



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 05:43 PM UTC

PDB ID : 1JCU / pdb_00001jcu
Title : Solution Structure of MTH1692 Protein from Methanobacterium thermoautotrophicum
Authors : Kozlov, G.; Ekiel, I.; Gehring, K.
Deposited on : 2001-06-11

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

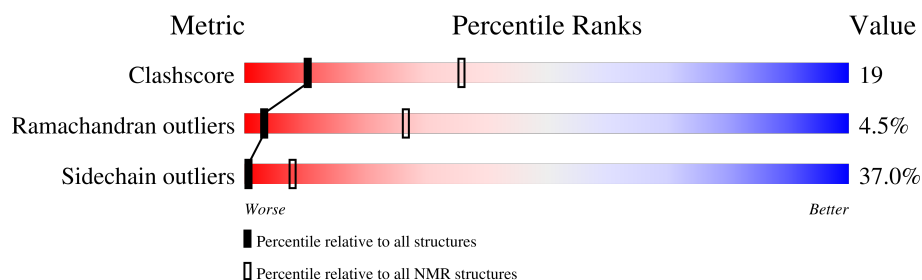
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	208	33% 44% 8% 16%

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:13-A:141, A:147-A:192 (175)	0.99	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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3219 atoms, of which 1636 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called conserved protein MTH1692.

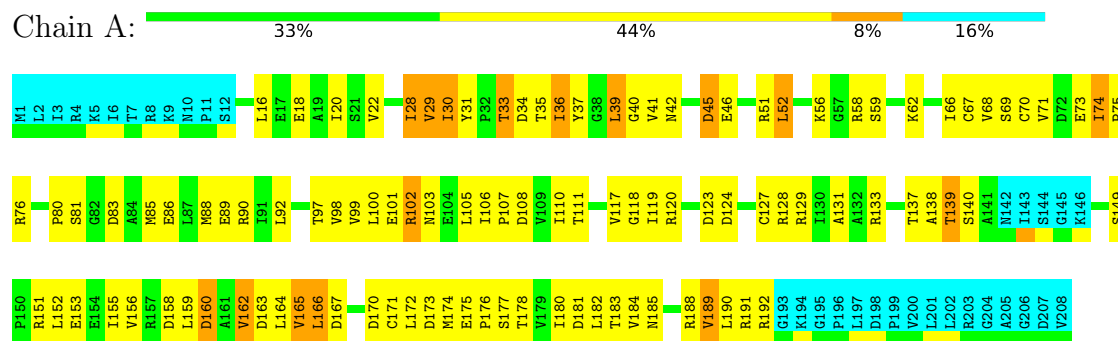
Mol	Chain	Residues	Atoms						Trace
1	A	208	Total	C	H	N	O	S	0
			3219	989	1636	284	301	9	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: conserved protein MTH1692

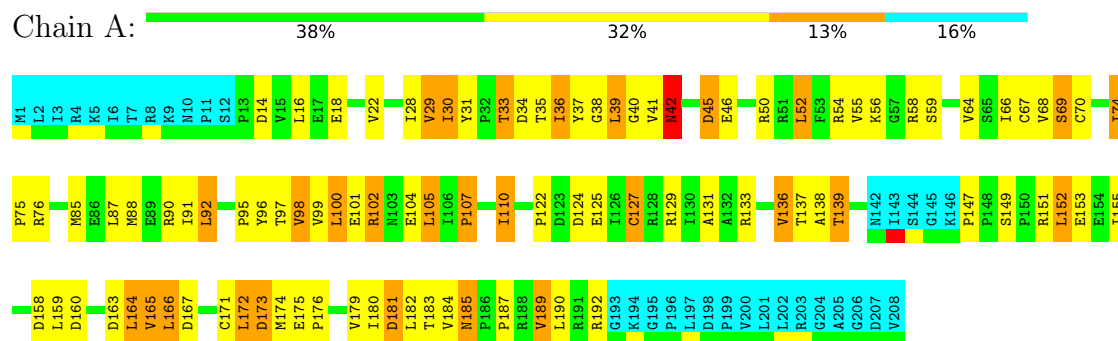


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

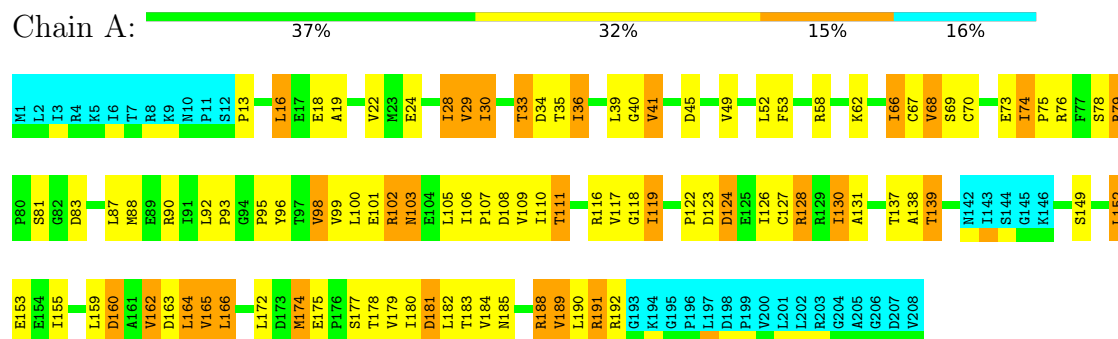
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: conserved protein MTH1692



