Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 03:19 PM BST

PDB ID	:	1IVM
Title	:	Solution structure of mouse lysozyme M
Authors	:	Ueda, T.; Obita, T.; Imoto, T.
Deposited on	:	2002-03-27

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:

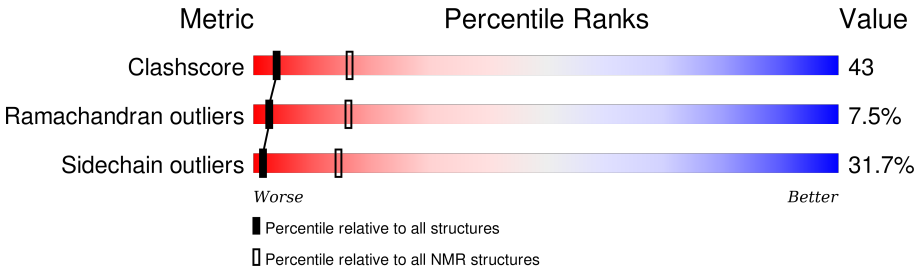
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 is 44%.

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	130	22% 66% 10%

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 20 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:2-A:130 (129)	0.57	9

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	4, 5, 6, 8, 9, 11, 12, 18, 19
2	1, 3, 7, 14, 16, 17
3	2, 10, 13, 15
Single-model clusters	20

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2024 atoms, of which 986 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called lysozyme M.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	130	2024	638	986	200	191	9	0

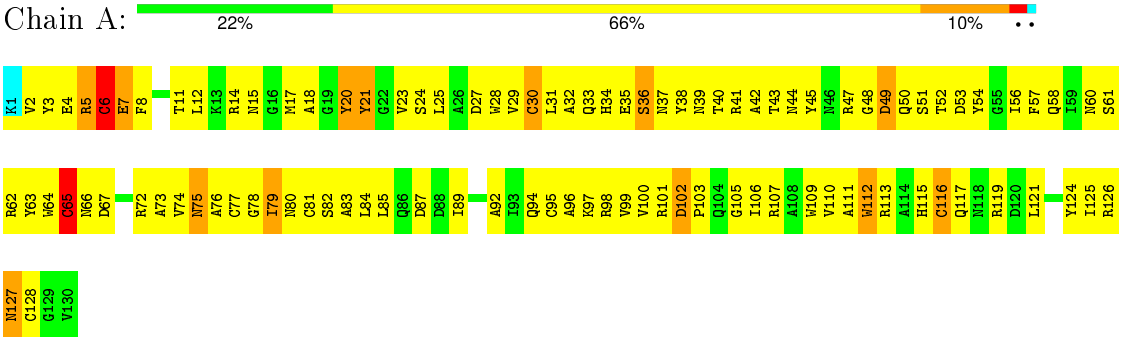
4 Residue-property plots

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: lysozyme M

Chain A:



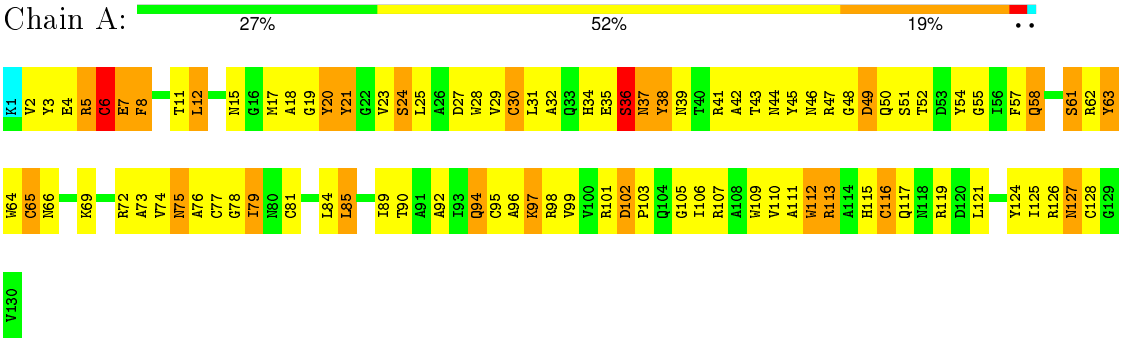
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: lysozyme M

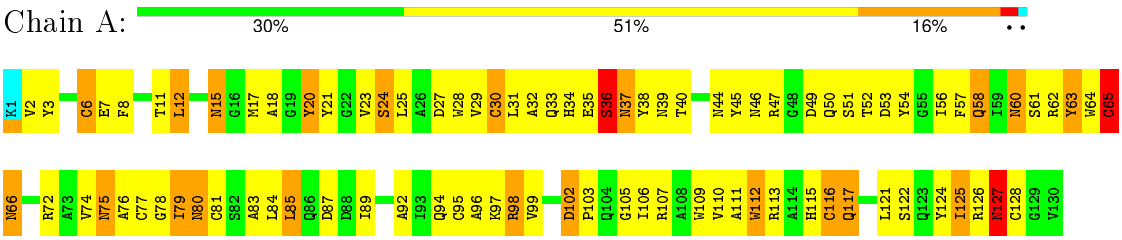
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: lysozyme M

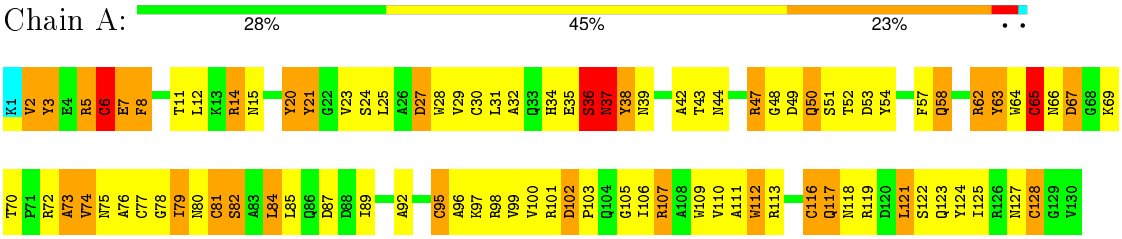
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: lysozyme M

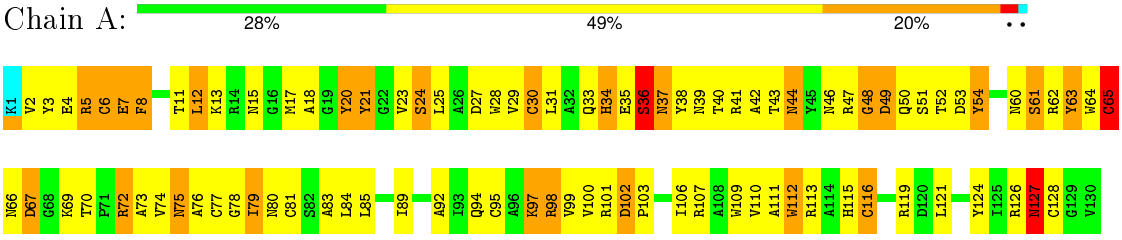
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: lysozyme M

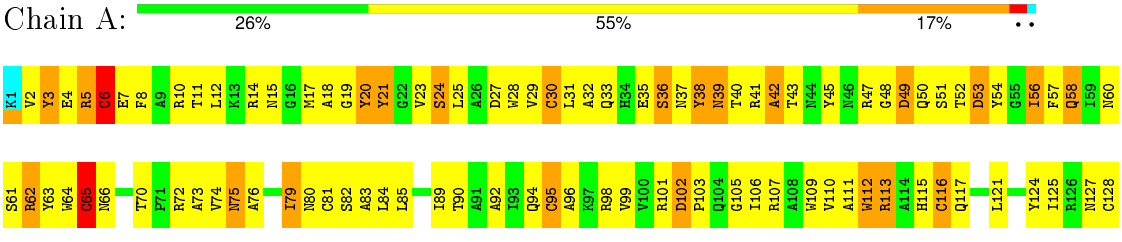
Chain A:



4.2.5 Score per residue for model 5

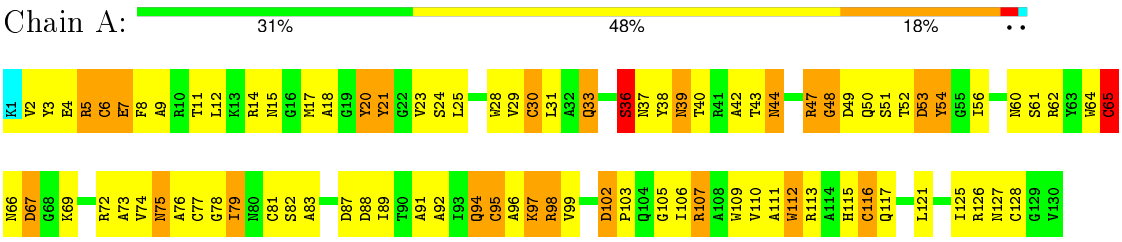
- Molecule 1: lysozyme M

Chain A:



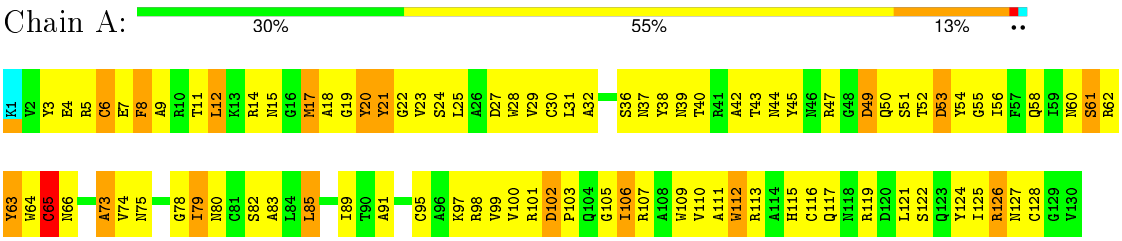
4.2.6 Score per residue for model 6

- Molecule 1: lysozyme M



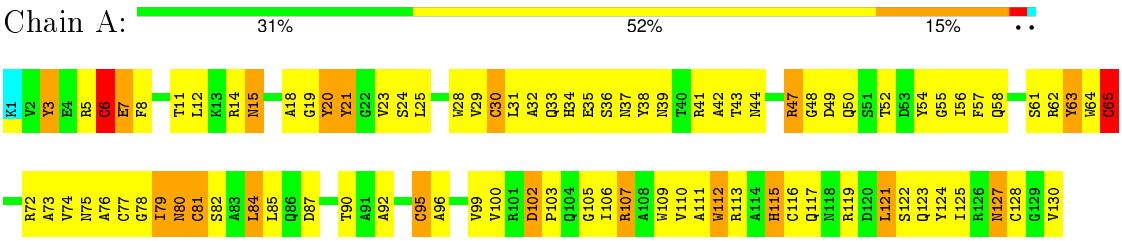
4.2.7 Score per residue for model 7

- Molecule 1: lysozyme M



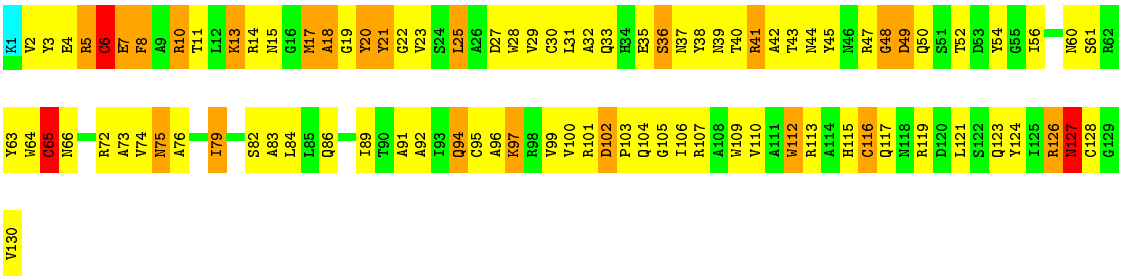
4.2.8 Score per residue for model 8

- Molecule 1: lysozyme M



4.2.9 Score per residue for model 9 (medoid)

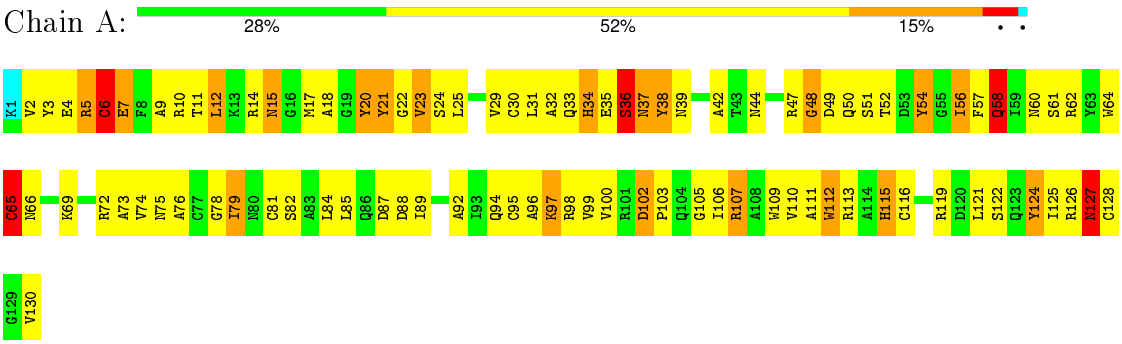
- Molecule 1: lysozyme M



4.2.10 Score per residue for model 10

- Molecule 1: lysozyme M

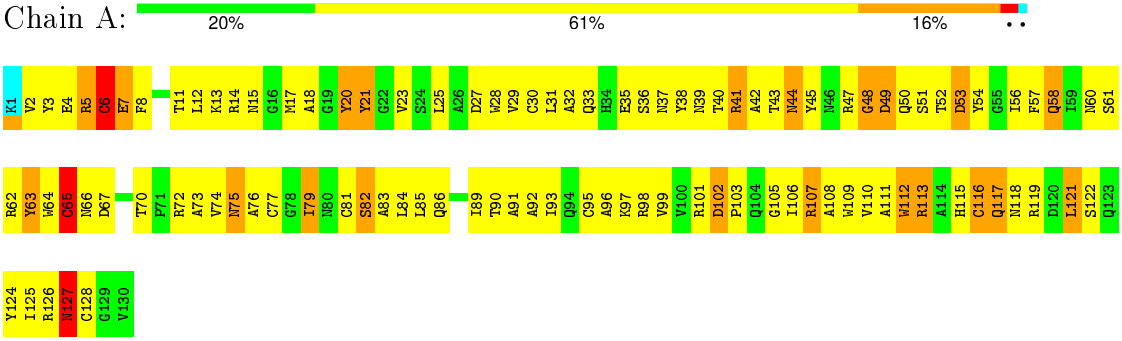
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: lysozyme M

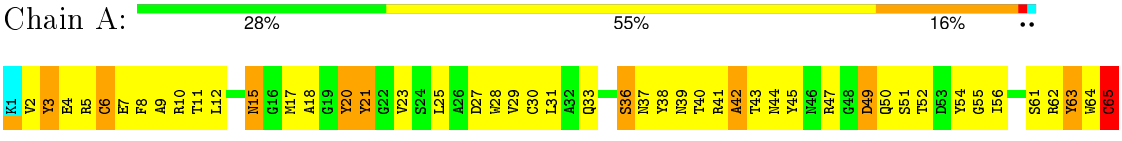
Chain A:

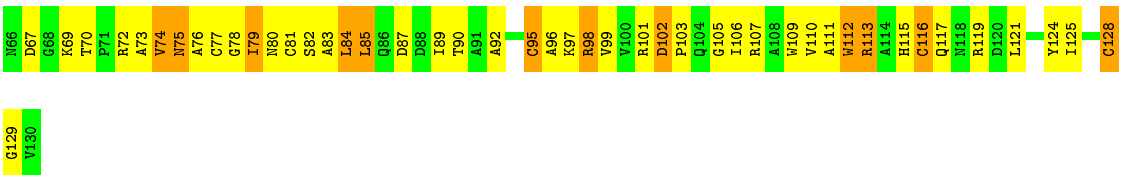


4.2.12 Score per residue for model 12

- Molecule 1: lysozyme M

Chain A:

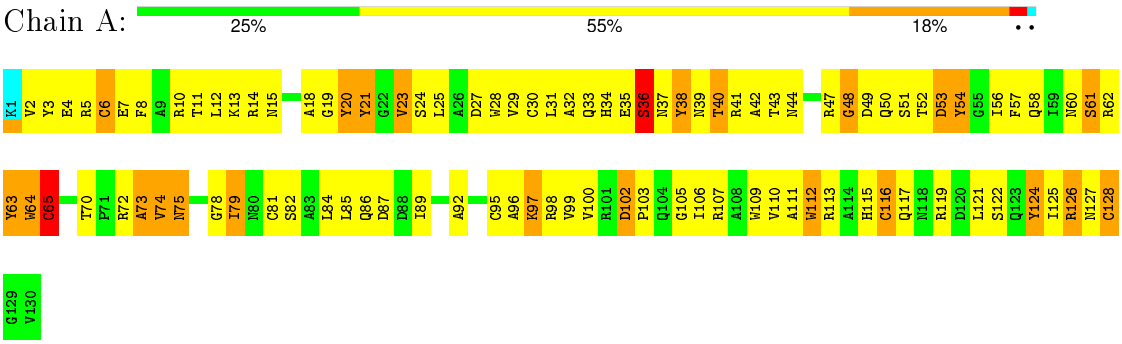




4.2.13 Score per residue for model 13

- Molecule 1: lysozyme M

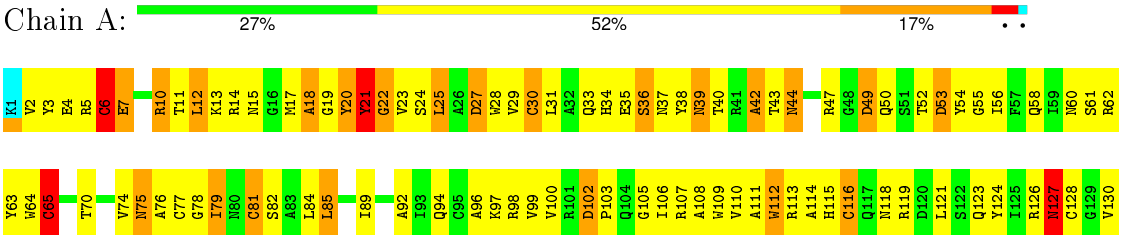
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: lysozyme M

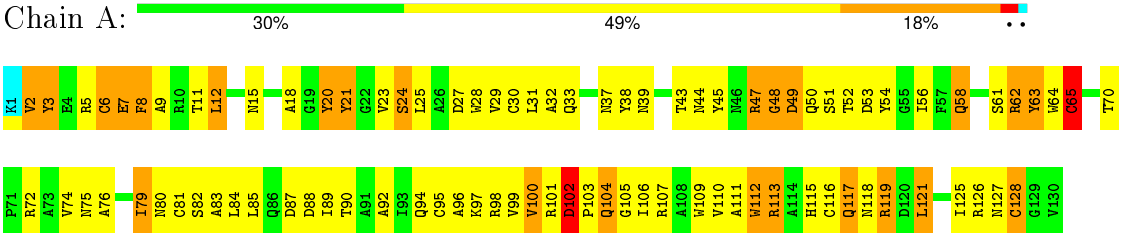
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: lysozyme M

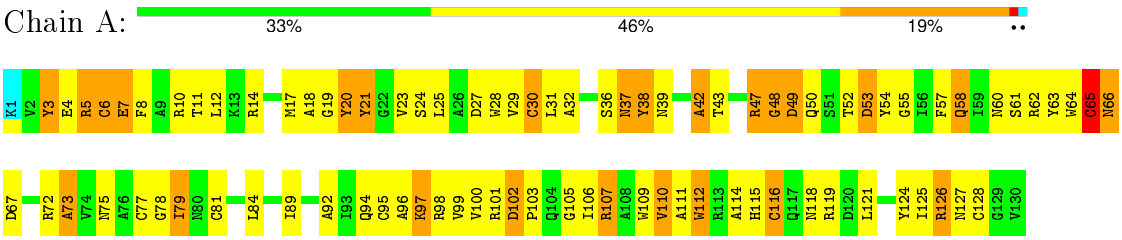
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: lysozyme M

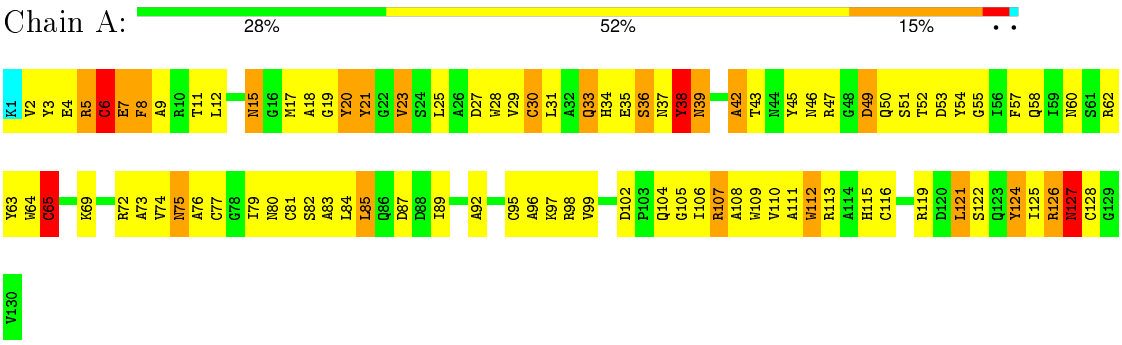
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: lysozyme M

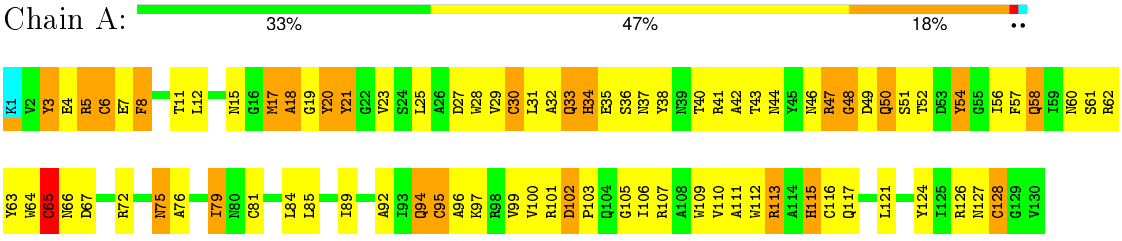
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: lysozyme M

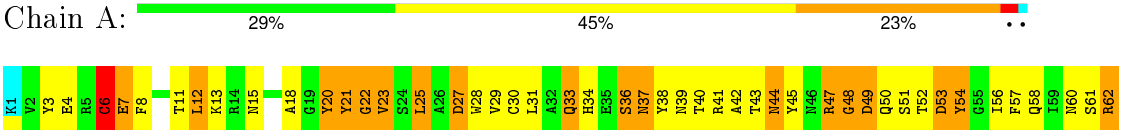
Chain A:

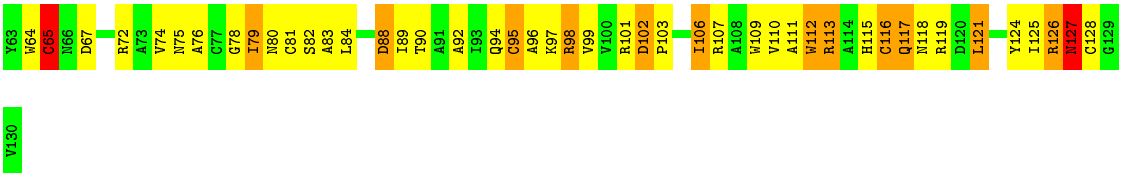


4.2.19 Score per residue for model 19

• Molecule 1: lysozyme M

Chain A:

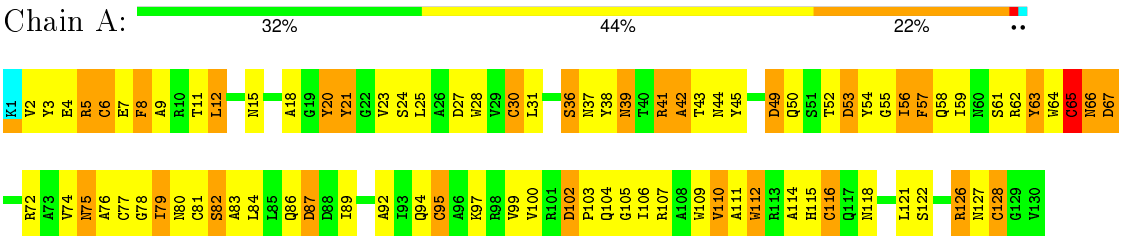




4.2.20 Score per residue for model 20

- Molecule 1: lysozyme M

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	1.5

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 4751
Number of chemical shift lists	1
Total number of shifts	836
Number of shifts mapped to atoms	836
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

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	1029	973	971	86±11
All	All	20580	19460	19420	1712

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 43.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ALA:HB1	1:A:25:LEU:HD22	1.09	1.11	19	6
1:A:40:THR:HG22	1:A:56:ILE:HD13	1.03	1.30	18	1
1:A:40:THR:HG22	1:A:56:ILE:HD12	1.01	1.30	12	4
1:A:3:TYR:CZ	1:A:89:ILE:HG22	0.97	1.93	19	1
1:A:43:THR:HG22	1:A:54:TYR:CD2	0.97	1.95	8	8
1:A:18:ALA:HB1	1:A:25:LEU:CD2	0.91	1.94	19	3
1:A:8:PHE:CE2	1:A:32:ALA:HB1	0.90	2.01	1	3
1:A:34:HIS:CD2	1:A:111:ALA:HB1	0.89	2.03	19	6
1:A:121:LEU:O	1:A:121:LEU:HD13	0.88	1.69	14	3
1:A:31:LEU:HD11	1:A:109:TRP:CE3	0.86	2.05	11	3
1:A:3:TYR:CE1	1:A:8:PHE:CG	0.85	2.64	18	4
1:A:31:LEU:HD11	1:A:109:TRP:CD2	0.85	2.06	19	5
1:A:116:CYS:SG	1:A:121:LEU:HD22	0.85	2.12	19	4
1:A:18:ALA:CB	1:A:25:LEU:HD13	0.84	2.02	16	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:TYR:CE2	1:A:56:ILE:HD13	0.83	2.08	8	2
1:A:64:TRP:CD1	1:A:99:VAL:HG22	0.83	2.08	15	5
1:A:43:THR:HG22	1:A:54:TYR:HB2	0.83	1.49	13	2
1:A:25:LEU:O	1:A:29:VAL:HG23	0.83	1.74	9	6
1:A:3:TYR:CE2	1:A:8:PHE:CE1	0.82	2.68	8	3
1:A:23:VAL:HG11	1:A:106:ILE:HG13	0.81	1.52	10	3
1:A:31:LEU:HD11	1:A:109:TRP:CG	0.81	2.11	16	6
1:A:121:LEU:HD13	1:A:121:LEU:O	0.81	1.74	13	5
1:A:30:CYS:HB3	1:A:121:LEU:HD12	0.81	1.53	18	4
1:A:43:THR:CG2	1:A:85:LEU:HD11	0.81	2.06	1	3
1:A:18:ALA:HB1	1:A:25:LEU:HD13	0.81	1.50	15	4
1:A:40:THR:CG2	1:A:56:ILE:HD13	0.80	2.06	18	1
1:A:64:TRP:CZ3	1:A:76:ALA:HB3	0.80	2.10	18	4
1:A:3:TYR:CD1	1:A:8:PHE:CD1	0.80	2.70	15	3
1:A:116:CYS:SG	1:A:121:LEU:HD13	0.80	2.17	11	2
1:A:8:PHE:CE1	1:A:89:ILE:HD13	0.79	2.13	15	1
1:A:2:VAL:HG13	1:A:38:TYR:O	0.78	1.78	12	4
1:A:64:TRP:CD2	1:A:99:VAL:HG22	0.78	2.13	9	2
1:A:83:ALA:HB1	1:A:91:ALA:CB	0.77	2.10	9	3
1:A:96:ALA:O	1:A:100:VAL:HG23	0.77	1.77	18	2
1:A:40:THR:HG22	1:A:56:ILE:CD1	0.77	2.09	18	2
1:A:23:VAL:HG11	1:A:28:TRP:CE2	0.77	2.14	5	14
1:A:18:ALA:HB1	1:A:25:LEU:HB2	0.77	1.55	7	8
1:A:3:TYR:CG	1:A:8:PHE:CD1	0.76	2.74	15	3
1:A:31:LEU:HD22	1:A:106:ILE:HD12	0.76	1.56	17	4
1:A:54:TYR:CE2	1:A:84:LEU:HD13	0.75	2.16	20	1
1:A:3:TYR:CE2	1:A:89:ILE:HG22	0.75	2.16	19	1
1:A:112:TRP:CE3	1:A:116:CYS:CB	0.74	2.70	11	4
1:A:31:LEU:HD22	1:A:106:ILE:CD1	0.74	2.13	9	6
1:A:52:THR:HG22	1:A:54:TYR:CD1	0.74	2.18	12	8
1:A:3:TYR:CZ	1:A:8:PHE:CD1	0.73	2.76	12	3
1:A:3:TYR:C	1:A:3:TYR:CD1	0.73	2.61	8	3
1:A:42:ALA:HB3	1:A:55:GLY:O	0.73	1.82	7	5
1:A:34:HIS:CE1	1:A:111:ALA:HB1	0.72	2.19	2	4
1:A:29:VAL:HG21	1:A:125:ILE:HG22	0.72	1.61	5	11
1:A:52:THR:CG2	1:A:54:TYR:CD1	0.71	2.73	8	7
1:A:3:TYR:OH	1:A:11:THR:HG21	0.71	1.84	16	1
1:A:3:TYR:CE1	1:A:8:PHE:CD1	0.71	2.79	12	4
1:A:37:ASN:O	1:A:38:TYR:HB3	0.71	1.83	17	2
1:A:8:PHE:CE1	1:A:89:ILE:CD1	0.71	2.72	15	1
1:A:95:CYS:O	1:A:99:VAL:HG23	0.71	1.84	20	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:CYS:HB3	1:A:121:LEU:HD22	0.70	1.62	5	4
1:A:43:THR:HG22	1:A:54:TYR:CB	0.69	2.15	13	2
1:A:8:PHE:CE2	1:A:32:ALA:CB	0.69	2.75	3	8
1:A:64:TRP:CZ3	1:A:76:ALA:CB	0.69	2.76	18	4
1:A:31:LEU:HD13	1:A:106:ILE:HD12	0.69	1.65	1	2
1:A:3:TYR:CZ	1:A:56:ILE:HD13	0.68	2.24	12	1
1:A:36:SER:O	1:A:38:TYR:CE1	0.68	2.47	17	1
1:A:31:LEU:HD13	1:A:31:LEU:C	0.68	2.09	2	1
1:A:116:CYS:O	1:A:118:ASN:N	0.68	2.26	19	7
1:A:31:LEU:C	1:A:31:LEU:HD23	0.67	2.09	19	2
1:A:23:VAL:CG1	1:A:28:TRP:CE2	0.67	2.77	5	14
1:A:30:CYS:CB	1:A:121:LEU:HD22	0.67	2.19	17	3
1:A:29:VAL:HG21	1:A:125:ILE:CG2	0.67	2.20	3	8
1:A:106:ILE:HG21	1:A:112:TRP:CZ3	0.67	2.24	16	2
1:A:106:ILE:HG21	1:A:112:TRP:CE3	0.66	2.25	16	3
1:A:32:ALA:HB2	1:A:57:PHE:CE1	0.66	2.26	3	3
1:A:30:CYS:CB	1:A:121:LEU:HD12	0.66	2.20	18	3
1:A:45:TYR:HA	1:A:52:THR:HG23	0.66	1.68	5	8
1:A:66:ASN:O	1:A:67:ASP:CB	0.65	2.45	16	1
1:A:31:LEU:CD1	1:A:109:TRP:CG	0.65	2.79	3	3
1:A:27:ASP:HB3	1:A:112:TRP:CZ2	0.65	2.26	14	3
1:A:106:ILE:CG2	1:A:112:TRP:CE3	0.65	2.80	14	3
1:A:3:TYR:CD2	1:A:8:PHE:CE1	0.65	2.85	18	2
1:A:65:CYS:HA	1:A:79:ILE:HD13	0.64	1.68	3	14
1:A:112:TRP:C	1:A:112:TRP:CD1	0.64	2.70	20	2
1:A:107:ARG:O	1:A:110:VAL:HG23	0.64	1.91	19	1
1:A:40:THR:HB	1:A:56:ILE:HD12	0.64	1.70	7	1
1:A:89:ILE:HD11	1:A:93:ILE:HD11	0.64	1.69	11	1
1:A:18:ALA:HB2	1:A:25:LEU:HD13	0.64	1.70	16	4
1:A:52:THR:HG21	1:A:54:TYR:CE2	0.64	2.27	6	2
1:A:3:TYR:CE2	1:A:56:ILE:HD11	0.64	2.28	18	1
1:A:92:ALA:O	1:A:96:ALA:HB2	0.64	1.92	8	17
1:A:23:VAL:HG22	1:A:28:TRP:CD1	0.64	2.27	9	3
1:A:8:PHE:CE1	1:A:12:LEU:CD1	0.64	2.81	19	1
1:A:80:ASN:O	1:A:83:ALA:HB3	0.64	1.93	4	5
1:A:33:GLN:NE2	1:A:38:TYR:CE2	0.64	2.66	14	1
1:A:3:TYR:CD1	1:A:3:TYR:C	0.63	2.71	12	1
1:A:3:TYR:OH	1:A:32:ALA:HB1	0.63	1.93	18	1
1:A:112:TRP:CE3	1:A:116:CYS:HB2	0.63	2.29	19	4
1:A:41:ARG:O	1:A:43:THR:HG23	0.63	1.94	13	4
1:A:12:LEU:HD21	1:A:28:TRP:CD1	0.63	2.28	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:TYR:CE2	1:A:56:ILE:CD1	0.63	2.80	8	2
1:A:31:LEU:C	1:A:31:LEU:HD13	0.63	2.13	8	1
1:A:81:CYS:HA	1:A:84:LEU:HD12	0.63	1.69	14	7
1:A:52:THR:CG2	1:A:54:TYR:CE2	0.63	2.82	6	2
1:A:37:ASN:O	1:A:38:TYR:CB	0.63	2.47	17	4
1:A:106:ILE:HG23	1:A:112:TRP:CE3	0.63	2.28	14	2
1:A:64:TRP:CE3	1:A:76:ALA:HB3	0.62	2.29	18	4
1:A:27:ASP:CB	1:A:112:TRP:CZ2	0.62	2.82	14	3
1:A:70:THR:O	1:A:70:THR:HG23	0.62	1.94	15	3
1:A:37:ASN:OD1	1:A:38:TYR:CD2	0.62	2.52	2	1
1:A:54:TYR:O	1:A:58:GLN:N	0.62	2.32	20	1
1:A:106:ILE:HD13	1:A:109:TRP:CZ3	0.62	2.29	7	9
1:A:43:THR:HG23	1:A:85:LEU:HD11	0.62	1.70	14	4
1:A:31:LEU:HD12	1:A:106:ILE:HD12	0.62	1.72	11	1
1:A:27:ASP:CB	1:A:112:TRP:CH2	0.62	2.83	14	3
1:A:37:ASN:O	1:A:39:ASN:N	0.61	2.33	11	12
1:A:3:TYR:N	1:A:3:TYR:CD1	0.61	2.69	5	1
1:A:36:SER:O	1:A:38:TYR:CD1	0.61	2.53	17	1
1:A:54:TYR:CE2	1:A:61:SER:OG	0.61	2.48	4	1
1:A:31:LEU:O	1:A:31:LEU:HD23	0.61	1.95	11	2
1:A:38:TYR:CD2	1:A:39:ASN:OD1	0.61	2.54	13	1
1:A:8:PHE:CD2	1:A:37:ASN:OD1	0.61	2.54	4	2
1:A:31:LEU:HD21	1:A:109:TRP:HB2	0.61	1.73	8	1
1:A:54:TYR:CE2	1:A:84:LEU:HB2	0.60	2.30	15	6
1:A:3:TYR:CZ	1:A:8:PHE:CE1	0.60	2.89	8	2
1:A:8:PHE:CE2	1:A:32:ALA:HB2	0.60	2.32	5	3
1:A:3:TYR:CD1	1:A:8:PHE:HB2	0.60	2.31	18	4
1:A:35:GLU:OE2	1:A:109:TRP:CD1	0.60	2.54	9	6
1:A:34:HIS:CE1	1:A:115:HIS:ND1	0.60	2.69	8	1
1:A:3:TYR:CE1	1:A:37:ASN:OD1	0.60	2.54	18	2
1:A:8:PHE:CE2	1:A:37:ASN:OD1	0.60	2.55	4	2
1:A:31:LEU:HD23	1:A:31:LEU:O	0.59	1.98	19	1
1:A:27:ASP:OD1	1:A:112:TRP:CH2	0.59	2.54	3	1
1:A:30:CYS:CB	1:A:121:LEU:HD23	0.59	2.27	4	3
1:A:31:LEU:CD1	1:A:109:TRP:CE3	0.59	2.86	19	2
1:A:23:VAL:HG11	1:A:106:ILE:CG1	0.59	2.27	19	3
1:A:43:THR:HG22	1:A:54:TYR:CE2	0.59	2.32	17	5
1:A:2:VAL:O	1:A:3:TYR:CD1	0.59	2.56	6	5
1:A:3:TYR:O	1:A:38:TYR:N	0.59	2.36	13	19
1:A:34:HIS:CD2	1:A:115:HIS:CE1	0.58	2.91	8	1
1:A:27:ASP:CG	1:A:112:TRP:CZ2	0.58	2.77	16	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:PHE:CE1	1:A:12:LEU:HD13	0.58	2.32	19	1
1:A:30:CYS:HB2	1:A:121:LEU:HD13	0.58	1.76	9	1
1:A:74:VAL:O	1:A:74:VAL:HG22	0.58	1.98	11	5
1:A:3:TYR:CE2	1:A:8:PHE:CD1	0.58	2.92	8	2
1:A:17:MET:SD	1:A:28:TRP:CZ2	0.58	2.96	7	1
1:A:17:MET:SD	1:A:20:TYR:CD1	0.58	2.97	14	2
1:A:55:GLY:O	1:A:57:PHE:N	0.58	2.36	20	1
1:A:37:ASN:O	1:A:37:ASN:CG	0.58	2.42	13	1
1:A:121:LEU:HD11	1:A:124:TYR:CD1	0.58	2.34	16	1
1:A:3:TYR:CE1	1:A:8:PHE:HB2	0.57	2.34	18	3
1:A:2:VAL:O	1:A:3:TYR:CD2	0.57	2.56	11	2
1:A:112:TRP:CD1	1:A:116:CYS:HB2	0.57	2.34	20	12
1:A:43:THR:CG2	1:A:54:TYR:CD2	0.57	2.81	8	4
1:A:5:ARG:CD	1:A:124:TYR:CE2	0.57	2.87	13	1
1:A:39:ASN:N	1:A:39:ASN:OD1	0.57	2.37	17	3
1:A:5:ARG:HA	1:A:29:VAL:HG13	0.57	1.76	3	1
1:A:55:GLY:O	1:A:56:ILE:C	0.57	2.43	20	1
1:A:3:TYR:OH	1:A:56:ILE:HD13	0.57	2.00	12	1
1:A:79:ILE:C	1:A:79:ILE:HD13	0.57	2.20	7	1
1:A:34:HIS:NE2	1:A:111:ALA:HB1	0.57	2.15	2	2
1:A:25:LEU:HD12	1:A:125:ILE:CD1	0.56	2.30	19	1
1:A:3:TYR:CE1	1:A:40:THR:HG21	0.56	2.34	19	1
1:A:27:ASP:OD2	1:A:112:TRP:CZ2	0.56	2.58	19	2
1:A:3:TYR:CD2	1:A:8:PHE:CD1	0.56	2.93	18	3
1:A:79:ILE:HD13	1:A:79:ILE:O	0.56	2.00	10	2
1:A:56:ILE:HG23	1:A:57:PHE:CD2	0.56	2.35	18	1
1:A:31:LEU:CD1	1:A:106:ILE:CD1	0.56	2.83	20	1
1:A:35:GLU:O	1:A:36:SER:CB	0.56	2.54	17	7
1:A:23:VAL:HG22	1:A:28:TRP:NE1	0.56	2.15	9	3
1:A:52:THR:CG2	1:A:54:TYR:CE1	0.56	2.88	1	6
1:A:79:ILE:O	1:A:79:ILE:HD13	0.56	2.01	3	4
1:A:45:TYR:CE2	1:A:52:THR:HG21	0.56	2.36	9	1
1:A:52:THR:CG2	1:A:54:TYR:CD2	0.56	2.88	4	3
1:A:112:TRP:CD1	1:A:112:TRP:C	0.56	2.79	14	1
1:A:3:TYR:OH	1:A:40:THR:HG21	0.55	2.01	5	1
1:A:31:LEU:CD1	1:A:57:PHE:CD1	0.55	2.89	13	1
1:A:3:TYR:CD1	1:A:8:PHE:CG	0.55	2.95	15	2
1:A:23:VAL:HG11	1:A:28:TRP:CD2	0.55	2.37	5	4
1:A:27:ASP:OD1	1:A:112:TRP:CD1	0.55	2.59	13	2
1:A:37:ASN:CG	1:A:38:TYR:N	0.55	2.59	15	2
1:A:3:TYR:CE1	1:A:89:ILE:HG22	0.55	2.33	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:THR:HG23	1:A:70:THR:O	0.55	2.01	12	1
1:A:12:LEU:HB3	1:A:18:ALA:HB2	0.55	1.79	1	4
1:A:3:TYR:CE2	1:A:37:ASN:HA	0.55	2.37	15	1
1:A:43:THR:CG2	1:A:54:TYR:CE2	0.55	2.90	1	7
1:A:37:ASN:O	1:A:38:TYR:HB2	0.55	2.02	2	12
1:A:37:ASN:HA	1:A:56:ILE:HD11	0.55	1.78	2	3
1:A:112:TRP:CZ3	1:A:116:CYS:CB	0.54	2.90	15	4
1:A:62:ARG:O	1:A:73:ALA:HB1	0.54	2.01	13	1
1:A:2:VAL:HG13	1:A:38:TYR:C	0.54	2.23	1	1
1:A:56:ILE:CG2	1:A:92:ALA:HB1	0.54	2.32	18	2
1:A:3:TYR:CE1	1:A:8:PHE:CB	0.54	2.90	18	3
1:A:64:TRP:NE1	1:A:99:VAL:HG22	0.54	2.16	19	1
1:A:92:ALA:O	1:A:96:ALA:CB	0.54	2.56	8	15
1:A:56:ILE:HG23	1:A:57:PHE:HD1	0.54	1.62	2	2
1:A:31:LEU:HD22	1:A:57:PHE:CD1	0.54	2.37	11	1
1:A:38:TYR:CD1	1:A:39:ASN:N	0.54	2.75	17	1
1:A:3:TYR:HE2	1:A:56:ILE:HD13	0.54	1.57	8	1
1:A:11:THR:O	1:A:15:ASN:N	0.54	2.41	19	19
1:A:23:VAL:HG11	1:A:28:TRP:CZ2	0.54	2.38	14	8
1:A:35:GLU:OE1	1:A:109:TRP:CD1	0.54	2.61	1	2
1:A:2:VAL:O	1:A:3:TYR:CG	0.54	2.60	6	2
1:A:3:TYR:N	1:A:38:TYR:O	0.53	2.41	5	15
1:A:3:TYR:HE2	1:A:56:ILE:HD11	0.53	1.63	18	1
1:A:52:THR:HG22	1:A:54:TYR:CD2	0.53	2.39	4	3
1:A:38:TYR:CZ	1:A:39:ASN:HB2	0.53	2.39	13	1
1:A:25:LEU:HG	1:A:125:ILE:HG21	0.53	1.80	3	2
1:A:52:THR:O	1:A:61:SER:N	0.53	2.41	10	12
1:A:27:ASP:HA	1:A:112:TRP:CZ3	0.53	2.39	19	4
1:A:40:THR:HG22	1:A:56:ILE:HB	0.53	1.81	9	1
1:A:77:CYS:HB3	1:A:79:ILE:HD12	0.53	1.80	1	9
1:A:31:LEU:HD12	1:A:57:PHE:CE2	0.53	2.39	2	1
1:A:2:VAL:CG1	1:A:38:TYR:O	0.53	2.55	12	2
1:A:9:ALA:CB	1:A:25:LEU:HD11	0.53	2.32	7	1
1:A:112:TRP:CZ3	1:A:116:CYS:HB3	0.53	2.39	19	3
1:A:5:ARG:HD2	1:A:124:TYR:CE2	0.53	2.38	13	3
1:A:27:ASP:OD2	1:A:106:ILE:HG21	0.53	2.03	15	1
1:A:3:TYR:OH	1:A:32:ALA:CB	0.53	2.56	8	3
1:A:102:ASP:CB	1:A:103:PRO:CD	0.53	2.87	13	19
1:A:110:VAL:O	1:A:113:ARG:N	0.53	2.42	11	17
1:A:6:CYS:O	1:A:7:GLU:C	0.53	2.48	15	20
1:A:31:LEU:CD1	1:A:106:ILE:HG23	0.53	2.33	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:TYR:CD2	1:A:52:THR:HG21	0.53	2.38	9	1
1:A:45:TYR:CA	1:A:52:THR:HG23	0.52	2.33	5	6
1:A:30:CYS:HB2	1:A:121:LEU:HD23	0.52	1.80	16	3
1:A:31:LEU:C	1:A:31:LEU:CD2	0.52	2.78	19	2
1:A:25:LEU:CD1	1:A:125:ILE:HD12	0.52	2.34	19	1
1:A:84:LEU:N	1:A:84:LEU:HD23	0.52	2.19	13	1
1:A:23:VAL:HG22	1:A:106:ILE:HG13	0.52	1.80	1	4
1:A:100:VAL:HG21	1:A:106:ILE:HG12	0.52	1.79	15	1
1:A:3:TYR:CD1	1:A:3:TYR:O	0.52	2.63	8	1
1:A:102:ASP:OD2	1:A:104:GLN:CG	0.52	2.58	9	1
1:A:28:TRP:CE3	1:A:57:PHE:CZ	0.52	2.97	5	1
1:A:3:TYR:CZ	1:A:8:PHE:CG	0.52	2.98	18	2
1:A:79:ILE:HD13	1:A:79:ILE:C	0.52	2.25	9	1
1:A:25:LEU:HD12	1:A:125:ILE:HD12	0.52	1.80	19	1
1:A:34:HIS:CG	1:A:111:ALA:HB1	0.52	2.40	13	1
1:A:29:VAL:O	1:A:33:GLN:N	0.52	2.43	8	14
1:A:38:TYR:CE2	1:A:39:ASN:HB2	0.52	2.40	13	1
1:A:83:ALA:HB1	1:A:91:ALA:HB1	0.51	1.79	9	1
1:A:106:ILE:HD13	1:A:109:TRP:CE3	0.51	2.41	7	6
1:A:121:LEU:HD23	1:A:121:LEU:O	0.51	2.06	9	2
1:A:3:TYR:OH	1:A:40:THR:CG2	0.51	2.59	5	1
1:A:66:ASN:OD1	1:A:73:ALA:HB3	0.51	2.06	16	2
1:A:31:LEU:HD13	1:A:106:ILE:CD1	0.51	2.35	1	3
1:A:34:HIS:ND1	1:A:111:ALA:HB1	0.51	2.20	14	1
1:A:31:LEU:CD1	1:A:31:LEU:C	0.51	2.79	8	2
1:A:31:LEU:HD21	1:A:109:TRP:CB	0.51	2.35	8	1
1:A:89:ILE:CD1	1:A:93:ILE:HD11	0.51	2.34	11	1
1:A:27:ASP:O	1:A:31:LEU:CB	0.51	2.58	3	10
1:A:34:HIS:NE2	1:A:115:HIS:CE1	0.51	2.78	8	1
1:A:126:ARG:O	1:A:127:ASN:CB	0.51	2.59	7	16
1:A:30:CYS:HB2	1:A:121:LEU:HD22	0.51	1.83	3	3
1:A:40:THR:CB	1:A:56:ILE:HD12	0.51	2.36	7	1
1:A:25:LEU:HD23	1:A:125:ILE:HD13	0.51	1.82	16	1
1:A:82:SER:O	1:A:86:GLN:CG	0.51	2.59	11	3
1:A:112:TRP:CD1	1:A:116:CYS:CB	0.51	2.94	20	6
1:A:43:THR:HB	1:A:54:TYR:CZ	0.51	2.41	17	6
1:A:54:TYR:CE1	1:A:84:LEU:HB2	0.51	2.41	2	1
1:A:25:LEU:HD12	1:A:29:VAL:HG23	0.51	1.82	3	1
1:A:35:GLU:CD	1:A:109:TRP:CD1	0.50	2.85	1	1
1:A:63:TYR:C	1:A:64:TRP:CE3	0.50	2.85	8	1
1:A:54:TYR:C	1:A:54:TYR:CD1	0.50	2.83	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:CD2	1:A:106:ILE:CD1	0.50	2.88	9	1
1:A:80:ASN:O	1:A:83:ALA:CB	0.50	2.60	5	4
1:A:38:TYR:N	1:A:38:TYR:CD1	0.50	2.79	17	1
1:A:70:THR:CG2	1:A:70:THR:O	0.50	2.59	12	1
1:A:70:THR:O	1:A:70:THR:CG2	0.50	2.60	15	1
1:A:8:PHE:CE1	1:A:56:ILE:HG21	0.50	2.42	13	1
1:A:112:TRP:CE3	1:A:113:ARG:N	0.50	2.80	9	12
1:A:54:TYR:CZ	1:A:84:LEU:HB2	0.50	2.41	18	3
1:A:8:PHE:CZ	1:A:57:PHE:CZ	0.50	3.00	17	3
1:A:2:VAL:HG22	1:A:38:TYR:O	0.50	2.06	15	2
1:A:102:ASP:OD2	1:A:104:GLN:CB	0.49	2.60	9	1
1:A:25:LEU:HG	1:A:125:ILE:HD13	0.49	1.81	6	2
1:A:42:ALA:CB	1:A:55:GLY:O	0.49	2.60	14	4
1:A:54:TYR:HE1	1:A:84:LEU:HD13	0.49	1.67	19	2
1:A:34:HIS:CG	1:A:115:HIS:CD2	0.49	3.01	8	1
1:A:95:CYS:O	1:A:99:VAL:N	0.49	2.46	5	18
1:A:3:TYR:CG	1:A:40:THR:HG22	0.49	2.42	19	1
1:A:38:TYR:CD1	1:A:38:TYR:C	0.49	2.86	17	1
1:A:30:CYS:SG	1:A:31:LEU:N	0.49	2.86	16	12
1:A:27:ASP:HA	1:A:112:TRP:CE3	0.49	2.42	11	3
1:A:56:ILE:HG23	1:A:57:PHE:CD1	0.49	2.43	19	1
1:A:116:CYS:SG	1:A:121:LEU:CB	0.49	3.00	3	2
1:A:37:ASN:HD22	1:A:37:ASN:N	0.49	2.05	3	1
1:A:63:TYR:HB3	1:A:64:TRP:CE3	0.48	2.42	20	2
1:A:74:VAL:O	1:A:76:ALA:N	0.48	2.43	12	16
1:A:63:TYR:O	1:A:74:VAL:O	0.48	2.31	3	11
1:A:44:ASN:N	1:A:53:ASP:O	0.48	2.45	7	10
1:A:64:TRP:CE2	1:A:99:VAL:HG22	0.48	2.43	9	2
1:A:109:TRP:O	1:A:110:VAL:C	0.48	2.52	20	6
1:A:49:ASP:O	1:A:50:GLN:C	0.48	2.51	17	20
1:A:17:MET:HE1	1:A:20:TYR:CG	0.48	2.44	18	1
1:A:54:TYR:O	1:A:58:GLN:CA	0.48	2.62	20	1
1:A:27:ASP:HB2	1:A:112:TRP:CZ2	0.48	2.43	11	1
1:A:64:TRP:O	1:A:65:CYS:C	0.48	2.52	13	1
1:A:63:TYR:CD1	1:A:64:TRP:CZ3	0.48	3.02	8	1
1:A:89:ILE:O	1:A:92:ALA:N	0.48	2.47	17	18
1:A:12:LEU:CD2	1:A:28:TRP:CD1	0.48	2.97	14	1
1:A:38:TYR:CG	1:A:39:ASN:N	0.48	2.81	17	2
1:A:54:TYR:O	1:A:54:TYR:CD1	0.48	2.67	10	1
1:A:74:VAL:HG22	1:A:74:VAL:O	0.48	2.09	1	1
1:A:20:TYR:O	1:A:22:GLY:N	0.48	2.47	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:THR:HG22	1:A:54:TYR:CG	0.48	2.44	7	1
1:A:54:TYR:CZ	1:A:61:SER:OG	0.48	2.59	4	1
1:A:47:ARG:O	1:A:49:ASP:N	0.48	2.47	13	10
1:A:54:TYR:CD1	1:A:54:TYR:N	0.47	2.81	6	2
1:A:32:ALA:O	1:A:37:ASN:N	0.47	2.47	3	1
1:A:109:TRP:C	1:A:111:ALA:N	0.47	2.66	11	17
1:A:4:GLU:O	1:A:5:ARG:C	0.47	2.52	17	12
1:A:38:TYR:CE1	1:A:39:ASN:O	0.47	2.67	17	1
1:A:37:ASN:C	1:A:38:TYR:CG	0.47	2.87	12	2
1:A:34:HIS:CD2	1:A:115:HIS:CG	0.47	3.02	10	2
1:A:3:TYR:CE2	1:A:89:ILE:HG12	0.47	2.44	10	1
1:A:62:ARG:CG	1:A:62:ARG:O	0.47	2.62	15	3
1:A:64:TRP:CD1	1:A:99:VAL:CG2	0.47	2.93	15	1
1:A:34:HIS:CD2	1:A:115:HIS:CD2	0.47	3.02	10	1
1:A:17:MET:HE2	1:A:20:TYR:CD1	0.47	2.45	18	1
1:A:66:ASN:CG	1:A:67:ASP:N	0.47	2.68	6	3
1:A:9:ALA:HA	1:A:25:LEU:HD11	0.47	1.86	20	3
1:A:20:TYR:O	1:A:21:TYR:C	0.47	2.52	9	19
1:A:33:GLN:HG3	1:A:124:TYR:CE2	0.47	2.44	13	2
1:A:37:ASN:C	1:A:37:ASN:ND2	0.47	2.67	3	1
1:A:53:ASP:N	1:A:53:ASP:OD1	0.47	2.48	16	1
1:A:19:GLY:O	1:A:20:TYR:O	0.47	2.33	14	10
1:A:50:GLN:CG	1:A:70:THR:HG21	0.47	2.39	11	2
1:A:97:LYS:HG3	1:A:98:ARG:N	0.47	2.24	11	14
1:A:3:TYR:CD1	1:A:40:THR:CG2	0.47	2.97	19	1
1:A:8:PHE:CD2	1:A:89:ILE:CD1	0.47	2.98	19	1
1:A:31:LEU:HD21	1:A:109:TRP:CG	0.47	2.43	2	2
1:A:121:LEU:O	1:A:121:LEU:CD1	0.47	2.54	14	2
1:A:12:LEU:HD21	1:A:28:TRP:CG	0.47	2.44	2	3
1:A:78:GLY:C	1:A:79:ILE:CG2	0.47	2.82	12	14
1:A:106:ILE:O	1:A:107:ARG:C	0.47	2.53	17	4
1:A:43:THR:HG21	1:A:85:LEU:HD11	0.47	1.86	12	1
1:A:57:PHE:O	1:A:58:GLN:C	0.47	2.53	10	7
1:A:25:LEU:HD23	1:A:25:LEU:H	0.47	1.69	9	1
1:A:112:TRP:C	1:A:114:ALA:N	0.47	2.69	20	2
1:A:27:ASP:HB3	1:A:112:TRP:CE2	0.47	2.45	20	3
1:A:106:ILE:O	1:A:108:ALA:N	0.46	2.48	17	2
1:A:109:TRP:O	1:A:111:ALA:N	0.46	2.47	20	11
1:A:40:THR:O	1:A:40:THR:OG1	0.46	2.33	13	1
1:A:17:MET:CE	1:A:20:TYR:CG	0.46	2.98	18	1
1:A:54:TYR:HE1	1:A:84:LEU:HD12	0.46	1.70	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:TYR:HB3	1:A:8:PHE:CD2	0.46	2.45	4	1
1:A:105:GLY:C	1:A:107:ARG:N	0.46	2.68	15	16
1:A:24:SER:O	1:A:27:ASP:N	0.46	2.49	4	6
1:A:31:LEU:CD1	1:A:106:ILE:HD12	0.46	2.40	20	1
1:A:23:VAL:HG22	1:A:106:ILE:CG1	0.46	2.40	12	1
1:A:34:HIS:ND1	1:A:115:HIS:CG	0.46	2.83	8	1
1:A:51:SER:CB	1:A:62:ARG:HB3	0.46	2.41	3	5
1:A:3:TYR:OH	1:A:8:PHE:CE1	0.46	2.69	12	1
1:A:47:ARG:O	1:A:48:GLY:C	0.46	2.54	10	14
1:A:50:GLN:HG2	1:A:70:THR:HG21	0.46	1.86	11	1
1:A:36:SER:HB2	1:A:42:ALA:HB2	0.46	1.88	5	1
1:A:44:ASN:O	1:A:53:ASP:N	0.46	2.48	20	1
1:A:111:ALA:O	1:A:114:ALA:C	0.46	2.54	14	1
1:A:79:ILE:O	1:A:79:ILE:CD1	0.46	2.64	3	1
1:A:55:GLY:O	1:A:58:GLN:N	0.46	2.49	16	4
1:A:51:SER:CB	1:A:62:ARG:HB2	0.46	2.40	13	6
1:A:60:ASN:ND2	1:A:64:TRP:CE3	0.46	2.83	2	1
1:A:30:CYS:HB3	1:A:121:LEU:HD23	0.46	1.88	12	1
1:A:31:LEU:HD22	1:A:57:PHE:CE1	0.46	2.46	11	1
1:A:110:VAL:O	1:A:113:ARG:CB	0.46	2.63	10	1
1:A:94:GLN:O	1:A:97:LYS:CG	0.46	2.64	4	12
1:A:27:ASP:N	1:A:27:ASP:OD1	0.46	2.46	19	1
1:A:33:GLN:NE2	1:A:38:TYR:OH	0.46	2.49	12	1
1:A:116:CYS:SG	1:A:121:LEU:CD2	0.46	2.99	3	2
1:A:37:ASN:ND2	1:A:38:TYR:CD2	0.46	2.84	15	1
1:A:3:TYR:O	1:A:38:TYR:CA	0.45	2.64	12	4
1:A:37:ASN:O	1:A:38:TYR:CD2	0.45	2.69	12	2
1:A:102:ASP:OD2	1:A:104:GLN:N	0.45	2.46	9	1
1:A:53:ASP:OD2	1:A:60:ASN:ND2	0.45	2.49	5	2
1:A:105:GLY:O	1:A:107:ARG:N	0.45	2.49	15	11
1:A:2:VAL:CG2	1:A:38:TYR:O	0.45	2.64	11	1
1:A:54:TYR:CE1	1:A:84:LEU:HD12	0.45	2.46	10	1
1:A:31:LEU:O	1:A:35:GLU:CG	0.45	2.64	9	1
1:A:17:MET:SD	1:A:28:TRP:CE2	0.45	3.10	18	1
1:A:116:CYS:C	1:A:118:ASN:N	0.45	2.69	15	2
1:A:116:CYS:O	1:A:119:ARG:N	0.45	2.49	15	1
1:A:102:ASP:CB	1:A:103:PRO:HD2	0.45	2.42	13	14
1:A:41:ARG:O	1:A:43:THR:N	0.45	2.50	5	5
1:A:54:TYR:N	1:A:54:TYR:CD1	0.45	2.85	5	2
1:A:3:TYR:CE1	1:A:40:THR:CG2	0.45	3.00	5	1
1:A:3:TYR:CE2	1:A:89:ILE:HG23	0.45	2.46	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:VAL:O	1:A:2:VAL:HG13	0.45	2.11	17	1
1:A:80:ASN:O	1:A:83:ALA:N	0.45	2.49	7	5
1:A:116:CYS:O	1:A:117:GLN:C	0.45	2.55	15	2
1:A:111:ALA:O	1:A:115:HIS:N	0.45	2.50	14	2
1:A:66:ASN:ND2	1:A:75:ASN:HD22	0.45	2.08	11	1
1:A:124:TYR:O	1:A:127:ASN:ND2	0.45	2.49	3	1
1:A:3:TYR:CD1	1:A:40:THR:HG21	0.45	2.47	19	1
1:A:63:TYR:O	1:A:76:ALA:N	0.45	2.49	17	1
1:A:35:GLU:OE2	1:A:109:TRP:NE1	0.45	2.50	5	3
1:A:75:ASN:N	1:A:75:ASN:OD1	0.45	2.50	5	3
1:A:54:TYR:CZ	1:A:61:SER:HB2	0.45	2.47	6	1
1:A:34:HIS:CG	1:A:115:HIS:CG	0.45	3.04	8	1
1:A:36:SER:CB	1:A:42:ALA:HB2	0.45	2.41	5	1
1:A:127:ASN:OD1	1:A:128:CYS:N	0.45	2.50	3	1
1:A:55:GLY:C	1:A:57:PHE:N	0.45	2.69	20	1
1:A:39:ASN:OD1	1:A:40:THR:N	0.45	2.49	12	1
1:A:3:TYR:OH	1:A:32:ALA:HB3	0.45	2.12	8	1
1:A:3:TYR:O	1:A:38:TYR:O	0.45	2.35	17	1
1:A:27:ASP:CG	1:A:112:TRP:CD1	0.45	2.91	9	1
1:A:30:CYS:CB	1:A:121:LEU:CD2	0.45	2.94	20	1
1:A:66:ASN:CG	1:A:73:ALA:HB3	0.45	2.32	16	1
1:A:11:THR:O	1:A:14:ARG:N	0.45	2.50	11	5
1:A:27:ASP:HB2	1:A:112:TRP:CH2	0.45	2.47	14	1
1:A:37:ASN:OD1	1:A:38:TYR:N	0.45	2.50	15	1
1:A:28:TRP:CZ3	1:A:106:ILE:HD11	0.44	2.47	19	2
1:A:64:TRP:O	1:A:65:CYS:O	0.44	2.35	3	18
1:A:107:ARG:O	1:A:110:VAL:N	0.44	2.50	3	4
1:A:54:TYR:OH	1:A:81:CYS:CA	0.44	2.65	15	2
1:A:8:PHE:CD2	1:A:89:ILE:HD12	0.44	2.47	19	1
1:A:113:ARG:NH1	1:A:117:GLN:NE2	0.44	2.65	15	1
1:A:74:VAL:O	1:A:75:ASN:C	0.44	2.56	14	6
1:A:45:TYR:CD2	1:A:52:THR:CG2	0.44	2.99	9	1
1:A:53:ASP:OD1	1:A:53:ASP:N	0.44	2.50	19	1
1:A:53:ASP:OD1	1:A:60:ASN:ND2	0.44	2.49	5	1
1:A:3:TYR:OH	1:A:89:ILE:CG2	0.44	2.66	5	1
1:A:3:TYR:CG	1:A:40:THR:CG2	0.44	2.99	19	1
1:A:32:ALA:HB2	1:A:57:PHE:HE1	0.44	1.72	13	2
1:A:27:ASP:OD1	1:A:27:ASP:N	0.44	2.51	3	1
1:A:43:THR:CG2	1:A:85:LEU:CD1	0.44	2.94	14	1
1:A:35:GLU:OE1	1:A:109:TRP:NE1	0.44	2.50	1	1
1:A:36:SER:O	1:A:37:ASN:O	0.44	2.35	1	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ALA:HB2	1:A:29:VAL:CG2	0.44	2.42	17	1
1:A:39:ASN:OD1	1:A:39:ASN:N	0.44	2.50	20	1
1:A:54:TYR:N	1:A:59:ILE:O	0.44	2.40	20	1
1:A:106:ILE:HD12	1:A:112:TRP:CZ3	0.44	2.47	20	1
1:A:23:VAL:HG13	1:A:112:TRP:CZ3	0.44	2.47	16	1
1:A:23:VAL:HG23	1:A:27:ASP:HB3	0.44	1.88	9	1
1:A:3:TYR:CE1	1:A:56:ILE:HD13	0.44	2.47	5	1
1:A:54:TYR:CE1	1:A:84:LEU:CB	0.44	3.00	2	1
1:A:23:VAL:CG2	1:A:28:TRP:CE2	0.44	3.01	17	1
1:A:42:ALA:O	1:A:55:GLY:N	0.44	2.48	20	1
1:A:111:ALA:O	1:A:115:HIS:HB2	0.44	2.12	20	3
1:A:100:VAL:HG22	1:A:106:ILE:HG12	0.43	1.90	13	1
1:A:25:LEU:HD12	1:A:25:LEU:O	0.43	2.13	4	1
1:A:17:MET:O	1:A:19:GLY:N	0.43	2.52	9	1
1:A:30:CYS:HB2	1:A:121:LEU:CD2	0.43	2.43	20	3
1:A:31:LEU:HD11	1:A:109:TRP:CD1	0.43	2.46	16	1
1:A:100:VAL:C	1:A:102:ASP:N	0.43	2.72	14	2
1:A:116:CYS:SG	1:A:121:LEU:CD1	0.43	3.05	3	1
1:A:79:ILE:HD12	1:A:95:CYS:SG	0.43	2.53	12	1
1:A:23:VAL:HG12	1:A:28:TRP:CE2	0.43	2.46	14	1
1:A:54:TYR:OH	1:A:65:CYS:SG	0.43	2.75	19	2
1:A:46:ASN:O	1:A:51:SER:O	0.43	2.37	18	5
1:A:36:SER:O	1:A:38:TYR:CD2	0.43	2.71	12	1
1:A:60:ASN:OD1	1:A:64:TRP:CZ3	0.43	2.72	14	1
1:A:61:SER:CB	1:A:81:CYS:SG	0.43	3.07	13	1
1:A:52:THR:CG2	1:A:53:ASP:N	0.43	2.81	20	3
1:A:2:VAL:C	1:A:3:TYR:CG	0.43	2.92	6	1
1:A:31:LEU:HD13	1:A:31:LEU:O	0.43	2.13	8	2
1:A:63:TYR:HB3	1:A:64:TRP:CD2	0.43	2.49	8	1
1:A:27:ASP:O	1:A:27:ASP:OD1	0.43	2.36	11	1
1:A:8:PHE:CE1	1:A:56:ILE:HG12	0.43	2.48	5	1
1:A:23:VAL:HG21	1:A:28:TRP:CE2	0.43	2.49	17	1
1:A:17:MET:CE	1:A:28:TRP:CZ2	0.43	3.01	17	1
1:A:58:GLN:NE2	1:A:58:GLN:HA	0.43	2.28	20	1
1:A:52:THR:HG23	1:A:54:TYR:CE1	0.43	2.49	8	1
1:A:13:LYS:HG2	1:A:18:ALA:HB3	0.43	1.90	9	1
1:A:65:CYS:C	1:A:81:CYS:SG	0.43	2.97	13	2
1:A:80:ASN:C	1:A:82:SER:N	0.43	2.71	12	3
1:A:106:ILE:C	1:A:108:ALA:N	0.43	2.72	11	2
1:A:66:ASN:O	1:A:81:CYS:SG	0.43	2.77	18	5
1:A:30:CYS:O	1:A:33:GLN:N	0.43	2.52	15	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:ASP:HB2	1:A:90:THR:HG22	0.43	1.91	19	1
1:A:54:TYR:OH	1:A:81:CYS:SG	0.43	2.77	6	2
1:A:18:ALA:HB1	1:A:25:LEU:CD1	0.43	2.35	15	1
1:A:64:TRP:O	1:A:65:CYS:SG	0.43	2.77	10	1
1:A:74:VAL:O	1:A:74:VAL:HG13	0.43	2.14	6	1
1:A:5:ARG:O	1:A:9:ALA:CB	0.42	2.67	10	1
1:A:3:TYR:CE2	1:A:8:PHE:CZ	0.42	3.07	18	1
1:A:75:ASN:OD1	1:A:75:ASN:N	0.42	2.51	17	1
1:A:54:TYR:CE1	1:A:84:LEU:HD13	0.42	2.49	2	1
1:A:75:ASN:CG	1:A:75:ASN:O	0.42	2.54	3	3
1:A:20:TYR:CG	1:A:21:TYR:N	0.42	2.87	11	2
1:A:45:TYR:OH	1:A:85:LEU:CD1	0.42	2.67	2	1
1:A:10:ARG:O	1:A:14:ARG:N	0.42	2.52	14	5
1:A:23:VAL:CG1	1:A:28:TRP:CD2	0.42	3.02	5	1
1:A:74:VAL:HG13	1:A:74:VAL:O	0.42	2.13	5	2
1:A:8:PHE:CZ	1:A:56:ILE:HG21	0.42	2.50	13	1
1:A:6:CYS:O	1:A:9:ALA:N	0.42	2.52	15	2
1:A:72:ARG:O	1:A:73:ALA:C	0.42	2.57	6	2
1:A:112:TRP:O	1:A:115:HIS:N	0.42	2.49	20	1
1:A:61:SER:CB	1:A:65:CYS:SG	0.42	3.07	19	2
1:A:79:ILE:HD11	1:A:84:LEU:HD11	0.42	1.91	2	1
1:A:39:ASN:OD1	1:A:41:ARG:N	0.42	2.51	12	1
1:A:5:ARG:HD3	1:A:124:TYR:CE2	0.42	2.49	13	1
1:A:70:THR:HG22	1:A:72:ARG:HB2	0.42	1.91	4	1
1:A:52:THR:O	1:A:60:ASN:HA	0.42	2.15	7	2
1:A:41:ARG:O	1:A:42:ALA:C	0.42	2.58	13	3
1:A:64:TRP:NE1	1:A:99:VAL:HG13	0.42	2.30	1	1
1:A:39:ASN:O	1:A:41:ARG:N	0.42	2.51	1	1
1:A:47:ARG:C	1:A:49:ASP:N	0.42	2.73	11	3
1:A:54:TYR:OH	1:A:81:CYS:O	0.42	2.36	5	1
1:A:67:ASP:OD1	1:A:67:ASP:C	0.42	2.58	19	2
1:A:66:ASN:C	1:A:81:CYS:SG	0.42	2.98	20	1
1:A:2:VAL:HA	1:A:38:TYR:O	0.42	2.14	15	2
1:A:75:ASN:O	1:A:75:ASN:OD1	0.42	2.38	13	1
1:A:30:CYS:CB	1:A:121:LEU:HD13	0.42	2.44	9	1
1:A:42:ALA:HB3	1:A:55:GLY:C	0.42	2.34	16	3
1:A:72:ARG:O	1:A:73:ALA:O	0.42	2.38	16	2
1:A:79:ILE:CD1	1:A:95:CYS:SG	0.42	3.08	12	1
1:A:20:TYR:C	1:A:22:GLY:N	0.41	2.72	14	2
1:A:8:PHE:HE1	1:A:89:ILE:HD13	0.41	1.68	15	1
1:A:66:ASN:ND2	1:A:75:ASN:CG	0.41	2.74	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:GLU:O	1:A:8:PHE:N	0.41	2.48	6	1
1:A:8:PHE:CZ	1:A:32:ALA:HB2	0.41	2.50	2	1
1:A:61:SER:HA	1:A:64:TRP:O	0.41	2.14	7	2
1:A:79:ILE:CG1	1:A:79:ILE:O	0.41	2.67	3	1
1:A:54:TYR:OH	1:A:81:CYS:CB	0.41	2.68	5	2
1:A:50:GLN:HG3	1:A:70:THR:HG21	0.41	1.91	5	1
1:A:53:ASP:CG	1:A:60:ASN:OD1	0.41	2.58	19	1
1:A:31:LEU:HD12	1:A:57:PHE:CE1	0.41	2.51	13	1
1:A:32:ALA:HB1	1:A:37:ASN:ND2	0.41	2.31	10	1
1:A:23:VAL:HG11	1:A:106:ILE:CB	0.41	2.45	19	1
1:A:3:TYR:CD1	1:A:8:PHE:CB	0.41	3.02	18	2
1:A:112:TRP:C	1:A:112:TRP:HD1	0.41	2.17	16	2
1:A:64:TRP:CE2	1:A:99:VAL:HG13	0.41	2.50	14	1
1:A:27:ASP:O	1:A:31:LEU:HB2	0.41	2.15	15	1
1:A:66:ASN:CG	1:A:75:ASN:CG	0.41	2.79	9	1
1:A:40:THR:OG1	1:A:40:THR:O	0.41	2.39	2	1
1:A:31:LEU:CD1	1:A:57:PHE:CE2	0.41	3.03	2	1
1:A:66:ASN:OD1	1:A:79:ILE:N	0.41	2.54	2	1
1:A:112:TRP:HD1	1:A:112:TRP:C	0.41	2.17	20	1
1:A:67:ASP:OD2	1:A:69:LYS:CB	0.41	2.68	12	1
1:A:105:GLY:O	1:A:108:ALA:N	0.41	2.48	14	1
1:A:77:CYS:SG	1:A:79:ILE:HD12	0.41	2.56	11	1
1:A:40:THR:CG2	1:A:56:ILE:HD12	0.41	2.45	9	1
1:A:53:ASP:OD2	1:A:60:ASN:OD1	0.41	2.38	5	1
1:A:104:GLN:O	1:A:107:ARG:NH1	0.41	2.53	20	1
1:A:61:SER:OG	1:A:61:SER:O	0.41	2.38	1	1
1:A:35:GLU:OE2	1:A:57:PHE:O	0.41	2.39	11	2
1:A:12:LEU:HD23	1:A:18:ALA:HB2	0.41	1.92	10	1
1:A:66:ASN:CB	1:A:75:ASN:HB3	0.41	2.45	9	2
1:A:18:ALA:CB	1:A:25:LEU:CD2	0.41	2.84	19	1
1:A:27:ASP:O	1:A:30:CYS:SG	0.41	2.79	13	1
1:A:75:ASN:O	1:A:75:ASN:CG	0.41	2.59	6	1
1:A:31:LEU:CD1	1:A:109:TRP:CB	0.41	2.98	16	1
1:A:5:ARG:HA	1:A:29:VAL:CG1	0.41	2.43	3	1
1:A:116:CYS:O	1:A:119:ARG:O	0.41	2.38	15	1
1:A:57:PHE:O	1:A:109:TRP:NE1	0.41	2.53	8	1
1:A:102:ASP:CG	1:A:103:PRO:HD2	0.41	2.36	13	1
1:A:6:CYS:SG	1:A:128:CYS:O	0.41	2.79	15	5
1:A:105:GLY:O	1:A:106:ILE:C	0.41	2.60	18	5
1:A:99:VAL:O	1:A:102:ASP:HB2	0.41	2.16	20	2
1:A:37:ASN:OD1	1:A:38:TYR:CE2	0.41	2.74	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:CD2	1:A:28:TRP:CG	0.41	3.04	2	2
1:A:61:SER:O	1:A:61:SER:OG	0.41	2.39	2	1
1:A:112:TRP:O	1:A:114:ALA:N	0.41	2.54	20	1
1:A:112:TRP:O	1:A:112:TRP:HD1	0.41	1.99	20	1
1:A:36:SER:O	1:A:38:TYR:CE2	0.41	2.74	12	1
1:A:112:TRP:CE3	1:A:116:CYS:SG	0.41	3.14	11	1
1:A:67:ASP:C	1:A:67:ASP:OD1	0.41	2.59	11	1
1:A:38:TYR:O	1:A:39:ASN:OD1	0.41	2.39	13	1
1:A:75:ASN:O	1:A:78:GLY:N	0.41	2.54	12	1
1:A:25:LEU:O	1:A:29:VAL:CG2	0.40	2.60	9	1
1:A:3:TYR:O	1:A:3:TYR:CD1	0.40	2.74	18	1
1:A:78:GLY:O	1:A:79:ILE:HG22	0.40	2.16	12	1
1:A:111:ALA:O	1:A:114:ALA:N	0.40	2.51	14	1
1:A:3:TYR:CB	1:A:56:ILE:HD12	0.40	2.45	19	1
1:A:79:ILE:CD1	1:A:79:ILE:C	0.40	2.87	7	1
1:A:17:MET:SD	1:A:28:TRP:CH2	0.40	3.14	7	1
1:A:8:PHE:CD2	1:A:37:ASN:CG	0.40	2.94	20	1
1:A:20:TYR:CD2	1:A:21:TYR:HB2	0.40	2.52	16	1
1:A:12:LEU:HD23	1:A:18:ALA:N	0.40	2.31	15	1
1:A:65:CYS:HA	1:A:79:ILE:CD1	0.40	2.46	9	2
1:A:117:GLN:OE1	1:A:117:GLN:CA	0.40	2.70	2	1
1:A:66:ASN:OD1	1:A:67:ASP:N	0.40	2.54	3	1
1:A:95:CYS:O	1:A:99:VAL:CG2	0.40	2.64	20	1
1:A:33:GLN:OE1	1:A:33:GLN:C	0.40	2.60	4	1
1:A:36:SER:O	1:A:37:ASN:CB	0.40	2.69	6	1
1:A:52:THR:C	1:A:53:ASP:OD1	0.40	2.60	20	1
1:A:77:CYS:HB3	1:A:79:ILE:CD1	0.40	2.46	12	1
1:A:110:VAL:O	1:A:111:ALA:C	0.40	2.59	14	1
1:A:66:ASN:ND2	1:A:75:ASN:ND2	0.40	2.69	11	1
1:A:84:LEU:HD23	1:A:84:LEU:N	0.40	2.31	10	1
1:A:8:PHE:CZ	1:A:57:PHE:CE1	0.40	3.09	19	1
1:A:83:ALA:O	1:A:91:ALA:HB3	0.40	2.16	7	1
1:A:116:CYS:SG	1:A:121:LEU:CG	0.40	3.10	3	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	128/130 (98%)	89±2 (69±2%)	30±3 (23±2%)	10±2 (8±2%)	3 16
All	All	2560/2600 (98%)	1774 (69%)	593 (23%)	193 (8%)	3 16

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

Mol	Chain	Res	Type	Models (Total)
1	A	65	CYS	20
1	A	20	TYR	20
1	A	6	CYS	19
1	A	75	ASN	18
1	A	36	SER	17
1	A	42	ALA	15
1	A	73	ALA	12
1	A	127	ASN	11
1	A	48	GLY	10
1	A	37	ASN	7
1	A	58	GLN	6
1	A	22	GLY	5
1	A	38	TYR	5
1	A	117	GLN	4
1	A	67	ASP	4
1	A	23	VAL	4
1	A	18	ALA	3
1	A	110	VAL	2
1	A	107	ARG	2
1	A	21	TYR	2
1	A	102	ASP	1
1	A	56	ILE	1
1	A	64	TRP	1
1	A	66	ASN	1
1	A	104	GLN	1
1	A	129	GLY	1
1	A	74	VAL	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	106/107 (99%)	72±4 (68±3%)	34±4 (32±3%)	1 14
All	All	2120/2140 (99%)	1447 (68%)	673 (32%)	1 14

All 83 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	102	ASP	20
1	A	128	CYS	20
1	A	112	TRP	20
1	A	79	ILE	20
1	A	65	CYS	19
1	A	21	TYR	19
1	A	12	LEU	18
1	A	116	CYS	18
1	A	115	HIS	16
1	A	5	ARG	16
1	A	85	LEU	15
1	A	124	TYR	15
1	A	72	ARG	15
1	A	63	TYR	15
1	A	119	ARG	15
1	A	24	SER	13
1	A	49	ASP	13
1	A	7	GLU	13
1	A	117	GLN	12
1	A	30	CYS	12
1	A	47	ARG	12
1	A	82	SER	12
1	A	101	ARG	12
1	A	62	ARG	12
1	A	36	SER	12
1	A	44	ASN	11
1	A	6	CYS	11
1	A	17	MET	11
1	A	58	GLN	11
1	A	87	ASP	10
1	A	53	ASP	10
1	A	8	PHE	9
1	A	127	ASN	9
1	A	60	ASN	9
1	A	122	SER	9
1	A	113	ARG	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	107	ARG	8
1	A	95	CYS	8
1	A	3	TYR	7
1	A	97	LYS	7
1	A	100	VAL	7
1	A	126	ARG	7
1	A	98	ARG	7
1	A	121	LEU	6
1	A	54	TYR	6
1	A	90	THR	6
1	A	69	LYS	6
1	A	61	SER	6
1	A	13	LYS	6
1	A	39	ASN	6
1	A	94	GLN	5
1	A	15	ASN	5
1	A	41	ARG	4
1	A	33	GLN	4
1	A	84	LEU	4
1	A	10	ARG	4
1	A	123	GLN	4
1	A	4	GLU	4
1	A	66	ASN	4
1	A	130	VAL	4
1	A	88	ASP	4
1	A	25	LEU	3
1	A	34	HIS	3
1	A	56	ILE	3
1	A	14	ARG	3
1	A	81	CYS	3
1	A	27	ASP	3
1	A	38	TYR	3
1	A	2	VAL	2
1	A	104	GLN	2
1	A	80	ASN	2
1	A	106	ILE	2
1	A	74	VAL	2
1	A	50	GLN	2
1	A	77	CYS	1
1	A	43	THR	1
1	A	37	ASN	1
1	A	45	TYR	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	86	GLN	1
1	A	57	PHE	1
1	A	40	THR	1
1	A	125	ILE	1
1	A	75	ASN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 44% for the well-defined parts and 44% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4751

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	836
Number of shifts mapped to atoms	836
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	0	—	—
^{15}N	127	0.98 ± 0.57	None needed (imprecise)

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 44%, i.e. 712 atoms were assigned a chemical shift out of a possible 1603. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	383/641 (60%)	256/256 (100%)	0/258 (0%)	127/127 (100%)
Sidechain	267/816 (33%)	267/479 (56%)	0/276 (0%)	0/61 (0%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	62/146 (42%)	62/74 (84%)	0/64 (0%)	0/8 (0%)
Overall	712/1603 (44%)	585/809 (72%)	0/598 (0%)	127/196 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 713 atoms were assigned a chemical shift out of a possible 1621. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	384/646 (59%)	257/258 (100%)	0/260 (0%)	127/128 (99%)
Sidechain	267/829 (32%)	267/487 (55%)	0/280 (0%)	0/62 (0%)
Aromatic	62/146 (42%)	62/74 (84%)	0/64 (0%)	0/8 (0%)
Overall	713/1621 (44%)	586/819 (72%)	0/604 (0%)	127/198 (64%)

7.1.4 Statistically unusual chemical shifts (i)

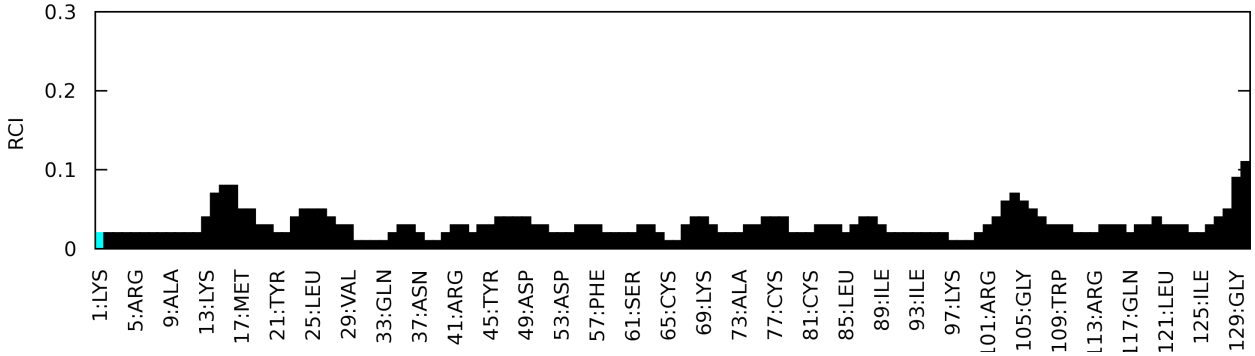
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	122	SER	HB2	1.59	5.18 – 2.58	-8.8
1	A	122	SER	HB3	1.59	5.25 – 2.45	-8.1
1	A	99	VAL	HG23	-0.63	2.20 – -0.60	-5.1
1	A	99	VAL	HG22	-0.63	2.20 – -0.60	-5.1
1	A	99	VAL	HG21	-0.63	2.20 – -0.60	-5.1

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.3
0.2
0.1
0
1:LYS
5:ARG
9:ALA
13:LYS
17:MET
21:TYR
25:LEU
29:VAL
33:GLN
37:ASN
41:ARG
45:TYR
49:ASP
53:ASP
57:PHE
61:SER
65:CYS
69:LYS
73:ALA
77:CYS
81:CYS
85:LEU
89:ILE
93:ILE
97:LYS
101:ARG
105:GLY
109:TRP
113:ARG
117:GLN
121:LEU
125:ILE
129:GLY