



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 03:54 AM BST

PDB ID : 2N3J
Title : Solution Structure of the alpha-crystallin domain from the redox-sensitive chaperone, HSPB1
Authors : Rajagopal, P.; Liu, Y.; Shi, L.; Klevit, R.E.
Deposited on : 2015-06-03

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

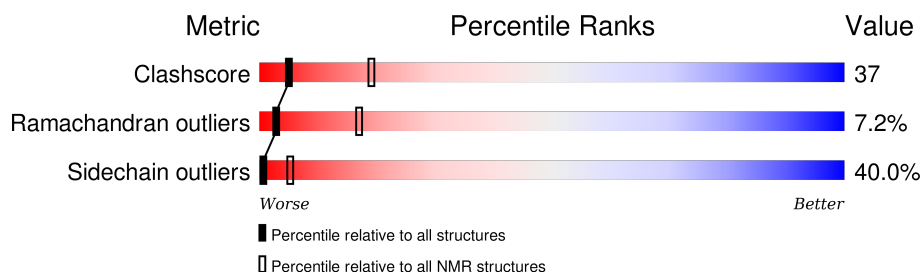
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 22%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	98	
1	B	98	

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:94-A:127, A:132-A:170, B:94-B:169 (149)	0.45	7

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3026 atoms, of which 1498 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock protein beta-1.

Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1513	472	749	135	154	3	
1	B	98	Total	C	H	N	O	S	0
			1513	472	749	135	154	3	

There are 2 discrepancies between the modelled and reference sequences:

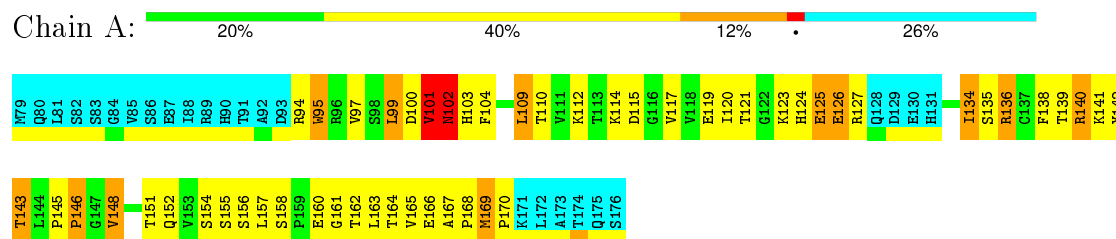
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	MET	-	INITIATING METHIONINE	UNP P04792
B	79	MET	-	INITIATING METHIONINE	UNP P04792

4 Residue-property plots

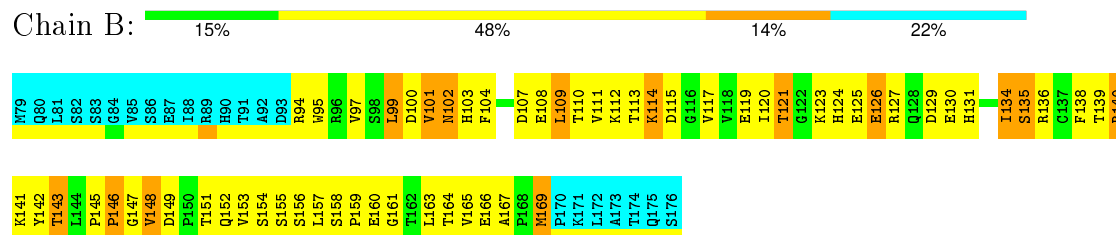
4.1 Average score per residue in the NMR ensemble

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: Heat shock protein beta-1



- Molecule 1: Heat shock protein beta-1

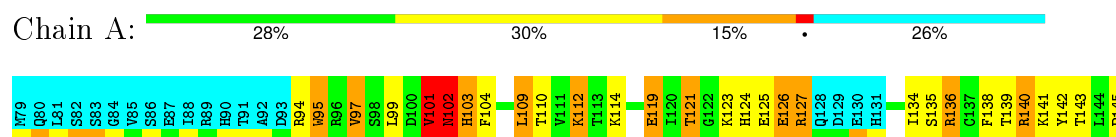


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

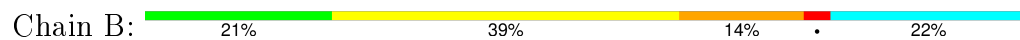
4.2.1 Score per residue for model 1

- Molecule 1: Heat shock protein beta-1



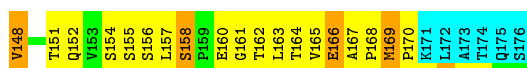
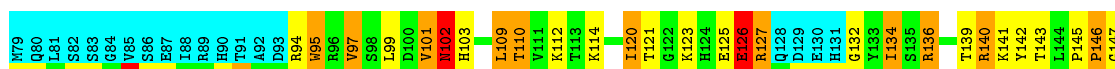
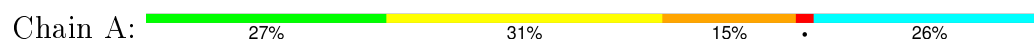


- Molecule 1: Heat shock protein beta-1

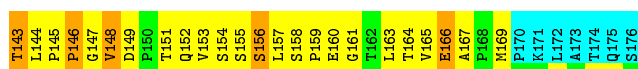
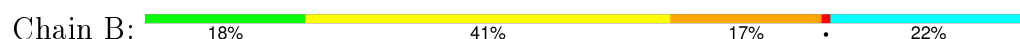


