Full wwPDB NMR Structure Validation Report (i)

Feb 3, 2021 – 10:06 AM EST

PDB ID	:	6U1O
Title	:	Structure of two-domain translational regulator Yih1 reveals a possible mechanism of action
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Deposited on	:	2019-08-16

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:

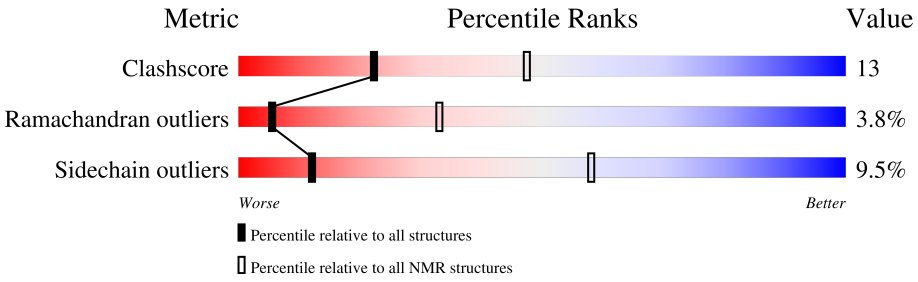
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.16
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 77%.

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	258	64% 26% • 9%

2 Ensemble composition and analysis (i)

This entry contains 12 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:4-A:68, A:76-A:112 (102)	0.55	4
2	A:127-A:258 (132)	0.58	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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 9, 10
2	8, 11
Single-model clusters	12

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3995 atoms, of which 1955 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein IMPACT homolog.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	258	3995	1286	1955	337	406	11	0

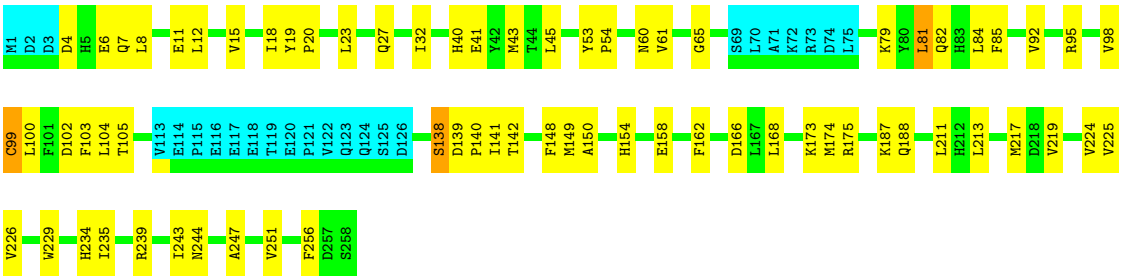
4 Residue-property plots

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: Protein IMPACT homolog

Chain A:



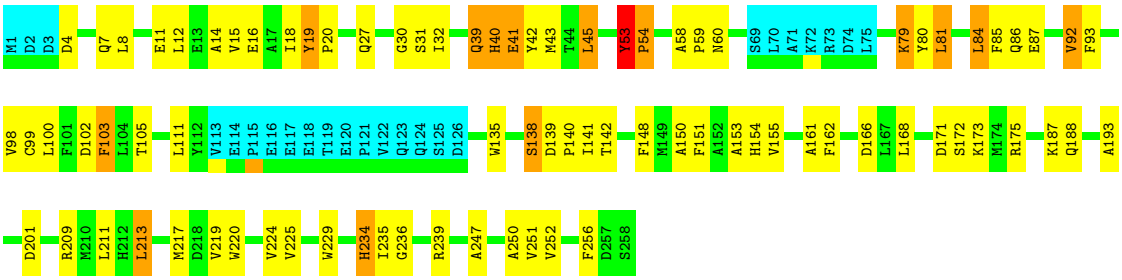
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Protein IMPACT homolog

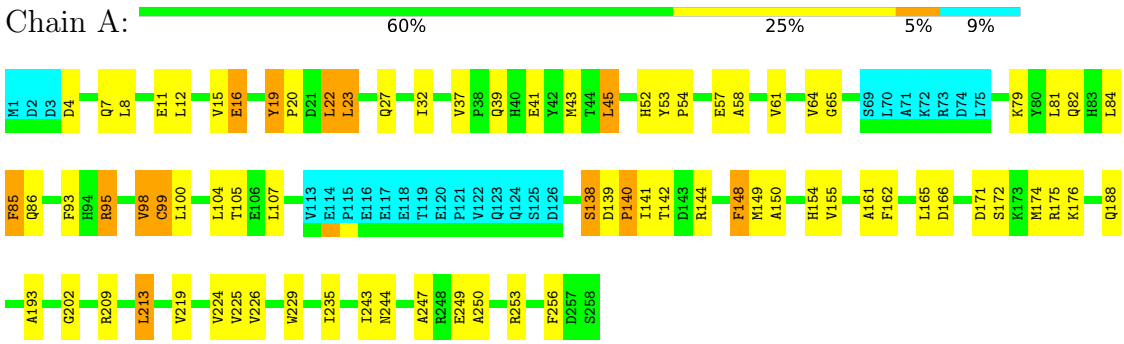
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Protein IMPACT homolog

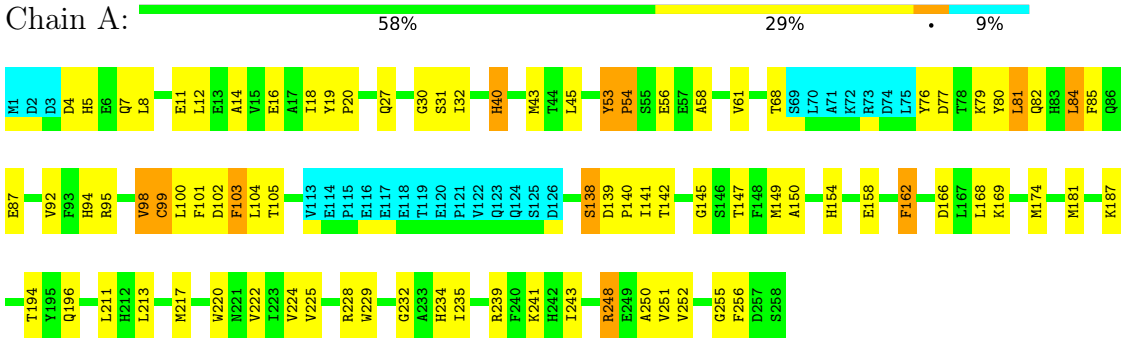
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Protein IMPACT homolog

