



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:01 PM BST

PDB ID : 1J0T
Title : The solution structure of molt-inhibiting hormone from the kuruma prawn
Authors : Katayama, H.; Nagata, K.; Ohira, T.; Yumoto, F.; Tanokura, M.; Nagasawa, H.
Deposited on : 2002-11-22

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

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

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

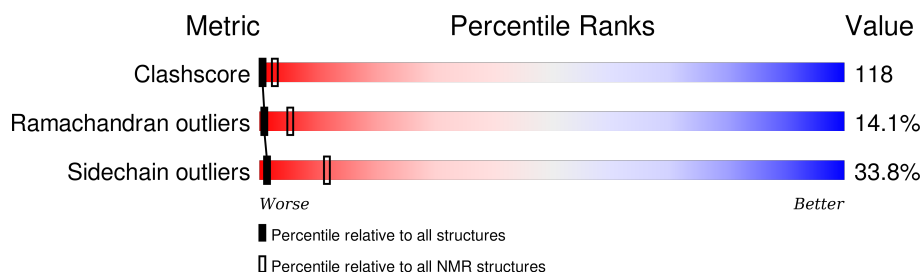
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	78	

2 Ensemble composition and analysis ⓘ

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

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:74 (71)	0.26	1

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

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

The models can be grouped into 1 clusters and 2 single-model clusters were found.

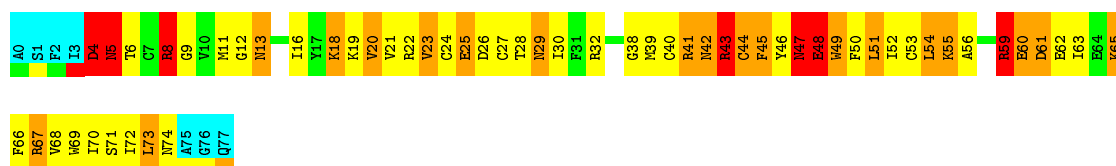
Cluster number	Models
1	1, 2, 3, 4, 5, 7, 8, 10
Single-model clusters	6; 9

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1264 atoms, of which 626 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MOLT-INHIBITING HORMONE.

Mol	Chain	Residues	Atoms						Trace
1	A	78	Total	C	H	N	O	S	0
			1264	401	626	116	113	8	



4.2.3 Score per residue for model 3

- Molecule 1: MOLT-INHIBITING HORMONE

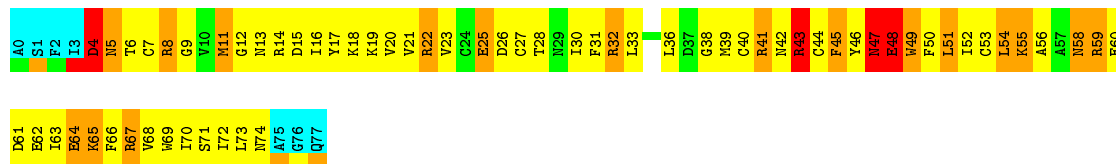
Chain A: 13% 49% 24% 5% 9%



4.2.4 Score per residue for model 4

- Molecule 1: MOLT-INHIBITING HORMONE

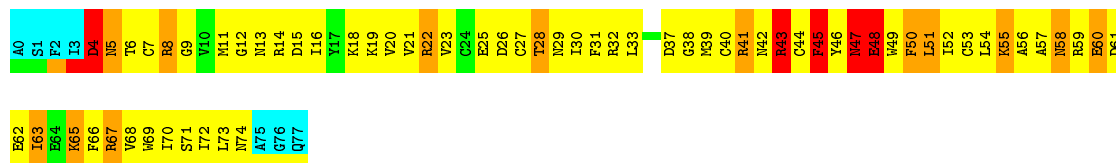
Chain A: 9% 55% 22% 5% 9%



4.2.5 Score per residue for model 5

- Molecule 1: MOLT-INHIBITING HORMONE

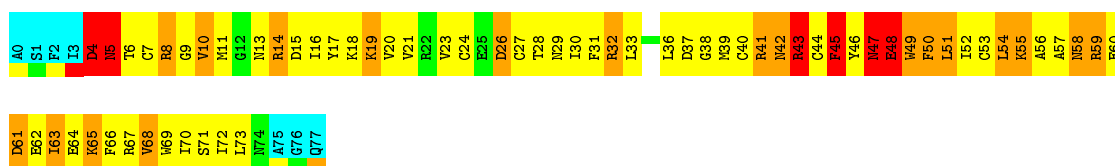
Chain A: 9% 59% 17% 6% 9%



4.2.6 Score per residue for model 6

- Molecule 1: MOLT-INHIBITING HORMONE

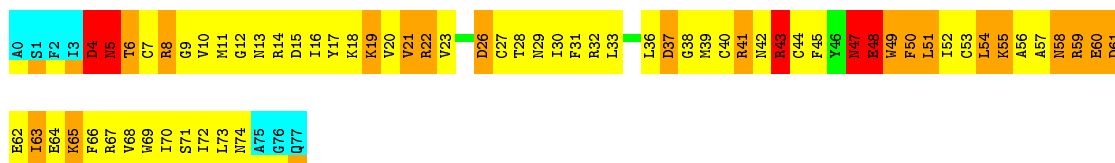
Chain A: 8% 51% 24% 8% 9%



4.2.7 Score per residue for model 7

- Molecule 1: MOLT-INHIBITING HORMONE

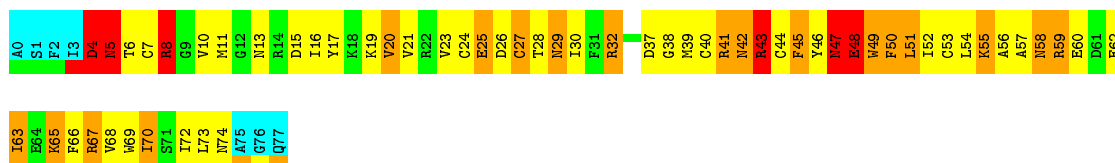
Chain A: 6% 54% 24% 6% 9%



4.2.8 Score per residue for model 8

- Molecule 1: MOLT-INHIBITING HORMONE

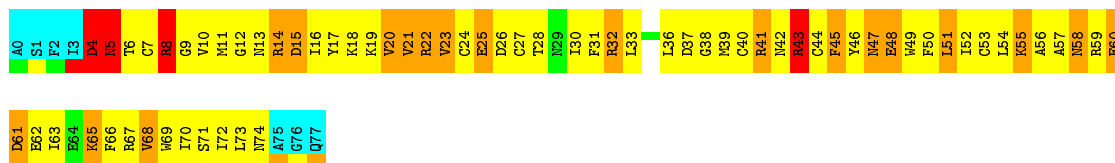
Chain A: 17% 44% 23% 8% 9%



4.2.9 Score per residue for model 9

- Molecule 1: MOLT-INHIBITING HORMONE

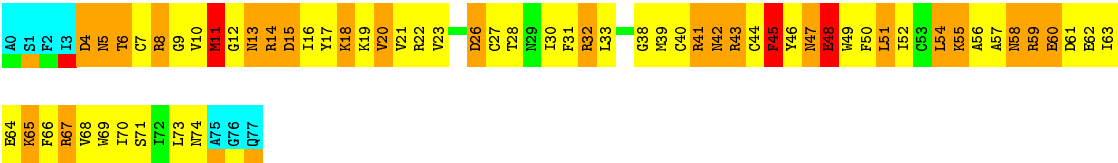
Chain A: 5% 56% 24% 5% 9%



4.2.10 Score per residue for model 10

- Molecule 1: MOLT-INHIBITING HORMONE

Chain A: 12% 46% 29% 9%



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DYANA	refinement	1.4

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 5653, BMRB entry 5633
Number of chemical shift lists	3
Total number of shifts	2032
Number of shifts mapped to atoms	2032
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	589	578	578	138±15
All	All	5890	5780	5780	1379

