Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 10:52 PM EST

PDB ID	:	2DKW
Title	:	Solution structure of the bromodomain of human protein KIAA1240
Authors	:	Sano, R.; Hayashi, F.; Kurosaki, C.; Yoshida, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-04-14

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
https://www.wwpdb.org/validation/2017/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:

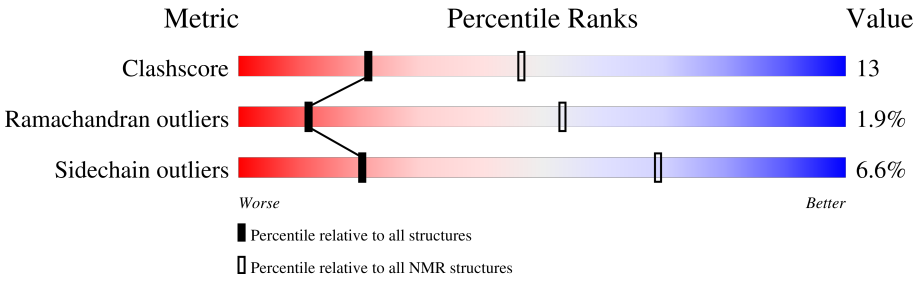
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	131	67% 18% 15%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:7-A:82, A:90-A:124 (111)	0.42	7

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2074 atoms, of which 1044 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical protein KIAA1240.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	131	2074	646	1044	177	203	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9ULI0
A	2	SER	-	cloning artifact	UNP Q9ULI0
A	3	SER	-	cloning artifact	UNP Q9ULI0
A	4	GLY	-	cloning artifact	UNP Q9ULI0
A	5	SER	-	cloning artifact	UNP Q9ULI0
A	6	SER	-	cloning artifact	UNP Q9ULI0
A	7	GLY	-	cloning artifact	UNP Q9ULI0
A	126	SER	-	cloning artifact	UNP Q9ULI0
A	127	GLY	-	cloning artifact	UNP Q9ULI0
A	128	PRO	-	cloning artifact	UNP Q9ULI0
A	129	SER	-	cloning artifact	UNP Q9ULI0
A	130	SER	-	cloning artifact	UNP Q9ULI0
A	131	GLY	-	cloning artifact	UNP Q9ULI0

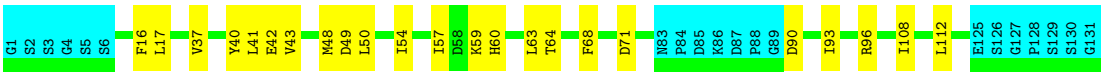
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: hypothetical protein KIAA1240

Chain A: 67% 18% 15%



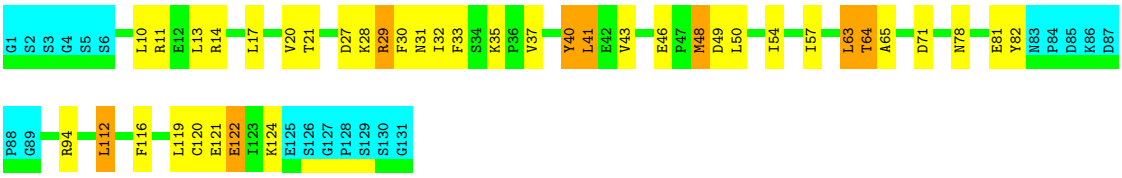
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: hypothetical protein KIAA1240

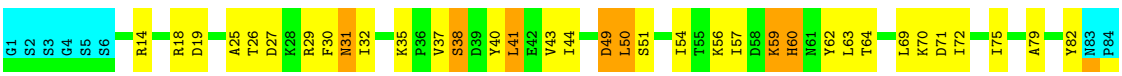
Chain A: 54% 24% 6% 15%



4.2.2 Score per residue for model 2

• Molecule 1: hypothetical protein KIAA1240

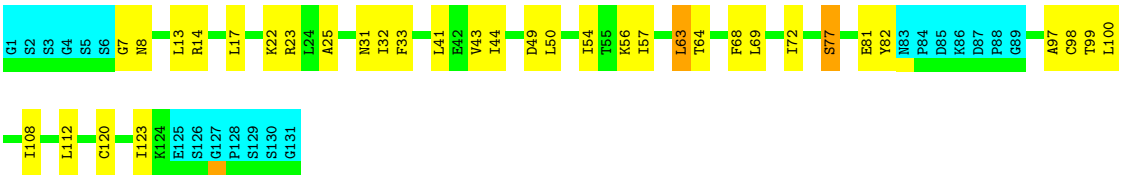
Chain A: 50% 29% 6% 15%



4.2.3 Score per residue for model 3

- Molecule 1: hypothetical protein KIAA1240

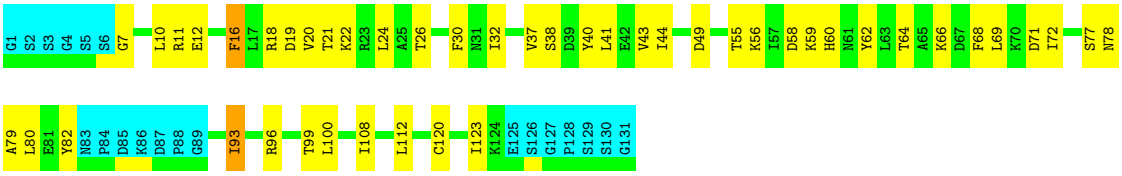
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: hypothetical protein KIAA1240

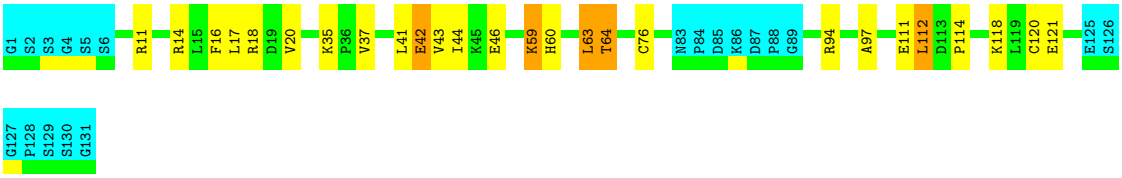
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: hypothetical protein KIAA1240

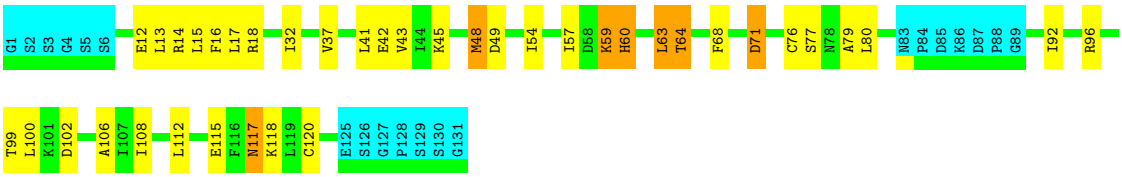
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: hypothetical protein KIAA1240

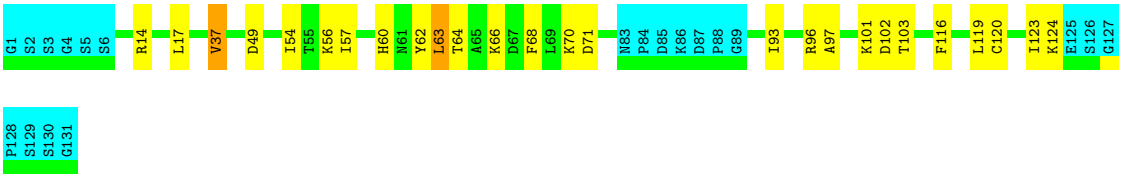
Chain A:



4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: hypothetical protein KIAA1240

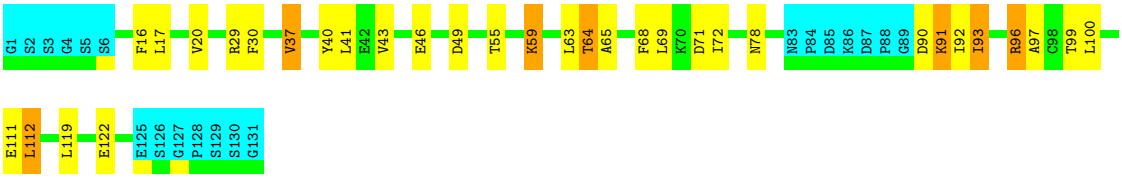
Chain A: 65% 18% • 15%



4.2.8 Score per residue for model 8

- Molecule 1: hypothetical protein KIAA1240

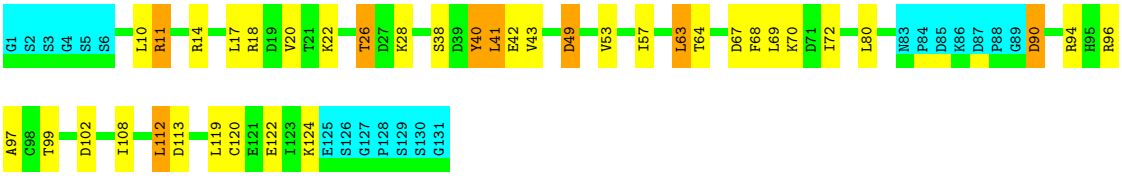
Chain A: 60% 20% 5% 15%



4.2.9 Score per residue for model 9

- Molecule 1: hypothetical protein KIAA1240

Chain A: 56% 23% 6% 15%



4.2.10 Score per residue for model 10

- Molecule 1: hypothetical protein KIAA1240

Chain A: 60% 23% • 15%

G1 S2 S3 G4 S5 S6 R14 L17 T21 K28 R29 F30 S38 D39 Y40 L41 E42 V43 I44 K45 E46 P47 M48 D49 L50 I57 T64 F68 D71 N78 A79 L80 E81 Y82 N83 P84 D85 K86 D87 P88 G89 D90 K91 H95 R96 A97 C98 E115

F116 C120 E125 S126 G127 P128 S129 S130 G131

4.2.11 Score per residue for model 11

- Molecule 1: hypothetical protein KIAA1240

Chain A: 62% 21% • 15%

G1 S2 S3 G4 S5 S6 T9 F16 L17 R18 K22 R23 L24 A25 T26 D27 K28 R29 F30 V37 L41 K45 D49 L50 I54 I57 D58 K59 H60 L63 T64 F68 I72 N83 P84 D85 K86 D87 P88 G89 H95 C98 F116 N117

K118 E121 E122 E125 S126 G127 P128 S129 S130 G131

4.2.12 Score per residue for model 12

- Molecule 1: hypothetical protein KIAA1240

Chain A: 53% 29% • 15%

G1 S2 S3 G4 S5 S6 G7 N8 T9 L10 F16 L17 V20 A25 T26 V37 S38 D39 Y40 L41 E42 V43 I44 K45 E46 D49 L50 V53 I54 L63 F68 L69 K70 D71 I72 C76 S77 N78 A79 L80 E81 Y82 N83 P84 D85 K86 D87 P88 G89 D90 K91