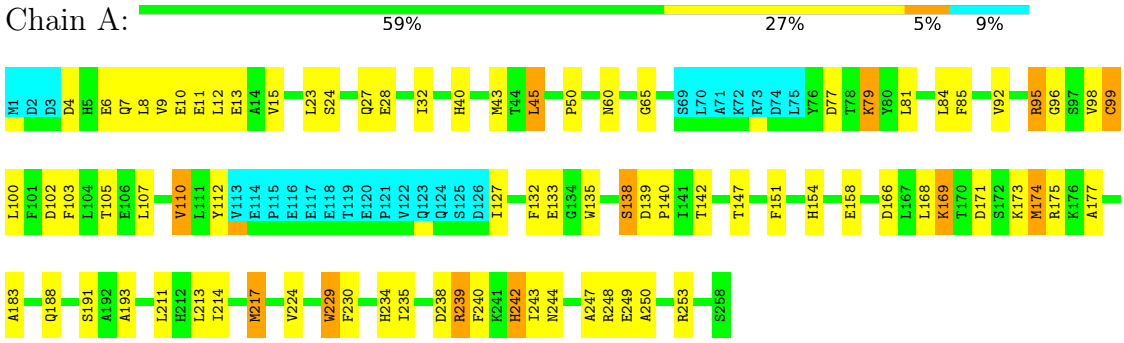
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Protein IMPACT homolog

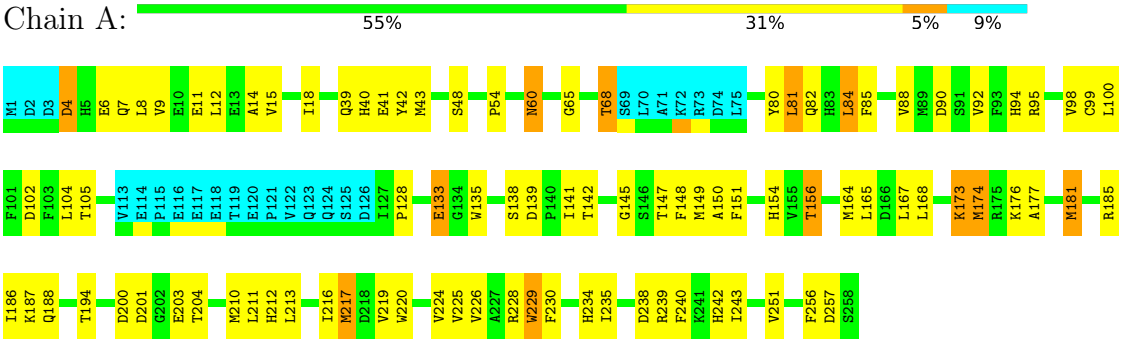
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Protein IMPACT homolog

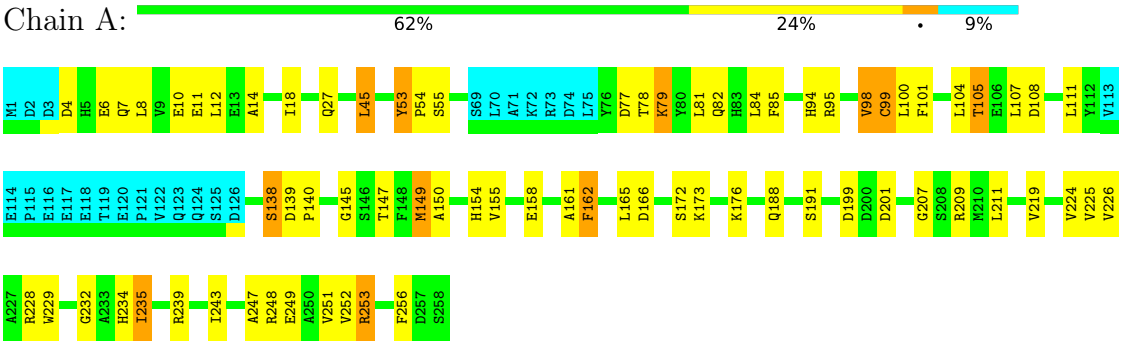
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Protein IMPACT homolog

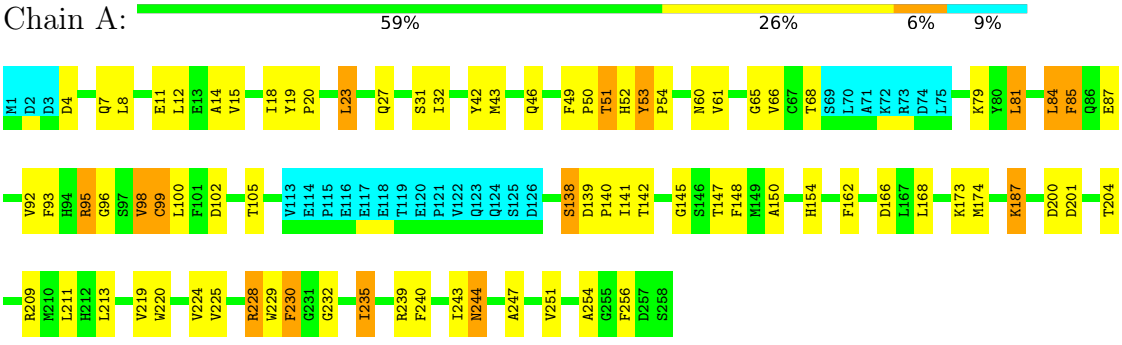
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Protein IMPACT homolog

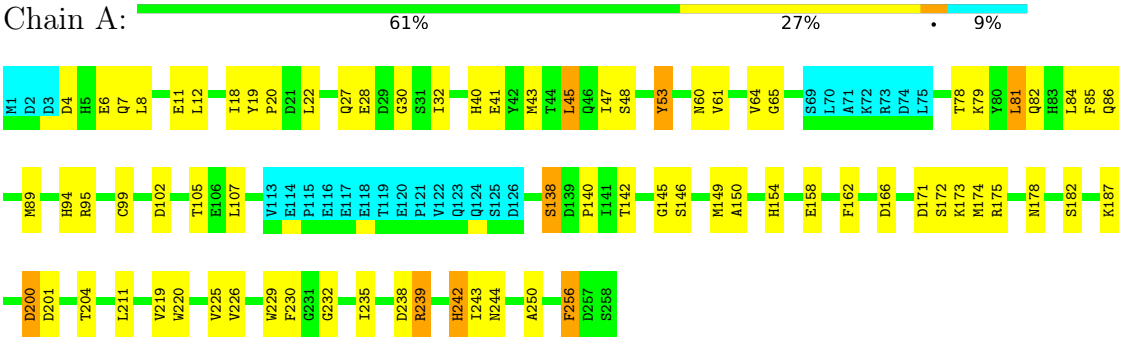
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Protein IMPACT homolog

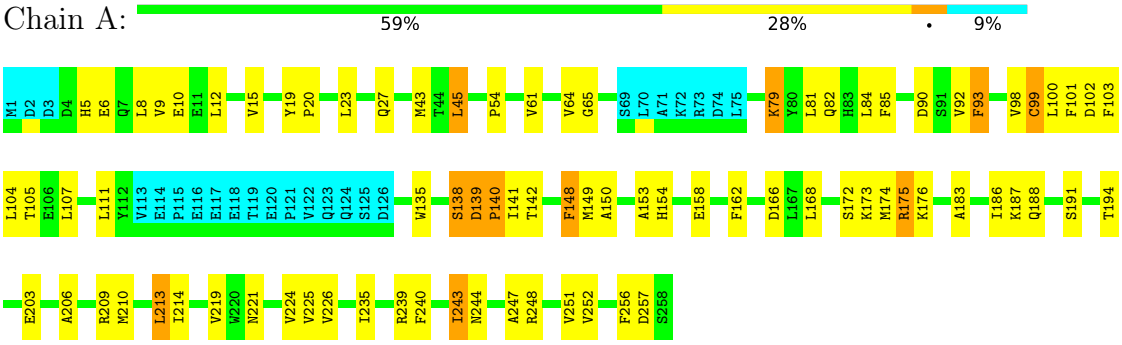
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Protein IMPACT homolog

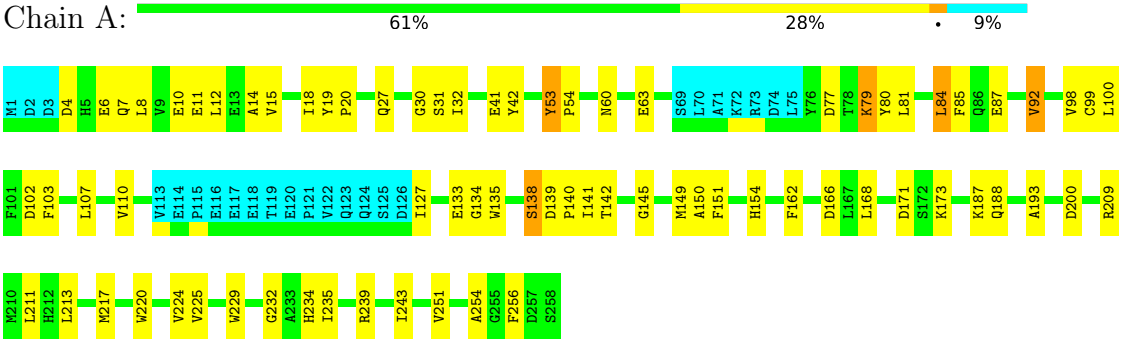
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Protein IMPACT homolog

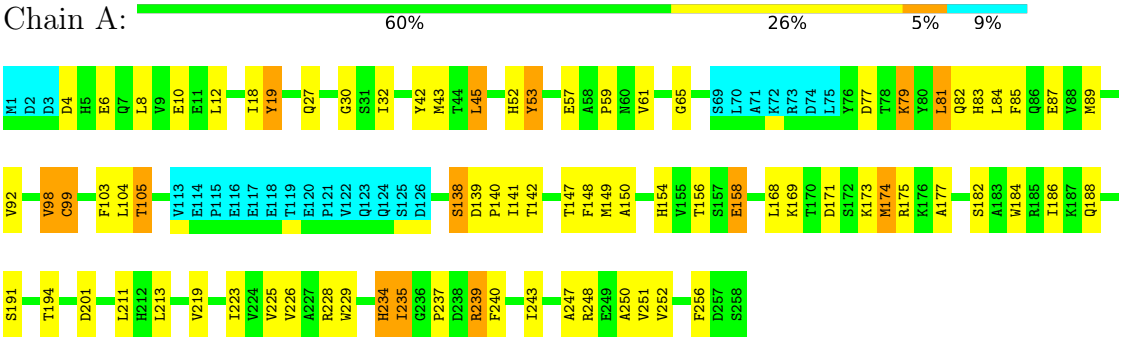
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Protein IMPACT homolog

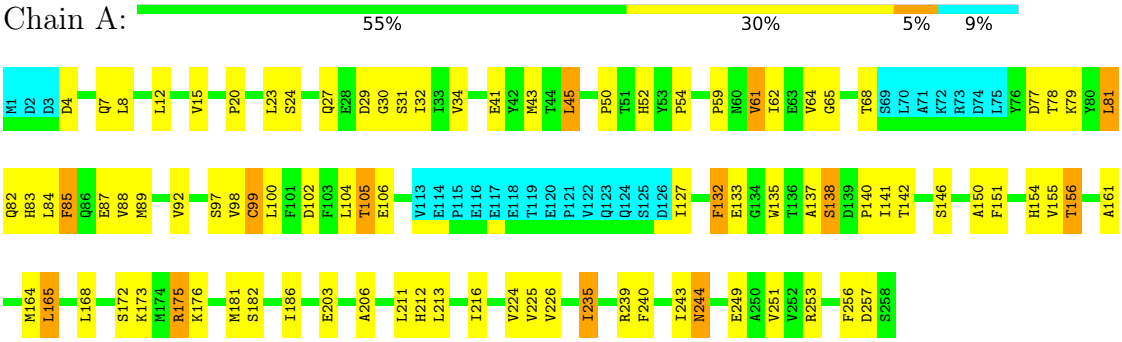
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Protein IMPACT homolog

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 12 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	structure calculation	
X-PLOR NIH	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2682
Number of shifts mapped to atoms	2682
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

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	1849	1780	1770	46±6
All	All	22188	21360	21240	551

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:MET:SD	1:A:81:LEU:HG	0.88	2.09	12	8
1:A:142:THR:HG23	1:A:235:ILE:HD12	0.76	1.57	12	11
1:A:52:HIS:O	1:A:57:GLU:HB3	0.74	1.83	11	2
1:A:141:ILE:HB	1:A:148:PHE:CE1	0.72	2.19	9	2
1:A:45:LEU:HG	1:A:85:PHE:CZ	0.69	2.22	8	3
1:A:187:LYS:HG3	1:A:220:TRP:CD1	0.68	2.24	7	3
1:A:82:GLN:HG2	1:A:85:PHE:CE2	0.66	2.26	2	1
1:A:45:LEU:HG	1:A:85:PHE:CE1	0.65	2.27	11	4
1:A:6:GLU:O	1:A:10:GLU:HB2	0.65	1.91	9	2
1:A:85:PHE:HD1	1:A:86:GLN:N	0.65	1.90	2	1
1:A:82:GLN:HA	1:A:85:PHE:CD2	0.64	2.27	2	1
1:A:92:VAL:O	1:A:95:ARG:HB2	0.64	1.91	4	2
1:A:100:LEU:HD23	1:A:100:LEU:H	0.63	1.53	9	2
1:A:4:ASP:HA	1:A:7:GLN:NE2	0.63	2.08	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ALA:HB2	1:A:151:PHE:HA	0.63	1.71	12	1
1:A:171:ASP:OD2	1:A:173:LYS:HG2	0.63	1.93	8	1
1:A:82:GLN:HA	1:A:85:PHE:CE2	0.62	2.30	2	1
1:A:239:ARG:O	1:A:243:ILE:HB	0.62	1.95	12	2
1:A:102:ASP:O	1:A:105:THR:HG22	0.61	1.94	3	4
1:A:212:HIS:O	1:A:216:ILE:HG13	0.61	1.95	12	2
1:A:171:ASP:OD1	1:A:173:LYS:HG2	0.60	1.97	10	3
1:A:172:SER:HA	1:A:175:ARG:HG2	0.60	1.74	8	1
1:A:8:LEU:O	1:A:11:GLU:HG2	0.60	1.97	1	9
1:A:173:LYS:HG3	1:A:174:MET:SD	0.59	2.37	4	2
1:A:213:LEU:O	1:A:217:MET:HB2	0.59	1.97	5	2
1:A:94:HIS:O	1:A:95:ARG:HD3	0.59	1.98	3	4
1:A:61:VAL:HG11	1:A:85:PHE:CD2	0.59	2.33	8	1
1:A:239:ARG:O	1:A:243:ILE:HG12	0.59	1.98	8	4
1:A:8:LEU:O	1:A:12:LEU:HG	0.59	1.98	5	12
1:A:206:ALA:O	1:A:210:MET:HG2	0.59	1.97	9	1
1:A:171:ASP:O	1:A:175:ARG:HB2	0.59	1.97	4	1
1:A:240:PHE:O	1:A:244:ASN:HB2	0.59	1.97	7	3
1:A:147:THR:HB	1:A:229:TRP:O	0.59	1.98	4	1
1:A:102:ASP:O	1:A:105:THR:HB	0.58	1.98	7	2
1:A:145:GLY:HA2	1:A:232:GLY:O	0.58	1.98	6	5
1:A:43:MET:HA	1:A:65:GLY:O	0.58	1.99	5	8
1:A:161:ALA:O	1:A:165:LEU:HB3	0.58	1.98	12	3
1:A:172:SER:O	1:A:176:LYS:HG2	0.58	1.99	2	2
1:A:173:LYS:O	1:A:176:LYS:HG3	0.58	1.99	12	2
1:A:188:GLN:HB2	1:A:193:ALA:O	0.58	1.99	2	1
1:A:85:PHE:CZ	1:A:107:LEU:HD21	0.58	2.34	8	1
1:A:181:MET:CG	1:A:226:VAL:HB	0.57	2.29	12	2
1:A:77:ASP:OD2	1:A:79:LYS:HG3	0.57	1.99	11	2
1:A:142:THR:HG21	1:A:234:HIS:O	0.57	1.99	10	5
1:A:84:LEU:O	1:A:87:GLU:HG2	0.57	2.00	10	3
1:A:89:MET:HA	1:A:92:VAL:HG13	0.57	1.75	12	1
1:A:176:LYS:HB2	1:A:229:TRP:CZ2	0.57	2.35	6	1
1:A:86:GLN:O	1:A:89:MET:HG2	0.57	2.00	8	1
1:A:150:ALA:HA	1:A:225:VAL:O	0.56	2.00	2	11
1:A:140:PRO:O	1:A:243:ILE:HG21	0.56	2.00	4	1
1:A:138:SER:C	1:A:140:PRO:HD3	0.56	2.21	1	9
1:A:209:ARG:O	1:A:213:LEU:HB2	0.56	2.00	9	5
1:A:251:VAL:O	1:A:256:PHE:HB2	0.56	2.00	6	6
1:A:15:VAL:HG11	1:A:23:LEU:HD13	0.56	1.77	12	1
1:A:219:VAL:HG21	1:A:256:PHE:HA	0.55	1.77	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:VAL:HG21	1:A:161:ALA:HB2	0.55	1.79	1	3
1:A:30:GLY:O	1:A:32:ILE:N	0.55	2.40	3	3
1:A:239:ARG:NE	1:A:239:ARG:HA	0.55	2.17	4	1
1:A:15:VAL:HB	1:A:100:LEU:CD1	0.55	2.31	7	3
1:A:50:PRO:C	1:A:52:HIS:H	0.55	2.04	7	2
1:A:85:PHE:CD1	1:A:86:GLN:N	0.55	2.74	2	1
1:A:138:SER:O	1:A:140:PRO:HD3	0.54	2.03	3	9
1:A:224:VAL:HB	1:A:256:PHE:CZ	0.54	2.37	2	9
1:A:162:PHE:O	1:A:166:ASP:HB2	0.54	2.02	1	8
1:A:52:HIS:HB3	1:A:57:GLU:CB	0.54	2.32	11	1
1:A:248:ARG:O	1:A:252:VAL:HG22	0.54	2.02	11	2
1:A:12:LEU:O	1:A:16:GLU:HB2	0.54	2.02	1	3
1:A:14:ALA:O	1:A:18:ILE:HG13	0.54	2.02	6	6
1:A:140:PRO:HD2	1:A:243:ILE:HG21	0.54	1.79	4	1
1:A:200:ASP:HB2	1:A:204:THR:HA	0.54	1.79	7	1
1:A:133:GLU:C	1:A:135:TRP:H	0.53	2.07	10	3
1:A:139:ASP:HA	1:A:247:ALA:CB	0.53	2.34	7	6
1:A:244:ASN:O	1:A:248:ARG:HG3	0.53	2.03	4	2
1:A:173:LYS:HG2	1:A:174:MET:SD	0.53	2.43	5	1
1:A:77:ASP:OD1	1:A:79:LYS:HG2	0.53	2.04	6	1
1:A:151:PHE:O	1:A:224:VAL:HA	0.53	2.04	5	4
1:A:12:LEU:O	1:A:15:VAL:HG12	0.53	2.04	5	5
1:A:61:VAL:HG22	1:A:82:GLN:OE1	0.53	2.04	11	3
1:A:183:ALA:HB1	1:A:214:ILE:HD13	0.52	1.81	4	2
1:A:42:TYR:O	1:A:66:VAL:HA	0.52	2.04	7	1
1:A:107:LEU:HA	1:A:110:VAL:HG12	0.52	1.79	4	2
1:A:133:GLU:O	1:A:133:GLU:HG3	0.52	2.04	4	1
1:A:138:SER:O	1:A:247:ALA:HA	0.52	2.05	2	2
1:A:15:VAL:HG13	1:A:23:LEU:HG	0.52	1.80	4	1
1:A:203:GLU:HB3	1:A:206:ALA:HB3	0.52	1.81	12	1
1:A:61:VAL:HG13	1:A:89:MET:SD	0.52	2.44	8	1
1:A:188:GLN:CB	1:A:191:SER:HB2	0.52	2.35	11	2
1:A:83:HIS:O	1:A:87:GLU:HG2	0.52	2.04	12	2
1:A:147:THR:O	1:A:228:ARG:HA	0.52	2.05	7	5
1:A:81:LEU:O	1:A:85:PHE:HB2	0.52	2.05	4	3
1:A:84:LEU:O	1:A:88:VAL:HG23	0.52	2.05	5	1
1:A:95:ARG:HG3	1:A:96:GLY:H	0.52	1.64	4	2
1:A:128:PRO:HD3	1:A:149:MET:SD	0.52	2.45	5	1
1:A:45:LEU:HD12	1:A:64:VAL:CG1	0.52	2.35	12	2
1:A:238:ASP:O	1:A:242:HIS:HB2	0.51	2.06	5	3
1:A:92:VAL:HG12	1:A:102:ASP:HB3	0.51	1.81	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:THR:OG1	1:A:235:ILE:HD11	0.51	2.06	4	1
1:A:52:HIS:HB3	1:A:57:GLU:HB3	0.51	1.80	11	1
1:A:199:ASP:OD2	1:A:207:GLY:HA3	0.51	2.04	6	1
1:A:142:THR:HG21	1:A:234:HIS:CD2	0.51	2.41	3	1
1:A:39:GLN:O	1:A:40:HIS:HB3	0.51	2.06	5	1
1:A:98:VAL:O	1:A:99:CYS:HB3	0.50	2.06	11	3
1:A:5:HIS:O	1:A:9:VAL:HG13	0.50	2.06	9	1
1:A:104:LEU:HD12	1:A:105:THR:N	0.50	2.21	9	5
1:A:92:VAL:HG21	1:A:99:CYS:HA	0.50	1.83	11	1
1:A:85:PHE:HA	1:A:88:VAL:HG22	0.50	1.83	12	1
1:A:27:GLN:HG2	1:A:32:ILE:HB	0.50	1.83	10	9
1:A:141:ILE:HG22	1:A:142:THR:N	0.50	2.22	11	4
1:A:141:ILE:HB	1:A:148:PHE:CD1	0.49	2.42	2	2
1:A:88:VAL:O	1:A:92:VAL:HG13	0.49	2.07	5	1
1:A:137:ALA:HB2	1:A:151:PHE:CG	0.49	2.42	12	1
1:A:249:GLU:O	1:A:253:ARG:HB2	0.49	2.07	6	4
1:A:177:ALA:HA	1:A:229:TRP:CD2	0.49	2.41	11	1
1:A:149:MET:O	1:A:226:VAL:HA	0.49	2.07	2	6
1:A:85:PHE:CE1	1:A:107:LEU:HD21	0.49	2.43	4	2
1:A:140:PRO:HD2	1:A:243:ILE:CG2	0.49	2.37	4	1
1:A:229:TRP:CE3	1:A:229:TRP:HA	0.49	2.42	5	1
1:A:100:LEU:H	1:A:100:LEU:HD23	0.49	1.68	12	3
1:A:92:VAL:HA	1:A:95:ARG:HD3	0.49	1.83	4	1
1:A:92:VAL:HG21	1:A:99:CYS:SG	0.49	2.48	12	3
1:A:61:VAL:HB	1:A:85:PHE:CE2	0.49	2.43	7	1
1:A:141:ILE:HB	1:A:148:PHE:HB2	0.49	1.85	11	2
1:A:173:LYS:H	1:A:173:LYS:HD2	0.48	1.68	5	1
1:A:169:LYS:HD2	1:A:182:SER:OG	0.48	2.08	11	1
1:A:6:GLU:O	1:A:10:GLU:HG2	0.48	2.07	11	1
1:A:79:LYS:HD3	1:A:80:TYR:N	0.48	2.23	1	2
1:A:79:LYS:HD2	1:A:79:LYS:C	0.48	2.29	4	1
1:A:251:VAL:HG22	1:A:256:PHE:CB	0.48	2.39	5	2
1:A:47:ILE:HG12	1:A:61:VAL:HG12	0.48	1.83	8	1
1:A:142:THR:H	1:A:240:PHE:HB3	0.48	1.68	4	1
1:A:137:ALA:CB	1:A:151:PHE:HA	0.48	2.37	12	1
1:A:140:PRO:O	1:A:141:ILE:HG12	0.48	2.08	12	3
1:A:92:VAL:HG11	1:A:103:PHE:CB	0.48	2.39	3	1
1:A:239:ARG:HA	1:A:239:ARG:CZ	0.48	2.39	4	1
1:A:140:PRO:HG2	1:A:243:ILE:CD1	0.48	2.37	9	3
1:A:138:SER:HB2	1:A:250:ALA:CB	0.48	2.39	4	5
1:A:127:ILE:HD13	1:A:239:ARG:HE	0.48	1.69	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:SER:HB3	1:A:102:ASP:OD2	0.48	2.08	12	1
1:A:9:VAL:O	1:A:13:GLU:HG3	0.48	2.08	4	1
1:A:229:TRP:HA	1:A:229:TRP:CE3	0.48	2.43	4	1
1:A:77:ASP:OD1	1:A:79:LYS:HE3	0.48	2.07	12	1
1:A:95:ARG:NE	1:A:95:ARG:HA	0.48	2.22	2	1
1:A:92:VAL:HA	1:A:95:ARG:HG2	0.48	1.86	3	1
1:A:219:VAL:HG21	1:A:256:PHE:CD2	0.48	2.43	5	2
1:A:188:GLN:HG2	1:A:193:ALA:O	0.47	2.09	10	2
1:A:222:VAL:HG11	1:A:255:GLY:O	0.47	2.09	3	1
1:A:158:GLU:O	1:A:162:PHE:HB2	0.47	2.09	6	1
1:A:54:PRO:HB3	1:A:98:VAL:O	0.47	2.09	6	2
1:A:51:THR:HA	1:A:53:TYR:CE1	0.47	2.43	7	1
1:A:15:VAL:CG1	1:A:23:LEU:HG	0.47	2.39	7	1
1:A:111:LEU:O	1:A:111:LEU:HD23	0.47	2.09	1	1
1:A:59:PRO:HG2	1:A:89:MET:SD	0.47	2.50	11	1
1:A:171:ASP:O	1:A:175:ARG:HG3	0.47	2.08	2	1
1:A:65:GLY:HA2	1:A:78:THR:HG22	0.47	1.86	12	1
1:A:135:TRP:CE3	1:A:153:ALA:HB2	0.47	2.44	1	2
1:A:58:ALA:HB1	1:A:59:PRO:HD2	0.47	1.87	1	1
1:A:61:VAL:HG12	1:A:89:MET:SD	0.47	2.49	12	1
1:A:100:LEU:HD23	1:A:100:LEU:N	0.47	2.23	7	3
1:A:251:VAL:HG22	1:A:256:PHE:HB2	0.47	1.86	5	3
1:A:166:ASP:O	1:A:169:LYS:HG3	0.47	2.08	4	1
1:A:140:PRO:HG2	1:A:243:ILE:HD13	0.47	1.84	11	1
1:A:181:MET:SD	1:A:206:ALA:HB1	0.47	2.50	12	1
1:A:15:VAL:HG11	1:A:23:LEU:HG	0.47	1.87	2	1
1:A:139:ASP:OD1	1:A:251:VAL:HB	0.47	2.10	3	1
1:A:78:THR:O	1:A:82:GLN:HB2	0.47	2.10	6	1
1:A:188:GLN:HA	1:A:188:GLN:OE1	0.46	2.10	5	2
1:A:145:GLY:O	1:A:230:PHE:HA	0.46	2.10	5	1
1:A:8:LEU:HD11	1:A:49:PHE:CD1	0.46	2.44	7	1
1:A:15:VAL:HG21	1:A:23:LEU:HD13	0.46	1.86	9	1
1:A:164:MET:O	1:A:167:LEU:HG	0.46	2.10	5	1
1:A:50:PRO:C	1:A:52:HIS:N	0.46	2.69	7	1
1:A:80:TYR:O	1:A:84:LEU:HD23	0.46	2.10	3	2
1:A:187:LYS:HA	1:A:194:THR:HG22	0.46	1.88	5	3
1:A:132:PHE:CB	1:A:135:TRP:HB2	0.46	2.41	4	1
1:A:100:LEU:N	1:A:100:LEU:HD23	0.46	2.26	10	3
1:A:85:PHE:CZ	1:A:103:PHE:CE1	0.46	3.03	3	1
1:A:39:GLN:HB3	1:A:41:GLU:OE1	0.46	2.11	1	1
1:A:37:VAL:HG23	1:A:43:MET:O	0.46	2.10	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:236:GLY:O	1:A:239:ARG:HB2	0.46	2.11	1	1
1:A:172:SER:HA	1:A:175:ARG:HB2	0.46	1.86	12	3
1:A:50:PRO:HG3	1:A:60:ASN:OD1	0.46	2.10	4	1
1:A:177:ALA:HA	1:A:229:TRP:NE1	0.46	2.26	5	1
1:A:48:SER:O	1:A:60:ASN:HB2	0.46	2.11	5	1
1:A:140:PRO:HD2	1:A:243:ILE:HD13	0.46	1.86	10	1
1:A:187:LYS:HB3	1:A:220:TRP:CD1	0.46	2.45	3	1
1:A:137:ALA:HB2	1:A:151:PHE:CA	0.46	2.41	12	1
1:A:19:TYR:HB2	1:A:22:LEU:HB3	0.45	1.88	2	2
1:A:140:PRO:HA	1:A:148:PHE:O	0.45	2.11	11	2
1:A:39:GLN:O	1:A:40:HIS:HB2	0.45	2.11	1	1
1:A:172:SER:HA	1:A:175:ARG:CG	0.45	2.41	8	1
1:A:142:THR:HB	1:A:240:PHE:CD2	0.45	2.46	11	1
1:A:241:LYS:C	1:A:241:LYS:HD3	0.45	2.32	3	1
1:A:99:CYS:SG	1:A:100:LEU:N	0.45	2.90	2	2
1:A:45:LEU:HD12	1:A:64:VAL:HG12	0.45	1.88	2	1
1:A:188:GLN:HB3	1:A:191:SER:HB2	0.45	1.88	11	4
1:A:187:LYS:CB	1:A:220:TRP:HB3	0.45	2.42	8	1
1:A:219:VAL:CG2	1:A:256:PHE:HA	0.44	2.42	1	1
1:A:148:PHE:O	1:A:148:PHE:HD1	0.44	1.94	2	2
1:A:61:VAL:CG1	1:A:85:PHE:CD1	0.44	3.00	2	1
1:A:90:ASP:HA	1:A:93:PHE:HB2	0.44	1.88	9	1
1:A:64:VAL:O	1:A:78:THR:HB	0.44	2.12	8	1
1:A:132:PHE:HB3	1:A:135:TRP:HB2	0.44	1.89	12	2
1:A:100:LEU:CD2	1:A:100:LEU:H	0.44	2.24	9	1
1:A:127:ILE:HG23	1:A:140:PRO:CB	0.44	2.42	12	1
1:A:140:PRO:HB2	1:A:239:ARG:NH2	0.44	2.28	10	1
1:A:101:PHE:O	1:A:104:LEU:HG	0.44	2.13	3	3
1:A:142:THR:HB	1:A:240:PHE:HB3	0.44	1.89	5	1
1:A:139:ASP:O	1:A:149:MET:HA	0.44	2.13	10	1
1:A:171:ASP:O	1:A:175:ARG:HG2	0.43	2.13	8	1
1:A:186:ILE:O	1:A:194:THR:HA	0.43	2.13	11	1
1:A:92:VAL:O	1:A:92:VAL:HG23	0.43	2.13	12	1
1:A:77:ASP:OD2	1:A:79:LYS:HE3	0.43	2.13	3	1
1:A:27:GLN:HA	1:A:27:GLN:NE2	0.43	2.28	12	1
1:A:187:LYS:CG	1:A:220:TRP:CD1	0.43	3.01	1	1
1:A:127:ILE:HD11	1:A:235:ILE:HD13	0.43	1.89	4	1
1:A:77:ASP:OD1	1:A:79:LYS:HG3	0.43	2.13	4	1
1:A:210:MET:HA	1:A:213:LEU:HB3	0.43	1.90	5	1
1:A:11:GLU:OE1	1:A:100:LEU:HD22	0.43	2.13	3	1
1:A:138:SER:HB2	1:A:250:ALA:HB2	0.43	1.89	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:THR:O	1:A:186:ILE:HD12	0.43	2.14	5	2
1:A:6:GLU:O	1:A:9:VAL:HG12	0.43	2.14	5	1
1:A:141:ILE:N	1:A:148:PHE:O	0.42	2.52	5	2
1:A:248:ARG:HH11	1:A:252:VAL:CG2	0.42	2.27	3	1
1:A:53:TYR:HB2	1:A:55:SER:OG	0.42	2.14	6	1
1:A:81:LEU:HA	1:A:84:LEU:HD21	0.42	1.90	3	2
1:A:18:ILE:HB	1:A:19:TYR:CD2	0.42	2.50	8	2
1:A:237:PRO:HA	1:A:240:PHE:CE2	0.42	2.49	11	1
1:A:89:MET:O	1:A:92:VAL:HG22	0.42	2.14	11	1
1:A:23:LEU:HD13	1:A:24:SER:N	0.42	2.30	4	1
1:A:92:VAL:HB	1:A:102:ASP:OD1	0.42	2.14	7	1
1:A:84:LEU:HA	1:A:87:GLU:HG2	0.42	1.92	3	1
1:A:50:PRO:HD2	1:A:59:PRO:HA	0.42	1.91	12	1
1:A:181:MET:HA	1:A:200:ASP:O	0.42	2.15	5	1
1:A:98:VAL:O	1:A:99:CYS:HB2	0.42	2.14	3	1
1:A:54:PRO:HA	1:A:58:ALA:HA	0.42	1.91	3	1
1:A:24:SER:O	1:A:34:VAL:HB	0.42	2.14	12	1
1:A:188:GLN:OE1	1:A:188:GLN:HA	0.41	2.15	9	1
1:A:102:ASP:O	1:A:106:GLU:HG2	0.41	2.15	12	1
1:A:155:VAL:HG12	1:A:164:MET:SD	0.41	2.56	12	1
1:A:61:VAL:HG13	1:A:85:PHE:CD1	0.41	2.50	2	1
1:A:185:ARG:HG2	1:A:220:TRP:HA	0.41	1.92	5	1
1:A:135:TRP:CE2	1:A:168:LEU:HD13	0.41	2.50	12	1
1:A:200:ASP:CB	1:A:204:THR:HA	0.41	2.46	5	1
1:A:210:MET:O	1:A:213:LEU:HB3	0.41	2.16	5	1
1:A:182:SER:HB3	1:A:225:VAL:HG22	0.41	1.92	12	1
1:A:146:SER:HA	1:A:230:PHE:HA	0.41	1.93	8	1
1:A:158:GLU:HA	1:A:186:ILE:CD1	0.41	2.45	9	1
1:A:139:ASP:OD2	1:A:247:ALA:HB1	0.41	2.16	6	3
1:A:85:PHE:CZ	1:A:103:PHE:HE1	0.41	2.34	1	1
1:A:151:PHE:CD2	1:A:168:LEU:HD11	0.41	2.51	5	1
1:A:107:LEU:O	1:A:111:LEU:HB2	0.41	2.15	6	2
1:A:15:VAL:HG23	1:A:19:TYR:CE1	0.41	2.50	1	1
1:A:251:VAL:HG13	1:A:252:VAL:N	0.41	2.31	3	3
1:A:140:PRO:HG2	1:A:243:ILE:HD11	0.41	1.91	2	1
1:A:187:LYS:HD2	1:A:194:THR:CG2	0.41	2.46	9	1
1:A:187:LYS:HB3	1:A:221:ASN:OD1	0.41	2.16	9	1
1:A:5:HIS:O	1:A:9:VAL:HG22	0.41	2.16	9	1
1:A:31:SER:O	1:A:32:ILE:HG12	0.41	2.16	12	1
1:A:45:LEU:HD12	1:A:64:VAL:HB	0.41	1.93	12	1
1:A:6:GLU:O	1:A:10:GLU:HG3	0.40	2.16	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:TRP:CB	1:A:223:ILE:HG22	0.40	2.46	11	1
1:A:95:ARG:CG	1:A:96:GLY:H	0.40	2.26	4	1
1:A:92:VAL:CB	1:A:99:CYS:HA	0.40	2.46	9	1
1:A:177:ALA:HA	1:A:229:TRP:CG	0.40	2.50	11	1
1:A:105:THR:O	1:A:108:ASP:HB3	0.40	2.16	6	1
1:A:200:ASP:HB2	1:A:204:THR:OG1	0.40	2.16	8	1
1:A:92:VAL:HB	1:A:99:CYS:HA	0.40	1.93	9	1
1:A:53:TYR:HB2	1:A:54:PRO:HD2	0.40	1.94	1	1
1:A:53:TYR:HB3	1:A:54:PRO:HD2	0.40	1.92	3	1
1:A:188:GLN:CG	1:A:193:ALA:HB3	0.40	2.46	4	1
1:A:79:LYS:HA	1:A:82:GLN:HB2	0.40	1.94	9	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	233/258 (90%)	195±5 (84±2%)	30±4 (13±2%)	9±2 (4±1%)	5	33
All	All	2796/3096 (90%)	2337 (84%)	354 (13%)	105 (4%)	5	33

All 30 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	99	CYS	12
1	A	138	SER	12
1	A	20	PRO	8
1	A	54	PRO	7
1	A	53	TYR	7
1	A	201	ASP	6
1	A	41	GLU	6
1	A	31	SER	4
1	A	42	TYR	4
1	A	235	ILE	4
1	A	40	HIS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	68	THR	3
1	A	30	GLY	3
1	A	257	ASP	3
1	A	158	GLU	3
1	A	254	ALA	2
1	A	200	ASP	2
1	A	156	THR	2
1	A	92	VAL	2
1	A	230	PHE	2
1	A	134	GLY	1
1	A	112	TYR	1
1	A	62	ILE	1
1	A	61	VAL	1
1	A	256	PHE	1
1	A	177	ALA	1
1	A	211	LEU	1
1	A	58	ALA	1
1	A	51	THR	1
1	A	202	GLY	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	201/224 (90%)	182±3 (90±1%)	19±3 (10±1%)	12 58
All	All	2412/2688 (90%)	2182 (90%)	230 (10%)	12 58

All 73 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	154	HIS	12
1	A	84	LEU	12
1	A	98	VAL	11
1	A	79	LYS	9
1	A	45	LEU	9
1	A	81	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	211	LEU	9
1	A	174	MET	8
1	A	229	TRP	8
1	A	168	LEU	7
1	A	19	TYR	7
1	A	213	LEU	6
1	A	103	PHE	6
1	A	217	MET	5
1	A	60	ASN	5
1	A	85	PHE	5
1	A	239	ARG	5
1	A	53	TYR	5
1	A	93	PHE	4
1	A	105	THR	4
1	A	234	HIS	4
1	A	244	ASN	4
1	A	95	ARG	3
1	A	173	LYS	3
1	A	82	GLN	3
1	A	175	ARG	3
1	A	149	MET	2
1	A	39	GLN	2
1	A	181	MET	2
1	A	242	HIS	2
1	A	40	HIS	2
1	A	203	GLU	2
1	A	28	GLU	2
1	A	4	ASP	2
1	A	165	LEU	2
1	A	140	PRO	2
1	A	158	GLU	2
1	A	148	PHE	2
1	A	27	GLN	2
1	A	139	ASP	2
1	A	169	LYS	2
1	A	162	PHE	2
1	A	23	LEU	2
1	A	22	LEU	1
1	A	187	LYS	1
1	A	133	GLU	1
1	A	243	ILE	1
1	A	196	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	107	LEU	1
1	A	63	GLU	1
1	A	86	GLN	1
1	A	146	SER	1
1	A	5	HIS	1
1	A	48	SER	1
1	A	68	THR	1
1	A	46	GLN	1
1	A	56	GLU	1
1	A	178	ASN	1
1	A	253	ARG	1
1	A	144	ARG	1
1	A	156	THR	1
1	A	132	PHE	1
1	A	90	ASP	1
1	A	235	ILE	1
1	A	16	GLU	1
1	A	248	ARG	1
1	A	209	ARG	1
1	A	182	SER	1
1	A	29	ASP	1
1	A	110	VAL	1
1	A	228	ARG	1
1	A	230	PHE	1
1	A	176	LYS	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *yih.str.txt*

