



Full wwPDB NMR Structure Validation Report ⓘ

Feb 9, 2017 – 11:06 am GMT

PDB ID : 2N8M
Title : Zipcode-binding-protein-1 KH3(DD)KH4 domains in complex with the KH4 RNA target
Authors : Nicastro, G.; Ramos, A.; Candel, A.; Hollingworth, D.
Deposited on : 2015-10-21

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : recalc28906
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28906

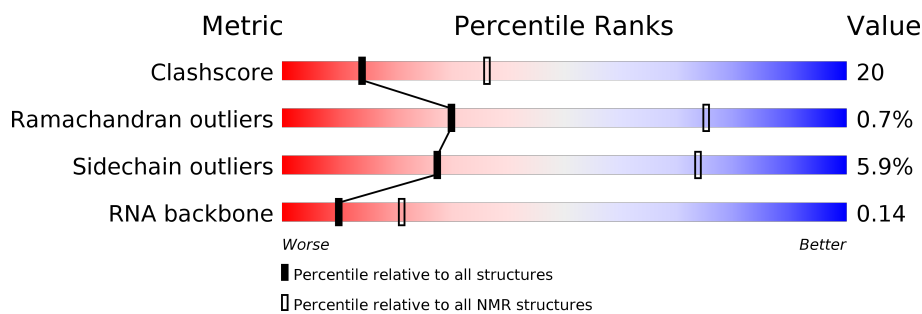
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 54%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367
RNA backbone	3398	623

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	191	
2	B	7	

2 Ensemble composition and analysis

This entry contains 12 models. Model 2 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:23-A:60, A:67-A:97, A:103-A:142, A:146-A:183 (147)	0.68	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3150 atoms, of which 1553 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin-like growth factor 2 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	191	Total	C	H	N	O	S	0
			2926	912	1477	261	272	4	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP O42254
A	2	ALA	-	EXPRESSION TAG	UNP O42254
A	3	MET	-	EXPRESSION TAG	UNP O42254
A	4	GLY	-	EXPRESSION TAG	UNP O42254
A	14	PHE	TYR	ENGINEERED MUTATION	UNP O42254
A	40	ASP	LYS	ENGINEERED MUTATION	UNP O42254
A	41	ASP	LYS	ENGINEERED MUTATION	UNP O42254

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3').

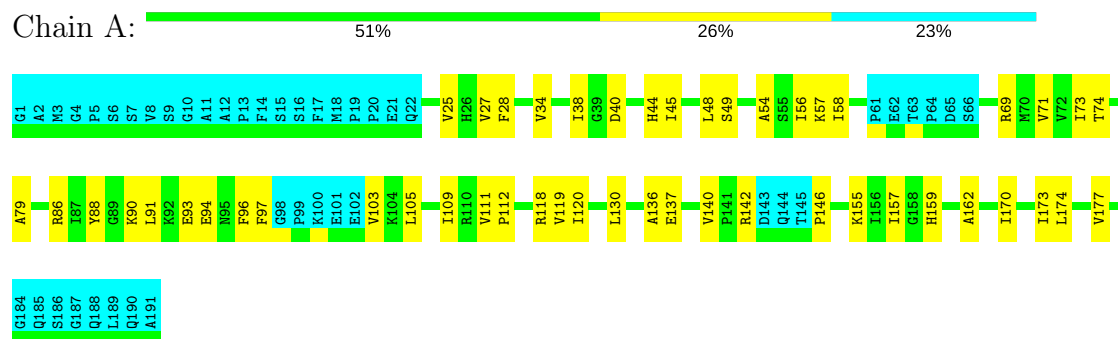
Mol	Chain	Residues	Atoms						Trace
2	B	7	Total	C	H	N	O	P	0
			224	66	76	25	50	7	

4 Residue-property plots [i](#)

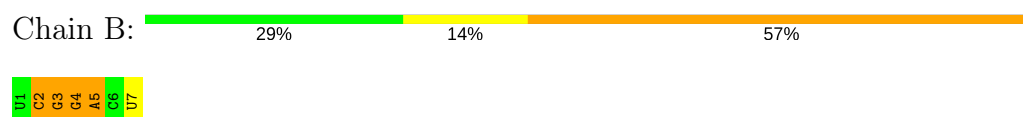
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

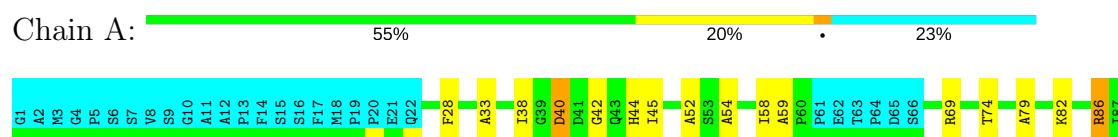


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1





- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

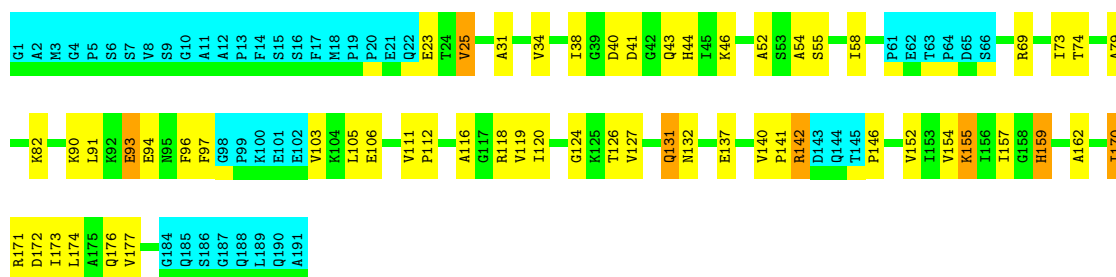
Chain B: 14% 29% 57%



4.2.2 Score per residue for model 2 (medoid)

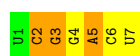
- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A: 47% 26% 23%



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

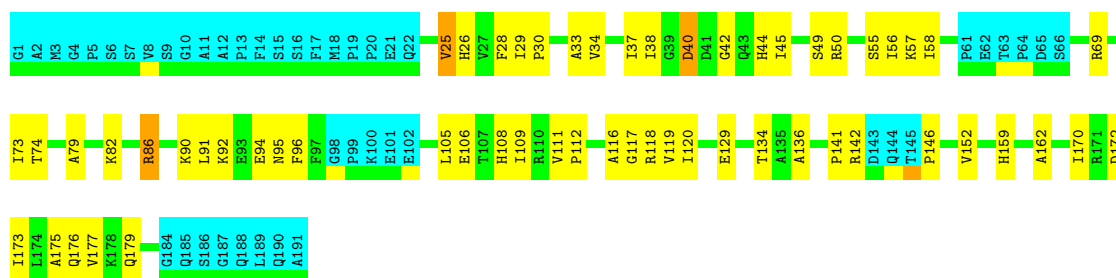
Chain B: 14% 43% 43%



4.2.3 Score per residue for model 3

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A: 47% 29% 23%



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

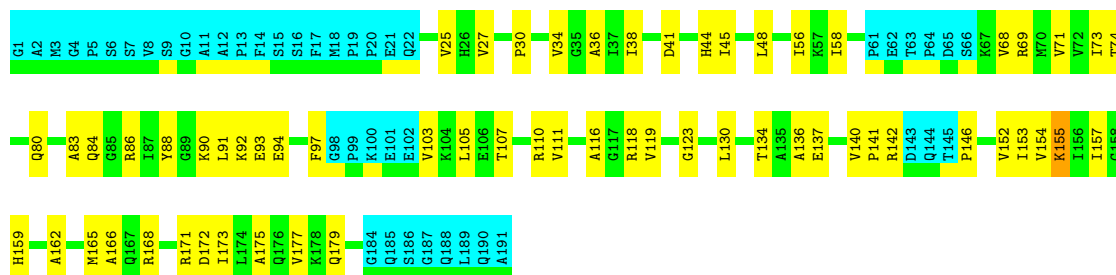
Chain B:  29% 14% 57%



4.2.4 Score per residue for model 4

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A:  45% 31% 23%



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

Chain B:  14% 43% 43%



4.2.5 Score per residue for model 5

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A:  49% 26% 23%



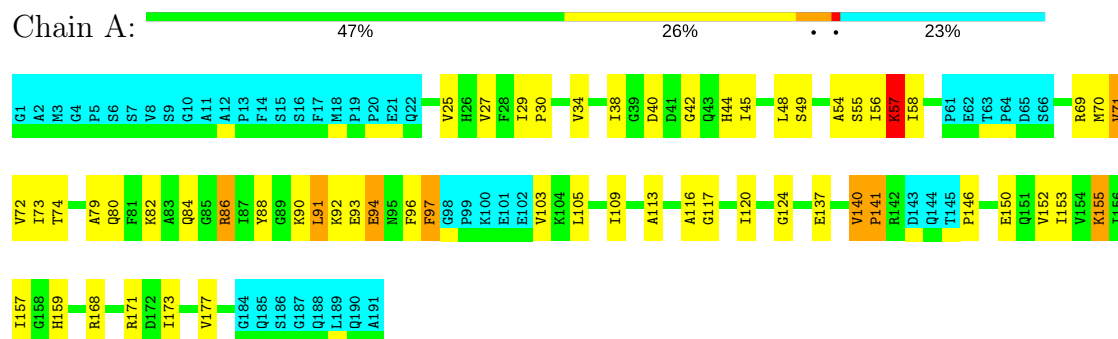
- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

Chain B:  14% 14% 71%

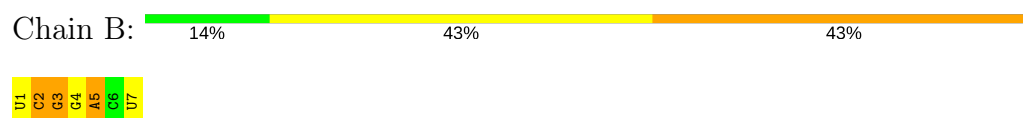


4.2.6 Score per residue for model 6

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

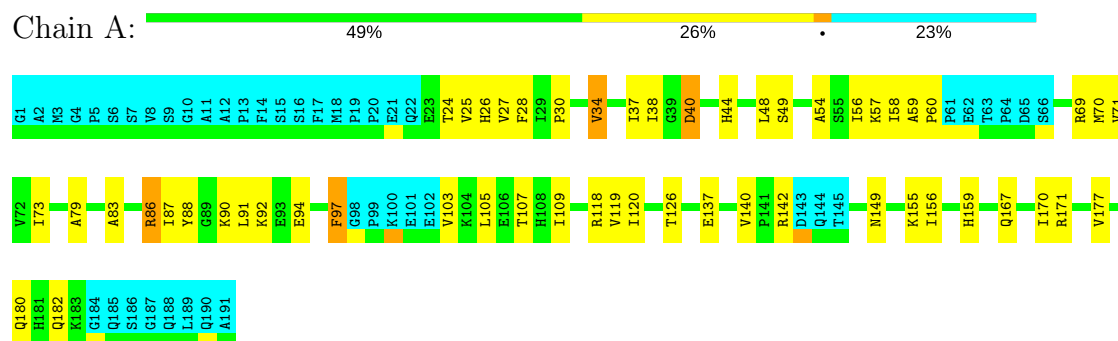


- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



4.2.7 Score per residue for model 7

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1



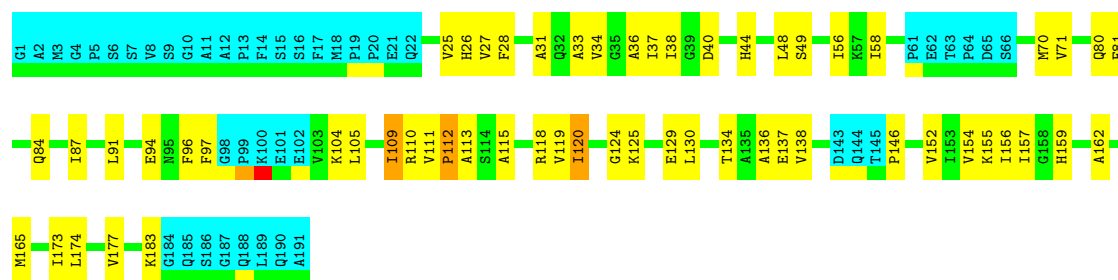
- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



4.2.8 Score per residue for model 8

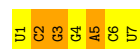
- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1





- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

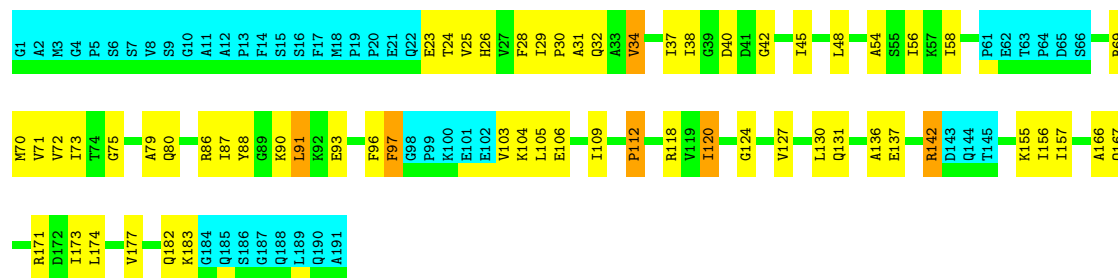
Chain B: 57% 43%



4.2.9 Score per residue for model 9

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A: 45% 29% 23%



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

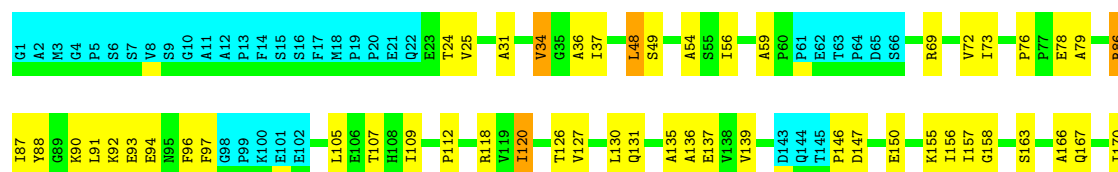
Chain B: 43% 57%

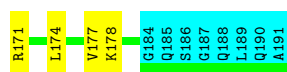


4.2.10 Score per residue for model 10

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

Chain A: 48% 27% 23%



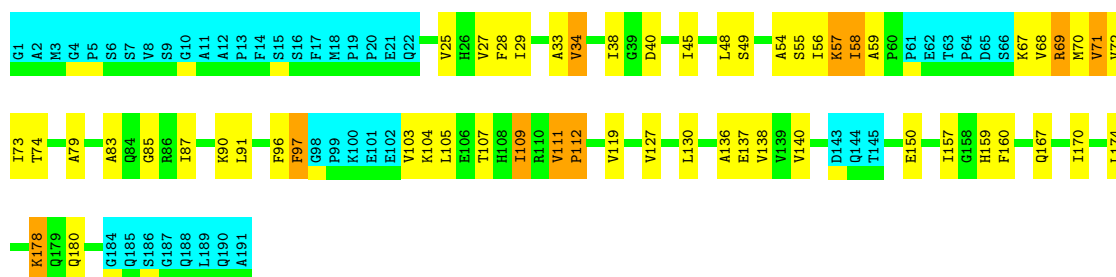


- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')

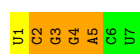


4.2.11 Score per residue for model 11

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1

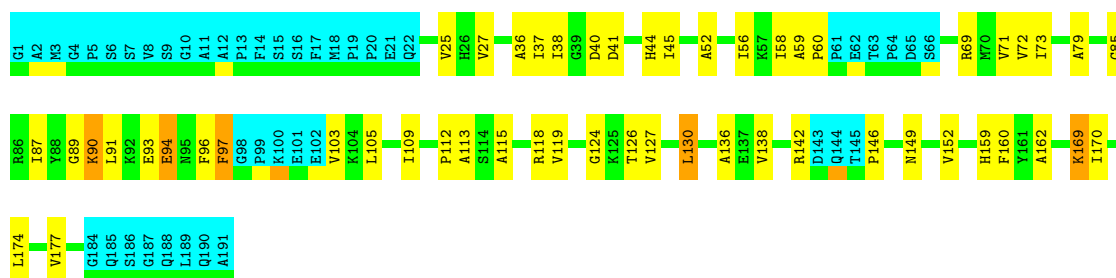


- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



4.2.12 Score per residue for model 12

- Molecule 1: Insulin-like growth factor 2 mRNA-binding protein 1



- Molecule 2: RNA (5'-R(P*UP*CP*GP*GP*AP*CP*U)-3')



5 Refinement protocol and experimental data overview

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

Of the 100 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
ARIA	structure solution	
ARIA	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)	2n8m_cs.str
Number of chemical shift lists	1
Total number of shifts	1440
Number of shifts mapped to atoms	1436
Number of unparsed shifts	4
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

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	0.2±0.4
All	All	0	3

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	57	LYS	Peptide	2
1	A	67	LYS	Peptide	1

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	1141	1198	1193	42±10
2	B	148	76	76	9±2
All	All	15468	15288	15228	603

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:ALA:HA	1:A:82:LYS:HD2	0.90	1.43	2	2
2:B:4:G:H4'	2:B:5:A:O5'	0.88	1.68	7	12
1:A:130:LEU:HG	1:A:136:ALA:HB3	0.86	1.48	10	3
1:A:56:ILE:HD12	1:A:57:LYS:HG2	0.85	1.46	11	1
1:A:56:ILE:HD12	1:A:57:LYS:HE3	0.81	1.52	6	1
2:B:3:G:H1'	2:B:4:G:N7	0.81	1.91	6	11
1:A:92:LYS:HD2	1:A:97:PHE:HZ	0.80	1.35	10	1
1:A:92:LYS:HD2	1:A:97:PHE:CZ	0.78	2.14	10	2
1:A:40:ASP:HB2	1:A:44:HIS:HB2	0.78	1.52	7	4
1:A:121:GLY:HA3	1:A:125:LYS:HB3	0.76	1.58	5	1
1:A:118:ARG:HG2	1:A:177:VAL:HG22	0.75	1.58	4	3
1:A:48:LEU:HD23	1:A:56:ILE:HD12	0.75	1.58	8	1
1:A:58:ILE:HG22	1:A:71:VAL:HA	0.75	1.59	6	1
1:A:117:GLY:HA3	2:B:4:G:C5	0.75	2.17	3	2
2:B:7:U:H2'	2:B:7:U:O2	0.74	1.83	3	3
1:A:97:PHE:CD1	1:A:103:VAL:HA	0.74	2.17	11	2
1:A:36:ALA:HB1	1:A:94:GLU:HG2	0.74	1.58	5	3
1:A:140:VAL:HG12	1:A:141:PRO:HD2	0.73	1.59	6	1
1:A:34:VAL:HG21	1:A:69:ARG:HD3	0.73	1.59	6	1
1:A:55:SER:HB2	1:A:74:THR:HB	0.73	1.61	6	3
1:A:131:GLN:HG3	1:A:137:GLU:HG2	0.73	1.60	1	1
1:A:25:VAL:HG12	1:A:109:ILE:HG22	0.73	1.60	11	5
1:A:56:ILE:O	1:A:72:VAL:HB	0.73	1.84	11	2
1:A:134:THR:HG22	1:A:162:ALA:HA	0.72	1.62	4	3
1:A:48:LEU:HD23	1:A:57:LYS:HG3	0.71	1.60	11	1
1:A:159:HIS:H	1:A:162:ALA:HB3	0.71	1.44	4	4
1:A:25:VAL:HG13	1:A:73:ILE:HG23	0.71	1.60	3	1
1:A:91:LEU:HA	1:A:94:GLU:OE2	0.71	1.85	6	1
1:A:49:SER:HB2	1:A:56:ILE:HD13	0.70	1.61	6	1
1:A:48:LEU:HG	1:A:57:LYS:HD2	0.69	1.63	6	1
1:A:34:VAL:HG11	1:A:69:ARG:HD3	0.68	1.63	4	1
1:A:91:LEU:HD11	1:A:105:LEU:HD21	0.68	1.65	2	4
1:A:91:LEU:HD22	1:A:105:LEU:HG	0.68	1.63	12	1
1:A:118:ARG:HD3	1:A:177:VAL:HG22	0.68	1.65	7	1
1:A:120:ILE:HG12	1:A:124:GLY:HA2	0.67	1.66	6	1
1:A:57:LYS:HA	1:A:72:VAL:H	0.67	1.49	11	2
1:A:118:ARG:HG2	1:A:177:VAL:CG2	0.67	2.19	10	5
1:A:141:PRO:HD3	1:A:153:ILE:O	0.67	1.89	6	1
1:A:118:ARG:HG2	1:A:177:VAL:HG21	0.66	1.66	10	3
1:A:56:ILE:HG12	1:A:73:ILE:HD13	0.66	1.63	3	1
1:A:107:THR:HG21	1:A:167:GLN:HE21	0.66	1.48	11	1
1:A:141:PRO:HG3	1:A:152:VAL:HB	0.65	1.66	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:VAL:HG21	1:A:69:ARG:HB3	0.65	1.69	4	1
1:A:104:LYS:HD2	1:A:157:ILE:HG22	0.65	1.69	9	1
1:A:90:LYS:O	1:A:94:GLU:HG3	0.65	1.91	6	1
1:A:40:ASP:HB3	1:A:44:HIS:HB2	0.64	1.69	1	2
1:A:112:PRO:HG2	1:A:174:LEU:HD22	0.64	1.67	9	2
1:A:91:LEU:CD2	1:A:105:LEU:HG	0.64	2.23	12	1
1:A:91:LEU:HA	1:A:96:PHE:CD1	0.63	2.27	12	1
1:A:56:ILE:CD1	1:A:57:LYS:HG2	0.63	2.23	11	1
1:A:130:LEU:HB3	1:A:136:ALA:HB3	0.63	1.69	11	2
1:A:169:LYS:HA	1:A:169:LYS:HE3	0.63	1.70	12	1
1:A:91:LEU:HD22	1:A:96:PHE:CE2	0.62	2.29	11	3
2:B:1:U:O2	2:B:1:U:H3'	0.62	1.94	6	1
1:A:88:TYR:CE1	1:A:105:LEU:HG	0.62	2.30	1	4
1:A:48:LEU:CG	1:A:57:LYS:HD2	0.62	2.24	6	1
1:A:27:VAL:HG12	1:A:71:VAL:HG22	0.62	1.72	7	3
1:A:25:VAL:HG13	1:A:73:ILE:HB	0.61	1.72	2	1
1:A:49:SER:N	1:A:56:ILE:HD13	0.61	2.10	11	1
2:B:7:U:O2	2:B:7:U:C2'	0.61	2.48	10	1
1:A:120:ILE:HD13	1:A:127:VAL:HG23	0.61	1.73	2	1
1:A:57:LYS:HE2	1:A:72:VAL:O	0.61	1.96	6	1
1:A:103:VAL:HG13	1:A:159:HIS:HD2	0.61	1.56	12	1
1:A:103:VAL:HG13	1:A:159:HIS:CD2	0.61	2.31	12	1
2:B:1:U:H2'	2:B:1:U:O2	0.60	1.95	8	1
1:A:91:LEU:HD22	1:A:105:LEU:CG	0.60	2.26	12	1
1:A:38:ILE:HD11	1:A:69:ARG:HH11	0.60	1.56	7	1
1:A:91:LEU:HB3	1:A:97:PHE:CE2	0.60	2.31	7	1
1:A:38:ILE:O	1:A:42:GLY:HA2	0.60	1.96	5	5
1:A:97:PHE:CD2	1:A:103:VAL:HG12	0.60	2.31	2	3
1:A:136:ALA:HA	1:A:157:ILE:O	0.60	1.97	8	2
1:A:54:ALA:HB2	1:A:79:ALA:HB1	0.60	1.71	7	6
1:A:97:PHE:CD2	1:A:103:VAL:HA	0.60	2.30	9	1
1:A:27:VAL:O	1:A:70:MET:HA	0.60	1.96	5	1
1:A:106:GLU:HG3	1:A:157:ILE:HD11	0.59	1.72	2	1
1:A:91:LEU:CD1	1:A:105:LEU:HD11	0.59	2.27	11	3
1:A:116:ALA:HB2	1:A:152:VAL:HG21	0.59	1.74	4	3
1:A:136:ALA:HB1	1:A:166:ALA:HB2	0.59	1.75	9	2
1:A:45:ILE:HG12	1:A:58:ILE:HG21	0.59	1.73	3	2
2:B:1:U:C2'	2:B:1:U:O2	0.59	2.50	7	3
1:A:173:ILE:O	1:A:177:VAL:HG23	0.59	1.98	4	6
1:A:134:THR:HG21	1:A:165:MET:HB3	0.59	1.75	4	1
1:A:105:LEU:O	1:A:157:ILE:HA	0.58	1.98	5	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:PHE:HB2	1:A:106:GLU:HG3	0.58	1.73	5	3
1:A:34:VAL:HG13	1:A:69:ARG:HE	0.58	1.56	2	1
1:A:167:GLN:O	1:A:171:ARG:HG2	0.58	1.98	9	2
1:A:73:ILE:HG21	1:A:80:GLN:HG2	0.58	1.74	4	1
1:A:34:VAL:HG21	1:A:69:ARG:HB2	0.58	1.75	3	2
2:B:1:U:O2	2:B:1:U:H2'	0.58	1.97	7	1
1:A:48:LEU:HB3	1:A:56:ILE:HG21	0.58	1.76	10	1
1:A:56:ILE:HA	1:A:72:VAL:O	0.57	1.99	5	4
1:A:123:GLY:HA3	2:B:4:G:OP1	0.57	1.98	4	1
1:A:91:LEU:HD11	1:A:105:LEU:HD11	0.57	1.75	10	2
1:A:136:ALA:HB2	1:A:162:ALA:HB1	0.57	1.76	12	3
1:A:127:VAL:O	1:A:131:GLN:HB3	0.57	2.00	10	1
1:A:103:VAL:O	1:A:159:HIS:HA	0.57	1.99	11	1
1:A:29:ILE:HG13	1:A:34:VAL:HG22	0.57	1.77	6	2
1:A:45:ILE:HD11	1:A:57:LYS:HB2	0.57	1.76	11	1
1:A:52:ALA:HA	1:A:82:LYS:HD3	0.57	1.77	5	1
1:A:45:ILE:HG12	1:A:58:ILE:CG2	0.57	2.30	4	3
1:A:34:VAL:O	1:A:38:ILE:HG12	0.57	1.99	5	5
1:A:137:GLU:O	1:A:156:ILE:HA	0.57	2.00	7	5
1:A:25:VAL:HG13	1:A:73:ILE:CG2	0.56	2.30	3	1
1:A:117:GLY:HA3	2:B:4:G:N7	0.56	2.14	5	1
1:A:58:ILE:HG13	1:A:69:ARG:HD3	0.56	1.76	11	1
1:A:56:ILE:HA	1:A:57:LYS:HE3	0.56	1.76	6	1
1:A:113:ALA:CB	1:A:146:PRO:HB3	0.55	2.31	5	3
1:A:87:ILE:O	1:A:91:LEU:HG	0.55	2.00	8	4
1:A:167:GLN:O	1:A:171:ARG:HG3	0.55	2.02	7	1
1:A:80:GLN:O	1:A:84:GLN:HB2	0.55	2.00	4	1
1:A:97:PHE:HB2	1:A:103:VAL:HG12	0.55	1.78	6	1
1:A:73:ILE:HD12	1:A:83:ALA:HB1	0.55	1.79	11	1
1:A:56:ILE:HA	1:A:57:LYS:CE	0.55	2.32	6	2
1:A:91:LEU:HB3	1:A:96:PHE:HB2	0.55	1.77	9	1
2:B:2:C:C5'	2:B:3:G:OP1	0.55	2.55	9	12
2:B:2:C:H5''	2:B:3:G:OP1	0.55	2.01	6	7
1:A:94:GLU:OE2	1:A:96:PHE:HD2	0.55	1.84	6	1
1:A:81:PHE:HA	1:A:84:GLN:HE21	0.54	1.62	8	1
1:A:113:ALA:HB1	1:A:146:PRO:HB3	0.54	1.78	5	1
1:A:171:ARG:HG3	1:A:172:ASP:N	0.54	2.17	4	2
1:A:58:ILE:HG13	1:A:58:ILE:O	0.54	2.02	4	1
1:A:171:ARG:HD3	1:A:174:LEU:HD12	0.54	1.80	10	1
1:A:57:LYS:HD3	1:A:73:ILE:CD1	0.54	2.32	6	1
1:A:80:GLN:O	1:A:84:GLN:HB3	0.54	2.03	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:LEU:HA	1:A:94:GLU:CD	0.54	2.21	6	1
1:A:139:VAL:HB	1:A:155:LYS:CG	0.54	2.32	10	1
2:B:7:U:C2'	2:B:7:U:O2	0.54	2.55	3	2
1:A:90:LYS:HA	1:A:93:GLU:HG2	0.54	1.79	1	6
1:A:26:HIS:HA	1:A:71:VAL:O	0.54	2.03	9	3
1:A:90:LYS:HD2	1:A:90:LYS:N	0.53	2.18	12	1
2:B:4:G:H4'	2:B:5:A:O4'	0.53	2.03	10	3
1:A:45:ILE:O	1:A:56:ILE:HD11	0.53	2.04	6	2
1:A:90:LYS:O	1:A:94:GLU:HB2	0.53	2.04	12	1
1:A:23:GLU:HG3	1:A:80:GLN:NE2	0.53	2.18	9	1
1:A:34:VAL:HG11	1:A:69:ARG:HD2	0.53	1.79	3	1
1:A:58:ILE:HB	1:A:70:MET:O	0.53	2.03	11	1
1:A:146:PRO:HB2	1:A:150:GLU:HA	0.53	1.79	6	1
2:B:1:U:O2	2:B:1:U:C3'	0.53	2.56	6	1
1:A:107:THR:O	1:A:155:LYS:HA	0.53	2.04	10	4
2:B:4:G:H4'	2:B:5:A:C5'	0.53	2.34	1	9
1:A:57:LYS:HD3	1:A:73:ILE:HD13	0.52	1.81	11	2
1:A:117:GLY:HA3	2:B:4:G:C6	0.52	2.39	3	1
1:A:91:LEU:HD12	1:A:103:VAL:HB	0.52	1.81	5	1
1:A:28:PHE:HB3	1:A:68:VAL:HB	0.52	1.80	11	1
1:A:120:ILE:HD13	1:A:140:VAL:HG23	0.52	1.81	7	1
1:A:118:ARG:HG3	1:A:173:ILE:CG2	0.52	2.35	9	2
1:A:52:ALA:HB1	1:A:79:ALA:HA	0.52	1.81	12	1
1:A:36:ALA:CB	1:A:94:GLU:HG2	0.52	2.34	5	2
1:A:28:PHE:HA	1:A:69:ARG:O	0.52	2.04	11	1
1:A:27:VAL:HG12	1:A:71:VAL:CG2	0.52	2.34	7	2
1:A:29:ILE:HG12	1:A:69:ARG:NE	0.51	2.20	11	1
1:A:172:ASP:O	1:A:176:GLN:HG2	0.51	2.04	3	1
1:A:41:ASP:HB3	1:A:44:HIS:HB2	0.51	1.80	2	3
1:A:146:PRO:HB3	1:A:150:GLU:HA	0.51	1.82	10	1
1:A:91:LEU:HD21	1:A:105:LEU:HD11	0.51	1.81	9	2
1:A:94:GLU:HG2	1:A:96:PHE:CE2	0.51	2.40	3	2
1:A:178:LYS:HA	1:A:178:LYS:HE2	0.51	1.82	11	1
1:A:82:LYS:O	1:A:86:ARG:HB2	0.51	2.05	6	2
1:A:31:ALA:O	1:A:34:VAL:HG22	0.51	2.06	9	3
1:A:27:VAL:HG13	1:A:71:VAL:CG2	0.51	2.36	6	1
1:A:59:ALA:HB1	1:A:69:ARG:HD2	0.51	1.83	5	1
1:A:27:VAL:HG13	1:A:71:VAL:HG22	0.51	1.81	6	2
1:A:91:LEU:HD22	1:A:96:PHE:CD2	0.51	2.41	10	3
1:A:110:ARG:HH11	1:A:110:ARG:HG3	0.51	1.64	8	1
1:A:172:ASP:O	1:A:176:GLN:HG3	0.51	2.06	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ILE:HA	1:A:57:LYS:HE2	0.51	1.81	11	1
1:A:119:VAL:HG11	1:A:154:VAL:HG11	0.51	1.83	4	1
1:A:90:LYS:O	1:A:93:GLU:HG2	0.51	2.06	4	2
1:A:116:ALA:O	1:A:119:VAL:HG12	0.50	2.06	4	3
2:B:4:G:H2'	2:B:4:G:N3	0.50	2.21	4	2
1:A:58:ILE:HG12	1:A:59:ALA:N	0.50	2.21	11	1
2:B:4:G:N3	2:B:4:G:H2'	0.50	2.21	6	3
1:A:170:ILE:O	1:A:174:LEU:HG	0.50	2.06	11	2
1:A:91:LEU:HB2	1:A:103:VAL:HG11	0.50	1.83	1	1
1:A:178:LYS:HA	1:A:178:LYS:CE	0.50	2.36	11	1
1:A:182:GLN:HG3	1:A:183:LYS:HG3	0.50	1.84	9	1
1:A:28:PHE:CE2	1:A:70:MET:HB3	0.50	2.42	7	3
2:B:1:U:O5'	2:B:2:C:H3'	0.50	2.07	6	1
1:A:137:GLU:HB3	1:A:157:ILE:HB	0.49	1.83	4	3
1:A:112:PRO:HD2	1:A:174:LEU:HD13	0.49	1.84	8	1
1:A:58:ILE:O	1:A:58:ILE:HG13	0.49	2.07	2	1
1:A:33:ALA:HB1	1:A:96:PHE:CE2	0.49	2.41	11	1
1:A:127:VAL:HG22	1:A:138:VAL:HB	0.49	1.83	12	1
1:A:58:ILE:HG22	1:A:71:VAL:HG12	0.49	1.83	12	1
1:A:91:LEU:HD12	1:A:96:PHE:CD2	0.49	2.42	9	1
1:A:150:GLU:O	1:A:150:GLU:HG3	0.49	2.05	11	1
1:A:124:GLY:HA3	2:B:5:A:O2'	0.49	2.06	12	1
1:A:155:LYS:HB3	1:A:157:ILE:HD11	0.49	1.84	9	1
1:A:118:ARG:CG	1:A:177:VAL:HG21	0.49	2.37	3	1
1:A:27:VAL:HB	1:A:71:VAL:CG2	0.49	2.37	12	1
1:A:118:ARG:HG3	1:A:173:ILE:HG22	0.49	1.83	8	1
1:A:104:LYS:HD3	1:A:157:ILE:CG2	0.49	2.38	11	1
1:A:24:THR:HA	1:A:73:ILE:O	0.49	2.08	10	3
1:A:134:THR:CG2	1:A:162:ALA:HA	0.49	2.37	3	2
2:B:6:C:C4	2:B:7:U:C5	0.48	3.01	1	1
1:A:146:PRO:HB3	1:A:152:VAL:HG13	0.48	1.85	8	1
1:A:33:ALA:HB1	1:A:96:PHE:CZ	0.48	2.43	11	2
1:A:142:ARG:HB2	2:B:5:A:H62	0.48	1.68	4	2
1:A:59:ALA:O	1:A:69:ARG:HD2	0.48	2.07	10	3
1:A:87:ILE:O	1:A:91:LEU:HD22	0.48	2.08	9	1
1:A:142:ARG:HG3	2:B:4:G:H21	0.48	1.67	5	1
1:A:25:VAL:CG2	1:A:73:ILE:HB	0.48	2.39	11	2
1:A:112:PRO:CD	1:A:174:LEU:HD21	0.48	2.39	1	1
1:A:25:VAL:HB	1:A:73:ILE:HB	0.48	1.86	12	1
1:A:91:LEU:HB3	1:A:97:PHE:CE1	0.48	2.43	5	1
1:A:36:ALA:O	1:A:40:ASP:HB2	0.48	2.08	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:PRO:CB	1:A:150:GLU:HA	0.47	2.38	6	2
1:A:111:VAL:HG11	1:A:170:ILE:HD11	0.47	1.83	2	1
1:A:58:ILE:HG22	1:A:71:VAL:CA	0.47	2.34	6	1
1:A:120:ILE:HD13	1:A:124:GLY:HA2	0.47	1.85	8	2
2:B:3:G:N3	2:B:4:G:C6	0.47	2.81	8	2
1:A:126:THR:O	1:A:130:LEU:HB2	0.47	2.08	12	1
1:A:37:ILE:HD11	1:A:87:ILE:HA	0.47	1.85	12	1
1:A:112:PRO:HD2	1:A:174:LEU:HD11	0.47	1.84	1	3
1:A:30:PRO:O	1:A:34:VAL:HG23	0.47	2.10	6	2
1:A:85:GLY:HA2	1:A:160:PHE:CE1	0.47	2.44	11	2
1:A:27:VAL:O	1:A:71:VAL:HG13	0.47	2.10	11	1
2:B:5:A:H2'	2:B:6:C:O4'	0.47	2.10	7	3
1:A:40:ASP:HB2	1:A:44:HIS:CB	0.47	2.39	5	2
1:A:90:LYS:O	1:A:93:GLU:HG3	0.47	2.09	2	1
1:A:58:ILE:HB	1:A:69:ARG:HD2	0.47	1.86	7	1
1:A:86:ARG:NE	1:A:86:ARG:HA	0.47	2.25	7	1
1:A:28:PHE:CE2	1:A:106:GLU:HB3	0.47	2.45	1	1
1:A:38:ILE:HD11	1:A:58:ILE:HD13	0.47	1.86	6	1
1:A:38:ILE:HD12	1:A:45:ILE:HG21	0.47	1.87	3	1
2:B:6:C:O2'	2:B:7:U:H5'	0.47	2.10	4	1
1:A:94:GLU:CD	1:A:96:PHE:CD2	0.47	2.87	6	1
1:A:131:GLN:HG2	1:A:137:GLU:HG3	0.47	1.85	2	1
1:A:130:LEU:HD21	1:A:166:ALA:HA	0.46	1.86	4	1
1:A:140:VAL:HB	1:A:141:PRO:HD2	0.46	1.86	2	2
1:A:120:ILE:HD11	1:A:124:GLY:HA2	0.46	1.86	2	1
1:A:127:VAL:O	1:A:131:GLN:HB2	0.46	2.09	9	1
1:A:142:ARG:HB2	2:B:5:A:N6	0.46	2.25	4	1
1:A:155:LYS:HD2	1:A:155:LYS:N	0.46	2.26	6	2
1:A:73:ILE:HD12	1:A:83:ALA:CB	0.46	2.39	11	1
1:A:88:TYR:O	1:A:92:LYS:HG2	0.46	2.10	10	1
1:A:85:GLY:HA2	1:A:160:PHE:HE1	0.46	1.70	11	1
1:A:120:ILE:HD13	1:A:120:ILE:O	0.46	2.10	8	2
1:A:119:VAL:CG2	1:A:170:ILE:HB	0.46	2.41	3	1
2:B:6:C:H2'	2:B:7:U:O4'	0.46	2.10	1	1
1:A:45:ILE:HG12	1:A:58:ILE:HD13	0.46	1.88	12	1
2:B:5:A:H8	2:B:5:A:O5'	0.46	1.94	7	1
1:A:54:ALA:HB2	1:A:79:ALA:CB	0.46	2.41	1	2
1:A:111:VAL:HG23	1:A:174:LEU:HD22	0.46	1.87	11	1
1:A:156:ILE:HD11	1:A:170:ILE:HD13	0.45	1.87	10	1
1:A:141:PRO:CG	1:A:152:VAL:HB	0.45	2.40	3	1
1:A:49:SER:HB2	1:A:56:ILE:HB	0.45	1.88	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:VAL:HG12	1:A:174:LEU:HD11	0.45	1.86	8	1
1:A:49:SER:HB2	1:A:56:ILE:HG22	0.45	1.89	10	1
1:A:135:ALA:O	1:A:158:GLY:HA3	0.45	2.10	10	1
1:A:96:PHE:HB3	1:A:97:PHE:CD2	0.45	2.47	1	1
1:A:112:PRO:HA	1:A:150:GLU:O	0.45	2.11	11	1
2:B:5:A:C6	2:B:6:C:N3	0.45	2.85	1	1
1:A:109:ILE:HG12	1:A:154:VAL:HG23	0.45	1.87	8	1
1:A:120:ILE:HA	1:A:126:THR:OG1	0.45	2.11	2	1
1:A:41:ASP:CB	1:A:44:HIS:HB2	0.45	2.42	2	1
1:A:140:VAL:HG12	1:A:154:VAL:HG12	0.45	1.88	4	1
1:A:37:ILE:O	1:A:44:HIS:HB3	0.45	2.11	12	2
1:A:57:LYS:CD	1:A:73:ILE:HD13	0.45	2.42	11	1
2:B:3:G:H1'	2:B:4:G:C5	0.45	2.47	6	3
1:A:56:ILE:CD1	1:A:57:LYS:H	0.45	2.25	11	1
1:A:56:ILE:CG1	1:A:57:LYS:H	0.45	2.24	11	1
1:A:58:ILE:O	1:A:60:PRO:HD3	0.45	2.12	12	1
1:A:26:HIS:O	1:A:108:HIS:HB2	0.44	2.12	3	1
1:A:112:PRO:CG	1:A:174:LEU:HD22	0.44	2.41	9	1
1:A:120:ILE:HD13	1:A:127:VAL:CG2	0.44	2.42	2	1
1:A:31:ALA:HA	1:A:34:VAL:HG23	0.44	1.88	2	2
1:A:90:LYS:O	1:A:90:LYS:HD3	0.44	2.12	1	4
1:A:125:LYS:O	1:A:129:GLU:HG3	0.44	2.13	8	1
1:A:111:VAL:HB	1:A:112:PRO:HD2	0.44	1.88	3	1
2:B:4:G:O2'	2:B:5:A:C8	0.44	2.67	11	1
1:A:120:ILE:O	1:A:126:THR:HB	0.44	2.12	10	1
1:A:40:ASP:HB3	1:A:44:HIS:HB3	0.44	1.90	2	1
1:A:142:ARG:HG3	2:B:5:A:H62	0.44	1.73	9	1
1:A:30:PRO:HA	1:A:68:VAL:HG12	0.44	1.89	4	1
1:A:90:LYS:HD3	1:A:90:LYS:O	0.44	2.12	10	1
1:A:117:GLY:O	1:A:120:ILE:HG22	0.44	2.13	6	2
1:A:79:ALA:HA	1:A:82:LYS:HG2	0.44	1.87	3	1
1:A:56:ILE:HD12	1:A:57:LYS:H	0.44	1.72	11	1
1:A:33:ALA:HB1	1:A:91:LEU:HD22	0.44	1.90	1	1
1:A:119:VAL:HG12	1:A:138:VAL:HG11	0.44	1.87	8	2
1:A:142:ARG:HG2	2:B:5:A:H62	0.44	1.72	2	1
1:A:50:ARG:N	1:A:50:ARG:HD2	0.44	2.27	3	1
1:A:86:ARG:O	1:A:86:ARG:HD3	0.44	2.13	3	2
1:A:140:VAL:CG1	1:A:141:PRO:HD2	0.44	2.38	6	1
1:A:127:VAL:HG13	1:A:137:GLU:HA	0.43	1.88	11	1
1:A:91:LEU:CD1	1:A:105:LEU:HD21	0.43	2.43	1	1
2:B:1:U:O4'	2:B:1:U:O2	0.43	2.36	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:ALA:O	1:A:179:GLN:HG3	0.43	2.13	3	2
1:A:112:PRO:HG3	1:A:178:LYS:HD3	0.43	1.88	10	1
1:A:30:PRO:HG2	1:A:97:PHE:CZ	0.43	2.48	7	1
1:A:49:SER:HB3	1:A:56:ILE:CG2	0.43	2.44	7	1
1:A:67:LYS:HB3	1:A:67:LYS:NZ	0.43	2.28	11	1
1:A:29:ILE:O	1:A:68:VAL:HB	0.43	2.12	5	1
1:A:90:LYS:HA	1:A:93:GLU:CG	0.43	2.43	5	1
1:A:34:VAL:CG1	1:A:69:ARG:HD3	0.43	2.43	7	1
1:A:73:ILE:CG2	1:A:80:GLN:HG2	0.43	2.43	4	1
1:A:49:SER:HB3	1:A:56:ILE:HG22	0.43	1.88	7	2
1:A:28:PHE:HB2	1:A:106:GLU:CG	0.43	2.43	3	1
1:A:56:ILE:O	1:A:72:VAL:CB	0.43	2.63	11	1
1:A:120:ILE:HG12	2:B:5:A:C2	0.43	2.48	7	1
2:B:3:G:O2'	2:B:4:G:C8	0.43	2.70	4	1
1:A:157:ILE:HD12	1:A:157:ILE:N	0.43	2.29	2	1
1:A:33:ALA:HA	1:A:96:PHE:CE2	0.43	2.49	3	1
1:A:23:GLU:HB3	1:A:75:GLY:O	0.43	2.13	9	1
1:A:38:ILE:HD11	1:A:58:ILE:CD1	0.43	2.43	6	1
1:A:38:ILE:HD11	1:A:69:ARG:NH1	0.43	2.27	7	1
1:A:155:LYS:HD3	1:A:155:LYS:N	0.43	2.28	4	1
1:A:80:GLN:O	1:A:84:GLN:HG2	0.43	2.14	8	1
1:A:29:ILE:HG22	1:A:105:LEU:HD13	0.43	1.91	3	1
1:A:120:ILE:HD13	1:A:140:VAL:HG13	0.43	1.91	1	1
1:A:48:LEU:HD23	1:A:56:ILE:CD1	0.43	2.43	9	1
1:A:168:ARG:O	1:A:171:ARG:HG2	0.43	2.14	6	1
1:A:94:GLU:CD	1:A:96:PHE:HD2	0.43	2.16	6	1
1:A:119:VAL:HG13	1:A:170:ILE:HG12	0.43	1.90	7	1
1:A:37:ILE:HD13	1:A:90:LYS:HG3	0.43	1.90	3	1
1:A:140:VAL:HG22	2:B:5:A:C2	0.42	2.48	11	1
1:A:34:VAL:HG13	1:A:69:ARG:HG2	0.42	1.90	11	1
2:B:5:A:C5	2:B:6:C:C4	0.42	3.07	1	1
1:A:87:ILE:HG22	1:A:105:LEU:HD11	0.42	1.90	12	1
2:B:1:U:O2	2:B:1:U:H5''	0.42	2.14	8	1
1:A:58:ILE:HA	1:A:70:MET:O	0.42	2.14	6	2
1:A:147:ASP:OD1	1:A:148:GLU:HG2	0.42	2.14	5	1
1:A:112:PRO:HG2	1:A:115:ALA:HB3	0.42	1.91	1	2
1:A:91:LEU:HD22	1:A:105:LEU:CD1	0.42	2.44	12	1
2:B:4:G:C4'	2:B:5:A:O5'	0.42	2.62	11	3
1:A:45:ILE:HD11	1:A:56:ILE:HG21	0.42	1.91	4	1
1:A:37:ILE:HG22	1:A:38:ILE:HD13	0.42	1.91	8	1
1:A:140:VAL:HG12	1:A:154:VAL:HG22	0.42	1.91	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ALA:CB	1:A:70:MET:HG2	0.42	2.45	7	1
1:A:37:ILE:HD13	1:A:90:LYS:HD2	0.42	1.90	9	2
1:A:118:ARG:HG3	1:A:177:VAL:HG21	0.42	1.90	3	1
1:A:38:ILE:HD11	1:A:58:ILE:HD12	0.42	1.92	11	1
1:A:160:PHE:O	1:A:164:GLN:HG2	0.42	2.15	1	1
1:A:38:ILE:HG23	1:A:45:ILE:HG21	0.42	1.91	9	1
1:A:57:LYS:HA	1:A:72:VAL:N	0.41	2.24	11	1
1:A:113:ALA:HB2	1:A:146:PRO:HB3	0.41	1.91	12	1
1:A:38:ILE:HD13	1:A:45:ILE:HB	0.41	1.92	12	1
1:A:43:GLN:HG2	1:A:46:LYS:HB2	0.41	1.91	2	1
1:A:97:PHE:CD1	1:A:103:VAL:HG12	0.41	2.49	1	1
1:A:111:VAL:HG23	1:A:152:VAL:HG23	0.41	1.91	4	1
2:B:4:G:O2'	2:B:5:A:P	0.41	2.78	4	1
1:A:25:VAL:HG22	1:A:73:ILE:HB	0.41	1.91	10	1
1:A:58:ILE:HB	1:A:70:MET:C	0.41	2.35	11	1
1:A:119:VAL:HG13	1:A:170:ILE:HB	0.41	1.91	12	1
2:B:4:G:HO2'	2:B:5:A:P	0.41	2.38	12	1
1:A:25:VAL:HG12	1:A:109:ILE:CG2	0.41	2.45	6	2
1:A:113:ALA:CB	1:A:152:VAL:HG13	0.41	2.46	8	1
1:A:89:GLY:O	1:A:93:GLU:HG2	0.41	2.16	12	1
1:A:163:SER:O	1:A:167:GLN:HG3	0.41	2.15	10	1
1:A:105:LEU:HA	1:A:105:LEU:HD23	0.41	1.74	12	1
1:A:37:ILE:HD13	1:A:37:ILE:HA	0.41	1.76	12	1
1:A:91:LEU:HB3	1:A:103:VAL:CG1	0.41	2.46	6	1
1:A:138:VAL:HA	1:A:155:LYS:O	0.41	2.15	8	1
1:A:57:LYS:HA	1:A:72:VAL:HB	0.41	1.92	6	1
1:A:97:PHE:HD2	1:A:103:VAL:HG12	0.41	1.73	7	1
1:A:83:ALA:O	1:A:87:ILE:HG13	0.41	2.16	7	1
1:A:92:LYS:HB3	1:A:92:LYS:NZ	0.41	2.30	4	1
1:A:120:ILE:CD1	1:A:124:GLY:HA2	0.41	2.44	8	1
1:A:58:ILE:HG13	1:A:69:ARG:CD	0.41	2.44	11	1
1:A:29:ILE:HB	1:A:30:PRO:CD	0.41	2.46	9	1
1:A:110:ARG:HH11	1:A:153:ILE:HD11	0.40	1.76	4	1
1:A:88:TYR:HA	1:A:91:LEU:CD2	0.40	2.46	9	1
1:A:97:PHE:CZ	1:A:103:VAL:CG1	0.40	3.04	4	1
1:A:76:PRO:HD2	1:A:79:ALA:HB3	0.40	1.93	10	1
1:A:86:ARG:C	1:A:86:ARG:HD3	0.40	2.37	10	1
1:A:56:ILE:CA	1:A:57:LYS:HE2	0.40	2.47	11	1
1:A:169:LYS:HE3	1:A:169:LYS:CA	0.40	2.44	12	1
1:A:83:ALA:O	1:A:86:ARG:HB3	0.40	2.17	4	1
1:A:23:GLU:O	1:A:74:THR:HA	0.40	2.17	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ILE:HB	1:A:30:PRO:HD2	0.40	1.91	9	1
1:A:90:LYS:O	1:A:94:GLU:HG2	0.40	2.16	7	1
1:A:130:LEU:HD21	1:A:166:ALA:CB	0.40	2.46	4	1
1:A:115:ALA:HB1	1:A:177:VAL:HG11	0.40	1.92	8	1
1:A:34:VAL:HG21	1:A:69:ARG:CB	0.40	2.45	4	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	147/191 (77%)	140±2 (95±1%)	6±2 (4±1%)	1±1 (1±1%)	30	75
All	All	1764/2292 (77%)	1680 (95%)	71 (4%)	13 (1%)	30	75

All 5 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	40	ASP	6
1	A	112	PRO	3
1	A	183	LYS	2
1	A	141	PRO	1
1	A	147	ASP	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	120/154 (78%)	113±2 (94±2%)	7±2 (6±2%)	27	73
All	All	1440/1848 (78%)	1355 (94%)	85 (6%)	27	73

All 42 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	86	ARG	7
1	A	97	PHE	5
1	A	34	VAL	4
1	A	109	ILE	4
1	A	120	ILE	4
1	A	159	HIS	4
1	A	155	LYS	4
1	A	25	VAL	3
1	A	48	LEU	3
1	A	57	LYS	3
1	A	142	ARG	3
1	A	58	ILE	3
1	A	91	LEU	3
1	A	71	VAL	2
1	A	69	ARG	2
1	A	94	GLU	2
1	A	92	LYS	2
1	A	147	ASP	2
1	A	149	ASN	2
1	A	104	LYS	1
1	A	93	GLU	1
1	A	165	MET	1
1	A	169	LYS	1
1	A	78	GLU	1
1	A	170	ILE	1
1	A	129	GLU	1
1	A	130	LEU	1
1	A	95	ASN	1
1	A	88	TYR	1
1	A	168	ARG	1
1	A	126	THR	1
1	A	111	VAL	1
1	A	178	LYS	1
1	A	32	GLN	1
1	A	90	LYS	1
1	A	152	VAL	1
1	A	140	VAL	1
1	A	134	THR	1
1	A	49	SER	1
1	A	131	GLN	1
1	A	132	ASN	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	182	GLN	1

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	6/7 (86%)	4±0 (68±8%)	0±0 (0±0%)	0.14±0.05
All	All	72/84 (86%)	49 (68%)	0 (0%)	0.14

The overall RNA backbone suiteness is 0.14.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	5	A	12
2	B	2	C	12
2	B	3	G	12
2	B	7	U	7
2	B	4	G	6

There are no RNA pucker outliers to report.

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

The completeness of assignment taking into account all chemical shift lists is 54% for the well-defined parts and 50% for the entire structure.

7.1 Chemical shift list 1

File name: 2n8m_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1440
Number of shifts mapped to atoms	1436
Number of unparsed shifts	4
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 4 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1385	A	57	LYS	HG2	1.294	0.003	.
1386	A	57	LYS	HG3	1.210	0.005	.
1400	A	30	PRO	HG2	2.093	0.001	.
1401	A	30	PRO	HG3	1.791	0.003	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	119	-0.30 ± 0.34	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	133	0.15 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

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 54%, i.e. 1064 atoms were assigned a chemical shift out of a possible 1982. 18 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	335/721 (46%)	230/287 (80%)	105/294 (36%)	0/140 (0%)
Sidechain	705/1020 (69%)	442/597 (74%)	263/369 (71%)	0/54 (0%)
Aromatic	24/110 (22%)	24/58 (41%)	0/42 (0%)	0/10 (0%)
Overall	1064/1982 (54%)	696/1017 (68%)	368/752 (49%)	0/213 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 1218 atoms were assigned a chemical shift out of a possible 2442. 18 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	381/927 (41%)	262/368 (71%)	119/382 (31%)	0/177 (0%)
Sidechain	809/1256 (64%)	514/741 (69%)	295/455 (65%)	0/60 (0%)
Aromatic	28/128 (22%)	28/68 (41%)	0/50 (0%)	0/10 (0%)
Overall	1218/2442 (50%)	804/1252 (64%)	414/934 (44%)	0/256 (0%)

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:

