



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:44 PM BST

PDB ID : 1RFL
Title : NMR data driven structural model of G-domain of MnmE protein
Authors : Monleon, D.; Esteve, V.; Martinez-Vicente, M.; Yim, L.; Armengod, M.E.; Celda, B.
Deposited on : 2003-11-10

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

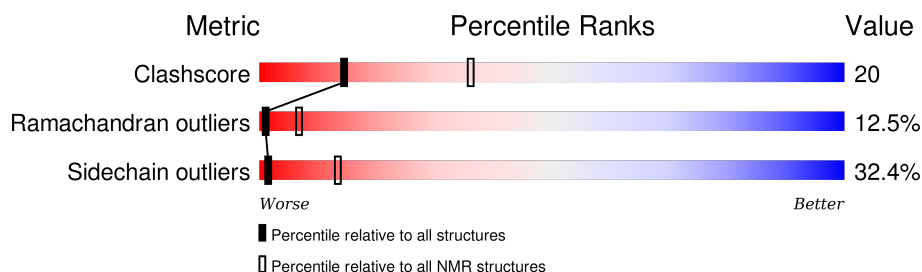
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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	172	 28% 65% . .

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:170 (167)	0.65	12

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2675 atoms, of which 1364 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Probable tRNA modification GTPase trmE.

Mol	Chain	Residues	Atoms						Trace
1	A	172	Total	C	H	N	O	S	0
			2675	812	1364	244	250	5	

There are 4 discrepancies between the modelled and reference sequences:

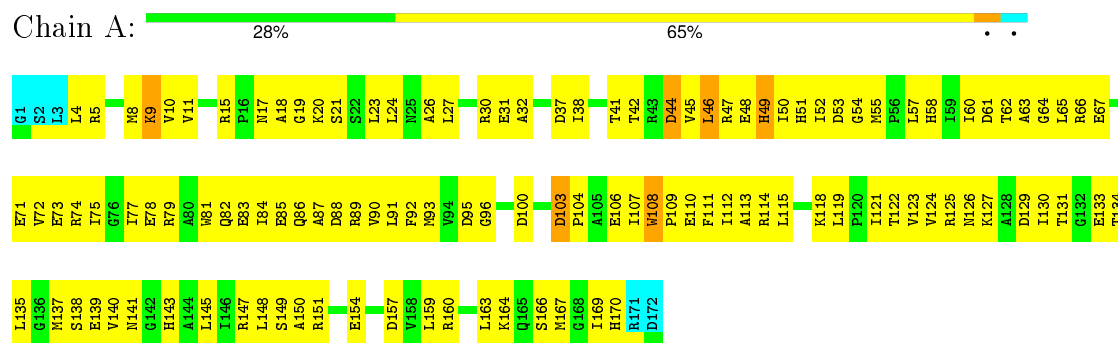
Chain	Residue	Modelled	Actual	Comment	Reference
A	169	ILE	-	CLONING ARTIFACT	UNP P25522
A	170	HIS	-	CLONING ARTIFACT	UNP P25522
A	171	ARG	-	CLONING ARTIFACT	UNP P25522
A	172	ASP	-	CLONING ARTIFACT	UNP P25522

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: Probable tRNA modification GTPase trmE