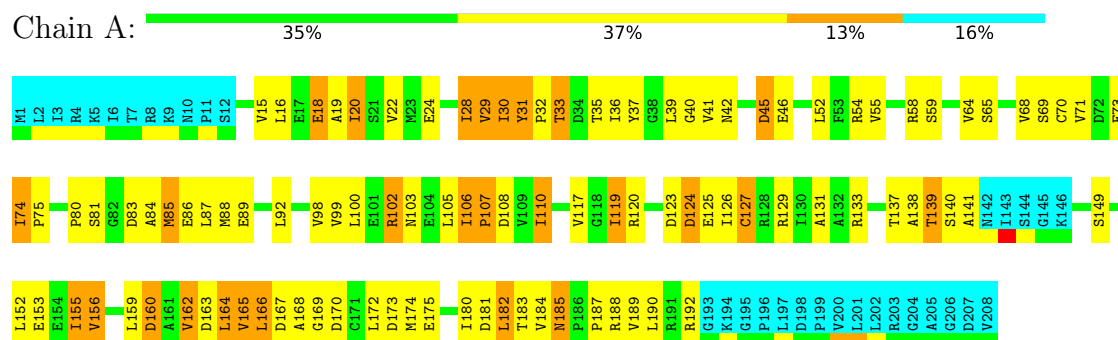
4.2.2 Score per residue for model 2

- Molecule 1: conserved protein MTH1692



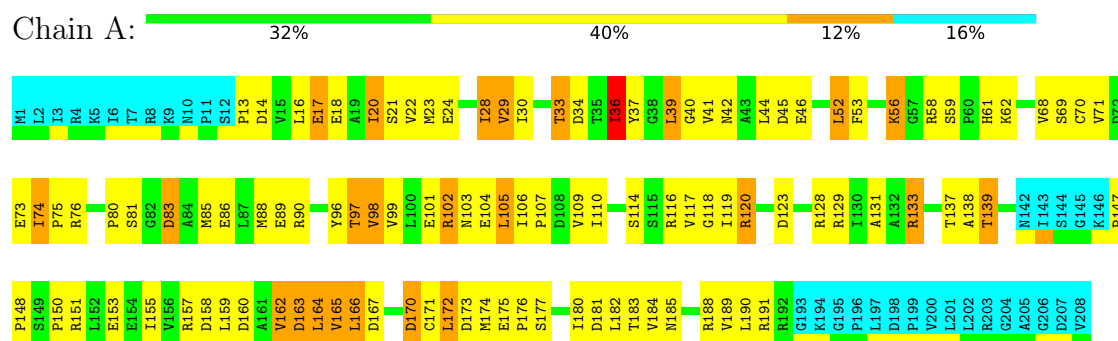
4.2.3 Score per residue for model 3

- Molecule 1: conserved protein MTH1692



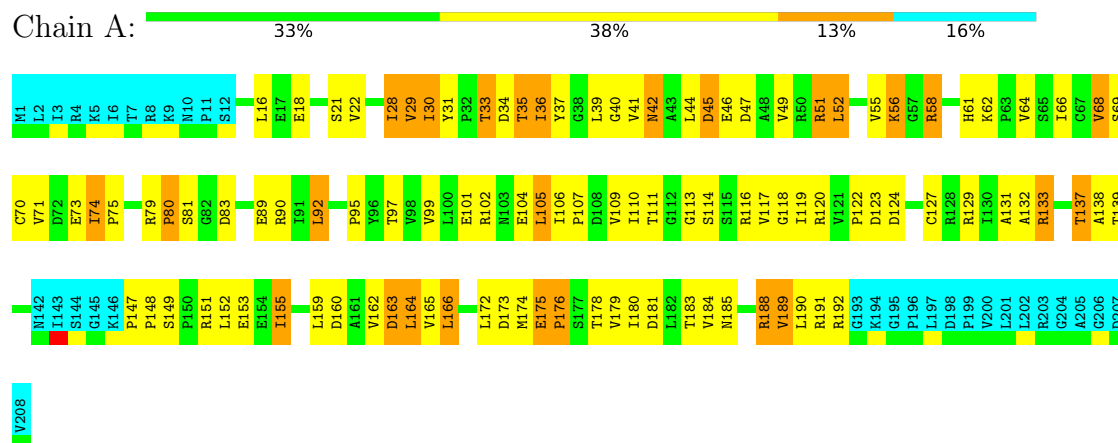
4.2.4 Score per residue for model 4

- Molecule 1: conserved protein MTH1692



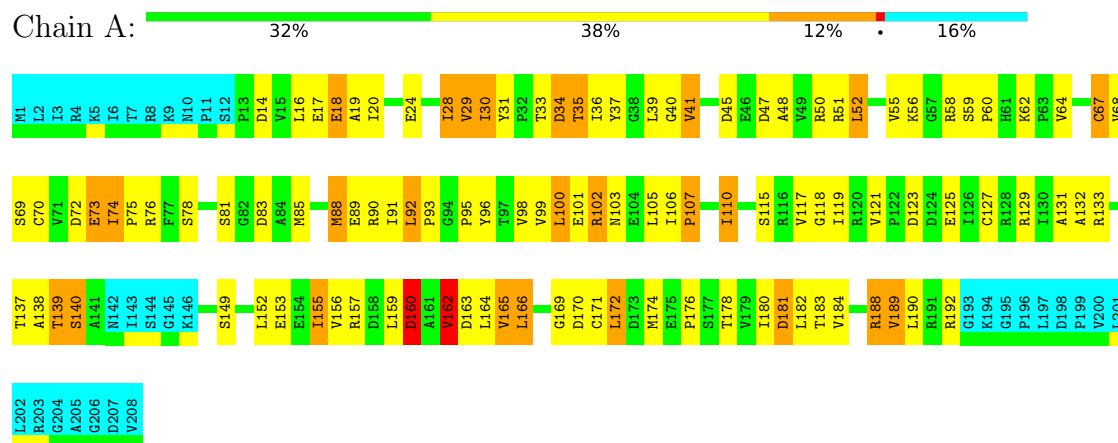
4.2.5 Score per residue for model 5

- Molecule 1: conserved protein MTH1692



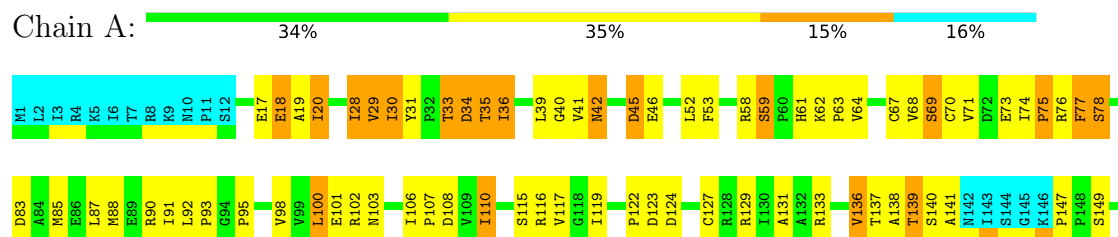
4.2.6 Score per residue for model 6

- Molecule 1: conserved protein MTH1692



4.2.7 Score per residue for model 7

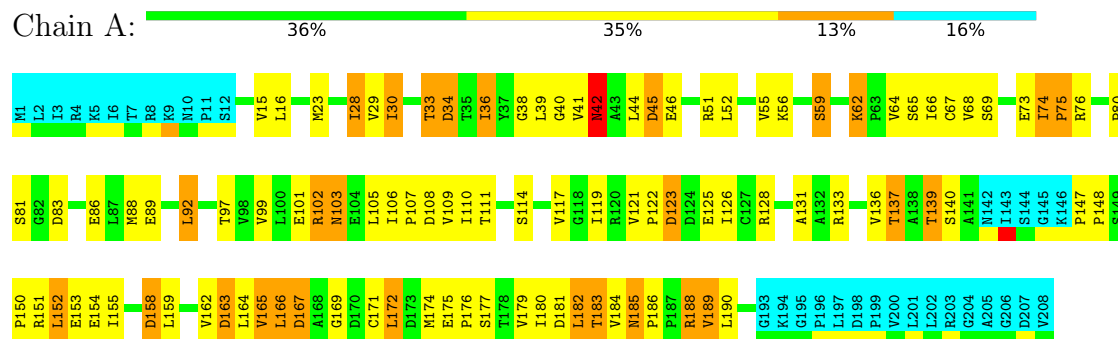
- Molecule 1: conserved protein MTH1692





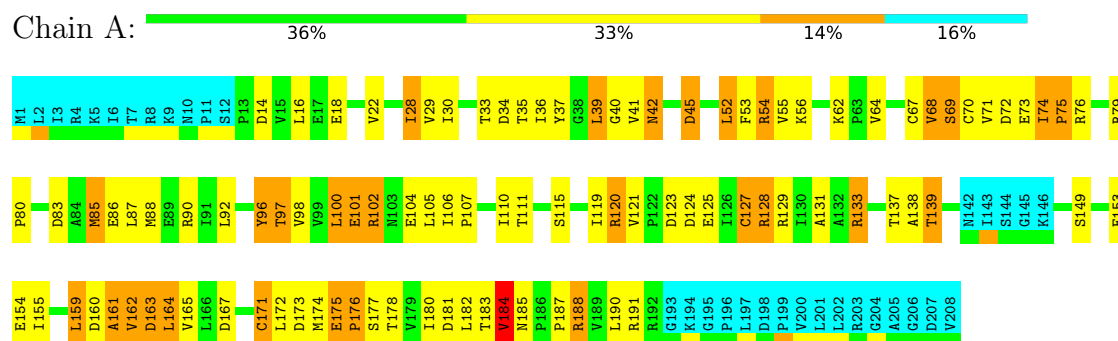
4.2.8 Score per residue for model 8

- Molecule 1: conserved protein MTH1692



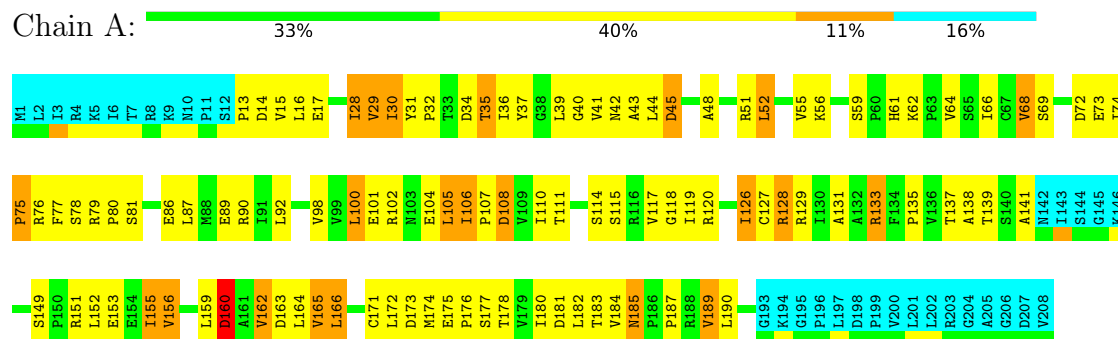
4.2.9 Score per residue for model 9

- Molecule 1: conserved protein MTH1692



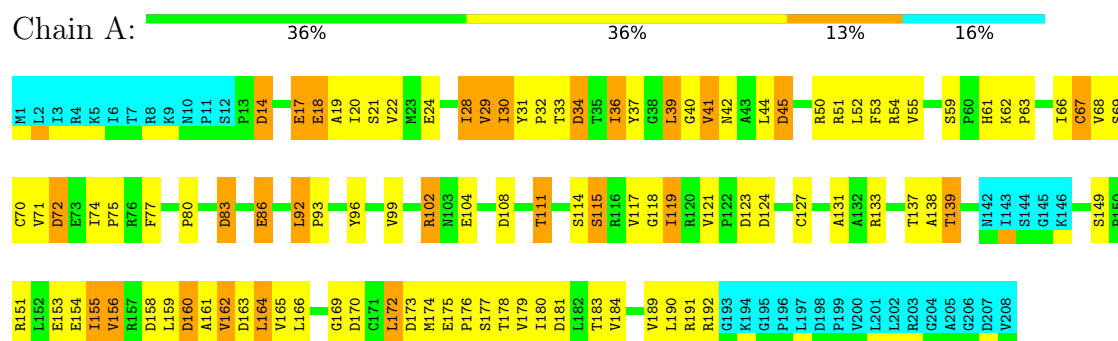
4.2.10 Score per residue for model 10

- Molecule 1: conserved protein MTH1692



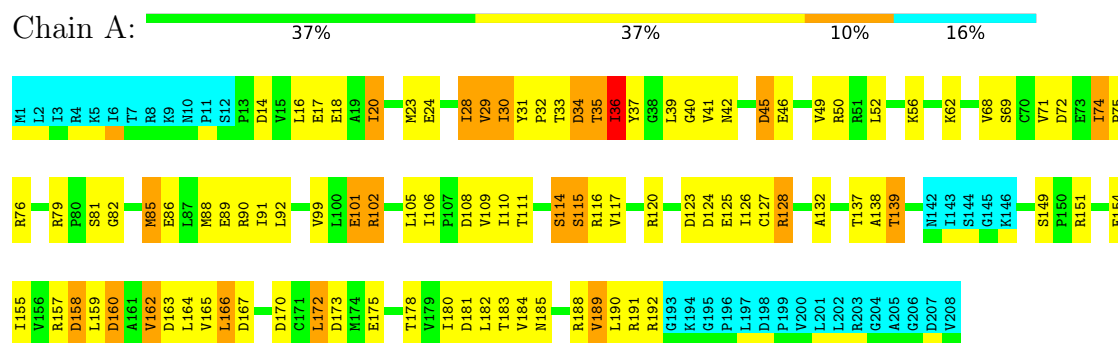
4.2.11 Score per residue for model 11

- Molecule 1: conserved protein MTH1692



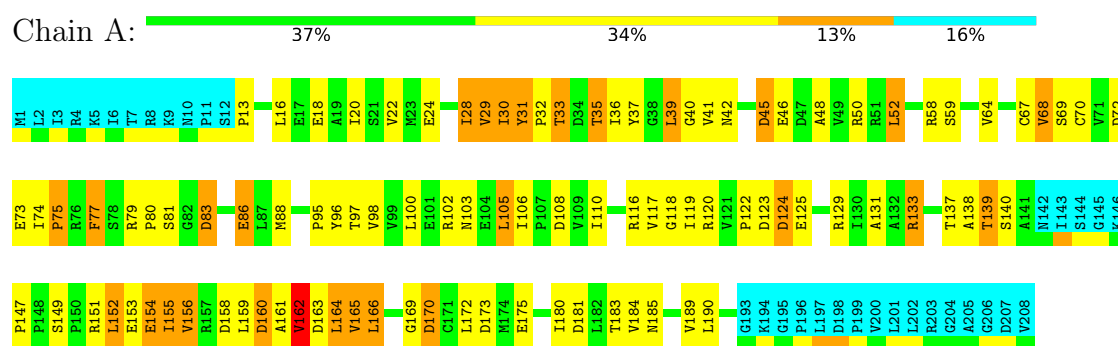
4.2.12 Score per residue for model 12

- Molecule 1: conserved protein MTH1692



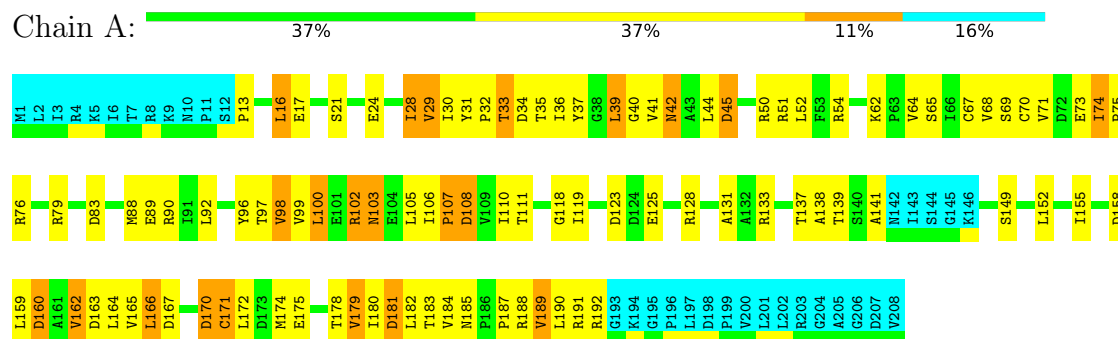
4.2.13 Score per residue for model 13

- Molecule 1: conserved protein MTH1692



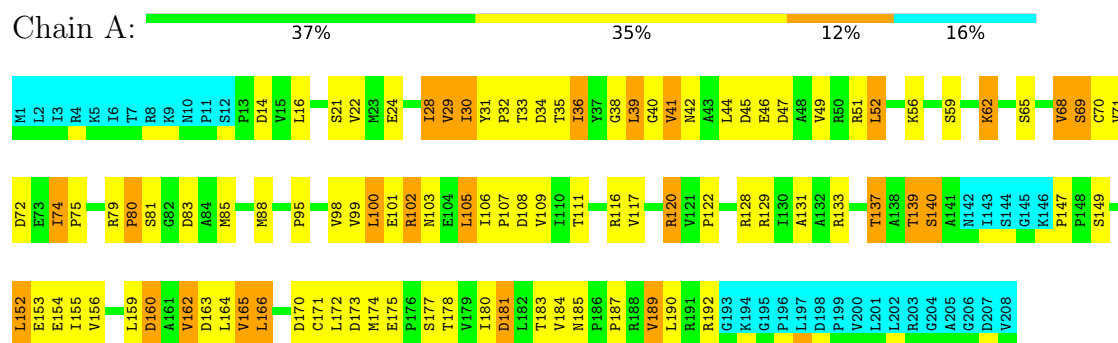
4.2.14 Score per residue for model 14

- Molecule 1: conserved protein MTH1692



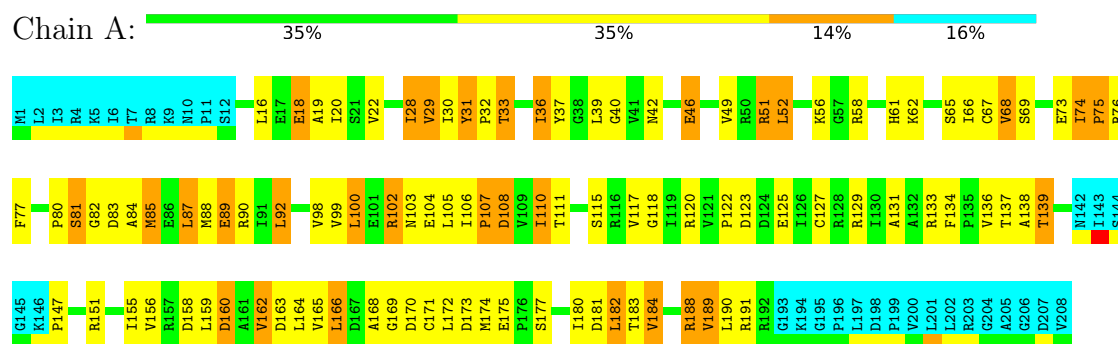
4.2.15 Score per residue for model 15

- Molecule 1: conserved protein MTH1692



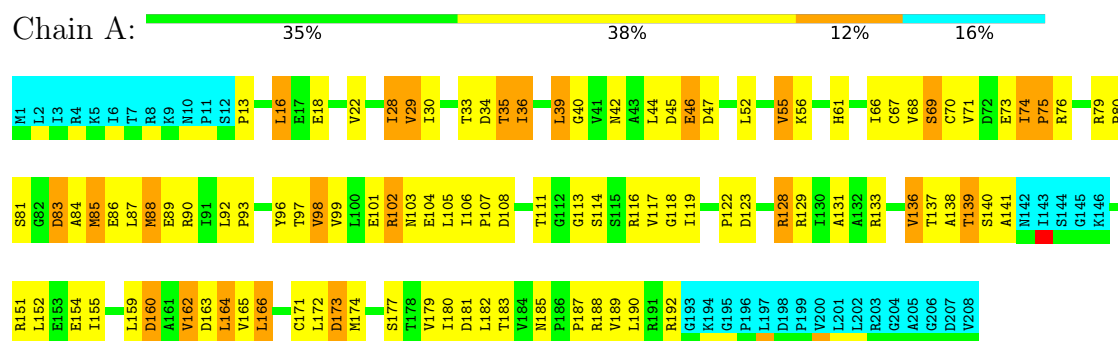
4.2.16 Score per residue for model 16

- Molecule 1: conserved protein MTH1692



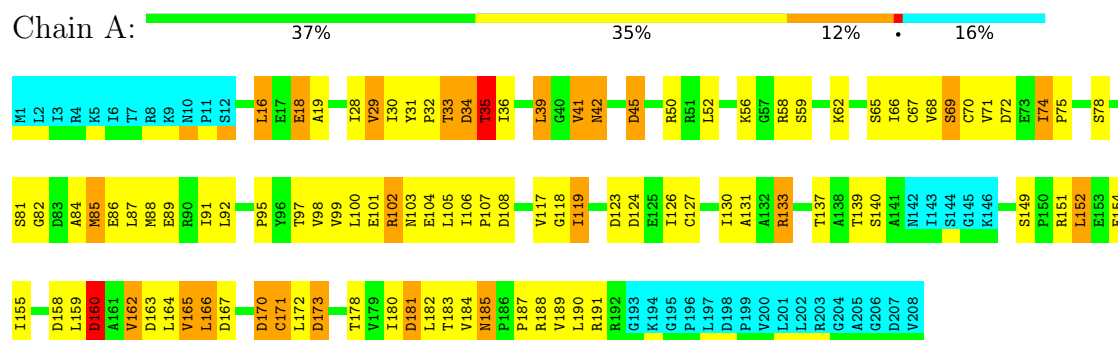
4.2.17 Score per residue for model 17

- Molecule 1: conserved protein MTH1692



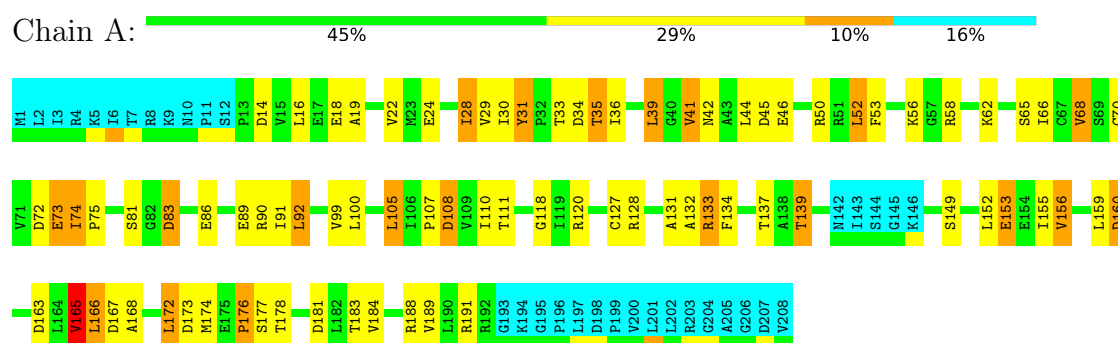
4.2.18 Score per residue for model 18

- Molecule 1: conserved protein MTH1692



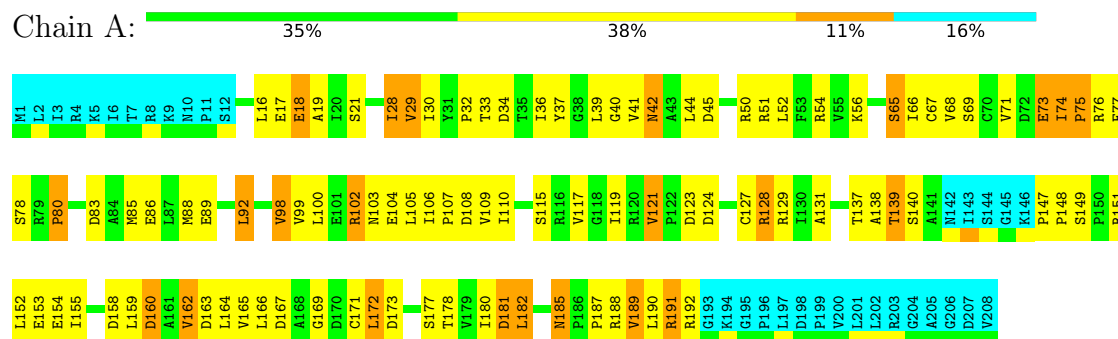
4.2.19 Score per residue for model 19

- Molecule 1: conserved protein MTH1692



4.2.20 Score per residue for model 20

- Molecule 1: conserved protein MTH1692



5 Refinement protocol and experimental data overview

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

Of the 100 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
CNS	refinement	0.9
ARIA	structure solution	0.9

No chemical shift data was provided.

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	1338	1361	1361	51±6
All	All	26760	27220	27220	1022

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ILE:HD12	1:A:165:VAL:HG23	0.80	1.50	16	13
1:A:16:LEU:HD11	1:A:126:ILE:HG22	0.79	1.55	12	1
1:A:159:LEU:HD13	1:A:163:ASP:HB3	0.75	1.56	2	3
1:A:152:LEU:HD22	1:A:166:LEU:HA	0.74	1.59	19	1
1:A:175:GLU:H	1:A:176:PRO:HA	0.73	1.43	9	1
1:A:68:VAL:HG21	1:A:74:ILE:HG23	0.73	1.60	16	12
1:A:81:SER:HB2	1:A:84:ALA:HB3	0.73	1.58	16	2
1:A:107:PRO:HB2	1:A:110:ILE:HB	0.72	1.60	19	2
1:A:81:SER:HB3	1:A:84:ALA:HB3	0.70	1.62	18	2
1:A:99:VAL:HB	1:A:181:ASP:HA	0.70	1.62	17	15
1:A:88:MET:HE3	1:A:98:VAL:HB	0.69	1.62	20	2
1:A:69:SER:HB3	1:A:73:GLU:HG3	0.68	1.65	14	7
1:A:67:CYS:HB2	1:A:138:ALA:HB2	0.68	1.64	20	7
1:A:92:LEU:HD21	1:A:121:VAL:HG21	0.68	1.66	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ILE:HD12	1:A:165:VAL:HG12	0.68	1.65	7	2
1:A:182:LEU:HA	1:A:187:PRO:HB3	0.68	1.64	20	1
1:A:33:THR:HG21	1:A:122:PRO:HB2	0.67	1.64	16	5
1:A:33:THR:HA	1:A:170:ASP:HB3	0.67	1.65	14	3
1:A:159:LEU:HD12	1:A:162:VAL:HB	0.67	1.65	9	1
1:A:166:LEU:HD23	1:A:169:GLY:H	0.66	1.49	6	2
1:A:68:VAL:HG11	1:A:74:ILE:HG12	0.66	1.67	15	7
1:A:33:THR:HA	1:A:171:CYS:H	0.65	1.50	18	2
1:A:166:LEU:N	1:A:166:LEU:HD13	0.65	2.04	6	9
1:A:105:LEU:HG	1:A:107:PRO:HD2	0.65	1.68	5	4
1:A:166:LEU:H	1:A:166:LEU:HD13	0.65	1.52	16	3
1:A:102:ARG:HB2	1:A:117:VAL:HG23	0.65	1.66	8	9
1:A:156:VAL:HG13	1:A:165:VAL:HG13	0.65	1.68	3	2
1:A:32:PRO:HB3	1:A:37:TYR:HA	0.64	1.70	12	7
1:A:124:ASP:HB3	1:A:127:CYS:HB3	0.64	1.67	12	3
1:A:30:ILE:HD11	1:A:163:ASP:HB2	0.64	1.70	15	1
1:A:49:VAL:HG13	1:A:109:VAL:HG21	0.64	1.69	12	2
1:A:159:LEU:HD21	1:A:165:VAL:HG13	0.64	1.68	7	2
1:A:88:MET:HB2	1:A:182:LEU:HD23	0.64	1.68	20	1
1:A:22:VAL:HG22	1:A:164:LEU:HD13	0.64	1.70	2	1
1:A:22:VAL:HG21	1:A:164:LEU:HG	0.64	1.68	16	1
1:A:102:ARG:HG2	1:A:117:VAL:HG23	0.64	1.70	11	2
1:A:180:ILE:HG12	1:A:189:VAL:HA	0.63	1.69	17	9
1:A:73:GLU:HG2	1:A:132:ALA:HA	0.63	1.69	5	3
1:A:36:ILE:HG23	1:A:174:MET:HG2	0.63	1.71	5	6
1:A:68:VAL:HA	1:A:131:ALA:HB1	0.63	1.71	6	18
1:A:71:VAL:HG11	1:A:85:MET:HG3	0.63	1.70	9	3
1:A:42:ASN:HB3	1:A:45:ASP:HB2	0.63	1.70	14	11
1:A:165:VAL:HG22	1:A:166:LEU:H	0.62	1.54	8	12
1:A:166:LEU:HD12	1:A:169:GLY:H	0.62	1.53	13	4
1:A:40:GLY:HA2	1:A:137:THR:O	0.62	1.94	15	18
1:A:73:GLU:C	1:A:75:PRO:HD3	0.62	2.18	13	7
1:A:97:THR:HG22	1:A:179:VAL:HA	0.62	1.71	1	1
1:A:181:ASP:HB2	1:A:188:ARG:HB2	0.62	1.72	16	10
1:A:38:GLY:HA2	1:A:140:SER:HA	0.62	1.71	8	2
1:A:178:THR:HG23	1:A:191:ARG:HB3	0.62	1.72	20	6
1:A:166:LEU:HD13	1:A:166:LEU:N	0.62	2.10	16	1
1:A:16:LEU:HD11	1:A:126:ILE:HG12	0.61	1.70	8	1
1:A:74:ILE:HD13	1:A:119:ILE:HD13	0.61	1.72	14	6
1:A:88:MET:HE2	1:A:98:VAL:HB	0.61	1.73	16	3
1:A:36:ILE:HG23	1:A:37:TYR:N	0.61	2.11	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:THR:HG23	1:A:95:PRO:HB2	0.61	1.71	7	6
1:A:159:LEU:HB3	1:A:162:VAL:HB	0.61	1.71	20	2
1:A:85:MET:HE3	1:A:100:LEU:HD21	0.61	1.71	18	1
1:A:180:ILE:HG23	1:A:189:VAL:HA	0.61	1.73	2	15
1:A:49:VAL:HG22	1:A:109:VAL:HG21	0.61	1.73	2	1
1:A:13:PRO:HB2	1:A:16:LEU:HB2	0.61	1.72	10	2
1:A:159:LEU:HB3	1:A:162:VAL:HG13	0.60	1.74	16	6
1:A:79:ARG:HB2	1:A:101:GLU:HB3	0.60	1.72	9	3
1:A:100:LEU:HD23	1:A:182:LEU:O	0.60	1.95	6	2
1:A:152:LEU:HD21	1:A:166:LEU:O	0.60	1.95	1	7
1:A:28:ILE:HD13	1:A:29:VAL:N	0.60	2.12	4	11
1:A:97:THR:HB	1:A:179:VAL:HA	0.60	1.72	5	4
1:A:22:VAL:HG11	1:A:164:LEU:HD13	0.59	1.72	4	1
1:A:22:VAL:HG21	1:A:164:LEU:HB2	0.59	1.72	5	5
1:A:15:VAL:HG11	1:A:126:ILE:HD13	0.59	1.72	3	2
1:A:92:LEU:HG	1:A:93:PRO:HA	0.59	1.74	11	3
1:A:69:SER:HB3	1:A:73:GLU:HG2	0.59	1.74	3	3
1:A:92:LEU:O	1:A:92:LEU:HD13	0.59	1.97	1	3
1:A:83:ASP:HA	1:A:86:GLU:HG3	0.59	1.74	11	5
1:A:107:PRO:HG2	1:A:111:THR:HB	0.59	1.74	2	2
1:A:13:PRO:HG2	1:A:16:LEU:HB2	0.58	1.75	13	3
1:A:35:THR:HB	1:A:95:PRO:HB2	0.58	1.76	6	1
1:A:109:VAL:HG13	1:A:110:ILE:HG13	0.58	1.76	4	3
1:A:184:VAL:HG13	1:A:185:ASN:H	0.58	1.59	9	1
1:A:85:MET:HE1	1:A:100:LEU:HD21	0.58	1.76	1	1
1:A:39:LEU:HB2	1:A:139:THR:HG23	0.58	1.76	3	7
1:A:33:THR:HA	1:A:170:ASP:HB2	0.57	1.75	13	1
1:A:34:ASP:HB2	1:A:95:PRO:HB3	0.57	1.75	15	2
1:A:51:ARG:NH2	1:A:139:THR:HG22	0.57	2.14	5	1
1:A:28:ILE:HG23	1:A:163:ASP:HA	0.57	1.77	9	7
1:A:30:ILE:O	1:A:166:LEU:HD12	0.57	2.00	6	8
1:A:175:GLU:N	1:A:176:PRO:HA	0.57	2.11	9	1
1:A:162:VAL:HG13	1:A:163:ASP:H	0.57	1.59	7	12
1:A:106:ILE:N	1:A:107:PRO:HD2	0.57	2.14	9	2
1:A:22:VAL:HB	1:A:164:LEU:HD22	0.57	1.77	13	1
1:A:49:VAL:HG21	1:A:109:VAL:HG22	0.57	1.76	15	1
1:A:159:LEU:HG	1:A:163:ASP:HB3	0.56	1.76	12	1
1:A:98:VAL:HG23	1:A:182:LEU:HB3	0.56	1.78	20	3
1:A:71:VAL:HG21	1:A:85:MET:SD	0.56	2.40	4	3
1:A:34:ASP:HB3	1:A:172:LEU:HB2	0.56	1.77	6	1
1:A:74:ILE:HG13	1:A:77:PHE:HB3	0.56	1.76	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:ASP:HA	1:A:111:THR:HG22	0.56	1.77	16	3
1:A:41:VAL:HG22	1:A:51:ARG:NH1	0.56	2.16	5	1
1:A:67:CYS:HB3	1:A:138:ALA:HB2	0.56	1.77	17	2
1:A:79:ARG:HG3	1:A:103:ASN:HA	0.56	1.77	2	1
1:A:105:LEU:HD13	1:A:107:PRO:HD2	0.55	1.77	4	1
1:A:22:VAL:HG21	1:A:164:LEU:HD22	0.55	1.78	9	1
1:A:30:ILE:HG22	1:A:31:TYR:H	0.55	1.61	19	1
1:A:28:ILE:HD13	1:A:29:VAL:H	0.55	1.60	15	8
1:A:184:VAL:HG22	1:A:185:ASN:N	0.55	2.16	9	1
1:A:92:LEU:HB2	1:A:93:PRO:HA	0.55	1.78	17	1
1:A:79:ARG:O	1:A:100:LEU:HD11	0.55	2.00	10	1
1:A:80:PRO:HA	1:A:100:LEU:HD22	0.55	1.77	15	1
1:A:35:THR:HB	1:A:95:PRO:HB3	0.55	1.77	13	1
1:A:39:LEU:HD12	1:A:139:THR:HG23	0.54	1.77	15	2
1:A:80:PRO:HA	1:A:100:LEU:HD11	0.54	1.78	20	1
1:A:158:ASP:HB3	1:A:159:LEU:HD22	0.54	1.80	8	6
1:A:159:LEU:O	1:A:160:ASP:C	0.54	2.50	11	16
1:A:71:VAL:HG11	1:A:85:MET:HE2	0.54	1.79	12	1
1:A:39:LEU:O	1:A:138:ALA:HA	0.54	2.02	11	15
1:A:124:ASP:HB3	1:A:127:CYS:HB2	0.54	1.80	2	4
1:A:102:ARG:HE	1:A:105:LEU:HB3	0.54	1.62	10	1
1:A:34:ASP:HA	1:A:172:LEU:HB2	0.54	1.80	8	5
1:A:152:LEU:O	1:A:156:VAL:HG23	0.54	2.01	6	2
1:A:16:LEU:HD11	1:A:130:ILE:HB	0.54	1.80	2	1
1:A:35:THR:HA	1:A:174:MET:HG3	0.54	1.78	17	1
1:A:30:ILE:HG23	1:A:39:LEU:HB3	0.54	1.80	19	1
1:A:18:GLU:HG3	1:A:19:ALA:N	0.53	2.18	16	7
1:A:41:VAL:O	1:A:136:VAL:HG12	0.53	2.03	7	2
1:A:32:PRO:O	1:A:170:ASP:HB2	0.53	2.03	13	5
1:A:166:LEU:HD22	1:A:166:LEU:O	0.53	2.04	16	4
1:A:159:LEU:HD22	1:A:163:ASP:O	0.53	2.02	6	4
1:A:74:ILE:N	1:A:75:PRO:HD3	0.53	2.19	13	2
1:A:34:ASP:HA	1:A:173:ASP:HB2	0.53	1.81	9	2
1:A:30:ILE:HB	1:A:165:VAL:HG13	0.53	1.79	19	1
1:A:89:GLU:HA	1:A:92:LEU:HD23	0.53	1.81	18	1
1:A:71:VAL:HA	1:A:74:ILE:HD11	0.53	1.80	5	3
1:A:96:TYR:HA	1:A:178:THR:HB	0.53	1.79	6	4
1:A:29:VAL:HG22	1:A:164:LEU:HD21	0.53	1.81	4	1
1:A:153:GLU:O	1:A:156:VAL:HG12	0.53	2.03	11	3
1:A:36:ILE:HG13	1:A:174:MET:HE3	0.53	1.80	15	1
1:A:28:ILE:HD12	1:A:29:VAL:N	0.53	2.19	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:HD22	1:A:107:PRO:HD2	0.53	1.79	20	2
1:A:75:PRO:HG3	1:A:80:PRO:HG3	0.52	1.81	5	1
1:A:42:ASN:HB2	1:A:45:ASP:HB2	0.52	1.79	7	2
1:A:36:ILE:HG12	1:A:37:TYR:H	0.52	1.62	14	2
1:A:87:LEU:HA	1:A:90:ARG:HD2	0.52	1.81	1	1
1:A:68:VAL:HG21	1:A:74:ILE:HB	0.52	1.81	10	1
1:A:166:LEU:HD22	1:A:166:LEU:H	0.52	1.64	7	3
1:A:155:ILE:O	1:A:159:LEU:HG	0.52	2.04	6	2
1:A:22:VAL:HG22	1:A:164:LEU:HG	0.52	1.82	11	1
1:A:118:GLY:C	1:A:119:ILE:HG13	0.52	2.30	11	5
1:A:88:MET:SD	1:A:182:LEU:HD23	0.52	2.45	17	2
1:A:51:ARG:HG3	1:A:52:LEU:N	0.52	2.20	16	2
1:A:99:VAL:HA	1:A:118:GLY:HA2	0.52	1.81	16	2
1:A:72:ASP:O	1:A:75:PRO:HD2	0.52	2.05	15	1
1:A:155:ILE:HG22	1:A:159:LEU:HD12	0.51	1.81	5	3
1:A:33:THR:HA	1:A:170:ASP:CB	0.51	2.35	3	1
1:A:85:MET:HE1	1:A:100:LEU:HD22	0.51	1.81	6	1
1:A:35:THR:HG22	1:A:176:PRO:O	0.51	2.05	19	3
1:A:105:LEU:HD13	1:A:106:ILE:N	0.51	2.20	10	1
1:A:36:ILE:HG23	1:A:174:MET:HB2	0.51	1.82	16	1
1:A:56:LYS:HE3	1:A:58:ARG:HB2	0.51	1.81	19	1
1:A:52:LEU:C	1:A:52:LEU:HD13	0.51	2.30	15	3
1:A:39:LEU:HB2	1:A:139:THR:O	0.51	2.05	4	7
1:A:61:HIS:HB3	1:A:113:GLY:HA3	0.51	1.83	5	1
1:A:81:SER:O	1:A:85:MET:HB3	0.51	2.05	16	1
1:A:71:VAL:O	1:A:75:PRO:HD3	0.51	2.05	15	2
1:A:16:LEU:O	1:A:20:ILE:HG23	0.51	2.05	3	2
1:A:14:ASP:HA	1:A:17:GLU:HG2	0.51	1.83	4	2
1:A:37:TYR:HB3	1:A:141:ALA:HB3	0.51	1.83	14	2
1:A:64:VAL:HG21	1:A:110:ILE:HG22	0.51	1.82	6	4
1:A:84:ALA:HB1	1:A:184:VAL:O	0.51	2.06	16	1
1:A:126:ILE:HD12	1:A:168:ALA:HB2	0.51	1.82	3	1
1:A:162:VAL:HG22	1:A:163:ASP:N	0.50	2.21	7	3
1:A:28:ILE:HD12	1:A:41:VAL:HG13	0.50	1.83	8	1
1:A:33:THR:C	1:A:171:CYS:HB2	0.50	2.31	4	1
1:A:102:ARG:HB3	1:A:117:VAL:HG23	0.50	1.84	7	2
1:A:100:LEU:HD23	1:A:182:LEU:HD12	0.50	1.84	16	1
1:A:159:LEU:HD13	1:A:164:LEU:HA	0.50	1.84	7	2
1:A:74:ILE:N	1:A:75:PRO:CD	0.50	2.74	5	3
1:A:98:VAL:HG12	1:A:180:ILE:HB	0.50	1.81	9	1
1:A:15:VAL:HG13	1:A:167:ASP:HB3	0.49	1.84	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:GLU:O	1:A:49:VAL:HG12	0.49	2.06	16	1
1:A:159:LEU:CD2	1:A:165:VAL:HG13	0.49	2.36	7	1
1:A:151:ARG:HG2	1:A:154:GLU:H	0.49	1.67	13	2
1:A:52:LEU:HD22	1:A:52:LEU:O	0.49	2.07	15	3
1:A:147:PRO:N	1:A:148:PRO:HD2	0.49	2.23	4	4
1:A:34:ASP:O	1:A:172:LEU:HB3	0.49	2.07	20	3
1:A:102:ARG:HG2	1:A:111:THR:HG23	0.49	1.84	8	1
1:A:64:VAL:HG12	1:A:110:ILE:O	0.49	2.07	9	6
1:A:33:THR:O	1:A:171:CYS:C	0.49	2.56	14	4
1:A:105:LEU:O	1:A:107:PRO:HD3	0.49	2.07	19	3
1:A:166:LEU:H	1:A:166:LEU:HD22	0.49	1.67	2	2
1:A:30:ILE:C	1:A:166:LEU:HD12	0.49	2.32	15	1
1:A:16:LEU:HD22	1:A:126:ILE:HG23	0.49	1.84	2	2
1:A:152:LEU:HD22	1:A:166:LEU:CA	0.49	2.36	19	1
1:A:41:VAL:HG22	1:A:42:ASN:H	0.49	1.66	15	6
1:A:166:LEU:N	1:A:166:LEU:CD1	0.49	2.76	6	4
1:A:166:LEU:HD23	1:A:169:GLY:HA2	0.49	1.84	7	2
1:A:120:ARG:O	1:A:122:PRO:HD3	0.48	2.08	5	2
1:A:78:SER:HB2	1:A:100:LEU:HD23	0.48	1.84	10	2
1:A:165:VAL:HG13	1:A:166:LEU:N	0.48	2.23	15	4
1:A:107:PRO:O	1:A:111:THR:HG22	0.48	2.08	19	1
1:A:166:LEU:C	1:A:166:LEU:HD13	0.48	2.32	19	1
1:A:43:ALA:HA	1:A:137:THR:OG1	0.48	2.08	10	1
1:A:88:MET:HB2	1:A:182:LEU:HD13	0.48	1.83	8	2
1:A:111:THR:HA	1:A:117:VAL:HG22	0.48	1.84	5	1
1:A:28:ILE:HG12	1:A:41:VAL:HG11	0.48	1.86	2	1
1:A:71:VAL:HG23	1:A:92:LEU:HD13	0.48	1.85	5	1
1:A:68:VAL:HG22	1:A:73:GLU:HB2	0.48	1.85	10	3
1:A:102:ARG:CZ	1:A:110:ILE:HG21	0.48	2.39	10	1
1:A:102:ARG:HH21	1:A:117:VAL:HG21	0.48	1.69	16	1
1:A:100:LEU:HG	1:A:101:GLU:O	0.48	2.09	10	1
1:A:152:LEU:O	1:A:165:VAL:HG11	0.48	2.08	3	1
1:A:159:LEU:O	1:A:161:ALA:N	0.48	2.47	7	4
1:A:102:ARG:HH11	1:A:117:VAL:HG21	0.48	1.69	10	1
1:A:28:ILE:HD11	1:A:39:LEU:HG	0.48	1.85	16	1
1:A:28:ILE:HB	1:A:51:ARG:HG2	0.47	1.84	10	1
1:A:28:ILE:O	1:A:163:ASP:HA	0.47	2.10	13	13
1:A:159:LEU:N	1:A:159:LEU:CD2	0.47	2.77	9	1
1:A:65:SER:HB2	1:A:138:ALA:O	0.47	2.09	20	1
1:A:100:LEU:HG	1:A:101:GLU:N	0.47	2.25	2	1
1:A:106:ILE:HB	1:A:107:PRO:HD3	0.47	1.85	20	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HG23	1:A:163:ASP:CA	0.47	2.39	9	2
1:A:32:PRO:HB2	1:A:170:ASP:HA	0.47	1.86	15	1
1:A:102:ARG:NH1	1:A:105:LEU:HD12	0.47	2.25	20	1
1:A:59:SER:HB3	1:A:62:LYS:HB2	0.47	1.87	15	2
1:A:36:ILE:HA	1:A:174:MET:HE3	0.47	1.87	2	1
1:A:28:ILE:HD12	1:A:29:VAL:H	0.47	1.68	16	3
1:A:69:SER:HB2	1:A:128:ARG:O	0.47	2.10	10	6
1:A:74:ILE:HG12	1:A:78:SER:HB2	0.47	1.86	7	1
1:A:15:VAL:HG22	1:A:167:ASP:HB3	0.47	1.87	8	1
1:A:87:LEU:O	1:A:90:ARG:HB3	0.47	2.10	16	1
1:A:81:SER:O	1:A:85:MET:HB2	0.47	2.10	18	1
1:A:28:ILE:HA	1:A:41:VAL:HG11	0.47	1.86	6	1
1:A:118:GLY:O	1:A:119:ILE:HG13	0.46	2.10	10	2
1:A:35:THR:OG1	1:A:36:ILE:HG13	0.46	2.09	12	1
1:A:19:ALA:O	1:A:22:VAL:HG12	0.46	2.09	19	1
1:A:20:ILE:HA	1:A:23:MET:HG2	0.46	1.86	12	1
1:A:61:HIS:HA	1:A:113:GLY:HA3	0.46	1.86	17	1
1:A:92:LEU:HD22	1:A:92:LEU:C	0.46	2.36	19	3
1:A:102:ARG:HB2	1:A:115:SER:C	0.46	2.35	20	2
1:A:28:ILE:HD11	1:A:39:LEU:HB2	0.46	1.87	18	1
1:A:29:VAL:HG13	1:A:164:LEU:CG	0.46	2.40	4	1
1:A:70:CYS:SG	1:A:92:LEU:HD21	0.46	2.51	5	1
1:A:48:ALA:HB1	1:A:137:THR:HG21	0.46	1.87	6	1
1:A:102:ARG:NH2	1:A:117:VAL:HG21	0.46	2.26	16	1
1:A:30:ILE:CB	1:A:165:VAL:HG13	0.46	2.40	19	1
1:A:68:VAL:HG22	1:A:69:SER:H	0.46	1.70	3	13
1:A:28:ILE:HD11	1:A:51:ARG:HH11	0.46	1.70	5	1
1:A:13:PRO:HG2	1:A:16:LEU:HD23	0.46	1.88	4	1
1:A:181:ASP:HB3	1:A:188:ARG:HG3	0.46	1.86	9	1
1:A:22:VAL:HB	1:A:164:LEU:HD13	0.46	1.86	17	1
1:A:30:ILE:HG22	1:A:31:TYR:N	0.46	2.26	19	1
1:A:71:VAL:HG21	1:A:85:MET:HE2	0.46	1.87	12	1
1:A:64:VAL:HG22	1:A:110:ILE:O	0.45	2.11	1	3
1:A:17:GLU:HG3	1:A:18:GLU:N	0.45	2.26	4	2
1:A:159:LEU:O	1:A:159:LEU:HD12	0.45	2.11	13	3
1:A:114:SER:HB2	1:A:116:ARG:HE	0.45	1.69	12	1
1:A:93:PRO:HB3	1:A:121:VAL:HG22	0.45	1.88	6	1
1:A:185:ASN:O	1:A:187:PRO:HD3	0.45	2.10	18	8
1:A:28:ILE:HG22	1:A:163:ASP:HA	0.45	1.87	2	1
1:A:102:ARG:CZ	1:A:117:VAL:HG21	0.45	2.41	3	1
1:A:88:MET:SD	1:A:98:VAL:HG21	0.45	2.51	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:HD11	1:A:155:ILE:HG21	0.45	1.87	12	1
1:A:166:LEU:O	1:A:166:LEU:HD13	0.45	2.12	14	2
1:A:87:LEU:HG	1:A:187:PRO:HG3	0.45	1.87	1	1
1:A:180:ILE:HG12	1:A:189:VAL:HG13	0.45	1.88	8	3
1:A:17:GLU:HA	1:A:20:ILE:HD12	0.45	1.88	7	1
1:A:72:ASP:O	1:A:75:PRO:HD3	0.45	2.10	11	3
1:A:182:LEU:HD13	1:A:187:PRO:HB3	0.45	1.87	17	3
1:A:31:TYR:CD1	1:A:166:LEU:HD13	0.45	2.47	13	2
1:A:71:VAL:O	1:A:74:ILE:HG13	0.45	2.12	5	2
1:A:36:ILE:HG12	1:A:174:MET:O	0.45	2.11	4	3
1:A:106:ILE:HG13	1:A:108:ASP:H	0.45	1.72	10	1
1:A:74:ILE:O	1:A:74:ILE:HG12	0.45	2.12	11	3
1:A:122:PRO:HG2	1:A:124:ASP:OD1	0.45	2.12	13	1
1:A:69:SER:HA	1:A:128:ARG:HE	0.45	1.71	17	1
1:A:66:ILE:HG12	1:A:118:GLY:O	0.45	2.11	18	2
1:A:100:LEU:HG	1:A:101:GLU:H	0.45	1.72	7	2
1:A:89:GLU:O	1:A:92:LEU:HD23	0.45	2.12	16	1
1:A:100:LEU:HD12	1:A:182:LEU:O	0.44	2.12	7	2
1:A:88:MET:SD	1:A:182:LEU:HD13	0.44	2.52	12	2
1:A:101:GLU:HA	1:A:116:ARG:HG2	0.44	1.89	7	1
1:A:36:ILE:CG2	1:A:37:TYR:N	0.44	2.80	9	1
1:A:159:LEU:CD1	1:A:162:VAL:HB	0.44	2.39	9	1
1:A:175:GLU:HB3	1:A:176:PRO:C	0.44	2.37	9	1
1:A:79:ARG:C	1:A:100:LEU:HD11	0.44	2.38	10	1
1:A:105:LEU:HD13	1:A:106:ILE:H	0.44	1.71	13	1
1:A:122:PRO:HD2	1:A:128:ARG:NH2	0.44	2.28	17	1
1:A:41:VAL:HG22	1:A:42:ASN:N	0.44	2.28	20	1
1:A:102:ARG:HE	1:A:106:ILE:HG12	0.44	1.72	2	1
1:A:35:THR:O	1:A:174:MET:HA	0.44	2.12	10	3
1:A:80:PRO:HB3	1:A:100:LEU:HD22	0.44	1.89	10	1
1:A:181:ASP:HB2	1:A:188:ARG:HD3	0.44	1.89	17	1
1:A:107:PRO:HA	1:A:111:THR:HG23	0.44	1.89	10	2
1:A:102:ARG:O	1:A:102:ARG:HG3	0.44	2.13	1	1
1:A:159:LEU:HD13	1:A:163:ASP:OD1	0.44	2.12	5	1
1:A:28:ILE:HG13	1:A:163:ASP:OD1	0.44	2.13	16	1
1:A:152:LEU:HD22	1:A:165:VAL:HG22	0.44	1.90	20	1
1:A:47:ASP:O	1:A:51:ARG:HB3	0.44	2.13	5	1
1:A:52:LEU:HG	1:A:139:THR:HG21	0.44	1.89	6	2
1:A:55:VAL:HG11	1:A:140:SER:O	0.44	2.12	6	1
1:A:69:SER:HA	1:A:128:ARG:HG2	0.44	1.88	10	2
1:A:85:MET:HE1	1:A:182:LEU:HG	0.44	1.90	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:LEU:HD23	1:A:169:GLY:N	0.44	2.23	6	2
1:A:155:ILE:HD12	1:A:165:VAL:CG2	0.44	2.42	13	1
1:A:159:LEU:HG	1:A:163:ASP:OD2	0.44	2.13	15	3
1:A:31:TYR:HE1	1:A:168:ALA:HB3	0.44	1.73	19	2
1:A:100:LEU:HG	1:A:182:LEU:O	0.43	2.12	14	2
1:A:159:LEU:HB3	1:A:163:ASP:H	0.43	1.72	1	3
1:A:52:LEU:O	1:A:56:LYS:HB2	0.43	2.13	4	1
1:A:34:ASP:HB3	1:A:173:ASP:O	0.43	2.13	17	2
1:A:32:PRO:HD2	1:A:166:LEU:CD1	0.43	2.42	11	2
1:A:48:ALA:O	1:A:52:LEU:HD13	0.43	2.13	13	1
1:A:66:ILE:HG13	1:A:119:ILE:HA	0.43	1.89	2	1
1:A:59:SER:HB3	1:A:61:HIS:NE2	0.43	2.28	7	1
1:A:102:ARG:HG2	1:A:115:SER:C	0.43	2.38	9	2
1:A:19:ALA:HA	1:A:22:VAL:HG12	0.43	1.89	2	1
1:A:166:LEU:CD1	1:A:166:LEU:N	0.43	2.81	4	2
1:A:54:ARG:HG3	1:A:55:VAL:N	0.43	2.27	9	1
1:A:102:ARG:HG2	1:A:103:ASN:O	0.43	2.14	14	2
1:A:74:ILE:HD13	1:A:119:ILE:HD12	0.43	1.88	18	1
1:A:20:ILE:HD12	1:A:21:SER:N	0.43	2.28	4	1
1:A:181:ASP:HB3	1:A:188:ARG:HE	0.43	1.74	6	1
1:A:67:CYS:SG	1:A:136:VAL:HB	0.43	2.53	8	2
1:A:96:TYR:HB3	1:A:178:THR:HB	0.43	1.89	9	1
1:A:71:VAL:HA	1:A:74:ILE:HG22	0.43	1.90	11	1
1:A:166:LEU:O	1:A:166:LEU:HD22	0.43	2.14	14	1
1:A:147:PRO:N	1:A:148:PRO:CD	0.43	2.81	20	1
1:A:41:VAL:HG13	1:A:42:ASN:N	0.43	2.28	15	1
1:A:102:ARG:HG2	1:A:103:ASN:N	0.43	2.28	18	1
1:A:166:LEU:CD1	1:A:166:LEU:H	0.43	2.27	4	1
1:A:159:LEU:HG	1:A:163:ASP:OD1	0.43	2.14	8	2
1:A:88:MET:SD	1:A:98:VAL:HG11	0.43	2.54	13	2
1:A:159:LEU:HD21	1:A:165:VAL:HB	0.43	1.90	13	1