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	2682
Number of shifts mapped to atoms	2682
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	249	2.60 ± 0.17	Should be applied
$^{13}C_{\beta}$	237	2.92 ± 0.08	Should be applied
$^{13}C'$	164	2.91 ± 0.22	Should be applied
^{15}N	238	0.17 ± 0.26	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 2168 atoms were assigned a chemical shift out of a possible 2825. 33 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1042/1152 (90%)	443/459 (97%)	381/468 (81%)	218/225 (97%)
Sidechain	1030/1381 (75%)	609/803 (76%)	417/529 (79%)	4/49 (8%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	96/292 (33%)	57/152 (38%)	37/116 (32%)	2/24 (8%)
Overall	2168/2825 (77%)	1109/1414 (78%)	835/1113 (75%)	224/298 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 2357 atoms were assigned a chemical shift out of a possible 3111. 34 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1134/1268 (89%)	483/505 (96%)	413/516 (80%)	238/247 (96%)
Sidechain	1127/1551 (73%)	668/902 (74%)	455/594 (77%)	4/55 (7%)
Aromatic	96/292 (33%)	57/152 (38%)	37/116 (32%)	2/24 (8%)
Overall	2357/3111 (76%)	1208/1559 (77%)	905/1226 (74%)	244/326 (75%)

7.1.4 Statistically unusual chemical shifts (i)

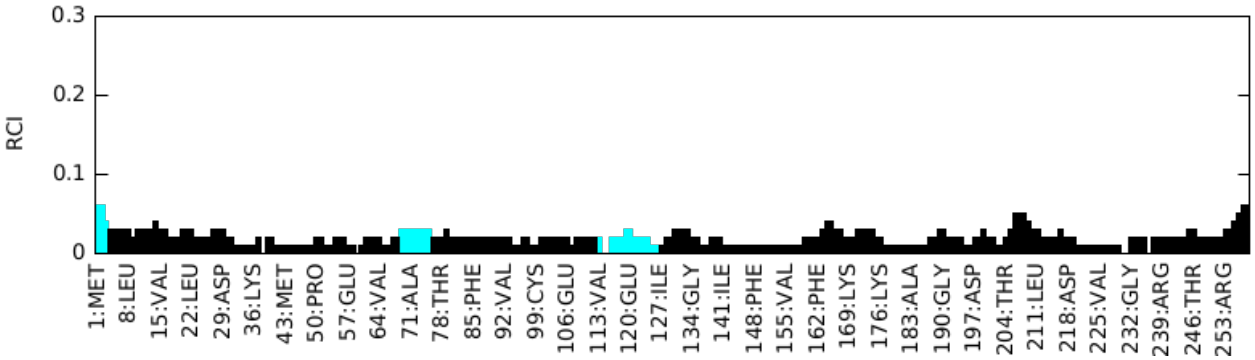
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	234	HIS	CE1	115.05	149.70 – 125.30	-9.2
1	A	168	LEU	HD11	-1.26	2.16 – -0.64	-7.2
1	A	168	LEU	HD13	-1.26	2.16 – -0.64	-7.2
1	A	168	LEU	HD12	-1.26	2.16 – -0.64	-7.2
1	A	168	LEU	HD21	-0.91	2.14 – -0.66	-5.9
1	A	168	LEU	HD22	-0.91	2.14 – -0.66	-5.9
1	A	168	LEU	HD23	-0.91	2.14 – -0.66	-5.9
1	A	54	PRO	CG	20.90	32.66 – 21.76	-5.8
1	A	253	ARG	CD	38.49	47.57 – 38.77	-5.3
1	A	145	GLY	N	129.71	129.07 – 90.27	5.2
1	A	109	GLY	N	129.54	129.07 – 90.27	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:


RCI
0.3
0.2
0.1
0
1:MET
8:LEU
15:VAL
22:LEU
29:ASP
36:LYS
43:MET
50:PRO
57:GLU
64:VAL
71:ALA
78:THR
85:PHE
92:VAL
99:CYS
106:GLU
113:VAL
120:GLU
127:ILE
134:GLY
141:ILE
148:PHE
155:VAL
162:PHE
169:LYS
176:LYS
183:ALA
190:GLY
197:ASP
204:THR
211:LEU
218:ASP
225:VAL
232:GLY
239:ARG
246:THR
253:ARG