I92 I93 R94 A97 K118 E122 E125 S126 G127 P128 S129 S130 G131

4.2.13 Score per residue for model 13

- Molecule 1: hypothetical protein KIAA1240

Chain A: 61% 21% • • 15%

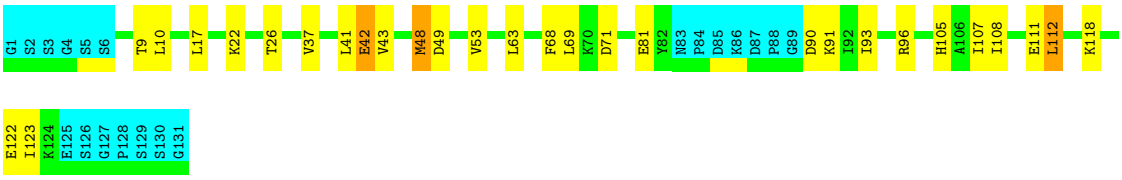
G1 S2 S3 G4 S5 S6 L10 R11 R14 L17 R18 K22 T26 R29 F30 N31 I32 F33 S38 D39 Y40 L41 E42 V43 I44 D49 L50 I57 L63 T64 L80 E81 Y82 N83 P84 D85 K86 D87 P88 G89 H95 R96 D102 I108 L112

L119 E122 E125 S126 G127 P128 S129 S130 G131

4.2.14 Score per residue for model 14

- Molecule 1: hypothetical protein KIAA1240

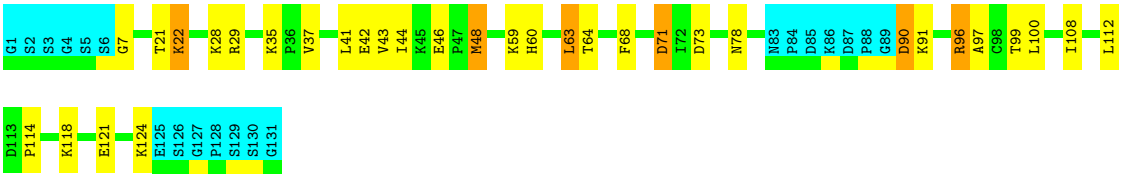
Chain A: 63% 20% • 15%



4.2.15 Score per residue for model 15

- Molecule 1: hypothetical protein KIAA1240

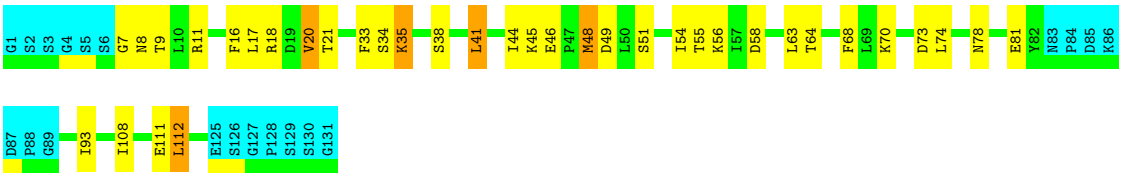
Chain A: 60% 21% 5% 15%



4.2.16 Score per residue for model 16

- Molecule 1: hypothetical protein KIAA1240

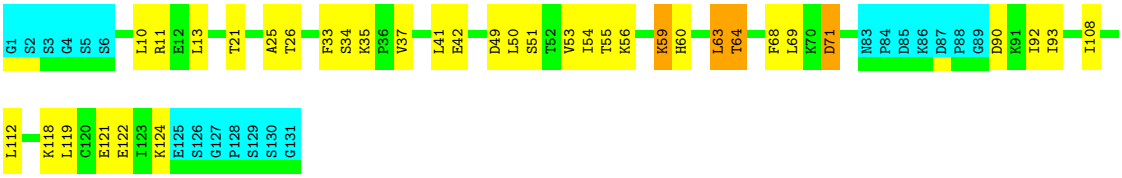
Chain A: 57% 24% • 15%



4.2.17 Score per residue for model 17

- Molecule 1: hypothetical protein KIAA1240

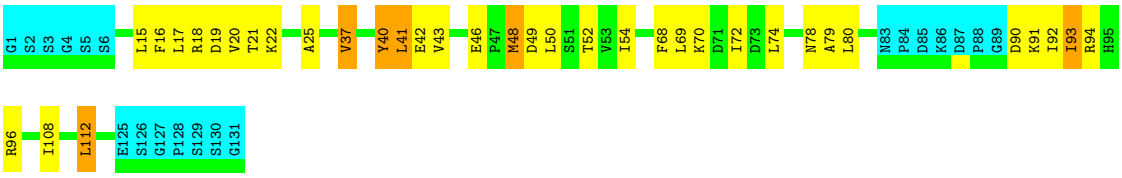
Chain A: 57% 24% • 15%



4.2.18 Score per residue for model 18

- Molecule 1: hypothetical protein KIAA1240

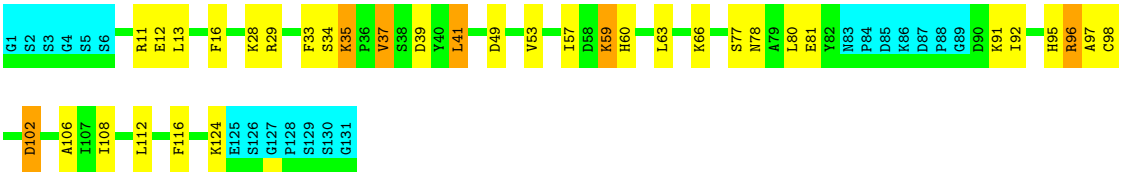
Chain A: 57% 23% 5% 15%



4.2.19 Score per residue for model 19

- Molecule 1: hypothetical protein KIAA1240

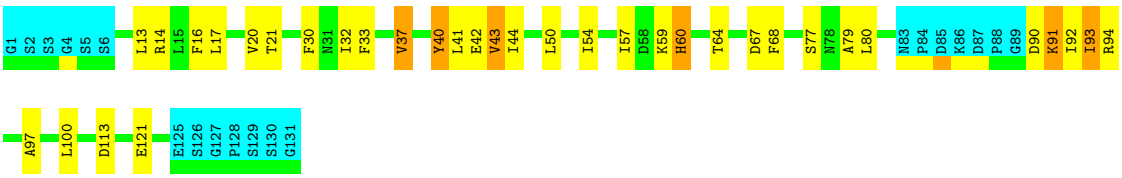
Chain A: 58% 22% 5% 15%



4.2.20 Score per residue for model 20

- Molecule 1: hypothetical protein KIAA1240

Chain A: 58% 22% 5% 15%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function,structures with the lowest energy,structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	905	940	937	24±4
All	All	18100	18800	18740	482

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD12	1:A:42:GLU:N	0.95	1.77	12	3
1:A:63:LEU:HD12	1:A:64:THR:HG23	0.89	1.41	16	4
1:A:49:ASP:O	1:A:53:VAL:HG23	0.84	1.70	12	5
1:A:22:LYS:O	1:A:26:THR:HG22	0.80	1.76	13	3
1:A:38:SER:OG	1:A:44:ILE:HD11	0.74	1.82	13	2
1:A:41:LEU:C	1:A:41:LEU:HD22	0.73	2.03	11	5
1:A:63:LEU:HD11	1:A:124:LYS:HB3	0.73	1.58	1	1
1:A:32:ILE:HG21	1:A:96:ARG:NH1	0.72	1.99	6	1
1:A:17:LEU:HD22	1:A:68:PHE:CG	0.72	2.18	12	8
1:A:49:ASP:O	1:A:52:THR:HG22	0.72	1.85	18	1
1:A:63:LEU:HD12	1:A:63:LEU:O	0.72	1.85	5	5
1:A:63:LEU:HD11	1:A:124:LYS:HB2	0.70	1.62	9	2
1:A:38:SER:CB	1:A:44:ILE:HD11	0.70	2.17	4	5
1:A:26:THR:HG23	1:A:26:THR:O	0.68	1.87	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:LYS:HG3	1:A:92:ILE:HD12	0.68	1.65	20	1
1:A:10:LEU:HD11	1:A:63:LEU:HD23	0.67	1.67	14	2
1:A:63:LEU:CD1	1:A:64:THR:HG23	0.66	2.20	16	4
1:A:21:THR:HG23	1:A:50:LEU:HD22	0.66	1.68	1	4
1:A:16:PHE:O	1:A:20:VAL:HG23	0.66	1.91	18	6
1:A:64:THR:HG22	1:A:120:CYS:SG	0.66	2.31	3	5
1:A:41:LEU:HD23	1:A:41:LEU:H	0.65	1.51	15	3
1:A:37:VAL:O	1:A:37:VAL:HG23	0.65	1.90	7	2
1:A:63:LEU:HD12	1:A:64:THR:N	0.65	2.06	11	2
1:A:17:LEU:HD22	1:A:68:PHE:CD1	0.63	2.29	16	2
1:A:54:ILE:HA	1:A:57:ILE:HD12	0.63	1.69	6	7
1:A:17:LEU:HD22	1:A:68:PHE:CD2	0.62	2.28	10	5
1:A:50:LEU:O	1:A:54:ILE:HD12	0.62	1.94	2	3
1:A:37:VAL:HG23	1:A:37:VAL:O	0.61	1.94	1	8
1:A:41:LEU:H	1:A:41:LEU:HD13	0.59	1.56	9	3
1:A:68:PHE:CZ	1:A:72:ILE:HD11	0.59	2.33	11	1
1:A:63:LEU:HD11	1:A:124:LYS:CB	0.58	2.28	1	1
1:A:63:LEU:HD12	1:A:64:THR:CG2	0.58	2.25	16	1
1:A:41:LEU:HD22	1:A:41:LEU:O	0.58	1.99	2	3
1:A:40:TYR:HB3	1:A:43:VAL:HG12	0.58	1.75	2	2
1:A:14:ARG:HG3	1:A:57:ILE:HG22	0.57	1.75	10	3
1:A:43:VAL:HG13	1:A:44:ILE:HD12	0.57	1.76	10	1
1:A:41:LEU:C	1:A:41:LEU:CD2	0.57	2.72	9	5
1:A:55:THR:HG22	1:A:59:LYS:HE2	0.57	1.75	8	1
1:A:63:LEU:HD21	1:A:124:LYS:HB2	0.56	1.76	1	1
1:A:44:ILE:HG23	1:A:82:TYR:CE2	0.56	2.36	10	1
1:A:18:ARG:HG3	1:A:54:ILE:HG23	0.56	1.77	18	1
1:A:43:VAL:HG22	1:A:43:VAL:O	0.56	2.00	8	3
1:A:40:TYR:O	1:A:43:VAL:HG12	0.56	2.01	20	2
1:A:92:ILE:HD12	1:A:92:ILE:N	0.55	2.17	19	2
1:A:9:THR:HG23	1:A:116:PHE:CE1	0.55	2.37	11	1
1:A:43:VAL:HG12	1:A:82:TYR:CE1	0.55	2.37	4	1
1:A:14:ARG:CD	1:A:60:HIS:CD2	0.55	2.90	5	1
1:A:44:ILE:HD12	1:A:44:ILE:H	0.55	1.61	13	2
1:A:48:MET:HE2	1:A:48:MET:HA	0.55	1.79	14	1
1:A:44:ILE:HG23	1:A:82:TYR:OH	0.55	2.01	3	1
1:A:41:LEU:HD12	1:A:41:LEU:C	0.54	2.23	6	4
1:A:93:ILE:O	1:A:97:ALA:HB2	0.54	2.02	7	1
1:A:29:ARG:CD	1:A:30:PHE:CD2	0.53	2.90	1	1
1:A:91:LYS:CG	1:A:92:ILE:HD12	0.53	2.34	20	1
1:A:40:TYR:O	1:A:42:GLU:N	0.52	2.43	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:SER:HB3	1:A:44:ILE:HD11	0.52	1.81	16	1
1:A:40:TYR:CD1	1:A:41:LEU:N	0.52	2.77	13	2
1:A:65:ALA:CB	1:A:112:LEU:HD13	0.52	2.35	8	1
1:A:43:VAL:HG13	1:A:44:ILE:CD1	0.52	2.34	10	1
1:A:112:LEU:HD21	1:A:117:ASN:OD1	0.51	2.06	6	1
1:A:90:ASP:CG	1:A:91:LYS:N	0.51	2.64	15	1
1:A:43:VAL:CG1	1:A:44:ILE:HD12	0.51	2.36	10	2
1:A:119:LEU:O	1:A:123:ILE:HD12	0.51	2.05	7	1
1:A:41:LEU:HD23	1:A:41:LEU:N	0.51	2.19	15	3
1:A:38:SER:HB2	1:A:44:ILE:HD11	0.51	1.83	12	2
1:A:18:ARG:CG	1:A:54:ILE:HG23	0.51	2.35	18	1
1:A:46:GLU:O	1:A:78:ASN:ND2	0.50	2.44	1	7
1:A:32:ILE:HD11	1:A:33:PHE:CE1	0.50	2.41	3	1
1:A:42:GLU:O	1:A:44:ILE:N	0.50	2.44	20	2
1:A:41:LEU:O	1:A:43:VAL:N	0.50	2.45	13	2
1:A:69:LEU:O	1:A:72:ILE:N	0.50	2.45	2	7
1:A:93:ILE:O	1:A:97:ALA:N	0.50	2.45	20	1
1:A:48:MET:HA	1:A:48:MET:HE2	0.49	1.83	1	6
1:A:38:SER:CB	1:A:43:VAL:HG11	0.49	2.37	10	1
1:A:43:VAL:O	1:A:43:VAL:CG2	0.49	2.59	8	1
1:A:24:LEU:HD22	1:A:100:LEU:HD12	0.49	1.83	4	1
1:A:41:LEU:O	1:A:42:GLU:C	0.49	2.51	13	2
1:A:27:ASP:OD2	1:A:29:ARG:NE	0.49	2.46	1	1
1:A:41:LEU:CD1	1:A:42:GLU:N	0.49	2.66	12	1
1:A:64:THR:HG22	1:A:120:CYS:HB3	0.49	1.84	10	1
1:A:40:TYR:HB3	1:A:43:VAL:HG23	0.48	1.84	4	2
1:A:17:LEU:O	1:A:20:VAL:N	0.48	2.46	18	4
1:A:49:ASP:OD1	1:A:49:ASP:N	0.48	2.46	4	2
1:A:32:ILE:CD1	1:A:93:ILE:HG23	0.48	2.37	4	1
1:A:65:ALA:CB	1:A:112:LEU:CD2	0.48	2.91	1	1
1:A:108:ILE:O	1:A:112:LEU:CB	0.48	2.61	3	8
1:A:96:ARG:O	1:A:99:THR:N	0.48	2.46	9	2
1:A:60:HIS:N	1:A:60:HIS:CD2	0.48	2.81	20	1
1:A:50:LEU:O	1:A:53:VAL:N	0.48	2.47	17	1
1:A:63:LEU:HD13	1:A:124:LYS:HB2	0.48	1.84	19	1
1:A:41:LEU:HD12	1:A:42:GLU:HB2	0.48	1.86	10	2
1:A:41:LEU:HD22	1:A:42:GLU:N	0.48	2.24	9	1
1:A:40:TYR:CE1	1:A:41:LEU:O	0.48	2.67	10	1
1:A:76:CYS:HB2	1:A:97:ALA:HB1	0.48	1.85	12	1
1:A:77:SER:O	1:A:81:GLU:N	0.47	2.47	3	1
1:A:119:LEU:O	1:A:122:GLU:N	0.47	2.47	9	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:PHE:CD1	1:A:69:LEU:N	0.47	2.82	4	1
1:A:119:LEU:O	1:A:122:GLU:CB	0.47	2.62	13	2
1:A:32:ILE:HD11	1:A:33:PHE:CE2	0.47	2.44	1	1
1:A:40:TYR:CD1	1:A:41:LEU:O	0.47	2.67	10	1
1:A:14:ARG:NH1	1:A:60:HIS:CD2	0.47	2.83	7	1
1:A:13:LEU:HD22	1:A:63:LEU:O	0.47	2.09	6	2
1:A:49:ASP:O	1:A:51:SER:N	0.47	2.48	2	1
1:A:50:LEU:O	1:A:54:ILE:CD1	0.47	2.61	2	3
1:A:14:ARG:HD2	1:A:60:HIS:CD2	0.47	2.44	5	1
1:A:32:ILE:HG21	1:A:96:ARG:HH12	0.47	1.64	6	1
1:A:79:ALA:O	1:A:81:GLU:N	0.47	2.47	12	2
1:A:116:PHE:HA	1:A:119:LEU:HD12	0.46	1.87	1	1
1:A:31:ASN:N	1:A:31:ASN:OD1	0.46	2.48	2	1
1:A:40:TYR:O	1:A:43:VAL:N	0.46	2.48	12	1
1:A:8:ASN:O	1:A:11:ARG:N	0.46	2.48	16	1
1:A:95:HIS:O	1:A:97:ALA:N	0.46	2.48	19	1
1:A:82:TYR:N	1:A:82:TYR:CD1	0.46	2.82	1	1
1:A:13:LEU:CD2	1:A:63:LEU:C	0.46	2.84	3	1
1:A:91:LYS:C	1:A:92:ILE:HD12	0.46	2.30	19	1
1:A:33:PHE:O	1:A:35:LYS:N	0.46	2.48	16	1
1:A:92:ILE:N	1:A:92:ILE:CD1	0.46	2.79	19	1
1:A:55:THR:HG22	1:A:59:LYS:CE	0.46	2.41	8	1
1:A:90:ASP:OD2	1:A:94:ARG:NE	0.46	2.47	2	1
1:A:92:ILE:O	1:A:93:ILE:C	0.46	2.54	8	4
1:A:32:ILE:HG13	1:A:33:PHE:CD1	0.46	2.46	3	1
1:A:69:LEU:HD13	1:A:105:HIS:CE1	0.46	2.46	14	1
1:A:49:ASP:O	1:A:50:LEU:C	0.46	2.55	11	2
1:A:8:ASN:O	1:A:10:LEU:N	0.46	2.48	12	1
1:A:50:LEU:O	1:A:51:SER:C	0.46	2.54	17	1
1:A:27:ASP:O	1:A:31:ASN:ND2	0.45	2.50	2	1
1:A:17:LEU:HB3	1:A:68:PHE:CE2	0.45	2.46	16	1
1:A:99:THR:O	1:A:100:LEU:C	0.45	2.55	15	5
1:A:56:LYS:NZ	1:A:62:TYR:CZ	0.45	2.84	7	1
1:A:33:PHE:O	1:A:34:SER:C	0.45	2.55	19	2
1:A:38:SER:HB3	1:A:43:VAL:HG11	0.45	1.87	10	1
1:A:57:ILE:O	1:A:60:HIS:N	0.45	2.50	19	1
1:A:76:CYS:SG	1:A:77:SER:N	0.45	2.89	6	1
1:A:118:LYS:O	1:A:122:GLU:CG	0.45	2.64	11	3
1:A:93:ILE:O	1:A:94:ARG:C	0.45	2.55	12	3
1:A:108:ILE:O	1:A:112:LEU:N	0.45	2.50	6	4
1:A:32:ILE:HD12	1:A:93:ILE:HG23	0.45	1.88	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:VAL:O	1:A:37:VAL:CG2	0.45	2.61	7	1
1:A:43:VAL:HG12	1:A:82:TYR:CE2	0.45	2.46	12	1
1:A:21:THR:HA	1:A:24:LEU:HD12	0.45	1.88	4	1
1:A:55:THR:O	1:A:56:LYS:C	0.45	2.55	17	3
1:A:102:ASP:O	1:A:106:ALA:HB2	0.45	2.12	6	2
1:A:33:PHE:HB2	1:A:50:LEU:HD12	0.45	1.89	20	1
1:A:29:ARG:N	1:A:31:ASN:OD1	0.45	2.50	2	1
1:A:30:PHE:CG	1:A:100:LEU:HD13	0.45	2.46	4	2
1:A:21:THR:O	1:A:22:LYS:C	0.45	2.56	15	2
1:A:32:ILE:O	1:A:37:VAL:CG1	0.44	2.65	2	2
1:A:59:LYS:O	1:A:60:HIS:C	0.44	2.55	15	8
1:A:77:SER:O	1:A:79:ALA:N	0.44	2.50	4	1
1:A:27:ASP:O	1:A:30:PHE:N	0.44	2.51	11	1
1:A:25:ALA:HB2	1:A:50:LEU:HD13	0.44	1.87	18	2
1:A:10:LEU:O	1:A:13:LEU:N	0.44	2.50	1	1
1:A:71:ASP:C	1:A:71:ASP:OD1	0.44	2.55	17	2
1:A:42:GLU:O	1:A:43:VAL:C	0.44	2.55	12	3
1:A:48:MET:SD	1:A:74:LEU:HD23	0.44	2.52	16	2
1:A:30:PHE:O	1:A:50:LEU:CD1	0.44	2.66	10	2
1:A:56:LYS:HB2	1:A:62:TYR:CE2	0.44	2.47	2	1
1:A:90:ASP:O	1:A:91:LYS:C	0.44	2.55	18	4
1:A:95:HIS:O	1:A:96:ARG:C	0.44	2.55	13	3
1:A:92:ILE:HG22	1:A:93:ILE:N	0.44	2.27	12	1
1:A:22:LYS:O	1:A:23:ARG:C	0.44	2.56	11	2
1:A:17:LEU:O	1:A:18:ARG:C	0.44	2.55	9	5
1:A:80:LEU:O	1:A:81:GLU:C	0.44	2.56	19	2
1:A:12:GLU:CD	1:A:116:PHE:CZ	0.44	2.91	19	1
1:A:64:THR:HG21	1:A:121:GLU:HA	0.44	1.89	20	1
1:A:79:ALA:O	1:A:80:LEU:C	0.44	2.56	18	3
1:A:96:ARG:O	1:A:97:ALA:C	0.44	2.56	15	3
1:A:8:ASN:O	1:A:9:THR:C	0.44	2.55	16	1
1:A:21:THR:HG23	1:A:50:LEU:CD2	0.44	2.41	1	1
1:A:102:ASP:OD1	1:A:103:THR:N	0.44	2.50	2	1
1:A:18:ARG:NH1	1:A:58:ASP:OD1	0.44	2.50	11	1
1:A:71:ASP:OD1	1:A:71:ASP:C	0.44	2.55	15	1
1:A:30:PHE:CD1	1:A:100:LEU:HD13	0.43	2.48	8	2
1:A:27:ASP:O	1:A:28:LYS:C	0.43	2.55	11	1
1:A:10:LEU:O	1:A:11:ARG:C	0.43	2.56	17	5
1:A:14:ARG:CZ	1:A:14:ARG:CB	0.43	2.96	5	2
1:A:69:LEU:O	1:A:70:LYS:C	0.43	2.57	9	2
1:A:31:ASN:OD1	1:A:32:ILE:N	0.43	2.52	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:THR:O	1:A:58:ASP:N	0.43	2.51	16	2
1:A:15:LEU:O	1:A:16:PHE:C	0.43	2.56	6	1
1:A:63:LEU:HD12	1:A:63:LEU:C	0.43	2.33	5	2
1:A:95:HIS:CD2	1:A:98:CYS:SG	0.43	3.12	11	1
1:A:81:GLU:HB3	1:A:82:TYR:CD1	0.43	2.49	1	1
1:A:25:ALA:O	1:A:26:THR:C	0.43	2.57	2	3
1:A:43:VAL:HG12	1:A:82:TYR:CD1	0.43	2.49	4	1
1:A:62:TYR:CZ	1:A:71:ASP:OD2	0.43	2.71	4	1
1:A:76:CYS:SG	1:A:97:ALA:HB1	0.43	2.54	5	1
1:A:26:THR:O	1:A:26:THR:CG2	0.43	2.59	14	1
1:A:59:LYS:N	1:A:59:LYS:HD2	0.43	2.29	5	1
1:A:60:HIS:CD2	1:A:60:HIS:N	0.43	2.87	6	1
1:A:101:LYS:O	1:A:102:ASP:C	0.43	2.57	7	1
1:A:40:TYR:O	1:A:41:LEU:C	0.43	2.57	8	3
1:A:77:SER:O	1:A:78:ASN:C	0.43	2.57	19	1
1:A:90:ASP:OD1	1:A:91:LYS:N	0.43	2.52	10	1
1:A:15:LEU:O	1:A:19:ASP:CB	0.43	2.67	18	1
1:A:13:LEU:O	1:A:14:ARG:C	0.43	2.57	20	1
1:A:41:LEU:HD12	1:A:41:LEU:O	0.43	2.14	1	2
1:A:43:VAL:HG12	1:A:82:TYR:CD2	0.43	2.49	1	1
1:A:90:ASP:O	1:A:93:ILE:N	0.43	2.52	2	2
1:A:22:LYS:O	1:A:25:ALA:N	0.43	2.51	3	2
1:A:77:SER:O	1:A:80:LEU:N	0.43	2.52	20	2
1:A:48:MET:HA	1:A:48:MET:CE	0.42	2.44	10	5
1:A:22:LYS:O	1:A:26:THR:HG23	0.42	2.14	4	1
1:A:75:ILE:O	1:A:79:ALA:HB2	0.42	2.13	2	1
1:A:14:ARG:HB3	1:A:14:ARG:CZ	0.42	2.44	3	1
1:A:97:ALA:O	1:A:98:CYS:C	0.42	2.58	10	2
1:A:114:PRO:O	1:A:118:LYS:CD	0.42	2.68	5	2
1:A:13:LEU:O	1:A:16:PHE:N	0.42	2.52	19	1
1:A:51:SER:O	1:A:54:ILE:N	0.42	2.52	16	1
1:A:7:GLY:O	1:A:8:ASN:C	0.42	2.57	3	1
1:A:63:LEU:CD1	1:A:120:CYS:O	0.42	2.68	7	1
1:A:8:ASN:C	1:A:10:LEU:N	0.42	2.73	12	1
1:A:107:ILE:CG2	1:A:111:GLU:OE2	0.42	2.67	14	1
1:A:43:VAL:O	1:A:43:VAL:CG1	0.42	2.67	1	1
1:A:77:SER:C	1:A:79:ALA:N	0.42	2.72	4	1
1:A:14:ARG:CZ	1:A:14:ARG:HB3	0.42	2.44	5	1
1:A:41:LEU:H	1:A:41:LEU:HD23	0.42	1.74	14	1
1:A:73:ASP:OD1	1:A:73:ASP:C	0.42	2.57	16	1
1:A:121:GLU:O	1:A:124:LYS:CB	0.42	2.68	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LYS:O	1:A:29:ARG:C	0.42	2.58	15	1
1:A:18:ARG:O	1:A:19:ASP:C	0.42	2.57	4	2
1:A:92:ILE:HD12	1:A:92:ILE:H	0.42	1.74	2	1
1:A:90:ASP:OD1	1:A:90:ASP:C	0.42	2.58	9	1
1:A:79:ALA:C	1:A:81:GLU:N	0.42	2.72	12	1
1:A:121:GLU:O	1:A:124:LYS:N	0.42	2.53	17	2
1:A:28:LYS:O	1:A:31:ASN:N	0.42	2.53	1	1
1:A:32:ILE:CG2	1:A:96:ARG:NH1	0.42	2.80	6	1
1:A:111:GLU:O	1:A:112:LEU:C	0.41	2.58	8	3
1:A:42:GLU:C	1:A:44:ILE:N	0.41	2.72	15	2
1:A:17:LEU:HD13	1:A:68:PHE:CD2	0.41	2.50	6	1
1:A:16:PHE:O	1:A:17:LEU:C	0.41	2.58	11	1
1:A:14:ARG:O	1:A:57:ILE:CG2	0.41	2.69	1	1
1:A:115:GLU:HG3	1:A:116:PHE:N	0.41	2.31	10	1
1:A:14:ARG:O	1:A:57:ILE:HG21	0.41	2.16	13	1
1:A:40:TYR:HB3	1:A:43:VAL:CG2	0.41	2.45	4	1
1:A:49:ASP:C	1:A:51:SER:N	0.41	2.73	2	1
1:A:32:ILE:O	1:A:37:VAL:HG13	0.41	2.15	20	1
1:A:102:ASP:O	1:A:103:THR:C	0.41	2.58	7	1
1:A:120:CYS:SG	1:A:121:GLU:N	0.41	2.94	5	1
1:A:95:HIS:C	1:A:97:ALA:N	0.41	2.73	19	1
1:A:17:LEU:HD13	1:A:68:PHE:HB2	0.41	1.92	3	1
1:A:116:PHE:C	1:A:116:PHE:CD1	0.41	2.94	7	1
1:A:68:PHE:CD1	1:A:68:PHE:C	0.41	2.94	12	2
1:A:32:ILE:HG13	1:A:33:PHE:N	0.41	2.31	13	1
1:A:69:LEU:HD21	1:A:108:ILE:HG13	0.41	1.93	17	1
1:A:67:ASP:O	1:A:68:PHE:C	0.41	2.58	20	1
1:A:30:PHE:CD1	1:A:100:LEU:HB2	0.41	2.51	2	1
1:A:123:ILE:O	1:A:124:LYS:C	0.41	2.59	2	1
1:A:95:HIS:O	1:A:98:CYS:N	0.41	2.54	19	1
1:A:80:LEU:HD21	1:A:94:ARG:CB	0.40	2.46	9	1
1:A:119:LEU:O	1:A:120:CYS:C	0.40	2.59	9	1
1:A:42:GLU:O	1:A:42:GLU:OE1	0.40	2.40	5	1
1:A:14:ARG:NE	1:A:18:ARG:NH2	0.40	2.70	6	1
1:A:21:THR:HG23	1:A:50:LEU:HD23	0.40	1.93	10	1
1:A:44:ILE:HG12	1:A:82:TYR:CZ	0.40	2.50	3	1
1:A:13:LEU:CD2	1:A:63:LEU:O	0.40	2.69	6	1
1:A:118:LYS:CB	1:A:118:LYS:NZ	0.40	2.84	14	1
1:A:20:VAL:O	1:A:21:THR:C	0.40	2.60	16	1
1:A:78:ASN:O	1:A:81:GLU:N	0.40	2.54	1	1
1:A:9:THR:HB	1:A:123:ILE:CD1	0.40	2.46	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:PHE:O	1:A:71:ASP:OD2	0.40	2.40	15	1
1:A:33:PHE:C	1:A:35:LYS:N	0.40	2.73	16	1
1:A:59:LYS:HD2	1:A:59:LYS:N	0.40	2.32	19	1
1:A:121:GLU:HG3	1:A:122:GLU:N	0.40	2.31	1	1
1:A:64:THR:CG2	1:A:121:GLU:HA	0.40	2.47	11	1
1:A:35:LYS:CD	1:A:35:LYS:H	0.40	2.30	19	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	111/131 (85%)	86±5 (78±4%)	22±4 (20±4%)	2±1 (2±1%)	11	53
All	All	2220/2620 (85%)	1729 (78%)	448 (20%)	43 (2%)	11	53

All 17 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	37	VAL	9
1	A	112	LEU	7
1	A	93	ILE	5
1	A	16	PHE	3
1	A	42	GLU	3
1	A	38	SER	2
1	A	80	LEU	2
1	A	7	GLY	2
1	A	43	VAL	2
1	A	50	LEU	1
1	A	60	HIS	1
1	A	78	ASN	1
1	A	9	THR	1
1	A	41	LEU	1
1	A	20	VAL	1
1	A	34	SER	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	96	ARG	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	102/117 (87%)	95±3 (93±3%)	7±3 (7±3%)	20 69
All	All	2040/2340 (87%)	1906 (93%)	134 (7%)	20 69

All 38 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	63	LEU	10
1	A	71	ASP	10
1	A	41	LEU	9
1	A	64	THR	9
1	A	49	ASP	8
1	A	35	LYS	7
1	A	48	MET	7
1	A	59	LYS	6
1	A	96	ARG	6
1	A	40	TYR	5
1	A	29	ARG	4
1	A	102	ASP	4
1	A	70	LYS	4
1	A	90	ASP	4
1	A	66	LYS	3
1	A	11	ARG	3
1	A	45	LYS	3
1	A	28	LYS	3
1	A	94	ARG	2
1	A	12	GLU	2
1	A	42	GLU	2
1	A	60	HIS	2
1	A	118	LYS	2
1	A	91	LYS	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	26	THR	2
1	A	113	ASP	2
1	A	81	GLU	2
1	A	122	GLU	1
1	A	31	ASN	1
1	A	56	LYS	1
1	A	77	SER	1
1	A	46	GLU	1
1	A	115	GLU	1
1	A	117	ASN	1
1	A	67	ASP	1
1	A	22	LYS	1
1	A	73	ASP	1
1	A	39	ASP	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

No chemical shift data were provided