



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:48 pm GMT

PDB ID : 1D1N  
Title : SOLUTION STRUCTURE OF THE FMET-TRNA<sup>FMET</sup> BINDING DOMAIN OF *BACILLUS STEAROTHERMOPHILLUS* TRANSLATION INITIATION FACTOR IF2  
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Deposited on : 1999-09-20

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

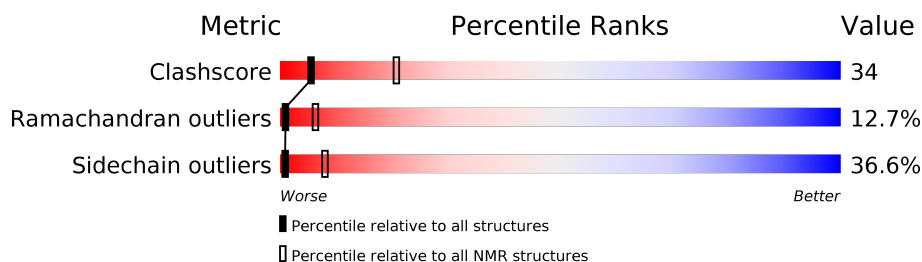
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 74%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	99	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 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:146-A:200, A:204-A:234 (86)	0.22	1

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 5 clusters and 3 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 1581 atoms, of which 797 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INITIATION FACTOR 2.

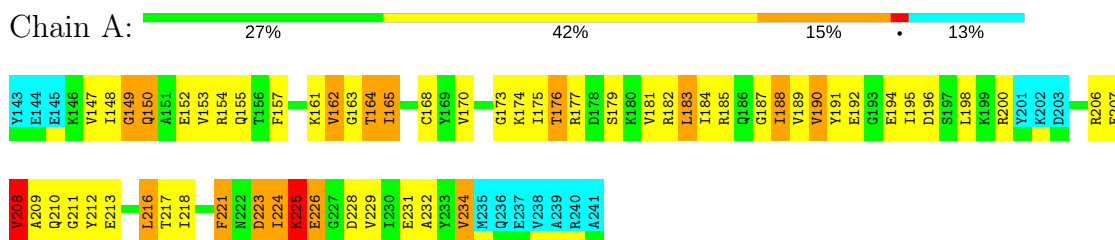
Mol	Chain	Residues	Atoms						Trace
1	A	99	Total	C	H	N	O	S	0
			1581	492	797	136	153	3	