4.2.2 Score per residue for model 2

- Molecule 1: Heat shock protein beta-1

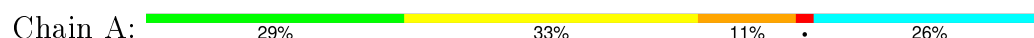


- Molecule 1: Heat shock protein beta-1

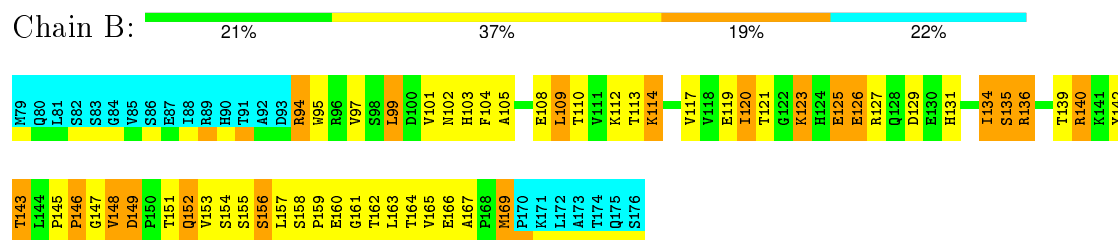


4.2.3 Score per residue for model 3

- Molecule 1: Heat shock protein beta-1

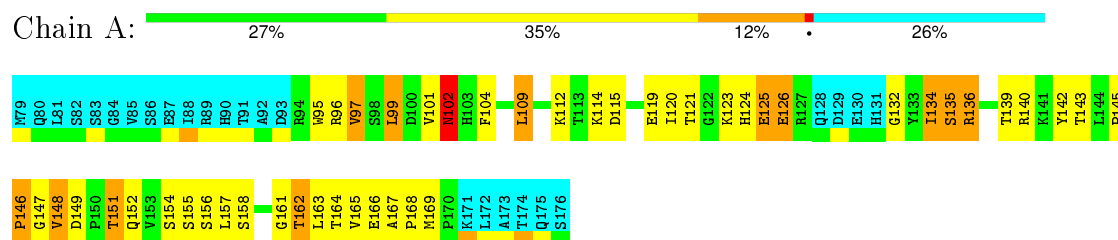


- Molecule 1: Heat shock protein beta-1

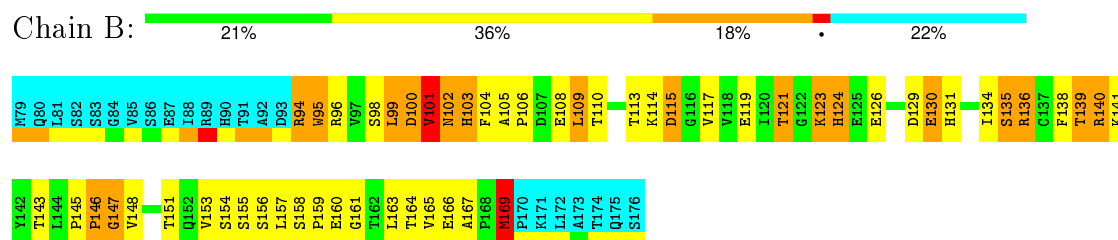


4.2.4 Score per residue for model 4

- Molecule 1: Heat shock protein beta-1

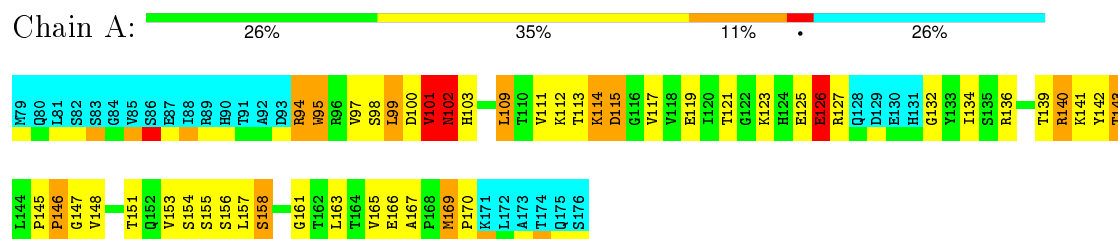


- Molecule 1: Heat shock protein beta-1

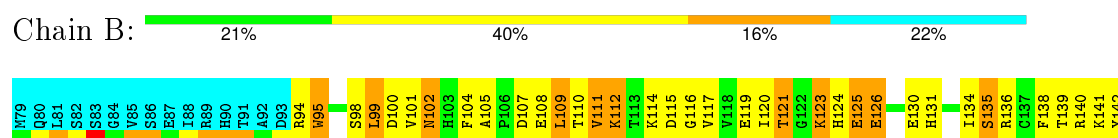


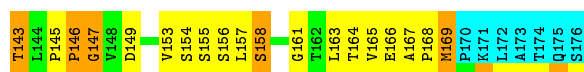
4.2.5 Score per residue for model 5

- Molecule 1: Heat shock protein beta-1



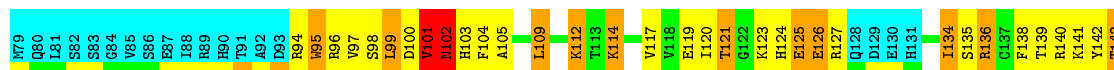
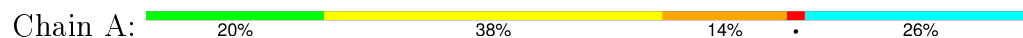
- Molecule 1: Heat shock protein beta-1



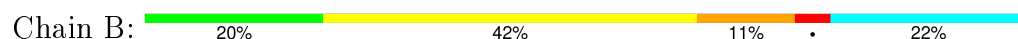


4.2.6 Score per residue for model 6

- Molecule 1: Heat shock protein beta-1

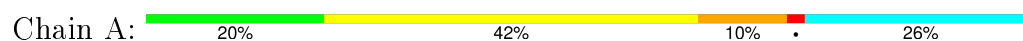


- Molecule 1: Heat shock protein beta-1

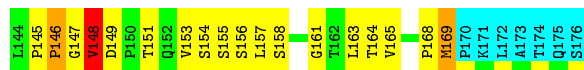
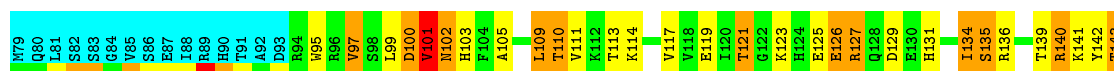