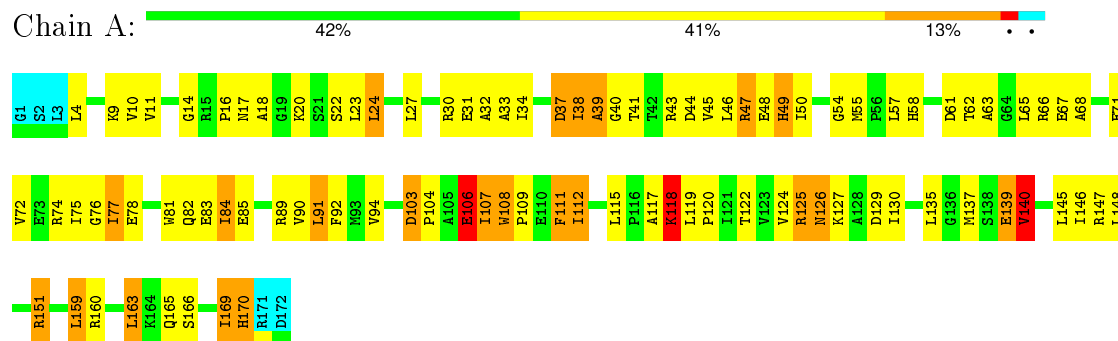


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

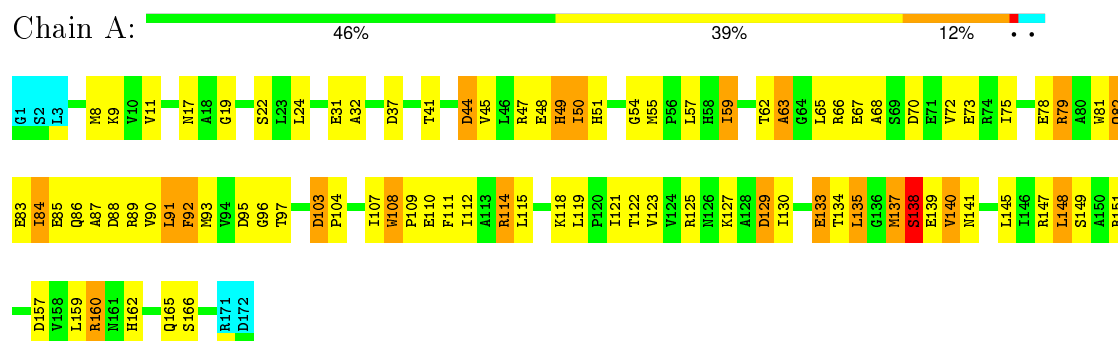
4.2.1 Score per residue for model 1

- Molecule 1: Probable tRNA modification GTPase trmE



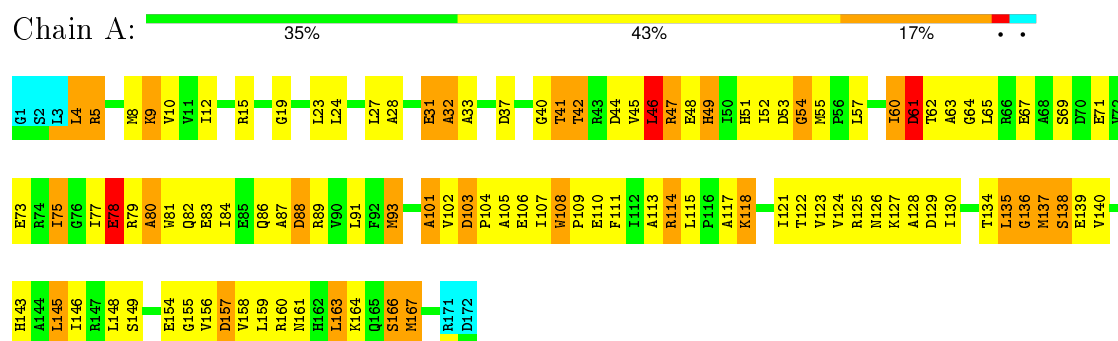
4.2.2 Score per residue for model 2

- Molecule 1: Probable tRNA modification GTPase trmE



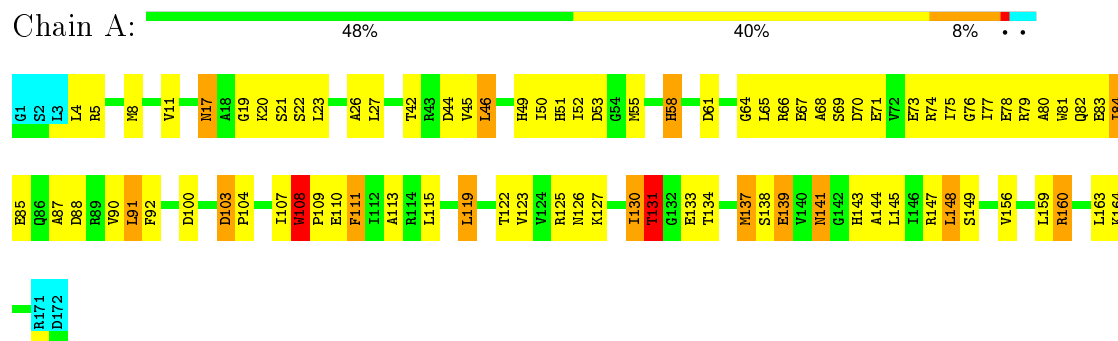
4.2.3 Score per residue for model 3

- Molecule 1: Probable tRNA modification GTPase trmE



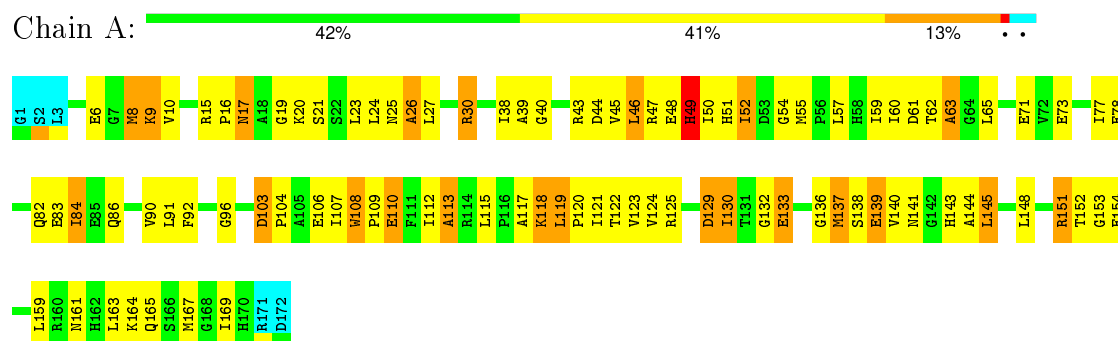
4.2.4 Score per residue for model 4

- Molecule 1: Probable tRNA modification GTPase trmE



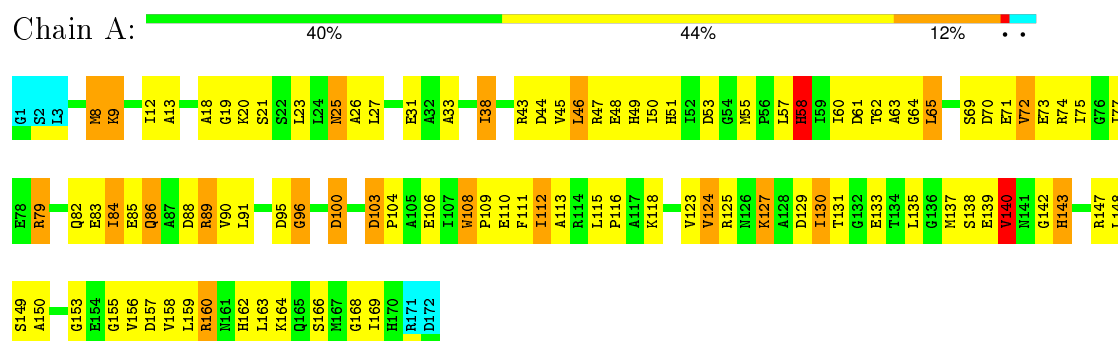
4.2.5 Score per residue for model 5

- Molecule 1: Probable tRNA modification GTPase trmE



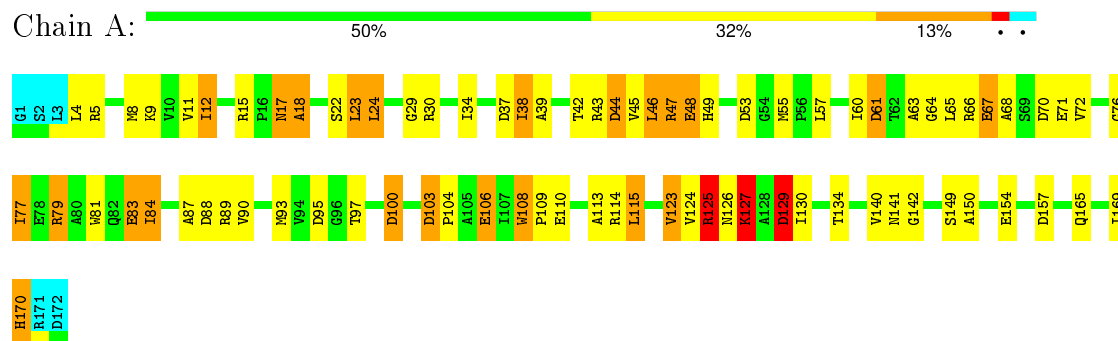
4.2.6 Score per residue for model 6

- Molecule 1: Probable tRNA modification GTPase trmE



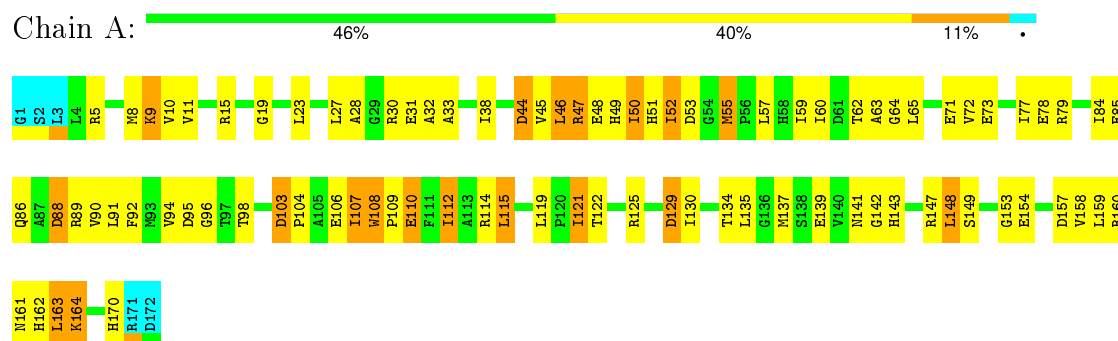
4.2.7 Score per residue for model 7

- Molecule 1: Probable tRNA modification GTPase trmE



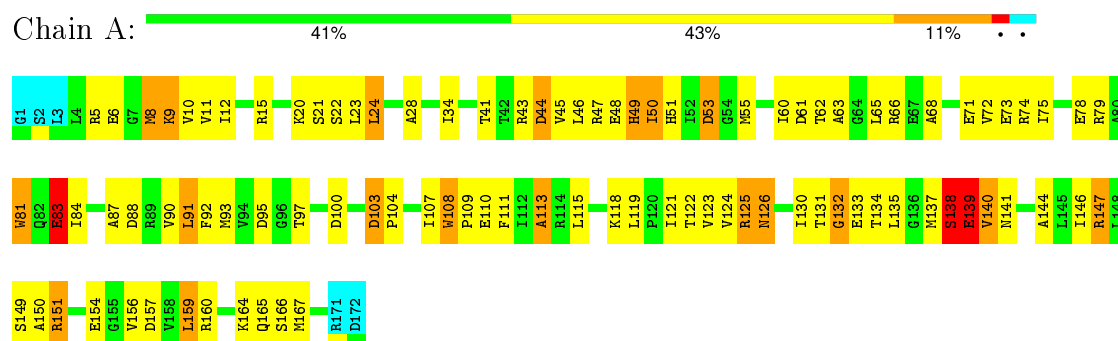
4.2.8 Score per residue for model 8

- Molecule 1: Probable tRNA modification GTPase trmE



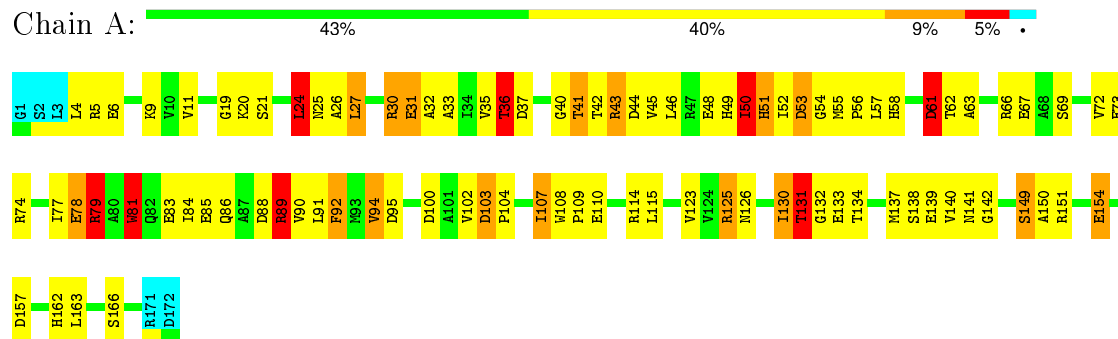
4.2.9 Score per residue for model 9

- Molecule 1: Probable tRNA modification GTPase trmE



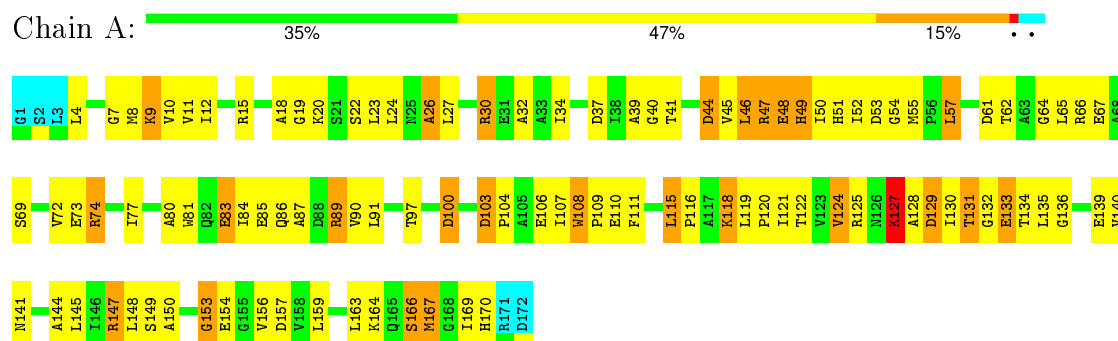
4.2.10 Score per residue for model 10

- Molecule 1: Probable tRNA modification GTPase trmE



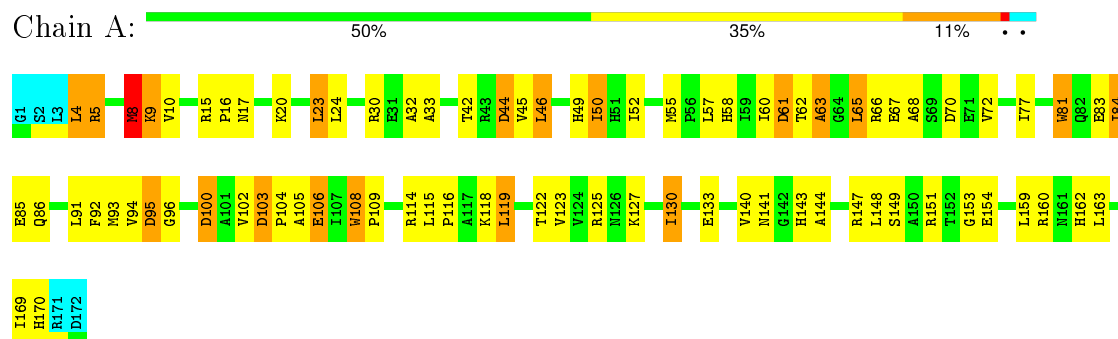
4.2.11 Score per residue for model 11

- Molecule 1: Probable tRNA modification GTPase trmE



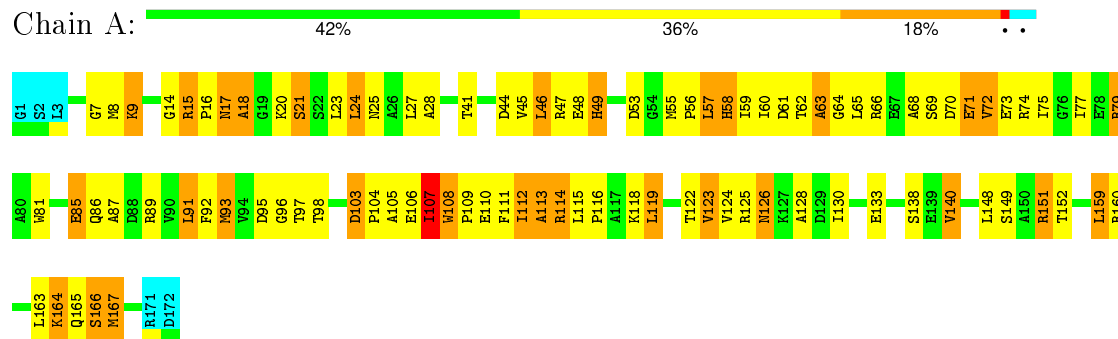
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Probable tRNA modification GTPase trmE



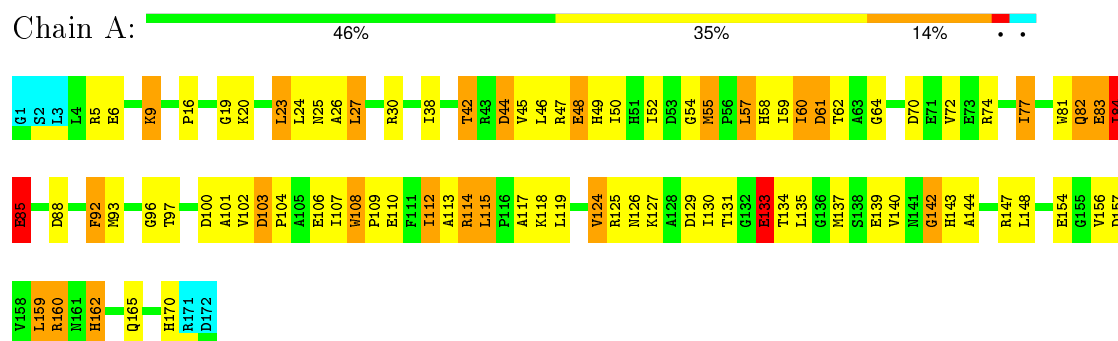
4.2.13 Score per residue for model 13

- Molecule 1: Probable tRNA modification GTPase trmE



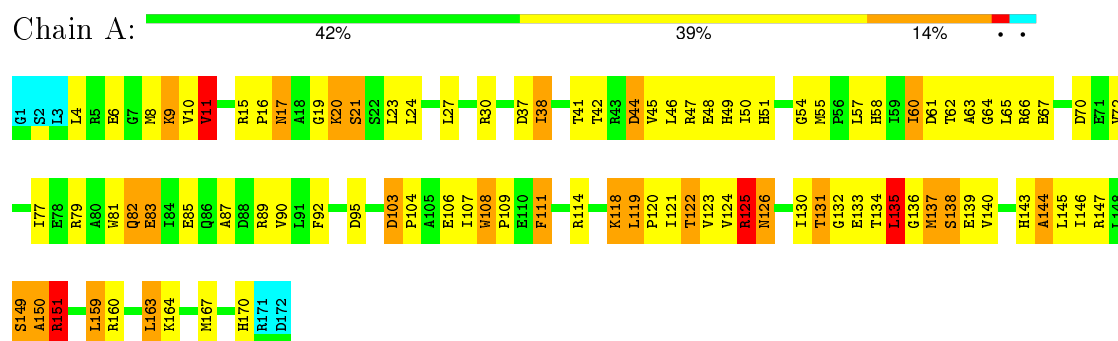
4.2.14 Score per residue for model 14

- Molecule 1: Probable tRNA modification GTPase trmE



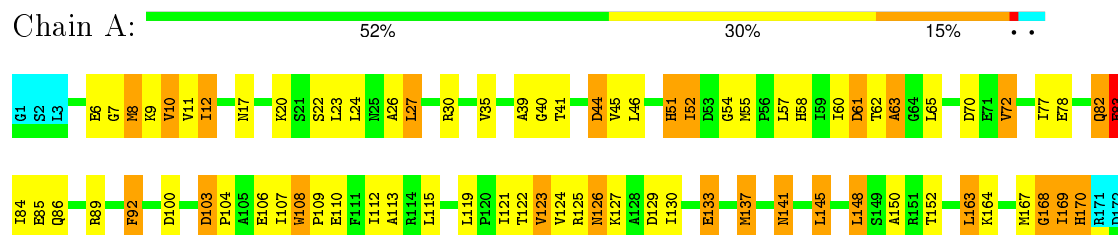
4.2.15 Score per residue for model 15

- Molecule 1: Probable tRNA modification GTPase trmE



4.2.16 Score per residue for model 16

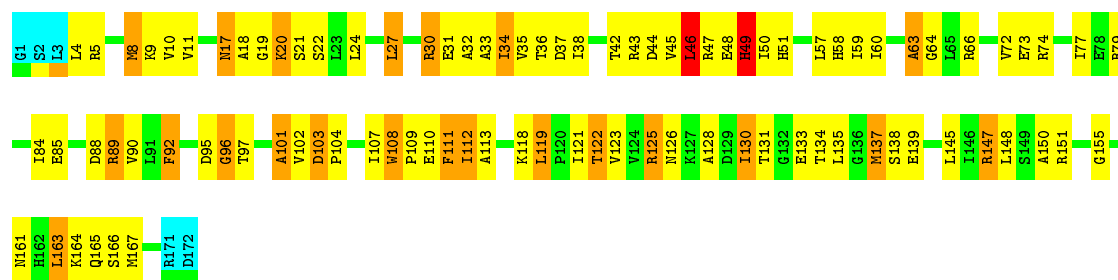
- Molecule 1: Probable tRNA modification GTPase trmE



4.2.17 Score per residue for model 17

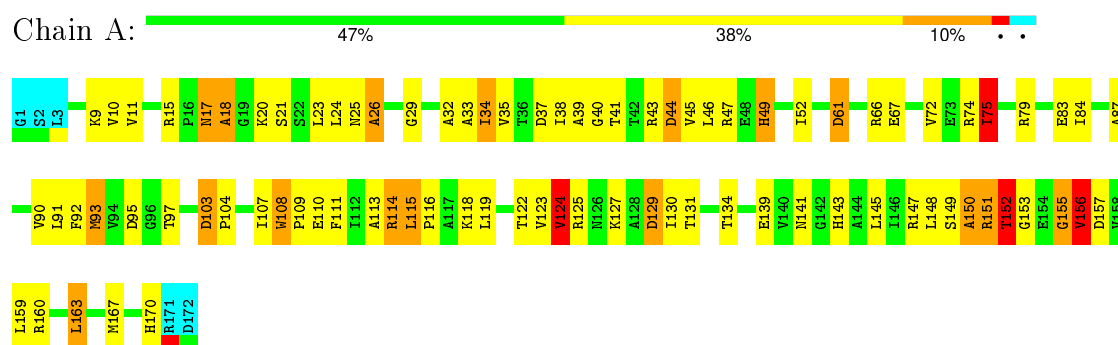
- Molecule 1: Probable tRNA modification GTPase trmE





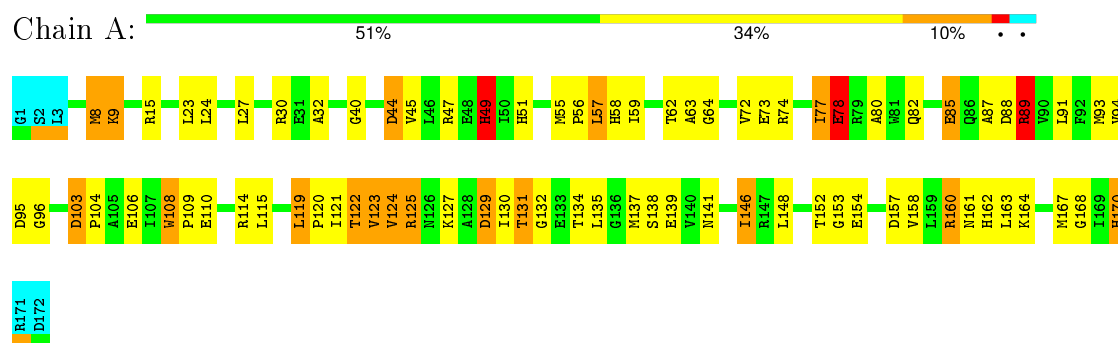
4.2.18 Score per residue for model 18

- Molecule 1: Probable tRNA modification GTPase trmE



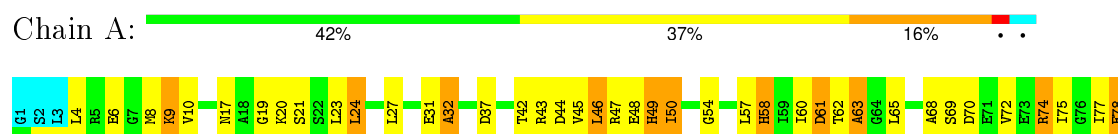
4.2.19 Score per residue for model 19

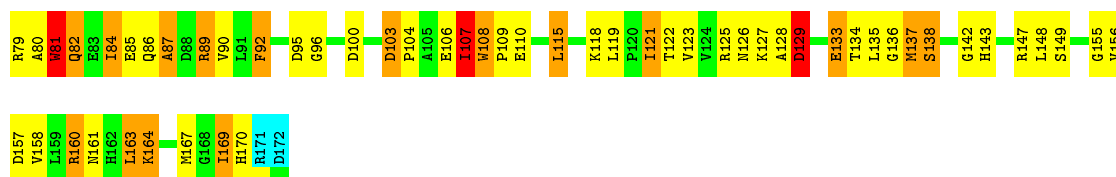
- Molecule 1: Probable tRNA modification GTPase trmE



4.2.20 Score per residue for model 20

- Molecule 1: Probable tRNA modification GTPase trmE





5 Refinement protocol and experimental data overview

The models were refined using the following method: *NMR restraints were obtained from the backbone assignment (TALOS analysis for dihedral angle constraints) and from the ¹⁵N-edited 3D NOESY. Additional structural information was obtained from the homologous GTPase protein structures..*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
DYANA	structure solution	2000
DYANA	refinement	2000

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 5861
Number of chemical shift lists	1
Total number of shifts	950
Number of shifts mapped to atoms	950
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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	1274	1327	1296	52±8
All	All	25480	26540	25920	1035