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

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

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: INITIATION FACTOR 2

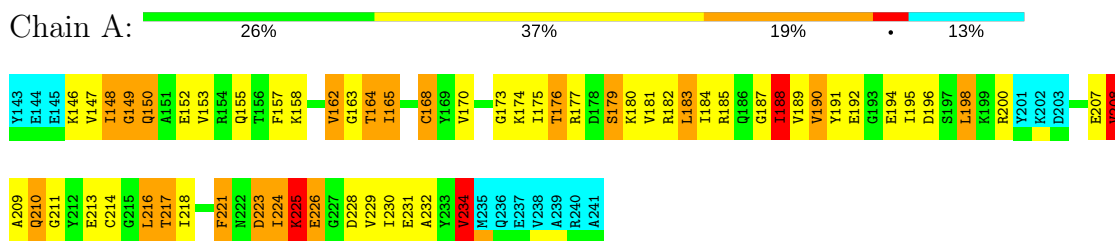


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

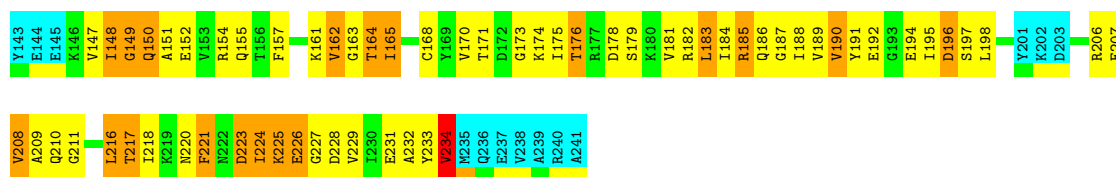
- Molecule 1: INITIATION FACTOR 2



#### 4.2.2 Score per residue for model 2

- Molecule 1: INITIATION FACTOR 2





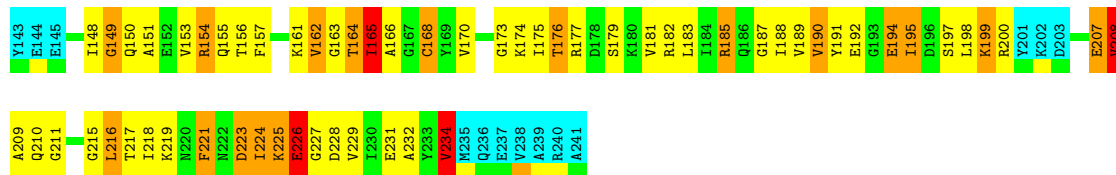
### 4.2.3 Score per residue for model 3

- Molecule 1: INITIATION FACTOR 2



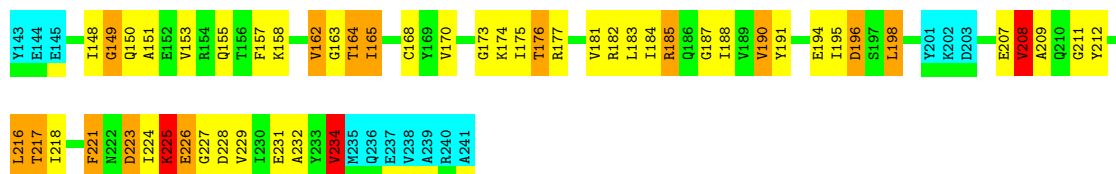
### 4.2.4 Score per residue for model 4

- Molecule 1: INITIATION FACTOR 2



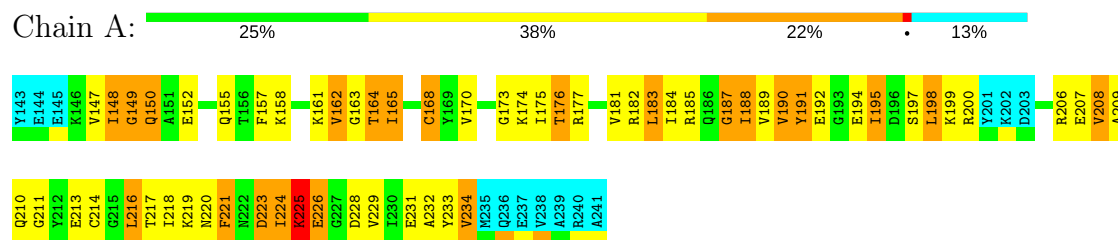
### 4.2.5 Score per residue for model 5

- Molecule 1: INITIATION FACTOR 2



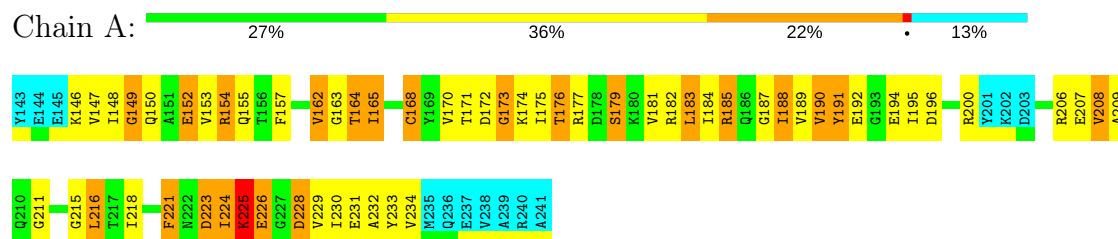
### 4.2.6 Score per residue for model 6

- Molecule 1: INITIATION FACTOR 2



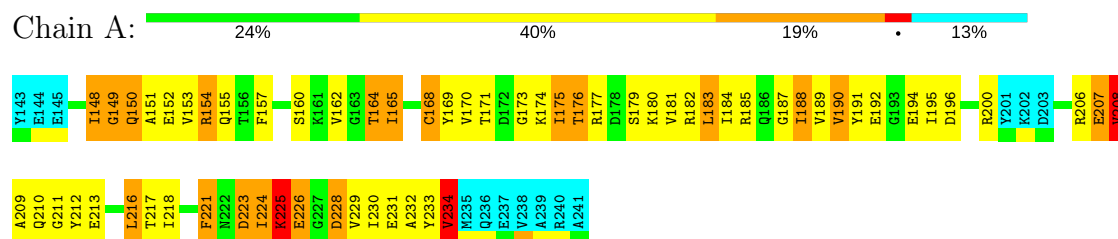
#### 4.2.7 Score per residue for model 7

- Molecule 1: INITIATION FACTOR 2



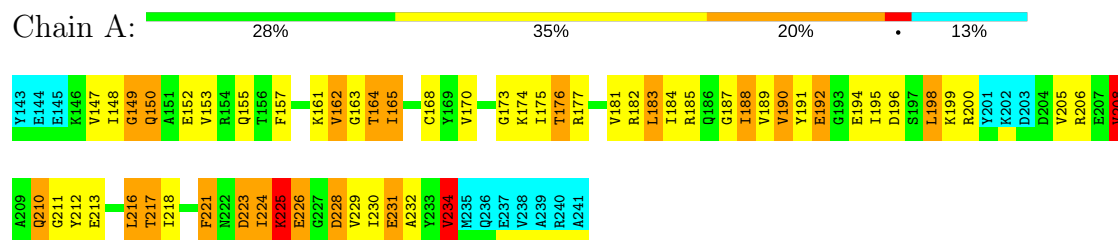
#### 4.2.8 Score per residue for model 8

- Molecule 1: INITIATION FACTOR 2



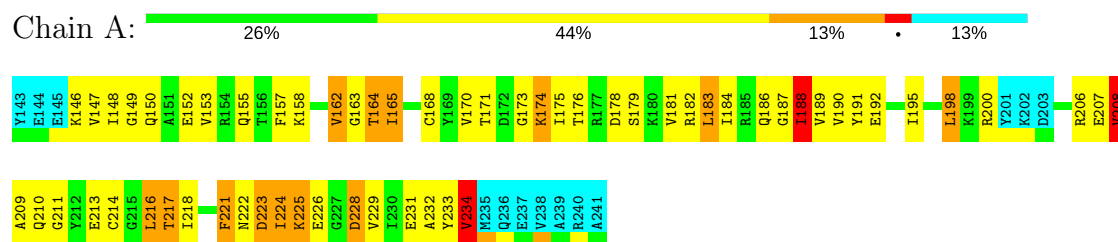
#### 4.2.9 Score per residue for model 9

- Molecule 1: INITIATION FACTOR 2



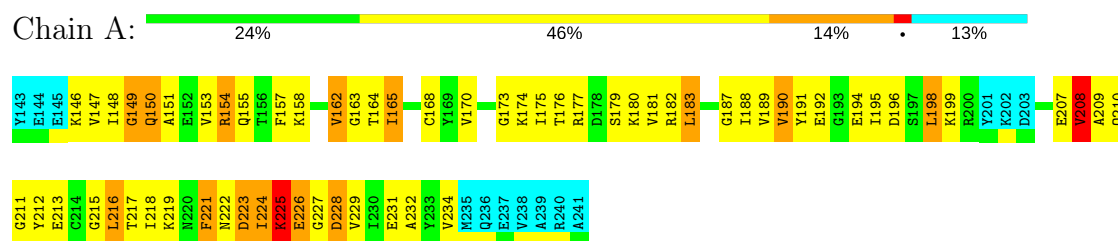
### 4.2.10 Score per residue for model 10

- Molecule 1: INITIATION FACTOR 2



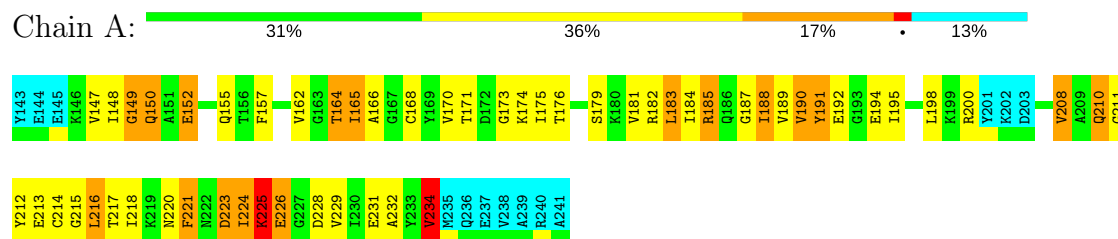
### 4.2.11 Score per residue for model 11

- Molecule 1: INITIATION FACTOR 2



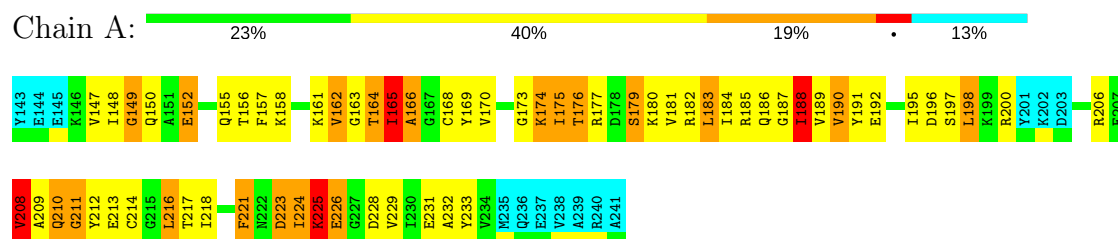
### 4.2.12 Score per residue for model 12

