W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 10:01 pm BST

PDB ID	:	2H3K
Title	:	Solution Structure of the first NEAT domain of IsdH
Authors	:	Pilpa, R.M.; Fadeev, E.A.; Villareal, V.A.; Wong, M.A.; Phillips, M.; Clubb, R.T.
Deposited on	:	2006-05-22

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 (i) symbol.

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

|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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.
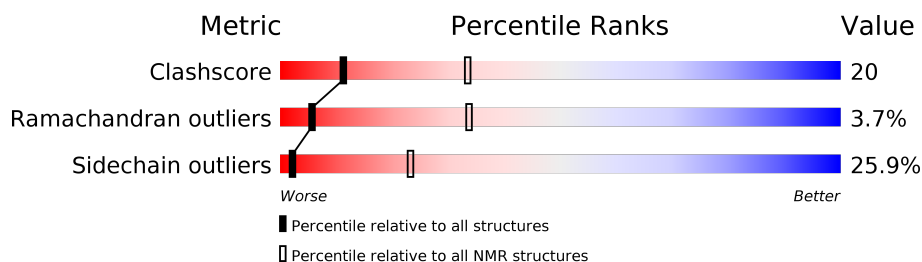
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	144	40%　　　47%　　　6%　8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 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,lowest energy,minimized average structure*.

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:3-A:37, A:45-A:141 (132)	0.33	5

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2319 atoms, of which 1135 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Haptoglobin-binding surface anchored protein.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	144	2319	754	1135	189	241	0

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.

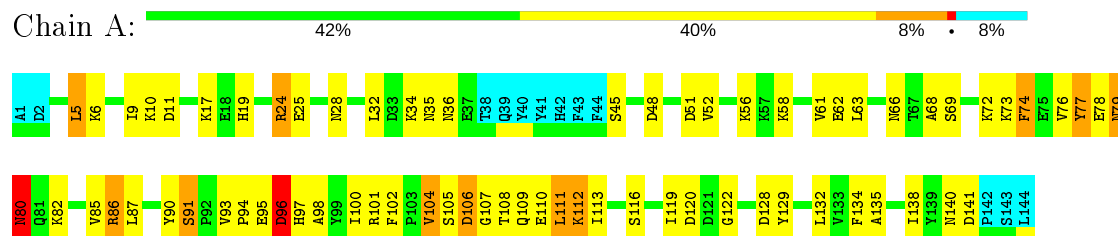• Molecule 1: Haptoglobin-binding surface anchored protein
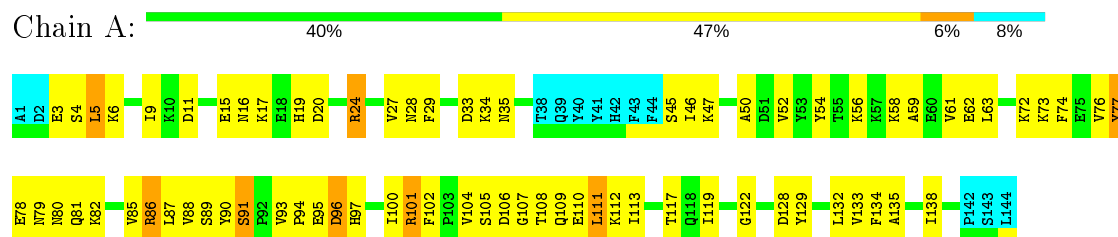
4.2   Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1   Score per residue for model 1

• Molecule 1: Haptoglobin-binding surface anchored protein

4.2.2   Score per residue for model 2

• Molecule 1: Haptoglobin-binding surface anchored protein

4.2.3 Score per residue for model 3

• Molecule 1: Haptoglobin-binding surface anchored protein

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Haptoglobin-binding surface anchored protein

Chain A:

4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Haptoglobin-binding surface anchored protein

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: Haptoglobin-binding surface anchored protein

4.2.7 Score per residue for model 7

• Molecule 1: Haptoglobin-binding surface anchored protein
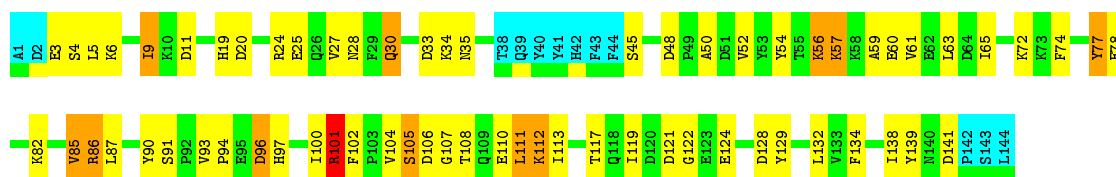

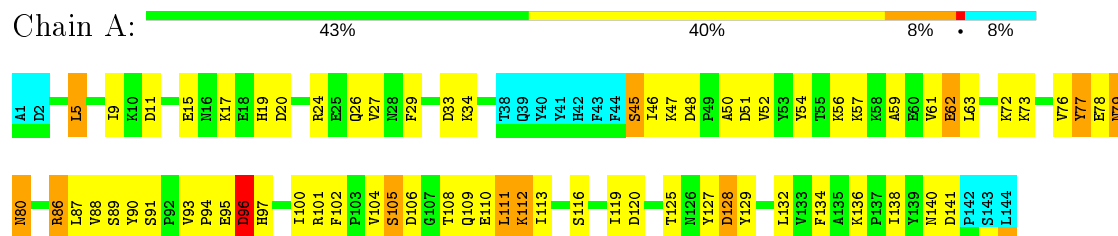### 4.2.8 Score per residue for model 8

• Molecule 1: Haptoglobin-binding surface anchored protein

4.2.9 Score per residue for model 9

• Molecule 1: Haptoglobin-binding surface anchored protein

L144

4.2.10 Score per residue for model 10

• Molecule 1: Haptoglobin-binding surface anchored protein

Chain A:

42% 42% 8% 8%

4.2.11 Score per residue for model 11

• Molecule 1: Haptoglobin-binding surface anchored protein

Chain A:

44% 36% 10% • 8%
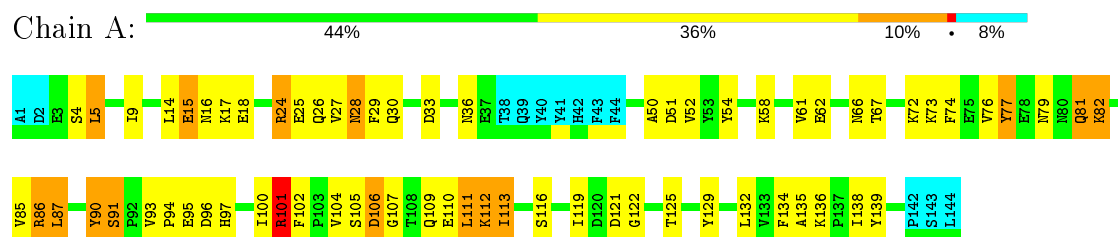
4.2.12 Score per residue for model 12

• Molecule 1: Haptoglobin-binding surface anchored protein

Chain A:

42% 40% 8% • 8%
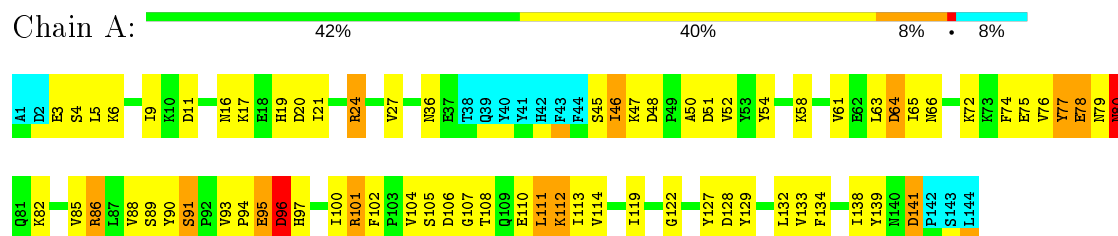
4.2.13 Score per residue for model 13

• Molecule 1: Haptoglobin-binding surface anchored protein

Chain A:

39% 46% 6% • 8%

4.2.14 Score per residue for model 14

• Molecule 1: Haptoglobin-binding surface anchored protein

4.2.15 Score per residue for model 15

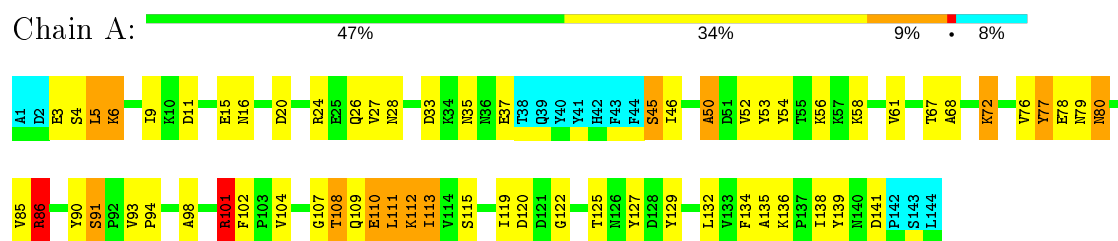• Molecule 1: Haptoglobin-binding surface anchored protein

4.2.16 Score per residue for model 16

• Molecule 1: Haptoglobin-binding surface anchored protein
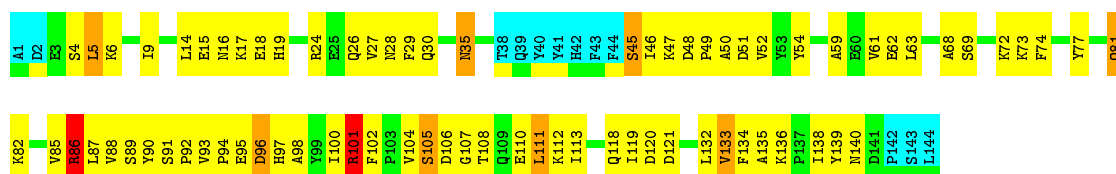
4.2.17 Score per residue for model 17
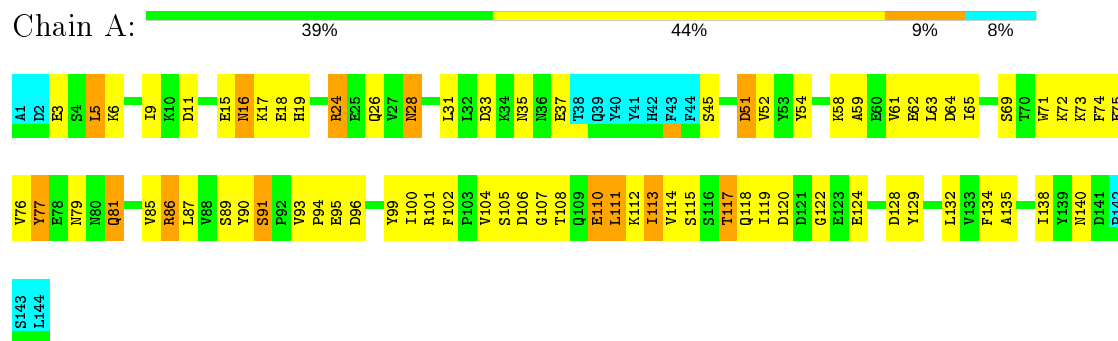
• Molecule 1: Haptoglobin-binding surface anchored protein
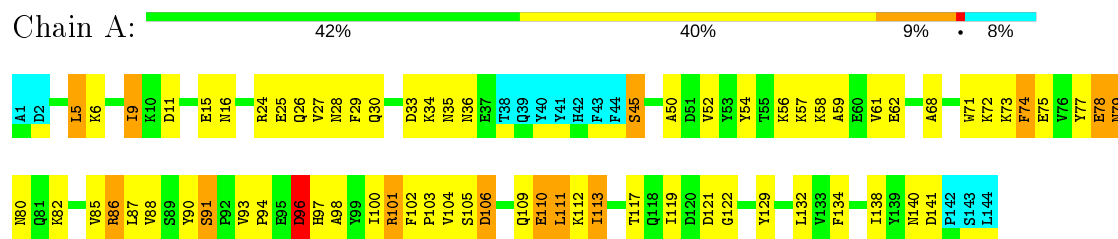
4.2.18 Score per residue for model 18