1:A:28:ILE:HD11	1:A:51:ARG:NH1	0.43	2.29	5	1
1:A:39:LEU:HD12	1:A:139:THR:O	0.43	2.13	5	1
1:A:32:PRO:HD2	1:A:166:LEU:HD11	0.43	1.89	11	1
1:A:111:THR:OG1	1:A:115:SER:HA	0.43	2.14	11	1
1:A:66:ILE:HD11	1:A:74:ILE:HD11	0.42	1.90	11	1
1:A:155:ILE:CD1	1:A:165:VAL:HG23	0.42	2.43	12	1
1:A:83:ASP:O	1:A:86:GLU:HB2	0.42	2.15	17	1
1:A:88:MET:HE1	1:A:180:ILE:HD13	0.42	1.91	18	1
1:A:102:ARG:HH11	1:A:111:THR:HG21	0.42	1.74	9	1
1:A:77:PHE:CE2	1:A:135:PRO:HG2	0.42	2.50	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:SER:HB2	1:A:100:LEU:CD2	0.42	2.45	10	1
1:A:79:ARG:N	1:A:80:PRO:HD3	0.42	2.30	10	1
1:A:34:ASP:O	1:A:173:ASP:HB2	0.42	2.14	18	1
1:A:92:LEU:HD13	1:A:121:VAL:HG21	0.42	1.90	20	1
1:A:147:PRO:HG2	1:A:148:PRO:HD3	0.42	1.89	20	1
1:A:30:ILE:HG22	1:A:38:GLY:O	0.42	2.14	1	1
1:A:180:ILE:HG23	1:A:189:VAL:CA	0.42	2.44	2	1
1:A:96:TYR:CE1	1:A:180:ILE:HD12	0.42	2.50	17	1
1:A:39:LEU:CB	1:A:139:THR:HG23	0.42	2.45	20	1
1:A:33:THR:HG23	1:A:170:ASP:HB3	0.42	1.89	14	2
1:A:99:VAL:HG13	1:A:118:GLY:HA2	0.42	1.91	17	2
1:A:68:VAL:CG1	1:A:74:ILE:HG12	0.42	2.41	15	1
1:A:119:ILE:HG22	1:A:120:ARG:H	0.42	1.74	3	1
1:A:102:ARG:NE	1:A:115:SER:HA	0.42	2.29	6	1
1:A:22:VAL:HG11	1:A:29:VAL:HG22	0.42	1.92	11	1
1:A:66:ILE:O	1:A:119:ILE:HA	0.42	2.14	11	2
1:A:30:ILE:HD12	1:A:165:VAL:HG22	0.42	1.92	19	1
1:A:22:VAL:HG11	1:A:164:LEU:CD1	0.42	2.43	4	1
1:A:35:THR:HB	1:A:36:ILE:H	0.42	1.49	5	1
1:A:111:THR:HG22	1:A:114:SER:O	0.42	2.14	8	1
1:A:166:LEU:H	1:A:166:LEU:CD1	0.42	2.27	12	1
1:A:29:VAL:H	1:A:41:VAL:HG13	0.42	1.73	6	1
1:A:41:VAL:HG22	1:A:42:ASN:ND2	0.42	2.30	7	1
1:A:97:THR:HA	1:A:120:ARG:HB3	0.42	1.90	4	1
1:A:33:THR:HG21	1:A:122:PRO:CB	0.42	2.45	5	1
1:A:30:ILE:HG12	1:A:163:ASP:OD2	0.42	2.15	11	1
1:A:118:GLY:O	1:A:119:ILE:HD13	0.42	2.15	2	1
1:A:44:LEU:HG	1:A:110:ILE:HD11	0.42	1.91	8	1
1:A:172:LEU:HB3	1:A:173:ASP:H	0.41	1.54	1	2
1:A:88:MET:HE2	1:A:98:VAL:HG22	0.41	1.91	4	2
1:A:79:ARG:H	1:A:100:LEU:HD21	0.41	1.75	10	1
1:A:17:GLU:O	1:A:20:ILE:HD13	0.41	2.14	12	1
1:A:34:ASP:N	1:A:171:CYS:HB2	0.41	2.30	6	1
1:A:102:ARG:HH22	1:A:110:ILE:HD12	0.41	1.75	16	1
1:A:175:GLU:HB2	1:A:176:PRO:HA	0.41	1.93	5	1
1:A:185:ASN:N	1:A:186:PRO:HD2	0.41	2.31	8	1
1:A:48:ALA:O	1:A:52:LEU:HB2	0.41	2.16	10	1
1:A:100:LEU:HD12	1:A:101:GLU:H	0.41	1.74	10	1
1:A:74:ILE:CG1	1:A:77:PHE:HB3	0.41	2.45	13	1
1:A:74:ILE:H	1:A:74:ILE:HG13	0.41	1.61	14	2
1:A:32:PRO:HD2	1:A:166:LEU:HG	0.41	1.92	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:VAL:HG13	1:A:119:ILE:HB	0.41	1.93	2	1
1:A:16:LEU:O	1:A:20:ILE:HG13	0.41	2.16	4	1
1:A:59:SER:N	1:A:60:PRO:HD3	0.41	2.30	6	1
1:A:28:ILE:HD12	1:A:41:VAL:CG1	0.41	2.46	8	1
1:A:36:ILE:HG13	1:A:37:TYR:H	0.41	1.75	9	1
1:A:67:CYS:O	1:A:131:ALA:HB1	0.41	2.14	11	3
1:A:128:ARG:NE	1:A:128:ARG:HA	0.41	2.30	17	1
1:A:120:ARG:C	1:A:122:PRO:HD3	0.41	2.41	5	1
1:A:88:MET:HG2	1:A:98:VAL:HG21	0.41	1.91	6	1
1:A:52:LEU:HD11	1:A:64:VAL:HG23	0.41	1.91	9	1
1:A:97:THR:HG23	1:A:120:ARG:HB3	0.41	1.92	9	1
1:A:165:VAL:HG22	1:A:166:LEU:N	0.41	2.29	11	1
1:A:107:PRO:CB	1:A:110:ILE:HB	0.41	2.45	2	1
1:A:88:MET:C	1:A:92:LEU:HD23	0.41	2.40	8	1
1:A:80:PRO:HB2	1:A:85:MET:SD	0.41	2.55	9	1
1:A:30:ILE:HG12	1:A:163:ASP:OD1	0.41	2.15	2	1
1:A:106:ILE:N	1:A:107:PRO:CD	0.41	2.84	16	2
1:A:152:LEU:HA	1:A:155:ILE:HD11	0.41	1.91	6	2
1:A:34:ASP:OD2	1:A:123:ASP:HB2	0.41	2.15	8	1
1:A:103:ASN:H	1:A:103:ASN:HD22	0.41	1.59	8	1
1:A:35:THR:HG23	1:A:36:ILE:H	0.41	1.76	12	1
1:A:85:MET:CE	1:A:100:LEU:HD21	0.41	2.46	15	1
1:A:173:ASP:C	1:A:175:GLU:H	0.41	2.22	16	1
1:A:159:LEU:HD22	1:A:159:LEU:N	0.41	2.31	8	2
1:A:39:LEU:HG	1:A:141:ALA:HB2	0.41	1.92	3	1
1:A:68:VAL:HG22	1:A:73:GLU:HB3	0.41	1.92	5	1
1:A:102:ARG:HD2	1:A:117:VAL:HG21	0.41	1.93	10	1
1:A:69:SER:HB2	1:A:132:ALA:HB2	0.41	1.93	12	1
1:A:159:LEU:HG	1:A:163:ASP:HB2	0.41	1.91	16	1
1:A:46:GLU:HG2	1:A:47:ASP:N	0.41	2.30	17	1
1:A:182:LEU:HD22	1:A:187:PRO:HG3	0.41	1.93	20	1
1:A:30:ILE:H	1:A:30:ILE:HG13	0.41	1.52	1	2
1:A:88:MET:HG2	1:A:98:VAL:HG11	0.41	1.93	1	1
1:A:105:LEU:HD23	1:A:107:PRO:HD2	0.41	1.91	1	1
1:A:98:VAL:HA	1:A:180:ILE:O	0.41	2.16	7	2
1:A:75:PRO:C	1:A:77:PHE:H	0.41	2.24	16	1
1:A:126:ILE:O	1:A:130:ILE:HG22	0.40	2.16	2	1
1:A:159:LEU:HG	1:A:163:ASP:CG	0.40	2.41	4	1
1:A:56:LYS:C	1:A:58:ARG:H	0.40	2.24	5	1
1:A:16:LEU:N	1:A:16:LEU:CD1	0.40	2.84	8	1
1:A:68:VAL:CG2	1:A:73:GLU:HB2	0.40	2.46	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ILE:HG23	1:A:159:LEU:HD12	0.40	1.91	2	1
1:A:181:ASP:HB3	1:A:188:ARG:HB2	0.40	1.94	7	1
1:A:102:ARG:HG2	1:A:117:VAL:CG2	0.40	2.47	20	2
1:A:30:ILE:HG12	1:A:163:ASP:HB2	0.40	1.93	13	1
1:A:39:LEU:CD1	1:A:141:ALA:HB2	0.40	2.46	17	1
1:A:22:VAL:HB	1:A:164:LEU:HG	0.40	1.92	1	1
1:A:16:LEU:HD22	1:A:16:LEU:N	0.40	2.31	6	1
1:A:63:PRO:HB3	1:A:116:ARG:O	0.40	2.15	7	1
1:A:141:ALA:HB1	1:A:147:PRO:HB3	0.40	1.93	7	1
1:A:85:MET:HE3	1:A:85:MET:HA	0.40	1.90	17	1
1:A:102:ARG:HG3	1:A:111:THR:HG21	0.40	1.93	15	1
1:A:78:SER:CB	1:A:100:LEU:HD23	0.40	2.46	20	1
1:A:33:THR:HG21	1:A:122:PRO:HB3	0.40	1.92	5	1
1:A:175:GLU:N	1:A:176:PRO:CA	0.40	2.83	9	1
1:A:34:ASP:HA	1:A:173:ASP:CB	0.40	2.46	17	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	175/208 (84%)	135±3 (77±2%)	32±3 (19±2%)	8±2 (4±1%)	3	27
All	All	3500/4160 (84%)	2694 (77%)	649 (19%)	157 (4%)	3	27

All 25 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	184	VAL	18
1	A	75	PRO	16
1	A	133	ARG	16
1	A	160	ASP	15
1	A	165	VAL	13
1	A	189	VAL	10
1	A	80	PRO	10

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Mol	Chain	Res	Type	Models (Total)
1	A	176	PRO	8
1	A	162	VAL	8
1	A	108	ASP	6
1	A	107	PRO	5
1	A	170	ASP	5
1	A	42	ASN	4
1	A	41	VAL	4
1	A	36	ILE	3
1	A	35	THR	3
1	A	82	GLY	3
1	A	103	ASN	2
1	A	150	PRO	2
1	A	183	THR	1
1	A	161	ALA	1
1	A	175	GLU	1
1	A	63	PRO	1
1	A	167	ASP	1
1	A	185	ASN	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	153/180 (85%)	96±4 (63±2%)	57±4 (37±2%)	1 8
All	All	3060/3600 (85%)	1927 (63%)	1133 (37%)	1 8

All 127 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	29	VAL	20
1	A	52	LEU	20
1	A	172	LEU	20
1	A	30	ILE	19
1	A	139	THR	19
1	A	183	THR	19
1	A	190	LEU	19

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Mol	Chain	Res	Type	Models (Total)
1	A	45	ASP	18
1	A	28	ILE	18
1	A	36	ILE	17
1	A	164	LEU	17
1	A	166	LEU	17
1	A	33	THR	16
1	A	74	ILE	16
1	A	102	ARG	16
1	A	149	SER	16
1	A	83	ASP	16
1	A	123	ASP	16
1	A	18	GLU	15
1	A	62	LYS	15
1	A	31	TYR	14
1	A	70	CYS	14
1	A	56	LYS	13
1	A	76	ARG	13
1	A	129	ARG	13
1	A	153	GLU	13
1	A	173	ASP	13
1	A	175	GLU	13
1	A	162	VAL	13
1	A	46	GLU	12
1	A	92	LEU	12
1	A	105	LEU	12
1	A	185	ASN	12
1	A	89	GLU	12
1	A	16	LEU	11
1	A	100	LEU	11
1	A	152	LEU	11
1	A	192	ARG	11
1	A	81	SER	11
1	A	90	ARG	11
1	A	177	SER	11
1	A	39	LEU	10
1	A	58	ARG	10
1	A	104	GLU	10
1	A	127	CYS	10
1	A	151	ARG	10
1	A	24	GLU	10
1	A	34	ASP	10
1	A	35	THR	10

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Mol	Chain	Res	Type	Models (Total)
1	A	50	ARG	9
1	A	59	SER	9
1	A	98	VAL	9
1	A	101	GLU	9
1	A	125	GLU	9
1	A	171	CYS	9
1	A	181	ASP	9
1	A	103	ASN	9
1	A	108	ASP	9
1	A	128	ARG	9
1	A	86	GLU	9
1	A	155	ILE	9
1	A	44	LEU	9
1	A	14	ASP	8
1	A	42	ASN	8
1	A	167	ASP	8
1	A	68	VAL	8
1	A	87	LEU	8
1	A	188	ARG	8
1	A	20	ILE	8
1	A	65	SER	8
1	A	140	SER	8
1	A	120	ARG	8
1	A	133	ARG	8
1	A	51	ARG	8
1	A	154	GLU	8
1	A	66	ILE	7
1	A	69	SER	7
1	A	41	VAL	7
1	A	191	ARG	7
1	A	156	VAL	7
1	A	158	ASP	7
1	A	54	ARG	6
1	A	91	ILE	6
1	A	110	ILE	6
1	A	160	ASP	6
1	A	53	PHE	6
1	A	116	ARG	6
1	A	124	ASP	6
1	A	174	MET	6
1	A	85	MET	6
1	A	182	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	17	GLU	6
1	A	114	SER	6
1	A	72	ASP	6
1	A	79	ARG	5
1	A	119	ILE	5
1	A	163	ASP	5
1	A	21	SER	5
1	A	137	THR	5
1	A	178	THR	5
1	A	37	TYR	4
1	A	96	TYR	4
1	A	136	VAL	4
1	A	78	SER	4
1	A	106	ILE	4
1	A	61	HIS	4
1	A	97	THR	4
1	A	170	ASP	4
1	A	67	CYS	4
1	A	77	PHE	4
1	A	115	SER	4
1	A	88	MET	3
1	A	111	THR	3
1	A	179	VAL	3
1	A	157	ARG	3
1	A	73	GLU	3
1	A	189	VAL	2
1	A	130	ILE	2
1	A	23	MET	2
1	A	165	VAL	2
1	A	47	ASP	2
1	A	121	VAL	2
1	A	134	PHE	2
1	A	159	LEU	1
1	A	184	VAL	1
1	A	126	ILE	1
1	A	55	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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

No chemical shift data were provided