4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Heat shock protein beta-1

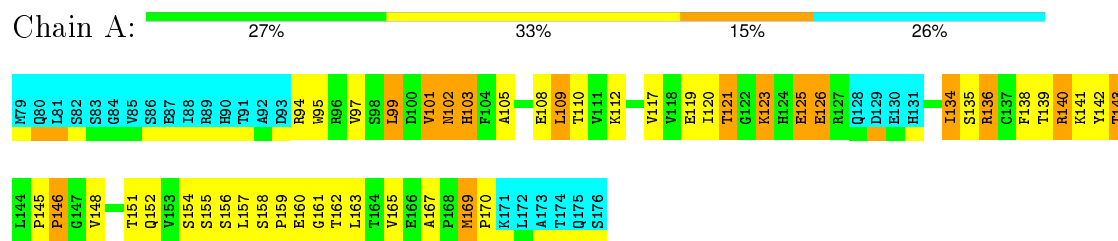


- Molecule 1: Heat shock protein beta-1

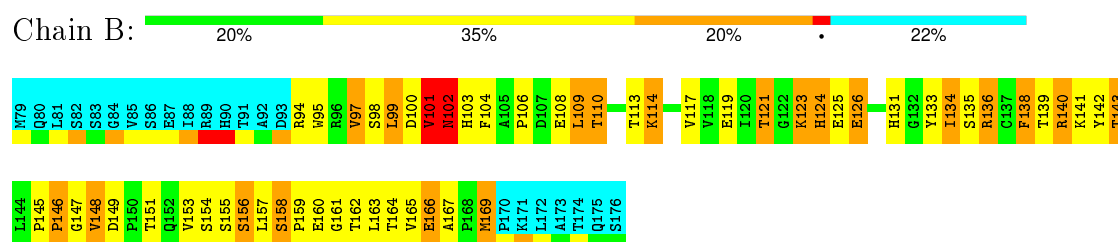


4.2.8 Score per residue for model 8

- Molecule 1: Heat shock protein beta-1

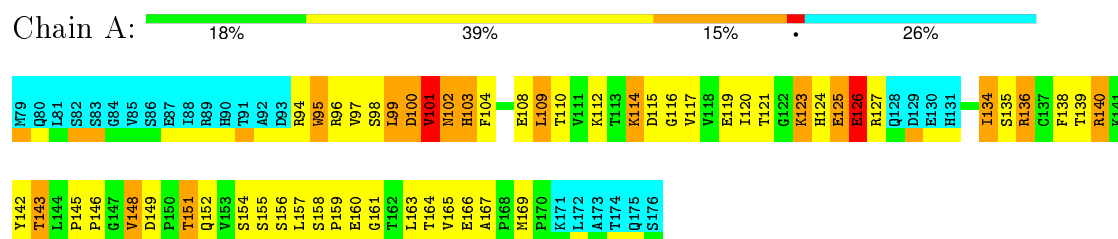


- Molecule 1: Heat shock protein beta-1

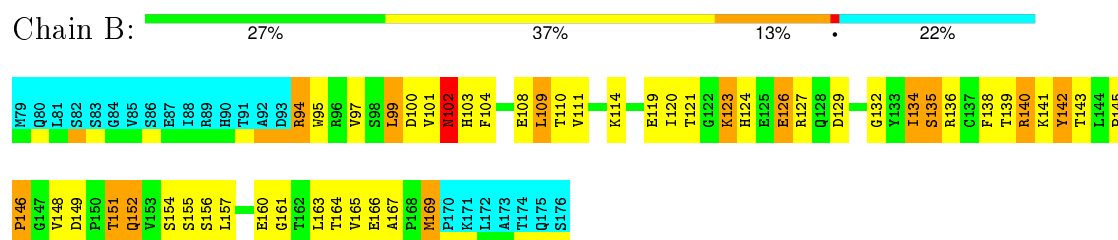


4.2.9 Score per residue for model 9

- Molecule 1: Heat shock protein beta-1

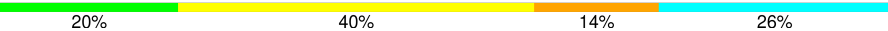


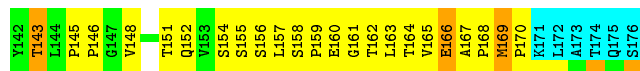
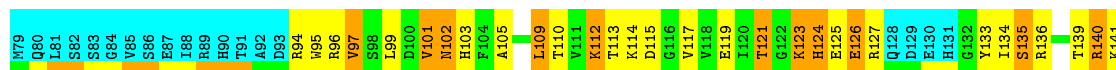
- Molecule 1: Heat shock protein beta-1




4.2.10 Score per residue for model 10

- Molecule 1: Heat shock protein beta-1

Chain A: 



● Molecule 1: Heat shock protein beta-1

Chain B: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 1000 calculated structures, 10 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
CS-Rosetta	structure solution	
X-PLOR NIH	structure solution	
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)	2n3j_cs.str
Number of chemical shift lists	1
Total number of shifts	490
Number of shifts mapped to atoms	490
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	22%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	571	565	565	43±7
1	B	600	583	583	47±6
All	All	11710	11480	11480	869

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:117:VAL:HG22	1:B:143:THR:HG23	0.85	1.47	4	6
1:A:102:ASN:HB3	1:A:109:LEU:HD13	0.79	1.53	1	4
1:B:99:LEU:HD22	1:B:120:ILE:HG12	0.79	1.52	6	3
1:B:102:ASN:HB3	1:B:109:LEU:HD13	0.76	1.57	1	4
1:B:109:LEU:HD22	1:B:157:LEU:HD22	0.74	1.59	8	9
1:A:99:LEU:HD23	1:A:140:ARG:NE	0.74	1.97	7	2
1:B:102:ASN:CB	1:B:109:LEU:HD13	0.73	2.14	5	8
1:A:102:ASN:HB2	1:A:109:LEU:HD13	0.71	1.61	9	2
1:A:109:LEU:HD22	1:A:157:LEU:HD22	0.70	1.61	2	10
1:B:102:ASN:HB2	1:B:109:LEU:HD13	0.69	1.63	2	3
1:A:99:LEU:HD22	1:A:120:ILE:HG13	0.69	1.62	2	1
1:A:127:ARG:HB3	1:A:127:ARG:CZ	0.69	2.16	2	2
1:B:99:LEU:HD22	1:B:120:ILE:HG13	0.68	1.65	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:VAL:HG22	1:A:143:THR:HG23	0.68	1.66	8	4
1:A:140:ARG:NH2	1:A:142:TYR:CD1	0.68	2.62	8	1
1:A:152:GLN:O	1:A:167:ALA:HB1	0.67	1.89	2	8
1:B:95:TRP:NE1	1:B:97:VAL:HG22	0.67	2.04	1	2
1:A:140:ARG:NH2	1:A:142:TYR:CE1	0.67	2.62	8	1
1:B:102:ASN:ND2	1:B:102:ASN:H	0.66	1.88	9	2
1:A:101:VAL:HG11	1:A:138:PHE:CD2	0.65	2.27	7	3
1:A:148:VAL:HA	1:A:169:MET:SD	0.65	2.31	3	2
1:B:102:ASN:OD1	1:B:157:LEU:HD11	0.65	1.91	5	3
1:A:95:TRP:CZ3	1:A:97:VAL:HG21	0.64	2.27	9	4
1:A:119:GLU:CD	1:A:141:LYS:NZ	0.64	2.51	1	2
1:B:109:LEU:CD2	1:B:157:LEU:HD22	0.63	2.23	8	4
1:A:127:ARG:CB	1:A:127:ARG:CZ	0.63	2.76	2	1
1:B:102:ASN:OD1	1:B:109:LEU:HD13	0.63	1.92	6	3
1:A:102:ASN:CB	1:A:109:LEU:HD13	0.63	2.24	1	7
1:A:109:LEU:CD2	1:A:157:LEU:HD22	0.62	2.25	7	5
1:A:102:ASN:ND2	1:A:102:ASN:H	0.62	1.92	1	2
1:A:167:ALA:HB3	1:A:169:MET:HE3	0.61	1.70	3	1
1:B:95:TRP:HB2	1:B:169:MET:SD	0.61	2.35	4	3
1:B:124:HIS:H	1:B:124:HIS:CD2	0.61	2.13	8	1
1:B:114:LYS:O	1:B:116:GLY:N	0.61	2.33	5	3
1:B:102:ASN:OD1	1:B:161:GLY:HA2	0.61	1.95	5	3
1:A:99:LEU:HD22	1:A:120:ILE:HG12	0.60	1.73	7	4
1:B:169:MET:SD	1:B:169:MET:N	0.60	2.74	7	1
1:A:166:GLU:O	1:A:167:ALA:HB2	0.60	1.95	1	7
1:A:102:ASN:OD1	1:A:109:LEU:HD13	0.60	1.96	7	6
1:A:119:GLU:CD	1:A:141:LYS:HZ2	0.60	2.00	7	1
1:A:142:TYR:CE1	1:B:132:GLY:HA3	0.60	2.32	9	2
1:A:99:LEU:HD22	1:A:120:ILE:CG1	0.60	2.27	4	3
1:B:102:ASN:ND2	1:B:102:ASN:N	0.59	2.48	9	2
1:B:140:ARG:NH1	1:B:142:TYR:OH	0.59	2.30	8	1
1:B:114:LYS:O	1:B:117:VAL:N	0.59	2.34	5	3
1:B:102:ASN:ND2	1:B:161:GLY:O	0.59	2.35	9	4
1:A:95:TRP:NE1	1:A:97:VAL:CG2	0.59	2.65	7	2
1:B:99:LEU:HD22	1:B:120:ILE:CG1	0.59	2.28	2	4
1:B:152:GLN:O	1:B:167:ALA:HB1	0.59	1.96	9	3
1:A:134:ILE:O	1:A:136:ARG:NH2	0.59	2.35	4	1
1:A:95:TRP:NE1	1:A:97:VAL:HG22	0.59	2.13	10	2
1:B:130:GLU:CD	1:B:130:GLU:N	0.59	2.56	10	1
1:B:99:LEU:HD23	1:B:140:ARG:NE	0.58	2.12	4	1
1:A:158:SER:O	1:A:161:GLY:N	0.58	2.36	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:163:LEU:C	1:B:163:LEU:HD13	0.58	2.18	2	4
1:B:99:LEU:HD23	1:B:140:ARG:HH11	0.58	1.59	8	1
1:B:99:LEU:HD21	1:B:142:TYR:CE1	0.58	2.33	9	1
1:B:145:PRO:O	1:B:147:GLY:N	0.58	2.37	10	9
1:B:163:LEU:HD13	1:B:163:LEU:C	0.58	2.18	1	6
1:A:134:ILE:HD12	1:B:140:ARG:NH1	0.58	2.14	2	1
1:A:140:ARG:NH2	1:A:142:TYR:OH	0.58	2.34	7	4
1:A:132:GLY:HA3	1:B:142:TYR:CE1	0.58	2.33	2	1
1:A:114:LYS:O	1:A:116:GLY:N	0.58	2.36	9	1
1:A:102:ASN:ND2	1:A:102:ASN:N	0.58	2.50	1	2
1:B:102:ASN:ND2	1:B:105:ALA:O	0.58	2.34	3	2
1:A:145:PRO:CD	1:A:146:PRO:HD3	0.57	2.29	1	10
1:A:102:ASN:O	1:A:102:ASN:ND2	0.57	2.34	9	4
1:A:99:LEU:HD23	1:A:140:ARG:HE	0.57	1.60	7	1
1:B:102:ASN:OD1	1:B:109:LEU:CD1	0.57	2.52	6	2
1:A:95:TRP:CH2	1:A:148:VAL:HG21	0.57	2.35	2	3
1:A:112:LYS:NZ	1:A:119:GLU:HB2	0.57	2.14	9	1
1:A:140:ARG:NE	1:A:142:TYR:OH	0.57	2.35	4	1
1:A:165:VAL:O	1:A:165:VAL:HG23	0.57	1.99	7	6
1:A:127:ARG:NH1	1:A:127:ARG:CB	0.57	2.68	2	2
1:A:145:PRO:HD2	1:A:146:PRO:CD	0.57	2.30	6	1
1:A:95:TRP:CB	1:A:169:MET:SD	0.57	2.93	5	1
1:A:102:ASN:ND2	1:A:161:GLY:O	0.56	2.37	1	5
1:B:145:PRO:HD2	1:B:146:PRO:CD	0.56	2.30	5	7
1:B:102:ASN:O	1:B:102:ASN:ND2	0.56	2.37	2	3
1:B:108:GLU:OE1	1:B:123:LYS:NZ	0.56	2.37	3	4
1:A:102:ASN:OD1	1:A:161:GLY:HA2	0.56	2.00	8	2
1:B:145:PRO:N	1:B:146:PRO:CD	0.56	2.68	1	9
1:A:140:ARG:NH1	1:A:142:TYR:OH	0.56	2.34	2	2
1:A:158:SER:HB2	1:A:162:THR:HG22	0.56	1.77	4	1
1:A:125:GLU:O	1:A:126:GLU:C	0.56	2.44	10	8
1:B:95:TRP:NE1	1:B:97:VAL:CG2	0.56	2.68	8	2
1:A:102:ASN:OD1	1:A:109:LEU:HD22	0.56	1.99	6	2
1:A:145:PRO:HD2	1:A:146:PRO:HD3	0.56	1.78	9	10
1:A:102:ASN:OD1	1:A:157:LEU:HD11	0.56	1.99	8	2
1:A:163:LEU:HD13	1:A:163:LEU:C	0.56	2.22	2	5
1:A:140:ARG:NH1	1:B:133:TYR:O	0.55	2.29	8	1
1:B:145:PRO:N	1:B:146:PRO:HD2	0.55	2.16	2	8
1:A:134:ILE:HD13	1:A:136:ARG:NH2	0.55	2.16	6	2
1:B:125:GLU:O	1:B:126:GLU:C	0.55	2.45	7	8
1:A:95:TRP:CZ2	1:A:148:VAL:CG2	0.55	2.89	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:LEU:CD2	1:A:140:ARG:HB3	0.55	2.31	8	1
1:B:127:ARG:NH1	1:B:127:ARG:HB2	0.55	2.17	7	1
1:A:108:GLU:OE1	1:A:123:LYS:NZ	0.54	2.38	3	1
1:B:99:LEU:O	1:B:140:ARG:NH2	0.54	2.32	3	2
1:A:112:LYS:NZ	1:A:119:GLU:CB	0.54	2.70	9	2
1:A:163:LEU:C	1:A:163:LEU:HD13	0.54	2.23	5	5
1:B:126:GLU:HA	1:B:135:SER:OG	0.54	2.02	1	6
1:A:114:LYS:O	1:A:117:VAL:HG23	0.54	2.03	5	3
1:B:102:ASN:OD1	1:B:157:LEU:CD1	0.54	2.55	5	1
1:B:95:TRP:CZ3	1:B:97:VAL:HG21	0.54	2.38	6	1
1:B:165:VAL:HG23	1:B:165:VAL:O	0.54	2.03	4	6
1:B:108:GLU:CD	1:B:123:LYS:NZ	0.54	2.61	5	2
1:A:165:VAL:HG23	1:A:165:VAL:O	0.54	2.03	4	4
1:A:124:HIS:ND1	1:A:125:GLU:N	0.54	2.56	6	1
1:B:145:PRO:CD	1:B:146:PRO:CD	0.54	2.85	5	6
1:A:102:ASN:H	1:A:102:ASN:HD22	0.54	1.46	3	1
1:B:114:LYS:CB	1:B:114:LYS:NZ	0.54	2.71	8	1
1:B:169:MET:N	1:B:169:MET:SD	0.53	2.78	3	1
1:B:149:ASP:O	1:B:153:VAL:HG23	0.53	2.03	7	6
1:A:95:TRP:CD1	1:A:95:TRP:C	0.53	2.81	1	4
1:A:142:TYR:CZ	1:B:131:HIS:O	0.53	2.61	2	6
1:B:102:ASN:ND2	1:B:102:ASN:C	0.53	2.62	10	2
1:A:100:ASP:C	1:A:101:VAL:HG22	0.53	2.23	9	3
1:B:148:VAL:O	1:B:148:VAL:CG1	0.53	2.56	10	4
1:A:142:TYR:CE1	1:B:131:HIS:O	0.53	2.61	8	2
1:A:102:ASN:OD1	1:A:109:LEU:CD1	0.53	2.56	7	3
1:B:102:ASN:HD22	1:B:102:ASN:C	0.53	2.07	10	2
1:B:145:PRO:CD	1:B:146:PRO:HD3	0.53	2.34	9	4
1:A:95:TRP:HB3	1:A:169:MET:SD	0.53	2.43	10	1
1:B:136:ARG:HD3	1:B:138:PHE:CE1	0.53	2.39	8	1
1:A:102:ASN:O	1:A:105:ALA:N	0.52	2.40	6	2
1:B:119:GLU:HG2	1:B:141:LYS:HA	0.52	1.82	6	2
1:A:134:ILE:CD1	1:A:136:ARG:NH2	0.52	2.72	6	1
1:A:141:LYS:NZ	1:B:126:GLU:OE1	0.52	2.42	2	2
1:B:129:ASP:CG	1:B:130:GLU:N	0.52	2.62	10	4
1:B:96:ARG:HB2	1:B:96:ARG:NH1	0.52	2.19	4	1
1:B:156:SER:O	1:B:163:LEU:HD22	0.52	2.04	3	4
1:A:101:VAL:HG11	1:A:138:PHE:CD1	0.52	2.40	1	1
1:B:108:GLU:OE2	1:B:123:LYS:NZ	0.52	2.41	4	4
1:A:127:ARG:CZ	1:A:127:ARG:HB3	0.52	2.34	6	1
1:A:127:ARG:NH1	1:A:127:ARG:HB2	0.52	2.19	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:104:PHE:HB2	1:B:124:HIS:CE1	0.52	2.40	2	1
1:A:112:LYS:NZ	1:A:121:THR:OG1	0.52	2.35	10	4
1:B:94:ARG:NH1	1:B:166:GLU:OE1	0.52	2.42	2	3
1:B:165:VAL:O	1:B:165:VAL:HG23	0.52	2.05	7	4
1:A:101:VAL:O	1:A:103:HIS:N	0.52	2.42	7	5
1:B:124:HIS:O	1:B:135:SER:CB	0.52	2.58	4	1
1:A:95:TRP:CH2	1:A:148:VAL:CG2	0.52	2.93	9	3
1:B:127:ARG:CB	1:B:127:ARG:CZ	0.52	2.88	7	1
1:B:153:VAL:HA	1:B:167:ALA:HB2	0.51	1.82	10	5
1:A:102:ASN:C	1:A:102:ASN:HD22	0.51	2.08	6	1
1:A:114:LYS:O	1:A:117:VAL:N	0.51	2.34	5	1
1:B:142:TYR:CD1	1:B:142:TYR:N	0.51	2.78	9	5
1:A:102:ASN:CG	1:A:109:LEU:HD13	0.51	2.25	5	5
1:B:140:ARG:HB3	1:B:140:ARG:CZ	0.51	2.34	8	1
1:B:102:ASN:CG	1:B:109:LEU:HD13	0.51	2.25	6	3
1:A:158:SER:HB3	1:A:162:THR:OG1	0.51	2.05	2	1
1:B:102:ASN:N	1:B:102:ASN:HD22	0.51	2.03	1	1
1:B:148:VAL:CG1	1:B:148:VAL:O	0.51	2.58	3	2
1:A:159:PRO:C	1:A:161:GLY:H	0.51	2.09	9	4
1:B:145:PRO:HD2	1:B:146:PRO:HD3	0.51	1.83	9	6
1:A:127:ARG:N	1:A:135:SER:OG	0.51	2.44	6	1
1:B:101:VAL:C	1:B:103:HIS:H	0.51	2.08	6	3
1:B:153:VAL:HG22	1:B:167:ALA:CB	0.51	2.36	4	5
1:B:143:THR:O	1:B:145:PRO:HD3	0.51	2.05	1	8
1:A:167:ALA:HB1	1:A:168:PRO:HD2	0.50	1.83	1	7
1:A:114:LYS:NZ	1:A:119:GLU:OE1	0.50	2.42	5	2
1:B:102:ASN:O	1:B:104:PHE:N	0.50	2.44	3	1
1:A:140:ARG:NH2	1:A:141:LYS:C	0.50	2.65	8	1
1:A:95:TRP:HB2	1:A:169:MET:SD	0.50	2.46	5	1
1:A:126:GLU:OE1	1:B:141:LYS:NZ	0.50	2.43	7	3
1:B:159:PRO:C	1:B:161:GLY:H	0.50	2.09	2	6
1:B:134:ILE:O	1:B:136:ARG:NH2	0.50	2.36	3	1
1:A:142:TYR:OH	1:B:131:HIS:O	0.50	2.26	7	1
1:A:167:ALA:HB3	1:A:169:MET:SD	0.50	2.47	8	1
1:A:140:ARG:NH1	1:A:140:ARG:HA	0.50	2.22	10	1
1:B:114:LYS:NZ	1:B:119:GLU:OE2	0.50	2.45	3	6
1:B:168:PRO:C	1:B:169:MET:HG3	0.50	2.28	6	1
1:B:100:ASP:C	1:B:101:VAL:HG22	0.50	2.26	1	6
1:A:101:VAL:HA	1:A:103:HIS:CE1	0.50	2.42	9	2
1:A:165:VAL:CG2	1:A:165:VAL:O	0.49	2.59	4	4
1:B:101:VAL:O	1:B:103:HIS:N	0.49	2.45	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:149:ASP:O	1:B:153:VAL:CG2	0.49	2.60	7	4
1:B:127:ARG:NH1	1:B:135:SER:HA	0.49	2.22	9	1
1:A:108:GLU:OE2	1:A:123:LYS:NZ	0.49	2.42	8	2
1:A:119:GLU:CD	1:A:141:LYS:HD3	0.49	2.27	10	1
1:A:157:LEU:HD12	1:A:158:SER:N	0.49	2.22	3	1
1:B:140:ARG:NH2	1:B:142:TYR:OH	0.49	2.37	7	3
1:B:114:LYS:NZ	1:B:115:ASP:OD1	0.49	2.45	4	1
1:A:104:PHE:O	1:A:124:HIS:ND1	0.49	2.34	1	2
1:A:101:VAL:HG11	1:A:138:PHE:CE2	0.49	2.42	7	1
1:B:102:ASN:HD22	1:B:102:ASN:N	0.49	2.05	9	1
1:A:95:TRP:CH2	1:A:97:VAL:HG21	0.49	2.42	1	1
1:A:169:MET:CB	1:A:170:PRO:CD	0.49	2.91	7	1
1:B:102:ASN:O	1:B:105:ALA:N	0.49	2.39	7	3
1:A:127:ARG:CZ	1:A:127:ARG:CB	0.49	2.89	6	1
1:A:101:VAL:HG21	1:A:138:PHE:CD2	0.49	2.43	8	1
1:A:103:HIS:N	1:A:161:GLY:HA3	0.49	2.23	10	2
1:A:153:VAL:HA	1:A:167:ALA:HB2	0.49	1.84	5	1
1:B:101:VAL:CG2	1:B:140:ARG:CZ	0.49	2.91	4	1
1:A:102:ASN:ND2	1:A:161:GLY:C	0.49	2.66	1	2
1:A:101:VAL:CG1	1:A:138:PHE:CD2	0.49	2.96	9	2
1:A:145:PRO:CD	1:A:146:PRO:CD	0.48	2.90	6	1
1:B:94:ARG:NH2	1:B:166:GLU:OE2	0.48	2.40	8	1
1:A:95:TRP:CG	1:A:96:ARG:N	0.48	2.81	10	1
1:A:142:TYR:CD1	1:A:142:TYR:N	0.48	2.80	1	1
1:B:100:ASP:O	1:B:101:VAL:HG22	0.48	2.08	4	1
1:A:145:PRO:CB	1:A:146:PRO:HD3	0.48	2.39	1	9
1:A:102:ASN:N	1:A:102:ASN:HD22	0.48	2.06	5	1
1:B:119:GLU:C	1:B:120:ILE:HD13	0.48	2.28	6	1
1:B:158:SER:O	1:B:161:GLY:N	0.48	2.45	10	3
1:A:134:ILE:HD13	1:A:136:ARG:HH21	0.48	1.69	4	1
1:B:107:ASP:OD1	1:B:107:ASP:N	0.48	2.46	6	1
1:B:128:GLN:HG2	1:B:129:ASP:N	0.48	2.24	6	1
1:A:166:GLU:O	1:A:167:ALA:CB	0.48	2.62	1	3
1:A:136:ARG:NH1	1:B:138:PHE:CZ	0.48	2.82	2	1
1:B:104:PHE:O	1:B:136:ARG:NH2	0.48	2.43	10	1
1:B:114:LYS:NZ	1:B:119:GLU:OE1	0.48	2.41	10	1
1:B:115:ASP:O	1:B:115:ASP:CG	0.48	2.50	4	1
1:A:165:VAL:O	1:A:165:VAL:CG2	0.48	2.61	3	5
1:A:101:VAL:C	1:A:103:HIS:H	0.48	2.11	7	3
1:A:102:ASN:HD22	1:A:102:ASN:N	0.47	2.06	1	1
1:A:115:ASP:CG	1:A:115:ASP:O	0.47	2.50	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:163:LEU:CD1	1:B:163:LEU:C	0.47	2.83	1	5
1:B:136:ARG:CZ	1:B:138:PHE:CZ	0.47	2.97	4	1
1:B:124:HIS:ND1	1:B:126:GLU:O	0.47	2.43	9	1
1:A:126:GLU:OE2	1:B:141:LYS:NZ	0.47	2.42	10	4
1:B:95:TRP:CB	1:B:169:MET:SD	0.47	3.02	4	2
1:B:145:PRO:C	1:B:147:GLY:N	0.47	2.67	7	6
1:B:134:ILE:HG23	1:B:134:ILE:O	0.47	2.09	2	2
1:B:168:PRO:O	1:B:169:MET:O	0.47	2.33	6	1
1:B:109:LEU:HD22	1:B:157:LEU:CD2	0.47	2.36	8	1
1:A:153:VAL:HG22	1:A:167:ALA:CB	0.47	2.40	5	1
1:B:166:GLU:O	1:B:167:ALA:HB2	0.47	2.10	1	1
1:B:165:VAL:CG2	1:B:165:VAL:O	0.47	2.63	1	5
1:B:101:VAL:N	1:B:103:HIS:CE1	0.47	2.83	1	1
1:B:94:ARG:HH12	1:B:166:GLU:CD	0.47	2.14	1	1
1:B:102:ASN:CG	1:B:161:GLY:HA2	0.47	2.30	5	3
1:A:100:ASP:OD1	1:A:140:ARG:NH2	0.47	2.44	6	1
1:B:127:ARG:NH2	1:B:136:ARG:O	0.47	2.47	9	1
1:B:163:LEU:C	1:B:163:LEU:CD1	0.46	2.84	5	4
1:A:117:VAL:HG13	1:A:143:THR:HG23	0.46	1.86	9	2
1:B:107:ASP:C	1:B:109:LEU:H	0.46	2.14	2	1
1:B:124:HIS:CD2	1:B:136:ARG:H	0.46	2.27	8	1
1:A:134:ILE:HD11	1:A:136:ARG:HH11	0.46	1.68	8	1
1:A:124:HIS:ND1	1:A:127:ARG:HG2	0.46	2.26	9	2
1:B:102:ASN:HD21	1:B:105:ALA:C	0.46	2.12	3	1
1:A:142:TYR:N	1:A:142:TYR:CD1	0.46	2.84	6	2
1:B:119:GLU:O	1:B:120:ILE:HD12	0.46	2.11	9	2
1:A:99:LEU:HD22	1:A:120:ILE:HB	0.46	1.86	8	1
1:B:165:VAL:O	1:B:165:VAL:CG2	0.46	2.63	2	4
1:B:100:ASP:C	1:B:101:VAL:CG2	0.46	2.84	4	1
1:A:117:VAL:HG22	1:A:143:THR:CG2	0.46	2.41	10	1
1:B:109:LEU:HD11	1:B:120:ILE:HG23	0.46	1.88	1	1
1:A:123:LYS:O	1:A:123:LYS:NZ	0.46	2.35	9	2
1:A:140:ARG:CZ	1:A:142:TYR:CZ	0.46	2.99	8	1
1:B:124:HIS:CD2	1:B:127:ARG:CZ	0.46	2.99	10	1
1:A:109:LEU:HD22	1:A:157:LEU:CD2	0.46	2.35	2	3
1:A:95:TRP:CZ3	1:A:97:VAL:CG2	0.46	2.99	2	3
1:B:145:PRO:CB	1:B:146:PRO:HD3	0.46	2.41	9	1
1:B:123:LYS:O	1:B:123:LYS:NZ	0.46	2.32	8	2
1:B:95:TRP:CD1	1:B:97:VAL:HG22	0.46	2.46	1	1
1:B:95:TRP:C	1:B:95:TRP:CD1	0.45	2.90	6	1
1:A:94:ARG:NH1	1:A:166:GLU:OE1	0.45	2.49	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:149:ASP:OD1	1:B:152:GLN:N	0.45	2.45	2	1
1:B:134:ILE:HD11	1:B:136:ARG:NH2	0.45	2.25	7	1
1:B:108:GLU:CD	1:B:123:LYS:HZ3	0.45	2.15	5	1
1:B:112:LYS:NZ	1:B:121:THR:OG1	0.45	2.40	10	2
1:A:102:ASN:CB	1:A:109:LEU:CD1	0.45	2.94	10	1
1:B:124:HIS:O	1:B:135:SER:HB3	0.45	2.11	4	2
1:A:162:THR:O	1:A:162:THR:CG2	0.45	2.65	4	1
1:A:108:GLU:N	1:A:108:GLU:CD	0.45	2.69	7	1
1:A:95:TRP:HE1	1:A:97:VAL:HG22	0.45	1.71	10	1
1:B:112:LYS:NZ	1:B:119:GLU:HB2	0.45	2.25	1	1
1:B:109:LEU:HA	1:B:121:THR:O	0.45	2.11	8	2
1:B:111:VAL:HG13	1:B:120:ILE:CD1	0.45	2.42	2	1
1:B:102:ASN:HB3	1:B:109:LEU:CD1	0.45	2.41	7	1
1:B:102:ASN:ND2	1:B:161:GLY:CA	0.45	2.79	1	2
1:A:126:GLU:HA	1:A:135:SER:OG	0.45	2.12	4	4
1:A:125:GLU:O	1:A:126:GLU:HB2	0.45	2.12	9	2
1:B:134:ILE:O	1:B:134:ILE:HG23	0.45	2.11	10	2
1:A:169:MET:SD	1:A:169:MET:N	0.45	2.90	1	1
1:B:109:LEU:HG	1:B:110:THR:N	0.45	2.27	6	2
1:A:119:GLU:HA	1:A:140:ARG:O	0.45	2.12	8	1
1:B:124:HIS:NE2	1:B:136:ARG:HG3	0.45	2.27	8	1
1:B:98:SER:HA	1:B:163:LEU:O	0.45	2.11	8	3
1:A:125:GLU:O	1:A:127:ARG:N	0.45	2.50	3	1
1:B:119:GLU:O	1:B:120:ILE:HD13	0.45	2.12	6	1
1:A:99:LEU:HD23	1:A:140:ARG:HG3	0.45	1.89	2	1
1:B:104:PHE:O	1:B:124:HIS:ND1	0.45	2.34	5	2
1:B:157:LEU:HD12	1:B:158:SER:N	0.45	2.27	1	1
1:B:103:HIS:N	1:B:161:GLY:HA3	0.44	2.28	7	2
1:A:169:MET:HB3	1:A:170:PRO:HD2	0.44	1.90	8	1
1:B:111:VAL:HG13	1:B:120:ILE:HD12	0.44	1.89	5	1
1:A:162:THR:HG23	1:A:162:THR:O	0.44	2.12	10	1
1:B:142:TYR:N	1:B:142:TYR:CD1	0.44	2.85	1	1
1:B:102:ASN:ND2	1:B:102:ASN:O	0.44	2.50	4	2
1:A:163:LEU:CD1	1:A:163:LEU:C	0.44	2.85	4	3
1:A:114:LYS:NZ	1:A:119:GLU:OE2	0.44	2.49	7	1
1:B:102:ASN:ND2	1:B:161:GLY:C	0.44	2.70	9	1
1:A:136:ARG:NH1	1:B:138:PHE:CE2	0.44	2.85	9	1
1:A:149:ASP:OD1	1:A:151:THR:N	0.44	2.51	9	2
1:A:163:LEU:C	1:A:163:LEU:CD1	0.44	2.85	3	4
1:A:141:LYS:NZ	1:B:126:GLU:OE2	0.44	2.42	3	1
1:B:99:LEU:CD2	1:B:140:ARG:HB2	0.44	2.42	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:102:ASN:C	1:B:104:PHE:N	0.44	2.69	5	2
1:A:102:ASN:ND2	1:A:105:ALA:O	0.44	2.45	8	3
1:B:147:GLY:O	1:B:149:ASP:N	0.44	2.51	10	1