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:VAL:HG12	1:A:130:ILE:HD11	0.86	1.47	1	1
1:A:107:ILE:O	1:A:107:ILE:HD13	0.86	1.71	1	3
1:A:130:ILE:HG23	1:A:134:THR:HG21	0.86	1.45	3	1
1:A:92:PHE:CE2	1:A:119:LEU:HD23	0.86	2.06	13	1
1:A:92:PHE:CE2	1:A:107:ILE:HG22	0.84	2.07	2	2
1:A:121:ILE:CG2	1:A:134:THR:HG23	0.82	2.05	20	1
1:A:75:ILE:HD13	1:A:75:ILE:O	0.82	1.75	3	1
1:A:68:ALA:O	1:A:72:VAL:HG23	0.81	1.73	12	3
1:A:130:ILE:HD12	1:A:131:THR:N	0.80	1.91	15	1
1:A:46:LEU:HD22	1:A:61:ASP:HA	0.78	1.55	15	4
1:A:63:ALA:HB3	1:A:86:GLN:OE1	0.78	1.78	12	1
1:A:11:VAL:CG1	1:A:90:VAL:HG22	0.77	2.09	4	4
1:A:88:ASP:C	1:A:115:LEU:HD12	0.77	2.00	8	1
1:A:46:LEU:HD12	1:A:62:THR:HG23	0.76	1.56	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ARG:HH21	1:A:49:HIS:CE1	0.76	1.98	1	1
1:A:4:LEU:HD21	1:A:169:ILE:HG22	0.76	1.56	20	1
1:A:121:ILE:HG21	1:A:134:THR:HG23	0.74	1.59	20	1
1:A:23:LEU:O	1:A:26:ALA:HB3	0.74	1.83	4	2
1:A:84:ILE:HD13	1:A:85:GLU:N	0.73	1.97	14	1
1:A:9:LYS:HB3	1:A:62:THR:HG22	0.73	1.59	9	2
1:A:91:LEU:O	1:A:91:LEU:HD13	0.73	1.83	1	1
1:A:124:VAL:HG22	1:A:125:ARG:N	0.73	1.98	18	2
1:A:97:THR:HG23	1:A:122:THR:HG21	0.72	1.59	9	1
1:A:144:ALA:O	1:A:145:LEU:HD23	0.71	1.84	5	2
1:A:57:LEU:C	1:A:57:LEU:HD22	0.71	2.06	19	1
1:A:130:ILE:O	1:A:130:ILE:HD12	0.71	1.85	7	1
1:A:140:VAL:HG23	1:A:141:ASN:N	0.71	2.00	9	1
1:A:63:ALA:HB2	1:A:72:VAL:HG21	0.71	1.61	16	4
1:A:148:LEU:O	1:A:148:LEU:HD13	0.71	1.86	2	1
1:A:92:PHE:CE2	1:A:119:LEU:HD13	0.70	2.21	18	1
1:A:50:ILE:N	1:A:50:ILE:HD13	0.70	2.02	9	3
1:A:61:ASP:HB2	1:A:72:VAL:HG11	0.70	1.64	14	1
1:A:130:ILE:CD1	1:A:134:THR:HG21	0.70	2.16	10	1
1:A:119:LEU:HD13	1:A:120:PRO:HD2	0.69	1.64	15	2
1:A:118:LYS:HG2	1:A:144:ALA:HB3	0.69	1.64	9	1
1:A:91:LEU:HD11	1:A:159:LEU:HD21	0.69	1.63	2	1
1:A:90:VAL:HG21	1:A:110:GLU:OE1	0.68	1.88	10	3
1:A:139:GLU:O	1:A:140:VAL:HG12	0.68	1.88	2	2
1:A:137:MET:SD	1:A:145:LEU:HD21	0.68	2.28	17	1
1:A:12:ILE:HG22	1:A:91:LEU:HB3	0.68	1.65	3	1
1:A:119:LEU:O	1:A:145:LEU:HD23	0.68	1.89	18	3
1:A:63:ALA:HB2	1:A:84:ILE:CG1	0.68	2.19	20	1
1:A:130:ILE:O	1:A:130:ILE:HG23	0.68	1.87	10	1
1:A:152:THR:HG22	1:A:152:THR:O	0.68	1.88	18	1
1:A:112:ILE:O	1:A:112:ILE:HG23	0.67	1.88	1	2
1:A:45:VAL:HG13	1:A:45:VAL:O	0.67	1.87	14	1
1:A:92:PHE:CE1	1:A:107:ILE:HG22	0.67	2.25	14	1
1:A:63:ALA:HB3	1:A:86:GLN:CD	0.67	2.09	12	1
1:A:24:LEU:HD21	1:A:48:GLU:HA	0.67	1.66	7	1
1:A:115:LEU:HD22	1:A:115:LEU:O	0.66	1.89	14	2
1:A:10:VAL:HG21	1:A:163:LEU:HD11	0.66	1.67	5	1
1:A:91:LEU:C	1:A:91:LEU:HD22	0.66	2.10	1	1
1:A:112:ILE:C	1:A:112:ILE:HD13	0.66	2.11	8	3
1:A:52:ILE:HG23	1:A:55:MET:O	0.66	1.88	8	2
1:A:114:ARG:C	1:A:115:LEU:HD22	0.66	2.11	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:VAL:HA	1:A:130:ILE:HG21	0.66	1.67	13	2
1:A:123:VAL:HG13	1:A:123:VAL:O	0.66	1.90	2	2
1:A:27:LEU:HD11	1:A:163:LEU:CD1	0.66	2.21	8	1
1:A:9:LYS:HB2	1:A:62:THR:HG22	0.66	1.66	8	3
1:A:130:ILE:C	1:A:130:ILE:HD13	0.66	2.11	4	1
1:A:134:THR:C	1:A:135:LEU:HD23	0.66	2.11	2	1
1:A:97:THR:HG22	1:A:97:THR:O	0.65	1.91	7	2
1:A:123:VAL:O	1:A:123:VAL:HG23	0.65	1.91	17	1
1:A:87:ALA:O	1:A:115:LEU:HD11	0.65	1.90	2	2
1:A:124:VAL:O	1:A:124:VAL:HG23	0.65	1.90	15	1
1:A:36:THR:HG23	1:A:37:ASP:N	0.65	2.05	10	1
1:A:97:THR:O	1:A:97:THR:HG22	0.65	1.91	17	1
1:A:12:ILE:O	1:A:12:ILE:HD12	0.65	1.92	9	1
1:A:24:LEU:HD11	1:A:49:HIS:NE2	0.65	2.07	20	1
1:A:122:THR:O	1:A:122:THR:HG23	0.65	1.92	16	1
1:A:90:VAL:HG13	1:A:90:VAL:O	0.65	1.92	1	1
1:A:101:ALA:C	1:A:102:VAL:HG23	0.65	2.11	17	2
1:A:115:LEU:O	1:A:115:LEU:HD22	0.65	1.92	20	1
1:A:89:ARG:NH1	1:A:143:HIS:CE1	0.65	2.65	15	2
1:A:112:ILE:HG22	1:A:112:ILE:O	0.65	1.90	16	1
1:A:91:LEU:HD13	1:A:159:LEU:HD21	0.64	1.65	13	1
1:A:69:SER:HB2	1:A:84:ILE:HG21	0.64	1.68	4	1
1:A:77:ILE:HG22	1:A:77:ILE:O	0.64	1.92	12	1
1:A:143:HIS:O	1:A:144:ALA:HB3	0.64	1.93	14	2
1:A:118:LYS:HD3	1:A:144:ALA:HB3	0.64	1.69	5	1
1:A:92:PHE:CZ	1:A:107:ILE:HD13	0.64	2.28	17	1
1:A:120:PRO:HB3	1:A:148:LEU:HD12	0.64	1.69	11	1
1:A:21:SER:HB2	1:A:35:VAL:HG21	0.64	1.67	18	1
1:A:10:VAL:HG11	1:A:163:LEU:HD21	0.64	1.68	1	4
1:A:24:LEU:HD23	1:A:24:LEU:C	0.64	2.12	2	1
1:A:112:ILE:O	1:A:112:ILE:HD13	0.63	1.93	8	1
1:A:94:VAL:HG22	1:A:120:PRO:HG2	0.63	1.69	1	1
1:A:122:THR:HG21	1:A:130:ILE:HG13	0.63	1.67	18	1
1:A:45:VAL:HG11	1:A:63:ALA:O	0.63	1.93	17	4
1:A:24:LEU:HD12	1:A:24:LEU:C	0.63	2.14	1	1
1:A:107:ILE:HG23	1:A:107:ILE:O	0.63	1.92	20	2
1:A:12:ILE:H	1:A:12:ILE:HD13	0.63	1.54	7	1
1:A:11:VAL:CG1	1:A:90:VAL:HG23	0.63	2.23	1	1
1:A:96:GLY:HA2	1:A:122:THR:HG21	0.63	1.68	17	2
1:A:124:VAL:HG13	1:A:129:ASP:HA	0.63	1.69	19	1
1:A:103:ASP:N	1:A:104:PRO:CD	0.62	2.62	12	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:THR:O	1:A:130:ILE:HG21	0.62	1.94	2	2
1:A:62:THR:O	1:A:62:THR:HG23	0.62	1.94	16	3
1:A:97:THR:CG2	1:A:122:THR:HG21	0.62	2.24	9	1
1:A:151:ARG:O	1:A:152:THR:HG23	0.62	1.93	13	1
1:A:30:ARG:NH2	1:A:49:HIS:CE1	0.62	2.67	1	3
1:A:92:PHE:HE1	1:A:107:ILE:HG22	0.62	1.54	14	1
1:A:122:THR:HG23	1:A:130:ILE:HD12	0.62	1.71	13	1
1:A:122:THR:O	1:A:130:ILE:HG23	0.62	1.94	12	1
1:A:112:ILE:O	1:A:113:ALA:HB2	0.62	1.93	13	3
1:A:46:LEU:HD22	1:A:60:ILE:O	0.62	1.95	13	3
1:A:77:ILE:O	1:A:77:ILE:HG22	0.62	1.94	16	2
1:A:149:SER:O	1:A:150:ALA:HB3	0.62	1.93	11	3
1:A:64:GLY:O	1:A:65:LEU:HD12	0.62	1.95	6	1
1:A:10:VAL:HG21	1:A:163:LEU:HD21	0.61	1.71	17	4
1:A:35:VAL:O	1:A:36:THR:HG22	0.61	1.94	10	1
1:A:123:VAL:O	1:A:123:VAL:HG13	0.61	1.95	12	3
1:A:50:ILE:HD13	1:A:60:ILE:HG21	0.61	1.71	14	1
1:A:113:ALA:HB1	1:A:115:LEU:HD11	0.61	1.72	14	1
1:A:12:ILE:HG22	1:A:91:LEU:HG	0.61	1.72	9	1
1:A:10:VAL:CG2	1:A:163:LEU:HD11	0.61	2.26	5	1
1:A:44:ASP:CB	1:A:72:VAL:HG23	0.61	2.26	6	1
1:A:97:THR:HG23	1:A:133:GLU:OE1	0.61	1.95	2	1
1:A:27:LEU:HD13	1:A:27:LEU:N	0.61	2.11	14	1
1:A:144:ALA:C	1:A:145:LEU:HD23	0.61	2.16	5	1
1:A:60:ILE:C	1:A:60:ILE:HD12	0.61	2.16	20	1
1:A:92:PHE:CD2	1:A:92:PHE:O	0.61	2.54	13	2
1:A:148:LEU:HD22	1:A:148:LEU:C	0.60	2.15	2	2
1:A:89:ARG:N	1:A:115:LEU:HD12	0.60	2.11	3	2
1:A:130:ILE:O	1:A:130:ILE:HD13	0.60	1.96	4	1
1:A:115:LEU:N	1:A:115:LEU:HD13	0.60	2.12	14	3
1:A:75:ILE:O	1:A:75:ILE:HG23	0.60	1.96	18	1
1:A:46:LEU:HD12	1:A:46:LEU:O	0.60	1.95	14	1
1:A:46:LEU:HD13	1:A:61:ASP:HA	0.60	1.72	20	2
1:A:113:ALA:HB3	1:A:115:LEU:CD2	0.60	2.27	9	1
1:A:32:ALA:O	1:A:33:ALA:HB3	0.60	1.96	3	5
1:A:18:ALA:HB3	1:A:93:MET:CE	0.60	2.27	13	1
1:A:12:ILE:HG22	1:A:12:ILE:O	0.60	1.97	6	1
1:A:52:ILE:O	1:A:52:ILE:HD12	0.59	1.97	18	1
1:A:113:ALA:HB1	1:A:115:LEU:HD21	0.59	1.73	7	1
1:A:46:LEU:HD13	1:A:62:THR:H	0.59	1.57	1	1
1:A:96:GLY:CA	1:A:122:THR:HG21	0.59	2.28	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ILE:HG21	1:A:60:ILE:H	0.59	1.57	20	1
1:A:108:TRP:CD1	1:A:108:TRP:C	0.59	2.76	16	1
1:A:113:ALA:HB3	1:A:115:LEU:HD11	0.59	1.74	18	1
1:A:118:LYS:HE2	1:A:159:LEU:HD11	0.58	1.73	15	1
1:A:17:ASN:O	1:A:18:ALA:HB3	0.58	1.99	7	1
1:A:11:VAL:HG13	1:A:90:VAL:HG22	0.58	1.76	8	4
1:A:50:ILE:HD13	1:A:50:ILE:H	0.58	1.57	2	2
1:A:86:GLN:NE2	1:A:87:ALA:HB2	0.58	2.13	20	1
1:A:159:LEU:HD12	1:A:160:ARG:N	0.58	2.13	4	1
1:A:67:GLU:O	1:A:68:ALA:HB3	0.58	1.97	12	1
1:A:51:HIS:CE1	1:A:160:ARG:HH21	0.58	2.17	2	2
1:A:23:LEU:CD2	1:A:148:LEU:HD11	0.58	2.29	4	1
1:A:92:PHE:CE2	1:A:107:ILE:CG2	0.58	2.87	18	1
1:A:59:ILE:HD13	1:A:59:ILE:C	0.58	2.20	2	1
1:A:112:ILE:HG23	1:A:112:ILE:O	0.57	1.99	14	1
1:A:25:ASN:O	1:A:26:ALA:HB2	0.57	1.99	5	1
1:A:24:LEU:O	1:A:28:ALA:HB2	0.57	2.00	3	1
1:A:92:PHE:O	1:A:92:PHE:CG	0.57	2.57	13	3
1:A:12:ILE:HD13	1:A:12:ILE:N	0.57	2.13	7	1
1:A:143:HIS:CE1	1:A:162:HIS:CE1	0.57	2.92	8	1
1:A:97:THR:CG2	1:A:130:ILE:HD13	0.57	2.29	13	1
1:A:28:ALA:HB2	1:A:49:HIS:CE1	0.57	2.35	13	1
1:A:24:LEU:HD21	1:A:48:GLU:C	0.56	2.21	14	1
1:A:104:PRO:HA	1:A:107:ILE:HG22	0.56	1.76	20	3
1:A:9:LYS:HZ2	1:A:87:ALA:HA	0.56	1.60	13	1
1:A:108:TRP:N	1:A:109:PRO:CD	0.56	2.69	10	15
1:A:46:LEU:HD22	1:A:61:ASP:HB3	0.56	1.77	20	1
1:A:72:VAL:HG11	1:A:84:ILE:CD1	0.56	2.30	12	1
1:A:42:THR:HG23	1:A:45:VAL:HA	0.56	1.77	14	1
1:A:44:ASP:O	1:A:45:VAL:HG12	0.56	1.99	6	7
1:A:118:LYS:CE	1:A:159:LEU:HD11	0.56	2.31	15	1
1:A:130:ILE:O	1:A:130:ILE:HG22	0.56	2.01	3	1
1:A:52:ILE:HG21	1:A:58:HIS:HB2	0.56	1.77	14	1
1:A:30:ARG:CZ	1:A:49:HIS:CE1	0.56	2.89	5	2
1:A:62:THR:HG23	1:A:62:THR:O	0.56	2.01	13	2
1:A:61:ASP:HB3	1:A:72:VAL:HG13	0.56	1.78	10	2
1:A:96:GLY:C	1:A:122:THR:HG21	0.56	2.22	17	1
1:A:133:GLU:O	1:A:134:THR:HG22	0.56	2.01	14	1
1:A:131:THR:HG22	1:A:132:GLY:N	0.55	2.16	10	1
1:A:59:ILE:HG23	1:A:59:ILE:O	0.55	2.01	2	1
1:A:118:LYS:HB2	1:A:144:ALA:HB3	0.55	1.77	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:ILE:O	1:A:131:THR:C	0.55	2.45	19	3
1:A:115:LEU:HD12	1:A:116:PRO:O	0.55	2.02	12	1
1:A:77:ILE:HD13	1:A:77:ILE:N	0.55	2.15	14	1
1:A:23:LEU:CD2	1:A:148:LEU:HD22	0.55	2.32	13	1
1:A:24:LEU:HD13	1:A:24:LEU:C	0.55	2.22	12	1
1:A:146:ILE:HD12	1:A:148:LEU:HD23	0.55	1.78	19	1
1:A:63:ALA:CB	1:A:72:VAL:HG21	0.55	2.32	15	2
1:A:72:VAL:HG12	1:A:73:GLU:N	0.55	2.16	13	1
1:A:160:ARG:HA	1:A:163:LEU:HD12	0.55	1.77	12	1
1:A:24:LEU:HD22	1:A:48:GLU:HA	0.54	1.79	15	1
1:A:11:VAL:HG13	1:A:90:VAL:HG23	0.54	1.79	1	4
1:A:97:THR:HG23	1:A:122:THR:CG2	0.54	2.31	9	1
1:A:91:LEU:HD22	1:A:92:PHE:N	0.54	2.18	1	1
1:A:31:GLU:O	1:A:32:ALA:HB2	0.54	2.02	20	1
1:A:90:VAL:HG21	1:A:110:GLU:CD	0.54	2.22	10	1
1:A:12:ILE:HD12	1:A:48:GLU:OE2	0.54	2.03	11	1
1:A:123:VAL:O	1:A:124:VAL:C	0.54	2.45	18	3
1:A:130:ILE:O	1:A:130:ILE:CG2	0.54	2.55	10	1
1:A:61:ASP:OD1	1:A:84:ILE:HD11	0.54	2.01	9	1
1:A:21:SER:CB	1:A:35:VAL:HG21	0.54	2.33	18	1
1:A:10:VAL:O	1:A:62:THR:HG21	0.54	2.03	1	1
1:A:46:LEU:CG	1:A:46:LEU:O	0.54	2.56	14	2
1:A:72:VAL:O	1:A:75:ILE:HG22	0.54	2.03	20	1
1:A:90:VAL:HG23	1:A:115:LEU:CD1	0.54	2.32	7	1
1:A:34:ILE:HD13	1:A:35:VAL:N	0.54	2.18	18	2
1:A:113:ALA:HB1	1:A:115:LEU:CD1	0.54	2.32	14	1
1:A:146:ILE:HG21	1:A:158:VAL:HG11	0.54	1.78	3	1
1:A:50:ILE:HB	1:A:60:ILE:HD12	0.54	1.80	6	1
1:A:88:ASP:O	1:A:115:LEU:HD12	0.54	2.02	8	1
1:A:92:PHE:O	1:A:92:PHE:CD2	0.54	2.60	9	1
1:A:38:ILE:N	1:A:38:ILE:HD13	0.53	2.18	1	1
1:A:84:ILE:HD13	1:A:84:ILE:C	0.53	2.23	14	1
1:A:124:VAL:HG12	1:A:125:ARG:N	0.53	2.18	19	1
1:A:38:ILE:HD13	1:A:38:ILE:H	0.53	1.63	6	1
1:A:140:VAL:CG2	1:A:141:ASN:N	0.53	2.70	9	1
1:A:44:ASP:HA	1:A:72:VAL:HG12	0.53	1.79	17	1
1:A:77:ILE:HG22	1:A:78:GLU:N	0.53	2.17	19	1
1:A:51:HIS:O	1:A:51:HIS:CG	0.53	2.62	16	2
1:A:111:PHE:CE1	1:A:140:VAL:HG23	0.53	2.39	6	1
1:A:27:LEU:HD23	1:A:27:LEU:O	0.53	2.04	10	1
1:A:26:ALA:HB1	1:A:156:VAL:HG21	0.53	1.81	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ILE:HD11	1:A:145:LEU:CB	0.53	2.34	3	2
1:A:97:THR:O	1:A:97:THR:HG23	0.53	2.03	14	1
1:A:11:VAL:HG12	1:A:90:VAL:HG22	0.53	1.81	9	2
1:A:92:PHE:CD1	1:A:107:ILE:HG22	0.53	2.39	15	1
1:A:69:SER:O	1:A:72:VAL:HG12	0.53	2.03	11	1
1:A:92:PHE:CZ	1:A:119:LEU:CD2	0.52	2.91	5	1
1:A:36:THR:CG2	1:A:37:ASP:N	0.52	2.73	10	1
1:A:122:THR:HG21	1:A:130:ILE:CG1	0.52	2.34	18	1
1:A:108:TRP:CB	1:A:109:PRO:HD3	0.52	2.35	20	12
1:A:152:THR:O	1:A:152:THR:CG2	0.52	2.58	18	1
1:A:90:VAL:HG21	1:A:110:GLU:OE2	0.52	2.04	4	2
1:A:97:THR:HG23	1:A:130:ILE:HD13	0.52	1.79	13	1
1:A:158:VAL:O	1:A:162:HIS:CD2	0.52	2.62	19	1
1:A:45:VAL:O	1:A:45:VAL:HG22	0.52	2.03	1	2
1:A:45:VAL:HG21	1:A:63:ALA:O	0.52	2.04	20	2
1:A:89:ARG:NH2	1:A:118:LYS:HZ2	0.52	2.03	3	1
1:A:94:VAL:HG12	1:A:96:GLY:H	0.52	1.65	8	1
1:A:94:VAL:HG12	1:A:95:ASP:H	0.52	1.64	10	1
1:A:111:PHE:CD1	1:A:140:VAL:HG21	0.52	2.40	15	1
1:A:111:PHE:CD1	1:A:140:VAL:CG2	0.52	2.93	15	2
1:A:111:PHE:CD1	1:A:111:PHE:C	0.52	2.83	13	1
1:A:112:ILE:O	1:A:112:ILE:CG2	0.51	2.58	1	2
1:A:140:VAL:HG22	1:A:141:ASN:H	0.51	1.65	2	1
1:A:50:ILE:HD13	1:A:50:ILE:N	0.51	2.19	2	1
1:A:26:ALA:HB3	1:A:27:LEU:HD13	0.51	1.82	14	1
1:A:111:PHE:HB3	1:A:140:VAL:HG23	0.51	1.81	11	1
1:A:63:ALA:HB2	1:A:72:VAL:CG2	0.51	2.35	1	1
1:A:139:GLU:O	1:A:140:VAL:CG1	0.51	2.58	2	1
1:A:92:PHE:CD2	1:A:117:ALA:HB1	0.51	2.40	14	1
1:A:123:VAL:O	1:A:123:VAL:HG12	0.51	2.04	5	1
1:A:124:VAL:HG22	1:A:125:ARG:HD3	0.51	1.82	7	1
1:A:119:LEU:HD23	1:A:120:PRO:HD2	0.51	1.82	19	1
1:A:92:PHE:HE2	1:A:119:LEU:HD13	0.51	1.64	18	1
1:A:124:VAL:O	1:A:124:VAL:HG13	0.51	2.05	7	1
1:A:45:VAL:CG1	1:A:45:VAL:O	0.51	2.58	14	1
1:A:113:ALA:CB	1:A:115:LEU:HD11	0.51	2.36	18	1
1:A:130:ILE:HD13	1:A:134:THR:HG21	0.51	1.81	10	1
1:A:52:ILE:HD12	1:A:53:ASP:N	0.51	2.19	10	1
1:A:46:LEU:CD1	1:A:46:LEU:O	0.51	2.58	14	1
1:A:143:HIS:O	1:A:144:ALA:CB	0.51	2.59	14	1
1:A:11:VAL:HG22	1:A:11:VAL:O	0.51	2.05	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ALA:O	1:A:152:THR:N	0.51	2.44	18	2
1:A:153:GLY:CA	1:A:156:VAL:HG13	0.51	2.35	11	1
1:A:52:ILE:HG21	1:A:56:PRO:HA	0.51	1.82	10	1
1:A:44:ASP:O	1:A:46:LEU:N	0.51	2.44	17	8
1:A:80:ALA:O	1:A:81:TRP:CG	0.51	2.64	20	1
1:A:149:SER:O	1:A:150:ALA:CB	0.51	2.59	11	1
1:A:59:ILE:C	1:A:59:ILE:CD1	0.51	2.80	2	1
1:A:20:LYS:O	1:A:24:LEU:HD13	0.51	2.06	10	1
1:A:112:ILE:O	1:A:113:ALA:CB	0.50	2.59	13	2
1:A:148:LEU:HD22	1:A:149:SER:N	0.50	2.21	2	1
1:A:137:MET:O	1:A:138:SER:CB	0.50	2.59	2	1
1:A:42:THR:HG23	1:A:45:VAL:N	0.50	2.21	15	2
1:A:112:ILE:CG2	1:A:112:ILE:O	0.50	2.59	13	3
1:A:50:ILE:HG22	1:A:52:ILE:CG1	0.50	2.35	4	1
1:A:35:VAL:O	1:A:36:THR:CB	0.50	2.59	10	1
1:A:107:ILE:CD1	1:A:107:ILE:O	0.50	2.59	20	1
1:A:42:THR:O	1:A:44:ASP:N	0.50	2.43	3	1
1:A:119:LEU:O	1:A:145:LEU:CB	0.50	2.60	5	1
1:A:12:ILE:CD1	1:A:48:GLU:OE2	0.50	2.60	11	1
1:A:44:ASP:O	1:A:45:VAL:C	0.50	2.50	14	3
1:A:115:LEU:O	1:A:115:LEU:HD12	0.50	2.07	5	2
1:A:87:ALA:O	1:A:115:LEU:HD22	0.50	2.06	11	1
1:A:103:ASP:N	1:A:104:PRO:HD2	0.50	2.21	12	15
1:A:124:VAL:HG22	1:A:125:ARG:H	0.50	1.67	16	5
1:A:107:ILE:CD1	1:A:110:GLU:CB	0.50	2.90	5	1
1:A:124:VAL:O	1:A:124:VAL:CG2	0.50	2.60	15	1
1:A:88:ASP:OD1	1:A:167:MET:CE	0.50	2.60	9	1
1:A:60:ILE:O	1:A:61:ASP:CB	0.50	2.59	3	2
1:A:62:THR:O	1:A:62:THR:CG2	0.50	2.60	12	2
1:A:57:LEU:O	1:A:57:LEU:HD22	0.50	2.06	19	1
1:A:169:ILE:O	1:A:170:HIS:CB	0.50	2.60	1	3
1:A:23:LEU:HD13	1:A:148:LEU:CD2	0.50	2.37	14	1
1:A:122:THR:O	1:A:130:ILE:HD13	0.50	2.07	5	1
1:A:111:PHE:CD1	1:A:140:VAL:HG23	0.50	2.42	1	1
1:A:89:ARG:CZ	1:A:166:SER:OG	0.49	2.60	17	3
1:A:115:LEU:C	1:A:115:LEU:HD22	0.49	2.26	20	1
1:A:92:PHE:CE2	1:A:119:LEU:CD2	0.49	2.89	13	1
1:A:91:LEU:HB2	1:A:118:LYS:HZ2	0.49	1.67	18	1
1:A:148:LEU:HD21	1:A:159:LEU:HD11	0.49	1.85	11	2
1:A:9:LYS:HG3	1:A:60:ILE:HD13	0.49	1.84	20	1
1:A:89:ARG:NH2	1:A:118:LYS:NZ	0.49	2.60	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:VAL:HG13	1:A:124:VAL:N	0.49	2.22	6	1
1:A:49:HIS:O	1:A:50:ILE:CG1	0.49	2.60	17	1
1:A:119:LEU:HD11	1:A:139:GLU:OE1	0.49	2.07	4	1
1:A:123:VAL:O	1:A:125:ARG:N	0.49	2.46	18	2
1:A:145:LEU:O	1:A:146:ILE:HD13	0.49	2.08	3	1
1:A:136:GLY:O	1:A:138:SER:N	0.49	2.46	15	2
1:A:84:ILE:O	1:A:85:GLU:CB	0.49	2.61	16	1
1:A:119:LEU:N	1:A:119:LEU:HD23	0.49	2.23	12	1
1:A:30:ARG:HB3	1:A:33:ALA:HB2	0.49	1.84	10	1
1:A:90:VAL:HG11	1:A:110:GLU:HG2	0.49	1.85	7	1
1:A:45:VAL:O	1:A:47:ARG:N	0.49	2.46	5	7
1:A:46:LEU:CD2	1:A:60:ILE:O	0.49	2.60	14	1
1:A:123:VAL:HG22	1:A:123:VAL:O	0.49	2.08	7	2
1:A:90:VAL:HG23	1:A:115:LEU:HD12	0.49	1.84	4	2
1:A:63:ALA:HB2	1:A:84:ILE:HD11	0.49	1.84	20	1
1:A:57:LEU:C	1:A:57:LEU:CD2	0.49	2.80	19	1
1:A:92:PHE:CD2	1:A:107:ILE:CG2	0.49	2.95	18	1
1:A:112:ILE:C	1:A:112:ILE:CD1	0.49	2.81	14	3
1:A:148:LEU:HD13	1:A:148:LEU:N	0.49	2.22	16	1
1:A:121:ILE:HD11	1:A:145:LEU:HB3	0.49	1.84	3	1
1:A:122:THR:HB	1:A:130:ILE:HG21	0.49	1.85	19	1
1:A:24:LEU:HD12	1:A:24:LEU:O	0.48	2.07	1	1
1:A:80:ALA:O	1:A:81:TRP:CB	0.48	2.59	20	1
1:A:121:ILE:CG1	1:A:145:LEU:HD22	0.48	2.38	2	1
1:A:75:ILE:O	1:A:75:ILE:CG2	0.48	2.61	18	1
1:A:50:ILE:CD1	1:A:58:HIS:O	0.48	2.60	6	2
1:A:92:PHE:CE1	1:A:110:GLU:HG3	0.48	2.43	20	1
1:A:113:ALA:HB1	1:A:115:LEU:CD2	0.48	2.37	7	2
1:A:151:ARG:O	1:A:152:THR:CG2	0.48	2.61	13	1
1:A:35:VAL:O	1:A:36:THR:CG2	0.48	2.60	10	1
1:A:50:ILE:HG23	1:A:50:ILE:O	0.48	2.08	10	1
1:A:121:ILE:O	1:A:147:ARG:CB	0.48	2.61	17	1
1:A:59:ILE:O	1:A:59:ILE:CG2	0.48	2.61	14	1
1:A:121:ILE:HG22	1:A:134:THR:HG23	0.48	1.83	20	1
1:A:8:MET:N	1:A:8:MET:SD	0.48	2.86	12	3
1:A:26:ALA:HB1	1:A:156:VAL:CG2	0.48	2.38	14	2
1:A:71:GLU:O	1:A:75:ILE:HG23	0.48	2.08	13	1
1:A:91:LEU:HD21	1:A:159:LEU:HD22	0.48	1.83	6	1
1:A:16:PRO:O	1:A:17:ASN:CB	0.48	2.60	12	5
1:A:92:PHE:CZ	1:A:119:LEU:HD21	0.48	2.43	5	1
1:A:123:VAL:CG1	1:A:123:VAL:O	0.48	2.60	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ASN:ND2	1:A:26:ALA:N	0.48	2.62	10	1
1:A:38:ILE:HD13	1:A:39:ALA:N	0.48	2.23	7	1
1:A:89:ARG:NH1	1:A:143:HIS:ND1	0.48	2.61	20	1
1:A:122:THR:CG2	1:A:124:VAL:HG22	0.48	2.38	5	1
1:A:50:ILE:HD13	1:A:51:HIS:N	0.48	2.23	10	1
1:A:62:THR:HG22	1:A:62:THR:O	0.48	2.09	3	1
1:A:114:ARG:N	1:A:115:LEU:HD13	0.48	2.24	14	1
1:A:25:ASN:OD1	1:A:33:ALA:HB1	0.48	2.09	6	1
1:A:23:LEU:HA	1:A:150:ALA:HB2	0.48	1.85	15	1
1:A:122:THR:CG2	1:A:122:THR:O	0.48	2.62	16	1
1:A:133:GLU:O	1:A:134:THR:CG2	0.48	2.62	14	1
1:A:59:ILE:O	1:A:59:ILE:HG23	0.48	2.09	14	1
1:A:63:ALA:HB2	1:A:84:ILE:CD1	0.48	2.38	20	1
1:A:72:VAL:CG1	1:A:84:ILE:HD11	0.48	2.39	6	1
1:A:50:ILE:C	1:A:50:ILE:CD1	0.48	2.82	10	1
1:A:166:SER:O	1:A:167:MET:C	0.48	2.51	13	2
1:A:121:ILE:HG22	1:A:122:THR:N	0.48	2.24	11	4
1:A:24:LEU:CD2	1:A:24:LEU:C	0.48	2.81	2	1
1:A:111:PHE:HB2	1:A:140:VAL:HG11	0.47	1.84	3	1
1:A:50:ILE:N	1:A:50:ILE:CD1	0.47	2.73	9	1
1:A:24:LEU:O	1:A:27:LEU:CB	0.47	2.62	1	1
1:A:45:VAL:O	1:A:46:LEU:C	0.47	2.52	13	8
1:A:97:THR:O	1:A:97:THR:CG2	0.47	2.60	7	2
1:A:130:ILE:O	1:A:131:THR:CB	0.47	2.63	4	1
1:A:27:LEU:HD21	1:A:159:LEU:HB2	0.47	1.86	11	1
1:A:51:HIS:CE1	1:A:160:ARG:NH2	0.47	2.82	9	1
1:A:44:ASP:O	1:A:45:VAL:CG1	0.47	2.62	6	3
1:A:124:VAL:O	1:A:125:ARG:CB	0.47	2.61	13	2
1:A:60:ILE:CD1	1:A:60:ILE:C	0.47	2.83	20	1
1:A:9:LYS:CG	1:A:60:ILE:HD13	0.47	2.39	20	1
1:A:38:ILE:HD11	1:A:47:ARG:HG3	0.47	1.84	15	1
1:A:89:ARG:NH2	1:A:116:PRO:CG	0.47	2.78	11	1
1:A:45:VAL:CG1	1:A:63:ALA:O	0.47	2.63	2	2
1:A:45:VAL:CG1	1:A:62:THR:O	0.47	2.63	11	2
1:A:72:VAL:HG11	1:A:84:ILE:HD11	0.47	1.85	6	1
1:A:90:VAL:HG11	1:A:110:GLU:OE2	0.47	2.09	18	1
1:A:42:THR:HG23	1:A:45:VAL:H	0.47	1.69	17	1
1:A:134:THR:HG23	1:A:135:LEU:N	0.47	2.25	2	3
1:A:107:ILE:CG2	1:A:107:ILE:O	0.47	2.63	20	1
1:A:9:LYS:HZ2	1:A:87:ALA:CA	0.47	2.22	13	1
1:A:92:PHE:CZ	1:A:110:GLU:HG2	0.47	2.45	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ILE:O	1:A:78:GLU:C	0.46	2.54	4	1
1:A:67:GLU:O	1:A:68:ALA:CB	0.46	2.63	12	1
1:A:121:ILE:CG2	1:A:122:THR:N	0.46	2.78	11	2
1:A:4:LEU:O	1:A:5:ARG:CB	0.46	2.62	12	1
1:A:50:ILE:C	1:A:50:ILE:HD13	0.46	2.29	10	1
1:A:122:THR:O	1:A:130:ILE:CD1	0.46	2.63	17	1
1:A:130:ILE:O	1:A:132:GLY:N	0.46	2.48	11	2
1:A:23:LEU:HD21	1:A:148:LEU:HD11	0.46	1.86	4	1
1:A:124:VAL:CG2	1:A:125:ARG:N	0.46	2.68	18	1
1:A:75:ILE:HD13	1:A:75:ILE:C	0.46	2.31	18	2
1:A:60:ILE:HG22	1:A:61:ASP:N	0.46	2.26	6	3
1:A:91:LEU:HD11	1:A:118:LYS:NZ	0.46	2.25	5	1
1:A:76:GLY:O	1:A:78:GLU:N	0.46	2.46	4	1
1:A:61:ASP:HB3	1:A:72:VAL:HG21	0.46	1.87	11	1
1:A:126:ASN:O	1:A:128:ALA:N	0.46	2.48	13	2
1:A:27:LEU:HD13	1:A:27:LEU:H	0.46	1.70	14	1
1:A:111:PHE:CG	1:A:140:VAL:HG21	0.46	2.45	15	1
1:A:69:SER:O	1:A:73:GLU:CG	0.46	2.64	3	1
1:A:136:GLY:O	1:A:137:MET:C	0.46	2.53	15	3
1:A:34:ILE:O	1:A:34:ILE:HG23	0.46	2.10	9	1
1:A:58:HIS:CD2	1:A:60:ILE:HG13	0.46	2.46	17	1
1:A:92:PHE:CD2	1:A:107:ILE:HG22	0.46	2.45	18	1
1:A:38:ILE:O	1:A:40:GLY:N	0.46	2.49	5	2
1:A:118:LYS:HZ3	1:A:159:LEU:HD23	0.46	1.71	3	1
1:A:81:TRP:O	1:A:81:TRP:CE3	0.46	2.69	4	1
1:A:134:THR:O	1:A:136:GLY:N	0.46	2.49	15	1
1:A:112:ILE:O	1:A:112:ILE:CD1	0.46	2.64	8	1
1:A:169:ILE:HG22	1:A:170:HIS:N	0.46	2.25	1	1
1:A:159:LEU:C	1:A:159:LEU:HD12	0.46	2.31	4	1
1:A:155:GLY:O	1:A:157:ASP:N	0.46	2.49	18	3
1:A:108:TRP:N	1:A:109:PRO:HD2	0.46	2.26	10	2
1:A:10:VAL:HG11	1:A:163:LEU:CD2	0.46	2.41	12	2
1:A:23:LEU:HD13	1:A:93:MET:SD	0.46	2.51	12	1
1:A:77:ILE:O	1:A:77:ILE:CG2	0.45	2.64	12	2
1:A:92:PHE:CE1	1:A:110:GLU:HG2	0.45	2.46	16	1
1:A:46:LEU:HD11	1:A:50:ILE:CG2	0.45	2.40	6	1
1:A:90:VAL:HG12	1:A:116:PRO:O	0.45	2.10	6	1
1:A:101:ALA:O	1:A:102:VAL:HG23	0.45	2.11	17	1
1:A:143:HIS:CG	1:A:143:HIS:O	0.45	2.69	14	1
1:A:143:HIS:O	1:A:144:ALA:HB2	0.45	2.12	15	2
1:A:50:ILE:CD1	1:A:50:ILE:N	0.45	2.76	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:ASP:N	1:A:103:ASP:OD1	0.45	2.50	7	1
1:A:91:LEU:C	1:A:91:LEU:CD2	0.45	2.82	1	1
1:A:38:ILE:C	1:A:40:GLY:N	0.45	2.69	1	1
1:A:121:ILE:N	1:A:146:ILE:O	0.45	2.50	15	1
1:A:9:LYS:CE	1:A:61:ASP:O	0.45	2.64	11	1
1:A:111:PHE:CG	1:A:140:VAL:HG11	0.45	2.45	9	1
1:A:134:THR:O	1:A:135:LEU:HD23	0.45	2.11	2	1
1:A:30:ARG:NH2	1:A:49:HIS:NE2	0.45	2.64	10	1
1:A:152:THR:O	1:A:154:GLU:N	0.45	2.49	5	2
1:A:148:LEU:HD13	1:A:159:LEU:HD12	0.45	1.87	8	1
1:A:103:ASP:O	1:A:107:ILE:CD1	0.45	2.65	9	1
1:A:92:PHE:CE1	1:A:107:ILE:HG12	0.45	2.47	1	2
1:A:103:ASP:CB	1:A:104:PRO:HD3	0.45	2.42	13	12
1:A:145:LEU:C	1:A:146:ILE:HD12	0.45	2.32	1	1
1:A:78:GLU:O	1:A:80:ALA:N	0.45	2.49	3	1
1:A:134:THR:CG2	1:A:135:LEU:N	0.45	2.80	11	2
1:A:17:ASN:O	1:A:18:ALA:HB2	0.45	2.12	18	1
1:A:58:HIS:O	1:A:58:HIS:ND1	0.45	2.50	13	1
1:A:9:LYS:HE3	1:A:60:ILE:HG22	0.45	1.89	15	1
1:A:121:ILE:HD11	1:A:145:LEU:O	0.45	2.12	16	1
1:A:90:VAL:C	1:A:91:LEU:HD22	0.45	2.32	8	1
1:A:104:PRO:HA	1:A:107:ILE:CG1	0.45	2.41	18	1
1:A:75:ILE:C	1:A:75:ILE:CD1	0.45	2.85	18	1
1:A:17:ASN:O	1:A:18:ALA:CB	0.45	2.65	7	1
1:A:101:ALA:O	1:A:102:VAL:CB	0.45	2.64	17	1
1:A:127:LYS:O	1:A:129:ASP:N	0.45	2.50	20	2
1:A:23:LEU:O	1:A:26:ALA:CB	0.45	2.61	4	1
1:A:91:LEU:O	1:A:91:LEU:HD12	0.45	2.12	13	1
1:A:130:ILE:CD1	1:A:131:THR:N	0.45	2.71	15	1
1:A:65:LEU:H	1:A:65:LEU:HD23	0.45	1.72	12	1
1:A:46:LEU:O	1:A:46:LEU:HD23	0.45	2.11	6	1
1:A:155:GLY:O	1:A:158:VAL:HG22	0.45	2.12	6	1
1:A:25:ASN:O	1:A:26:ALA:CB	0.44	2.65	5	1
1:A:122:THR:O	1:A:130:ILE:CG2	0.44	2.66	5	1
1:A:149:SER:O	1:A:151:ARG:N	0.44	2.50	15	2
1:A:88:ASP:O	1:A:89:ARG:CB	0.44	2.65	19	1
1:A:111:PHE:C	1:A:111:PHE:CD1	0.44	2.88	17	3
1:A:89:ARG:NH1	1:A:143:HIS:CG	0.44	2.85	20	1
1:A:164:LYS:O	1:A:167:MET:N	0.44	2.50	20	1
1:A:68:ALA:O	1:A:72:VAL:N	0.44	2.49	9	3
1:A:149:SER:O	1:A:153:GLY:N	0.44	2.51	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:VAL:O	1:A:125:ARG:C	0.44	2.55	7	1
1:A:115:LEU:N	1:A:115:LEU:CD1	0.44	2.81	20	1
1:A:9:LYS:CG	1:A:62:THR:HB	0.44	2.43	5	1
1:A:103:ASP:N	1:A:103:ASP:OD1	0.44	2.50	15	1
1:A:9:LYS:CE	1:A:60:ILE:HG22	0.44	2.42	15	1
1:A:122:THR:HG23	1:A:130:ILE:HB	0.44	1.88	8	1
1:A:61:ASP:HB3	1:A:72:VAL:HG22	0.44	1.90	10	1
1:A:63:ALA:HB2	1:A:72:VAL:HG11	0.44	1.89	7	1
1:A:104:PRO:O	1:A:106:GLU:N	0.44	2.50	1	1
1:A:18:ALA:HB3	1:A:93:MET:HE1	0.44	1.89	13	1
1:A:39:ALA:O	1:A:41:THR:N	0.44	2.50	11	3
1:A:102:VAL:O	1:A:105:ALA:HB3	0.44	2.12	3	1
1:A:135:LEU:O	1:A:136:GLY:C	0.44	2.56	15	2
1:A:61:ASP:CB	1:A:72:VAL:HG11	0.44	2.38	14	1
1:A:160:ARG:O	1:A:163:LEU:N	0.44	2.51	20	1
1:A:19:GLY:O	1:A:21:SER:N	0.44	2.51	15	2
1:A:120:PRO:CB	1:A:148:LEU:HD12	0.44	2.42	11	1
1:A:45:VAL:HG12	1:A:46:LEU:N	0.44	2.28	12	1
1:A:89:ARG:NH1	1:A:162:HIS:O	0.44	2.50	19	4
1:A:32:ALA:O	1:A:33:ALA:CB	0.44	2.62	3	2
1:A:140:VAL:O	1:A:142:GLY:N	0.44	2.50	7	3
1:A:124:VAL:O	1:A:130:ILE:HD11	0.44	2.13	5	1
1:A:24:LEU:O	1:A:26:ALA:N	0.44	2.50	18	2
1:A:41:THR:CG2	1:A:41:THR:O	0.44	2.66	18	1
1:A:168:GLY:O	1:A:169:ILE:C	0.44	2.56	16	1
1:A:55:MET:SD	1:A:55:MET:N	0.44	2.90	16	1
1:A:30:ARG:NH1	1:A:49:HIS:NE2	0.44	2.66	11	1
1:A:157:ASP:O	1:A:160:ARG:N	0.44	2.50	6	1
1:A:78:GLU:O	1:A:79:ARG:CG	0.44	2.65	10	1
1:A:58:HIS:CD2	1:A:60:ILE:CG1	0.44	3.01	17	1
1:A:130:ILE:O	1:A:130:ILE:CD1	0.44	2.66	4	1
1:A:90:VAL:HG13	1:A:117:ALA:CB	0.44	2.43	5	1
1:A:52:ILE:HG21	1:A:58:HIS:HB3	0.44	1.89	4	1
1:A:60:ILE:HG22	1:A:61:ASP:H	0.44	1.73	9	1
1:A:61:ASP:OD1	1:A:84:ILE:CD1	0.44	2.65	9	1
1:A:161:ASN:O	1:A:164:LYS:N	0.44	2.50	8	2
1:A:37:ASP:O	1:A:38:ILE:C	0.43	2.54	1	2
1:A:86:GLN:CD	1:A:87:ALA:N	0.43	2.72	20	1
1:A:79:ARG:O	1:A:81:TRP:N	0.43	2.51	9	1
1:A:24:LEU:O	1:A:24:LEU:HD13	0.43	2.12	12	1
1:A:155:GLY:C	1:A:156:VAL:CG2	0.43	2.86	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:ILE:CG1	1:A:134:THR:HG21	0.43	2.43	10	1
1:A:73:GLU:O	1:A:78:GLU:N	0.43	2.50	5	1
1:A:35:VAL:O	1:A:35:VAL:HG23	0.43	2.13	16	1
1:A:110:GLU:O	1:A:113:ALA:N	0.43	2.50	9	1
1:A:4:LEU:HD21	1:A:169:ILE:CG2	0.43	2.38	20	1
1:A:9:LYS:CB	1:A:62:THR:HG22	0.43	2.37	9	1
1:A:31:GLU:O	1:A:33:ALA:N	0.43	2.52	1	2
1:A:61:ASP:O	1:A:63:ALA:N	0.43	2.50	3	1
1:A:46:LEU:HG	1:A:46:LEU:O	0.43	2.13	14	1
1:A:92:PHE:CE1	1:A:119:LEU:CD2	0.43	3.01	5	1
1:A:117:ALA:O	1:A:143:HIS:N	0.43	2.51	5	1
1:A:21:SER:O	1:A:24:LEU:N	0.43	2.51	13	1
1:A:52:ILE:O	1:A:52:ILE:CG2	0.43	2.66	16	1
1:A:139:GLU:O	1:A:140:VAL:O	0.43	2.37	9	2
1:A:129:ASP:O	1:A:133:GLU:N	0.43	2.50	6	1
1:A:129:ASP:C	1:A:131:THR:N	0.43	2.70	19	2
1:A:52:ILE:O	1:A:53:ASP:CB	0.43	2.66	8	1
1:A:52:ILE:O	1:A:54:GLY:N	0.43	2.51	5	2
1:A:68:ALA:O	1:A:72:VAL:CG2	0.43	2.65	9	1
1:A:46:LEU:HD23	1:A:62:THR:HB	0.43	1.91	12	1
1:A:52:ILE:HD12	1:A:53:ASP:C	0.43	2.34	10	1
1:A:27:LEU:N	1:A:27:LEU:CD1	0.43	2.80	14	1
1:A:27:LEU:HD22	1:A:27:LEU:H	0.43	1.73	14	1
1:A:42:THR:HG1	1:A:44:ASP:CG	0.43	2.17	20	1
1:A:82:GLN:O	1:A:83:GLU:CB	0.43	2.66	16	1
1:A:133:GLU:O	1:A:136:GLY:N	0.43	2.52	11	1
1:A:107:ILE:O	1:A:108:TRP:C	0.43	2.57	18	2
1:A:24:LEU:O	1:A:28:ALA:N	0.43	2.50	9	1
1:A:73:GLU:OE1	1:A:82:GLN:CG	0.43	2.67	2	1
1:A:47:ARG:O	1:A:47:ARG:CG	0.43	2.66	7	1
1:A:48:GLU:O	1:A:49:HIS:C	0.43	2.57	20	1
1:A:108:TRP:CB	1:A:109:PRO:CD	0.43	2.97	12	2
1:A:112:ILE:CD1	1:A:112:ILE:C	0.43	2.87	13	1
1:A:61:ASP:HB2	1:A:72:VAL:HG13	0.43	1.90	16	1
1:A:139:GLU:CG	1:A:139:GLU:O	0.43	2.66	6	1
1:A:8:MET:SD	1:A:9:LYS:N	0.43	2.91	19	1
1:A:97:THR:CG2	1:A:97:THR:O	0.43	2.63	2	1
1:A:12:ILE:CD1	1:A:12:ILE:N	0.43	2.80	7	1
1:A:90:VAL:HG12	1:A:91:LEU:N	0.43	2.29	4	1
1:A:130:ILE:HD12	1:A:130:ILE:C	0.43	2.34	15	1
1:A:131:THR:O	1:A:135:LEU:HD12	0.43	2.13	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LYS:C	1:A:10:VAL:CG1	0.43	2.87	9	1
1:A:100:ASP:O	1:A:104:PRO:CD	0.43	2.66	12	1
1:A:105:ALA:O	1:A:106:GLU:CB	0.43	2.67	12	1
1:A:92:PHE:CZ	1:A:106:GLU:OE2	0.43	2.71	12	1
1:A:114:ARG:C	1:A:115:LEU:HD13	0.43	2.34	18	1
1:A:130:ILE:CG2	1:A:131:THR:N	0.43	2.82	17	1
1:A:88:ASP:OD1	1:A:88:ASP:N	0.43	2.52	3	1
1:A:113:ALA:HB1	1:A:115:LEU:HD23	0.43	1.91	4	1
1:A:137:MET:O	1:A:139:GLU:N	0.43	2.51	4	1
1:A:59:ILE:HG22	1:A:59:ILE:O	0.43	2.14	13	1
1:A:45:VAL:HG13	1:A:62:THR:HG23	0.43	1.90	10	1
1:A:130:ILE:CD1	1:A:130:ILE:O	0.43	2.65	7	1
1:A:84:ILE:CG2	1:A:84:ILE:O	0.42	2.66	17	1
1:A:90:VAL:O	1:A:90:VAL:CG1	0.42	2.63	1	1
1:A:125:ARG:O	1:A:127:LYS:N	0.42	2.48	6	2
1:A:84:ILE:CD1	1:A:84:ILE:C	0.42	2.87	14	1
1:A:52:ILE:HG21	1:A:58:HIS:CB	0.42	2.44	14	2
1:A:127:LYS:O	1:A:130:ILE:CG1	0.42	2.66	14	1
1:A:46:LEU:HD13	1:A:61:ASP:CA	0.42	2.44	4	1
1:A:139:GLU:O	1:A:140:VAL:C	0.42	2.57	9	1
1:A:87:ALA:O	1:A:115:LEU:CD2	0.42	2.67	19	1
1:A:51:HIS:NE2	1:A:160:ARG:NH2	0.42	2.66	2	2
1:A:97:THR:HG21	1:A:127:LYS:HD2	0.42	1.90	18	1
1:A:73:GLU:OE1	1:A:81:TRP:N	0.42	2.52	10	1
1:A:63:ALA:HB1	1:A:68:ALA:CB	0.42	2.44	1	1
1:A:23:LEU:O	1:A:26:ALA:N	0.42	2.51	14	2
1:A:122:THR:HG23	1:A:130:ILE:HA	0.42	1.91	9	1
1:A:123:VAL:O	1:A:123:VAL:CG1	0.42	2.66	12	1
1:A:68:ALA:O	1:A:72:VAL:HG13	0.42	2.14	7	1
1:A:122:THR:O	1:A:124:VAL:N	0.42	2.50	16	1
1:A:131:THR:O	1:A:132:GLY:C	0.42	2.57	9	1
1:A:118:LYS:NZ	1:A:159:LEU:HD12	0.42	2.30	1	1
1:A:46:LEU:HD12	1:A:46:LEU:C	0.42	2.34	14	1
1:A:156:VAL:O	1:A:159:LEU:N	0.42	2.51	9	1
1:A:146:ILE:CG2	1:A:147:ARG:N	0.42	2.83	9	1
1:A:72:VAL:HG23	1:A:73:GLU:N	0.42	2.29	8	1
1:A:149:SER:O	1:A:150:ALA:O	0.42	2.37	18	1
1:A:42:THR:OG1	1:A:43:ARG:N	0.42	2.52	10	1
1:A:117:ALA:O	1:A:118:LYS:CB	0.42	2.66	1	1
1:A:41:THR:HG22	1:A:47:ARG:NH2	0.42	2.29	1	1
1:A:130:ILE:C	1:A:132:GLY:N	0.42	2.72	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:PRO:O	1:A:107:ILE:N	0.42	2.52	13	1
1:A:65:LEU:O	1:A:68:ALA:N	0.42	2.52	13	1
1:A:89:ARG:NH1	1:A:116:PRO:O	0.42	2.53	13	1
1:A:30:ARG:NH1	1:A:49:HIS:CE1	0.42	2.87	11	1
1:A:8:MET:HG2	1:A:9:LYS:N	0.42	2.30	12	1
1:A:60:ILE:CG2	1:A:61:ASP:N	0.42	2.83	6	1
1:A:27:LEU:HD11	1:A:163:LEU:HD13	0.42	1.90	17	1
1:A:121:ILE:HD11	1:A:145:LEU:HB2	0.42	1.91	5	1
1:A:130:ILE:C	1:A:130:ILE:CD1	0.42	2.84	4	1
1:A:127:LYS:O	1:A:128:ALA:C	0.42	2.57	11	1
1:A:8:MET:CE	1:A:8:MET:O	0.42	2.67	9	1
1:A:92:PHE:CZ	1:A:107:ILE:HG12	0.42	2.50	8	1
1:A:62:THR:O	1:A:64:GLY:N	0.42	2.52	15	1
1:A:85:GLU:O	1:A:86:GLN:CB	0.42	2.67	6	1
1:A:9:LYS:NZ	1:A:85:GLU:O	0.42	2.53	19	1
1:A:24:LEU:HD12	1:A:48:GLU:HA	0.42	1.92	2	1
1:A:92:PHE:CE2	1:A:119:LEU:HB2	0.42	2.50	18	1
1:A:116:PRO:HB3	1:A:143:HIS:CD2	0.42	2.50	18	1
1:A:107:ILE:CD1	1:A:110:GLU:HB3	0.42	2.45	5	1
1:A:125:ARG:O	1:A:126:ASN:C	0.42	2.58	10	2
1:A:113:ALA:CB	1:A:115:LEU:CD1	0.42	2.97	18	1
1:A:90:VAL:CG2	1:A:110:GLU:OE1	0.42	2.64	10	1
1:A:38:ILE:O	1:A:39:ALA:C	0.42	2.58	1	1
1:A:23:LEU:O	1:A:24:LEU:C	0.42	2.58	14	3
1:A:102:VAL:O	1:A:103:ASP:C	0.42	2.58	14	1
1:A:61:ASP:OD2	1:A:72:VAL:HG13	0.42	2.15	20	1
1:A:8:MET:HB3	1:A:167:MET:CB	0.42	2.45	17	1
1:A:107:ILE:CG2	1:A:108:TRP:N	0.42	2.83	13	2
1:A:122:THR:HG22	1:A:124:VAL:HG12	0.42	1.91	3	1
1:A:121:ILE:HG21	1:A:134:THR:CG2	0.42	2.40	20	1
1:A:26:ALA:HB1	1:A:156:VAL:HG11	0.42	1.91	6	1
1:A:115:LEU:HD22	1:A:115:LEU:C	0.42	2.34	18	1
1:A:115:LEU:CD1	1:A:115:LEU:N	0.42	2.83	18	1
1:A:20:LYS:O	1:A:21:SER:CB	0.41	2.68	17	1
1:A:68:ALA:O	1:A:69:SER:C	0.41	2.58	20	1
1:A:89:ARG:CZ	1:A:143:HIS:CE1	0.41	3.02	15	1
1:A:148:LEU:C	1:A:148:LEU:CD2	0.41	2.88	16	1
1:A:59:ILE:CG2	1:A:59:ILE:O	0.41	2.68	2	1
1:A:12:ILE:CD1	1:A:48:GLU:OE1	0.41	2.68	7	1
1:A:112:ILE:O	1:A:113:ALA:HB3	0.41	2.14	17	1
1:A:81:TRP:O	1:A:82:GLN:CB	0.41	2.67	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ILE:HD13	1:A:47:ARG:HD2	0.41	1.91	5	1
1:A:113:ALA:CB	1:A:115:LEU:CD2	0.41	2.98	16	1
1:A:121:ILE:HD13	1:A:134:THR:HG23	0.41	1.92	9	1
1:A:10:VAL:HG11	1:A:163:LEU:HD22	0.41	1.92	12	1
1:A:60:ILE:O	1:A:61:ASP:O	0.41	2.37	12	1
1:A:98:THR:O	1:A:98:THR:CG2	0.41	2.69	8	1
1:A:24:LEU:HD21	1:A:48:GLU:CA	0.41	2.42	7	1
1:A:17:ASN:O	1:A:18:ALA:C	0.41	2.58	17	1
1:A:9:LYS:HE3	1:A:87:ALA:HB2	0.41	1.90	3	1
1:A:61:ASP:OD2	1:A:72:VAL:CG1	0.41	2.69	20	1
1:A:130:ILE:O	1:A:133:GLU:N	0.41	2.53	5	1
1:A:104:PRO:C	1:A:106:GLU:N	0.41	2.73	13	1
1:A:7:GLY:HA2	1:A:167:MET:CG	0.41	2.46	13	1
1:A:94:VAL:O	1:A:96:GLY:N	0.41	2.53	19	1
1:A:131:THR:CG2	1:A:132:GLY:N	0.41	2.84	10	1
1:A:95:ASP:O	1:A:96:GLY:C	0.41	2.59	6	2
1:A:111:PHE:CD1	1:A:111:PHE:O	0.41	2.74	1	1
1:A:137:MET:O	1:A:138:SER:C	0.41	2.59	3	1
1:A:117:ALA:O	1:A:143:HIS:CB	0.41	2.68	3	1
1:A:81:TRP:CG	1:A:82:GLN:N	0.41	2.88	14	1
1:A:44:ASP:C	1:A:46:LEU:N	0.41	2.72	4	3
1:A:8:MET:SD	1:A:8:MET:N	0.41	2.93	17	2
1:A:159:LEU:O	1:A:160:ARG:C	0.41	2.59	14	1
1:A:31:GLU:O	1:A:32:ALA:CB	0.41	2.68	20	1
1:A:10:VAL:HG13	1:A:163:LEU:HD11	0.41	1.92	15	1
1:A:53:ASP:OD1	1:A:54:GLY:N	0.41	2.54	11	1
1:A:83:GLU:OE1	1:A:83:GLU:N	0.41	2.53	9	1
1:A:129:ASP:O	1:A:130:ILE:C	0.41	2.58	6	1
1:A:130:ILE:HG12	1:A:134:THR:CG2	0.41	2.46	10	1
1:A:138:SER:O	1:A:139:GLU:C	0.41	2.59	9	1
1:A:23:LEU:HD23	1:A:24:LEU:N	0.41	2.31	7	1
1:A:115:LEU:CD2	1:A:115:LEU:C	0.41	2.89	20	1
1:A:48:GLU:O	1:A:49:HIS:O	0.41	2.38	9	3
1:A:24:LEU:CD1	1:A:24:LEU:C	0.41	2.89	12	1
1:A:102:VAL:O	1:A:106:GLU:CD	0.41	2.59	12	1
1:A:44:ASP:HB3	1:A:72:VAL:HG22	0.41	1.92	19	1
1:A:30:ARG:NE	1:A:49:HIS:CE1	0.41	2.89	10	1
1:A:93:MET:SD	1:A:93:MET:N	0.41	2.93	3	1
1:A:42:THR:OG1	1:A:44:ASP:CG	0.41	2.59	20	1
1:A:108:TRP:CE3	1:A:108:TRP:HA	0.41	2.50	20	1
1:A:104:PRO:O	1:A:105:ALA:C	0.41	2.59	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:LYS:C	1:A:129:ASP:N	0.41	2.72	7	2
1:A:130:ILE:O	1:A:134:THR:CB	0.41	2.69	9	1
1:A:30:ARG:O	1:A:31:GLU:C	0.41	2.59	10	1
1:A:125:ARG:CG	1:A:126:ASN:N	0.41	2.82	7	1
1:A:40:GLY:O	1:A:41:THR:C	0.41	2.60	3	1
1:A:95:ASP:O	1:A:98:THR:CB	0.41	2.69	13	1
1:A:30:ARG:O	1:A:32:ALA:N	0.41	2.52	11	1
1:A:64:GLY:O	1:A:65:LEU:CD1	0.41	2.66	6	1
1:A:44:ASP:HB2	1:A:72:VAL:HG23	0.41	1.90	6	1
1:A:96:GLY:HA3	1:A:122:THR:HG21	0.41	1.92	2	1
1:A:107:ILE:O	1:A:107:ILE:CD1	0.41	2.58	10	1
1:A:76:GLY:O	1:A:77:ILE:C	0.41	2.59	7	2
1:A:52:ILE:O	1:A:52:ILE:HG23	0.41	2.15	3	1
1:A:77:ILE:H	1:A:77:ILE:HD13	0.41	1.74	14	1
1:A:104:PRO:HA	1:A:107:ILE:CG2	0.41	2.46	13	1
1:A:24:LEU:HD11	1:A:48:GLU:CB	0.41	2.46	11	1
1:A:134:THR:O	1:A:135:LEU:C	0.41	2.57	2	1
1:A:96:GLY:O	1:A:122:THR:CB	0.41	2.69	8	1
1:A:124:VAL:HG13	1:A:127:LYS:CB	0.41	2.46	7	1
1:A:76:GLY:C	1:A:77:ILE:CG1	0.41	2.90	7	1
1:A:88:ASP:OD2	1:A:166:SER:O	0.40	2.39	17	1
1:A:25:ASN:O	1:A:26:ALA:C	0.40	2.59	14	1
1:A:50:ILE:CG1	1:A:51:HIS:N	0.40	2.84	5	1
1:A:97:THR:HG23	1:A:130:ILE:CD1	0.40	2.46	13	1
1:A:164:LYS:O	1:A:166:SER:N	0.40	2.51	13	1
1:A:24:LEU:HD23	1:A:24:LEU:O	0.40	2.16	2	1
1:A:40:GLY:O	1:A:41:THR:O	0.40	2.39	10	1
1:A:128:ALA:O	1:A:131:THR:N	0.40	2.53	17	1
1:A:73:GLU:C	1:A:78:GLU:O	0.40	2.59	4	1
1:A:92:PHE:CZ	1:A:119:LEU:HD23	0.40	2.48	13	1
1:A:11:VAL:O	1:A:12:ILE:CG2	0.40	2.70	16	1
1:A:83:GLU:C	1:A:84:ILE:HD12	0.40	2.37	11	1
1:A:124:VAL:HG13	1:A:125:ARG:H	0.40	1.76	18	1
1:A:107:ILE:O	1:A:110:GLU:CB	0.40	2.69	18	1
1:A:53:ASP:O	1:A:54:GLY:C	0.40	2.60	11	2
1:A:51:HIS:CD2	1:A:51:HIS:O	0.40	2.74	16	1
1:A:149:SER:OG	1:A:154:GLU:N	0.40	2.54	11	1
1:A:24:LEU:O	1:A:27:LEU:N	0.40	2.54	1	1
1:A:119:LEU:O	1:A:145:LEU:CA	0.40	2.69	5	1
1:A:12:ILE:CG1	1:A:12:ILE:O	0.40	2.70	16	1
1:A:166:SER:OG	1:A:167:MET:N	0.40	2.53	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:THR:O	1:A:132:GLY:O	0.40	2.39	9	1
1:A:154:GLU:O	1:A:154:GLU:CG	0.40	2.69	9	1
1:A:94:VAL:O	1:A:95:ASP:O	0.40	2.38	12	1
1:A:109:PRO:O	1:A:110:GLU:CG	0.40	2.70	8	1
1:A:126:ASN:O	1:A:127:LYS:C	0.40	2.59	7	1
1:A:150:ALA:O	1:A:151:ARG:C	0.40	2.59	17	1
1:A:78:GLU:O	1:A:79:ARG:C	0.40	2.60	20	1
1:A:18:ALA:O	1:A:93:MET:SD	0.40	2.80	13	1
1:A:122:THR:C	1:A:124:VAL:N	0.40	2.75	11	1
1:A:10:VAL:HG13	1:A:89:ARG:O	0.40	2.16	11	1
1:A:44:ASP:O	1:A:45:VAL:HB	0.40	2.17	8	1
1:A:155:GLY:O	1:A:156:VAL:C	0.40	2.59	18	1
1:A:153:GLY:O	1:A:156:VAL:HG22	0.40	2.16	18	1
1:A:29:GLY:O	1:A:30:ARG:C	0.40	2.60	7	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	167/172 (97%)	100±6 (60±4%)	46±5 (27±3%)	21±4 (12±2%)	1	7
All	All	3340/3440 (97%)	2008 (60%)	916 (27%)	416 (12%)	1	7

All 124 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	49	HIS	17
1	A	63	ALA	12
1	A	77	ILE	12
1	A	84	ILE	11
1	A	19	GLY	10
1	A	125	ARG	9
1	A	129	ASP	9
1	A	64	GLY	9

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Mol	Chain	Res	Type	Models (Total)
1	A	83	GLU	9
1	A	46	LEU	8
1	A	17	ASN	8
1	A	140	VAL	7
1	A	141	ASN	7
1	A	54	GLY	7
1	A	85	GLU	7
1	A	123	VAL	6
1	A	18	ALA	6
1	A	87	ALA	6
1	A	41	THR	6
1	A	32	ALA	6
1	A	139	GLU	6
1	A	106	GLU	6
1	A	137	MET	6
1	A	126	ASN	6
1	A	96	GLY	6
1	A	79	ARG	6
1	A	61	ASP	5
1	A	124	VAL	5
1	A	138	SER	5
1	A	131	THR	5
1	A	166	SER	4
1	A	80	ALA	4
1	A	151	ARG	4
1	A	169	ILE	4
1	A	74	ARG	4
1	A	153	GLY	4
1	A	40	GLY	4
1	A	50	ILE	4
1	A	133	GLU	4
1	A	113	ALA	4
1	A	142	GLY	4
1	A	51	HIS	4
1	A	150	ALA	4
1	A	57	LEU	3
1	A	26	ALA	3
1	A	30	ARG	3
1	A	132	GLY	3
1	A	4	LEU	3
1	A	58	HIS	3
1	A	168	GLY	3

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Mol	Chain	Res	Type	Models (Total)
1	A	156	VAL	3
1	A	154	GLU	3
1	A	101	ALA	3
1	A	81	TRP	3
1	A	31	GLU	3
1	A	130	ILE	3
1	A	110	GLU	3
1	A	89	ARG	3
1	A	42	THR	2
1	A	60	ILE	2
1	A	82	GLN	2
1	A	135	LEU	2
1	A	39	ALA	2
1	A	167	MET	2
1	A	95	ASP	2
1	A	56	PRO	2
1	A	52	ILE	2
1	A	5	ARG	2
1	A	24	LEU	2
1	A	14	GLY	2
1	A	20	LYS	2
1	A	122	THR	2
1	A	38	ILE	2
1	A	100	ASP	2
1	A	7	GLY	2
1	A	112	ILE	2
1	A	127	LYS	2
1	A	155	GLY	2
1	A	158	VAL	2
1	A	134	THR	2
1	A	6	GLU	2
1	A	107	ILE	2
1	A	78	GLU	2
1	A	28	ALA	1
1	A	67	GLU	1
1	A	72	VAL	1
1	A	92	PHE	1
1	A	15	ARG	1
1	A	114	ARG	1
1	A	147	ARG	1
1	A	94	VAL	1
1	A	36	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	143	HIS	1
1	A	68	ALA	1
1	A	75	ILE	1
1	A	121	ILE	1
1	A	29	GLY	1
1	A	16	PRO	1
1	A	118	LYS	1
1	A	136	GLY	1
1	A	8	MET	1
1	A	25	ASN	1
1	A	11	VAL	1
1	A	65	LEU	1
1	A	59	ILE	1
1	A	13	ALA	1
1	A	12	ILE	1
1	A	86	GLN	1
1	A	162	HIS	1
1	A	128	ALA	1
1	A	149	SER	1
1	A	170	HIS	1
1	A	66	ARG	1
1	A	53	ASP	1
1	A	27	LEU	1
1	A	33	ALA	1
1	A	152	THR	1
1	A	97	THR	1
1	A	144	ALA	1
1	A	108	TRP	1
1	A	70	ASP	1
1	A	119	LEU	1
1	A	93	MET	1
1	A	10	VAL	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/138 (97%)	91±5 (68±3%)	43±5 (32±3%)	1	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2680/2760 (97%)	1812 (68%)	868 (32%)	1 13

All 116 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	103	ASP	20
1	A	9	LYS	19
1	A	108	TRP	19
1	A	57	LEU	17
1	A	55	MET	16
1	A	8	MET	16
1	A	163	LEU	14
1	A	147	ARG	13
1	A	44	ASP	13
1	A	65	LEU	13
1	A	20	LYS	13
1	A	119	LEU	13
1	A	164	LYS	12
1	A	160	ARG	12
1	A	118	LYS	12
1	A	133	GLU	12
1	A	27	LEU	12
1	A	47	ARG	11
1	A	15	ARG	11
1	A	114	ARG	11
1	A	23	LEU	11
1	A	83	GLU	11
1	A	66	ARG	11
1	A	148	LEU	11
1	A	81	TRP	11
1	A	137	MET	11
1	A	82	GLN	10
1	A	74	ARG	10
1	A	100	ASP	10
1	A	79	ARG	10
1	A	48	GLU	10
1	A	67	GLU	9
1	A	151	ARG	9
1	A	129	ASP	9
1	A	139	GLU	9
1	A	91	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	106	GLU	9
1	A	24	LEU	9
1	A	135	LEU	9
1	A	157	ASP	9
1	A	43	ARG	9
1	A	71	GLU	9
1	A	170	HIS	9
1	A	138	SER	9
1	A	127	LYS	9
1	A	70	ASP	9
1	A	78	GLU	9
1	A	88	ASP	8
1	A	61	ASP	8
1	A	5	ARG	8
1	A	125	ARG	8
1	A	86	GLN	8
1	A	22	SER	8
1	A	115	LEU	8
1	A	58	HIS	8
1	A	37	ASP	8
1	A	85	GLU	8
1	A	165	GLN	8
1	A	93	MET	8
1	A	92	PHE	7
1	A	49	HIS	7
1	A	95	ASP	7
1	A	75	ILE	7
1	A	21	SER	7
1	A	46	LEU	7
1	A	159	LEU	7
1	A	110	GLU	7
1	A	89	ARG	7
1	A	84	ILE	7
1	A	107	ILE	7
1	A	167	MET	6
1	A	30	ARG	6
1	A	111	PHE	6
1	A	4	LEU	6
1	A	149	SER	6
1	A	53	ASP	6
1	A	38	ILE	6
1	A	126	ASN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	34	ILE	5
1	A	73	GLU	5
1	A	6	GLU	5
1	A	141	ASN	5
1	A	50	ILE	5
1	A	112	ILE	5
1	A	161	ASN	4
1	A	51	HIS	4
1	A	145	LEU	4
1	A	154	GLU	4
1	A	59	ILE	4
1	A	122	THR	4
1	A	130	ILE	4
1	A	42	THR	3
1	A	69	SER	3
1	A	140	VAL	3
1	A	169	ILE	3
1	A	52	ILE	3
1	A	162	HIS	3
1	A	31	GLU	3
1	A	17	ASN	3
1	A	131	THR	3
1	A	134	THR	3
1	A	166	SER	2
1	A	60	ILE	2
1	A	72	VAL	2
1	A	36	THR	2
1	A	25	ASN	2
1	A	124	VAL	1
1	A	143	HIS	1
1	A	121	ILE	1
1	A	11	VAL	1
1	A	12	ILE	1
1	A	146	ILE	1
1	A	102	VAL	1
1	A	156	VAL	1
1	A	152	THR	1
1	A	77	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 46% for the well-defined parts and 46% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5861

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	950
Number of shifts mapped to atoms	950
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
$^{13}\text{C}_\alpha$	168	0.02 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	137	0.10 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	157	-0.45 ± 0.14	None needed (< 0.5 ppm)
^{15}N	159	-0.03 ± 0.53	None needed (< 0.5 ppm)

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 46%, i.e. 930 atoms were assigned a chemical shift out of a possible 2016. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	796/823 (97%)	321/328 (98%)	319/334 (96%)	156/161 (97%)
Sidechain	134/1103 (12%)	0/637 (0%)	134/411 (33%)	0/55 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/90 (0%)	0/46 (0%)	0/30 (0%)	0/14 (0%)
Overall	930/2016 (46%)	321/1011 (32%)	453/775 (58%)	156/230 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 949 atoms were assigned a chemical shift out of a possible 2075. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	812/848 (96%)	328/338 (97%)	325/344 (94%)	159/166 (96%)
Sidechain	137/1137 (12%)	0/657 (0%)	137/422 (32%)	0/58 (0%)
Aromatic	0/90 (0%)	0/46 (0%)	0/30 (0%)	0/14 (0%)
Overall	949/2075 (46%)	328/1041 (32%)	462/796 (58%)	159/238 (67%)

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:

