Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 02:54 PM BST

PDB ID	:	1FI6
Title	:	SOLUTION STRUCTURE OF THE REPS1 EH DOMAIN
Authors	:	Kim, S.; Baleja, J.D.
Deposited on	:	2000-08-03

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 (i) symbol.

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

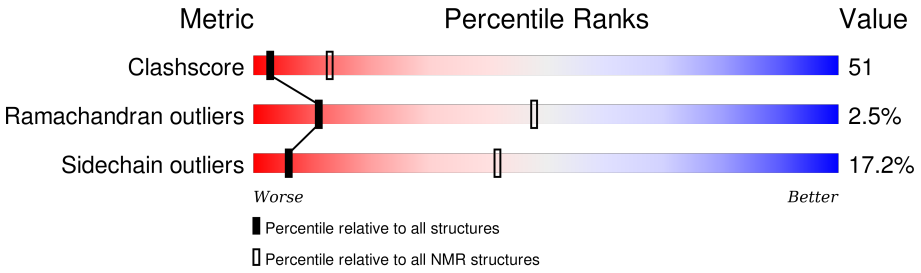
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	92	17% 59% • 20%

2 Ensemble composition and analysis

This entry contains 30 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:8-A:81 (74)	0.45	20

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 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 6, 7, 12, 13, 15, 16, 17, 20, 21, 22, 23, 24, 27, 29, 30
2	5, 9, 10, 18, 25, 28
3	3, 11
4	4, 19
Single-model clusters	2; 8; 14; 26

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1497 atoms, of which 743 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called EH DOMAIN PROTEIN REPS1.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1496	491	743	120	140	2	

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

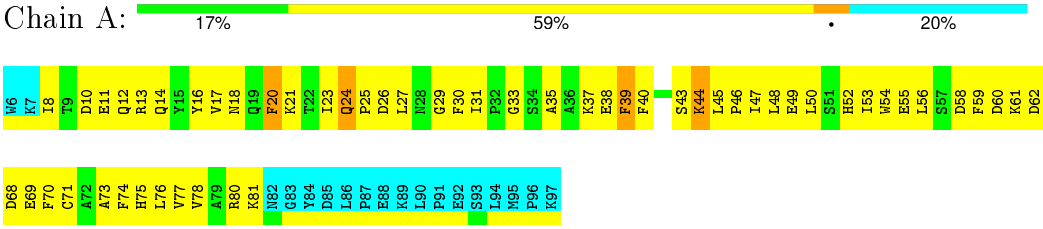
4 Residue-property plots

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: EH DOMAIN PROTEIN REPS1

Chain A:



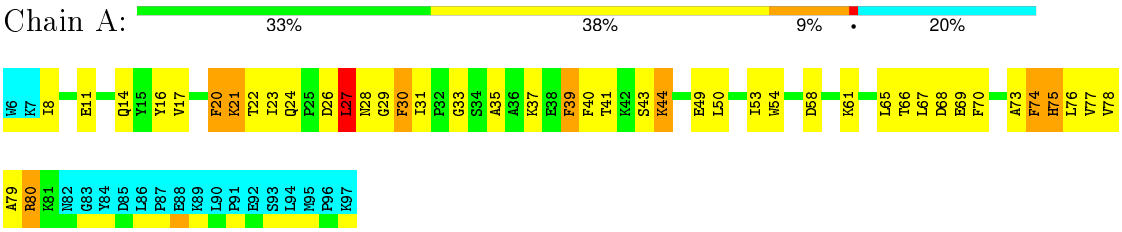
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: EH DOMAIN PROTEIN REPS1

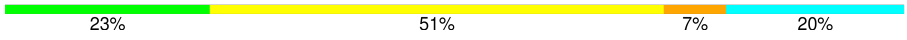
Chain A:

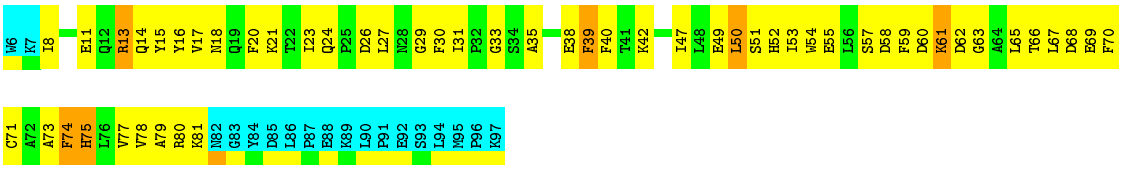


4.2.2 Score per residue for model 2

• Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

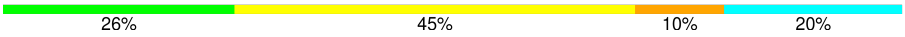


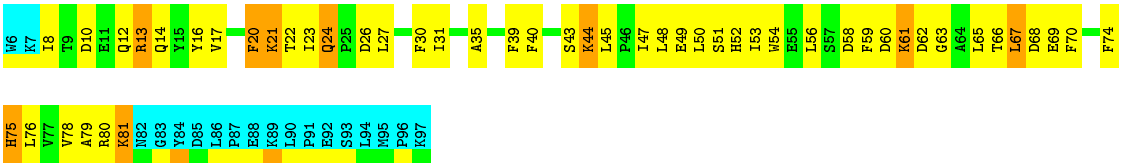


4.2.3 Score per residue for model 3

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

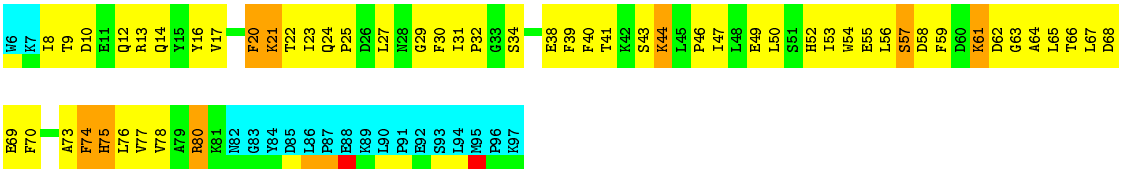




4.2.4 Score per residue for model 4

- Molecule 1: EH DOMAIN PROTEIN REPS1

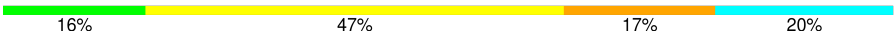
Chain A:

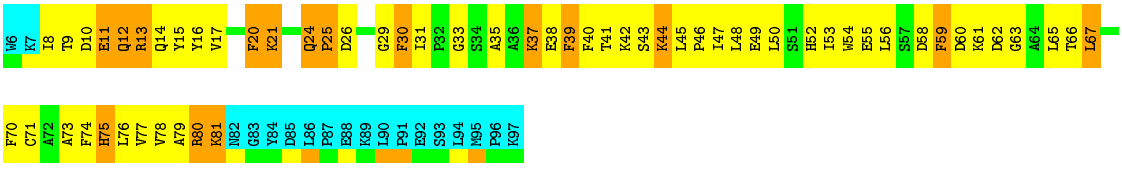


4.2.5 Score per residue for model 5

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

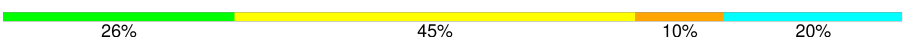


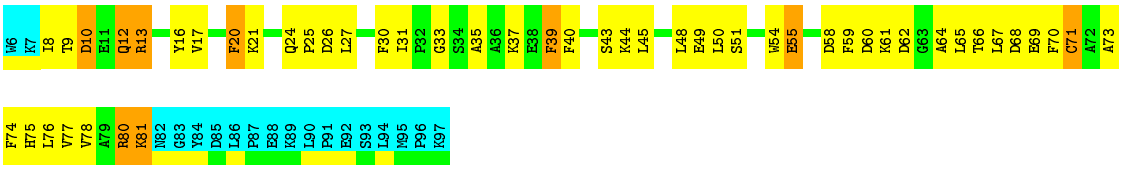


4.2.6 Score per residue for model 6

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

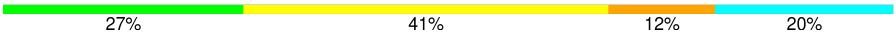


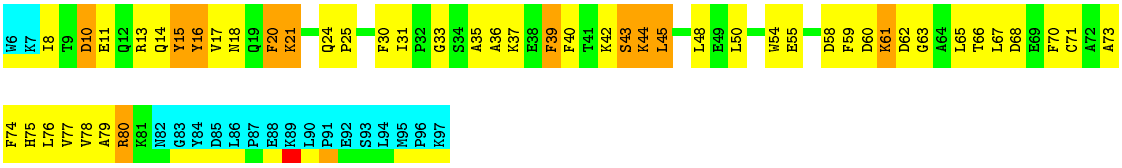


4.2.7 Score per residue for model 7

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

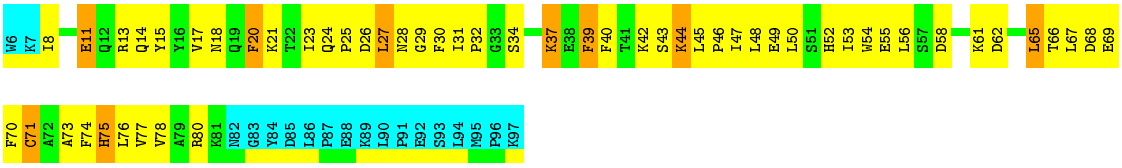




4.2.8 Score per residue for model 8

- Molecule 1: EH DOMAIN PROTEIN REPS1

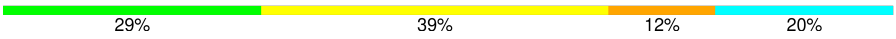
Chain A:

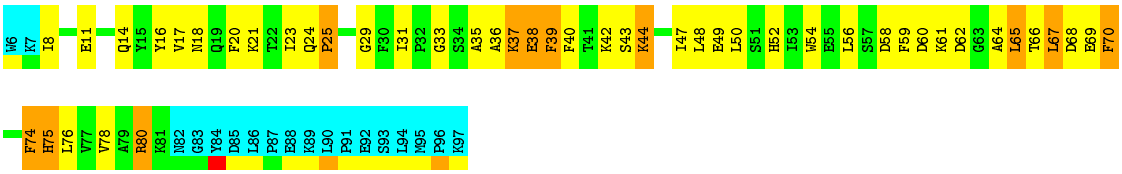


4.2.9 Score per residue for model 9

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

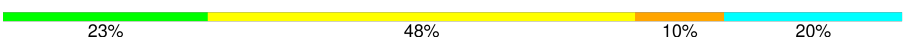


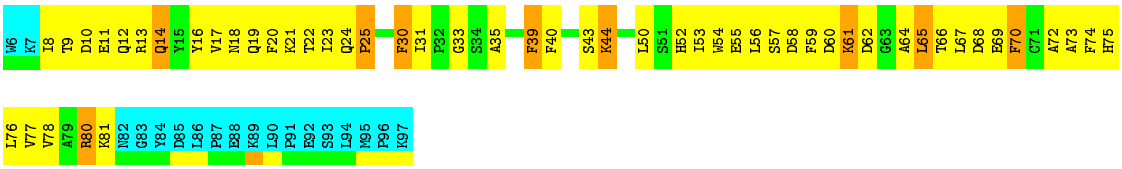


4.2.10 Score per residue for model 10

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

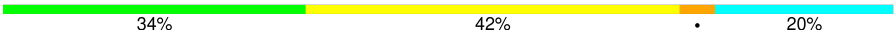


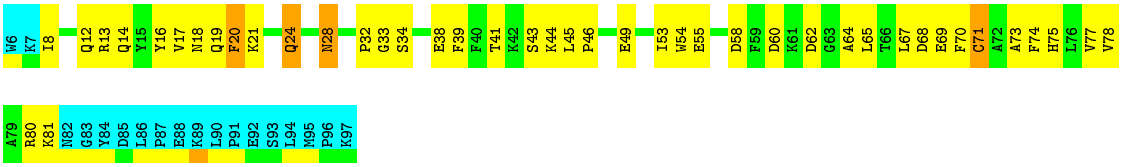


4.2.11 Score per residue for model 11

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

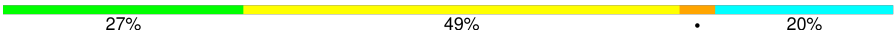


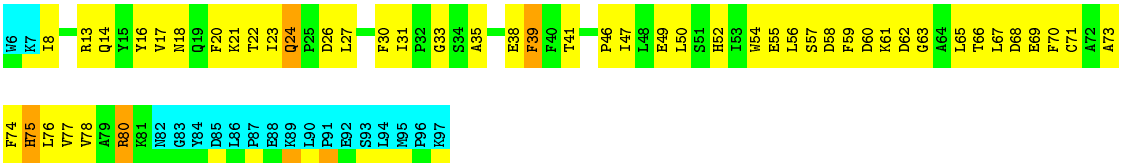


4.2.12 Score per residue for model 12

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

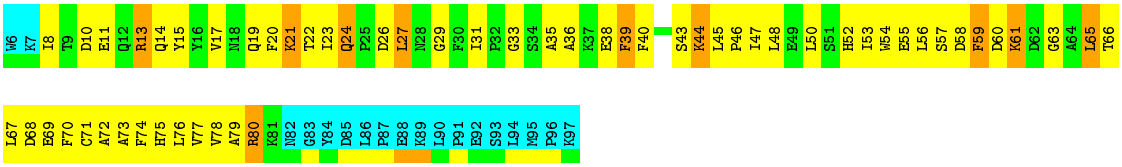




4.2.13 Score per residue for model 13

- Molecule 1: EH DOMAIN PROTEIN REPS1

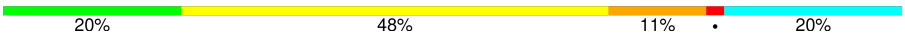
Chain A:

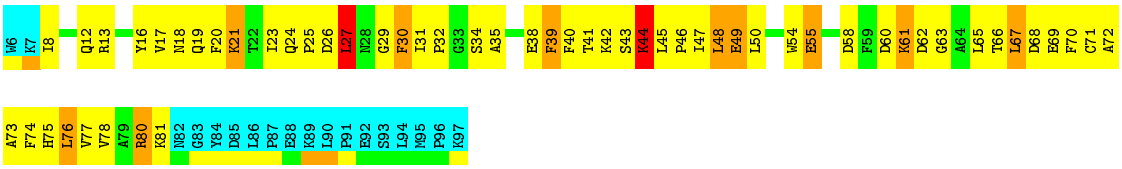


4.2.14 Score per residue for model 14

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

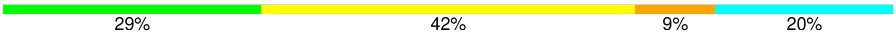


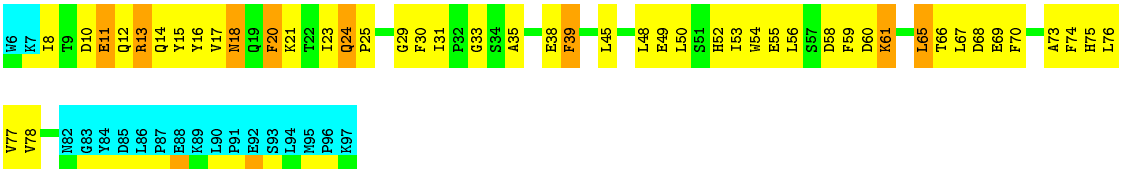


4.2.15 Score per residue for model 15

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

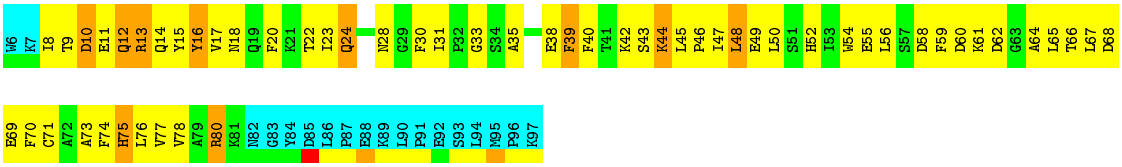




4.2.16 Score per residue for model 16

- Molecule 1: EH DOMAIN PROTEIN REPS1

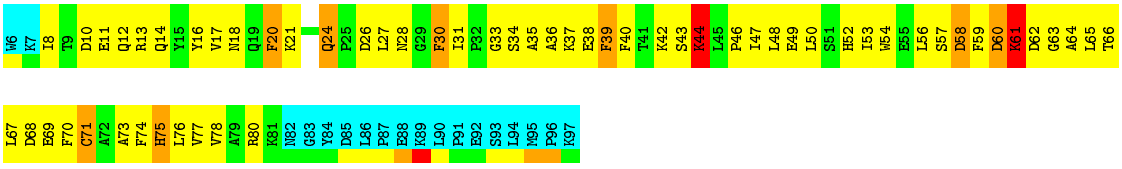
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: EH DOMAIN PROTEIN REPS1

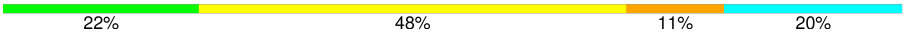
Chain A:

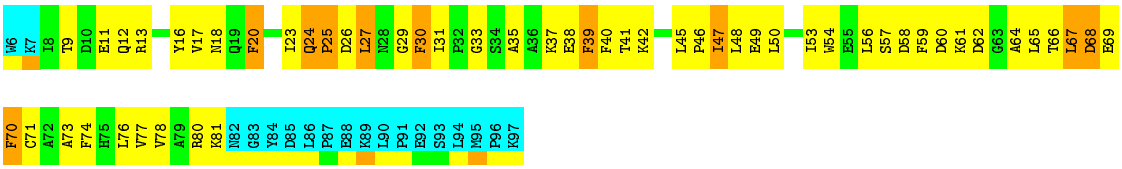


4.2.18 Score per residue for model 18

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

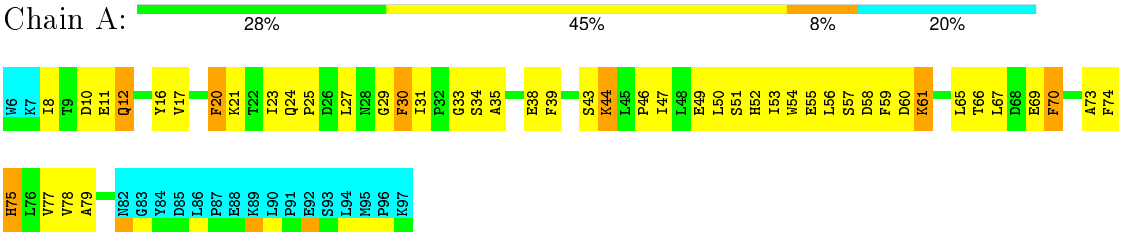




4.2.19 Score per residue for model 19

- Molecule 1: EH DOMAIN PROTEIN REPS1

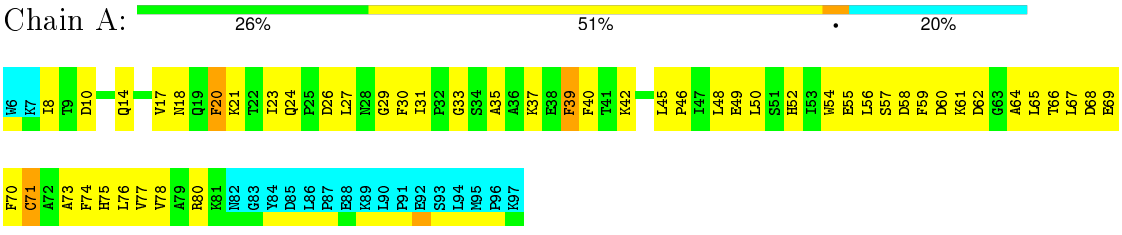
Chain A:



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: EH DOMAIN PROTEIN REPS1

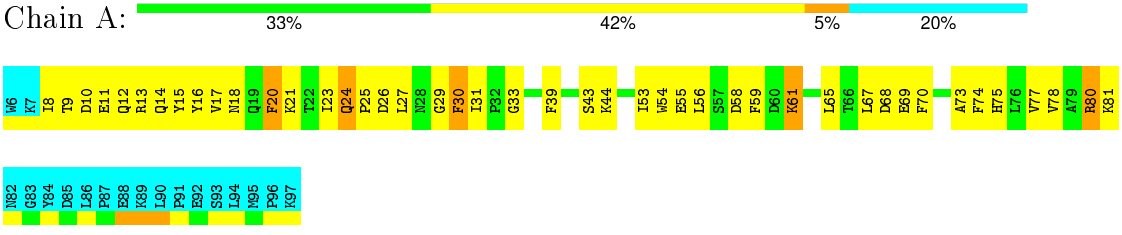
Chain A:



4.2.21 Score per residue for model 21

- Molecule 1: EH DOMAIN PROTEIN REPS1

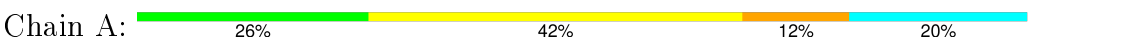
Chain A:

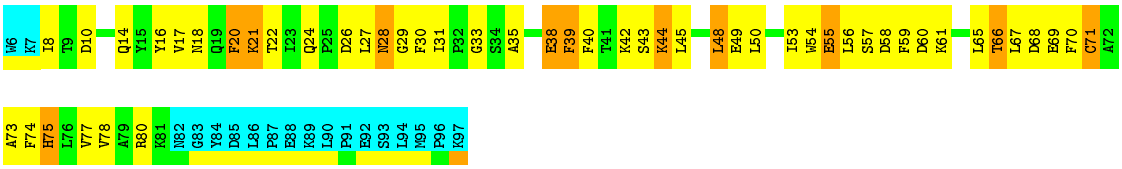


4.2.22 Score per residue for model 22

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

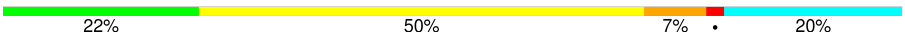


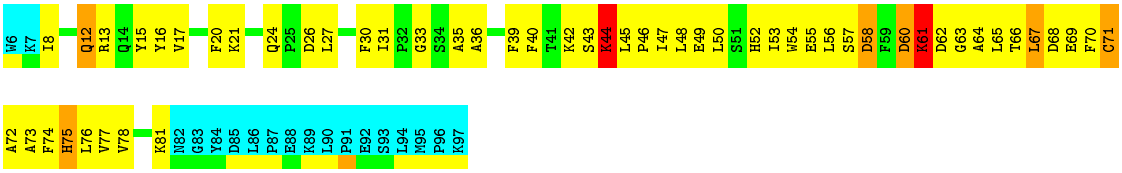


4.2.23 Score per residue for model 23

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

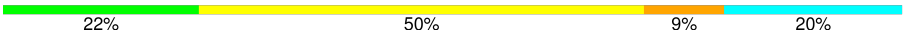


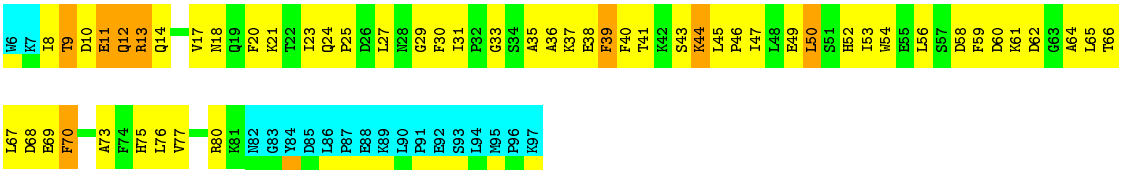


4.2.24 Score per residue for model 24

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

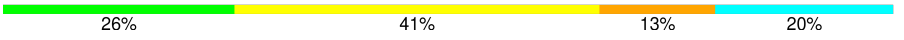


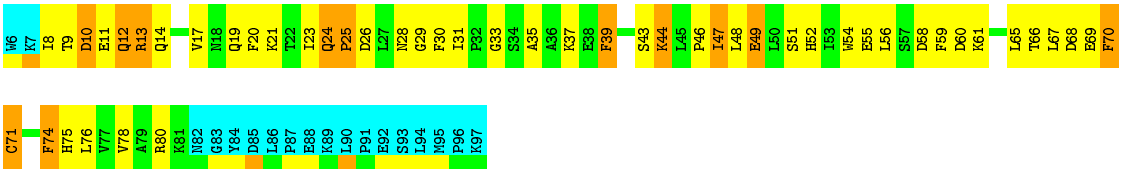


4.2.25 Score per residue for model 25

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:

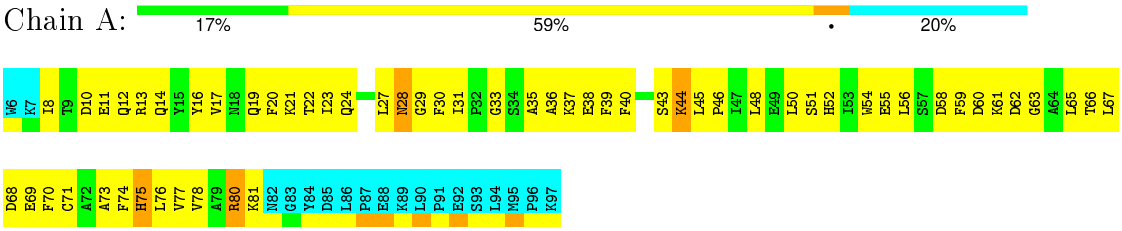




4.2.26 Score per residue for model 26

- Molecule 1: EH DOMAIN PROTEIN REPS1

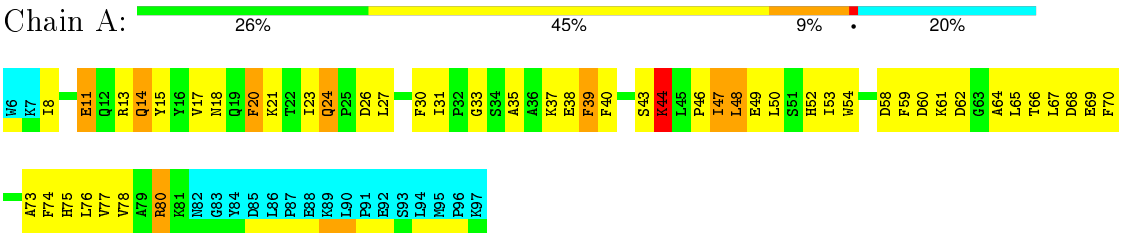
Chain A:



4.2.27 Score per residue for model 27

- Molecule 1: EH DOMAIN PROTEIN REPS1

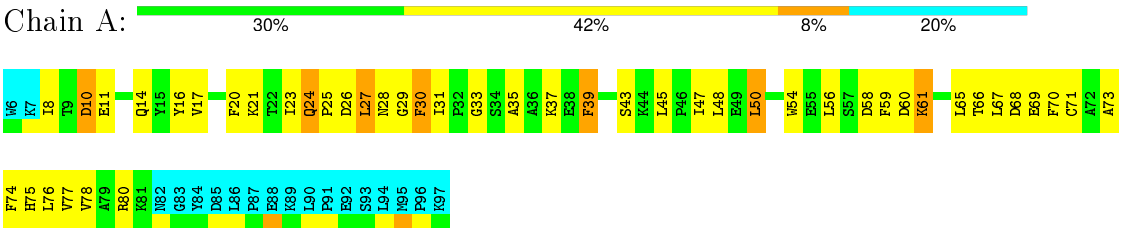
Chain A:



4.2.28 Score per residue for model 28

- Molecule 1: EH DOMAIN PROTEIN REPS1

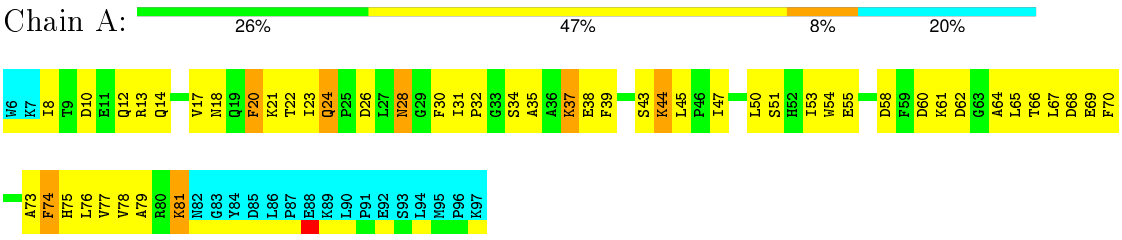
Chain A:



4.2.29 Score per residue for model 29

- Molecule 1: EH DOMAIN PROTEIN REPS1

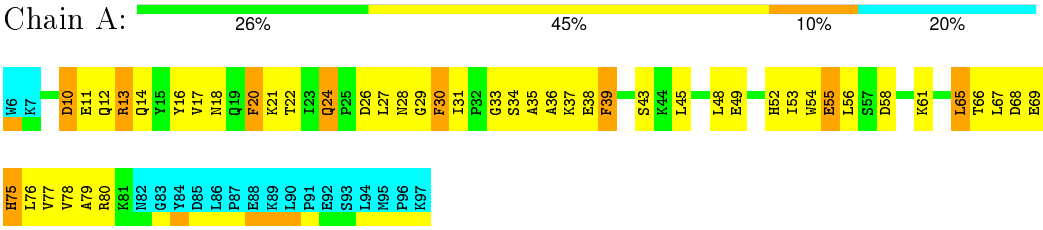
Chain A:



4.2.30 Score per residue for model 30

- Molecule 1: EH DOMAIN PROTEIN REPS1

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 30 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
X-plor	structure solution	3.1
X-plor	refinement	3.1

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)	BMRB entry 4778
Number of chemical shift lists	1
Total number of shifts	533
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	533
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	602	590	590	61±7
All	All	18090	17700	17700	1820

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 51.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:HD13	1:A:77:VAL:HG22	1.03	1.30	13	15
1:A:50:LEU:HD13	1:A:53:ILE:HD12	0.98	1.33	10	2
1:A:53:ILE:HD12	1:A:77:VAL:HG22	0.96	1.36	23	1
1:A:30:PHE:CD1	1:A:66:THR:HG22	0.91	2.01	12	8
1:A:47:ILE:HD12	1:A:47:ILE:H	0.91	1.22	27	8
1:A:45:LEU:HD21	1:A:80:ARG:HG2	0.91	1.41	18	2
1:A:54:TRP:CH2	1:A:65:LEU:HD13	0.90	2.02	26	29
1:A:31:ILE:HG23	1:A:35:ALA:HB3	0.86	1.47	22	21
1:A:81:LYS:HA	1:A:81:LYS:HE2	0.85	1.47	29	1
1:A:44:LYS:HA	1:A:44:LYS:HE2	0.85	1.47	17	1
1:A:54:TRP:CZ3	1:A:65:LEU:HD13	0.84	2.08	25	27
1:A:65:LEU:HG	1:A:69:GLU:HB3	0.84	1.49	26	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:GLU:OE1	1:A:42:LYS:NZ	0.84	2.10	17	1
1:A:17:VAL:HG12	1:A:21:LYS:CG	0.84	2.02	24	7
1:A:8:ILE:HG23	1:A:75:HIS:CD2	0.83	2.09	4	14
1:A:43:SER:HB3	1:A:45:LEU:HD13	0.83	1.50	30	2
1:A:66:THR:HG23	1:A:69:GLU:OE2	0.83	1.73	2	1
1:A:73:ALA:O	1:A:77:VAL:HG23	0.82	1.74	21	27
1:A:46:PRO:HG2	1:A:49:GLU:OE1	0.81	1.74	4	5
1:A:65:LEU:HA	1:A:69:GLU:OE1	0.81	1.75	30	20
1:A:13:ARG:O	1:A:17:VAL:HG23	0.81	1.74	7	19
1:A:74:PHE:O	1:A:78:VAL:HG23	0.81	1.76	11	28
1:A:52:HIS:CE1	1:A:56:LEU:HD11	0.80	2.12	12	10
1:A:37:LYS:HE3	1:A:50:LEU:HB3	0.80	1.53	20	1
1:A:10:ASP:OD1	1:A:13:ARG:NH1	0.78	2.16	6	3
1:A:21:LYS:HD2	1:A:22:THR:N	0.78	1.92	13	3
1:A:55:GLU:OE2	1:A:61:LYS:HE2	0.78	1.78	30	2
1:A:21:LYS:HD3	1:A:25:PRO:HB3	0.78	1.53	25	1
1:A:55:GLU:OE2	1:A:61:LYS:NZ	0.77	2.17	10	1
1:A:55:GLU:OE2	1:A:61:LYS:CE	0.77	2.33	30	1
1:A:20:PHE:CG	1:A:70:PHE:CZ	0.77	2.73	25	30
1:A:17:VAL:HG12	1:A:21:LYS:HG3	0.76	1.54	24	10
1:A:42:LYS:HB3	1:A:42:LYS:NZ	0.76	1.95	23	2
1:A:58:ASP:OD2	1:A:61:LYS:HA	0.75	1.82	26	17
1:A:9:THR:HG22	1:A:11:GLU:OE1	0.75	1.82	10	3
1:A:46:PRO:O	1:A:50:LEU:HD13	0.75	1.81	19	7
1:A:67:LEU:HD13	1:A:67:LEU:O	0.74	1.82	21	7
1:A:38:GLU:OE2	1:A:42:LYS:NZ	0.74	2.20	9	1
1:A:42:LYS:NZ	1:A:42:LYS:HB3	0.74	1.98	2	2
1:A:45:LEU:HD21	1:A:80:ARG:NH2	0.74	1.98	5	1
1:A:47:ILE:H	1:A:47:ILE:HD12	0.74	1.42	16	1
1:A:40:PHE:CB	1:A:50:LEU:HD11	0.73	2.12	14	4
1:A:80:ARG:NH1	1:A:80:ARG:HG3	0.73	1.97	26	1
1:A:43:SER:HB2	1:A:45:LEU:HD13	0.72	1.60	11	1
1:A:37:LYS:HG3	1:A:47:ILE:HG13	0.72	1.61	8	1
1:A:43:SER:O	1:A:44:LYS:HB2	0.72	1.82	26	16
1:A:40:PHE:CE1	1:A:77:VAL:HG21	0.72	2.19	17	5
1:A:37:LYS:NZ	1:A:50:LEU:O	0.72	2.23	20	1
1:A:80:ARG:HH11	1:A:80:ARG:HG3	0.72	1.45	26	1
1:A:46:PRO:HG2	1:A:49:GLU:OE2	0.72	1.85	12	1
1:A:30:PHE:CE1	1:A:66:THR:HG22	0.71	2.20	26	2
1:A:48:LEU:HD23	1:A:48:LEU:C	0.71	2.04	15	3
1:A:80:ARG:HE	1:A:80:ARG:HA	0.71	1.43	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:TYR:CD1	1:A:17:VAL:N	0.71	2.59	16	8
1:A:54:TRP:CZ2	1:A:65:LEU:HD13	0.71	2.20	26	9
1:A:20:PHE:HB3	1:A:70:PHE:CZ	0.71	2.19	26	2
1:A:45:LEU:HD21	1:A:80:ARG:CZ	0.71	2.15	5	1
1:A:49:GLU:OE2	1:A:80:ARG:NH1	0.70	2.23	5	2
1:A:55:GLU:OE1	1:A:61:LYS:NZ	0.70	2.19	21	2
1:A:61:LYS:NZ	1:A:61:LYS:HB3	0.70	2.01	2	2
1:A:33:GLY:HA2	1:A:54:TRP:CZ3	0.70	2.21	24	24
1:A:8:ILE:HG12	1:A:75:HIS:CD2	0.70	2.21	8	18
1:A:78:VAL:O	1:A:81:LYS:HG3	0.70	1.86	11	1
1:A:65:LEU:HG	1:A:69:GLU:CB	0.70	2.16	2	7
1:A:81:LYS:CA	1:A:81:LYS:HE2	0.70	2.17	29	1
1:A:40:PHE:HB2	1:A:50:LEU:HD11	0.69	1.64	18	2
1:A:49:GLU:OE1	1:A:49:GLU:HA	0.69	1.87	2	2
1:A:65:LEU:HD12	1:A:69:GLU:OE1	0.69	1.87	30	5
1:A:17:VAL:O	1:A:21:LYS:HG3	0.69	1.88	24	6
1:A:13:ARG:HD2	1:A:71:CYS:SG	0.69	2.28	6	2
1:A:57:SER:O	1:A:69:GLU:HG2	0.69	1.86	17	6
1:A:21:LYS:NZ	1:A:25:PRO:O	0.68	2.26	21	1
1:A:66:THR:HG22	1:A:69:GLU:HG3	0.68	1.63	4	3
1:A:26:ASP:C	1:A:67:LEU:HD12	0.68	2.09	23	3
1:A:30:PHE:HD2	1:A:66:THR:HG22	0.68	1.48	7	3
1:A:44:LYS:HD3	1:A:44:LYS:O	0.68	1.87	11	1
1:A:40:PHE:CE2	1:A:77:VAL:HG21	0.68	2.24	1	4
1:A:9:THR:HB	1:A:12:GLN:OE1	0.68	1.89	4	1
1:A:17:VAL:HG13	1:A:25:PRO:HA	0.68	1.66	10	3
1:A:20:PHE:HB3	1:A:70:PHE:CE2	0.67	2.24	26	4
1:A:60:ASP:O	1:A:61:LYS:HB2	0.67	1.89	2	16
1:A:20:PHE:CB	1:A:70:PHE:CZ	0.67	2.77	26	30
1:A:47:ILE:HA	1:A:50:LEU:HD22	0.67	1.67	9	4
1:A:62:ASP:OD2	1:A:64:ALA:HB3	0.67	1.90	9	9
1:A:10:ASP:OD2	1:A:14:GLN:NE2	0.67	2.27	10	2
1:A:14:GLN:OE1	1:A:18:ASN:ND2	0.67	2.28	8	2
1:A:8:ILE:HG23	1:A:75:HIS:CE1	0.67	2.25	24	2
1:A:21:LYS:HG2	1:A:25:PRO:HB3	0.67	1.66	10	2
1:A:8:ILE:HA	1:A:75:HIS:NE2	0.67	2.05	5	9
1:A:30:PHE:CD2	1:A:66:THR:HG22	0.66	2.24	17	4
1:A:17:VAL:HG12	1:A:21:LYS:HG2	0.66	1.67	25	2
1:A:24:GLN:NE2	1:A:29:GLY:C	0.66	2.49	25	12
1:A:67:LEU:HD13	1:A:67:LEU:C	0.66	2.11	4	4
1:A:18:ASN:O	1:A:21:LYS:HE2	0.66	1.90	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:GLN:OE1	1:A:29:GLY:HA3	0.66	1.90	22	4
1:A:8:ILE:HG23	1:A:75:HIS:NE2	0.66	2.06	1	3
1:A:24:GLN:HE21	1:A:24:GLN:HA	0.66	1.51	11	7
1:A:10:ASP:O	1:A:14:GLN:HG2	0.66	1.91	28	7
1:A:67:LEU:O	1:A:67:LEU:HD13	0.65	1.90	7	6
1:A:81:LYS:HD3	1:A:81:LYS:C	0.65	2.10	3	1
1:A:52:HIS:O	1:A:56:LEU:HD13	0.65	1.91	20	4
1:A:66:THR:CG2	1:A:69:GLU:HG3	0.65	2.21	24	3
1:A:30:PHE:CD1	1:A:30:PHE:N	0.65	2.65	19	7
1:A:11:GLU:O	1:A:14:GLN:HG3	0.65	1.91	7	4
1:A:67:LEU:HD23	1:A:67:LEU:O	0.65	1.92	26	2
1:A:40:PHE:HB3	1:A:50:LEU:HD21	0.65	1.69	3	2
1:A:21:LYS:HD2	1:A:21:LYS:C	0.65	2.12	1	1
1:A:58:ASP:OD1	1:A:61:LYS:N	0.65	2.30	27	4
1:A:56:LEU:O	1:A:59:PHE:CE1	0.64	2.50	10	9
1:A:24:GLN:OE1	1:A:31:ILE:HG13	0.64	1.92	26	5
1:A:41:THR:N	1:A:50:LEU:HD21	0.64	2.07	1	3
1:A:37:LYS:HD3	1:A:47:ILE:HD11	0.64	1.68	9	1
1:A:47:ILE:N	1:A:47:ILE:HD12	0.64	2.07	17	1
1:A:47:ILE:CD1	1:A:47:ILE:H	0.64	2.06	2	5
1:A:54:TRP:CE2	1:A:65:LEU:HD13	0.64	2.27	24	2
1:A:51:SER:O	1:A:55:GLU:HG3	0.64	1.93	25	2
1:A:67:LEU:O	1:A:70:PHE:HB3	0.64	1.92	8	8
1:A:47:ILE:HD12	1:A:47:ILE:N	0.64	2.08	2	5
1:A:11:GLU:O	1:A:14:GLN:HG2	0.63	1.92	17	7
1:A:67:LEU:C	1:A:67:LEU:HD13	0.63	2.13	15	6
1:A:53:ILE:CD1	1:A:77:VAL:HG22	0.63	2.17	13	1
1:A:46:PRO:C	1:A:50:LEU:HD13	0.63	2.13	23	1
1:A:72:ALA:O	1:A:76:LEU:HB2	0.63	1.93	14	4
1:A:55:GLU:N	1:A:55:GLU:OE1	0.63	2.32	15	2
1:A:20:PHE:HB2	1:A:70:PHE:CZ	0.63	2.28	15	26
1:A:66:THR:N	1:A:69:GLU:OE1	0.63	2.32	29	5
1:A:16:TYR:OH	1:A:78:VAL:HG21	0.63	1.93	11	3
1:A:20:PHE:CD2	1:A:70:PHE:CE1	0.63	2.86	2	3
1:A:46:PRO:HG2	1:A:49:GLU:CG	0.63	2.23	11	2
1:A:57:SER:OG	1:A:73:ALA:HB2	0.62	1.94	12	5
1:A:80:ARG:O	1:A:80:ARG:NE	0.62	2.32	7	4
1:A:58:ASP:HA	1:A:69:GLU:OE2	0.62	1.93	13	7
1:A:55:GLU:O	1:A:61:LYS:NZ	0.62	2.32	29	3
1:A:41:THR:HA	1:A:45:LEU:O	0.62	1.94	14	2
1:A:17:VAL:CG1	1:A:21:LYS:HG3	0.62	2.24	14	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ASP:CG	1:A:14:GLN:NE2	0.62	2.53	10	1
1:A:40:PHE:O	1:A:43:SER:HB3	0.62	1.93	24	7
1:A:80:ARG:HG2	1:A:80:ARG:HH11	0.62	1.54	25	3
1:A:49:GLU:O	1:A:53:ILE:HG13	0.62	1.95	11	4
1:A:81:LYS:HD2	1:A:81:LYS:C	0.62	2.15	10	1
1:A:54:TRP:O	1:A:58:ASP:N	0.62	2.33	24	19
1:A:37:LYS:NZ	1:A:51:SER:HA	0.62	2.10	6	1
1:A:58:ASP:OD2	1:A:61:LYS:CA	0.61	2.48	26	7
1:A:49:GLU:N	1:A:49:GLU:OE1	0.61	2.33	24	2
1:A:28:ASN:O	1:A:28:ASN:ND2	0.61	2.33	26	2
1:A:33:GLY:O	1:A:37:LYS:HB2	0.61	1.95	30	7
1:A:20:PHE:CB	1:A:70:PHE:CE2	0.61	2.82	7	21
1:A:58:ASP:O	1:A:61:LYS:NZ	0.61	2.32	7	3
1:A:45:LEU:CD1	1:A:77:VAL:HG13	0.61	2.25	24	2
1:A:24:GLN:OE1	1:A:67:LEU:HA	0.61	1.94	20	2
1:A:24:GLN:HA	1:A:24:GLN:HE21	0.61	1.54	17	2
1:A:16:TYR:CD1	1:A:70:PHE:CE2	0.61	2.87	7	5
1:A:10:ASP:O	1:A:13:ARG:HB3	0.61	1.96	26	4
1:A:49:GLU:OE1	1:A:80:ARG:NH1	0.61	2.34	5	2
1:A:21:LYS:C	1:A:21:LYS:HD2	0.61	2.15	13	3
1:A:70:PHE:CD1	1:A:70:PHE:C	0.61	2.74	9	7
1:A:10:ASP:OD1	1:A:14:GLN:NE2	0.61	2.34	10	1
1:A:43:SER:O	1:A:44:LYS:CB	0.61	2.49	16	13
1:A:62:ASP:OD1	1:A:63:GLY:N	0.60	2.34	5	6
1:A:27:LEU:HD12	1:A:67:LEU:HD13	0.60	1.72	19	3
1:A:38:GLU:O	1:A:42:LYS:HG3	0.60	1.96	22	2
1:A:49:GLU:O	1:A:53:ILE:HG12	0.60	1.95	3	1
1:A:16:TYR:CE2	1:A:71:CYS:SG	0.60	2.95	22	1
1:A:17:VAL:CG1	1:A:21:LYS:HG2	0.60	2.26	6	2
1:A:52:HIS:O	1:A:56:LEU:HD23	0.60	1.95	16	2
1:A:12:GLN:O	1:A:15:TYR:HB3	0.60	1.96	21	1
1:A:26:ASP:CA	1:A:67:LEU:HD13	0.60	2.26	18	1
1:A:46:PRO:CG	1:A:49:GLU:OE2	0.60	2.50	12	1
1:A:38:GLU:N	1:A:38:GLU:OE1	0.60	2.34	14	1
1:A:13:ARG:HG2	1:A:13:ARG:HH11	0.60	1.56	2	1
1:A:31:ILE:HG22	1:A:36:ALA:HB2	0.60	1.73	30	1
1:A:18:ASN:O	1:A:21:LYS:HE3	0.60	1.97	12	2
1:A:24:GLN:NE2	1:A:29:GLY:O	0.60	2.34	8	8
1:A:48:LEU:HD23	1:A:48:LEU:O	0.60	1.97	28	3
1:A:12:GLN:NE2	1:A:75:HIS:NE2	0.59	2.50	15	3
1:A:24:GLN:HG2	1:A:67:LEU:HD23	0.59	1.73	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:LEU:O	1:A:67:LEU:HD23	0.59	1.97	19	5
1:A:27:LEU:N	1:A:27:LEU:HD12	0.59	2.12	4	2
1:A:42:LYS:HB3	1:A:42:LYS:HZ3	0.59	1.58	14	2
1:A:26:ASP:O	1:A:27:LEU:O	0.58	2.21	14	2
1:A:19:GLN:O	1:A:22:THR:HG22	0.58	1.97	26	1
1:A:22:THR:HG23	1:A:23:ILE:HG13	0.58	1.75	1	3
1:A:24:GLN:HE22	1:A:29:GLY:C	0.58	2.02	4	1
1:A:42:LYS:NZ	1:A:42:LYS:CB	0.58	2.67	14	2
1:A:16:TYR:CE1	1:A:17:VAL:HG22	0.58	2.33	23	8
1:A:22:THR:HB	1:A:23:ILE:HD12	0.58	1.74	12	1
1:A:47:ILE:O	1:A:50:LEU:HB2	0.58	1.99	9	3
1:A:21:LYS:HG2	1:A:25:PRO:HA	0.58	1.73	14	2
1:A:52:HIS:CE1	1:A:56:LEU:CD1	0.58	2.86	12	7
1:A:26:ASP:CG	1:A:27:LEU:H	0.58	2.01	6	5
1:A:31:ILE:HG23	1:A:35:ALA:CB	0.58	2.26	6	2
1:A:24:GLN:NE2	1:A:29:GLY:HA3	0.58	2.12	9	4
1:A:27:LEU:N	1:A:67:LEU:CD1	0.58	2.66	18	1
1:A:24:GLN:CG	1:A:67:LEU:HG	0.58	2.29	8	1
1:A:24:GLN:NE2	1:A:29:GLY:CA	0.58	2.67	9	5
1:A:49:GLU:HG2	1:A:80:ARG:CD	0.58	2.29	14	1
1:A:49:GLU:CD	1:A:80:ARG:NH1	0.58	2.56	5	1
1:A:54:TRP:CE3	1:A:65:LEU:HD13	0.58	2.34	19	3
1:A:34:SER:O	1:A:38:GLU:HB2	0.57	1.99	17	3
1:A:53:ILE:HD11	1:A:80:ARG:HH21	0.57	1.60	24	1
1:A:16:TYR:CE1	1:A:17:VAL:CG2	0.57	2.88	23	3
1:A:24:GLN:OE1	1:A:31:ILE:N	0.57	2.37	13	2
1:A:52:HIS:HA	1:A:55:GLU:OE1	0.57	1.98	23	2
1:A:46:PRO:O	1:A:48:LEU:N	0.57	2.38	25	3
1:A:76:LEU:HD23	1:A:76:LEU:O	0.57	2.00	20	7
1:A:16:TYR:C	1:A:16:TYR:CD1	0.57	2.78	16	5
1:A:17:VAL:HG12	1:A:21:LYS:HB3	0.57	1.75	8	2
1:A:47:ILE:H	1:A:47:ILE:CD1	0.57	2.02	27	3
1:A:42:LYS:HB3	1:A:42:LYS:HZ2	0.57	1.60	23	1
1:A:30:PHE:N	1:A:30:PHE:CD1	0.57	2.73	21	8
1:A:23:ILE:HG21	1:A:31:ILE:HG12	0.57	1.77	27	15
1:A:10:ASP:OD1	1:A:13:ARG:HD2	0.57	2.00	10	2
1:A:58:ASP:O	1:A:61:LYS:HD2	0.57	2.00	29	2
1:A:51:SER:HB3	1:A:55:GLU:OE2	0.57	2.00	19	1
1:A:35:ALA:O	1:A:39:PHE:HB2	0.56	1.99	15	14
1:A:11:GLU:O	1:A:15:TYR:HB2	0.56	2.00	2	4
1:A:62:ASP:OD1	1:A:64:ALA:N	0.56	2.39	17	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:SER:O	1:A:45:LEU:HD12	0.56	2.00	7	1
1:A:18:ASN:HB3	1:A:19:GLN:NE2	0.56	2.15	14	1
1:A:54:TRP:NE1	1:A:58:ASP:OD2	0.56	2.38	30	2
1:A:80:ARG:NE	1:A:80:ARG:O	0.56	2.38	21	1
1:A:54:TRP:HZ2	1:A:63:GLY:C	0.56	2.04	17	5
1:A:10:ASP:CG	1:A:13:ARG:HH21	0.56	2.03	24	1
1:A:78:VAL:O	1:A:81:LYS:HG2	0.56	2.00	18	1
1:A:49:GLU:CD	1:A:80:ARG:NE	0.56	2.59	30	1
1:A:52:HIS:HA	1:A:55:GLU:OE2	0.56	1.99	13	1
1:A:78:VAL:O	1:A:81:LYS:HB3	0.56	2.00	23	3
1:A:24:GLN:OE1	1:A:29:GLY:CA	0.56	2.54	21	4
1:A:62:ASP:CG	1:A:63:GLY:N	0.56	2.59	14	2
1:A:60:ASP:OD1	1:A:61:LYS:N	0.56	2.39	6	9
1:A:53:ILE:CG1	1:A:80:ARG:NH2	0.56	2.69	24	1
1:A:30:PHE:CE2	1:A:66:THR:HG22	0.56	2.36	3	1
1:A:27:LEU:H	1:A:27:LEU:HD12	0.56	1.60	4	1
1:A:55:GLU:O	1:A:61:LYS:HE2	0.56	2.01	26	1
1:A:24:GLN:HE21	1:A:24:GLN:CA	0.56	2.13	29	3
1:A:23:ILE:HD12	1:A:23:ILE:N	0.56	2.16	12	1
1:A:23:ILE:N	1:A:23:ILE:HD12	0.56	2.15	2	3
1:A:61:LYS:HZ2	1:A:61:LYS:HB3	0.56	1.58	2	1
1:A:23:ILE:HD11	1:A:39:PHE:CZ	0.56	2.36	2	1
1:A:17:VAL:HG12	1:A:21:LYS:HE3	0.56	1.78	10	1
1:A:48:LEU:CD2	1:A:48:LEU:C	0.55	2.75	15	2
1:A:48:LEU:HB3	1:A:49:GLU:OE1	0.55	2.02	9	1
1:A:10:ASP:CG	1:A:14:GLN:HE22	0.55	2.04	10	1
1:A:8:ILE:HG12	1:A:75:HIS:NE2	0.55	2.17	21	2
1:A:45:LEU:CB	1:A:50:LEU:HD11	0.55	2.31	15	2
1:A:76:LEU:O	1:A:76:LEU:HD23	0.55	2.02	27	10
1:A:75:HIS:O	1:A:78:VAL:HB	0.55	2.02	5	10
1:A:13:ARG:HH11	1:A:13:ARG:CG	0.55	2.15	25	2
1:A:48:LEU:C	1:A:48:LEU:HD23	0.55	2.22	18	3
1:A:53:ILE:HG21	1:A:77:VAL:HG22	0.55	1.79	27	1
1:A:56:LEU:O	1:A:59:PHE:CD1	0.55	2.60	17	5
1:A:20:PHE:CE1	1:A:39:PHE:CD1	0.55	2.94	28	6
1:A:49:GLU:HG2	1:A:80:ARG:HD3	0.55	1.78	14	1
1:A:31:ILE:CG2	1:A:36:ALA:HB2	0.55	2.32	30	1
1:A:38:GLU:O	1:A:41:THR:HB	0.55	2.02	11	3
1:A:12:GLN:O	1:A:16:TYR:CD2	0.54	2.60	30	2
1:A:13:ARG:HD3	1:A:26:ASP:OD2	0.54	2.01	5	1
1:A:46:PRO:CG	1:A:49:GLU:OE1	0.54	2.55	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:CYS:O	1:A:75:HIS:HB2	0.54	2.03	11	2
1:A:78:VAL:O	1:A:81:LYS:HB2	0.54	2.01	14	1
1:A:22:THR:CG2	1:A:23:ILE:HD12	0.54	2.32	26	1
1:A:8:ILE:HG12	1:A:75:HIS:CG	0.54	2.38	6	1
1:A:52:HIS:CD2	1:A:80:ARG:CZ	0.54	2.91	2	1
1:A:58:ASP:O	1:A:61:LYS:HD3	0.54	2.03	19	1
1:A:58:ASP:OD2	1:A:62:ASP:N	0.54	2.41	11	3
1:A:13:ARG:HG3	1:A:71:CYS:SG	0.54	2.43	8	2
1:A:26:ASP:C	1:A:67:LEU:HD13	0.54	2.23	18	1
1:A:13:ARG:HG3	1:A:13:ARG:HH11	0.54	1.61	16	1
1:A:24:GLN:CA	1:A:24:GLN:HE21	0.54	2.15	3	2
1:A:49:GLU:OE2	1:A:80:ARG:NE	0.54	2.41	20	2
1:A:24:GLN:HE22	1:A:30:PHE:HA	0.54	1.63	23	1
1:A:58:ASP:O	1:A:61:LYS:CE	0.54	2.56	7	1
1:A:10:ASP:HA	1:A:13:ARG:HB2	0.54	1.80	24	1
1:A:13:ARG:CG	1:A:13:ARG:NH1	0.54	2.70	25	2
1:A:17:VAL:O	1:A:21:LYS:CG	0.53	2.56	8	6
1:A:20:PHE:CD2	1:A:70:PHE:CZ	0.53	2.96	2	10
1:A:80:ARG:HH11	1:A:80:ARG:CG	0.53	2.15	26	1
1:A:18:ASN:O	1:A:21:LYS:NZ	0.53	2.29	8	1
1:A:24:GLN:HG2	1:A:67:LEU:HA	0.53	1.79	8	1
1:A:16:TYR:CE2	1:A:74:PHE:HD2	0.53	2.21	19	1
1:A:21:LYS:HG2	1:A:25:PRO:CA	0.53	2.33	14	2
1:A:11:GLU:O	1:A:14:GLN:CG	0.53	2.56	1	3
1:A:31:ILE:CG2	1:A:35:ALA:HB3	0.53	2.33	18	4
1:A:70:PHE:C	1:A:70:PHE:CD1	0.53	2.82	18	8
1:A:40:PHE:CD2	1:A:77:VAL:HG21	0.53	2.37	1	1
1:A:53:ILE:HD13	1:A:77:VAL:CG2	0.53	2.21	13	3
1:A:44:LYS:CE	1:A:44:LYS:O	0.53	2.56	3	1
1:A:61:LYS:NZ	1:A:61:LYS:CB	0.53	2.71	2	2
1:A:60:ASP:O	1:A:61:LYS:CB	0.53	2.57	17	3
1:A:20:PHE:CE1	1:A:39:PHE:CD2	0.53	2.97	25	11
1:A:12:GLN:HB3	1:A:16:TYR:CZ	0.53	2.39	3	1
1:A:43:SER:CB	1:A:45:LEU:HD13	0.53	2.29	30	3
1:A:18:ASN:O	1:A:21:LYS:CE	0.53	2.57	11	1
1:A:12:GLN:NE2	1:A:75:HIS:CE1	0.53	2.77	29	3
1:A:16:TYR:CG	1:A:74:PHE:CD1	0.53	2.97	28	1
1:A:49:GLU:OE2	1:A:80:ARG:NH2	0.53	2.41	20	3
1:A:24:GLN:NE2	1:A:24:GLN:HA	0.53	2.19	30	4
1:A:10:ASP:HA	1:A:13:ARG:HB3	0.53	1.81	15	2
1:A:37:LYS:HE3	1:A:47:ILE:CG2	0.52	2.34	24	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LYS:HG2	1:A:47:ILE:HG23	0.52	1.80	29	1
1:A:26:ASP:O	1:A:67:LEU:HD12	0.52	2.04	6	1
1:A:61:LYS:HB3	1:A:61:LYS:HZ2	0.52	1.63	30	1
1:A:24:GLN:HG3	1:A:67:LEU:HD23	0.52	1.80	5	3
1:A:81:LYS:C	1:A:81:LYS:HD2	0.52	2.25	6	1
1:A:66:THR:HG22	1:A:69:GLU:CG	0.52	2.34	10	1
1:A:12:GLN:HE22	1:A:75:HIS:CE1	0.52	2.23	25	3
1:A:53:ILE:HG13	1:A:80:ARG:NH2	0.52	2.19	24	1
1:A:27:LEU:HD12	1:A:27:LEU:N	0.52	2.19	23	5
1:A:26:ASP:O	1:A:28:ASN:N	0.52	2.43	8	1
1:A:13:ARG:HH11	1:A:13:ARG:CB	0.52	2.18	25	1
1:A:16:TYR:CE1	1:A:70:PHE:CE2	0.52	2.98	16	1
1:A:17:VAL:O	1:A:21:LYS:HB3	0.52	2.05	13	7
1:A:27:LEU:HD23	1:A:27:LEU:H	0.52	1.65	28	1
1:A:16:TYR:CE1	1:A:74:PHE:CD1	0.52	2.98	30	4
1:A:27:LEU:H	1:A:27:LEU:CD1	0.52	2.18	4	1
1:A:46:PRO:O	1:A:47:ILE:C	0.51	2.49	25	3
1:A:36:ALA:O	1:A:40:PHE:HD2	0.51	1.89	9	3
1:A:40:PHE:O	1:A:43:SER:N	0.51	2.43	24	4
1:A:23:ILE:O	1:A:25:PRO:HD3	0.51	2.05	8	2
1:A:49:GLU:CG	1:A:80:ARG:HD2	0.51	2.35	14	1
1:A:10:ASP:OD1	1:A:13:ARG:HD3	0.51	2.05	21	1
1:A:66:THR:HG22	1:A:69:GLU:OE1	0.51	2.05	22	2
1:A:58:ASP:C	1:A:60:ASP:N	0.51	2.64	23	9
1:A:48:LEU:HD22	1:A:49:GLU:OE2	0.51	2.06	9	1
1:A:49:GLU:OE1	1:A:80:ARG:NE	0.51	2.42	30	3
1:A:38:GLU:O	1:A:42:LYS:HG2	0.51	2.05	16	1
1:A:24:GLN:HA	1:A:24:GLN:OE1	0.51	2.05	6	3
1:A:58:ASP:O	1:A:60:ASP:N	0.51	2.43	16	6
1:A:27:LEU:HA	1:A:67:LEU:HD12	0.51	1.82	24	3
1:A:14:GLN:NE2	1:A:15:TYR:N	0.51	2.59	13	2
1:A:44:LYS:HE3	1:A:44:LYS:O	0.51	2.06	3	1
1:A:76:LEU:C	1:A:76:LEU:HD23	0.51	2.26	12	11
1:A:22:THR:HG23	1:A:23:ILE:HD12	0.51	1.82	26	1
1:A:57:SER:O	1:A:69:GLU:CG	0.51	2.59	10	1
1:A:37:LYS:HE3	1:A:47:ILE:HG23	0.50	1.82	24	1
1:A:57:SER:CB	1:A:65:LEU:HD11	0.50	2.37	23	1
1:A:58:ASP:O	1:A:61:LYS:CD	0.50	2.59	29	1
1:A:17:VAL:O	1:A:21:LYS:HB2	0.50	2.05	20	2
1:A:30:PHE:CD2	1:A:66:THR:HB	0.50	2.41	18	1
1:A:16:TYR:CD1	1:A:16:TYR:N	0.50	2.78	10	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLU:OE1	1:A:80:ARG:HD2	0.50	2.05	12	1
1:A:60:ASP:N	1:A:60:ASP:OD1	0.50	2.42	19	4
1:A:18:ASN:O	1:A:21:LYS:HG2	0.50	2.06	30	2
1:A:28:ASN:ND2	1:A:28:ASN:O	0.50	2.44	29	3
1:A:17:VAL:O	1:A:21:LYS:CB	0.50	2.60	5	5
1:A:45:LEU:HD11	1:A:77:VAL:HG13	0.50	1.84	24	1
1:A:23:ILE:CG2	1:A:31:ILE:HG12	0.50	2.36	4	3
1:A:46:PRO:HG2	1:A:49:GLU:HG3	0.50	1.84	11	1
1:A:23:ILE:O	1:A:25:PRO:HD2	0.50	2.07	4	3
1:A:54:TRP:CD2	1:A:65:LEU:HD13	0.50	2.42	16	2
1:A:53:ILE:HG21	1:A:77:VAL:CG2	0.50	2.36	27	2
1:A:81:LYS:HD2	1:A:81:LYS:O	0.50	2.07	6	1
1:A:16:TYR:CZ	1:A:78:VAL:HG21	0.49	2.42	28	1
1:A:23:ILE:C	1:A:25:PRO:HD3	0.49	2.27	4	3
1:A:11:GLU:OE1	1:A:11:GLU:N	0.49	2.43	21	2
1:A:10:ASP:OD1	1:A:13:ARG:CD	0.49	2.59	3	1
1:A:52:HIS:NE2	1:A:56:LEU:HD11	0.49	2.21	15	2
1:A:46:PRO:HG2	1:A:49:GLU:CD	0.49	2.27	18	1
1:A:37:LYS:O	1:A:50:LEU:CD2	0.49	2.60	1	1
1:A:45:LEU:HD12	1:A:45:LEU:H	0.49	1.66	29	1
1:A:66:THR:O	1:A:69:GLU:N	0.49	2.45	2	11
1:A:23:ILE:C	1:A:25:PRO:CD	0.49	2.80	4	2
1:A:54:TRP:CZ2	1:A:65:LEU:CD1	0.49	2.94	26	1
1:A:49:GLU:OE1	1:A:80:ARG:NH2	0.49	2.43	6	2
1:A:31:ILE:HD12	1:A:70:PHE:CG	0.49	2.42	26	1
1:A:37:LYS:CG	1:A:47:ILE:HG13	0.49	2.35	8	1
1:A:65:LEU:HG	1:A:69:GLU:HB2	0.49	1.83	1	1
1:A:13:ARG:NH1	1:A:13:ARG:HG2	0.49	2.22	25	1
1:A:52:HIS:CE1	1:A:56:LEU:HD21	0.49	2.42	16	2
1:A:61:LYS:CD	1:A:61:LYS:O	0.49	2.61	23	1
1:A:30:PHE:HD1	1:A:66:THR:HG22	0.49	1.67	20	3
1:A:45:LEU:HD21	1:A:77:VAL:HG13	0.49	1.82	20	1
1:A:11:GLU:N	1:A:11:GLU:OE1	0.49	2.44	25	2
1:A:40:PHE:O	1:A:43:SER:HB2	0.49	2.08	14	2
1:A:12:GLN:OE1	1:A:75:HIS:CE1	0.49	2.66	19	1
1:A:24:GLN:OE1	1:A:29:GLY:C	0.49	2.51	21	2
1:A:22:THR:HG23	1:A:23:ILE:CD1	0.48	2.38	26	1
1:A:49:GLU:CG	1:A:80:ARG:CD	0.48	2.91	14	1
1:A:36:ALA:O	1:A:40:PHE:CD2	0.48	2.66	7	3
1:A:9:THR:O	1:A:12:GLN:N	0.48	2.46	24	3
1:A:16:TYR:HB3	1:A:70:PHE:CZ	0.48	2.43	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASP:OD1	1:A:60:ASP:N	0.48	2.46	29	3
1:A:54:TRP:CZ3	1:A:65:LEU:HD22	0.48	2.43	8	2
1:A:42:LYS:HZ2	1:A:42:LYS:HB3	0.48	1.67	2	1
1:A:16:TYR:N	1:A:16:TYR:CD1	0.48	2.77	28	3
1:A:80:ARG:HG3	1:A:80:ARG:HH11	0.48	1.68	30	1
1:A:76:LEU:HD23	1:A:76:LEU:C	0.48	2.29	23	4
1:A:24:GLN:HB2	1:A:70:PHE:CD2	0.48	2.43	26	1
1:A:67:LEU:C	1:A:67:LEU:CD1	0.48	2.82	4	5
1:A:57:SER:O	1:A:69:GLU:HB3	0.48	2.09	20	1
1:A:55:GLU:HA	1:A:55:GLU:OE1	0.48	2.08	10	1
1:A:25:PRO:HD2	1:A:27:LEU:CD2	0.48	2.39	18	1
1:A:66:THR:O	1:A:67:LEU:C	0.48	2.51	26	22
1:A:24:GLN:OE1	1:A:31:ILE:CG1	0.48	2.61	28	1
1:A:67:LEU:HD22	1:A:70:PHE:HD2	0.48	1.68	22	3
1:A:27:LEU:HA	1:A:67:LEU:CD1	0.48	2.38	24	2
1:A:24:GLN:CD	1:A:29:GLY:O	0.48	2.52	26	2
1:A:80:ARG:O	1:A:81:LYS:C	0.48	2.52	6	1
1:A:61:LYS:O	1:A:61:LYS:HD2	0.48	2.09	17	1
1:A:21:LYS:C	1:A:21:LYS:CD	0.47	2.82	3	1
1:A:26:ASP:CA	1:A:67:LEU:CD1	0.47	2.92	18	1
1:A:16:TYR:CD1	1:A:16:TYR:C	0.47	2.87	14	2
1:A:49:GLU:OE1	1:A:49:GLU:N	0.47	2.41	8	2
1:A:14:GLN:OE1	1:A:15:TYR:N	0.47	2.47	27	1
1:A:10:ASP:CG	1:A:13:ARG:HH22	0.47	2.11	5	1
1:A:13:ARG:CD	1:A:26:ASP:OD2	0.47	2.63	5	1
1:A:16:TYR:OH	1:A:71:CYS:SG	0.47	2.72	17	2
1:A:66:THR:OG1	1:A:69:GLU:HG3	0.47	2.09	1	2
1:A:37:LYS:NZ	1:A:54:TRP:CB	0.47	2.78	18	1
1:A:26:ASP:N	1:A:67:LEU:HD11	0.47	2.24	18	1
1:A:26:ASP:HA	1:A:67:LEU:HD13	0.47	1.85	18	1
1:A:66:THR:HG23	1:A:69:GLU:H	0.47	1.69	14	3
1:A:81:LYS:CE	1:A:81:LYS:CA	0.47	2.91	29	1
1:A:29:GLY:C	1:A:30:PHE:CD1	0.47	2.88	2	4
1:A:26:ASP:OD1	1:A:27:LEU:N	0.47	2.48	8	5
1:A:25:PRO:HG2	1:A:27:LEU:CD2	0.47	2.39	28	1
1:A:17:VAL:O	1:A:21:LYS:N	0.47	2.45	19	4
1:A:16:TYR:CB	1:A:74:PHE:CE2	0.47	2.98	5	1
1:A:50:LEU:CD1	1:A:53:ILE:HD12	0.47	2.22	10	1
1:A:27:LEU:N	1:A:67:LEU:HD13	0.47	2.24	18	1
1:A:54:TRP:O	1:A:57:SER:N	0.47	2.48	23	1
1:A:26:ASP:CA	1:A:67:LEU:HD12	0.47	2.40	29	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:GLN:HG3	1:A:67:LEU:HG	0.47	1.87	8	2
1:A:52:HIS:CD2	1:A:80:ARG:NH1	0.47	2.83	2	1
1:A:14:GLN:CD	1:A:15:TYR:N	0.46	2.68	8	1
1:A:12:GLN:HA	1:A:15:TYR:HB3	0.46	1.86	16	1
1:A:58:ASP:C	1:A:60:ASP:H	0.46	2.14	17	3
1:A:44:LYS:HE3	1:A:44:LYS:C	0.46	2.30	3	1
1:A:37:LYS:NZ	1:A:54:TRP:HB2	0.46	2.25	20	2
1:A:45:LEU:CD2	1:A:77:VAL:HG13	0.46	2.41	20	1
1:A:27:LEU:N	1:A:27:LEU:CD1	0.46	2.79	4	1
1:A:45:LEU:O	1:A:50:LEU:HD11	0.46	2.09	23	1
1:A:81:LYS:HD3	1:A:81:LYS:O	0.46	2.10	3	1
1:A:11:GLU:OE2	1:A:14:GLN:NE2	0.46	2.47	5	1
1:A:73:ALA:O	1:A:77:VAL:CG2	0.46	2.60	23	1
1:A:33:GLY:N	1:A:54:TRP:CH2	0.46	2.83	17	3
1:A:49:GLU:N	1:A:49:GLU:CD	0.46	2.69	22	1
1:A:16:TYR:CG	1:A:17:VAL:N	0.46	2.83	16	3
1:A:26:ASP:C	1:A:28:ASN:H	0.46	2.14	1	2
1:A:16:TYR:CD1	1:A:74:PHE:CD2	0.46	3.04	11	1
1:A:58:ASP:OD1	1:A:61:LYS:CA	0.46	2.64	19	1
1:A:16:TYR:HB3	1:A:74:PHE:CE2	0.46	2.46	12	1
1:A:21:LYS:HA	1:A:25:PRO:HA	0.46	1.87	7	1
1:A:37:LYS:HG3	1:A:47:ILE:HG23	0.46	1.87	5	1
1:A:21:LYS:HD3	1:A:22:THR:N	0.46	2.25	22	1
1:A:14:GLN:HG3	1:A:15:TYR:N	0.46	2.25	15	1
1:A:76:LEU:CD2	1:A:76:LEU:C	0.46	2.84	6	3
1:A:65:LEU:HA	1:A:69:GLU:CD	0.46	2.31	2	2
1:A:70:PHE:O	1:A:74:PHE:HB2	0.46	2.11	11	1
1:A:45:LEU:CD2	1:A:80:ARG:HG2	0.46	2.29	18	1
1:A:60:ASP:C	1:A:61:LYS:HG3	0.46	2.32	23	2
1:A:8:ILE:CG1	1:A:75:HIS:CD2	0.46	2.99	12	3
1:A:20:PHE:O	1:A:23:ILE:N	0.45	2.49	24	4
1:A:24:GLN:NE2	1:A:30:PHE:HA	0.45	2.26	20	1
1:A:33:GLY:O	1:A:37:LYS:HE2	0.45	2.11	5	1
1:A:52:HIS:O	1:A:55:GLU:CG	0.45	2.64	4	1
1:A:41:THR:O	1:A:44:LYS:N	0.45	2.48	14	1
1:A:80:ARG:HG3	1:A:80:ARG:NH1	0.45	2.25	30	1
1:A:24:GLN:CB	1:A:70:PHE:CD2	0.45	3.00	26	1
1:A:32:PRO:O	1:A:34:SER:N	0.45	2.49	11	4
1:A:46:PRO:O	1:A:49:GLU:N	0.45	2.49	25	1
1:A:49:GLU:H	1:A:49:GLU:CD	0.45	2.14	22	1
1:A:18:ASN:HA	1:A:21:LYS:HD3	0.45	1.88	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:CD1	1:A:80:ARG:HH21	0.45	2.25	24	1
1:A:40:PHE:CB	1:A:50:LEU:HD21	0.45	2.41	3	2
1:A:17:VAL:HG22	1:A:25:PRO:O	0.45	2.11	5	1
1:A:8:ILE:HA	1:A:75:HIS:CE1	0.45	2.47	10	1
1:A:24:GLN:OE1	1:A:24:GLN:HA	0.45	2.10	21	3
1:A:30:PHE:HD1	1:A:66:THR:HA	0.45	1.71	26	1
1:A:10:ASP:O	1:A:13:ARG:N	0.45	2.50	24	1
1:A:54:TRP:NE1	1:A:58:ASP:CG	0.45	2.70	24	1
1:A:26:ASP:CG	1:A:27:LEU:N	0.45	2.69	6	2
1:A:60:ASP:O	1:A:61:LYS:HB3	0.45	2.11	23	2
1:A:80:ARG:NH1	1:A:80:ARG:HG2	0.45	2.26	28	3
1:A:23:ILE:O	1:A:25:PRO:CD	0.45	2.65	28	3
1:A:32:PRO:C	1:A:34:SER:H	0.45	2.15	29	2
1:A:16:TYR:CE1	1:A:74:PHE:CD2	0.45	3.05	26	1
1:A:31:ILE:HG22	1:A:31:ILE:O	0.45	2.11	8	1
1:A:41:THR:OG1	1:A:50:LEU:HD22	0.45	2.11	1	1
1:A:44:LYS:O	1:A:44:LYS:HD3	0.45	2.12	3	1
1:A:24:GLN:HE21	1:A:29:GLY:C	0.45	2.16	20	1
1:A:45:LEU:CD2	1:A:80:ARG:HD3	0.45	2.42	13	1
1:A:13:ARG:O	1:A:16:TYR:CD2	0.45	2.70	16	1
1:A:67:LEU:CD1	1:A:67:LEU:C	0.44	2.85	27	3
1:A:54:TRP:CD1	1:A:58:ASP:HB2	0.44	2.48	24	1
1:A:20:PHE:CD2	1:A:70:PHE:CE2	0.44	3.05	5	2
1:A:76:LEU:O	1:A:79:ALA:HB3	0.44	2.12	29	1
1:A:55:GLU:OE1	1:A:61:LYS:HD3	0.44	2.12	16	1
1:A:49:GLU:CD	1:A:80:ARG:HH21	0.44	2.14	16	1
1:A:54:TRP:O	1:A:58:ASP:HB2	0.44	2.12	24	1
1:A:44:LYS:O	1:A:44:LYS:CD	0.44	2.65	3	1
1:A:16:TYR:O	1:A:20:PHE:HB2	0.44	2.12	2	1
1:A:46:PRO:HG2	1:A:49:GLU:HG2	0.44	1.87	11	1
1:A:42:LYS:C	1:A:44:LYS:H	0.44	2.15	7	1
1:A:58:ASP:OD2	1:A:61:LYS:N	0.44	2.51	14	1
1:A:52:HIS:HD2	1:A:80:ARG:CZ	0.44	2.25	2	1
1:A:16:TYR:CD1	1:A:70:PHE:CZ	0.44	3.06	22	2
1:A:80:ARG:HD3	1:A:80:ARG:C	0.44	2.33	22	1
1:A:13:ARG:HA	1:A:16:TYR:CE2	0.44	2.48	23	1
1:A:36:ALA:O	1:A:40:PHE:HD1	0.44	1.94	13	2
1:A:44:LYS:HE3	1:A:44:LYS:CA	0.44	2.43	3	1
1:A:33:GLY:CA	1:A:54:TRP:CH2	0.44	3.01	17	1
1:A:52:HIS:ND1	1:A:55:GLU:OE2	0.44	2.45	12	1
1:A:46:PRO:O	1:A:50:LEU:HD23	0.44	2.12	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:HIS:HA	1:A:55:GLU:HG2	0.44	1.89	12	1
1:A:20:PHE:CE2	1:A:31:ILE:HD13	0.44	2.48	12	2
1:A:45:LEU:HB3	1:A:50:LEU:CD1	0.44	2.42	7	1
1:A:51:SER:O	1:A:54:TRP:N	0.44	2.50	6	2
1:A:40:PHE:HB2	1:A:50:LEU:HD21	0.44	1.90	2	2
1:A:12:GLN:OE1	1:A:15:TYR:CD2	0.43	2.71	23	1
1:A:67:LEU:HD23	1:A:67:LEU:C	0.43	2.33	26	1
1:A:40:PHE:O	1:A:43:SER:CB	0.43	2.67	27	3
1:A:16:TYR:CD2	1:A:74:PHE:HB3	0.43	2.48	10	1
1:A:52:HIS:HA	1:A:55:GLU:CD	0.43	2.33	13	1
1:A:30:PHE:CB	1:A:64:ALA:HB1	0.43	2.43	18	1
1:A:16:TYR:CE1	1:A:74:PHE:CE1	0.43	3.06	6	1
1:A:77:VAL:O	1:A:80:ARG:CB	0.43	2.66	27	1
1:A:10:ASP:O	1:A:11:GLU:C	0.43	2.56	24	1
1:A:45:LEU:HB3	1:A:50:LEU:HD11	0.43	1.90	15	1
1:A:28:ASN:ND2	1:A:30:PHE:CZ	0.43	2.87	26	1
1:A:21:LYS:CD	1:A:21:LYS:C	0.43	2.86	4	1
1:A:18:ASN:O	1:A:21:LYS:CG	0.43	2.66	22	1
1:A:20:PHE:CE2	1:A:31:ILE:CD1	0.43	3.01	22	1
1:A:55:GLU:OE1	1:A:61:LYS:CD	0.43	2.67	16	1
1:A:22:THR:O	1:A:22:THR:HG22	0.43	2.12	16	1
1:A:21:LYS:HG2	1:A:25:PRO:CB	0.43	2.44	9	2
1:A:31:ILE:CG2	1:A:36:ALA:N	0.43	2.82	30	1
1:A:8:ILE:HG13	1:A:75:HIS:CD2	0.43	2.48	12	1
1:A:67:LEU:HD23	1:A:70:PHE:CD2	0.43	2.49	18	1
1:A:13:ARG:C	1:A:13:ARG:HD2	0.43	2.34	7	1
1:A:53:ILE:O	1:A:57:SER:N	0.43	2.50	18	1
1:A:11:GLU:CD	1:A:11:GLU:N	0.43	2.72	25	1
1:A:23:ILE:CG2	1:A:31:ILE:CG1	0.43	2.97	19	2
1:A:32:PRO:HA	1:A:64:ALA:HA	0.43	1.89	4	1
1:A:20:PHE:CG	1:A:70:PHE:CE1	0.42	3.06	28	2
1:A:23:ILE:H	1:A:23:ILE:HD12	0.42	1.74	2	1
1:A:13:ARG:O	1:A:16:TYR:CE2	0.42	2.73	12	1
1:A:47:ILE:HA	1:A:50:LEU:HD13	0.42	1.91	28	1
1:A:58:ASP:O	1:A:61:LYS:N	0.42	2.52	16	3
1:A:12:GLN:O	1:A:15:TYR:N	0.42	2.51	5	1
1:A:17:VAL:HG13	1:A:25:PRO:CA	0.42	2.42	10	1
1:A:43:SER:OG	1:A:44:LYS:N	0.42	2.52	29	1
1:A:44:LYS:HA	1:A:44:LYS:CE	0.42	2.32	17	1
1:A:47:ILE:HA	1:A:50:LEU:HB2	0.42	1.92	12	1
1:A:51:SER:C	1:A:55:GLU:OE1	0.42	2.58	26	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HA	1:A:67:LEU:HB3	0.42	1.90	1	1
1:A:81:LYS:CE	1:A:81:LYS:HA	0.42	2.27	29	1
1:A:43:SER:OG	1:A:45:LEU:HG	0.42	2.15	28	1
1:A:81:LYS:O	1:A:81:LYS:HE2	0.42	2.14	29	1
1:A:37:LYS:CG	1:A:47:ILE:HG23	0.42	2.44	5	1
1:A:80:ARG:O	1:A:80:ARG:CD	0.42	2.67	16	1
1:A:60:ASP:OD1	1:A:62:ASP:N	0.42	2.52	2	1
1:A:13:ARG:NH2	1:A:26:ASP:OD2	0.42	2.48	18	1
1:A:80:ARG:CG	1:A:80:ARG:HH11	0.42	2.26	25	1
1:A:16:TYR:CD2	1:A:74:PHE:CD2	0.42	3.07	21	1
1:A:62:ASP:OD2	1:A:64:ALA:N	0.42	2.49	24	1
1:A:24:GLN:OE1	1:A:70:PHE:CB	0.42	2.68	20	1
1:A:23:ILE:CG2	1:A:31:ILE:HD11	0.42	2.44	2	1
1:A:24:GLN:HE22	1:A:29:GLY:HA3	0.42	1.75	9	1
1:A:34:SER:OG	1:A:35:ALA:N	0.42	2.53	29	1
1:A:37:LYS:CE	1:A:50:LEU:HB3	0.42	2.36	20	1
1:A:26:ASP:HA	1:A:67:LEU:HD12	0.42	1.92	13	1
1:A:46:PRO:HD2	1:A:49:GLU:OE1	0.42	2.15	23	1
1:A:76:LEU:C	1:A:76:LEU:CD2	0.42	2.88	7	3
1:A:26:ASP:CA	1:A:67:LEU:HD11	0.42	2.45	25	1
1:A:24:GLN:CD	1:A:67:LEU:HA	0.42	2.35	20	1
1:A:8:ILE:HG23	1:A:75:HIS:HD2	0.42	1.67	4	1
1:A:26:ASP:C	1:A:28:ASN:N	0.41	2.72	8	1
1:A:10:ASP:OD2	1:A:13:ARG:NH2	0.41	2.50	5	1
1:A:52:HIS:CE1	1:A:56:LEU:CD2	0.41	3.03	16	1
1:A:54:TRP:CZ2	1:A:63:GLY:C	0.41	2.93	23	1
1:A:80:ARG:CG	1:A:80:ARG:NH1	0.41	2.82	28	1
1:A:45:LEU:HB2	1:A:50:LEU:HD11	0.41	1.91	26	2
1:A:37:LYS:HA	1:A:50:LEU:HD23	0.41	1.90	1	1
1:A:23:ILE:CG2	1:A:31:ILE:CD1	0.41	2.99	2	1
1:A:57:SER:HB3	1:A:65:LEU:HD11	0.41	1.93	23	1
1:A:8:ILE:CG1	1:A:75:HIS:HD2	0.41	2.28	9	1
1:A:81:LYS:CD	1:A:81:LYS:C	0.41	2.84	3	1
1:A:50:LEU:O	1:A:53:ILE:N	0.41	2.53	29	1
1:A:52:HIS:O	1:A:55:GLU:HG2	0.41	2.16	13	1
1:A:43:SER:O	1:A:44:LYS:HB3	0.41	2.16	6	2
1:A:8:ILE:CD1	1:A:75:HIS:HB2	0.41	2.46	6	1
1:A:58:ASP:O	1:A:61:LYS:HE2	0.41	2.15	7	1
1:A:26:ASP:OD1	1:A:27:LEU:CD1	0.41	2.69	21	1
1:A:16:TYR:HD1	1:A:70:PHE:CE2	0.41	2.33	7	1
1:A:27:LEU:HA	1:A:67:LEU:CB	0.41	2.45	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ILE:CD1	1:A:47:ILE:N	0.41	2.76	17	2
1:A:33:GLY:HA2	1:A:54:TRP:CH2	0.41	2.50	5	2
1:A:78:VAL:O	1:A:81:LYS:CB	0.41	2.69	5	1
1:A:24:GLN:HE22	1:A:29:GLY:CA	0.41	2.29	4	1
1:A:27:LEU:HD23	1:A:27:LEU:N	0.41	2.29	28	1
1:A:28:ASN:OD1	1:A:30:PHE:CZ	0.41	2.74	28	1
1:A:24:GLN:HG2	1:A:67:LEU:CD2	0.41	2.46	7	1
1:A:24:GLN:NE2	1:A:24:GLN:CA	0.41	2.83	29	2
1:A:43:SER:HB2	1:A:45:LEU:HG	0.41	1.92	3	1
1:A:54:TRP:O	1:A:55:GLU:C	0.41	2.59	29	1
1:A:43:SER:O	1:A:45:LEU:CD1	0.41	2.69	6	1
1:A:47:ILE:O	1:A:51:SER:CB	0.41	2.68	3	1
1:A:47:ILE:N	1:A:47:ILE:CD1	0.41	2.78	27	1
1:A:30:PHE:HA	1:A:65:LEU:O	0.41	2.15	10	1
1:A:33:GLY:O	1:A:37:LYS:HG3	0.41	2.16	17	1
1:A:37:LYS:HZ1	1:A:54:TRP:CB	0.41	2.29	18	1
1:A:61:LYS:C	1:A:61:LYS:HD2	0.41	2.35	23	1
1:A:21:LYS:CG	1:A:25:PRO:HB3	0.41	2.46	9	1
1:A:21:LYS:O	1:A:25:PRO:HD3	0.41	2.15	24	1
1:A:28:ASN:OD1	1:A:28:ASN:O	0.40	2.38	1	1
1:A:19:GLN:HA	1:A:19:GLN:NE2	0.40	2.31	11	1
1:A:14:GLN:NE2	1:A:15:TYR:CA	0.40	2.85	13	1
1:A:23:ILE:O	1:A:24:GLN:NE2	0.40	2.53	16	1
1:A:42:LYS:HZ3	1:A:42:LYS:HB3	0.40	1.76	20	1
1:A:67:LEU:C	1:A:67:LEU:HD23	0.40	2.36	19	1
1:A:24:GLN:HB2	1:A:31:ILE:HD11	0.40	1.94	5	1
1:A:21:LYS:HG3	1:A:22:THR:N	0.40	2.31	30	1
1:A:21:LYS:CD	1:A:25:PRO:HB3	0.40	2.46	9	1
1:A:41:THR:O	1:A:42:LYS:C	0.40	2.59	14	1
1:A:13:ARG:NH1	1:A:13:ARG:CG	0.40	2.83	15	1
1:A:66:THR:C	1:A:68:ASP:N	0.40	2.74	18	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	74/92 (80%)	63±3 (85±3%)	9±2 (12±3%)	2±1 (2±2%)	11 48
All	All	2220/2760 (80%)	1896 (85%)	269 (12%)	55 (2%)	11 48

All 9 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	44	LYS	18
1	A	59	PHE	8
1	A	48	LEU	8
1	A	27	LEU	6
1	A	25	PRO	6
1	A	61	LYS	4
1	A	47	ILE	3
1	A	43	SER	1
1	A	33	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	65/82 (79%)	54±2 (83±4%)	11±2 (17±4%)	6 42
All	All	1950/2460 (79%)	1615 (83%)	335 (17%)	6 42

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	39	PHE	30
1	A	68	ASP	28
1	A	20	PHE	18
1	A	71	CYS	18
1	A	24	GLN	16
1	A	75	HIS	15
1	A	80	ARG	14
1	A	18	ASN	12
1	A	12	GLN	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	61	LYS	11
1	A	13	ARG	11
1	A	10	ASP	10
1	A	38	GLU	10
1	A	30	PHE	10
1	A	21	LYS	9
1	A	67	LEU	8
1	A	14	GLN	8
1	A	59	PHE	8
1	A	11	GLU	7
1	A	48	LEU	7
1	A	37	LYS	6
1	A	65	LEU	6
1	A	28	ASN	6
1	A	74	PHE	6
1	A	44	LYS	6
1	A	70	PHE	6
1	A	81	LYS	5
1	A	55	GLU	4
1	A	27	LEU	3
1	A	9	THR	3
1	A	50	LEU	3
1	A	49	GLU	3
1	A	19	GLN	3
1	A	42	LYS	2
1	A	60	ASP	2
1	A	58	ASP	2
1	A	76	LEU	2
1	A	16	TYR	2
1	A	57	SER	1
1	A	45	LEU	1
1	A	66	THR	1
1	A	15	TYR	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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4778

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	533
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	533
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 533 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	140	ILE	H	9.19	0.04	1
UNMAPPED	181	GLU	H	7.37	0.04	1
UNMAPPED	93	PHE	H	7.43	0.04	1
UNMAPPED	73	LEU	CB	40.16	0.2	1
UNMAPPED	56	LEU	N	135.82	0.15	1
UNMAPPED	82	LEU	H	8.78	0.04	1
UNMAPPED	124	ASN	CB	38.85	0.2	1
UNMAPPED	98	GLU	N	117.54	0.15	1
UNMAPPED	135	GLN	CA	54.88	0.2	1
UNMAPPED	24	ILE	CA	65.56	0.2	1
UNMAPPED	73	LEU	N	123.33	0.15	1
UNMAPPED	28	THR	N	114.81	0.15	1
UNMAPPED	78	THR	CA	66.57	0.2	1
UNMAPPED	13	GLY	H	6.62	0.04	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	109	PRO	CB	30.64	0.2	1
UNMAPPED	46	THR	H	8.59	0.04	1
UNMAPPED	125	ASP	CA	53.32	0.2	1
UNMAPPED	54	PHE	CB	42.39	0.2	1
UNMAPPED	24	ILE	N	126.05	0.15	1
UNMAPPED	89	SER	H	7.99	0.04	1
UNMAPPED	33	ALA	CA	52.66	0.2	1
UNMAPPED	92	SER	H	8.13	0.04	1
UNMAPPED	53	PRO	CB	31.98	0.2	1
UNMAPPED	141	THR	H	8.31	0.04	1
UNMAPPED	96	VAL	CB	30.53	0.2	1
UNMAPPED	27	THR	H	7.83	0.04	1
UNMAPPED	149	ALA	CA	55.05	0.2	1
UNMAPPED	127	VAL	N	125.13	0.15	1
UNMAPPED	105	HIS	H	8.45	0.04	1
UNMAPPED	47	VAL	CB	34.38	0.2	1
UNMAPPED	122	LEU	CA	55.06	0.2	1
UNMAPPED	66	ASP	H	8.58	0.04	1
UNMAPPED	39	VAL	H	5.71	0.04	1
UNMAPPED	77	SER	CA	58.98	0.2	1
UNMAPPED	128	ILE	N	127.53	0.15	1
UNMAPPED	20	THR	N	123.55	0.15	1
UNMAPPED	128	ILE	CB	35.83	0.2	1
UNMAPPED	129	LEU	CA	58.22	0.2	1
UNMAPPED	113	ILE	CA	59.58	0.2	1
UNMAPPED	149	ALA	N	123.12	0.15	1
UNMAPPED	79	ASP	H	8.75	0.04	1
UNMAPPED	177	VAL	N	120.91	0.15	1
UNMAPPED	57	GLY	H	9.68	0.04	1
UNMAPPED	157	TYR	H	8.57	0.04	1
UNMAPPED	4	MET	CA	55.22	0.2	1
UNMAPPED	116	VAL	CB	33.3	0.2	1
UNMAPPED	95	ASN	N	119.51	0.15	1
UNMAPPED	175	ALA	CA	55.2	0.2	1
UNMAPPED	116	VAL	N	133.04	0.15	1
UNMAPPED	176	ILE	CA	65.49	0.2	1
UNMAPPED	105	HIS	CA	57.18	0.2	1
UNMAPPED	122	LEU	H	7.81	0.04	1
UNMAPPED	95	ASN	CB	37.66	0.2	1
UNMAPPED	22	LEU	N	126.82	0.15	1
UNMAPPED	6	THR	N	121.34	0.15	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	177	VAL	CB	31.03	0.2	1
UNMAPPED	35	TYR	H	7.81	0.04	1
UNMAPPED	150	LYS	H	7.65	0.04	1
UNMAPPED	22	LEU	CB	41.02	0.2	1
UNMAPPED	155	VAL	N	125.06	0.15	1
UNMAPPED	137	LEU	CB	46.25	0.2	1
UNMAPPED	28	THR	CA	62.03	0.2	1
UNMAPPED	8	LYS	N	136.05	0.15	1
UNMAPPED	26	TYR	H	7.95	0.04	1
UNMAPPED	86	SER	N	117.9	0.15	1
UNMAPPED	29	SER	CB	62.31	0.2	1
UNMAPPED	25	SER	H	8.81	0.04	1
UNMAPPED	146	GLU	H	8.19	0.04	1
UNMAPPED	29	SER	N	118.97	0.15	1
UNMAPPED	178	ALA	CB	18.36	0.2	1
UNMAPPED	152	LEU	CA	53.84	0.2	1
UNMAPPED	88	ILE	N	112.03	0.15	1
UNMAPPED	178	ALA	N	124.36	0.15	1
UNMAPPED	147	LYS	H	8.05	0.04	1
UNMAPPED	179	ALA	CA	53.44	0.2	1
UNMAPPED	93	PHE	CB	38.65	0.2	1
UNMAPPED	99	LYS	N	120.84	0.15	1
UNMAPPED	82	LEU	CB	40.88	0.2	1
UNMAPPED	145	GLY	N	113.98	0.15	1
UNMAPPED	124	ASN	H	7.23	0.04	1
UNMAPPED	163	LEU	H	7.32	0.04	1
UNMAPPED	133	HIS	N	124.64	0.15	1
UNMAPPED	56	LEU	H	9.46	0.04	1
UNMAPPED	82	LEU	N	124.07	0.15	1
UNMAPPED	133	HIS	CB	29.38	0.2	1
UNMAPPED	165	GLN	CB	25.12	0.2	1
UNMAPPED	161	SER	H	7.82	0.04	1
UNMAPPED	54	PHE	H	9.23	0.04	1
UNMAPPED	92	SER	N	120.54	0.15	1
UNMAPPED	46	THR	N	126.12	0.15	1
UNMAPPED	92	SER	CB	63.91	0.2	1
UNMAPPED	164	THR	CA	61.45	0.2	1
UNMAPPED	9	CYS	CA	55.76	0.2	1
UNMAPPED	121	ASP	H	8.58	0.04	1
UNMAPPED	72	PRO	CB	29.61	0.2	1
UNMAPPED	83	VAL	CA	60.65	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	132	LEU	CA	57.87	0.2	1
UNMAPPED	47	VAL	H	9.37	0.04	1
UNMAPPED	85	PHE	H	8.97	0.04	1
UNMAPPED	34	ASP	N	120.54	0.15	1
UNMAPPED	55	THR	CB	69.35	0.2	1
UNMAPPED	128	ILE	H	8.1	0.04	1
UNMAPPED	55	THR	N	122.32	0.15	1
UNMAPPED	177	VAL	CA	66.21	0.2	1
UNMAPPED	166	ARG	CA	57.71	0.2	1
UNMAPPED	162	ALA	H	9.25	0.04	1
UNMAPPED	34	ASP	CA	54.55	0.2	1
UNMAPPED	49	ILE	N	131.11	0.15	1
UNMAPPED	33	ALA	CB	19.36	0.2	1
UNMAPPED	53	PRO	CA	61.86	0.2	1
UNMAPPED	170	THR	N	118.78	0.15	1
UNMAPPED	75	TYR	N	124.87	0.15	1
UNMAPPED	126	ASP	CB	41.17	0.2	1
UNMAPPED	23	LEU	CA	57.56	0.2	1
UNMAPPED	126	ASP	N	130.88	0.15	1
UNMAPPED	167	GLY	N	120.67	0.15	1
UNMAPPED	122	LEU	CB	42.02	0.2	1
UNMAPPED	45	VAL	CA	59.41	0.2	1
UNMAPPED	22	LEU	H	8.15	0.04	1
UNMAPPED	142	GLN	N	126.64	0.15	1
UNMAPPED	17	VAL	CA	61.86	0.2	1
UNMAPPED	35	TYR	N	124.62	0.15	1
UNMAPPED	137	LEU	H	8.05	0.04	1
UNMAPPED	31	PHE	CA	55.25	0.2	1
UNMAPPED	26	TYR	CB	39.81	0.2	1
UNMAPPED	29	SER	H	7.43	0.04	1
UNMAPPED	23	LEU	N	122.83	0.15	1
UNMAPPED	7	ILE	CA	59.61	0.2	1
UNMAPPED	146	GLU	CB	28.96	0.2	1
UNMAPPED	181	GLU	N	129.82	0.15	1
UNMAPPED	114	ILE	H	8.8	0.04	1
UNMAPPED	48	MET	CA	53.03	0.2	1
UNMAPPED	146	GLU	N	125.47	0.15	1
UNMAPPED	117	GLY	CA	44.09	0.2	1
UNMAPPED	127	VAL	H	7.97	0.04	1
UNMAPPED	181	GLU	CA	58.87	0.2	1
UNMAPPED	6	THR	CA	61.26	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	155	VAL	CA	65.79	0.2	1
UNMAPPED	20	THR	H	9.21	0.04	1
UNMAPPED	130	GLN	CA	58.9	0.2	1
UNMAPPED	153	ARG	CB	25.6	0.2	1
UNMAPPED	133	HIS	H	8.87	0.04	1
UNMAPPED	165	GLN	H	7.5	0.04	1
UNMAPPED	161	SER	CB	64.74	0.2	1
UNMAPPED	21	CYS	H	9.26	0.04	1
UNMAPPED	29	SER	CA	60.51	0.2	1
UNMAPPED	158	VAL	CA	58.53	0.2	1
UNMAPPED	130	GLN	N	122.66	0.15	1
UNMAPPED	81	PHE	CA	56.61	0.2	1
UNMAPPED	48	MET	H	8.45	0.04	1
UNMAPPED	19	LYS	CA	60.54	0.2	1
UNMAPPED	121	ASP	CB	40.02	0.2	1
UNMAPPED	119	GLN	H	9.43	0.04	1
UNMAPPED	117	GLY	H	8.7	0.04	1
UNMAPPED	179	ALA	N	122.37	0.15	1
UNMAPPED	15	GLY	CA	46.54	0.2	1
UNMAPPED	145	GLY	CA	46.61	0.2	1
UNMAPPED	93	PHE	CA	59.65	0.2	1
UNMAPPED	55	THR	H	8.8	0.04	1
UNMAPPED	115	ILE	CA	60.15	0.2	1
UNMAPPED	74	SER	CA	60.33	0.2	1
UNMAPPED	24	ILE	H	8.73	0.04	1
UNMAPPED	148	LEU	CA	57.41	0.2	1
UNMAPPED	162	ALA	CB	18.84	0.2	1
UNMAPPED	97	LYS	CA	58.44	0.2	1
UNMAPPED	12	VAL	CA	58.09	0.2	1
UNMAPPED	33	ALA	H	7.9	0.04	1
UNMAPPED	168	LEU	CA	58.43	0.2	1
UNMAPPED	19	LYS	H	9.48	0.04	1
UNMAPPED	65	GLU	H	9.08	0.04	1
UNMAPPED	126	ASP	H	8.73	0.04	1
UNMAPPED	88	ILE	H	7.44	0.04	1
UNMAPPED	151	GLU	CB	29.43	0.2	1
UNMAPPED	11	VAL	H	8.29	0.04	1
UNMAPPED	118	THR	H	9.29	0.04	1
UNMAPPED	158	VAL	N	126.99	0.15	1
UNMAPPED	50	GLY	N	123.9	0.15	1
UNMAPPED	83	VAL	CB	31.33	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	151	GLU	N	126.12	0.15	1
UNMAPPED	115	ILE	H	8.21	0.04	1
UNMAPPED	98	GLU	CB	30.2	0.2	1
UNMAPPED	91	ALA	CA	55.26	0.2	1
UNMAPPED	28	THR	CB	72.02	0.2	1
UNMAPPED	54	PHE	N	126.6	0.15	1
UNMAPPED	154	ALA	H	8.53	0.04	1
UNMAPPED	170	THR	CA	65.91	0.2	1
UNMAPPED	5	GLN	H	8.48	0.04	1
UNMAPPED	136	LYS	CA	57.15	0.2	1
UNMAPPED	110	GLY	N	115.12	0.15	1
UNMAPPED	21	CYS	CA	65.49	0.2	1
UNMAPPED	10	VAL	CA	60.44	0.2	1
UNMAPPED	167	GLY	CA	46.09	0.2	1
UNMAPPED	127	VAL	CB	30.44	0.2	1
UNMAPPED	64	GLN	CA	60.21	0.2	1
UNMAPPED	47	VAL	N	131.62	0.15	1
UNMAPPED	140	ILE	CA	58.49	0.2	1
UNMAPPED	142	GLN	CA	58.78	0.2	1
UNMAPPED	25	SER	CA	61.38	0.2	1
UNMAPPED	30	LYS	N	125.28	0.15	1
UNMAPPED	35	TYR	CA	57.84	0.2	1
UNMAPPED	14	ASP	N	123.12	0.15	1
UNMAPPED	14	ASP	CB	40.69	0.2	1
UNMAPPED	120	THR	CA	64.77	0.2	1
UNMAPPED	26	TYR	CA	60.47	0.2	1
UNMAPPED	89	SER	CA	53.04	0.2	1
UNMAPPED	125	ASP	H	7.24	0.04	1
UNMAPPED	21	CYS	N	123.68	0.15	1
UNMAPPED	49	ILE	H	8.88	0.04	1
UNMAPPED	48	MET	CB	30.98	0.2	1
UNMAPPED	27	THR	CA	60.5	0.2	1
UNMAPPED	160	CYS	N	117.56	0.15	1
UNMAPPED	117	GLY	N	119.79	0.15	1
UNMAPPED	119	GLN	CB	24.31	0.2	1
UNMAPPED	10	VAL	H	7.47	0.04	1
UNMAPPED	178	ALA	H	8.01	0.04	1
UNMAPPED	77	SER	H	9.03	0.04	1
UNMAPPED	66	ASP	CA	55.63	0.2	1
UNMAPPED	171	VAL	CB	31.13	0.2	1
UNMAPPED	171	VAL	N	124.27	0.15	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	111	VAL	N	128.3	0.15	1
UNMAPPED	67	TYR	H	7.89	0.04	1
UNMAPPED	153	ARG	H	7.67	0.04	1
UNMAPPED	161	SER	CA	55.78	0.2	1
UNMAPPED	79	ASP	CA	55.85	0.2	1
UNMAPPED	173	ASP	CA	57.53	0.2	1
UNMAPPED	114	ILE	N	131.44	0.15	1
UNMAPPED	11	VAL	N	131.35	0.15	1
UNMAPPED	175	ALA	H	7.75	0.04	1
UNMAPPED	160	CYS	CB	31.25	0.2	1
UNMAPPED	88	ILE	CB	36.33	0.2	1
UNMAPPED	153	ARG	CA	57.15	0.2	1
UNMAPPED	102	PRO	CA	65.87	0.2	1
UNMAPPED	65	GLU	N	126.97	0.15	1
UNMAPPED	80	VAL	N	120.94	0.15	1
UNMAPPED	83	VAL	H	8.75	0.04	1
UNMAPPED	104	VAL	H	8.35	0.04	1
UNMAPPED	90	PRO	CA	65.22	0.2	1
UNMAPPED	103	GLU	N	122.56	0.15	1
UNMAPPED	123	ARG	N	120.32	0.15	1
UNMAPPED	180	LEU	CA	54.75	0.2	1
UNMAPPED	115	ILE	N	130.84	0.15	1
UNMAPPED	150	LYS	CA	58.77	0.2	1
UNMAPPED	159	GLU	CA	53.43	0.2	1
UNMAPPED	51	ASP	CA	54.14	0.2	1
UNMAPPED	148	LEU	N	126.34	0.15	1
UNMAPPED	115	ILE	CB	37.98	0.2	1
UNMAPPED	98	GLU	H	7.77	0.04	1
UNMAPPED	169	LYS	CB	31.41	0.2	1
UNMAPPED	105	HIS	N	120.82	0.15	1
UNMAPPED	157	TYR	CB	40.73	0.2	1
UNMAPPED	148	LEU	CB	40.51	0.2	1
UNMAPPED	95	ASN	H	7.95	0.04	1
UNMAPPED	84	CYS	N	128.87	0.15	1
UNMAPPED	157	TYR	N	126.23	0.15	1
UNMAPPED	165	GLN	N	118.29	0.15	1
UNMAPPED	97	LYS	N	120.15	0.15	1
UNMAPPED	84	CYS	CB	30.13	0.2	1
UNMAPPED	154	ALA	CB	19.39	0.2	1
UNMAPPED	168	LEU	N	125.47	0.15	1
UNMAPPED	112	PRO	CA	63.38	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	131	ARG	CB	29.5	0.2	1
UNMAPPED	141	THR	N	123.38	0.15	1
UNMAPPED	163	LEU	N	122.86	0.15	1
UNMAPPED	138	SER	CA	56.34	0.2	1
UNMAPPED	130	GLN	H	8.11	0.04	1
UNMAPPED	147	LYS	CA	59.56	0.2	1
UNMAPPED	176	ILE	N	120.76	0.15	1
UNMAPPED	149	ALA	CB	17.83	0.2	1
UNMAPPED	73	LEU	CA	56.9	0.2	1
UNMAPPED	56	LEU	CA	53.36	0.2	1
UNMAPPED	51	ASP	H	8.71	0.04	1
UNMAPPED	124	ASN	CA	51.57	0.2	1
UNMAPPED	98	GLU	CA	57.72	0.2	1
UNMAPPED	91	ALA	CB	17.7	0.2	1
UNMAPPED	14	ASP	H	8.26	0.04	1
UNMAPPED	78	THR	CB	67.76	0.2	1
UNMAPPED	125	ASP	N	126.66	0.15	1
UNMAPPED	109	PRO	CA	63.83	0.2	1
UNMAPPED	125	ASP	CB	43.11	0.2	1
UNMAPPED	164	THR	H	7.99	0.04	1
UNMAPPED	49	ILE	CB	36.06	0.2	1
UNMAPPED	33	ALA	N	130.56	0.15	1
UNMAPPED	34	ASP	CB	41.13	0.2	1
UNMAPPED	52	GLU	H	7.9	0.04	1
UNMAPPED	96	VAL	CA	68.6	0.2	1
UNMAPPED	77	SER	CB	60.79	0.2	1
UNMAPPED	122	LEU	N	122.73	0.15	1
UNMAPPED	77	SER	N	118.47	0.15	1
UNMAPPED	155	VAL	CB	31.66	0.2	1
UNMAPPED	171	VAL	H	7.26	0.04	1
UNMAPPED	94	GLU	H	8.21	0.04	1
UNMAPPED	129	LEU	N	124.09	0.15	1
UNMAPPED	177	VAL	H	7.33	0.04	1
UNMAPPED	113	ILE	N	123.41	0.15	1
UNMAPPED	86	SER	H	8.09	0.04	1
UNMAPPED	136	LYS	CB	27.91	0.2	1
UNMAPPED	175	ALA	CB	16.99	0.2	1
UNMAPPED	110	GLY	H	8.7	0.04	1
UNMAPPED	116	VAL	CA	59.01	0.2	1
UNMAPPED	175	ALA	N	128.02	0.15	1
UNMAPPED	23	LEU	H	7.4	0.04	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	58	LEU	CA	53.59	0.2	1
UNMAPPED	176	ILE	CB	36.88	0.2	1
UNMAPPED	45	VAL	H	8.72	0.04	1
UNMAPPED	104	VAL	N	121.92	0.15	1
UNMAPPED	171	VAL	CA	67.1	0.2	1
UNMAPPED	111	VAL	CA	60.62	0.2	1
UNMAPPED	30	LYS	H	7.79	0.04	1
UNMAPPED	169	LYS	H	8.48	0.04	1
UNMAPPED	148	LEU	H	7.84	0.04	1
UNMAPPED	137	LEU	CA	52.69	0.2	1
UNMAPPED	8	LYS	CA	55.94	0.2	1
UNMAPPED	7	ILE	H	8.99	0.04	1
UNMAPPED	84	CYS	H	8.95	0.04	1
UNMAPPED	118	THR	N	121.08	0.15	1
UNMAPPED	114	ILE	CA	59.47	0.2	1
UNMAPPED	173	ASP	CB	39.6	0.2	1
UNMAPPED	152	LEU	N	119.32	0.15	1
UNMAPPED	57	GLY	N	120.65	0.15	1
UNMAPPED	65	GLU	CA	58.12	0.2	1
UNMAPPED	18	GLY	N	113.33	0.15	1
UNMAPPED	121	ASP	N	123.48	0.15	1
UNMAPPED	172	PHE	H	6.33	0.04	1
UNMAPPED	123	ARG	H	7.22	0.04	1
UNMAPPED	90	PRO	CB	31.2	0.2	1
UNMAPPED	179	ALA	CB	19.39	0.2	1
UNMAPPED	136	LYS	H	8.02	0.04	1
UNMAPPED	99	LYS	CA	57.19	0.2	1
UNMAPPED	6	THR	H	8.18	0.04	1
UNMAPPED	161	SER	N	114.22	0.15	1
UNMAPPED	149	ALA	H	8.15	0.04	1
UNMAPPED	76	PRO	CA	65.91	0.2	1
UNMAPPED	82	LEU	CA	52.79	0.2	1
UNMAPPED	51	ASP	CB	40.53	0.2	1
UNMAPPED	16	ALA	H	9.4	0.04	1
UNMAPPED	91	ALA	H	8.99	0.04	1
UNMAPPED	78	THR	H	7.39	0.04	1
UNMAPPED	172	PHE	CA	61.68	0.2	1
UNMAPPED	46	THR	CA	62.32	0.2	1
UNMAPPED	92	SER	CA	61.16	0.2	1
UNMAPPED	141	THR	CA	60.17	0.2	1
UNMAPPED	164	THR	N	111.33	0.15	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	34	ASP	H	8.13	0.04	1
UNMAPPED	132	LEU	N	124.1	0.15	1
UNMAPPED	80	VAL	H	7.49	0.04	1
UNMAPPED	83	VAL	N	128.59	0.15	1
UNMAPPED	174	GLU	N	121.34	0.15	1
UNMAPPED	15	GLY	H	8.62	0.04	1
UNMAPPED	178	ALA	CA	53.87	0.2	1
UNMAPPED	99	LYS	H	8.2	0.04	1
UNMAPPED	174	GLU	CB	26.93	0.2	1
UNMAPPED	124	ASN	N	115.68	0.15	1
UNMAPPED	55	THR	CA	62.3	0.2	1
UNMAPPED	94	GLU	CB	28.38	0.2	1
UNMAPPED	74	SER	H	7.94	0.04	1
UNMAPPED	87	VAL	CA	63.68	0.2	1
UNMAPPED	113	ILE	H	8.02	0.04	1
UNMAPPED	94	GLU	N	124.91	0.15	1
UNMAPPED	97	LYS	H	6.74	0.04	1
UNMAPPED	152	LEU	CB	40.37	0.2	1
UNMAPPED	156	LYS	H	7.08	0.04	1
UNMAPPED	49	ILE	CA	59.78	0.2	1
UNMAPPED	96	VAL	N	129.72	0.15	1
UNMAPPED	75	TYR	CA	55.89	0.2	1
UNMAPPED	126	ASP	CA	58.22	0.2	1
UNMAPPED	151	GLU	H	8.23	0.04	1
UNMAPPED	45	VAL	CB	35.08	0.2	1
UNMAPPED	45	VAL	N	123.14	0.15	1
UNMAPPED	30	LYS	CB	34.41	0.2	1
UNMAPPED	87	VAL	H	8.7	0.04	1
UNMAPPED	13	GLY	CA	43.03	0.2	1
UNMAPPED	31	PHE	N	130.49	0.15	1
UNMAPPED	7	ILE	CB	40.23	0.2	1
UNMAPPED	50	GLY	H	8.95	0.04	1
UNMAPPED	7	ILE	N	131.61	0.15	1
UNMAPPED	146	GLU	CA	59.5	0.2	1
UNMAPPED	173	ASP	H	8.14	0.04	1
UNMAPPED	18	GLY	H	8.38	0.04	1
UNMAPPED	48	MET	N	127.15	0.15	1
UNMAPPED	152	LEU	H	8.04	0.04	1
UNMAPPED	52	GLU	N	126.19	0.15	1
UNMAPPED	176	ILE	H	7.68	0.04	1
UNMAPPED	119	GLN	N	113.44	0.15	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	167	GLY	H	9.16	0.04	1
UNMAPPED	104	VAL	CA	66.27	0.2	1
UNMAPPED	179	ALA	H	7.78	0.04	1
UNMAPPED	6	THR	CB	70.52	0.2	1
UNMAPPED	180	LEU	H	7.33	0.04	1
UNMAPPED	142	GLN	H	9.06	0.04	1
UNMAPPED	137	LEU	N	122.75	0.15	1
UNMAPPED	118	THR	CB	70.05	0.2	1
UNMAPPED	120	THR	H	8.05	0.04	1
UNMAPPED	16	ALA	N	127.82	0.15	1
UNMAPPED	129	LEU	H	8.72	0.04	1
UNMAPPED	58	LEU	N	130.21	0.15	1
UNMAPPED	174	GLU	H	8.16	0.04	1
UNMAPPED	73	LEU	H	7.46	0.04	1
UNMAPPED	57	GLY	CA	44.93	0.2	1
UNMAPPED	81	PHE	CB	42.91	0.2	1
UNMAPPED	180	LEU	CB	42.36	0.2	1
UNMAPPED	18	GLY	CA	44.79	0.2	1
UNMAPPED	121	ASP	CA	55.12	0.2	1
UNMAPPED	81	PHE	N	127.87	0.15	1
UNMAPPED	19	LYS	N	130.6	0.15	1
UNMAPPED	80	VAL	CB	31.7	0.2	1
UNMAPPED	93	PHE	N	130.55	0.15	1
UNMAPPED	85	PHE	CA	56.43	0.2	1
UNMAPPED	15	GLY	N	109.92	0.15	1
UNMAPPED	74	SER	N	117.11	0.15	1
UNMAPPED	74	SER	CB	63.69	0.2	1
UNMAPPED	169	LYS	N	121.32	0.15	1
UNMAPPED	172	PHE	N	118.75	0.15	1
UNMAPPED	67	TYR	CA	57.92	0.2	1
UNMAPPED	162	ALA	CA	54.38	0.2	1
UNMAPPED	172	PHE	CB	38.99	0.2	1
UNMAPPED	97	LYS	CB	32.9	0.2	1
UNMAPPED	174	GLU	CA	57.72	0.2	1
UNMAPPED	154	ALA	N	124.83	0.15	1
UNMAPPED	168	LEU	CB	42.85	0.2	1
UNMAPPED	156	LYS	CB	34.99	0.2	1
UNMAPPED	166	ARG	H	7.89	0.04	1
UNMAPPED	12	VAL	N	121.71	0.15	1
UNMAPPED	5	GLN	N	126.73	0.15	1
UNMAPPED	156	LYS	N	114.7	0.15	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	32	PRO	CA	61.93	0.2	1
UNMAPPED	157	TYR	CA	55.95	0.2	1
UNMAPPED	139	PRO	CB	32.1	0.2	1
UNMAPPED	151	GLU	CA	59.16	0.2	1
UNMAPPED	134	ARG	CA	59.06	0.2	1
UNMAPPED	50	GLY	CA	47.1	0.2	1
UNMAPPED	39	VAL	N	109.67	0.15	1
UNMAPPED	164	THR	CB	69.39	0.2	1
UNMAPPED	28	THR	H	8.12	0.04	1
UNMAPPED	159	GLU	H	7.9	0.04	1
UNMAPPED	135	GLN	CB	29.43	0.2	1
UNMAPPED	87	VAL	N	125.69	0.15	1
UNMAPPED	94	GLU	CA	58.71	0.2	1
UNMAPPED	135	GLN	N	121.26	0.15	1
UNMAPPED	91	ALA	N	125.09	0.15	1
UNMAPPED	95	ASN	CA	54.43	0.2	1
UNMAPPED	78	THR	N	122.52	0.15	1
UNMAPPED	54	PHE	CA	56.72	0.2	1
UNMAPPED	170	THR	CB	68.89	0.2	1
UNMAPPED	9	CYS	H	9.39	0.04	1
UNMAPPED	110	GLY	CA	45.31	0.2	1
UNMAPPED	160	CYS	H	8.86	0.04	1
UNMAPPED	158	VAL	H	8.26	0.04	1
UNMAPPED	163	LEU	CA	57.29	0.2	1
UNMAPPED	138	SER	H	7.74	0.04	1
UNMAPPED	132	LEU	H	8.49	0.04	1
UNMAPPED	10	VAL	N	133.56	0.15	1
UNMAPPED	166	ARG	N	128.54	0.15	1
UNMAPPED	47	VAL	CA	60.14	0.2	1
UNMAPPED	127	VAL	CA	66.33	0.2	1
UNMAPPED	44	ALA	CA	50.68	0.2	1
UNMAPPED	140	ILE	N	128.08	0.15	1
UNMAPPED	128	ILE	CA	63.14	0.2	1
UNMAPPED	155	VAL	H	9.11	0.04	1
UNMAPPED	163	LEU	CB	42.82	0.2	1
UNMAPPED	13	GLY	N	111.92	0.15	1
UNMAPPED	20	THR	CA	66.82	0.2	1
UNMAPPED	30	LYS	CA	54.55	0.2	1
UNMAPPED	14	ASP	CA	55.73	0.2	1
UNMAPPED	58	LEU	H	8.65	0.04	1
UNMAPPED	120	THR	CB	67.92	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	129	LEU	CB	40.86	0.2	1
UNMAPPED	26	TYR	N	122.6	0.15	1
UNMAPPED	89	SER	N	116.27	0.15	1
UNMAPPED	5	GLN	CA	56.15	0.2	1
UNMAPPED	120	THR	N	109.95	0.15	1
UNMAPPED	25	SER	N	123.71	0.15	1
UNMAPPED	136	LYS	N	119.22	0.15	1
UNMAPPED	81	PHE	H	8.38	0.04	1
UNMAPPED	27	THR	N	111.86	0.15	1
UNMAPPED	52	GLU	CA	52.86	0.2	1
UNMAPPED	96	VAL	H	7.93	0.04	1
UNMAPPED	5	GLN	CB	28.86	0.2	1
UNMAPPED	119	GLN	CA	55.78	0.2	1
UNMAPPED	27	THR	CB	68.93	0.2	1
UNMAPPED	160	CYS	CA	55.69	0.2	1
UNMAPPED	123	ARG	CA	60.21	0.2	1
UNMAPPED	144	GLN	CA	59.04	0.2	1
UNMAPPED	66	ASP	CB	39.31	0.2	1
UNMAPPED	103	GLU	H	7.55	0.04	1
UNMAPPED	66	ASP	N	122.59	0.15	1
UNMAPPED	145	GLY	H	7.86	0.04	1
UNMAPPED	22	LEU	CA	59.28	0.2	1
UNMAPPED	16	ALA	CA	53.1	0.2	1
UNMAPPED	118	THR	CA	59.45	0.2	1
UNMAPPED	75	TYR	H	7.22	0.04	1
UNMAPPED	31	PHE	H	8.48	0.04	1
UNMAPPED	79	ASP	CB	43.92	0.2	1
UNMAPPED	138	SER	N	118.0	0.15	1
UNMAPPED	12	VAL	H	8.83	0.04	1
UNMAPPED	86	SER	CA	55.09	0.2	1
UNMAPPED	79	ASP	N	127.7	0.15	1
UNMAPPED	168	LEU	H	7.39	0.04	1
UNMAPPED	173	ASP	N	126.07	0.15	1
UNMAPPED	116	VAL	H	8.94	0.04	1
UNMAPPED	11	VAL	CA	60.88	0.2	1
UNMAPPED	88	ILE	CA	58.92	0.2	1
UNMAPPED	153	ARG	N	119.29	0.15	1
UNMAPPED	80	VAL	CA	60.39	0.2	1
UNMAPPED	158	VAL	CB	34.38	0.2	1
UNMAPPED	85	PHE	N	122.98	0.15	1
UNMAPPED	103	GLU	CA	60.55	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	150	LYS	N	121.54	0.15	1
UNMAPPED	159	GLU	CB	31.08	0.2	1
UNMAPPED	180	LEU	N	120.92	0.15	1
UNMAPPED	135	GLN	H	7.44	0.04	1
UNMAPPED	169	LYS	CA	60.04	0.2	1
UNMAPPED	150	LYS	CB	31.73	0.2	1
UNMAPPED	159	GLU	N	118.97	0.15	1
UNMAPPED	51	ASP	N	127.37	0.15	1
UNMAPPED	111	VAL	H	7.28	0.04	1
UNMAPPED	67	TYR	N	121.39	0.15	1
UNMAPPED	133	HIS	CA	59.06	0.2	1
UNMAPPED	162	ALA	N	137.04	0.15	1
UNMAPPED	165	GLN	CA	58.43	0.2	1
UNMAPPED	84	CYS	CA	57.13	0.2	1
UNMAPPED	154	ALA	CA	51.33	0.2	1
UNMAPPED	8	LYS	H	10.57	0.04	1
UNMAPPED	112	PRO	CB	32.92	0.2	1
UNMAPPED	170	THR	H	7.64	0.04	1
UNMAPPED	156	LYS	CA	54.85	0.2	1
UNMAPPED	9	CYS	CB	28.61	0.2	1
UNMAPPED	131	ARG	CA	59.38	0.2	1
UNMAPPED	72	PRO	CA	63.4	0.2	1
UNMAPPED	9	CYS	N	135.77	0.15	1
UNMAPPED	139	PRO	CA	62.72	0.2	1
UNMAPPED	147	LYS	N	125.17	0.15	1
UNMAPPED	132	LEU	CB	40.63	0.2	1
UNMAPPED	147	LYS	CB	31.62	0.2	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	155	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	98	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	140	0.00 ± 0.00	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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 937. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/364 (0%)	0/145 (0%)	0/148 (0%)	0/71 (0%)
Sidechain	0/468 (0%)	0/274 (0%)	0/176 (0%)	0/18 (0%)
Aromatic	0/105 (0%)	0/57 (0%)	0/45 (0%)	0/3 (0%)
Overall	0/937 (0%)	0/476 (0%)	0/369 (0%)	0/92 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1176. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/448 (0%)	0/178 (0%)	0/184 (0%)	0/86 (0%)
Sidechain	0/603 (0%)	0/356 (0%)	0/225 (0%)	0/22 (0%)
Aromatic	0/125 (0%)	0/67 (0%)	0/54 (0%)	0/4 (0%)
Overall	0/1176 (0%)	0/601 (0%)	0/463 (0%)	0/112 (0%)

7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.