• Molecule 1: Haptoglobin-binding surface anchored protein
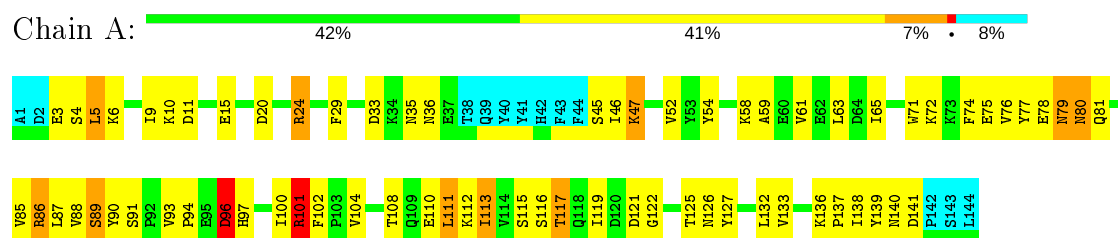
4.2.19 Score per residue for model 19

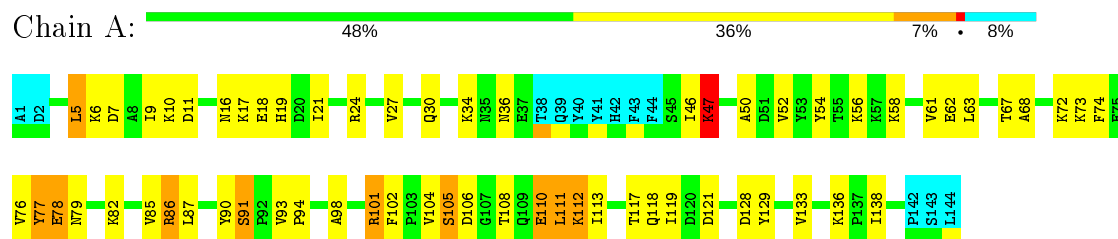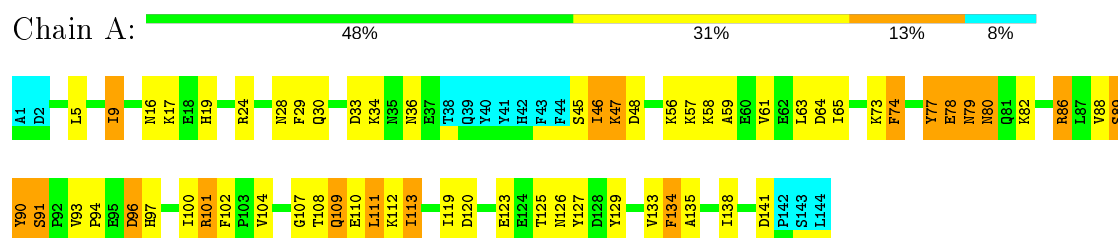• Molecule 1: Haptoglobin-binding surface anchored protein
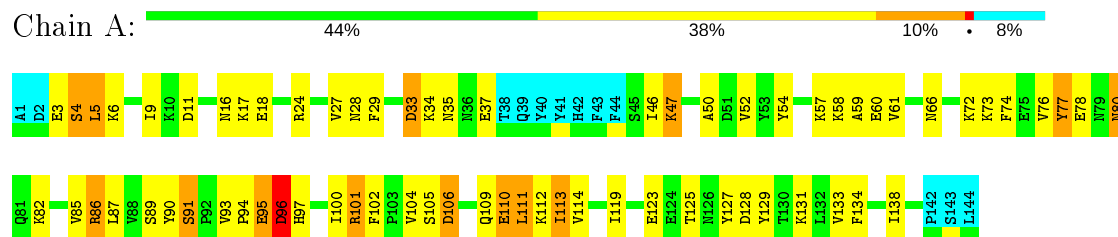
4.2.20 Score per residue for model 20

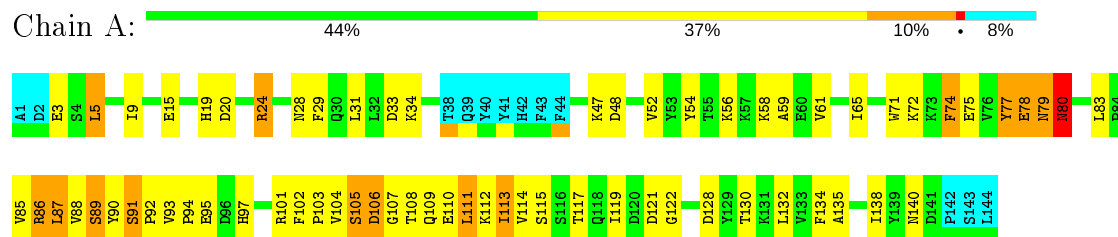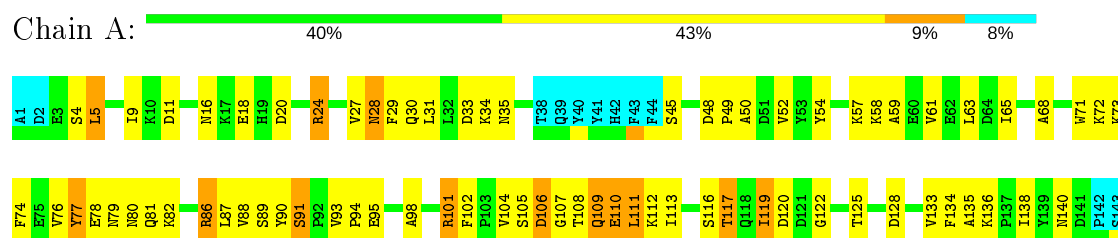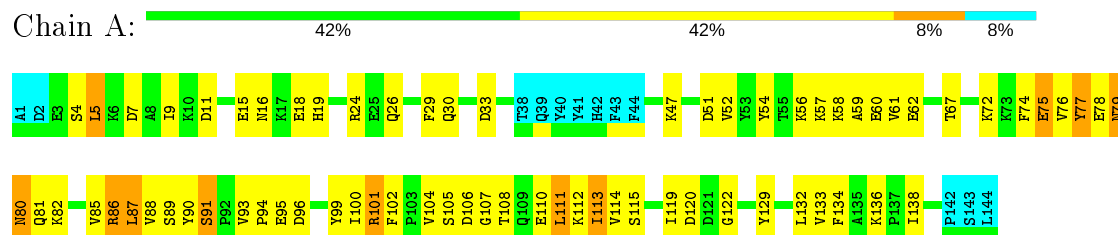• Molecule 1: Haptoglobin-binding surface anchored protein
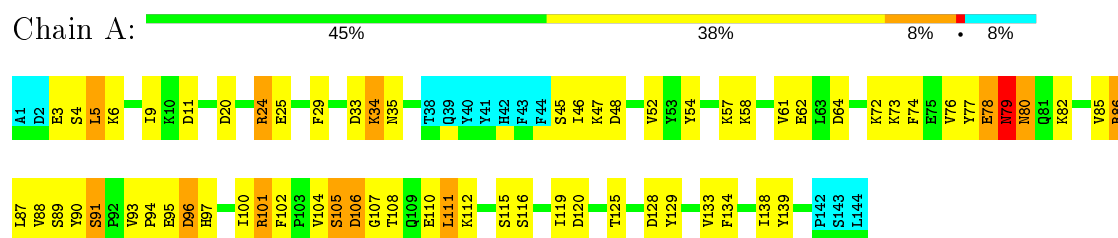
5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry*.

Of the 200 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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1508
Number of shifts mapped to atoms	1508
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0 ± 0.0	3.0 ± 0.0
All	All	0	60

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	86	ARG	Sidechain	20
1	A	101	ARG	Sidechain	20
1	A	24	ARG	Sidechain	20

6.2 Too-close contacts (i)

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	1077	1043	1043	43 ± 6
All	All	21540	20860	20860	857

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:52:VAL:HG11	1:A:54:TYR:CZ	0.83	2.09	20	16
1:A:61:VAL:HG11	1:A:134:PHE:CZ	0.79	2.13	12	14
1:A:74:PHE:CE2	1:A:85:VAL:HG21	0.79	2.13	16	9
1:A:110:GLU:C	1:A:111:LEU:HD23	0.76	2.01	17	20
1:A:104:VAL:HG21	1:A:138:ILE:CG2	0.76	2.09	9	16
1:A:5:LEU:O	1:A:9:ILE:HG23	0.76	1.80	9	20
1:A:28:ASN:OD1	1:A:135:ALA:HB2	0.76	1.81	9	3
1:A:132:LEU:O	1:A:132:LEU:HD23	0.73	1.83	1	7
1:A:68:ALA:HB2	1:A:98:ALA:HB2	0.72	1.61	4	4
1:A:61:VAL:HG11	1:A:134:PHE:CE1	0.71	2.20	16	4
1:A:132:LEU:HD23	1:A:132:LEU:O	0.70	1.87	10	6
1:A:104:VAL:HG21	1:A:138:ILE:HG21	0.67	1.67	11	16
1:A:87:LEU:HD23	1:A:99:TYR:O	0.66	1.89	10	1
1:A:78:GLU:OE1	1:A:108:THR:HG23	0.66	1.89	2	3
1:A:62:GLU:O	1:A:63:LEU:HD12	0.66	1.91	16	2
1:A:61:VAL:HG21	1:A:134:PHE:CZ	0.66	2.26	9	2
1:A:54:TYR:CD1	1:A:59:ALA:HB2	0.65	2.26	19	5
1:A:64:ASP:C	1:A:65:ILE:HD12	0.64	2.12	5	3
1:A:14:LEU:HD12	1:A:87:LEU:CD2	0.62	2.24	15	1
1:A:110:GLU:HG3	1:A:133:VAL:HG12	0.62	1.71	10	1
1:A:78:GLU:OE1	1:A:108:THR:HG21	0.62	1.94	18	1
1:A:74:PHE:CE2	1:A:85:VAL:HG11	0.62	2.29	12	2
1:A:119:ILE:HD12	1:A:119:ILE:N	0.61	2.10	16	4
1:A:108:THR:HG22	1:A:111:LEU:HD22	0.61	1.71	3	6
1:A:74:PHE:CE1	1:A:113:ILE:HG23	0.61	2.30	6	7
1:A:76:VAL:HG22	1:A:113:ILE:HG13	0.61	1.73	4	6
1:A:59:ALA:HB3	1:A:104:VAL:CG2	0.61	2.25	15	7
1:A:104:VAL:O	1:A:104:VAL:HG23	0.60	1.96	11	5
1:A:104:VAL:HG23	1:A:104:VAL:O	0.60	1.97	7	11
1:A:119:ILE:HG22	1:A:119:ILE:O	0.60	1.96	13	10
1:A:104:VAL:HG21	1:A:138:ILE:HG22	0.60	1.72	10	5
1:A:110:GLU:HG2	1:A:133:VAL:HG22	0.59	1.73	12	2
1:A:63:LEU:N	1:A:63:LEU:HD12	0.58	2.14	3	1
1:A:74:PHE:CE1	1:A:76:VAL:HG23	0.58	2.34	6	4
1:A:20:ASP:C	1:A:21:ILE:HD13	0.57	2.19	12	1
1:A:52:VAL:HG11	1:A:54:TYR:CE1	0.57	2.34	13	10
1:A:78:GLU:OE2	1:A:108:THR:HG21	0.57	1.99	6	1
1:A:61:VAL:HG11	1:A:102:PHE:CE2	0.57	2.34	9	2
1:A:28:ASN:HB3	1:A:135:ALA:HB2	0.57	1.77	8	7
1:A:62:GLU:C	1:A:63:LEU:HD12	0.57	2.20	13	1
1:A:74:PHE:CD2	1:A:85:VAL:HG21	0.57	2.34	6	3
1:A:83:LEU:HD22	1:A:103:PRO:HG2	0.56	1.77	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:ILE:O	1:A:119:ILE:HG22	0.56	2.00	10	6
1:A:111:LEU:HD23	1:A:111:LEU:N	0.56	2.15	19	13
1:A:5:LEU:HG	1:A:87:LEU:HD11	0.56	1.77	8	1
1:A:100:ILE:C	1:A:100:ILE:HD12	0.56	2.21	2	5
1:A:71:TRP:HA	1:A:117:THR:HG22	0.56	1.78	15	2
1:A:74:PHE:HE2	1:A:85:VAL:HG11	0.55	1.61	12	1
1:A:68:ALA:CB	1:A:98:ALA:HB2	0.55	2.31	4	7
1:A:100:ILE:HD12	1:A:100:ILE:C	0.55	2.21	20	4
1:A:61:VAL:HG11	1:A:134:PHE:HZ	0.55	1.56	12	8
1:A:14:LEU:HD12	1:A:87:LEU:HD23	0.55	1.78	15	1
1:A:111:LEU:N	1:A:111:LEU:HD23	0.55	2.17	13	7
1:A:61:VAL:HG21	1:A:134:PHE:CE1	0.54	2.37	9	1
1:A:71:TRP:CE3	1:A:117:THR:HG22	0.54	2.37	17	4
1:A:59:ALA:HB3	1:A:104:VAL:HG23	0.54	1.80	8	4
1:A:90:TYR:CZ	1:A:91:SER:O	0.53	2.61	7	20
1:A:52:VAL:HG22	1:A:61:VAL:HG22	0.53	1.80	12	3
1:A:87:LEU:HG	1:A:100:ILE:HG22	0.53	1.81	11	1
1:A:102:PHE:N	1:A:102:PHE:CD1	0.53	2.77	10	11
1:A:108:THR:CG2	1:A:111:LEU:HD22	0.53	2.34	3	3
1:A:102:PHE:CD1	1:A:102:PHE:N	0.52	2.77	16	5
1:A:52:VAL:CG1	1:A:54:TYR:CZ	0.52	2.93	8	6
1:A:87:LEU:HD12	1:A:100:ILE:HG22	0.52	1.81	14	2
1:A:71:TRP:CZ3	1:A:74:PHE:CD2	0.52	2.97	8	1
1:A:52:VAL:CG1	1:A:54:TYR:CE1	0.51	2.93	4	9
1:A:71:TRP:CE3	1:A:117:THR:CG2	0.51	2.93	17	2
1:A:85:VAL:HG22	1:A:102:PHE:HB3	0.51	1.82	11	1
1:A:74:PHE:HE2	1:A:100:ILE:HD13	0.51	1.66	12	5
1:A:110:GLU:HB3	1:A:133:VAL:HG22	0.51	1.81	6	2
1:A:21:ILE:N	1:A:21:ILE:HD13	0.51	2.21	12	1
1:A:54:TYR:CE1	1:A:59:ALA:HB2	0.51	2.41	16	4
1:A:110:GLU:CG	1:A:133:VAL:HG22	0.51	2.35	12	1
1:A:54:TYR:CD1	1:A:59:ALA:CB	0.51	2.94	19	3
1:A:61:VAL:CG2	1:A:138:ILE:HG21	0.50	2.36	5	4
1:A:14:LEU:HD22	1:A:88:VAL:O	0.50	2.06	13	1
1:A:133:VAL:HG23	1:A:133:VAL:O	0.50	2.05	10	2
1:A:74:PHE:CD2	1:A:85:VAL:HG11	0.50	2.42	10	3
1:A:74:PHE:HE2	1:A:85:VAL:HG21	0.50	1.65	10	2
1:A:111:LEU:CD2	1:A:111:LEU:N	0.50	2.75	11	11
1:A:85:VAL:HG13	1:A:85:VAL:O	0.50	2.07	5	2
1:A:133:VAL:HG12	1:A:133:VAL:O	0.50	2.06	14	2
1:A:111:LEU:N	1:A:111:LEU:CD2	0.49	2.75	7	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:VAL:HG12	1:A:89:SER:N	0.49	2.23	3	2
1:A:88:VAL:HG11	1:A:101:ARG:HD3	0.49	1.84	9	1
1:A:76:VAL:HG12	1:A:113:ILE:HG13	0.49	1.85	19	2
1:A:61:VAL:HG23	1:A:138:ILE:HG21	0.49	1.84	14	1
1:A:61:VAL:HG23	1:A:104:VAL:HG21	0.48	1.85	1	4
1:A:74:PHE:HE1	1:A:113:ILE:HG23	0.48	1.68	13	3
1:A:71:TRP:CZ3	1:A:117:THR:CG2	0.48	2.96	18	2
1:A:96:ASP:O	1:A:97:HIS:CG	0.48	2.66	13	13
1:A:46:ILE:HG22	1:A:47:LYS:N	0.48	2.24	20	6
1:A:29:PHE:CZ	1:A:46:ILE:HG21	0.48	2.43	15	2
1:A:90:TYR:CE2	1:A:91:SER:O	0.48	2.67	15	13
1:A:74:PHE:HB3	1:A:85:VAL:HG11	0.48	1.86	14	1
1:A:50:ALA:HB1	1:A:61:VAL:CG1	0.48	2.38	16	1
1:A:129:TYR:CD2	1:A:129:TYR:O	0.47	2.67	4	5
1:A:19:HIS:O	1:A:19:HIS:CG	0.47	2.67	10	5
1:A:29:PHE:O	1:A:29:PHE:CD1	0.47	2.67	15	7
1:A:90:TYR:CE1	1:A:91:SER:O	0.47	2.67	11	4
1:A:61:VAL:CG2	1:A:104:VAL:HG11	0.47	2.39	13	2
1:A:45:SER:OG	1:A:46:ILE:HD12	0.47	2.09	13	1
1:A:29:PHE:CD1	1:A:29:PHE:O	0.47	2.68	13	7
1:A:77:TYR:O	1:A:77:TYR:CG	0.47	2.67	15	11
1:A:129:TYR:O	1:A:129:TYR:CD2	0.47	2.67	14	7
1:A:14:LEU:HD13	1:A:89:SER:HA	0.47	1.85	15	1
1:A:19:HIS:CG	1:A:19:HIS:O	0.47	2.68	7	6
1:A:66:ASN:OD1	1:A:97:HIS:CE1	0.47	2.67	19	3
1:A:86:ARG:CB	1:A:86:ARG:CZ	0.47	2.92	13	1
1:A:112:LYS:CG	1:A:129:TYR:CE1	0.47	2.98	1	2
1:A:19:HIS:CE1	1:A:89:SER:OG	0.46	2.68	16	1
1:A:108:THR:HG22	1:A:111:LEU:CD2	0.46	2.40	3	2
1:A:77:TYR:CD2	1:A:112:LYS:HB2	0.46	2.45	4	6
1:A:88:VAL:HG23	1:A:101:ARG:HG2	0.46	1.87	12	2
1:A:77:TYR:CG	1:A:77:TYR:O	0.46	2.68	2	1
1:A:125:THR:HG22	1:A:127:TYR:CE1	0.46	2.45	4	1
1:A:88:VAL:CG2	1:A:89:SER:N	0.46	2.78	18	5
1:A:54:TYR:CE1	1:A:59:ALA:CB	0.46	2.99	16	3
1:A:119:ILE:N	1:A:119:ILE:CD1	0.46	2.78	16	2
1:A:88:VAL:HG13	1:A:89:SER:OG	0.46	2.10	8	1
1:A:100:ILE:HD12	1:A:101:ARG:N	0.46	2.26	11	1
1:A:138:ILE:N	1:A:138:ILE:HD13	0.46	2.26	14	1
1:A:93:VAL:N	1:A:94:PRO:HD2	0.45	2.26	7	20
1:A:85:VAL:HG21	1:A:100:ILE:HD13	0.45	1.87	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:ILE:CD1	1:A:119:ILE:N	0.45	2.78	18	1
1:A:34:LYS:HG3	1:A:129:TYR:CD2	0.45	2.46	20	1
1:A:77:TYR:CD1	1:A:78:GLU:N	0.45	2.84	7	1
1:A:65:ILE:O	1:A:65:ILE:HG22	0.45	2.10	18	2
1:A:54:TYR:CE1	1:A:139:TYR:O	0.45	2.69	13	1
1:A:62:GLU:CG	1:A:63:LEU:N	0.45	2.79	16	1
1:A:78:GLU:O	1:A:79:ASN:CB	0.45	2.65	3	10
1:A:88:VAL:HG23	1:A:89:SER:N	0.45	2.26	9	4
1:A:51:ASP:OD1	1:A:53:TYR:CE2	0.45	2.70	15	1
1:A:56:LYS:CD	1:A:57:LYS:N	0.45	2.80	2	1
1:A:34:LYS:CG	1:A:129:TYR:CD2	0.45	3.00	20	1
1:A:111:LEU:HD21	1:A:134:PHE:CD2	0.45	2.47	4	3
1:A:74:PHE:CE1	1:A:76:VAL:CG2	0.45	3.00	1	2
1:A:65:ILE:HD12	1:A:65:ILE:N	0.44	2.27	16	1
1:A:5:LEU:HD23	1:A:9:ILE:CG2	0.44	2.42	1	1
1:A:77:TYR:CE1	1:A:112:LYS:HB2	0.44	2.48	3	1
1:A:125:THR:HG22	1:A:127:TYR:CZ	0.44	2.47	19	2
1:A:133:VAL:O	1:A:133:VAL:HG12	0.44	2.12	12	2
1:A:119:ILE:N	1:A:119:ILE:HD12	0.44	2.28	13	1
1:A:78:GLU:O	1:A:80:ASN:N	0.44	2.51	12	14
1:A:91:SER:OG	1:A:95:GLU:CB	0.44	2.66	5	10
1:A:3:GLU:CG	1:A:4:SER:N	0.44	2.78	19	1
1:A:105:SER:O	1:A:106:ASP:CB	0.44	2.66	11	16
1:A:77:TYR:CD1	1:A:77:TYR:O	0.44	2.70	3	1
1:A:31:LEU:CD2	1:A:132:LEU:HD12	0.44	2.43	5	1
1:A:90:TYR:O	1:A:90:TYR:CD2	0.44	2.71	7	1
1:A:68:ALA:HB1	1:A:98:ALA:HB2	0.44	1.89	13	1
1:A:102:PHE:N	1:A:102:PHE:CD2	0.43	2.86	7	2
1:A:61:VAL:HG13	1:A:61:VAL:O	0.43	2.13	9	1
1:A:61:VAL:CG1	1:A:102:PHE:CE2	0.43	3.02	10	2
1:A:46:ILE:N	1:A:46:ILE:HD13	0.43	2.29	7	1
1:A:85:VAL:HG11	1:A:100:ILE:HD13	0.43	1.88	1	1
1:A:76:VAL:HG13	1:A:111:LEU:HB2	0.43	1.90	10	1
1:A:109:GLN:O	1:A:134:PHE:N	0.43	2.52	4	6
1:A:74:PHE:CE2	1:A:100:ILE:HD13	0.43	2.48	7	1
1:A:102:PHE:CD2	1:A:102:PHE:N	0.43	2.85	20	1
1:A:32:LEU:HD22	1:A:36:ASN:C	0.43	2.33	1	1
1:A:46:ILE:H	1:A:46:ILE:HD12	0.43	1.73	6	2
1:A:73:LYS:O	1:A:115:SER:CB	0.43	2.67	5	1
1:A:82:LYS:HE3	1:A:114:VAL:HG21	0.43	1.89	19	1
1:A:61:VAL:O	1:A:101:ARG:CB	0.43	2.67	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:VAL:O	1:A:50:ALA:N	0.43	2.52	9	8
1:A:127:TYR:O	1:A:128:ASP:CB	0.43	2.67	3	2
1:A:127:TYR:O	1:A:129:TYR:N	0.43	2.52	12	3
1:A:85:VAL:CG1	1:A:85:VAL:O	0.43	2.67	4	1
1:A:107:GLY:O	1:A:108:THR:C	0.43	2.57	7	11
1:A:74:PHE:CZ	1:A:76:VAL:CG2	0.43	3.02	9	1
1:A:28:ASN:O	1:A:135:ALA:N	0.42	2.52	7	2
1:A:29:PHE:CE2	1:A:49:PRO:HA	0.42	2.49	13	2
1:A:75:GLU:O	1:A:114:VAL:N	0.42	2.52	12	2
1:A:85:VAL:O	1:A:85:VAL:CG1	0.42	2.67	16	1
1:A:107:GLY:HA3	1:A:139:TYR:CE1	0.42	2.49	20	3
1:A:27:VAL:N	1:A:50:ALA:O	0.42	2.52	17	5
1:A:61:VAL:HG23	1:A:104:VAL:CG2	0.42	2.44	4	1
1:A:19:HIS:O	1:A:19:HIS:ND1	0.42	2.52	1	4
1:A:45:SER:C	1:A:46:ILE:HD12	0.42	2.34	12	1
1:A:107:GLY:N	1:A:139:TYR:CE1	0.42	2.87	4	1
1:A:77:TYR:CE2	1:A:112:LYS:HB2	0.42	2.50	12	1
1:A:107:GLY:HA3	1:A:139:TYR:CZ	0.42	2.49	4	3
1:A:78:GLU:OE2	1:A:108:THR:CG2	0.42	2.68	6	1
1:A:19:HIS:ND1	1:A:19:HIS:O	0.42	2.52	7	1
1:A:52:VAL:HG21	1:A:138:ILE:HD12	0.42	1.92	12	1
1:A:15:GLU:O	1:A:16:ASN:CB	0.42	2.68	11	3
1:A:24:ARG:O	1:A:25:GLU:CG	0.42	2.68	11	1
1:A:54:TYR:CG	1:A:141:ASP:OD1	0.42	2.73	18	1
1:A:119:ILE:O	1:A:120:ASP:CB	0.42	2.67	7	1
1:A:6:LYS:CD	1:A:6:LYS:O	0.42	2.68	16	1
1:A:18:GLU:O	1:A:18:GLU:CG	0.42	2.68	10	1
1:A:14:LEU:N	1:A:14:LEU:CD1	0.42	2.82	11	1
1:A:103:PRO:C	1:A:104:VAL:HG13	0.42	2.35	17	1
1:A:88:VAL:HG11	1:A:101:ARG:NE	0.42	2.30	17	2
1:A:109:GLN:NE2	1:A:133:VAL:CG1	0.42	2.83	19	1
1:A:34:LYS:O	1:A:35:ASN:ND2	0.42	2.53	1	1
1:A:133:VAL:O	1:A:133:VAL:CG2	0.42	2.68	10	1
1:A:89:SER:OG	1:A:99:TYR:CD2	0.42	2.73	5	1
1:A:14:LEU:CD2	1:A:14:LEU:N	0.42	2.83	15	1
1:A:46:ILE:CG2	1:A:47:LYS:N	0.42	2.83	19	3
1:A:65:ILE:N	1:A:65:ILE:HD12	0.42	2.30	2	1
1:A:51:ASP:O	1:A:62:GLU:N	0.42	2.52	3	2
1:A:107:GLY:HA3	1:A:139:TYR:CE2	0.42	2.50	4	1
1:A:75:GLU:O	1:A:114:VAL:CG2	0.42	2.68	8	2
1:A:77:TYR:O	1:A:77:TYR:CD2	0.42	2.73	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:19:HIS:CD2	1:A:19:HIS:N	0.42	2.87	16	1
1:A:133:VAL:CG2	1:A:133:VAL:O	0.42	2.68	18	1
1:A:76:VAL:HG13	1:A:112:LYS:O	0.42	2.15	3	1
1:A:63:LEU:N	1:A:63:LEU:CD1	0.42	2.83	3	1
1:A:65:ILE:O	1:A:97:HIS:ND1	0.42	2.53	8	2
1:A:109:GLN:NE2	1:A:134:PHE:O	0.42	2.53	17	1
1:A:32:LEU:HD22	1:A:36:ASN:HA	0.42	1.91	1	1
1:A:28:ASN:OD1	1:A:30:GLN:NE2	0.41	2.53	2	1
1:A:28:ASN:OD1	1:A:29:PHE:N	0.41	2.53	17	2
1:A:61:VAL:HG11	1:A:102:PHE:CZ	0.41	2.50	9	1
1:A:88:VAL:HG11	1:A:101:ARG:HG2	0.41	1.92	18	1
1:A:112:LYS:HG3	1:A:129:TYR:CE1	0.41	2.50	1	1
1:A:91:SER:CB	1:A:95:GLU:HB3	0.41	2.45	14	6
1:A:90:TYR:O	1:A:90:TYR:CD1	0.41	2.73	20	1
1:A:112:LYS:HG3	1:A:129:TYR:CD1	0.41	2.50	1	1
1:A:6:LYS:O	1:A:9:ILE:CG1	0.41	2.68	4	1
1:A:91:SER:HB3	1:A:95:GLU:CB	0.41	2.45	13	3
1:A:24:ARG:HB3	1:A:53:TYR:CD1	0.41	2.50	15	1
1:A:5:LEU:O	1:A:9:ILE:CG2	0.41	2.68	16	2
1:A:95:GLU:O	1:A:97:HIS:CD2	0.41	2.74	8	2
1:A:113:ILE:HD11	1:A:132:LEU:HD13	0.41	1.91	1	1
1:A:9:ILE:HD12	1:A:90:TYR:CZ	0.41	2.50	1	1
1:A:9:ILE:HB	1:A:90:TYR:CG	0.41	2.51	2	1
1:A:91:SER:N	1:A:97:HIS:O	0.41	2.51	7	1
1:A:104:VAL:CG2	1:A:138:ILE:HG21	0.41	2.45	12	1
1:A:125:THR:CG2	1:A:127:TYR:CZ	0.41	3.04	19	1
1:A:53:TYR:CB	1:A:101:ARG:NH2	0.41	2.84	4	1
1:A:115:SER:O	1:A:127:TYR:N	0.41	2.54	4	1
1:A:77:TYR:CD1	1:A:77:TYR:C	0.41	2.92	6	1
1:A:9:ILE:HB	1:A:90:TYR:CE1	0.41	2.51	6	2
1:A:92:PRO:O	1:A:95:GLU:N	0.41	2.53	8	2
1:A:14:LEU:HD13	1:A:87:LEU:CD2	0.41	2.46	14	1
1:A:137:PRO:HB2	1:A:139:TYR:CE2	0.41	2.51	18	1
1:A:17:LYS:CG	1:A:18:GLU:N	0.41	2.84	19	1
1:A:78:GLU:HG3	1:A:108:THR:HG23	0.41	1.93	10	1
1:A:86:ARG:CG	1:A:101:ARG:O	0.41	2.69	4	1
1:A:61:VAL:HB	1:A:102:PHE:CE2	0.41	2.50	4	1
1:A:77:TYR:CD2	1:A:112:LYS:CB	0.41	3.04	4	1
1:A:66:ASN:ND2	1:A:97:HIS:CE1	0.41	2.89	11	1
1:A:78:GLU:OE1	1:A:79:ASN:CB	0.41	2.69	17	1
1:A:119:ILE:HD12	1:A:119:ILE:H	0.41	1.76	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:GLU:HG3	1:A:4:SER:N	0.41	2.32	4	1
1:A:20:ASP:OD1	1:A:20:ASP:N	0.41	2.53	9	1
1:A:104:VAL:CG2	1:A:104:VAL:O	0.40	2.68	7	1
1:A:24:ARG:HB3	1:A:53:TYR:CE1	0.40	2.51	15	1
1:A:90:TYR:CD2	1:A:90:TYR:O	0.40	2.74	16	1
1:A:64:ASP:OD1	1:A:99:TYR:CE2	0.40	2.75	16	1
1:A:112:LYS:HG2	1:A:129:TYR:CE1	0.40	2.51	2	1
1:A:59:ALA:N	1:A:140:ASN:OD1	0.40	2.54	5	1
1:A:119:ILE:H	1:A:119:ILE:HD12	0.40	1.71	18	1
1:A:54:TYR:HD1	1:A:59:ALA:HB2	0.40	1.74	19	1
1:A:130:THR:O	1:A:130:THR:HG22	0.40	2.15	8	1
1:A:82:LYS:HE2	1:A:114:VAL:HG21	0.40	1.93	12	1
1:A:88:VAL:HG12	1:A:101:ARG:HE	0.40	1.76	14	1
1:A:34:LYS:O	1:A:34:LYS:CG	0.40	2.69	2	1
1:A:90:TYR:CD1	1:A:90:TYR:O	0.40	2.74	11	1
1:A:45:SER:OG	1:A:46:ILE:N	0.40	2.54	13	1
1:A:119:ILE:O	1:A:119:ILE:CG2	0.40	2.69	4	1
1:A:4:SER:OG	1:A:72:LYS:CE	0.40	2.69	4	1
1:A:79:ASN:N	1:A:79:ASN:OD1	0.40	2.55	6	1
1:A:52:VAL:HG13	1:A:138:ILE:HG23	0.40	1.94	14	1
1:A:54:TYR:CD1	1:A:140:ASN:HA	0.40	2.52	15	1
1:A:110:GLU:HG2	1:A:133:VAL:HG13	0.40	1.92	16	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	132/144 (92%)	105±3 (80±2%)	22±3 (17±2%)	5±2 (4±1%)	6	34
All	All	2640/2880 (92%)	2099 (80%)	443 (17%)	98 (4%)	6	34

All 22 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	33	ASP	16
1	A	96	ASP	14
1	A	122	GLY	12
1	A	80	ASN	10
1	A	45	SER	7
1	A	79	ASN	6
1	A	15	GLU	5
1	A	16	ASN	5
1	A	140	ASN	4
1	A	81	GLN	3
1	A	47	LYS	3
1	A	17	LYS	2
1	A	46	ILE	2
1	A	82	LYS	1
1	A	20	ASP	1
1	A	134	PHE	1
1	A	50	ALA	1
1	A	35	ASN	1
1	A	119	ILE	1
1	A	125	THR	1
1	A	9	ILE	1
1	A	108	THR	1

6.3.2 Protein sidechains (i)

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	122/133 (92%)	90±3 (74±3%)	32±3 (26±3%)	2	23
All	All	2440/2660 (92%)	1807 (74%)	633 (26%)	2	23

All 85 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	111	LEU	20
1	A	77	TYR	20
1	A	86	ARG	20
1	A	112	LYS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	72	LYS	19
1	A	58	LYS	17
1	A	5	LEU	17
1	A	11	ASP	16
1	A	87	LEU	16
1	A	91	SER	15
1	A	6	LYS	14
1	A	113	ILE	14
1	A	82	LYS	12
1	A	128	ASP	11
1	A	17	LYS	10
1	A	101	ARG	10
1	A	4	SER	10
1	A	48	ASP	10
1	A	63	LEU	10
1	A	73	LYS	10
1	A	79	ASN	10
1	A	56	LYS	10
1	A	35	ASN	10
1	A	120	ASP	9
1	A	96	ASP	9
1	A	30	GLN	9
1	A	57	LYS	9
1	A	3	GLU	9
1	A	45	SER	9
1	A	136	LYS	9
1	A	26	GLN	9
1	A	141	ASP	8
1	A	24	ARG	8
1	A	106	ASP	8
1	A	78	GLU	8
1	A	47	LYS	8
1	A	116	SER	8
1	A	34	LYS	8
1	A	89	SER	7
1	A	81	GLN	7
1	A	20	ASP	7
1	A	121	ASP	7
1	A	16	ASN	7
1	A	36	ASN	7
1	A	62	GLU	7
1	A	110	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	51	ASP	6
1	A	105	SER	6
1	A	117	THR	6
1	A	74	PHE	6
1	A	28	ASN	5
1	A	25	GLU	5
1	A	18	GLU	5
1	A	10	LYS	5
1	A	75	GLU	5
1	A	95	GLU	5
1	A	115	SER	5
1	A	126	ASN	4
1	A	15	GLU	4
1	A	125	THR	4
1	A	85	VAL	4
1	A	69	SER	4
1	A	80	ASN	4
1	A	37	GLU	4
1	A	67	THR	3
1	A	109	GLN	3
1	A	60	GLU	3
1	A	90	TYR	3
1	A	118	GLN	3
1	A	140	ASN	3
1	A	123	GLU	2
1	A	124	GLU	2
1	A	64	ASP	2
1	A	133	VAL	2
1	A	7	ASP	2
1	A	9	ILE	2
1	A	52	VAL	2
1	A	33	ASP	2
1	A	21	ILE	1
1	A	131	LYS	1
1	A	88	VAL	1
1	A	114	VAL	1
1	A	104	VAL	1
1	A	132	LEU	1
1	A	102	PHE	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 (i)

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping (i)

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	1508
Number of shifts mapped to atoms	1508
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}\text{C}_\alpha$	139	0.50 ± 0.16	Should be applied
$^{13}\text{C}_\beta$	136	0.31 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	114	0.28 ± 0.13	None needed (< 0.5 ppm)
^{15}N	122	0.03 ± 0.31	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1285 atoms were assigned a chemical shift out of a possible 1658. 19 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	598/644 (93%)	244/256 (95%)	238/264 (90%)	116/124 (94%)
Sidechain	635/888 (72%)	372/519 (72%)	263/332 (79%)	0/37 (0%)

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	Total	**^{1}H**	**^{13}C**	**^{15}N**
Aromatic	52/126 (41%)	26/66 (39%)	25/57 (44%)	1/3 (33%)
Overall	1285/1658 (78%)	642/841 (76%)	526/653 (81%)	117/164 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 1356 atoms were assigned a chemical shift out of a possible 1813. 20 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	633/702 (90%)	258/279 (92%)	253/288 (88%)	122/135 (90%)
Sidechain	667/944 (71%)	390/553 (71%)	277/353 (78%)	0/38 (0%)
Aromatic	56/167 (34%)	28/88 (32%)	27/75 (36%)	1/4 (25%)
Overall	1356/1813 (75%)	676/920 (73%)	557/716 (78%)	123/177 (69%)

7.1.4　Statistically unusual chemical shifts ⓘ

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	102	PHE	CE1	117.34	137.92 − 123.42	-9.2
1	A	71	TRP	CE3	131.04	129.06 − 111.96	6.2
1	A	71	TRP	CZ3	129.85	129.20 − 113.60	5.4

7.1.5　Random Coil Index (RCI) plots ⓘ

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: