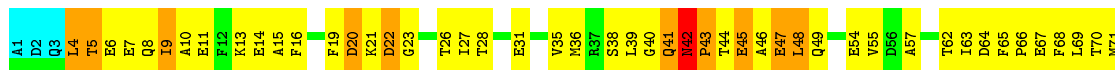


• Molecule 2: PROTEIN (CALCIUM PUMP)

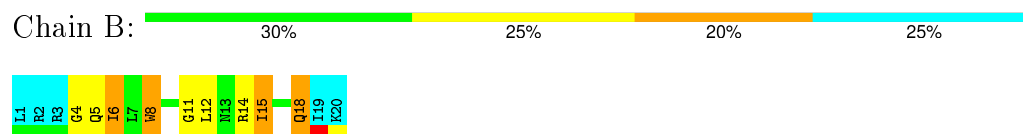


4.2.25 Score per residue for model 25

• Molecule 1: PROTEIN (CALMODULIN)

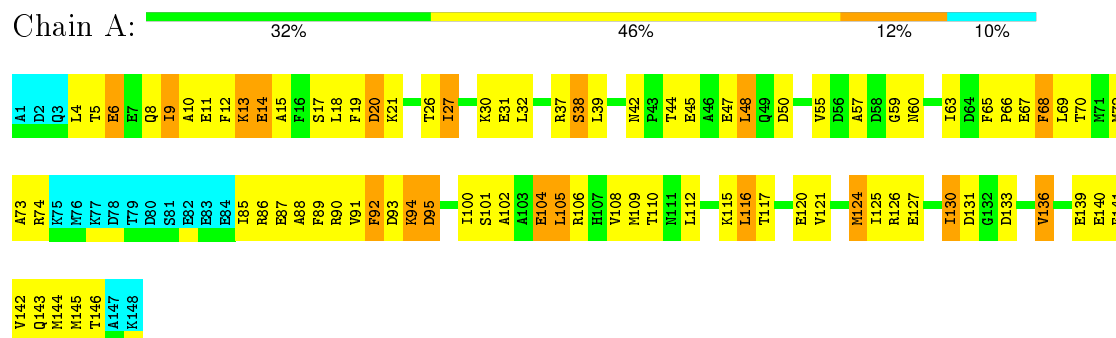


• Molecule 2: PROTEIN (CALCIUM PUMP)

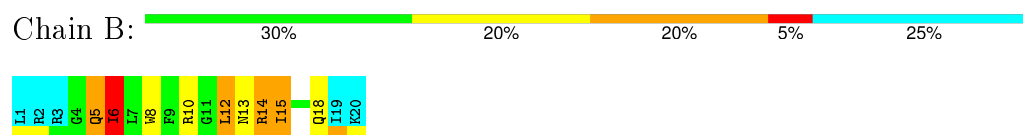


4.2.26 Score per residue for model 26

• Molecule 1: PROTEIN (CALMODULIN)