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 118.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:HG21	1:A:56:ALA:HB1	1.06	1.18	10	5
1:A:20:VAL:HG22	1:A:50:PHE:CZ	1.03	1.88	6	7
1:A:49:TRP:HA	1:A:52:ILE:HD13	1.01	1.32	1	10
1:A:13:ASN:ND2	1:A:73:LEU:HD22	0.98	1.73	1	1
1:A:51:LEU:HD12	1:A:63:ILE:HG21	0.97	1.36	8	6
1:A:43:ARG:NE	1:A:47:ASN:HD22	0.95	1.59	10	2
1:A:54:LEU:HD22	1:A:63:ILE:HD13	0.93	1.37	7	3
1:A:16:ILE:HD13	1:A:69:TRP:HB3	0.92	1.42	1	10
1:A:42:ASN:ND2	1:A:43:ARG:H	0.90	1.63	6	5
1:A:42:ASN:HD22	1:A:43:ARG:N	0.90	1.63	2	6
1:A:69:TRP:HA	1:A:72:ILE:HD12	0.89	1.45	7	7
1:A:52:ILE:HD12	1:A:52:ILE:H	0.88	1.29	8	6
1:A:43:ARG:HE	1:A:47:ASN:HD22	0.87	1.06	3	2
1:A:54:LEU:HD13	1:A:63:ILE:HD13	0.87	1.41	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ILE:H	1:A:52:ILE:HD12	0.87	1.30	7	4
1:A:43:ARG:HE	1:A:47:ASN:ND2	0.86	1.67	10	1
1:A:20:VAL:HG23	1:A:21:VAL:H	0.85	1.30	7	3
1:A:66:PHE:O	1:A:70:ILE:HD12	0.85	1.69	4	4
1:A:20:VAL:HG13	1:A:50:PHE:CE1	0.85	2.05	5	5
1:A:20:VAL:HG11	1:A:45:PHE:CD2	0.85	2.06	1	7
1:A:43:ARG:NH2	1:A:49:TRP:HE1	0.85	1.70	1	7
1:A:42:ASN:HD22	1:A:43:ARG:H	0.84	1.09	6	3
1:A:48:GLU:CD	1:A:52:ILE:HD11	0.83	1.94	7	8
1:A:54:LEU:HD13	1:A:63:ILE:CD1	0.82	2.04	3	5
1:A:50:PHE:O	1:A:54:LEU:HD12	0.81	1.75	8	7
1:A:20:VAL:HG23	1:A:21:VAL:N	0.81	1.91	7	3
1:A:31:PHE:O	1:A:33:LEU:HD12	0.81	1.76	6	6
1:A:43:ARG:HH21	1:A:49:TRP:HE1	0.80	1.18	2	2
1:A:16:ILE:O	1:A:20:VAL:HG23	0.80	1.75	5	7
1:A:54:LEU:HD11	1:A:66:PHE:CD2	0.79	2.13	3	1
1:A:49:TRP:CA	1:A:52:ILE:HD13	0.78	2.08	7	10
1:A:20:VAL:HG21	1:A:45:PHE:CD2	0.78	2.14	10	4
1:A:4:ASP:O	1:A:6:THR:N	0.78	2.17	7	7
1:A:19:LYS:HE3	1:A:69:TRP:CZ3	0.78	2.12	9	3
1:A:51:LEU:CD1	1:A:63:ILE:HG21	0.77	2.10	8	4
1:A:16:ILE:HG21	1:A:69:TRP:HB3	0.77	1.56	9	10
1:A:5:ASN:N	1:A:5:ASN:HD22	0.76	1.75	7	4
1:A:20:VAL:HG12	1:A:50:PHE:CE1	0.76	2.14	9	2
1:A:50:PHE:CE2	1:A:66:PHE:CD2	0.76	2.73	6	3
1:A:66:PHE:CE1	1:A:69:TRP:CZ3	0.76	2.73	6	8
1:A:10:VAL:HA	1:A:13:ASN:HD22	0.76	1.38	10	2
1:A:48:GLU:OE2	1:A:52:ILE:HD11	0.76	1.81	8	2
1:A:52:ILE:N	1:A:52:ILE:HD12	0.76	1.95	7	4
1:A:52:ILE:HD12	1:A:52:ILE:N	0.76	1.95	2	6
1:A:13:ASN:HD22	1:A:73:LEU:CD2	0.76	1.93	8	2
1:A:20:VAL:O	1:A:23:VAL:HG12	0.75	1.80	4	3
1:A:20:VAL:HG12	1:A:50:PHE:CZ	0.75	2.17	7	1
1:A:10:VAL:HG23	1:A:13:ASN:HD21	0.75	1.40	10	1
1:A:42:ASN:HD21	1:A:43:ARG:CD	0.75	1.94	10	1
1:A:23:VAL:HG22	1:A:59:ARG:NH2	0.75	1.95	10	1
1:A:36:LEU:HD12	1:A:39:MET:HE1	0.74	1.59	1	3
1:A:70:ILE:HD13	1:A:70:ILE:N	0.74	1.95	3	1
1:A:16:ILE:HD12	1:A:73:LEU:HD21	0.74	1.60	1	1
1:A:13:ASN:CG	1:A:73:LEU:HD23	0.74	2.03	7	4
1:A:13:ASN:ND2	1:A:73:LEU:HD23	0.74	1.98	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:ASN:HA	1:A:44:CYS:H	0.74	1.40	3	6
1:A:19:LYS:NZ	1:A:66:PHE:CD1	0.74	2.56	2	2
1:A:16:ILE:HD13	1:A:69:TRP:CB	0.72	2.14	4	10
1:A:19:LYS:HE3	1:A:20:VAL:N	0.72	2.00	7	1
1:A:43:ARG:NH2	1:A:49:TRP:CD1	0.72	2.57	4	1
1:A:54:LEU:HD11	1:A:66:PHE:HD2	0.72	1.43	3	1
1:A:42:ASN:HD21	1:A:47:ASN:ND2	0.72	1.82	10	1
1:A:16:ILE:O	1:A:20:VAL:HG13	0.72	1.84	7	3
1:A:45:PHE:HB2	1:A:70:ILE:HD12	0.72	1.62	10	5
1:A:13:ASN:HD22	1:A:73:LEU:HD23	0.72	1.45	6	1
1:A:42:ASN:HD22	1:A:43:ARG:HD3	0.71	1.45	7	4
1:A:45:PHE:N	1:A:45:PHE:CD1	0.71	2.57	1	4
1:A:5:ASN:N	1:A:5:ASN:ND2	0.71	2.38	2	4
1:A:10:VAL:HG23	1:A:13:ASN:ND2	0.71	2.00	10	1
1:A:4:ASP:C	1:A:5:ASN:HD22	0.71	1.89	2	3
1:A:42:ASN:ND2	1:A:43:ARG:N	0.71	2.39	9	6
1:A:5:ASN:H	1:A:43:ARG:HA	0.71	1.46	10	3
1:A:43:ARG:NH2	1:A:49:TRP:NE1	0.71	2.37	10	6
1:A:42:ASN:ND2	1:A:47:ASN:ND2	0.71	2.39	10	1
1:A:41:ARG:CB	1:A:45:PHE:CE2	0.70	2.74	4	1
1:A:50:PHE:CD2	1:A:54:LEU:CD1	0.70	2.75	4	3
1:A:65:LYS:O	1:A:68:VAL:HG12	0.70	1.86	7	8
1:A:5:ASN:H	1:A:43:ARG:N	0.70	1.83	9	1
1:A:20:VAL:HG11	1:A:45:PHE:CE2	0.70	2.22	10	2
1:A:5:ASN:ND2	1:A:5:ASN:N	0.70	2.40	3	5
1:A:20:VAL:HG21	1:A:45:PHE:CE2	0.70	2.22	4	4
1:A:19:LYS:NZ	1:A:66:PHE:CZ	0.70	2.56	6	1
1:A:52:ILE:CD1	1:A:52:ILE:H	0.69	1.99	2	6
1:A:45:PHE:CD1	1:A:45:PHE:N	0.69	2.58	5	5
1:A:30:ILE:HG12	1:A:56:ALA:HB1	0.69	1.64	1	6
1:A:42:ASN:HD21	1:A:47:ASN:HD22	0.69	1.27	10	1
1:A:16:ILE:O	1:A:20:VAL:HG22	0.69	1.88	7	3
1:A:39:MET:HE3	1:A:49:TRP:CZ2	0.69	2.23	5	3
1:A:20:VAL:HG22	1:A:50:PHE:CE1	0.69	2.23	1	3
1:A:60:GLU:HA	1:A:63:ILE:HD11	0.68	1.64	5	6
1:A:30:ILE:HG21	1:A:56:ALA:CB	0.68	2.10	10	2
1:A:42:ASN:ND2	1:A:43:ARG:CD	0.68	2.56	10	2
1:A:42:ASN:HD22	1:A:42:ASN:C	0.68	1.92	2	2
1:A:31:PHE:CZ	1:A:56:ALA:HB2	0.68	2.24	6	3
1:A:50:PHE:CE2	1:A:66:PHE:CG	0.67	2.82	4	5
1:A:70:ILE:HA	1:A:73:LEU:HD12	0.67	1.66	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:GLY:HA2	1:A:41:ARG:HH11	0.67	1.50	9	1
1:A:19:LYS:NZ	1:A:66:PHE:CE2	0.67	2.63	6	1
1:A:17:TYR:O	1:A:21:VAL:HG12	0.67	1.89	1	3
1:A:20:VAL:CG2	1:A:45:PHE:CE2	0.66	2.77	4	2
1:A:30:ILE:CG2	1:A:56:ALA:HB1	0.66	2.11	10	3
1:A:54:LEU:HD13	1:A:63:ILE:HD12	0.66	1.68	1	4
1:A:47:ASN:C	1:A:49:TRP:H	0.66	1.94	3	10
1:A:52:ILE:H	1:A:52:ILE:CD1	0.66	2.03	7	3
1:A:50:PHE:CD2	1:A:54:LEU:HD11	0.66	2.25	1	2
1:A:20:VAL:CG2	1:A:21:VAL:H	0.65	2.02	7	3
1:A:47:ASN:O	1:A:49:TRP:N	0.65	2.29	3	10
1:A:13:ASN:ND2	1:A:73:LEU:CD2	0.65	2.60	6	2
1:A:42:ASN:ND2	1:A:43:ARG:HG2	0.65	2.06	10	1
1:A:10:VAL:CA	1:A:13:ASN:HD22	0.65	2.03	10	1
1:A:19:LYS:C	1:A:19:LYS:HE3	0.65	2.12	7	1
1:A:54:LEU:HD22	1:A:63:ILE:CD1	0.65	2.21	1	3
1:A:39:MET:CE	1:A:49:TRP:CZ2	0.64	2.80	5	2
1:A:19:LYS:HE2	1:A:69:TRP:CZ3	0.64	2.28	5	1
1:A:5:ASN:HD22	1:A:5:ASN:N	0.64	1.89	2	5
1:A:31:PHE:HB3	1:A:33:LEU:HD13	0.64	1.67	4	6
1:A:59:ARG:HG3	1:A:59:ARG:HH11	0.64	1.52	4	1
1:A:51:LEU:HD12	1:A:63:ILE:CG2	0.64	2.20	8	3
1:A:39:MET:SD	1:A:49:TRP:CZ2	0.64	2.91	2	5
1:A:41:ARG:CB	1:A:45:PHE:CE1	0.63	2.81	7	2
1:A:48:GLU:O	1:A:52:ILE:HD12	0.63	1.93	9	10
1:A:19:LYS:NZ	1:A:69:TRP:CH2	0.63	2.60	5	1
1:A:43:ARG:NE	1:A:47:ASN:ND2	0.63	2.39	10	1
1:A:41:ARG:HA	1:A:45:PHE:CD1	0.63	2.29	1	4
1:A:13:ASN:CG	1:A:14:ARG:N	0.63	2.51	10	1
1:A:54:LEU:HD23	1:A:59:ARG:O	0.62	1.94	6	1
1:A:6:THR:O	1:A:6:THR:HG23	0.62	1.94	2	2
1:A:19:LYS:HZ1	1:A:50:PHE:HZ	0.62	1.36	6	1
1:A:70:ILE:N	1:A:70:ILE:HD13	0.62	2.09	5	1
1:A:45:PHE:O	1:A:70:ILE:HG21	0.62	1.94	5	4
1:A:40:CYS:SG	1:A:53:CYS:SG	0.62	2.97	8	4
1:A:42:ASN:HD22	1:A:43:ARG:CD	0.62	2.08	9	3
1:A:17:TYR:CE1	1:A:41:ARG:NH2	0.62	2.68	1	1
1:A:50:PHE:CD2	1:A:70:ILE:HD11	0.62	2.30	8	1
1:A:42:ASN:O	1:A:45:PHE:N	0.62	2.33	6	5
1:A:45:PHE:CB	1:A:70:ILE:HD12	0.62	2.25	9	1
1:A:6:THR:HG23	1:A:6:THR:O	0.61	1.95	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LYS:O	1:A:21:VAL:HG12	0.61	1.95	10	4
1:A:19:LYS:HE2	1:A:20:VAL:N	0.61	2.11	3	2
1:A:27:CYS:SG	1:A:28:THR:N	0.61	2.74	9	5
1:A:20:VAL:CG2	1:A:21:VAL:N	0.61	2.62	7	3
1:A:43:ARG:HE	1:A:47:ASN:CB	0.61	2.09	7	4
1:A:19:LYS:CE	1:A:69:TRP:CZ3	0.61	2.84	5	3
1:A:39:MET:SD	1:A:49:TRP:CE2	0.61	2.94	8	4
1:A:47:ASN:O	1:A:48:GLU:CG	0.60	2.49	10	10
1:A:51:LEU:CD2	1:A:55:LYS:CD	0.60	2.79	4	4
1:A:43:ARG:HG2	1:A:47:ASN:ND2	0.60	2.11	10	2
1:A:54:LEU:HD21	1:A:66:PHE:CE2	0.60	2.32	3	4
1:A:68:VAL:CG1	1:A:69:TRP:N	0.60	2.63	9	2
1:A:5:ASN:CA	1:A:44:CYS:H	0.60	2.10	2	3
1:A:51:LEU:HD21	1:A:55:LYS:NZ	0.60	2.12	7	5
1:A:41:ARG:HB3	1:A:45:PHE:CE2	0.60	2.32	4	2
1:A:20:VAL:HG11	1:A:45:PHE:CG	0.60	2.31	10	7
1:A:26:ASP:O	1:A:30:ILE:HD13	0.60	1.97	2	3
1:A:39:MET:CE	1:A:49:TRP:CH2	0.60	2.85	5	1
1:A:13:ASN:CG	1:A:73:LEU:HD22	0.59	2.18	1	1
1:A:42:ASN:O	1:A:43:ARG:C	0.59	2.41	4	5
1:A:58:ASN:C	1:A:60:GLU:H	0.59	2.01	6	2
1:A:47:ASN:C	1:A:49:TRP:N	0.59	2.56	9	10
1:A:54:LEU:HD23	1:A:59:ARG:HB3	0.59	1.74	4	1
1:A:13:ASN:OD1	1:A:16:ILE:HD12	0.59	1.98	3	1
1:A:48:GLU:O	1:A:52:ILE:CD1	0.59	2.51	1	10
1:A:42:ASN:ND2	1:A:43:ARG:CG	0.59	2.65	10	1
1:A:5:ASN:C	1:A:7:CYS:H	0.59	2.01	10	1
1:A:42:ASN:ND2	1:A:43:ARG:HD3	0.59	2.12	10	7
1:A:21:VAL:HB	1:A:41:ARG:HH21	0.59	1.56	3	2
1:A:39:MET:HA	1:A:43:ARG:NH2	0.58	2.13	4	2
1:A:65:LYS:HG3	1:A:66:PHE:H	0.58	1.58	9	4
1:A:50:PHE:CE2	1:A:54:LEU:HD11	0.58	2.32	4	2
1:A:63:ILE:N	1:A:63:ILE:HD13	0.58	2.13	1	2
1:A:16:ILE:HA	1:A:19:LYS:HE2	0.58	1.74	9	2
1:A:58:ASN:C	1:A:58:ASN:ND2	0.58	2.57	8	6
1:A:64:GLU:CG	1:A:65:LYS:N	0.58	2.66	10	3
1:A:20:VAL:HG13	1:A:50:PHE:HE1	0.58	1.58	2	3
1:A:42:ASN:C	1:A:42:ASN:ND2	0.58	2.57	3	1
1:A:25:GLU:O	1:A:28:THR:HG22	0.58	1.99	5	2
1:A:42:ASN:ND2	1:A:42:ASN:C	0.57	2.57	2	1
1:A:5:ASN:N	1:A:43:ARG:HA	0.57	2.13	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ASN:ND2	1:A:30:ILE:HD12	0.57	2.14	2	2
1:A:64:GLU:HG2	1:A:65:LYS:H	0.57	1.59	10	2
1:A:50:PHE:CE2	1:A:66:PHE:CD1	0.57	2.93	5	4
1:A:19:LYS:NZ	1:A:69:TRP:CE3	0.57	2.73	1	3
1:A:42:ASN:C	1:A:43:ARG:HG2	0.57	2.20	9	5
1:A:62:GLU:O	1:A:66:PHE:CG	0.57	2.58	10	4
1:A:43:ARG:NE	1:A:47:ASN:HB3	0.57	2.15	10	1
1:A:10:VAL:HA	1:A:13:ASN:ND2	0.57	2.14	1	2
1:A:13:ASN:HD22	1:A:73:LEU:HD21	0.57	1.60	8	1
1:A:50:PHE:CE2	1:A:66:PHE:HB3	0.57	2.35	3	6
1:A:39:MET:HE3	1:A:49:TRP:CH2	0.56	2.35	5	2
1:A:19:LYS:HZ1	1:A:69:TRP:HH2	0.56	1.34	5	1
1:A:38:GLY:HA2	1:A:41:ARG:NE	0.56	2.15	8	1
1:A:19:LYS:NZ	1:A:69:TRP:CZ3	0.56	2.73	1	3
1:A:50:PHE:CZ	1:A:66:PHE:CD1	0.56	2.92	4	2
1:A:59:ARG:O	1:A:60:GLU:C	0.56	2.43	10	8
1:A:4:ASP:C	1:A:6:THR:H	0.56	2.01	7	1
1:A:23:VAL:HG11	1:A:50:PHE:CE1	0.56	2.36	2	5
1:A:51:LEU:CD2	1:A:55:LYS:NZ	0.56	2.69	6	2
1:A:28:THR:HG21	1:A:37:ASP:OD1	0.56	2.01	7	1
1:A:26:ASP:HA	1:A:29:ASN:ND2	0.56	2.16	7	3
1:A:24:CYS:SG	1:A:37:ASP:HA	0.56	2.40	9	1
1:A:43:ARG:HH21	1:A:47:ASN:ND2	0.56	1.98	7	2
1:A:65:LYS:HD2	1:A:66:PHE:CD1	0.55	2.36	3	5
1:A:20:VAL:O	1:A:23:VAL:N	0.55	2.40	2	10
1:A:23:VAL:CG1	1:A:24:CYS:N	0.55	2.69	9	1
1:A:9:GLY:C	1:A:13:ASN:ND2	0.55	2.60	1	1
1:A:57:ALA:C	1:A:59:ARG:H	0.55	2.04	3	6
1:A:41:ARG:HB2	1:A:45:PHE:CE1	0.55	2.37	5	7
1:A:13:ASN:HD22	1:A:13:ASN:H	0.55	1.44	3	1
1:A:31:PHE:CD2	1:A:36:LEU:CD2	0.55	2.89	3	1
1:A:39:MET:CG	1:A:43:ARG:NH2	0.55	2.69	9	1
1:A:73:LEU:HD23	1:A:73:LEU:N	0.55	2.16	2	2
1:A:50:PHE:CZ	1:A:66:PHE:CE1	0.55	2.94	4	1
1:A:51:LEU:CD2	1:A:55:LYS:HE2	0.55	2.32	4	2
1:A:28:THR:HG23	1:A:33:LEU:O	0.55	2.02	3	2
1:A:58:ASN:ND2	1:A:58:ASN:C	0.55	2.60	3	3
1:A:5:ASN:ND2	1:A:42:ASN:HA	0.55	2.17	4	4
1:A:5:ASN:HA	1:A:44:CYS:N	0.55	2.15	2	4
1:A:54:LEU:CD2	1:A:63:ILE:HD13	0.54	2.23	7	1
1:A:65:LYS:HG3	1:A:66:PHE:N	0.54	2.17	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:TYR:CZ	1:A:41:ARG:NH2	0.54	2.75	1	2
1:A:27:CYS:CB	1:A:53:CYS:HA	0.54	2.33	9	2
1:A:62:GLU:O	1:A:66:PHE:CD2	0.54	2.60	8	5
1:A:37:ASP:C	1:A:41:ARG:HE	0.54	2.05	8	1
1:A:38:GLY:O	1:A:42:ASN:N	0.54	2.41	7	10
1:A:43:ARG:CG	1:A:47:ASN:ND2	0.54	2.71	10	1
1:A:51:LEU:HD21	1:A:55:LYS:HE2	0.54	1.79	4	2
1:A:62:GLU:HB2	1:A:66:PHE:CE2	0.54	2.37	1	3
1:A:55:LYS:CG	1:A:60:GLU:CD	0.53	2.76	7	6
1:A:42:ASN:HD22	1:A:42:ASN:H	0.53	1.45	10	1
1:A:5:ASN:O	1:A:7:CYS:N	0.53	2.41	7	4
1:A:65:LYS:NZ	1:A:69:TRP:CH2	0.53	2.75	9	2
1:A:39:MET:HG2	1:A:43:ARG:HH22	0.53	1.62	4	1
1:A:31:PHE:CE2	1:A:56:ALA:HB2	0.53	2.39	6	1
1:A:41:ARG:HB2	1:A:45:PHE:CE2	0.53	2.39	4	1
1:A:42:ASN:HD22	1:A:42:ASN:N	0.53	2.00	10	1
1:A:43:ARG:HD2	1:A:47:ASN:ND2	0.53	2.18	9	1
1:A:48:GLU:C	1:A:50:PHE:N	0.53	2.62	1	9
1:A:33:LEU:HD12	1:A:33:LEU:H	0.53	1.63	4	3
1:A:13:ASN:ND2	1:A:73:LEU:HG	0.53	2.19	6	2
1:A:42:ASN:O	1:A:44:CYS:N	0.53	2.42	8	9
1:A:24:CYS:SG	1:A:41:ARG:CG	0.53	2.96	2	2
1:A:43:ARG:NE	1:A:47:ASN:CB	0.52	2.71	10	1
1:A:47:ASN:ND2	1:A:47:ASN:N	0.52	2.54	8	1
1:A:59:ARG:HG3	1:A:59:ARG:NH1	0.52	2.20	4	1
1:A:65:LYS:O	1:A:69:TRP:CG	0.52	2.62	8	3
1:A:42:ASN:HD21	1:A:43:ARG:NE	0.52	2.03	10	1
1:A:43:ARG:NH2	1:A:47:ASN:HB2	0.52	2.19	10	1
1:A:58:ASN:O	1:A:58:ASN:ND2	0.52	2.42	7	1
1:A:48:GLU:HA	1:A:67:ARG:NH2	0.52	2.19	8	2
1:A:65:LYS:HD2	1:A:66:PHE:CE1	0.52	2.40	2	3
1:A:48:GLU:O	1:A:50:PHE:N	0.52	2.42	1	7
1:A:39:MET:HB3	1:A:49:TRP:CD1	0.52	2.40	8	8
1:A:25:GLU:HG3	1:A:26:ASP:H	0.52	1.63	4	1
1:A:43:ARG:NE	1:A:47:ASN:CG	0.52	2.63	7	3
1:A:57:ALA:CB	1:A:59:ARG:HD2	0.52	2.35	7	1
1:A:48:GLU:C	1:A:50:PHE:H	0.52	2.08	1	7
1:A:16:ILE:HG23	1:A:69:TRP:CE3	0.52	2.40	1	4
1:A:5:ASN:H	1:A:5:ASN:ND2	0.52	1.99	7	1
1:A:25:GLU:HG3	1:A:26:ASP:N	0.52	2.18	2	2
1:A:20:VAL:HG22	1:A:50:PHE:HZ	0.52	1.61	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ASN:O	1:A:60:GLU:N	0.52	2.43	7	2
1:A:5:ASN:N	1:A:42:ASN:O	0.52	2.43	10	3
1:A:20:VAL:CG2	1:A:50:PHE:CZ	0.52	2.85	8	1
1:A:4:ASP:HB3	1:A:5:ASN:ND2	0.51	2.21	10	1
1:A:23:VAL:HG22	1:A:59:ARG:HH22	0.51	1.65	10	1
1:A:27:CYS:O	1:A:30:ILE:N	0.51	2.43	9	3
1:A:16:ILE:HG23	1:A:69:TRP:HE3	0.51	1.65	1	1
1:A:13:ASN:ND2	1:A:13:ASN:H	0.51	2.02	3	1
1:A:41:ARG:HB3	1:A:45:PHE:CZ	0.51	2.40	9	1
1:A:44:CYS:O	1:A:46:TYR:N	0.51	2.44	6	6
1:A:47:ASN:N	1:A:47:ASN:OD1	0.51	2.42	3	1
1:A:13:ASN:O	1:A:15:ASP:N	0.51	2.44	10	6
1:A:43:ARG:HE	1:A:47:ASN:CG	0.51	2.09	7	2
1:A:51:LEU:CD2	1:A:55:LYS:HD2	0.51	2.36	5	8
1:A:10:VAL:O	1:A:13:ASN:ND2	0.51	2.44	10	1
1:A:10:VAL:HG13	1:A:11:MET:N	0.51	2.20	8	2
1:A:66:PHE:CD1	1:A:69:TRP:CZ3	0.51	3.00	3	6
1:A:65:LYS:O	1:A:69:TRP:CD1	0.51	2.64	3	3
1:A:9:GLY:C	1:A:11:MET:N	0.50	2.65	6	5
1:A:10:VAL:CG2	1:A:17:TYR:CD2	0.50	2.95	7	2
1:A:16:ILE:HA	1:A:19:LYS:CE	0.50	2.36	8	3
1:A:57:ALA:O	1:A:59:ARG:NE	0.50	2.45	6	1
1:A:5:ASN:ND2	1:A:42:ASN:O	0.50	2.44	10	2
1:A:9:GLY:N	1:A:73:LEU:O	0.50	2.45	4	8
1:A:41:ARG:HB3	1:A:45:PHE:CE1	0.50	2.41	7	1
1:A:64:GLU:HG3	1:A:65:LYS:N	0.50	2.21	7	2
1:A:26:ASP:HA	1:A:29:ASN:HD22	0.50	1.66	7	2
1:A:47:ASN:HB3	1:A:49:TRP:CD1	0.50	2.41	9	3
1:A:42:ASN:HD21	1:A:43:ARG:CG	0.50	2.18	10	1
1:A:62:GLU:HB3	1:A:65:LYS:HE3	0.50	1.82	7	5
1:A:30:ILE:HD12	1:A:30:ILE:N	0.50	2.21	4	3
1:A:39:MET:HB3	1:A:49:TRP:CG	0.50	2.42	5	6
1:A:43:ARG:CZ	1:A:47:ASN:HB3	0.50	2.36	10	1
1:A:20:VAL:CG1	1:A:45:PHE:CE2	0.50	2.95	10	1
1:A:4:ASP:HA	1:A:43:ARG:HA	0.50	1.84	10	2
1:A:59:ARG:O	1:A:61:ASP:N	0.50	2.45	3	7
1:A:48:GLU:HG3	1:A:49:TRP:N	0.50	2.21	3	4
1:A:20:VAL:CG1	1:A:45:PHE:CD2	0.50	2.92	10	1
1:A:65:LYS:HD2	1:A:66:PHE:CD2	0.49	2.41	9	2
1:A:31:PHE:CD2	1:A:36:LEU:HD13	0.49	2.41	6	1
1:A:16:ILE:HG23	1:A:19:LYS:NZ	0.49	2.21	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:LYS:HD2	1:A:66:PHE:CZ	0.49	2.41	7	2
1:A:10:VAL:HA	1:A:73:LEU:CD2	0.49	2.37	8	1
1:A:19:LYS:C	1:A:19:LYS:CE	0.49	2.80	7	1
1:A:13:ASN:ND2	1:A:73:LEU:HA	0.49	2.23	7	1
1:A:19:LYS:HE3	1:A:69:TRP:CE3	0.49	2.41	9	2
1:A:17:TYR:CE2	1:A:41:ARG:NH2	0.49	2.80	10	1
1:A:13:ASN:CG	1:A:73:LEU:CD2	0.49	2.80	7	6
1:A:57:ALA:HB1	1:A:59:ARG:HD2	0.49	1.84	7	1
1:A:23:VAL:HG13	1:A:40:CYS:SG	0.49	2.47	4	1
1:A:41:ARG:HA	1:A:45:PHE:CD2	0.49	2.42	4	1
1:A:8:ARG:N	1:A:73:LEU:O	0.49	2.46	8	4
1:A:9:GLY:O	1:A:11:MET:N	0.49	2.46	1	4
1:A:58:ASN:C	1:A:60:GLU:N	0.49	2.66	6	2
1:A:43:ARG:HD3	1:A:43:ARG:H	0.49	1.67	1	2
1:A:43:ARG:NH2	1:A:47:ASN:ND2	0.49	2.61	6	2
1:A:11:MET:HG3	1:A:12:GLY:N	0.49	2.23	7	4
1:A:20:VAL:O	1:A:22:ARG:N	0.49	2.45	7	2
1:A:55:LYS:NZ	1:A:60:GLU:OE2	0.49	2.46	2	3
1:A:43:ARG:O	1:A:46:TYR:N	0.49	2.42	3	3
1:A:25:GLU:O	1:A:29:ASN:ND2	0.49	2.46	1	2
1:A:9:GLY:O	1:A:12:GLY:N	0.48	2.44	9	5
1:A:31:PHE:C	1:A:33:LEU:HD12	0.48	2.28	3	2
1:A:31:PHE:CD1	1:A:36:LEU:CD2	0.48	2.96	7	1
1:A:40:CYS:HB2	1:A:53:CYS:SG	0.48	2.48	5	6
1:A:13:ASN:ND2	1:A:73:LEU:CG	0.48	2.76	6	1
1:A:51:LEU:HD23	1:A:55:LYS:HZ3	0.48	1.67	6	1
1:A:41:ARG:CB	1:A:45:PHE:CD1	0.48	2.95	7	1
1:A:9:GLY:C	1:A:13:ASN:HD22	0.48	2.10	7	3
1:A:11:MET:HA	1:A:11:MET:CE	0.48	2.39	6	1
1:A:54:LEU:O	1:A:59:ARG:N	0.48	2.47	6	1
1:A:19:LYS:NZ	1:A:66:PHE:CE1	0.48	2.80	2	2
1:A:64:GLU:HG3	1:A:65:LYS:H	0.48	1.69	7	1
1:A:13:ASN:C	1:A:15:ASP:N	0.48	2.66	9	6
1:A:40:CYS:HA	1:A:49:TRP:HB3	0.48	1.85	6	4
1:A:62:GLU:CD	1:A:65:LYS:HE2	0.48	2.29	8	1
1:A:58:ASN:OD1	1:A:59:ARG:NH1	0.48	2.47	7	1
1:A:50:PHE:CD2	1:A:66:PHE:HB3	0.48	2.43	5	4
1:A:43:ARG:CD	1:A:47:ASN:HD22	0.48	2.21	10	1
1:A:30:ILE:CG1	1:A:56:ALA:HB1	0.48	2.39	5	4
1:A:4:ASP:CA	1:A:42:ASN:O	0.48	2.62	10	1
1:A:50:PHE:O	1:A:54:LEU:CD1	0.48	2.62	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:GLY:O	1:A:13:ASN:ND2	0.48	2.47	6	2
1:A:44:CYS:C	1:A:46:TYR:N	0.48	2.65	10	6
1:A:39:MET:HB3	1:A:49:TRP:CD2	0.48	2.44	5	2
1:A:5:ASN:ND2	1:A:42:ASN:HD22	0.48	2.07	8	1
1:A:16:ILE:CG2	1:A:69:TRP:HB3	0.48	2.38	8	2
1:A:43:ARG:NE	1:A:47:ASN:OD1	0.48	2.47	7	3
1:A:4:ASP:C	1:A:6:THR:N	0.48	2.63	7	8
1:A:39:MET:O	1:A:47:ASN:ND2	0.48	2.46	10	1
1:A:10:VAL:CG2	1:A:13:ASN:ND2	0.47	2.73	10	1
1:A:62:GLU:OE1	1:A:65:LYS:HE2	0.47	2.09	8	1
1:A:51:LEU:HD12	1:A:63:ILE:HG13	0.47	1.86	7	2
1:A:16:ILE:HD13	1:A:69:TRP:CG	0.47	2.44	5	1
1:A:10:VAL:O	1:A:12:GLY:N	0.47	2.47	10	1
1:A:16:ILE:HA	1:A:19:LYS:HZ1	0.47	1.69	8	1
1:A:5:ASN:C	1:A:7:CYS:N	0.47	2.67	10	1
1:A:4:ASP:HA	1:A:43:ARG:CA	0.47	2.38	9	1
1:A:23:VAL:HG11	1:A:50:PHE:CZ	0.47	2.44	4	1
1:A:41:ARG:CA	1:A:45:PHE:CD1	0.47	2.97	1	2
1:A:38:GLY:O	1:A:41:ARG:N	0.47	2.47	3	5
1:A:20:VAL:HB	1:A:45:PHE:CD2	0.47	2.45	4	1
1:A:28:THR:O	1:A:32:ARG:N	0.47	2.47	9	5
1:A:5:ASN:HD22	1:A:42:ASN:HA	0.47	1.67	9	1
1:A:64:GLU:CG	1:A:65:LYS:H	0.47	2.22	10	2
1:A:10:VAL:CA	1:A:13:ASN:ND2	0.47	2.78	1	1
1:A:39:MET:CG	1:A:43:ARG:HH22	0.47	2.23	9	2
1:A:73:LEU:CD2	1:A:73:LEU:N	0.47	2.76	2	1
1:A:42:ASN:OD1	1:A:43:ARG:NH1	0.47	2.48	3	1
1:A:4:ASP:CA	1:A:43:ARG:HA	0.46	2.39	9	1
1:A:22:ARG:C	1:A:22:ARG:HD2	0.46	2.31	1	1
1:A:57:ALA:O	1:A:58:ASN:CB	0.46	2.63	8	2
1:A:16:ILE:HA	1:A:19:LYS:NZ	0.46	2.25	8	1
1:A:38:GLY:HA2	1:A:41:ARG:HD3	0.46	1.87	9	1
1:A:24:CYS:SG	1:A:41:ARG:HG3	0.46	2.51	8	2
1:A:63:ILE:O	1:A:67:ARG:N	0.46	2.49	10	5
1:A:37:ASP:CG	1:A:38:GLY:N	0.46	2.69	1	1
1:A:20:VAL:CB	1:A:45:PHE:CE2	0.46	2.98	10	1
1:A:4:ASP:O	1:A:6:THR:HG23	0.46	2.11	9	1
1:A:43:ARG:O	1:A:45:PHE:N	0.46	2.48	2	1
1:A:42:ASN:OD1	1:A:43:ARG:CZ	0.46	2.64	3	1
1:A:51:LEU:HD21	1:A:55:LYS:HD2	0.46	1.88	5	1
1:A:9:GLY:C	1:A:11:MET:H	0.46	2.14	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ARG:CZ	1:A:47:ASN:CB	0.46	2.93	10	1
1:A:66:PHE:CD1	1:A:69:TRP:CE3	0.46	3.04	9	1
1:A:31:PHE:C	1:A:33:LEU:H	0.46	2.15	9	3
1:A:16:ILE:HG12	1:A:19:LYS:NZ	0.46	2.25	4	2
1:A:16:ILE:HD12	1:A:73:LEU:CD2	0.46	2.39	1	1
1:A:16:ILE:O	1:A:20:VAL:CG2	0.46	2.64	6	7
1:A:51:LEU:CD2	1:A:55:LYS:HZ3	0.46	2.24	7	2
1:A:13:ASN:O	1:A:14:ARG:CG	0.46	2.64	6	1
1:A:27:CYS:HB2	1:A:53:CYS:HA	0.45	1.88	9	3
1:A:44:CYS:O	1:A:45:PHE:C	0.45	2.54	4	4
1:A:69:TRP:O	1:A:72:ILE:N	0.45	2.47	9	4
1:A:42:ASN:ND2	1:A:43:ARG:NH1	0.45	2.64	9	1
1:A:28:THR:O	1:A:32:ARG:CA	0.45	2.64	6	3
1:A:31:PHE:CD2	1:A:36:LEU:CD1	0.45	2.99	6	1
1:A:10:VAL:C	1:A:12:GLY:N	0.45	2.69	10	1
1:A:5:ASN:H	1:A:43:ARG:CA	0.45	2.21	10	1
1:A:30:ILE:CD1	1:A:30:ILE:N	0.45	2.79	4	2
1:A:5:ASN:ND2	1:A:42:ASN:OD1	0.45	2.50	5	1
1:A:63:ILE:HG22	1:A:67:ARG:CD	0.45	2.41	2	1
1:A:57:ALA:C	1:A:59:ARG:N	0.45	2.70	5	6
1:A:43:ARG:C	1:A:45:PHE:N	0.45	2.70	2	1
1:A:4:ASP:C	1:A:43:ARG:HA	0.45	2.32	7	1
1:A:55:LYS:CG	1:A:60:GLU:OE1	0.45	2.65	5	2
1:A:4:ASP:HA	1:A:43:ARG:H	0.45	1.70	9	1
1:A:41:ARG:HB3	1:A:45:PHE:CD1	0.45	2.47	7	1
1:A:42:ASN:HB3	1:A:43:ARG:NE	0.45	2.27	4	1
1:A:39:MET:HG2	1:A:43:ARG:NH2	0.45	2.27	9	2
1:A:21:VAL:CB	1:A:41:ARG:HE	0.45	2.24	3	1
1:A:59:ARG:CG	1:A:59:ARG:NH1	0.44	2.80	4	1
1:A:57:ALA:O	1:A:59:ARG:N	0.44	2.50	3	4
1:A:10:VAL:HG23	1:A:17:TYR:CD1	0.44	2.47	9	1
1:A:27:CYS:HB3	1:A:53:CYS:CA	0.44	2.40	2	1
1:A:13:ASN:OD1	1:A:72:ILE:CG2	0.44	2.66	7	1
1:A:51:LEU:HD21	1:A:55:LYS:HZ2	0.44	1.70	6	2
1:A:60:GLU:CA	1:A:63:ILE:HD11	0.44	2.41	5	1
1:A:43:ARG:CD	1:A:43:ARG:H	0.44	2.22	1	3
1:A:20:VAL:HG21	1:A:45:PHE:CE1	0.44	2.47	7	1
1:A:23:VAL:CG1	1:A:50:PHE:CE1	0.44	3.00	7	1
1:A:13:ASN:HD22	1:A:73:LEU:CG	0.44	2.25	8	1
1:A:4:ASP:HB2	1:A:5:ASN:ND2	0.44	2.26	3	1
1:A:54:LEU:HB3	1:A:63:ILE:HD11	0.44	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ASN:HB3	1:A:43:ARG:CZ	0.44	2.43	4	1
1:A:51:LEU:HD21	1:A:55:LYS:CE	0.44	2.43	4	1
1:A:21:VAL:CG1	1:A:22:ARG:N	0.44	2.80	5	1
1:A:58:ASN:ND2	1:A:58:ASN:O	0.44	2.50	8	1
1:A:49:TRP:HA	1:A:52:ILE:CD1	0.44	2.28	9	1
1:A:16:ILE:O	1:A:20:VAL:CG1	0.44	2.66	9	2
1:A:44:CYS:O	1:A:70:ILE:CG2	0.44	2.66	3	1
1:A:10:VAL:N	1:A:13:ASN:ND2	0.44	2.65	1	1
1:A:20:VAL:C	1:A:22:ARG:N	0.44	2.71	9	3
1:A:64:GLU:HG2	1:A:65:LYS:N	0.44	2.25	10	2
1:A:42:ASN:ND2	1:A:42:ASN:H	0.44	2.10	10	1
1:A:55:LYS:CE	1:A:60:GLU:OE2	0.44	2.66	7	1
1:A:36:LEU:HA	1:A:39:MET:SD	0.44	2.53	4	1
1:A:70:ILE:HA	1:A:73:LEU:CD1	0.43	2.40	7	1
1:A:62:GLU:HB3	1:A:65:LYS:CD	0.43	2.43	4	2
1:A:20:VAL:HA	1:A:50:PHE:CE1	0.43	2.48	9	3
1:A:21:VAL:HG23	1:A:41:ARG:HE	0.43	1.73	5	1
1:A:19:LYS:O	1:A:22:ARG:N	0.43	2.51	2	2
1:A:18:LYS:O	1:A:21:VAL:CG1	0.43	2.66	2	2
1:A:16:ILE:HG22	1:A:20:VAL:CG1	0.43	2.43	7	1
1:A:51:LEU:CD2	1:A:55:LYS:CE	0.43	2.96	4	1
1:A:31:PHE:HB2	1:A:36:LEU:CD1	0.43	2.43	6	1
1:A:39:MET:HA	1:A:42:ASN:CG	0.43	2.34	10	1
1:A:62:GLU:CB	1:A:66:PHE:CE2	0.43	3.01	1	1
1:A:19:LYS:O	1:A:19:LYS:NZ	0.43	2.46	7	1
1:A:17:TYR:CD2	1:A:45:PHE:CE2	0.43	3.07	7	1
1:A:17:TYR:HA	1:A:20:VAL:CG2	0.43	2.43	4	2
1:A:42:ASN:CG	1:A:43:ARG:HD3	0.43	2.33	10	3
1:A:36:LEU:O	1:A:40:CYS:CB	0.43	2.66	6	1
1:A:63:ILE:CD1	1:A:63:ILE:N	0.43	2.73	1	1
1:A:62:GLU:HB3	1:A:65:LYS:CE	0.43	2.43	9	2
1:A:55:LYS:HG3	1:A:60:GLU:CD	0.43	2.33	10	6
1:A:55:LYS:CD	1:A:60:GLU:OE2	0.43	2.66	6	1
1:A:45:PHE:O	1:A:70:ILE:CG2	0.43	2.66	2	2
1:A:8:ARG:O	1:A:8:ARG:CD	0.43	2.66	8	1
1:A:17:TYR:CD1	1:A:45:PHE:CZ	0.43	3.06	3	1
1:A:4:ASP:HA	1:A:43:ARG:N	0.43	2.28	9	1
1:A:8:ARG:HD3	1:A:8:ARG:C	0.43	2.33	5	1
1:A:8:ARG:CB	1:A:73:LEU:O	0.43	2.67	5	1
1:A:33:LEU:H	1:A:33:LEU:HD12	0.43	1.74	6	1
1:A:11:MET:N	1:A:11:MET:SD	0.43	2.87	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:MET:SD	1:A:11:MET:N	0.43	2.91	8	1
1:A:20:VAL:HG12	1:A:50:PHE:HZ	0.43	1.66	7	1
1:A:37:ASP:O	1:A:41:ARG:CD	0.43	2.67	9	1
1:A:43:ARG:HD2	1:A:47:ASN:HD22	0.43	1.73	9	1
1:A:38:GLY:HA2	1:A:41:ARG:HD2	0.43	1.90	2	1
1:A:16:ILE:HA	1:A:19:LYS:HZ3	0.42	1.74	3	1
1:A:43:ARG:H	1:A:43:ARG:CD	0.42	2.27	7	1
1:A:4:ASP:CB	1:A:42:ASN:O	0.42	2.67	10	1
1:A:13:ASN:HD21	1:A:72:ILE:CG2	0.42	2.27	2	1
1:A:47:ASN:ND2	1:A:49:TRP:HB2	0.42	2.29	8	1
1:A:31:PHE:HB3	1:A:33:LEU:HD12	0.42	1.91	1	1
1:A:17:TYR:O	1:A:20:VAL:CG2	0.42	2.66	4	1
1:A:41:ARG:C	1:A:41:ARG:HD3	0.42	2.35	7	1
1:A:31:PHE:HB3	1:A:33:LEU:CD1	0.42	2.42	5	4
1:A:24:CYS:SG	1:A:41:ARG:HG2	0.42	2.54	6	2
1:A:7:CYS:SG	1:A:73:LEU:CB	0.42	3.08	10	1
1:A:68:VAL:HG13	1:A:69:TRP:N	0.42	2.29	9	1
1:A:5:ASN:ND2	1:A:42:ASN:ND2	0.42	2.67	8	1
1:A:4:ASP:O	1:A:43:ARG:HA	0.42	2.15	7	1
1:A:45:PHE:HB2	1:A:70:ILE:CD1	0.42	2.40	10	2
1:A:28:THR:CG2	1:A:37:ASP:OD1	0.42	2.66	7	1
1:A:10:VAL:HG23	1:A:17:TYR:CD2	0.42	2.50	6	1
1:A:39:MET:HA	1:A:42:ASN:HB2	0.42	1.92	8	1
1:A:5:ASN:CA	1:A:42:ASN:O	0.42	2.68	3	1
1:A:30:ILE:N	1:A:30:ILE:HD12	0.42	2.30	9	1
1:A:55:LYS:C	1:A:57:ALA:N	0.42	2.73	1	4
1:A:59:ARG:C	1:A:61:ASP:N	0.42	2.72	5	2
1:A:42:ASN:N	1:A:42:ASN:ND2	0.42	2.68	10	1
1:A:23:VAL:HG21	1:A:66:PHE:HE2	0.42	1.75	3	1
1:A:13:ASN:OD1	1:A:73:LEU:HD22	0.42	2.15	2	1
1:A:10:VAL:HA	1:A:73:LEU:HD23	0.41	1.91	8	1
1:A:54:LEU:CB	1:A:63:ILE:CD1	0.41	2.98	7	1
1:A:51:LEU:HD21	1:A:55:LYS:CD	0.41	2.45	4	1
1:A:54:LEU:O	1:A:60:GLU:N	0.41	2.53	6	1
1:A:21:VAL:HB	1:A:41:ARG:NH2	0.41	2.28	3	1
1:A:24:CYS:HB3	1:A:37:ASP:HA	0.41	1.93	3	1
1:A:47:ASN:O	1:A:48:GLU:HG3	0.41	2.15	1	4
1:A:65:LYS:HD3	1:A:69:TRP:CZ2	0.41	2.50	3	1
1:A:20:VAL:CG2	1:A:45:PHE:CE1	0.41	3.03	7	1
1:A:38:GLY:O	1:A:39:MET:C	0.41	2.58	9	4
1:A:36:LEU:HD12	1:A:39:MET:CE	0.41	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:GLU:CG	1:A:52:ILE:HD11	0.41	2.45	10	1
1:A:7:CYS:SG	1:A:73:LEU:HB3	0.41	2.55	10	2
1:A:24:CYS:O	1:A:27:CYS:SG	0.41	2.79	9	1
1:A:11:MET:SD	1:A:12:GLY:N	0.41	2.93	1	1
1:A:37:ASP:OD1	1:A:38:GLY:N	0.41	2.52	1	1
1:A:22:ARG:C	1:A:22:ARG:CD	0.41	2.89	1	2
1:A:6:THR:O	1:A:6:THR:CG2	0.41	2.65	2	2
1:A:10:VAL:O	1:A:10:VAL:HG22	0.41	2.16	6	1
1:A:50:PHE:HE2	1:A:66:PHE:CD2	0.41	2.34	10	1
1:A:66:PHE:HE1	1:A:69:TRP:CZ3	0.41	2.31	2	1
1:A:10:VAL:CG1	1:A:11:MET:N	0.41	2.84	8	1
1:A:14:ARG:O	1:A:18:LYS:CD	0.41	2.69	1	1
1:A:48:GLU:O	1:A:51:LEU:N	0.40	2.47	6	1
1:A:24:CYS:O	1:A:25:GLU:C	0.40	2.58	9	1
1:A:50:PHE:O	1:A:54:LEU:HD13	0.40	2.16	7	1
1:A:31:PHE:O	1:A:32:ARG:CB	0.40	2.69	4	1
1:A:11:MET:O	1:A:14:ARG:CD	0.40	2.70	9	1
1:A:13:ASN:HD21	1:A:73:LEU:HA	0.40	1.77	7	1
1:A:13:ASN:CB	1:A:73:LEU:HD23	0.40	2.46	7	1
1:A:17:TYR:CE2	1:A:45:PHE:CZ	0.40	3.09	4	1
1:A:25:GLU:CG	1:A:26:ASP:N	0.40	2.84	4	1
1:A:13:ASN:HB3	1:A:73:LEU:HD23	0.40	1.92	10	1
1:A:65:LYS:HD3	1:A:69:TRP:CH2	0.40	2.51	8	1
1:A:25:GLU:HA	1:A:28:THR:CG2	0.40	2.46	2	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	71/78 (91%)	44±2 (61±3%)	17±2 (25±3%)	10±1 (14±2%)	1	5
All	All	710/780 (91%)	436 (61%)	174 (25%)	100 (14%)	1	5

All 20 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	48	GLU	10
1	A	47	ASN	10
1	A	4	ASP	10
1	A	43	ARG	9
1	A	60	GLU	7
1	A	49	TRP	7
1	A	45	PHE	6
1	A	5	ASN	6
1	A	14	ARG	6
1	A	59	ARG	5
1	A	8	ARG	4
1	A	20	VAL	4
1	A	7	CYS	3
1	A	13	ASN	3
1	A	6	THR	3
1	A	10	VAL	2
1	A	21	VAL	2
1	A	11	MET	1
1	A	44	CYS	1
1	A	37	ASP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	65/69 (94%)	43±2 (66±3%)	22±2 (34±3%)	1	11
All	All	650/690 (94%)	430 (66%)	220 (34%)	1	11

All 39 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	51	LEU	10
1	A	65	LYS	10
1	A	41	ARG	10
1	A	5	ASN	10
1	A	55	LYS	10
1	A	43	ARG	10

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Mol	Chain	Res	Type	Models (Total)
1	A	32	ARG	9
1	A	58	ASN	9
1	A	71	SER	9
1	A	8	ARG	9
1	A	48	GLU	9
1	A	4	ASP	9
1	A	18	LYS	8
1	A	47	ASN	7
1	A	67	ARG	7
1	A	61	ASP	7
1	A	54	LEU	6
1	A	45	PHE	6
1	A	50	PHE	6
1	A	22	ARG	5
1	A	42	ASN	5
1	A	63	ILE	5
1	A	27	CYS	5
1	A	25	GLU	4
1	A	23	VAL	4
1	A	26	ASP	4
1	A	11	MET	4
1	A	19	LYS	4
1	A	59	ARG	3
1	A	15	ASP	3
1	A	73	LEU	2
1	A	68	VAL	2
1	A	29	ASN	2
1	A	37	ASP	2
1	A	13	ASN	1
1	A	28	THR	1
1	A	62	GLU	1
1	A	70	ILE	1
1	A	64	GLU	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 [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5633

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	964
Number of shifts mapped to atoms	964
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	78	-1.27 ± 0.46	Should be applied
$^{13}\text{C}_\beta$	73	0.32 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	76	-1.01 ± 0.34	Should be applied
^{15}N	76	1.07 ± 0.34	Should be applied

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 86%, i.e. 806 atoms were assigned a chemical shift out of a possible 940. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	349/353 (99%)	139/141 (99%)	140/142 (99%)	70/70 (100%)
Sidechain	404/511 (79%)	240/300 (80%)	150/176 (85%)	14/35 (40%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	53/76 (70%)	29/40 (72%)	22/34 (65%)	2/2 (100%)
Overall	806/940 (86%)	408/481 (85%)	312/352 (89%)	86/107 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 869 atoms were assigned a chemical shift out of a possible 1013. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	381/388 (98%)	151/155 (97%)	154/156 (99%)	76/77 (99%)
Sidechain	431/540 (80%)	255/317 (80%)	161/187 (86%)	15/36 (42%)
Aromatic	57/85 (67%)	31/45 (69%)	24/38 (63%)	2/2 (100%)
Overall	869/1013 (86%)	437/517 (85%)	339/381 (89%)	93/115 (81%)

7.1.4 Statistically unusual chemical shifts ⓘ

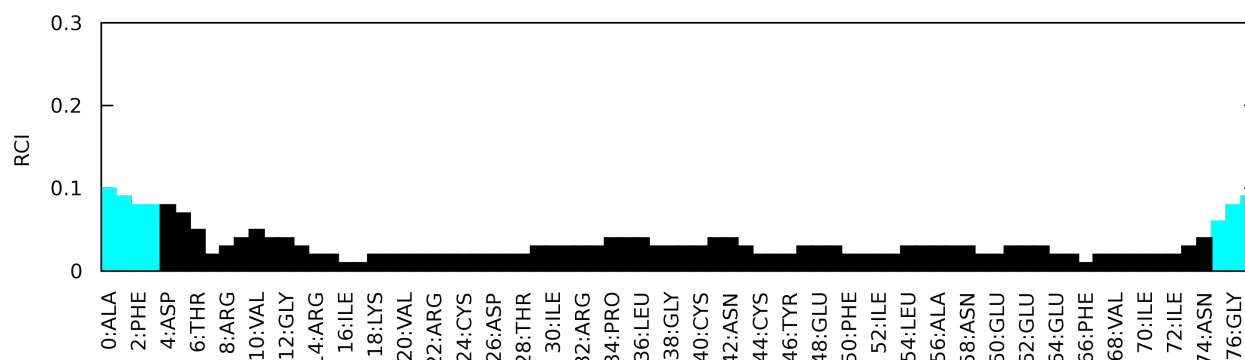
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	22	ARG	NE	122.72	92.63 – 76.73	23.9
1	A	41	ARG	NE	121.66	92.63 – 76.73	23.3
1	A	32	ARG	NE	121.13	92.63 – 76.73	22.9
1	A	59	ARG	NE	120.94	92.63 – 76.73	22.8
1	A	43	ARG	NE	120.89	92.63 – 76.73	22.8
1	A	8	ARG	NE	120.14	92.63 – 76.73	22.3
1	A	67	ARG	NE	119.58	92.63 – 76.73	22.0
1	A	49	TRP	CZ2	102.41	121.76 – 106.66	-7.8
1	A	65	LYS	HG2	-0.16	2.67 – 0.07	-5.9

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5653

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 Bookkeeping [i](#)

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

Total number of shifts	964
Number of shifts mapped to atoms	964
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	78	-1.23 ± 0.52	Should be applied
$^{13}\text{C}_\beta$	73	0.31 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}'$	76	-1.02 ± 0.31	Should be applied
^{15}N	76	1.09 ± 0.30	Should be applied

7.2.3 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 86%, i.e. 806 atoms were assigned a chemical shift out of a possible 940. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	349/353 (99%)	139/141 (99%)	140/142 (99%)	70/70 (100%)
Sidechain	404/511 (79%)	240/300 (80%)	150/176 (85%)	14/35 (40%)
Aromatic	53/76 (70%)	29/40 (72%)	22/34 (65%)	2/2 (100%)
Overall	806/940 (86%)	408/481 (85%)	312/352 (89%)	86/107 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 869 atoms were assigned a chemical shift out of a possible 1013. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	381/388 (98%)	151/155 (97%)	154/156 (99%)	76/77 (99%)
Sidechain	431/540 (80%)	255/317 (80%)	161/187 (86%)	15/36 (42%)
Aromatic	57/85 (67%)	31/45 (69%)	24/38 (63%)	2/2 (100%)
Overall	869/1013 (86%)	437/517 (85%)	339/381 (89%)	93/115 (81%)

7.2.4 Statistically unusual chemical shifts ⓘ

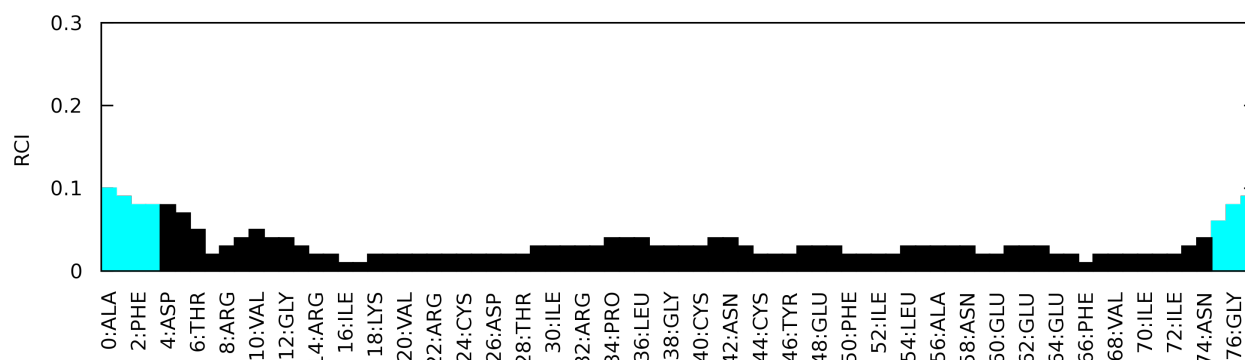
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	22	ARG	NE	122.72	92.63 – 76.73	23.9
1	A	41	ARG	NE	121.66	92.63 – 76.73	23.3
1	A	32	ARG	NE	121.13	92.63 – 76.73	22.9
1	A	59	ARG	NE	120.94	92.63 – 76.73	22.8
1	A	43	ARG	NE	120.89	92.63 – 76.73	22.8
1	A	8	ARG	NE	120.14	92.63 – 76.73	22.3
1	A	67	ARG	NE	119.58	92.63 – 76.73	22.0
1	A	49	TRP	CZ2	102.41	121.76 – 106.66	-7.8
1	A	65	LYS	HG2	-0.16	2.67 – 0.07	-5.9

7.2.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



7.3 Chemical shift list 3

File name: BMRB entry 5633

Chemical shift list name: *assigned_chem_shift_list_2*

7.3.1 Bookkeeping [i](#)

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

Total number of shifts	104
Number of shifts mapped to atoms	104
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.3.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.3.3 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 9%, i.e. 85 atoms were assigned a chemical shift out of a possible 940. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	64/353 (18%)	64/141 (45%)	0/142 (0%)	0/70 (0%)

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	Total	¹H	¹³C	¹⁵N
Sidechain	21/511 (4%)	18/300 (6%)	0/176 (0%)	3/35 (9%)
Aromatic	0/76 (0%)	0/40 (0%)	0/34 (0%)	0/2 (0%)
Overall	85/940 (9%)	82/481 (17%)	0/352 (0%)	3/107 (3%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 94 atoms were assigned a chemical shift out of a possible 1013. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	69/388 (18%)	69/155 (45%)	0/156 (0%)	0/77 (0%)
Sidechain	25/540 (5%)	21/317 (7%)	0/187 (0%)	4/36 (11%)
Aromatic	0/85 (0%)	0/45 (0%)	0/38 (0%)	0/2 (0%)
Overall	94/1013 (9%)	90/517 (17%)	0/381 (0%)	4/115 (3%)

7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_2). RCI is only applicable to proteins.