1:A:141:LYS:HB2	1:A:141:LYS:HZ3	0.44	1.73	6	1
1:B:95:TRP:CE2	1:B:97:VAL:HG22	0.44	2.47	8	1
1:A:114:LYS:HB3	1:A:117:VAL:HB	0.44	1.89	6	4
1:A:143:THR:O	1:A:145:PRO:HD3	0.44	2.12	6	2
1:A:112:LYS:HZ3	1:A:119:GLU:HB2	0.44	1.69	9	1
1:B:149:ASP:OD1	1:B:151:THR:N	0.44	2.48	9	1
1:B:99:LEU:HD23	1:B:140:ARG:NH1	0.44	2.28	8	1
1:A:109:LEU:HG	1:A:110:THR:N	0.43	2.27	2	1
1:A:140:ARG:NH2	1:A:141:LYS:O	0.43	2.46	8	1
1:A:140:ARG:CZ	1:A:140:ARG:HB3	0.43	2.43	2	1
1:A:95:TRP:CZ2	1:A:165:VAL:HG23	0.43	2.49	2	1
1:A:102:ASN:OD1	1:A:161:GLY:CA	0.43	2.67	8	2
1:B:149:ASP:OD1	1:B:149:ASP:N	0.43	2.49	1	2
1:A:167:ALA:HB3	1:A:169:MET:CE	0.43	2.42	3	1
1:B:104:PHE:CE2	1:B:136:ARG:NH2	0.43	2.86	8	1
1:A:140:ARG:NH2	1:B:131:HIS:ND1	0.43	2.66	4	1
1:A:96:ARG:HB3	1:A:96:ARG:CZ	0.43	2.44	9	1
1:B:104:PHE:CD2	1:B:136:ARG:NH2	0.43	2.86	8	1
1:A:102:ASN:HB3	1:A:109:LEU:CD1	0.43	2.43	10	1
1:A:101:VAL:C	1:A:103:HIS:N	0.43	2.70	6	1
1:A:100:ASP:O	1:A:101:VAL:HG22	0.43	2.14	9	1
1:A:140:ARG:CZ	1:A:142:TYR:CE1	0.43	3.01	8	1
1:A:140:ARG:NH2	1:A:141:LYS:N	0.43	2.66	8	1
1:B:140:ARG:CZ	1:B:140:ARG:CB	0.43	2.97	8	1
1:B:103:HIS:ND1	1:B:103:HIS:N	0.43	2.67	4	1
1:B:102:ASN:OD1	1:B:157:LEU:HD13	0.43	2.13	9	2
1:B:134:ILE:HD11	1:B:136:ARG:NH1	0.43	2.29	9	1
1:A:102:ASN:C	1:A:102:ASN:ND2	0.43	2.73	6	1
1:A:141:LYS:NZ	1:A:141:LYS:HB2	0.43	2.28	1	1
1:B:104:PHE:HB3	1:B:136:ARG:CZ	0.43	2.44	10	1
1:A:134:ILE:HA	1:B:139:THR:O	0.42	2.13	4	1
1:A:94:ARG:NH2	1:A:166:GLU:OE2	0.42	2.44	2	1
1:B:117:VAL:HG13	1:B:143:THR:HG23	0.42	1.89	5	1
1:B:119:GLU:HG2	1:B:141:LYS:CB	0.42	2.45	4	1
1:A:95:TRP:O	1:A:166:GLU:HA	0.42	2.13	7	1
1:B:136:ARG:NE	1:B:136:ARG:O	0.42	2.48	10	1
1:B:101:VAL:C	1:B:103:HIS:N	0.42	2.73	6	1
1:A:127:ARG:O	1:A:134:ILE:N	0.42	2.47	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:TYR:O	1:B:141:LYS:N	0.42	2.46	10	1
1:A:149:ASP:OD2	1:A:152:GLN:N	0.42	2.45	1	1
1:B:160:GLU:H	1:B:160:GLU:CD	0.42	2.18	1	1
1:A:104:PHE:CE2	1:A:136:ARG:NH2	0.42	2.88	1	1
1:A:169:MET:CB	1:A:170:PRO:HD2	0.42	2.45	8	1
1:B:95:TRP:N	1:B:167:ALA:O	0.42	2.52	2	1
1:B:157:LEU:HD12	1:B:158:SER:H	0.42	1.75	8	1
1:A:124:HIS:HB3	1:A:127:ARG:NH2	0.42	2.30	7	1
1:A:140:ARG:HH22	1:A:141:LYS:C	0.42	2.18	8	1
1:B:104:PHE:HB3	1:B:136:ARG:NH1	0.42	2.30	10	1
1:B:127:ARG:CB	1:B:127:ARG:NH1	0.41	2.82	7	1
1:A:140:ARG:NE	1:A:142:TYR:CZ	0.41	2.88	8	1
1:B:95:TRP:CB	1:B:169:MET:HG2	0.41	2.45	8	1
1:A:124:HIS:CD2	1:A:127:ARG:HG3	0.41	2.50	10	1
1:B:145:PRO:C	1:B:147:GLY:H	0.41	2.18	3	1
1:A:101:VAL:N	1:A:103:HIS:CE1	0.41	2.88	3	1
1:B:158:SER:HB2	1:B:162:THR:CG2	0.41	2.45	8	1
1:B:108:GLU:HB3	1:B:123:LYS:O	0.41	2.15	10	1
1:A:99:LEU:HD23	1:A:140:ARG:HD3	0.41	1.93	4	1
1:B:117:VAL:CG1	1:B:141:LYS:HG3	0.41	2.46	7	1
1:A:140:ARG:NH1	1:B:134:ILE:HB	0.41	2.30	10	2
1:A:135:SER:OG	1:A:136:ARG:N	0.41	2.54	3	1
1:B:102:ASN:O	1:B:102:ASN:CG	0.41	2.58	3	1
1:B:148:VAL:O	1:B:149:ASP:C	0.41	2.59	3	1
1:A:119:GLU:HG2	1:A:141:LYS:CB	0.41	2.45	3	2
1:B:95:TRP:O	1:B:166:GLU:HA	0.41	2.16	2	1
1:A:114:LYS:O	1:A:115:ASP:C	0.41	2.59	4	1
1:A:104:PHE:CZ	1:A:136:ARG:NH1	0.41	2.89	6	1
1:A:158:SER:C	1:A:160:GLU:N	0.41	2.74	2	1
1:A:99:LEU:CD2	1:A:140:ARG:CB	0.41	2.98	8	1
1:A:102:ASN:HB3	1:A:161:GLY:O	0.41	2.15	6	1
1:A:124:HIS:CD2	1:A:127:ARG:CG	0.41	3.03	1	1
1:B:114:LYS:O	1:B:115:ASP:C	0.41	2.59	1	1
1:B:100:ASP:CG	1:B:103:HIS:HE2	0.41	2.19	2	1
1:A:160:GLU:O	1:A:162:THR:N	0.41	2.54	7	1
1:B:119:GLU:CD	1:B:141:LYS:HZ2	0.41	2.16	9	1
1:B:160:GLU:N	1:B:160:GLU:CD	0.41	2.74	9	1
1:A:132:GLY:HA3	1:B:142:TYR:CZ	0.41	2.50	5	1
1:B:104:PHE:CE1	1:B:127:ARG:NH1	0.41	2.89	2	2
1:A:134:ILE:HD12	1:B:140:ARG:CZ	0.41	2.45	2	1
1:B:110:THR:N	1:B:121:THR:O	0.41	2.53	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:102:ASN:HD21	1:B:106:PRO:HA	0.41	1.75	10	1
1:A:124:HIS:CG	1:A:127:ARG:HD3	0.41	2.51	10	1
1:B:157:LEU:HD12	1:B:162:THR:O	0.41	2.16	3	1
1:B:157:LEU:HD11	1:B:161:GLY:HA2	0.41	1.91	3	1
1:B:114:LYS:O	1:B:117:VAL:CB	0.41	2.68	7	1
1:B:127:ARG:NH1	1:B:134:ILE:HG23	0.40	2.31	7	1
1:A:100:ASP:C	1:A:101:VAL:CG2	0.40	2.88	9	1
1:A:119:GLU:HG2	1:A:141:LYS:HA	0.40	1.92	8	1
1:A:141:LYS:HB2	1:A:141:LYS:NZ	0.40	2.29	6	1
1:B:100:ASP:OD2	1:B:103:HIS:NE2	0.40	2.45	7	1
1:A:119:GLU:HG2	1:A:141:LYS:HB2	0.40	1.94	8	1
1:B:124:HIS:CD2	1:B:124:HIS:N	0.40	2.82	8	1
1:B:145:PRO:CD	1:B:146:PRO:HD2	0.40	2.46	5	1
1:B:124:HIS:O	1:B:135:SER:OG	0.40	2.35	4	1
1:A:95:TRP:CD1	1:A:95:TRP:O	0.40	2.74	6	1
1:A:149:ASP:OD1	1:A:152:GLN:N	0.40	2.49	9	1
1:A:162:THR:O	1:A:162:THR:HG23	0.40	2.17	8	1
1:B:144:LEU:C	1:B:146:PRO:HD2	0.40	2.37	2	1
1:B:136:ARG:HD2	1:B:138:PHE:CE2	0.40	2.51	5	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/98 (74%)	58±2 (80±3%)	10±2 (13±3%)	5±1 (7±2%)	3	18
1	B	76/98 (78%)	61±2 (81±3%)	9±2 (12±3%)	6±1 (8±2%)	3	16
All	All	1490/1960 (76%)	1197 (80%)	185 (12%)	108 (7%)	3	17

All 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	146	PRO	10
1	A	126	GLU	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	101	VAL	9
1	B	101	VAL	9
1	B	126	GLU	8
1	A	146	PRO	7
1	A	102	ASN	7
1	B	160	GLU	5
1	B	102	ASN	5
1	A	160	GLU	4
1	A	147	GLY	4
1	B	106	PRO	3
1	B	94	ARG	3
1	B	147	GLY	3
1	B	115	ASP	3
1	A	94	ARG	3
1	A	170	PRO	2
1	B	169	MET	2
1	B	148	VAL	2
1	B	100	ASP	2
1	A	161	GLY	1
1	A	115	ASP	1
1	B	103	HIS	1
1	A	150	PRO	1
1	A	106	PRO	1
1	B	161	GLY	1
1	A	167	ALA	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	66/88 (75%)	40±2 (61±4%)	26±2 (39±4%)	1	6
1	B	69/88 (78%)	41±3 (59±4%)	28±3 (41±4%)	0	4
All	All	1350/1760 (77%)	810 (60%)	540 (40%)	1	5

All 92 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	139	THR	10
1	B	99	LEU	10
1	B	154	SER	10
1	A	151	THR	10
1	B	135	SER	10
1	B	134	ILE	10
1	B	109	LEU	10
1	B	139	THR	10
1	A	123	LYS	10
1	B	156	SER	10
1	A	154	SER	10
1	B	164	THR	10
1	A	102	ASN	10
1	A	121	THR	10
1	B	121	THR	10
1	A	143	THR	10
1	A	134	ILE	10
1	B	140	ARG	10
1	A	156	SER	10
1	A	109	LEU	10
1	A	148	VAL	10
1	B	123	LYS	9
1	B	148	VAL	9
1	B	102	ASN	9
1	A	136	ARG	9
1	B	151	THR	9
1	B	143	THR	9
1	A	155	SER	9
1	A	99	LEU	9
1	B	169	MET	9
1	B	155	SER	9
1	B	110	THR	9
1	A	169	MET	8
1	A	158	SER	8
1	B	158	SER	8
1	A	101	VAL	8
1	B	101	VAL	7
1	A	97	VAL	7
1	A	95	TRP	7
1	A	110	THR	7
1	A	114	LYS	7
1	B	95	TRP	7
1	B	113	THR	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	140	ARG	6
1	B	97	VAL	6
1	B	166	GLU	6
1	B	129	ASP	6
1	A	164	THR	6
1	A	135	SER	5
1	B	125	GLU	5
1	B	138	PHE	5
1	A	112	LYS	5
1	A	125	GLU	5
1	B	114	LYS	5
1	B	111	VAL	4
1	B	136	ARG	4
1	A	103	HIS	4
1	A	166	GLU	4
1	B	130	GLU	4
1	B	126	GLU	4
1	A	113	THR	4
1	A	127	ARG	4
1	B	103	HIS	3
1	B	112	LYS	3
1	B	107	ASP	3
1	A	126	GLU	3
1	A	104	PHE	3
1	B	127	ARG	3
1	B	124	HIS	3
1	A	115	ASP	3
1	A	98	SER	3
1	B	94	ARG	3
1	A	100	ASP	2
1	B	104	PHE	2
1	B	108	GLU	2
1	B	115	ASP	2
1	B	149	ASP	2
1	A	96	ARG	2
1	B	100	ASP	2
1	B	152	GLN	2
1	A	111	VAL	1
1	A	162	THR	1
1	B	128	GLN	1
1	A	94	ARG	1
1	B	142	TYR	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	138	PHE	1
1	B	120	ILE	1
1	A	120	ILE	1
1	A	124	HIS	1
1	A	152	GLN	1
1	A	119	GLU	1
1	A	149	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 22% for the well-defined parts and 21% for the entire structure.

7.1 Chemical shift list 1

File name: 2n3j_cs.str

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	490
Number of shifts mapped to atoms	490
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	90	0.40 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	84	0.84 ± 0.21	Should be applied
$^{13}\text{C}'$	0	—	—
^{15}N	77	-0.47 ± 0.40	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 22%, i.e. 395 atoms were assigned a chemical shift out of a possible 1815. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	219/719 (30%)	83/285 (29%)	72/298 (24%)	64/136 (47%)
Sidechain	174/969 (18%)	104/570 (18%)	68/356 (19%)	2/43 (5%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	2/127 (2%)	1/68 (1%)	0/52 (0%)	1/7 (14%)
Overall	395/1815 (22%)	188/923 (20%)	140/706 (20%)	67/186 (36%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 21%, i.e. 486 atoms were assigned a chemical shift out of a possible 2362. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	269/952 (28%)	102/378 (27%)	90/392 (23%)	77/182 (42%)
Sidechain	215/1262 (17%)	126/742 (17%)	86/464 (19%)	3/56 (5%)
Aromatic	2/148 (1%)	1/80 (1%)	0/58 (0%)	1/10 (10%)
Overall	486/2362 (21%)	229/1200 (19%)	176/914 (19%)	81/248 (33%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