• Molecule 2: PROTEIN (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	

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

Chemical shift file(s)	BMRB entry 5480
Number of chemical shift lists	2
Total number of shifts	1962
Number of shifts mapped to atoms	1832
Number of unparsed shifts	0
Number of shifts with mapping errors	130
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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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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:26:THR:HG22	1:A:63:ILE:O	0.69	1.87	11	5
1:A:104:GLU:O	1:A:108:VAL:HG22	0.69	1.87	14	6
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:C	1:A:18:LEU:HD13	0.67	2.09	4	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: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
2:B:12:LEU:HD13	2:B:12:LEU:C	0.65	2.11	9	2
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: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
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: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	6
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	5
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
1:A:39:LEU:HD22	1:A:39:LEU:N	0.59	2.12	21	9
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:112:LEU:HD11	2:B:15:ILE:HG12	0.59	1.73	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:4:LEU:CG	1:A:69:LEU:HD21	0.58	2.28	21	5
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: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:29:THR:HG22	1:A:52:ILE:HG13	0.58	1.76	9	4
1:A:9:ILE:HG13	1:A:69:LEU:HD13	0.58	1.74	3	11
1:A:32:LEU:O	1:A:32:LEU:HD13	0.58	1.98	26	3
1:A:112:LEU:HD21	2:B:11:GLY:CA	0.58	2.27	6	2
1:A:105:LEU:HD21	2:B:8:TRP:CE3	0.58	2.34	15	3
1:A:112:LEU:HD23	2:B:15:ILE:HG23	0.58	1.75	3	1
1:A:62:THR:HG23	1:A:63:ILE:N	0.58	2.13	23	1
1:A:109:MET:HB3	1:A:116:LEU:HD21	0.58	1.74	15	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:27:ILE:HD13	1:A:27:ILE:N	0.58	2.12	3	4
1:A:107:HIS:O	1:A:110:THR:HG22	0.58	1.98	20	3
1:A:69:LEU:O	1:A:69:LEU:HD12	0.57	1.99	12	2
1:A:106:ARG:CG	1:A:121:VAL:HG11	0.57	2.29	2	2
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:100:ILE:H	1:A:136:VAL:HG13	0.56	1.59	23	2
1:A:55:VAL:O	1:A:55:VAL:HG22	0.56	2.00	17	6
1:A:35:VAL:HA	1:A:39:LEU:HD23	0.56	1.77	22	6
1:A:4:LEU:HD21	1:A:69:LEU:CD2	0.56	2.30	7	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
2:B:7:LEU:C	2:B:7:LEU:HD13	0.56	2.21	18	8
1:A:4:LEU:H	1:A:4:LEU:HD13	0.56	1.60	25	1
1:A:4:LEU:HD22	1:A:4:LEU:C	0.56	2.21	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:92:PHE:CZ	2:B:12:LEU:CD2	0.55	2.90	1	2
1:A:105:LEU:CD2	2:B:8:TRP:CZ3	0.55	2.90	3	2
2:B:12:LEU:HD22	2:B:12:LEU:C	0.55	2.21	3	2
1:A:4:LEU:C	1:A:4:LEU:HD22	0.55	2.22	3	2
2:B:6:ILE:O	2:B:6:ILE:HG23	0.55	2.01	12	4
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: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
1:A:55:VAL:HG22	1:A:55:VAL:O	0.55	2.02	13	3
1:A:69:LEU:HD12	1:A:69:LEU:C	0.54	2.20	12	4
2:B:5:GLN:O	2:B:6:ILE:HG22	0.54	2.02	17	4
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: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	1
1:A:117:THR:O	1:A:118:ASP:CB	0.54	2.56	20	2
1:A:92:PHE:HB3	1:A:100:ILE:HD11	0.54	1.79	25	6
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: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:63:ILE:CG2	1:A:68:PHE:CD2	0.53	2.92	23	4
1:A:29:THR:HB	1:A:48:LEU:HD11	0.53	1.79	7	1
1:A:136:VAL:HG13	1:A:136:VAL:O	0.53	2.01	3	2
1:A:124:MET:CE	2:B:8:TRP:CD1	0.53	2.90	9	9
1:A:63:ILE:N	1:A:63:ILE:HD13	0.53	2.19	5	1
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:16:PHE:CE1	1:A:27:ILE:HD11	0.53	2.38	21	2
1:A:16:PHE:CZ	1:A:65:PHE:N	0.53	2.76	13	2
1:A:39:LEU:N	1:A:39:LEU:CD1	0.53	2.72	4	1
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:87:GLU:O	1:A:91:VAL:HB	0.53	2.04	24	1
1:A:101:SER:O	1:A:102:ALA:HB2	0.53	2.04	21	9
1:A:13:LYS:CG	1:A:65:PHE:CD1	0.53	2.92	15	5
1:A:4:LEU:HD22	1:A:5:THR:O	0.53	2.03	1	3
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
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
2:B:15:ILE:HD12	2:B:15:ILE:C	0.51	2.26	20	1
1:A:27:ILE:CG2	1:A:32:LEU:HD23	0.51	2.35	15	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	13
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:26:THR:HB	1:A:62:THR:HG22	0.51	1.83	23	1
1:A:142:VAL:CG2	1:A:146:THR:OG1	0.51	2.59	11	1
1:A:100:ILE:CG2	1:A:105:LEU:CD2	0.51	2.89	11	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:109:MET:CG	1:A:116:LEU:HD12	0.50	2.36	7	1
1:A:26:THR:C	1:A:27:ILE:HD13	0.50	2.27	5	1
1:A:124:MET:HE1	2:B:8:TRP:CD1	0.50	2.42	17	1
1:A:4:LEU:HD13	1:A:4:LEU:H	0.49	1.65	22	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:103:ALA:O	1:A:106:ARG:HG3	0.49	2.07	20	2
1:A:32:LEU:O	1:A:35:VAL:HG12	0.49	2.07	14	3
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:28:THR:CG2	1:A:62:THR:CG2	0.49	2.90	8	2
1:A:125:ILE:CG2	1:A:136:VAL:CG2	0.49	2.91	20	4
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	2
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
2:B:7:LEU:HD13	2:B:7:LEU:C	0.49	2.28	19	1
1:A:39:LEU:CD2	1:A:39:LEU:N	0.49	2.75	18	7
1:A:65:PHE:N	1:A:66:PRO:CD	0.49	2.76	23	9
1:A:106:ARG:HG2	1:A:107:HIS:N	0.49	2.23	5	1
1:A:61:GLY:O	1:A:62:THR:HG23	0.49	2.08	16	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:B:7:LEU:C	2:B:7:LEU:HD12	0.48	2.28	9	2
1:A:144:MET:CE	2:B:9:PHE:CZ	0.48	2.96	3	2
1:A:114:GLU:CG	1:A:116:LEU:CD2	0.48	2.91	1	1
1:A:105:LEU:CB	1:A:121:VAL:CG2	0.48	2.91	19	5
1:A:48:LEU:N	1:A:48:LEU:HD23	0.48	2.23	15	2
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: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: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:4:LEU:HD21	1:A:69:LEU:HD21	0.47	1.86	7	1
1:A:13:LYS:HG3	1:A:65:PHE:CD1	0.47	2.44	5	2
1:A:18:LEU:C	1:A:18:LEU:CD1	0.47	2.81	4	2
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:9:ILE:CD1	1:A:69:LEU:HD23	0.47	2.39	9	2
1:A:44:THR:OG1	1:A:47:GLU:CB	0.47	2.63	13	13
1:A:89:PHE:HA	1:A:92:PHE:CE1	0.47	2.45	19	1
1:A:105:LEU:O	1:A:109:MET:CB	0.47	2.63	22	17
1:A:116:LEU:HD13	1:A:124:MET:SD	0.47	2.50	3	1
1:A:145:MET:HG3	2:B:9:PHE:CE2	0.47	2.45	22	1
1:A:94:LYS:CB	1:A:104:GLU:CG	0.47	2.93	5	3
1:A:55:VAL:HG23	1:A:71:MET:HG3	0.47	1.87	20	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
1:A:63:ILE:CD1	1:A:63:ILE:N	0.47	2.78	5	1
1:A:92:PHE:CE1	2:B:12:LEU:HD11	0.47	2.45	24	1

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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:9:ILE:O	1:A:12:PHE:N	0.47	2.48	20	21
2:B:6:ILE:O	2:B:6:ILE:CG2	0.47	2.62	19	4
2:B:12:LEU:HA	2:B:15:ILE:HD12	0.47	1.86	7	2
1:A:6:GLU:HA	1:A:9:ILE:HG22	0.47	1.87	7	3
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:145:MET:CG	2:B:9:PHE:CE2	0.46	2.97	22	1
1:A:13:LYS:HG2	1:A:65:PHE:CD1	0.46	2.45	15	2
1:A:108:VAL:HG23	1:A:109:MET:N	0.46	2.25	26	2
2:B:15:ILE:O	2:B:17:THR:N	0.46	2.48	16	3
1:A:4:LEU:CD2	1:A:69:LEU:HD21	0.46	2.41	7	2
1:A:114:GLU:CG	1:A:116:LEU:HD21	0.46	2.40	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
2:B:6:ILE:HG22	2:B:10:ARG:HD2	0.46	1.88	1	1
1:A:125:ILE:HG23	1:A:136:VAL:HB	0.46	1.88	23	2
1:A:65:PHE:O	1:A:69:LEU:CB	0.46	2.64	6	10
1:A:99:TYR:CE1	1:A:137:ASN:HB3	0.46	2.46	3	3
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:100:ILE:O	1:A:135:GLN:NE2	0.45	2.48	21	2
1:A:101:SER:CB	1:A:135:GLN:NE2	0.45	2.79	4	1
1:A:124:MET:HE1	2:B:8:TRP:CG	0.45	2.46	11	2
1:A:100:ILE:HB	1:A:136:VAL:HG11	0.45	1.88	10	2
1:A:106:ARG:O	1:A:110:THR:CG2	0.45	2.65	2	10
1:A:35:VAL:HG22	1:A:39:LEU:HD22	0.45	1.88	14	1
1:A:104:GLU:O	1:A:108:VAL:CG2	0.45	2.63	11	6
1:A:29:THR:HB	1:A:48:LEU:CD1	0.45	2.41	12	4
1:A:106:ARG:C	1:A:106:ARG:CD	0.45	2.84	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:VAL:CG2	1:A:55:VAL:O	0.45	2.64	14	1
1:A:102:ALA:O	1:A:121:VAL:HG21	0.45	2.12	19	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: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:122:ASP:OD1	1:A:126:ARG:NE	0.45	2.50	12	1
1:A:112:LEU:CD1	2:B:15:ILE:CG1	0.45	2.94	10	1
1:A:45:GLU:O	1:A:48:LEU:CD1	0.45	2.64	3	13
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:124:MET:CE	2:B:8:TRP:CG	0.45	2.99	2	3
1:A:116:LEU:HD22	1:A:121:VAL:CG2	0.45	2.33	15	1
1:A:4:LEU:C	1:A:4:LEU:HD12	0.45	2.32	12	2
1:A:46:ALA:O	1:A:49:GLN:N	0.45	2.50	8	7
1:A:4:LEU:HD23	1:A:5:THR:O	0.45	2.12	17	2
2:B:7:LEU:O	2:B:7:LEU:HD13	0.45	2.12	4	1
1:A:4:LEU:O	1:A:5:THR:O	0.45	2.34	25	1
1:A:116:LEU:CD1	1:A:116:LEU:O	0.45	2.64	15	2
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:122:ASP:O	1:A:126:ARG:CD	0.45	2.64	12	2
1:A:136:VAL:CG1	1:A:136:VAL:O	0.45	2.65	3	6
1:A:112:LEU:HD11	2:B:15:ILE:HG13	0.45	1.89	11	3
1:A:105:LEU:O	1:A:109:MET:N	0.45	2.46	24	6
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:112:LEU:CD2	2:B:15:ILE:HG12	0.44	2.42	20	1
1:A:35:VAL:HA	1:A:39:LEU:HD13	0.44	1.88	15	1
1:A:48:LEU:HD23	1:A:48:LEU:N	0.44	2.27	9	3
1:A:95:ASP:OD2	1:A:97:ASN:ND2	0.44	2.50	23	1
1:A:54:GLU:CA	1:A:54:GLU:OE1	0.44	2.65	6	1
2:B:14:ARG:O	2:B:18:GLN:N	0.44	2.49	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:12:LEU:CD1	2:B:12:LEU:O	0.44	2.66	17	1
1:A:104:GLU:O	1:A:108:VAL:CB	0.44	2.65	20	4
1:A:92:PHE:CD1	1:A:100:ILE:CD1	0.44	2.88	19	1
1:A:106:ARG:O	1:A:110:THR:HB	0.44	2.11	25	2
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:64:ASP:N	1:A:67:GLU:OE1	0.44	2.50	17	3
1:A:4:LEU:HD11	1:A:9:ILE:CG1	0.44	2.42	21	1
1:A:102:ALA:O	1:A:106:ARG:N	0.44	2.50	5	3
1:A:89:PHE:CE2	1:A:90:ARG:NE	0.44	2.85	22	1
1:A:32:LEU:HA	1:A:35:VAL:CG2	0.44	2.42	16	1
1:A:85:ILE:O	1:A:89:PHE:CB	0.44	2.65	8	2
1:A:55:VAL:O	1:A:57:ALA:N	0.44	2.49	5	7
1:A:138:TYR:CE1	1:A:141:PHE:CD2	0.44	3.05	24	1
1:A:4:LEU:HD11	1:A:69:LEU:HG	0.44	1.88	9	1
1:A:38:SER:OG	1:A:39:LEU:HD22	0.44	2.13	19	1
1:A:44:THR:O	1:A:47:GLU:CG	0.44	2.66	22	4
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:117:THR:O	1:A:121:VAL:CG1	0.44	2.66	16	5
1:A:40:GLY:O	1:A:41:GLN:C	0.44	2.56	3	8
1:A:130:ILE:HG22	1:A:131:ASP:N	0.44	2.27	10	1
1:A:10:ALA:O	1:A:13:LYS:CB	0.44	2.66	9	9
1:A:118:ASP:HA	1:A:121:VAL:HG12	0.44	1.89	21	3
1:A:37:ARG:O	1:A:41:GLN:CG	0.44	2.66	2	1
1:A:115:LYS:O	1:A:115:LYS:CG	0.44	2.65	16	4
1:A:95:ASP:OD1	1:A:95:ASP:N	0.43	2.50	19	2
1:A:105:LEU:HB3	1:A:121:VAL:CG2	0.43	2.43	6	4
1:A:64:ASP:N	1:A:67:GLU:OE2	0.43	2.51	10	1
1:A:35:VAL:O	1:A:39:LEU:HD23	0.43	2.13	2	1
1:A:144:MET:CG	2:B:9:PHE:CZ	0.43	3.01	6	1
1:A:42:ASN:N	1:A:43:PRO:HD2	0.43	2.28	14	3
1:A:38:SER:OG	1:A:39:LEU:CD2	0.43	2.66	19	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:4:LEU:O	1:A:4:LEU:HD22	0.43	2.13	16	1
1:A:20:ASP:O	1:A:31:GLU:CG	0.43	2.65	16	1
1:A:137:ASN:O	1:A:139:GLU:N	0.43	2.51	13	3
1:A:61:GLY:O	1:A:62:THR:CG2	0.43	2.67	16	3
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: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:16:PHE:CE2	1:A:27:ILE:HD11	0.43	2.48	20	1
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:104:GLU:O	1:A:108:VAL:CG1	0.43	2.65	11	2
1:A:13:LYS:HG3	1:A:65:PHE:CG	0.43	2.48	5	1
1:A:87:GLU:O	1:A:91:VAL:N	0.43	2.46	24	1
1:A:63:ILE:N	1:A:63:ILE:CD1	0.43	2.80	23	1
1:A:20:ASP:OD1	1:A:31:GLU:CB	0.43	2.67	26	1
1:A:137:ASN:ND2	1:A:139:GLU:HG3	0.43	2.28	4	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: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:88:ALA:HA	1:A:91:VAL:CG1	0.43	2.43	24	1
1:A:112:LEU:HD21	2:B:12:LEU:HA	0.43	1.88	9	1
2:B:7:LEU:HD22	2:B:7:LEU:C	0.43	2.33	6	1
1:A:64:ASP:N	1:A:64:ASP:OD1	0.43	2.51	25	1
1:A:54:GLU:N	1:A:54:GLU:OE1	0.43	2.52	19	1
1:A:33:GLY:O	1:A:37:ARG:N	0.43	2.52	8	2
1:A:18:LEU:O	1:A:21:LYS:N	0.43	2.50	21	4
1:A:138:TYR:O	1:A:141:PHE:N	0.43	2.51	11	3
1:A:138:TYR:CD2	1:A:142:VAL:HG13	0.43	2.49	9	1
1:A:85:ILE:O	1:A:89:PHE:N	0.43	2.48	6	2
1:A:136:VAL:O	1:A:136:VAL:CG1	0.43	2.65	4	1
1:A:137:ASN:N	1:A:140:GLU:OE2	0.43	2.50	25	1
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:50:ASP:O	1:A:54:GLU:CG	0.43	2.67	22	6
1:A:65:PHE:CZ	1:A:69:LEU:HD22	0.43	2.49	8	1
1:A:13:LYS:O	1:A:17:SER:N	0.43	2.52	26	5
1:A:124:MET:O	1:A:128:ALA:CB	0.43	2.67	1	1
1:A:69:LEU:O	1:A:73:ALA:CB	0.43	2.67	26	1
1:A:32:LEU:O	1:A:35:VAL:CG2	0.43	2.67	16	1
1:A:9:ILE:CD1	1:A:69:LEU:CD1	0.43	2.95	19	4
1:A:5:THR:O	1:A:9:ILE:CD1	0.43	2.67	22	1
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
1:A:60:ASN:OD1	1:A:60:ASN:N	0.43	2.52	14	1
1:A:58:ASP:OD1	1:A:59:GLY:N	0.43	2.52	19	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:ARG:O	1:A:90:ARG:CG	0.43	2.66	19	1
1:A:20:ASP:OD1	1:A:22:ASP:CB	0.43	2.67	18	2
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:122:ASP:OD1	1:A:123:GLU:N	0.43	2.52	18	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:88:ALA:O	1:A:92:PHE:CD2	0.43	2.72	19	1
1:A:137:ASN:OD1	1:A:138:TYR:N	0.43	2.52	10	4
1:A:85:ILE:CG2	1:A:88:ALA:HB3	0.43	2.43	21	2
1:A:29:THR:HB	1:A:48:LEU:CG	0.43	2.44	7	1
1:A:105:LEU:HD11	2:B:8:TRP:CE3	0.43	2.49	22	1
1:A:115:LYS:O	1:A:117:THR:N	0.43	2.52	4	1
1:A:55:VAL:HG22	1:A:63:ILE:CD1	0.43	2.44	15	1
1:A:128:ALA:O	1:A:130:ILE:N	0.42	2.52	7	6
1:A:94:LYS:CB	1:A:104:GLU:HG2	0.42	2.44	15	5
1:A:62:THR:CG2	1:A:63:ILE:N	0.42	2.80	23	1
1:A:44:THR:O	1:A:48:LEU:CD1	0.42	2.67	26	3
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:47:GLU:OE1	1:A:48:LEU:N	0.42	2.52	20	1
1:A:74:ARG:CG	1:A:74:ARG:O	0.42	2.67	24	3
1:A:67:GLU:CG	1:A:68:PHE:N	0.42	2.82	21	2
1:A:121:VAL:CG1	1:A:122:ASP:N	0.42	2.82	3	1
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:104:GLU:O	1:A:108:VAL:HB	0.42	2.14	20	2
1:A:144:MET:HG3	2:B:9:PHE:CZ	0.42	2.50	10	2
1:A:39:LEU:O	1:A:41:GLN:CG	0.42	2.68	3	2
1:A:27:ILE:O	1:A:63:ILE:HG12	0.42	2.14	7	4
1:A:13:LYS:HB2	1:A:65:PHE:CE1	0.42	2.49	18	6
2:B:11:GLY:O	2:B:14:ARG:N	0.42	2.52	9	2
1:A:116:LEU:HD22	1:A:116:LEU:N	0.42	2.29	1	1
1:A:44:THR:O	1:A:48:LEU:CG	0.42	2.66	23	1
1:A:60:ASN:N	1:A:60:ASN:OD1	0.42	2.53	23	2
1:A:28:THR:HA	1:A:52:ILE:HD12	0.42	1.90	18	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:29:THR:O	1:A:48:LEU:HD12	0.42	2.14	19	1
1:A:105:LEU:HB2	1:A:121:VAL:CG2	0.42	2.44	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:THR:OG1	1:A:47:GLU:HB2	0.42	2.14	10	5
1:A:4:LEU:CD2	1:A:69:LEU:CD2	0.42	2.96	7	1
1:A:93:ASP:O	1:A:96:GLY:N	0.42	2.52	22	1
1:A:4:LEU:C	1:A:4:LEU:HD23	0.42	2.35	9	1
1:A:92:PHE:CZ	1:A:105:LEU:HD22	0.42	2.48	8	3
1:A:100:ILE:O	1:A:136:VAL:CG1	0.42	2.68	11	3
1:A:99:TYR:OH	1:A:137:ASN:ND2	0.42	2.52	8	1
1:A:27:ILE:CD1	1:A:27:ILE:N	0.42	2.80	21	1
1:A:131:ASP:OD1	1:A:131:ASP:N	0.42	2.52	22	2
1:A:137:ASN:N	1:A:140:GLU:OE1	0.42	2.52	9	3
1:A:28:THR:O	1:A:32:LEU:CB	0.42	2.68	9	1
1:A:36:MET:O	1:A:40:GLY:CA	0.42	2.67	2	1
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:137:ASN:ND2	1:A:140:GLU:OE1	0.42	2.52	4	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:28:THR:HG23	1:A:62:THR:CB	0.42	2.45	9	1
1:A:9:ILE:CG1	1:A:65:PHE:CZ	0.42	3.02	17	3
1:A:131:ASP:N	1:A:131:ASP:OD1	0.42	2.53	10	3
1:A:47:GLU:O	1:A:51:MET:N	0.42	2.50	20	7
1:A:137:ASN:ND2	1:A:139:GLU:HG2	0.42	2.30	15	4
1:A:4:LEU:CD2	1:A:5:THR:O	0.42	2.67	3	2
1:A:108:VAL:O	1:A:112:LEU:N	0.42	2.51	26	2
1:A:45:GLU:O	1:A:48:LEU:CG	0.42	2.67	4	2
2:B:5:GLN:HB2	2:B:9:PHE:CE2	0.42	2.49	15	1
1:A:16:PHE:CE2	1:A:27:ILE:HG12	0.42	2.50	15	1
1:A:63:ILE:HG21	1:A:68:PHE:CG	0.42	2.49	11	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:46:ALA:O	1:A:50:ASP:N	0.42	2.52	2	2
2:B:12:LEU:HD13	2:B:15:ILE:CG1	0.42	2.45	17	1
1:A:99:TYR:HB3	1:A:135:GLN:NE2	0.42	2.29	16	1
1:A:115:LYS:CG	1:A:115:LYS:O	0.42	2.68	10	2
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:105:LEU:O	1:A:116:LEU:CD1	0.42	2.67	25	1
1:A:4:LEU:HD11	1:A:9:ILE:CD1	0.42	2.26	19	1
1:A:105:LEU:CB	1:A:121:VAL:HG23	0.42	2.42	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:GLU:O	1:A:91:VAL:CG2	0.42	2.66	10	2
1:A:6:GLU:O	1:A:10:ALA:N	0.42	2.53	16	2
1:A:101:SER:O	1:A:102:ALA:CB	0.42	2.68	21	2
1:A:109:MET:HG3	1:A:116:LEU:CD2	0.42	2.45	1	1
1:A:44:THR:OG1	1:A:47:GLU:N	0.42	2.51	9	1
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:114:GLU:N	1:A:114:GLU:OE1	0.41	2.53	19	1
1:A:100:ILE:CG2	1:A:105:LEU:HG	0.41	2.45	10	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:61:GLY:O	1:A:62:THR:HG22	0.41	2.15	23	1
1:A:109:MET:CG	1:A:114:GLU:OE2	0.41	2.68	16	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:99:TYR:CE1	1:A:137:ASN:HA	0.41	2.49	5	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:88:ALA:HA	1:A:91:VAL:HG12	0.41	1.93	24	1
1:A:55:VAL:O	1:A:67:GLU:CG	0.41	2.68	2	1
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:142:VAL:CG1	1:A:143:GLN:N	0.41	2.83	21	1
1:A:112:LEU:HD11	2:B:15:ILE:HG23	0.41	1.92	6	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:105:LEU:CD1	1:A:121:VAL:CG2	0.41	2.98	20	1
1:A:116:LEU:HD13	1:A:116:LEU:O	0.41	2.15	15	1
1:A:88:ALA:HB2	2:B:12:LEU:HD21	0.41	1.89	3	1
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:94:LYS:O	1:A:95:ASP:HB3	0.41	2.15	6	2
1:A:42:ASN:N	1:A:43:PRO:CD	0.41	2.83	6	1
1:A:85:ILE:O	1:A:87:GLU:N	0.41	2.53	26	1
1:A:88:ALA:HB1	2:B:12:LEU:CG	0.41	2.40	7	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:106:ARG:CD	1:A:121:VAL:HG11	0.41	2.45	9	1
1:A:109:MET:HE3	2:B:8:TRP:HA	0.41	1.91	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LYS:HG3	1:A:65:PHE:CE1	0.41	2.51	23	2
1:A:124:MET:HE3	2:B:8:TRP:CG	0.41	2.50	15	2
1:A:92:PHE:O	1:A:104:GLU:OE1	0.41	2.38	13	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: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: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:125:ILE:O	1:A:129:ASP:N	0.41	2.52	25	1
1:A:32:LEU:O	1:A:35:VAL:CG1	0.41	2.69	14	1
1:A:100:ILE:HB	1:A:136:VAL:CG1	0.41	2.45	10	2
1:A:118:ASP:OD1	1:A:119:GLU:N	0.41	2.54	8	1
1:A:16:PHE:O	1:A:27:ILE:CD1	0.41	2.68	6	1
1:A:109:MET:HE2	1:A:114:GLU:HG3	0.41	1.92	21	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:109:MET:HB3	1:A:116:LEU:HD11	0.41	1.92	25	1
1:A:34:THR:O	1:A:38:SER:CB	0.41	2.68	14	1
1:A:102:ALA:O	1:A:105:LEU:N	0.41	2.54	11	1
1:A:64:ASP:OD1	1:A:67:GLU:CB	0.41	2.68	13	2
1:A:18:LEU:HD13	1:A:18:LEU:O	0.41	2.16	13	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:42:ASN:CB	1:A:43:PRO:HD3	0.41	2.46	8	3
2:B:15:ILE:O	2:B:16:GLN:C	0.41	2.59	22	1
1:A:105:LEU:HB3	1:A:121:VAL:HG21	0.41	1.93	20	1
1:A:55:VAL:HB	1:A:63:ILE:CD1	0.41	2.46	16	1
1:A:69:LEU:CD1	1:A:73:ALA:HB2	0.40	2.46	10	1
1:A:55:VAL:CG1	1:A:63:ILE:CG1	0.40	2.99	10	1
1:A:10:ALA:O	1:A:13:LYS:N	0.40	2.54	21	1
1:A:145:MET:HB2	2:B:9:PHE:CE2	0.40	2.51	7	1
1:A:39:LEU:O	1:A:41:GLN:HG2	0.40	2.16	3	1
1:A:32:LEU:HD13	1:A:32:LEU:O	0.40	2.15	5	1
1:A:105:LEU:O	1:A:109:MET:HB2	0.40	2.16	7	2
1:A:94:LYS:HB2	1:A:104:GLU:HG2	0.40	1.93	5	1
1:A:142:VAL:CG2	1:A:143:GLN:N	0.40	2.84	1	1
1:A:9:ILE:HG12	1:A:65:PHE:CE1	0.40	2.51	9	1
1:A:20:ASP:OD1	1:A:20:ASP:O	0.40	2.39	9	1
1:A:55:VAL:CG1	1:A:55:VAL:O	0.40	2.67	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:B:12:LEU:HD22	2:B:12:LEU:H	0.40	1.76	14	1
1:A:51:MET:HG3	1:A:52:ILE:N	0.40	2.30	14	1
1:A:48:LEU:N	1:A:48:LEU:CD2	0.40	2.85	19	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:N	0.40	2.52	22	1
1:A:124:MET:HG3	1:A:125:ILE:N	0.40	2.32	1	1
1:A:4:LEU:C	1:A:4:LEU:HD13	0.40	2.37	24	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:20:ASP:OD2	1:A:24:ASP:CB	0.40	2.69	10	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:120:GLU:CG	1:A:121:VAL:N	0.40	2.84	7	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:92:PHE:CE1	2:B:8:TRP:CE3	0.40	3.10	20	1
1:A:20:ASP:OD2	1:A:24:ASP:N	0.40	2.53	10	1
1:A:40:GLY:O	1:A:43:PRO:CD	0.40	2.70	3	1
1:A:101:SER:HA	1:A:135:GLN:NE2	0.40	2.32	23	1
1:A:29:THR:CG2	1:A:48:LEU:HD13	0.40	2.45	14	1
1:A:48:LEU:HD12	1:A:48:LEU:N	0.40	2.32	13	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	133/148 (90%)	102±3 (77±2%)	22±3 (17±2%)	9±3 (7±2%)	3	19
2	B	15/20 (75%)	10±1 (66±7%)	3±1 (22±6%)	2±1 (12±5%)	1	7
All	All	3848/4368 (88%)	2915 (76%)	658 (17%)	275 (7%)	3	17

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%)	2 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	13/18 (72%)	10±2 (76±12%)	3±2 (24±12%)	3	28
All	All	3276/3744 (88%)	2292 (70%)	984 (30%)	2	17

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
1	A	106	ARG	13
1	A	126	ARG	13

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Mol	Chain	Res	Type	Models (Total)
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
1	A	137	ASN	4
1	A	131	ASP	4

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Mol	Chain	Res	Type	Models (Total)
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

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5480

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1832
Number of shifts mapped to atoms	1832
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	148	-0.16 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	137	0.26 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	148	-0.51 ± 0.07	Should be applied
^{15}N	145	0.76 ± 0.19	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1472 atoms were assigned a chemical shift out of a possible 1799. 16 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	661/736 (90%)	264/294 (90%)	266/296 (90%)	131/146 (90%)
Sidechain	730/947 (77%)	434/547 (79%)	285/356 (80%)	11/44 (25%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	81/116 (70%)	46/63 (73%)	35/51 (69%)	0/2 (0%)
Overall	1472/1799 (82%)	744/904 (82%)	586/703 (83%)	142/192 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1638 atoms were assigned a chemical shift out of a possible 2067. 16 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	734/836 (88%)	293/334 (88%)	296/336 (88%)	145/166 (87%)
Sidechain	823/1115 (74%)	492/646 (76%)	319/414 (77%)	12/55 (22%)
Aromatic	81/116 (70%)	46/63 (73%)	35/51 (69%)	0/2 (0%)
Overall	1638/2067 (79%)	831/1043 (80%)	650/801 (81%)	157/223 (70%)

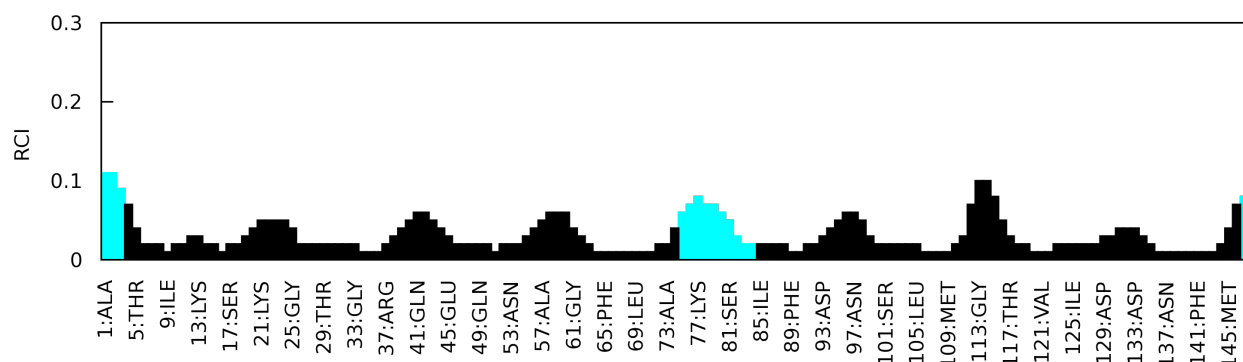
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5480

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping

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

Total number of shifts	130
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	130
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 130 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	17	LEU	HD22	0.874	0.05	2
UNMAPPED	3	ARG	HA	4.245	0.05	1
UNMAPPED	7	PHE	HZ	6.748	0.05	1
UNMAPPED	26	ARG	HB2	1.735	0.05	2
UNMAPPED	1	GLN	HG3	2.258	0.05	1
UNMAPPED	5	GLY	HA2	3.991	0.05	2
UNMAPPED	22	TYR	HB2	3.067	0.05	2
UNMAPPED	25	PHE	HD1	6.857	0.05	3
UNMAPPED	16	VAL	HA	3.675	0.05	1
UNMAPPED	15	GLY	HA2	3.981	0.05	2
UNMAPPED	22	TYR	HE2	6.695	0.05	1
UNMAPPED	16	VAL	HG21	1.008	0.05	2
UNMAPPED	26	ARG	HG3	1.329	0.05	2
UNMAPPED	2	GLN	H	8.449	0.05	1
UNMAPPED	20	TRP	H	8.392	0.05	1
UNMAPPED	6	GLY	H	8.472	0.05	1
UNMAPPED	3	ARG	HB2	1.771	0.05	2
UNMAPPED	7	PHE	HB3	3.071	0.05	2
UNMAPPED	14	VAL	H	8.412	0.05	1
UNMAPPED	11	ALA	H	8.882	0.05	1
UNMAPPED	7	PHE	HE1	6.402	0.05	1
UNMAPPED	26	ARG	HB3	1.594	0.05	2
UNMAPPED	22	TYR	H	7.847	0.05	1
UNMAPPED	5	GLY	H	9.029	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	19	GLU	HG2	2.397	0.05	2
UNMAPPED	17	LEU	HD12	1.011	0.05	2
UNMAPPED	11	ALA	HB2	1.365	0.05	1
UNMAPPED	11	ALA	HA	4.323	0.05	1
UNMAPPED	11	ALA	HB1	1.365	0.05	1
UNMAPPED	21	ALA	HA	3.875	0.05	1
UNMAPPED	17	LEU	H	8.496	0.05	1
UNMAPPED	3	ARG	H	8.349	0.05	1
UNMAPPED	22	TYR	HD2	7.058	0.05	1
UNMAPPED	3	ARG	HG2	1.536	0.05	2
UNMAPPED	6	GLY	HA2	3.945	0.05	2
UNMAPPED	2	GLN	HB2	1.899	0.05	2
UNMAPPED	22	TYR	HD1	7.058	0.05	1
UNMAPPED	2	GLN	HA	4.22	0.05	1
UNMAPPED	20	TRP	HB2	3.48	0.05	2
UNMAPPED	20	TRP	HE1	9.742	0.05	3
UNMAPPED	21	ALA	HB3	1.169	0.05	1
UNMAPPED	17	LEU	HD23	0.874	0.05	2
UNMAPPED	16	VAL	HG13	0.861	0.05	2
UNMAPPED	1	GLN	HB2	1.981	0.05	2
UNMAPPED	20	TRP	HH2	6.62	0.05	1
UNMAPPED	1	GLN	HG2	2.258	0.05	1
UNMAPPED	5	GLY	HA3	3.899	0.05	2
UNMAPPED	19	GLU	HB3	1.902	0.05	2
UNMAPPED	22	TYR	HB3	3.002	0.05	2
UNMAPPED	12	ARG	H	7.913	0.05	1
UNMAPPED	16	VAL	HB	2.27	0.05	1
UNMAPPED	15	GLY	HA3	3.784	0.05	2
UNMAPPED	4	ARG	HA	4.311	0.05	1
UNMAPPED	19	GLU	H	7.872	0.05	1
UNMAPPED	18	ARG	H	8.334	0.05	1
UNMAPPED	4	ARG	HG2	1.56	0.05	2
UNMAPPED	22	TYR	HE1	6.695	0.05	1
UNMAPPED	14	VAL	HG13	1.087	0.05	2
UNMAPPED	14	VAL	HG22	0.894	0.05	2
UNMAPPED	16	VAL	HG23	1.008	0.05	2
UNMAPPED	20	TRP	HZ3	6.5	0.05	3
UNMAPPED	25	PHE	HB3	2.934	0.05	2
UNMAPPED	7	PHE	HD1	7.227	0.05	1
UNMAPPED	14	VAL	HA	3.535	0.05	1
UNMAPPED	14	VAL	HB	2.381	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	21	ALA	H	8.01	0.05	1
UNMAPPED	14	VAL	HG21	0.894	0.05	2
UNMAPPED	17	LEU	HA	4.236	0.05	1
UNMAPPED	2	GLN	HG2	2.269	0.05	1
UNMAPPED	8	ARG	HB2	1.615	0.05	2
UNMAPPED	24	ASN	HB3	2.324	0.05	2
UNMAPPED	26	ARG	HA	4.049	0.05	1
UNMAPPED	14	VAL	HG12	1.087	0.05	2
UNMAPPED	17	LEU	HD11	1.011	0.05	2
UNMAPPED	20	TRP	HA	4.218	0.05	1
UNMAPPED	24	ASN	H	7.816	0.05	1
UNMAPPED	20	TRP	HE3	7.173	0.05	3
UNMAPPED	14	VAL	HG11	1.087	0.05	2
UNMAPPED	12	ARG	HA	4.092	0.05	1
UNMAPPED	8	ARG	HA	3.51	0.05	1
UNMAPPED	14	VAL	HG23	0.894	0.05	2
UNMAPPED	4	ARG	H	8.285	0.05	1
UNMAPPED	25	PHE	H	7.745	0.05	1
UNMAPPED	26	ARG	H	7.835	0.05	1
UNMAPPED	10	ILE	HB	1.91	0.05	1
UNMAPPED	1	GLN	H	8.225	0.05	1
UNMAPPED	21	ALA	HB1	1.169	0.05	1
UNMAPPED	4	ARG	HB2	1.8	0.05	2
UNMAPPED	10	ILE	HG22	1.153	0.05	1
UNMAPPED	15	GLY	H	8.142	0.05	1
UNMAPPED	18	ARG	HA	3.871	0.05	1
UNMAPPED	1	GLN	HB3	1.859	0.05	2
UNMAPPED	22	TYR	HA	4.204	0.05	1
UNMAPPED	24	ASN	HA	4.603	0.05	1
UNMAPPED	8	ARG	H	8.501	0.05	1
UNMAPPED	19	GLU	HB2	2.116	0.05	2
UNMAPPED	1	GLN	HA	4.18	0.05	1
UNMAPPED	16	VAL	HG22	1.008	0.05	2
UNMAPPED	26	ARG	HG2	1.461	0.05	2
UNMAPPED	20	TRP	HZ2	7.004	0.05	3
UNMAPPED	25	PHE	HB2	3.105	0.05	2
UNMAPPED	9	ARG	H	7.712	0.05	1
UNMAPPED	3	ARG	HB3	1.678	0.05	2
UNMAPPED	7	PHE	HD2	7.227	0.05	1
UNMAPPED	7	PHE	HB2	3.361	0.05	2
UNMAPPED	16	VAL	H	7.978	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	7	PHE	HE2	6.402	0.05	1
UNMAPPED	2	GLN	HG3	2.269	0.05	1
UNMAPPED	19	GLU	HA	4.047	0.05	1
UNMAPPED	8	ARG	HB3	1.703	0.05	2
UNMAPPED	20	TRP	HD1	7.233	0.05	1
UNMAPPED	24	ASN	HB2	2.577	0.05	2
UNMAPPED	17	LEU	HD13	1.011	0.05	2
UNMAPPED	11	ALA	HB3	1.365	0.05	1
UNMAPPED	16	VAL	HG11	0.861	0.05	2
UNMAPPED	10	ILE	H	8.379	0.05	1
UNMAPPED	16	VAL	HG12	0.861	0.05	2
UNMAPPED	10	ILE	HG21	1.153	0.05	1
UNMAPPED	6	GLY	HA3	3.776	0.05	2
UNMAPPED	7	PHE	HA	4.58	0.05	1
UNMAPPED	7	PHE	H	9.52	0.05	1
UNMAPPED	10	ILE	HG23	1.153	0.05	1
UNMAPPED	2	GLN	HB3	1.991	0.05	2
UNMAPPED	20	TRP	HB3	3.208	0.05	2
UNMAPPED	10	ILE	HA	3.979	0.05	1
UNMAPPED	25	PHE	HA	4.565	0.05	1
UNMAPPED	21	ALA	HB2	1.169	0.05	1
UNMAPPED	4	ARG	HB3	1.72	0.05	2
UNMAPPED	13	LEU	H	7.706	0.05	1
UNMAPPED	17	LEU	HD21	0.874	0.05	2

7.2.2 Chemical shift referencing ⓘ

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1799. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/736 (0%)	0/294 (0%)	0/296 (0%)	0/146 (0%)
Sidechain	0/947 (0%)	0/547 (0%)	0/356 (0%)	0/44 (0%)
Aromatic	0/116 (0%)	0/63 (0%)	0/51 (0%)	0/2 (0%)
Overall	0/1799 (0%)	0/904 (0%)	0/703 (0%)	0/192 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2067. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/836 (0%)	0/334 (0%)	0/336 (0%)	0/166 (0%)
Sidechain	0/1115 (0%)	0/646 (0%)	0/414 (0%)	0/55 (0%)
Aromatic	0/116 (0%)	0/63 (0%)	0/51 (0%)	0/2 (0%)
Overall	0/2067 (0%)	0/1043 (0%)	0/801 (0%)	0/223 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_2). RCI is only applicable to proteins.