- Molecule 1: INITIATION FACTOR 2



### 4.2.13 Score per residue for model 13

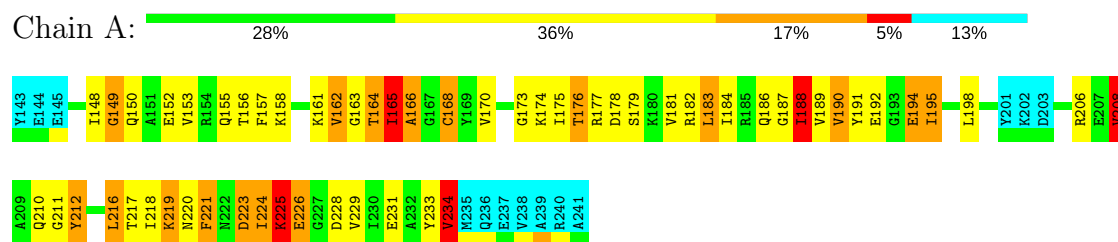
- Molecule 1: INITIATION FACTOR 2





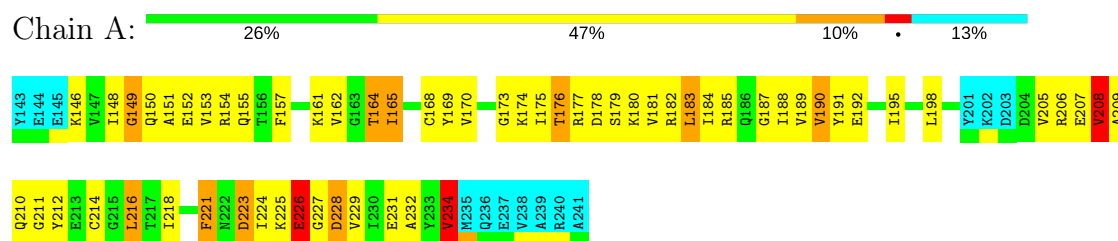
### 4.2.14 Score per residue for model 14

- Molecule 1: INITIATION FACTOR 2



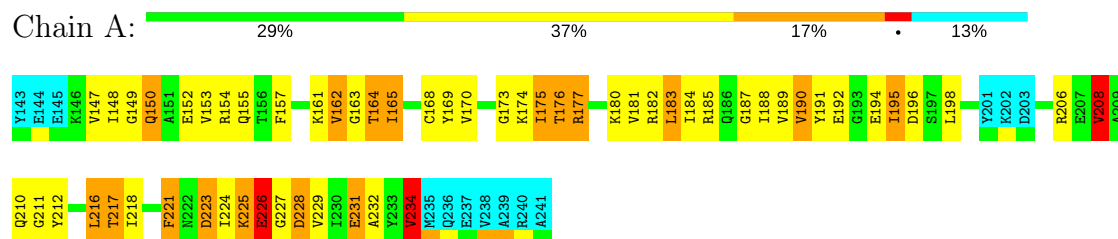
### 4.2.15 Score per residue for model 15

- Molecule 1: INITIATION FACTOR 2



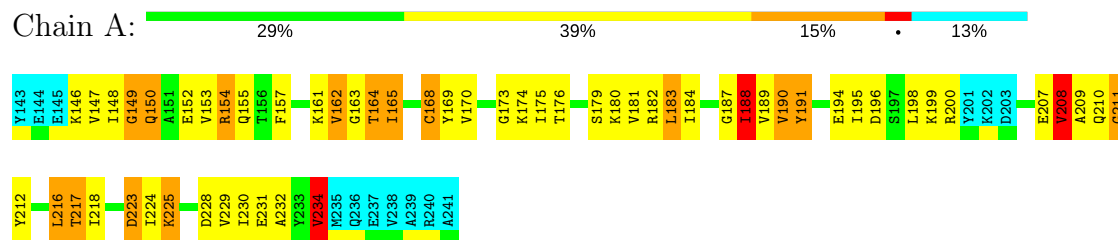
### 4.2.16 Score per residue for model 16

- Molecule 1: INITIATION FACTOR 2



### 4.2.17 Score per residue for model 17

- Molecule 1: INITIATION FACTOR 2



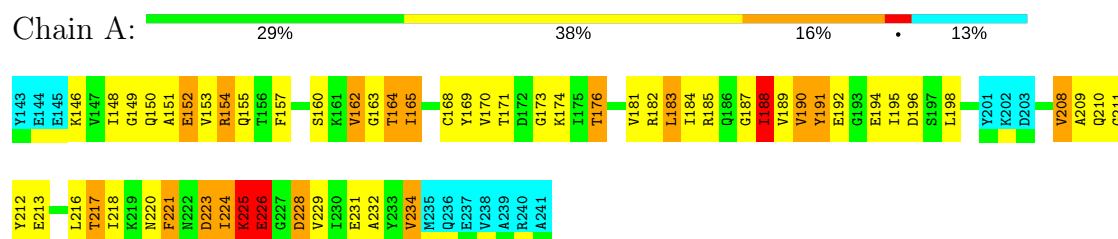
## 4.2.18 Score per residue for model 18

- Molecule 1: INITIATION FACTOR 2



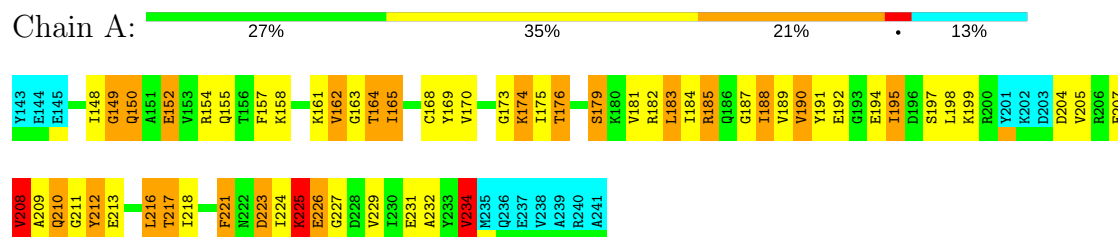
## 4.2.19 Score per residue for model 19

- Molecule 1: INITIATION FACTOR 2



## 4.2.20 Score per residue for model 20

- Molecule 1: INITIATION FACTOR 2



## 5 Refinement protocol and experimental data overview

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURES WITH ACCEPTABLE COVALENT GEOMETRY, STRUCTURES WITH FAVORABLE NON-BOND ENERGY, STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS, STRUCTURES WITH THE LOWEST ENERGY.*

The authors did not provide any information on software used for structure solution, optimization or refinement.

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

Chemical shift file(s)	BMRB entry 4697
Number of chemical shift lists	1
Total number of shifts	1101
Number of shifts mapped to atoms	1028
Number of unparsed shifts	0
Number of shifts with mapping errors	73
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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	672	693	693	47±5
All	All	13440	13860	13860	940

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:ILE:HD11	1:A:216:LEU:HD13	1.10	1.10	6	3
1:A:148:ILE:HG21	1:A:234:VAL:HG12	1.01	1.29	6	10
1:A:164:THR:HG21	1:A:224:ILE:HG21	0.92	1.38	4	8
1:A:198:LEU:CD1	1:A:216:LEU:HD23	0.80	2.06	18	1
1:A:190:VAL:HG12	1:A:223:ASP:OD2	0.80	1.76	15	13
1:A:198:LEU:HD13	1:A:216:LEU:HD23	0.79	1.52	17	2
1:A:181:VAL:CG1	1:A:195:ILE:HD12	0.79	2.08	3	1
1:A:198:LEU:CD1	1:A:216:LEU:HD22	0.78	2.08	3	5
1:A:176:THR:O	1:A:195:ILE:HD13	0.77	1.80	8	3
1:A:166:ALA:O	1:A:216:LEU:HD12	0.77	1.80	4	1
1:A:152:GLU:CG	1:A:229:VAL:HG22	0.76	2.10	18	9
1:A:158:LYS:CB	1:A:224:ILE:HD13	0.76	2.11	5	1
1:A:184:ILE:HG23	1:A:188:ILE:O	0.75	1.81	17	12
1:A:195:ILE:HD12	1:A:216:LEU:HD13	0.75	1.57	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:ILE:CD1	1:A:216:LEU:HD13	0.74	2.03	6	2
1:A:179:SER:O	1:A:195:ILE:HD12	0.74	1.83	7	7
1:A:175:ILE:CG2	1:A:216:LEU:HD21	0.73	2.12	4	1
1:A:183:LEU:HD13	1:A:191:TYR:HB3	0.73	1.61	4	3
1:A:148:ILE:HD13	1:A:234:VAL:HG12	0.72	1.61	17	1
1:A:170:VAL:HG21	1:A:208:VAL:O	0.72	1.84	16	18
1:A:152:GLU:HG2	1:A:229:VAL:HG22	0.72	1.58	15	14
1:A:198:LEU:HD13	1:A:216:LEU:HD22	0.72	1.62	3	3
1:A:195:ILE:HD13	1:A:217:THR:O	0.71	1.84	16	2
1:A:195:ILE:HG12	1:A:216:LEU:HD13	0.70	1.61	12	2
1:A:168:CYS:SG	1:A:216:LEU:HD11	0.70	2.26	18	6
1:A:195:ILE:HD11	1:A:216:LEU:CD1	0.70	2.16	20	4
1:A:190:VAL:HG21	1:A:228:ASP:CB	0.70	2.17	13	5
1:A:148:ILE:HD13	1:A:234:VAL:CG1	0.70	2.16	17	1
1:A:189:VAL:HG11	1:A:192:GLU:CG	0.70	2.17	16	18
1:A:185:ARG:NH2	1:A:190:VAL:HG13	0.69	2.01	6	1
1:A:198:LEU:HD12	1:A:216:LEU:HD23	0.69	1.62	18	1
1:A:183:LEU:HD22	1:A:221:PHE:CZ	0.69	2.22	5	3
1:A:174:LYS:CG	1:A:209:ALA:HB2	0.69	2.18	18	10
1:A:190:VAL:HG21	1:A:228:ASP:HB2	0.68	1.64	14	2
1:A:184:ILE:N	1:A:190:VAL:HG23	0.68	2.04	13	5
1:A:176:THR:O	1:A:195:ILE:HD12	0.68	1.88	5	1
1:A:164:THR:HG21	1:A:224:ILE:CG2	0.67	2.18	4	9
1:A:147:VAL:O	1:A:148:ILE:HD13	0.67	1.90	16	3
1:A:162:VAL:HG11	1:A:165:ILE:HD12	0.67	1.65	10	4
1:A:183:LEU:HD13	1:A:221:PHE:CZ	0.67	2.25	3	7
1:A:174:LYS:HG3	1:A:209:ALA:HB2	0.67	1.65	18	4
1:A:181:VAL:HG21	1:A:218:ILE:HD12	0.67	1.65	12	2
1:A:189:VAL:HG11	1:A:192:GLU:CD	0.66	2.10	12	3
1:A:198:LEU:HG	1:A:216:LEU:HD23	0.66	1.68	4	1
1:A:162:VAL:CG1	1:A:165:ILE:HD12	0.65	2.21	5	4
1:A:174:LYS:HG2	1:A:209:ALA:HB2	0.65	1.69	19	11
1:A:233:TYR:O	1:A:234:VAL:HG23	0.64	1.93	8	2
1:A:158:LYS:HB2	1:A:224:ILE:HD13	0.64	1.69	5	1
1:A:195:ILE:CG1	1:A:216:LEU:HD13	0.63	2.22	12	2
1:A:194:GLU:O	1:A:218:ILE:HG23	0.63	1.93	12	3
1:A:181:VAL:HG21	1:A:218:ILE:HG23	0.62	1.71	17	8
1:A:147:VAL:HG11	1:A:150:GLN:HB2	0.62	1.71	3	10
1:A:152:GLU:HG3	1:A:229:VAL:HG22	0.62	1.69	20	6
1:A:224:ILE:HD12	1:A:225:LYS:HG2	0.62	1.69	5	2
1:A:208:VAL:HG12	1:A:212:TYR:HB3	0.61	1.70	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:ILE:HD11	1:A:216:LEU:HD12	0.61	1.72	3	3
1:A:176:THR:HG22	1:A:207:GLU:HB3	0.61	1.73	20	7
1:A:175:ILE:O	1:A:198:LEU:HD11	0.60	1.96	5	1
1:A:175:ILE:HG23	1:A:175:ILE:O	0.60	1.96	17	3
1:A:188:ILE:HG23	1:A:189:VAL:N	0.60	2.12	13	6
1:A:217:THR:O	1:A:218:ILE:HD13	0.60	1.96	17	1
1:A:198:LEU:HD12	1:A:216:LEU:HD22	0.60	1.72	15	1
1:A:183:LEU:O	1:A:184:ILE:HD13	0.60	1.97	18	3
1:A:189:VAL:HG11	1:A:192:GLU:HG3	0.59	1.74	6	7
1:A:224:ILE:HD13	1:A:224:ILE:N	0.59	2.13	7	6
1:A:195:ILE:HD11	1:A:216:LEU:HB2	0.59	1.75	16	1
1:A:175:ILE:O	1:A:175:ILE:HG23	0.59	1.98	20	5
1:A:148:ILE:HD13	1:A:179:SER:OG	0.58	1.98	14	2
1:A:165:ILE:HD12	1:A:215:GLY:O	0.58	1.98	4	3
1:A:189:VAL:HG11	1:A:192:GLU:HG2	0.58	1.74	11	5
1:A:153:VAL:HB	1:A:230:ILE:HD11	0.58	1.75	1	3
1:A:190:VAL:HG21	1:A:228:ASP:CG	0.58	2.19	4	3
1:A:168:CYS:HB3	1:A:230:ILE:HD13	0.58	1.76	8	4
1:A:183:LEU:HD12	1:A:191:TYR:HB3	0.58	1.74	15	6
1:A:191:TYR:CE1	1:A:218:ILE:HG22	0.57	2.34	18	1
1:A:195:ILE:CD1	1:A:216:LEU:HD22	0.57	2.30	4	1
1:A:198:LEU:HD22	1:A:216:LEU:HB3	0.57	1.76	1	2
1:A:148:ILE:HD11	1:A:179:SER:HB3	0.57	1.75	12	5
1:A:224:ILE:N	1:A:224:ILE:HD13	0.57	2.15	14	8
1:A:189:VAL:HG11	1:A:192:GLU:OE2	0.56	1.99	10	1
1:A:149:GLY:HA3	1:A:232:ALA:HB3	0.56	1.77	9	1
1:A:195:ILE:HD11	1:A:216:LEU:HD22	0.56	1.76	17	2
1:A:183:LEU:C	1:A:184:ILE:HD12	0.56	2.20	1	6
1:A:218:ILE:HG22	1:A:218:ILE:O	0.56	2.01	9	9
1:A:181:VAL:HG22	1:A:194:GLU:CA	0.56	2.31	5	12
1:A:218:ILE:O	1:A:218:ILE:HG22	0.55	2.01	1	6
1:A:198:LEU:HD13	1:A:216:LEU:HB3	0.55	1.78	14	1
1:A:176:THR:C	1:A:198:LEU:HD11	0.55	2.22	19	1
1:A:183:LEU:HD21	1:A:221:PHE:CZ	0.55	2.37	10	8
1:A:181:VAL:HG21	1:A:218:ILE:CD1	0.54	2.33	12	1
1:A:184:ILE:CA	1:A:190:VAL:HG23	0.54	2.33	20	9
1:A:200:ARG:NH1	1:A:205:VAL:HG11	0.54	2.17	9	1
1:A:164:THR:CG2	1:A:224:ILE:HG22	0.54	2.33	10	3
1:A:170:VAL:HG22	1:A:175:ILE:CG1	0.53	2.34	11	5
1:A:175:ILE:CG2	1:A:208:VAL:HG23	0.53	2.33	3	2
1:A:148:ILE:HG21	1:A:234:VAL:O	0.52	2.04	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:TYR:CB	1:A:221:PHE:CE1	0.52	2.92	10	1
1:A:216:LEU:HD12	1:A:218:ILE:HD11	0.52	1.80	5	5
1:A:166:ALA:HB3	1:A:218:ILE:HD13	0.52	1.82	3	1
1:A:148:ILE:HD12	1:A:233:TYR:C	0.52	2.24	2	2
1:A:157:PHE:HB2	1:A:165:ILE:HB	0.52	1.82	13	13
1:A:183:LEU:O	1:A:189:VAL:HG13	0.52	2.05	2	7
1:A:148:ILE:O	1:A:148:ILE:HD13	0.52	2.05	1	1
1:A:216:LEU:HD12	1:A:218:ILE:CD1	0.51	2.34	15	6
1:A:182:ARG:NH1	1:A:184:ILE:HD11	0.51	2.20	2	1
1:A:165:ILE:O	1:A:165:ILE:HG22	0.51	2.06	15	11
1:A:198:LEU:HD22	1:A:216:LEU:CB	0.51	2.35	1	1
1:A:175:ILE:HG22	1:A:175:ILE:O	0.51	2.06	7	3
1:A:175:ILE:O	1:A:198:LEU:HD21	0.51	2.06	11	1
1:A:148:ILE:HG13	1:A:234:VAL:HG12	0.51	1.81	2	1
1:A:187:GLY:C	1:A:188:ILE:HD13	0.51	2.26	6	1
1:A:157:PHE:CD1	1:A:165:ILE:HG22	0.51	2.41	13	1
1:A:170:VAL:HG22	1:A:175:ILE:HG13	0.51	1.83	1	5
1:A:198:LEU:HD21	1:A:205:VAL:O	0.51	2.06	20	2
1:A:198:LEU:CD2	1:A:205:VAL:HG23	0.51	2.35	15	1
1:A:157:PHE:CE2	1:A:165:ILE:HG21	0.51	2.41	14	1
1:A:225:LYS:O	1:A:227:GLY:N	0.50	2.45	20	8
1:A:181:VAL:HG13	1:A:195:ILE:HD12	0.50	1.79	3	1
1:A:198:LEU:HD11	1:A:205:VAL:O	0.50	2.07	20	1
1:A:165:ILE:HG22	1:A:165:ILE:O	0.50	2.07	16	6
1:A:181:VAL:HG11	1:A:195:ILE:HD12	0.50	1.82	3	1
1:A:198:LEU:HD11	1:A:216:LEU:HD22	0.50	1.83	10	2
1:A:195:ILE:HG23	1:A:216:LEU:HB2	0.50	1.84	12	1
1:A:223:ASP:OD1	1:A:223:ASP:N	0.49	2.43	5	4
1:A:224:ILE:H	1:A:224:ILE:HD13	0.49	1.67	8	5
1:A:175:ILE:O	1:A:175:ILE:HG22	0.49	2.08	15	2
1:A:198:LEU:HD11	1:A:206:ARG:C	0.49	2.27	9	1
1:A:175:ILE:HB	1:A:208:VAL:HG23	0.49	1.84	7	1
1:A:149:GLY:O	1:A:175:ILE:HD11	0.49	2.06	14	2
1:A:224:ILE:HD13	1:A:224:ILE:H	0.49	1.68	1	7
1:A:149:GLY:CA	1:A:232:ALA:HB3	0.49	2.38	9	8
1:A:185:ARG:N	1:A:190:VAL:HG22	0.49	2.23	2	10
1:A:148:ILE:HG22	1:A:232:ALA:O	0.49	2.08	19	1
1:A:175:ILE:HG21	1:A:216:LEU:HD11	0.48	1.83	9	1
1:A:164:THR:CG2	1:A:224:ILE:HG21	0.48	2.37	14	9
1:A:183:LEU:CD2	1:A:221:PHE:CZ	0.48	2.96	10	11
1:A:196:ASP:HB3	1:A:217:THR:HG23	0.48	1.85	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:LEU:CD1	1:A:221:PHE:CZ	0.48	2.96	3	6
1:A:175:ILE:HG22	1:A:198:LEU:HD11	0.48	1.85	14	1
1:A:181:VAL:HG11	1:A:218:ILE:HG13	0.48	1.84	20	2
1:A:175:ILE:HD12	1:A:232:ALA:HB2	0.48	1.84	10	3
1:A:191:TYR:CZ	1:A:218:ILE:CG2	0.48	2.96	15	1
1:A:183:LEU:HA	1:A:229:VAL:O	0.48	2.09	6	10
1:A:191:TYR:CD2	1:A:218:ILE:CG2	0.47	2.97	2	6
1:A:148:ILE:O	1:A:148:ILE:HG22	0.47	2.08	11	3
1:A:198:LEU:HD22	1:A:206:ARG:C	0.47	2.29	13	1
1:A:194:GLU:CG	1:A:195:ILE:N	0.47	2.78	14	4
1:A:198:LEU:HD23	1:A:205:VAL:O	0.47	2.09	18	1
1:A:148:ILE:HG12	1:A:234:VAL:HG12	0.47	1.86	4	4
1:A:154:ARG:O	1:A:226:GLU:HB3	0.47	2.10	20	7
1:A:191:TYR:CD1	1:A:192:GLU:N	0.47	2.82	18	1
1:A:148:ILE:CD1	1:A:234:VAL:HG12	0.47	2.38	17	1
1:A:224:ILE:HD12	1:A:225:LYS:CG	0.47	2.39	20	1
1:A:184:ILE:HA	1:A:190:VAL:HG23	0.47	1.86	17	7
1:A:148:ILE:HG22	1:A:232:ALA:C	0.47	2.31	19	1
1:A:221:PHE:CE1	1:A:223:ASP:HB3	0.47	2.45	10	1
1:A:182:ARG:N	1:A:231:GLU:O	0.47	2.48	20	20
1:A:176:THR:HG22	1:A:207:GLU:CB	0.47	2.40	18	1
1:A:181:VAL:HG13	1:A:195:ILE:CD1	0.46	2.40	11	1
1:A:175:ILE:HG23	1:A:208:VAL:HG23	0.46	1.87	20	2
1:A:221:PHE:CZ	1:A:223:ASP:OD1	0.46	2.68	10	1
1:A:149:GLY:O	1:A:232:ALA:HB3	0.46	2.10	3	9
1:A:177:ARG:HB2	1:A:198:LEU:HD22	0.46	1.88	9	1
1:A:162:VAL:HG12	1:A:163:GLY:N	0.46	2.26	16	17
1:A:221:PHE:CD1	1:A:223:ASP:O	0.46	2.68	19	16
1:A:148:ILE:O	1:A:174:LYS:O	0.46	2.33	18	7
1:A:191:TYR:CD2	1:A:192:GLU:N	0.46	2.84	15	1
1:A:148:ILE:HG21	1:A:234:VAL:CG1	0.46	2.41	18	1
1:A:223:ASP:N	1:A:223:ASP:OD1	0.46	2.47	19	2
1:A:198:LEU:HD22	1:A:206:ARG:O	0.46	2.10	13	1
1:A:162:VAL:HG12	1:A:165:ILE:HD13	0.46	1.87	2	2
1:A:165:ILE:HD13	1:A:217:THR:OG1	0.46	2.11	6	1
1:A:198:LEU:HD23	1:A:199:LYS:N	0.46	2.25	4	1
1:A:223:ASP:OD1	1:A:224:ILE:N	0.45	2.49	17	1
1:A:191:TYR:CE2	1:A:220:ASN:O	0.45	2.70	6	3
1:A:208:VAL:HG21	1:A:214:CYS:HB3	0.45	1.87	12	2
1:A:148:ILE:HD13	1:A:179:SER:HB3	0.45	1.89	20	1
1:A:157:PHE:CD1	1:A:165:ILE:CG2	0.45	3.00	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:THR:HA	1:A:166:ALA:HA	0.45	1.89	14	2
1:A:170:VAL:HG12	1:A:212:TYR:N	0.45	2.27	14	3
1:A:217:THR:C	1:A:218:ILE:HD12	0.45	2.32	10	2
1:A:221:PHE:CZ	1:A:223:ASP:CG	0.45	2.90	10	1
1:A:147:VAL:HG11	1:A:150:GLN:HG3	0.45	1.88	7	1
1:A:153:VAL:HB	1:A:228:ASP:O	0.44	2.13	14	3
1:A:175:ILE:HD11	1:A:181:VAL:CG1	0.44	2.43	10	1
1:A:164:THR:HG22	1:A:224:ILE:CG2	0.44	2.42	8	4
1:A:152:GLU:CD	1:A:229:VAL:HG22	0.44	2.33	2	1
1:A:208:VAL:HG12	1:A:212:TYR:O	0.44	2.12	14	1
1:A:177:ARG:CB	1:A:198:LEU:HD22	0.44	2.42	9	1
1:A:195:ILE:HG22	1:A:196:ASP:N	0.44	2.27	19	1
1:A:230:ILE:N	1:A:230:ILE:HD12	0.44	2.28	1	1
1:A:148:ILE:CG2	1:A:234:VAL:HG12	0.44	2.42	18	2
1:A:218:ILE:N	1:A:218:ILE:HD12	0.44	2.28	3	1
1:A:218:ILE:O	1:A:220:ASN:N	0.44	2.51	14	3
1:A:230:ILE:HD12	1:A:230:ILE:N	0.44	2.28	8	1
1:A:165:ILE:HG23	1:A:215:GLY:C	0.44	2.33	7	1
1:A:176:THR:HB	1:A:206:ARG:O	0.44	2.13	13	5
1:A:164:THR:CG2	1:A:224:ILE:CG2	0.44	2.96	1	13
1:A:151:ALA:O	1:A:229:VAL:HG13	0.44	2.12	15	6
1:A:191:TYR:HB2	1:A:221:PHE:CE1	0.44	2.48	4	10
1:A:181:VAL:HG22	1:A:194:GLU:C	0.43	2.33	17	5
1:A:223:ASP:C	1:A:223:ASP:OD1	0.43	2.56	10	1
1:A:147:VAL:HG22	1:A:231:GLU:OE2	0.43	2.12	11	1
1:A:188:ILE:CG2	1:A:189:VAL:N	0.43	2.81	10	2
1:A:148:ILE:HD13	1:A:232:ALA:C	0.43	2.34	2	2
1:A:181:VAL:HG13	1:A:195:ILE:HD11	0.43	1.90	12	1
1:A:177:ARG:O	1:A:195:ILE:HG22	0.43	2.13	16	1
1:A:148:ILE:HD12	1:A:149:GLY:N	0.43	2.29	20	1
1:A:158:LYS:HG3	1:A:224:ILE:HD13	0.43	1.89	20	1
1:A:183:LEU:N	1:A:183:LEU:HD12	0.43	2.28	18	1
1:A:200:ARG:NH1	1:A:212:TYR:CD1	0.43	2.87	17	1
1:A:152:GLU:HG3	1:A:229:VAL:HG13	0.43	1.89	13	1
1:A:208:VAL:HG12	1:A:212:TYR:CB	0.43	2.43	15	1
1:A:172:ASP:O	1:A:173:GLY:O	0.43	2.37	7	1
1:A:191:TYR:CE2	1:A:218:ILE:CG2	0.43	3.01	14	2
1:A:152:GLU:N	1:A:169:TYR:O	0.43	2.52	15	5
1:A:184:ILE:HD12	1:A:184:ILE:N	0.43	2.28	15	1
1:A:208:VAL:HG21	1:A:214:CYS:CB	0.42	2.44	18	3
1:A:153:VAL:HG12	1:A:228:ASP:O	0.42	2.13	11	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:TYR:CD2	1:A:213:GLU:CG	0.42	3.02	18	1
1:A:225:LYS:O	1:A:226:GLU:C	0.42	2.58	6	12
1:A:233:TYR:O	1:A:233:TYR:CD1	0.42	2.72	13	2
1:A:148:ILE:HG22	1:A:148:ILE:O	0.42	2.13	9	1
1:A:183:LEU:CD1	1:A:191:TYR:HB3	0.42	2.44	15	4
1:A:218:ILE:HD12	1:A:218:ILE:N	0.42	2.29	14	1
1:A:195:ILE:HD12	1:A:216:LEU:CD1	0.42	2.45	9	1
1:A:156:THR:OG1	1:A:225:LYS:N	0.42	2.50	4	1
1:A:154:ARG:CA	1:A:154:ARG:NE	0.42	2.83	4	4
1:A:226:GLU:CG	1:A:226:GLU:O	0.42	2.68	18	3
1:A:165:ILE:HD12	1:A:217:THR:HG23	0.42	1.90	9	1
1:A:218:ILE:O	1:A:218:ILE:CG2	0.42	2.67	9	3
1:A:181:VAL:HG21	1:A:218:ILE:HG13	0.42	1.91	7	1
1:A:175:ILE:HG21	1:A:216:LEU:HD21	0.42	1.92	12	1
1:A:181:VAL:HG11	1:A:195:ILE:CD1	0.42	2.45	18	1
1:A:154:ARG:NE	1:A:154:ARG:CA	0.42	2.83	19	2
1:A:183:LEU:HB2	1:A:229:VAL:O	0.42	2.13	10	1
1:A:191:TYR:CE2	1:A:218:ILE:HG22	0.42	2.50	13	3
1:A:218:ILE:CD1	1:A:218:ILE:N	0.42	2.83	3	2
1:A:183:LEU:CB	1:A:230:ILE:HA	0.42	2.45	8	2
1:A:157:PHE:CG	1:A:165:ILE:HB	0.42	2.50	15	2
1:A:150:GLN:CG	1:A:231:GLU:CG	0.41	2.99	20	3
1:A:218:ILE:CG2	1:A:218:ILE:O	0.41	2.68	13	4
1:A:185:ARG:N	1:A:190:VAL:CG2	0.41	2.84	5	3
1:A:198:LEU:HD13	1:A:216:LEU:CD2	0.41	2.34	17	1
1:A:151:ALA:HB1	1:A:169:TYR:O	0.41	2.16	19	3
1:A:224:ILE:CD1	1:A:224:ILE:N	0.41	2.83	13	3
1:A:181:VAL:CG1	1:A:195:ILE:CD1	0.41	2.99	19	1
1:A:183:LEU:HD21	1:A:191:TYR:CB	0.41	2.45	17	1
1:A:195:ILE:HD13	1:A:216:LEU:HD13	0.41	1.93	5	1
1:A:191:TYR:CD1	1:A:223:ASP:OD1	0.41	2.74	12	2
1:A:175:ILE:HG22	1:A:216:LEU:HD21	0.41	1.90	4	1
1:A:224:ILE:O	1:A:225:LYS:O	0.41	2.39	11	1
1:A:157:PHE:CD2	1:A:165:ILE:CG2	0.41	3.03	15	1
1:A:191:TYR:CE2	1:A:192:GLU:O	0.41	2.74	15	1
1:A:183:LEU:HB3	1:A:190:VAL:HG23	0.41	1.93	16	2
1:A:169:TYR:CE1	1:A:211:GLY:O	0.41	2.74	18	2
1:A:157:PHE:CD2	1:A:165:ILE:HB	0.41	2.51	8	2
1:A:148:ILE:HD12	1:A:148:ILE:C	0.41	2.37	20	1
1:A:176:THR:HA	1:A:206:ARG:O	0.41	2.16	14	1
1:A:233:TYR:O	1:A:234:VAL:CG2	0.41	2.69	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:ALA:N	1:A:216:LEU:O	0.41	2.54	12	1
1:A:153:VAL:CG1	1:A:226:GLU:HA	0.41	2.46	18	2
1:A:195:ILE:HD12	1:A:195:ILE:N	0.41	2.31	10	1
1:A:195:ILE:HD11	1:A:216:LEU:CD2	0.41	2.46	17	1
1:A:169:TYR:CE1	1:A:170:VAL:O	0.40	2.74	15	2
1:A:165:ILE:O	1:A:216:LEU:O	0.40	2.39	14	1
1:A:198:LEU:CD1	1:A:216:LEU:CD2	0.40	2.99	12	1
1:A:226:GLU:O	1:A:226:GLU:CG	0.40	2.69	11	1
1:A:191:TYR:CE1	1:A:221:PHE:HA	0.40	2.52	3	1
1:A:164:THR:HG22	1:A:224:ILE:HG22	0.40	1.93	10	1
1:A:175:ILE:CG2	1:A:175:ILE:O	0.40	2.68	17	1
1:A:169:TYR:CE2	1:A:211:GLY:O	0.40	2.75	17	1
1:A:157:PHE:O	1:A:163:GLY:O	0.40	2.39	13	1
1:A:148:ILE:HD13	1:A:232:ALA:O	0.40	2.17	6	1
1:A:221:PHE:CG	1:A:223:ASP:O	0.40	2.74	14	1
1:A:169:TYR:CD2	1:A:213:GLU:HG2	0.40	2.51	18	1
1:A:153:VAL:CG1	1:A:153:VAL:O	0.40	2.70	11	1
1:A:224:ILE:N	1:A:224:ILE:CD1	0.40	2.83	6	1
1:A:181:VAL:HG22	1:A:194:GLU:HA	0.40	1.93	12	1
1:A:146:LYS:HG3	1:A:147:VAL:HG23	0.40	1.92	10	1
1:A:183:LEU:HD11	1:A:190:VAL:HB	0.40	1.92	9	1
1:A:153:VAL:O	1:A:153:VAL:CG1	0.40	2.70	7	1
1:A:195:ILE:CD1	1:A:218:ILE:CD1	0.40	3.00	18	1
1:A:148:ILE:HD13	1:A:148:ILE:C	0.40	2.37	8	1
1:A:216:LEU:CD1	1:A:218:ILE:HD11	0.40	2.47	8	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	86/99 (87%)	58±3 (67±3%)	17±2 (20±3%)	11±1 (13±2%)	1	6
All	All	1720/1980 (87%)	1157 (67%)	344 (20%)	219 (13%)	1	6

All 15 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	173	GLY	20
1	A	211	GLY	20
1	A	187	GLY	20
1	A	165	ILE	20
1	A	162	VAL	20
1	A	225	LYS	19
1	A	226	GLU	19
1	A	149	GLY	18
1	A	208	VAL	18
1	A	234	VAL	16
1	A	210	GLN	16
1	A	188	ILE	6
1	A	219	LYS	3
1	A	146	LYS	2
1	A	166	ALA	2

### 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	73/84 (87%)	46±3 (63±4%)	27±3 (37±4%)	1	8
All	All	1460/1680 (87%)	926 (63%)	534 (37%)	1	8

All 57 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	188	ILE	20
1	A	164	THR	20
1	A	155	GLN	20
1	A	216	LEU	20
1	A	223	ASP	20
1	A	168	CYS	20
1	A	190	VAL	20
1	A	176	THR	20
1	A	221	PHE	19
1	A	150	GLN	17
1	A	183	LEU	17

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Mol	Chain	Res	Type	Models (Total)
1	A	208	VAL	17
1	A	217	THR	17
1	A	225	LYS	15
1	A	224	ILE	15
1	A	234	VAL	15
1	A	177	ARG	13
1	A	228	ASP	13
1	A	161	LYS	11
1	A	196	ASP	11
1	A	213	GLU	11
1	A	200	ARG	9
1	A	212	TYR	9
1	A	174	LYS	9
1	A	185	ARG	9
1	A	171	THR	8
1	A	210	GLN	8
1	A	180	LYS	8
1	A	157	PHE	7
1	A	207	GLU	7
1	A	198	LEU	7
1	A	158	LYS	7
1	A	199	LYS	6
1	A	154	ARG	6
1	A	152	GLU	6
1	A	179	SER	6
1	A	195	ILE	6
1	A	226	GLU	5
1	A	197	SER	5
1	A	175	ILE	5
1	A	206	ARG	5
1	A	191	TYR	5
1	A	219	LYS	4
1	A	186	GLN	4
1	A	194	GLU	4
1	A	146	LYS	4
1	A	148	ILE	4
1	A	222	ASN	3
1	A	231	GLU	3
1	A	165	ILE	3
1	A	214	CYS	3
1	A	160	SER	2
1	A	178	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	192	GLU	1
1	A	204	ASP	1
1	A	220	ASN	1
1	A	181	VAL	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.6 Ligand geometry [i](#)

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 74% for the well-defined parts and 74% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 4697

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	1101
Number of shifts mapped to atoms	1028
Number of unparsed shifts	0
Number of shifts with mapping errors	73
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

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

- Residue not found in structure. All 73 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	4	ALA	HB1	1.881	-1.0	1
A	12	PRO	C	176.099	-1.0	1
A	4	ALA	HB2	1.881	-1.0	1
A	9	MET	H	7.969	-1.0	1
A	8	GLY	N	110.33	-1.0	1
A	7	LYS	HA	4.237	-1.0	1
A	1	GLU	H	8.733	-1.0	1
A	9	MET	C	175.787	-1.0	1
A	3	GLU	HB2	1.987	-1.0	1
A	2	ILE	H	8.118	-1.0	1
A	6	MET	HA	4.35	-1.0	1
A	8	GLY	HA3	3.909	-1.0	1
A	4	ALA	N	124.649	-1.0	1
A	1	GLU	HA	4.098	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	5	ALA	CA	53.278	-1.0	1
A	8	GLY	H	8.208	-1.0	1
A	3	GLU	H	8.081	-1.0	1
A	6	MET	N	119.102	-1.0	1
A	8	GLY	CA	45.576	-1.0	1
A	6	MET	CB	30.248	-1.0	1
A	1	GLU	N	122.631	-1.0	1
A	13	GLU	HB2	1.834	-1.0	1
A	12	PRO	CA	63.259	-1.0	1
A	3	GLU	HB3	2.272	-1.0	1
A	2	ILE	HB	2.359	-1.0	1
A	10	LEU	N	123.276	-1.0	1
A	4	ALA	CA	53.67	-1.0	1
A	5	ALA	N	122.658	-1.0	1
A	2	ILE	C	176.313	-1.0	1
A	6	MET	HB3	2.431	-1.0	1
A	2	ILE	CA	58.753	-1.0	1
A	7	LYS	C	177.077	-1.0	1
A	5	ALA	HA	4.239	-1.0	1
A	13	GLU	HB3	1.943	-1.0	1
A	3	GLU	N	122.646	-1.0	1
A	7	LYS	CA	57.08	-1.0	1
A	8	GLY	C	174.171	-1.0	1
A	5	ALA	H	7.952	-1.0	1
A	13	GLU	H	8.267	-1.0	1
A	4	ALA	HA	3.963	-1.0	1
A	13	GLU	CA	55.917	-1.0	1
A	5	ALA	C	178.446	-1.0	1
A	6	MET	HB2	2.525	-1.0	1
A	13	GLU	N	121.039	-1.0	1
A	6	MET	HG2	2.019	-1.0	1
A	2	ILE	N	121.449	-1.0	1
A	13	GLU	HG3	2.271	-1.0	1
A	7	LYS	N	122.156	-1.0	1
A	9	MET	N	120.525	-1.0	1
A	3	GLU	HA	4.089	-1.0	1
A	13	GLU	HA	4.32	-1.0	1
A	4	ALA	HB3	1.881	-1.0	1
A	4	ALA	H	8.1	-1.0	1
A	6	MET	HG3	1.992	-1.0	1
A	1	GLU	C	176.807	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	6	MET	CA	56.032	-1.0	1
A	3	GLU	HG3	1.623	-1.0	1
A	1	GLU	CA	58.32	-1.0	1
A	6	MET	H	7.91	-1.0	1
A	10	LEU	HA	4.346	-1.0	1
A	13	GLU	HG2	2.151	-1.0	1
A	10	LEU	H	8.007	-1.0	1
A	2	ILE	HA	4.494	-1.0	1
A	13	GLU	C	175.219	-1.0	1
A	10	LEU	CA	54.907	-1.0	1
A	7	LYS	H	7.958	-1.0	1
A	4	ALA	CB	32.985	-1.0	1
A	6	MET	C	178.309	-1.0	1
A	9	MET	CA	55.794	-1.0	1
A	3	GLU	CA	57.531	-1.0	1
A	3	GLU	C	176.955	-1.0	1
A	9	MET	CB	41.6	-1.0	1
A	4	ALA	C	178.311	-1.0	1

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	109	$-0.32 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	68	$-0.52 \pm 0.18$	Should be applied
$^{13}\text{C}'$	109	$0.39 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	110	$-1.59 \pm 0.34$	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 74%, i.e. 784 atoms were assigned a chemical shift out of a possible 1060. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	424/430 (99%)	168/172 (98%)	170/172 (99%)	86/86 (100%)
Sidechain	335/580 (58%)	264/334 (79%)	61/214 (29%)	10/32 (31%)
Aromatic	25/50 (50%)	25/26 (96%)	0/24 (0%)	0/0 (—%)
Overall	784/1060 (74%)	457/532 (86%)	231/410 (56%)	96/118 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 911 atoms were assigned a chemical shift out of a possible 1231. 1 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	488/495 (99%)	194/198 (98%)	195/198 (98%)	99/99 (100%)
Sidechain	394/670 (59%)	312/387 (81%)	70/246 (28%)	12/37 (32%)
Aromatic	29/66 (44%)	29/34 (85%)	0/32 (0%)	0/0 (—%)
Overall	911/1231 (74%)	535/619 (86%)	265/476 (56%)	111/136 (82%)

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

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	206	ARG	NE	136.16	92.63 – 76.73	32.4
1	A	240	ARG	NE	126.09	92.63 – 76.73	26.0
1	A	185	ARG	NE	125.85	92.63 – 76.73	25.9
1	A	177	ARG	NE	125.37	92.63 – 76.73	25.6
1	A	154	ARG	NE	125.12	92.63 – 76.73	25.4
1	A	182	ARG	NE	123.72	92.63 – 76.73	24.6
1	A	4	ALA	CB	32.98	28.03 – 9.93	7.7
1	A	180	LYS	HB3	0.27	3.10 – 0.40	-5.5
1	A	223	ASP	H	5.43	11.17 – 5.47	-5.1

#### 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:

