Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 06:15 PM BST

PDB ID	:	1X50
Title	:	Solution structure of the C-terminal gal-bind lectin domain from human galectin-4
Authors	:	Tomizawa, T.; Kigawa, T.; Saito, K.; Koshiba, S.; Inoue, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-05-15

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

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

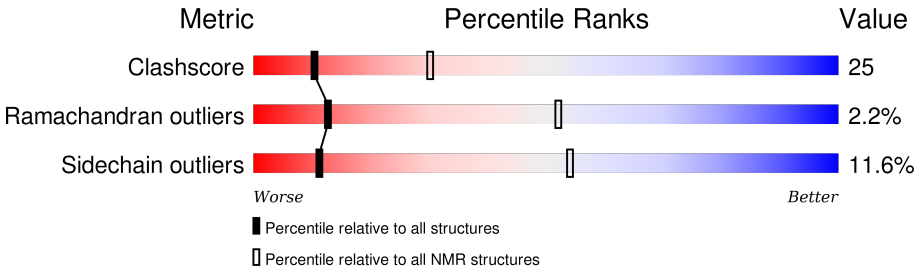
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	164	50% 27% • 18%

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:22-A:76, A:80-A:158 (134)	0.14	18

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2481 atoms, of which 1231 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Galectin-4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	164	2481	791	1231	225	231	3	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P56470
A	2	SER	-	CLONING ARTIFACT	UNP P56470
A	3	SER	-	CLONING ARTIFACT	UNP P56470
A	4	GLY	-	CLONING ARTIFACT	UNP P56470
A	5	SER	-	CLONING ARTIFACT	UNP P56470
A	6	SER	-	CLONING ARTIFACT	UNP P56470
A	7	GLY	-	CLONING ARTIFACT	UNP P56470
A	159	SER	-	CLONING ARTIFACT	UNP P56470
A	160	GLY	-	CLONING ARTIFACT	UNP P56470
A	161	PRO	-	CLONING ARTIFACT	UNP P56470
A	162	SER	-	CLONING ARTIFACT	UNP P56470
A	163	SER	-	CLONING ARTIFACT	UNP P56470
A	164	GLY	-	CLONING ARTIFACT	UNP P56470

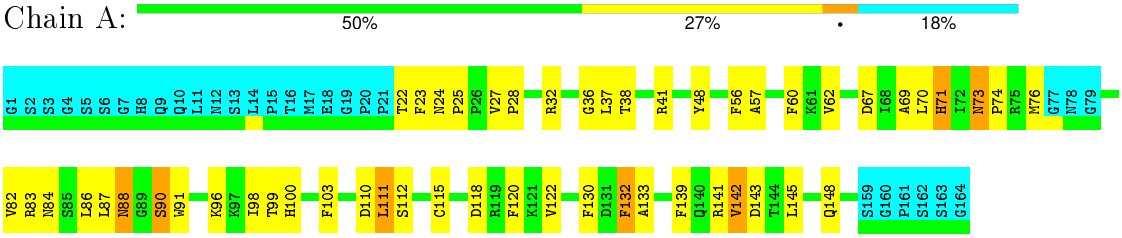
4 Residue-property plots

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: Galectin-4

Chain A:



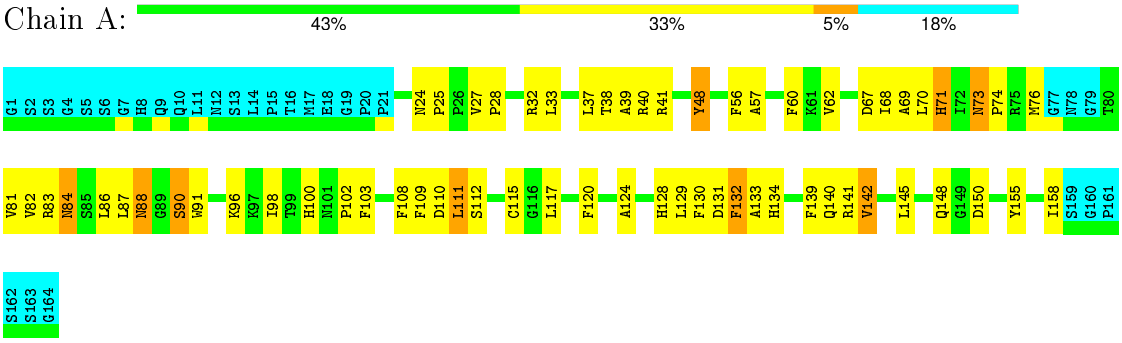
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

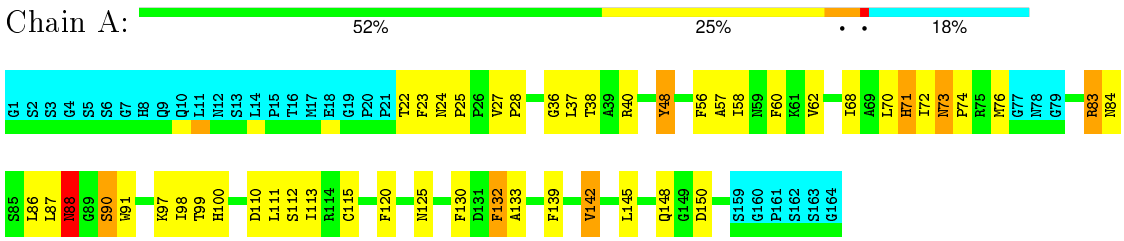
- Molecule 1: Galectin-4

Chain A:



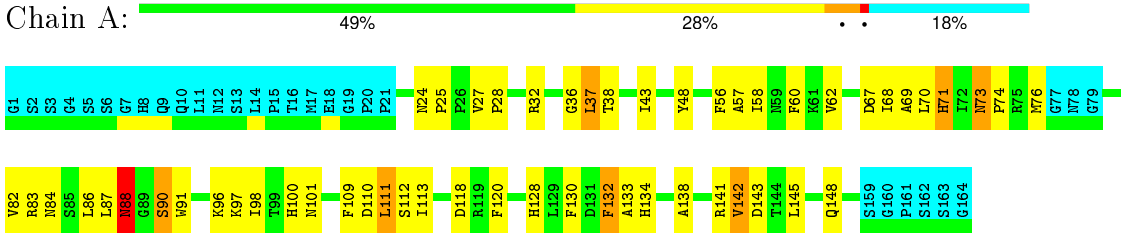
4.2.2 Score per residue for model 2

- Molecule 1: Galectin-4



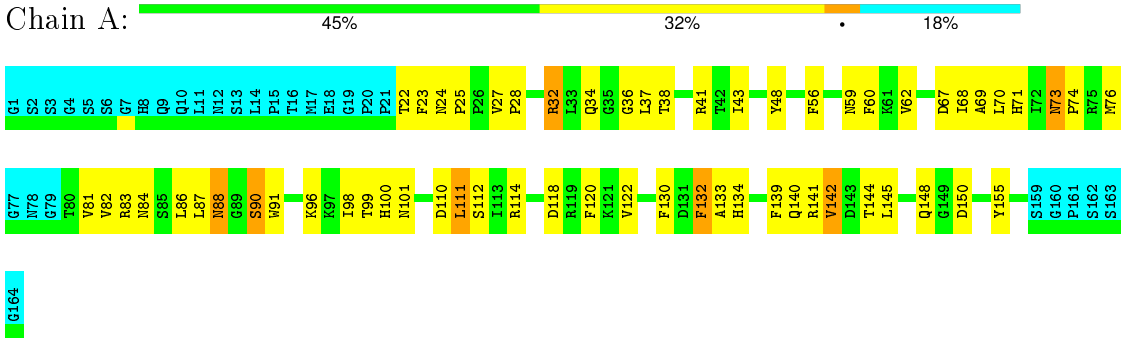
4.2.3 Score per residue for model 3

- Molecule 1: Galectin-4



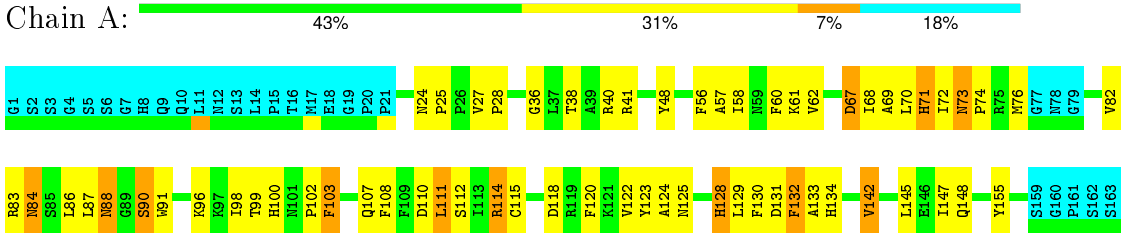
4.2.4 Score per residue for model 4

- Molecule 1: Galectin-4



4.2.5 Score per residue for model 5

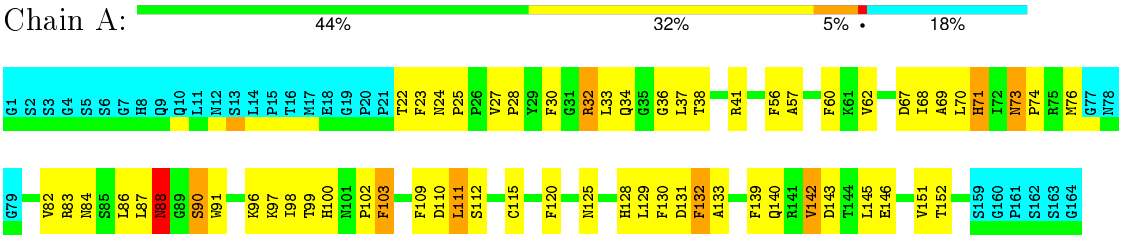
- Molecule 1: Galectin-4



4.2.6 Score per residue for model 6

- Molecule 1: Galectin-4

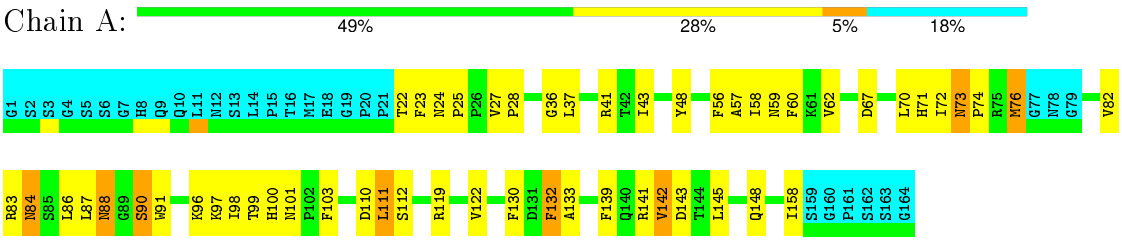
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Galectin-4

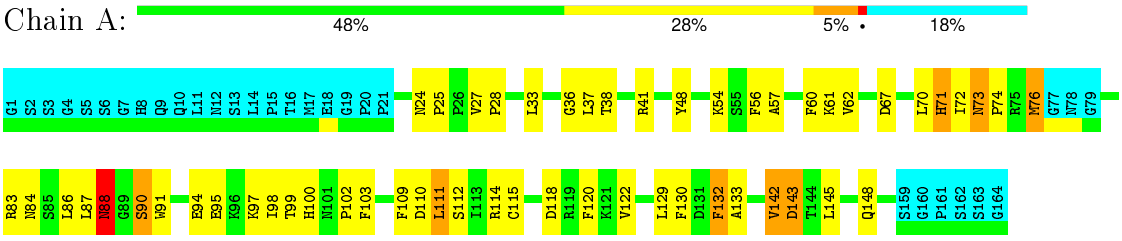
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Galectin-4

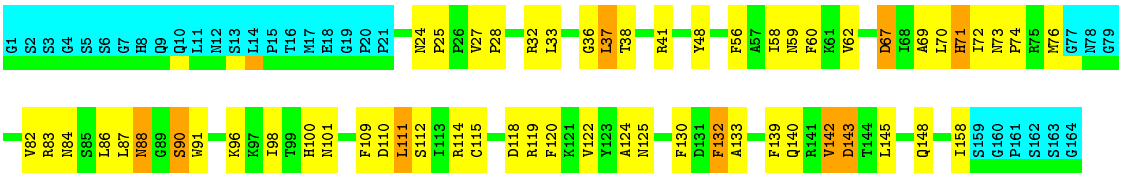
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Galectin-4

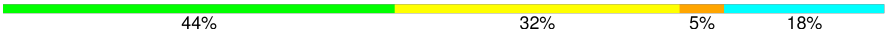
Chain A:

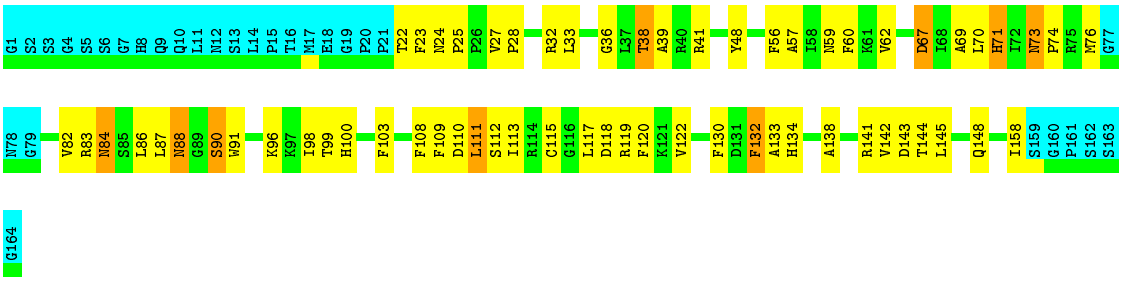


4.2.10 Score per residue for model 10

- Molecule 1: Galectin-4

Chain A:

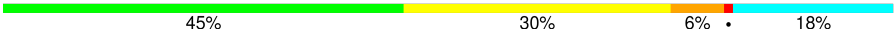


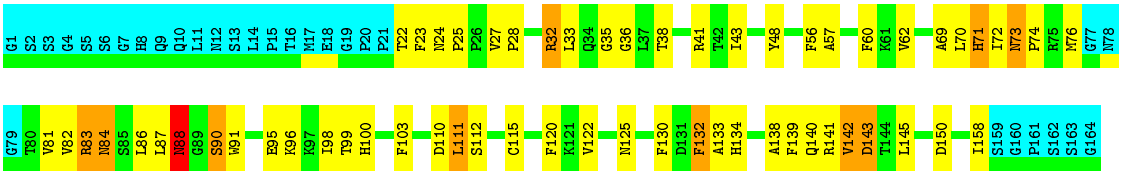


4.2.11 Score per residue for model 11

- Molecule 1: Galectin-4

Chain A:

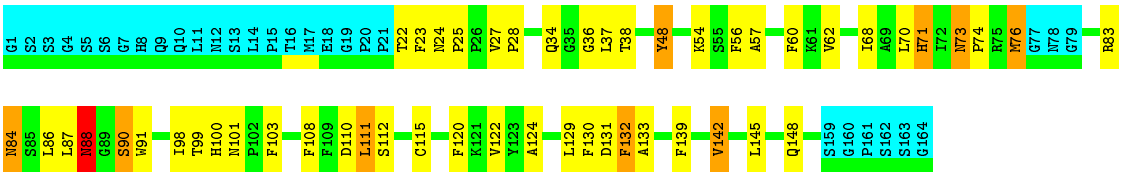




4.2.12 Score per residue for model 12

- Molecule 1: Galectin-4

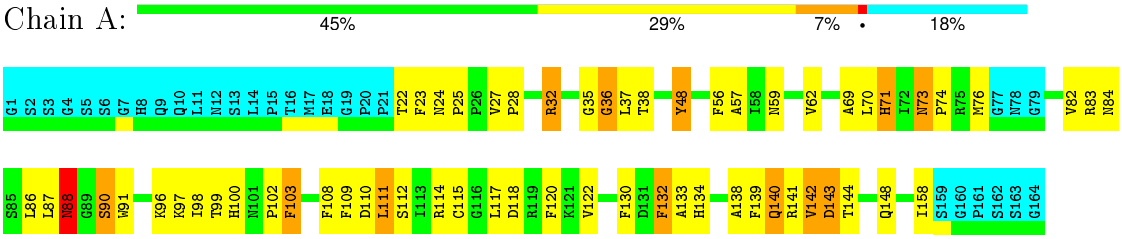
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: Galectin-4

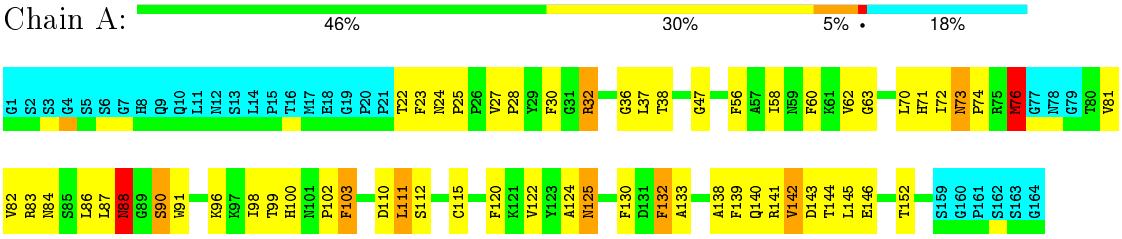
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Galectin-4

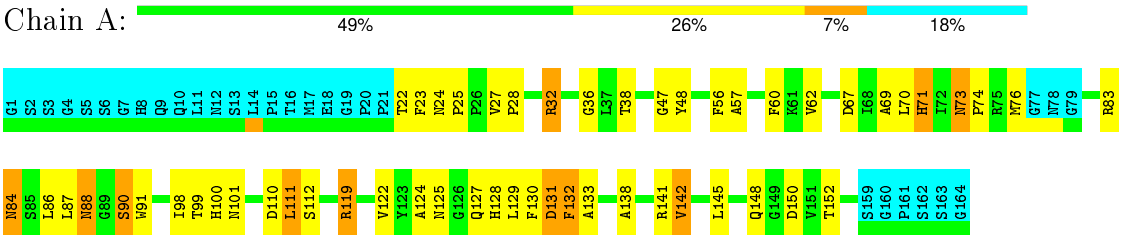
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Galectin-4

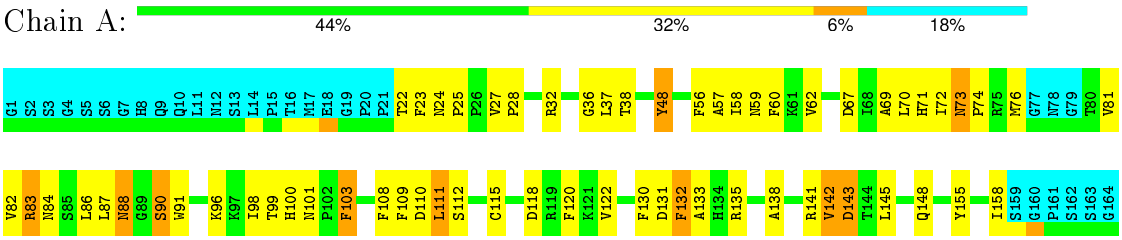
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Galectin-4

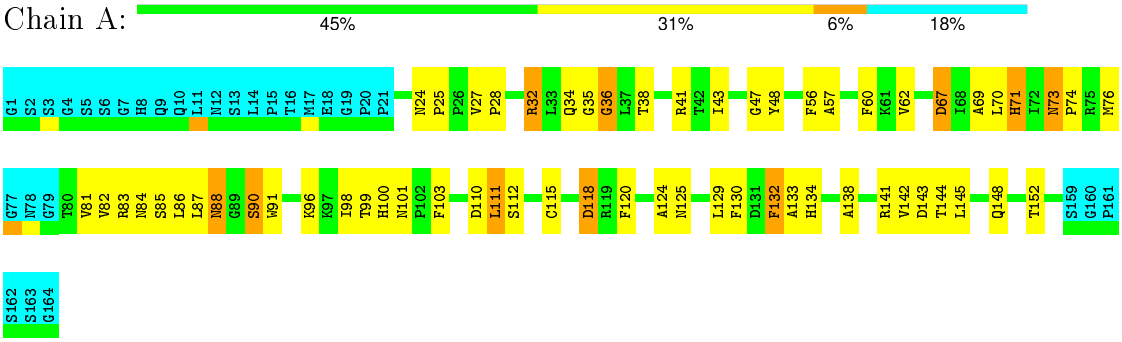
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Galectin-4

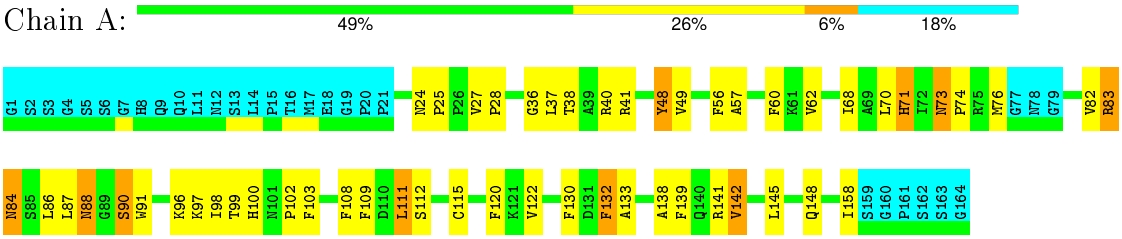
Chain A:



4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Galectin-4

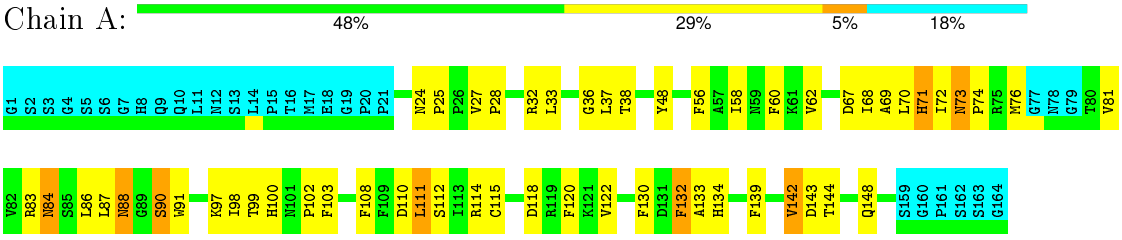
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Galectin-4

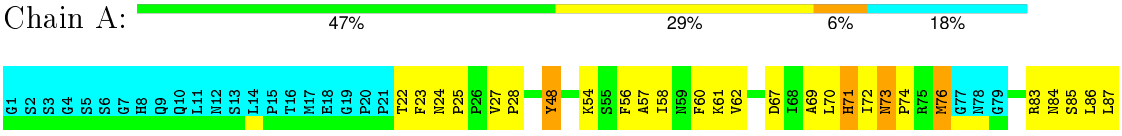
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Galectin-4

Chain A:




N88
G89
S90
W91
K97
I98
T99
H100
N101
P102
F103
F108
F109
D110
L111
S112
I113
R114
C115
F120
K121
V122
Y123
A124
L129
F130
D131
F132
A133
H134
R135
F139
Q140
R141
V142
L145
Q148
Y155
Y156
Q157
I158
S159
G160
P161
S162
S163
G164

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, restrainted molecular 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. 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	1058	1059	1055	52±5
All	All	21160	21180	21100	1042

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ALA:HB2	1:A:73:ASN:OD1	0.87	1.68	8	16
1:A:36:GLY:O	1:A:38:THR:HG23	0.85	1.71	6	14
1:A:86:LEU:HD12	1:A:90:SER:O	0.84	1.72	8	20
1:A:98:ILE:HD11	1:A:100:HIS:O	0.83	1.74	6	20
1:A:86:LEU:HD13	1:A:91:TRP:NE1	0.81	1.90	20	20
1:A:60:PHE:CE2	1:A:145:LEU:HD13	0.81	2.11	11	18
1:A:111:LEU:HD13	1:A:112:SER:N	0.79	1.92	14	20
1:A:86:LEU:HD13	1:A:91:TRP:CE2	0.78	2.13	5	20
1:A:41:ARG:CZ	1:A:43:ILE:HD11	0.73	2.13	17	2
1:A:111:LEU:HD11	1:A:122:VAL:HG13	0.69	1.64	14	14
1:A:111:LEU:HD11	1:A:122:VAL:CG1	0.67	2.19	7	5
1:A:33:LEU:HD23	1:A:158:ILE:HG12	0.67	1.66	1	2
1:A:62:VAL:HG13	1:A:141:ARG:O	0.66	1.90	17	5
1:A:41:ARG:NH1	1:A:43:ILE:HD11	0.65	2.06	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:ARG:NH1	1:A:130:PHE:CD2	0.65	2.65	14	3
1:A:41:ARG:NH2	1:A:43:ILE:HD11	0.65	2.07	11	2
1:A:82:VAL:HG22	1:A:96:LYS:CE	0.65	2.22	16	1
1:A:70:LEU:HD22	1:A:132:PHE:CD2	0.64	2.27	15	18
1:A:41:ARG:NH1	1:A:158:ILE:HG22	0.64	2.07	10	1
1:A:60:PHE:CZ	1:A:145:LEU:HD13	0.63	2.27	4	7
1:A:69:ALA:CB	1:A:142:VAL:HG21	0.63	2.24	13	13
1:A:62:VAL:HG22	1:A:142:VAL:HA	0.62	1.69	19	18
1:A:58:ILE:HG22	1:A:60:PHE:CE1	0.61	2.31	5	6
1:A:132:PHE:CE1	1:A:133:ALA:O	0.60	2.54	15	20
1:A:118:ASP:O	1:A:134:HIS:CD2	0.60	2.54	4	5
1:A:24:ASN:N	1:A:25:PRO:CD	0.60	2.64	2	20
1:A:114:ARG:O	1:A:120:PHE:CD2	0.60	2.55	13	4
1:A:82:VAL:HG22	1:A:96:LYS:HE3	0.59	1.73	16	1
1:A:70:LEU:HD21	1:A:72:ILE:HD11	0.59	1.74	9	9
1:A:70:LEU:HD13	1:A:132:PHE:CG	0.58	2.33	17	11
1:A:82:VAL:HG22	1:A:96:LYS:HD3	0.58	1.75	17	13
1:A:86:LEU:HD13	1:A:91:TRP:CD1	0.57	2.34	18	20
1:A:74:PRO:HA	1:A:81:VAL:HG22	0.57	1.77	1	3
1:A:98:ILE:HD11	1:A:100:HIS:C	0.57	2.18	5	7
1:A:37:LEU:HD23	1:A:41:ARG:CZ	0.57	2.30	8	1
1:A:37:LEU:HD23	1:A:41:ARG:NH1	0.57	2.14	8	1
1:A:41:ARG:NH1	1:A:158:ILE:HG23	0.57	2.14	7	2
1:A:70:LEU:HD13	1:A:132:PHE:CD1	0.56	2.34	20	8
1:A:132:PHE:CD1	1:A:132:PHE:C	0.56	2.79	11	10
1:A:132:PHE:C	1:A:132:PHE:CD1	0.56	2.78	3	6
1:A:62:VAL:HG22	1:A:142:VAL:CA	0.56	2.31	19	5
1:A:22:THR:CG2	1:A:23:PHE:N	0.56	2.68	20	7
1:A:27:VAL:HG13	1:A:28:PRO:HA	0.55	1.77	14	20
1:A:74:PRO:HB3	1:A:103:PHE:CD2	0.55	2.36	7	6
1:A:82:VAL:HG22	1:A:96:LYS:CG	0.55	2.30	3	3
1:A:118:ASP:C	1:A:134:HIS:CD2	0.55	2.80	13	7
1:A:99:THR:HG23	1:A:100:HIS:N	0.55	2.16	15	11
1:A:37:LEU:HD12	1:A:139:PHE:O	0.55	2.01	2	8
1:A:39:ALA:HB2	1:A:117:LEU:HD21	0.55	1.77	10	1
1:A:109:PHE:O	1:A:109:PHE:CD1	0.54	2.59	16	2
1:A:37:LEU:HD22	1:A:120:PHE:CZ	0.54	2.38	18	6
1:A:22:THR:O	1:A:23:PHE:CD1	0.54	2.61	7	10
1:A:69:ALA:HB2	1:A:142:VAL:HG21	0.53	1.81	17	1
1:A:87:LEU:N	1:A:90:SER:O	0.53	2.42	20	20
1:A:37:LEU:HD22	1:A:120:PHE:HZ	0.53	1.61	18	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ILE:HD13	1:A:101:ASN:ND2	0.53	2.18	17	1
1:A:37:LEU:HD23	1:A:41:ARG:HE	0.53	1.62	7	1
1:A:41:ARG:NH2	1:A:43:ILE:CG1	0.53	2.72	17	1
1:A:38:THR:HG23	1:A:41:ARG:HB2	0.53	1.80	10	1
1:A:138:ALA:HB1	1:A:141:ARG:HG3	0.53	1.79	15	5
1:A:98:ILE:HD13	1:A:101:ASN:CG	0.52	2.24	17	2
1:A:71:HIS:N	1:A:84:ASN:O	0.52	2.43	9	20
1:A:36:GLY:O	1:A:38:THR:HG22	0.52	2.03	10	1
1:A:111:LEU:HD12	1:A:113:ILE:HD11	0.52	1.81	2	2
1:A:56:PHE:CZ	1:A:74:PRO:HG3	0.52	2.40	11	19
1:A:83:ARG:HH12	1:A:97:LYS:N	0.52	2.02	3	1
1:A:56:PHE:O	1:A:73:ASN:ND2	0.51	2.42	17	20
1:A:115:CYS:SG	1:A:120:PHE:CZ	0.51	3.03	5	3
1:A:32:ARG:O	1:A:32:ARG:CD	0.51	2.58	14	2
1:A:59:ASN:OD1	1:A:71:HIS:CG	0.51	2.62	16	5
1:A:33:LEU:N	1:A:143:ASP:O	0.51	2.44	6	4
1:A:109:PHE:CD1	1:A:109:PHE:O	0.51	2.64	3	2
1:A:138:ALA:HB1	1:A:141:ARG:HD2	0.51	1.82	16	3
1:A:115:CYS:HA	1:A:120:PHE:CE1	0.51	2.41	5	11
1:A:115:CYS:SG	1:A:120:PHE:CE1	0.51	3.03	5	3
1:A:62:VAL:HG23	1:A:67:ASP:O	0.51	2.06	3	4
1:A:36:GLY:N	1:A:143:ASP:OD2	0.51	2.44	16	3
1:A:41:ARG:NH1	1:A:158:ILE:CG2	0.50	2.74	18	2
1:A:38:THR:O	1:A:41:ARG:N	0.50	2.45	1	2
1:A:74:PRO:HB3	1:A:103:PHE:CE2	0.50	2.42	7	3
1:A:47:GLY:CA	1:A:152:THR:O	0.50	2.60	15	3
1:A:139:PHE:CE1	1:A:140:GLN:HG3	0.50	2.42	13	1
1:A:41:ARG:HH12	1:A:158:ILE:HG22	0.50	1.63	10	1
1:A:124:ALA:O	1:A:125:ASN:ND2	0.50	2.45	9	2
1:A:69:ALA:HB3	1:A:142:VAL:HG21	0.50	1.83	1	7
1:A:87:LEU:O	1:A:90:SER:N	0.50	2.44	8	17
1:A:59:ASN:ND2	1:A:71:HIS:ND1	0.50	2.60	9	1
1:A:111:LEU:HD13	1:A:112:SER:H	0.50	1.63	16	8
1:A:56:PHE:CZ	1:A:109:PHE:CZ	0.49	3.00	3	2
1:A:82:VAL:HG22	1:A:96:LYS:CD	0.49	2.37	3	2
1:A:36:GLY:N	1:A:143:ASP:OD1	0.49	2.45	14	1
1:A:36:GLY:O	1:A:41:ARG:NE	0.49	2.45	9	3
1:A:114:ARG:HD3	1:A:123:TYR:CD1	0.49	2.43	5	1
1:A:130:PHE:CD1	1:A:130:PHE:C	0.49	2.86	17	8
1:A:115:CYS:HA	1:A:120:PHE:CE2	0.49	2.43	8	2
1:A:111:LEU:HD21	1:A:129:LEU:HD22	0.49	1.83	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:CYS:HB2	1:A:120:PHE:CZ	0.49	2.43	16	5
1:A:138:ALA:HB1	1:A:141:ARG:CD	0.49	2.38	10	6
1:A:67:ASP:OD2	1:A:88:ASN:ND2	0.49	2.45	16	4
1:A:115:CYS:HB2	1:A:120:PHE:CE2	0.49	2.43	10	3
1:A:128:HIS:CE1	1:A:131:ASP:OD2	0.49	2.65	5	1
1:A:86:LEU:HB2	1:A:91:TRP:CZ2	0.49	2.43	9	20
1:A:32:ARG:O	1:A:32:ARG:CG	0.49	2.60	14	2
1:A:32:ARG:NH1	1:A:34:GLN:NE2	0.49	2.61	6	1
1:A:48:TYR:HB2	1:A:108:PHE:CD2	0.48	2.43	16	8
1:A:107:GLN:NE2	1:A:108:PHE:O	0.48	2.46	5	1
1:A:56:PHE:CE2	1:A:58:ILE:HD11	0.48	2.43	14	4
1:A:130:PHE:C	1:A:130:PHE:CD1	0.48	2.86	19	11
1:A:98:ILE:CG1	1:A:99:THR:N	0.48	2.75	17	7
1:A:32:ARG:O	1:A:34:GLN:NE2	0.48	2.46	4	1
1:A:131:ASP:OD1	1:A:132:PHE:N	0.48	2.47	15	1
1:A:103:PHE:CZ	1:A:129:LEU:HD21	0.48	2.44	1	4
1:A:124:ALA:CB	1:A:129:LEU:HD13	0.47	2.39	5	3
1:A:83:ARG:NH1	1:A:130:PHE:CG	0.47	2.81	16	1
1:A:86:LEU:HB2	1:A:91:TRP:CH2	0.47	2.44	14	16
1:A:115:CYS:HA	1:A:120:PHE:CD1	0.47	2.45	5	5
1:A:35:GLY:O	1:A:38:THR:HG23	0.47	2.09	17	2
1:A:109:PHE:O	1:A:109:PHE:CD2	0.47	2.68	6	1
1:A:36:GLY:CA	1:A:143:ASP:OD1	0.47	2.62	7	5
1:A:41:ARG:NH2	1:A:43:ILE:CD1	0.47	2.77	17	1
1:A:139:PHE:CG	1:A:140:GLN:N	0.47	2.82	4	7
1:A:68:ILE:HD12	1:A:86:LEU:HB3	0.47	1.87	1	9
1:A:115:CYS:CB	1:A:120:PHE:CZ	0.46	2.98	5	1
1:A:155:TYR:C	1:A:155:TYR:CD1	0.46	2.89	16	2
1:A:109:PHE:CG	1:A:109:PHE:O	0.46	2.67	13	2
1:A:56:PHE:N	1:A:56:PHE:CD1	0.46	2.83	7	3
1:A:139:PHE:CD1	1:A:140:GLN:OE1	0.46	2.68	13	1
1:A:87:LEU:O	1:A:90:SER:O	0.46	2.33	8	20
1:A:27:VAL:HA	1:A:28:PRO:C	0.46	2.31	6	20
1:A:109:PHE:O	1:A:109:PHE:CG	0.46	2.68	6	5
1:A:48:TYR:O	1:A:48:TYR:CD1	0.46	2.69	20	2
1:A:32:ARG:NH1	1:A:34:GLN:OE1	0.46	2.49	17	1
1:A:132:PHE:CG	1:A:132:PHE:O	0.45	2.70	12	2
1:A:24:ASN:N	1:A:25:PRO:HD3	0.45	2.26	2	9
1:A:49:VAL:HG23	1:A:109:PHE:CD2	0.45	2.47	18	1
1:A:102:PRO:O	1:A:103:PHE:C	0.45	2.54	8	9
1:A:73:ASN:C	1:A:73:ASN:ND2	0.45	2.69	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:PHE:O	1:A:132:PHE:CG	0.45	2.70	2	4
1:A:99:THR:CG2	1:A:100:HIS:N	0.45	2.80	15	3
1:A:100:HIS:O	1:A:100:HIS:CG	0.45	2.70	4	4
1:A:124:ALA:O	1:A:125:ASN:CG	0.45	2.55	9	2
1:A:72:ILE:CG2	1:A:81:VAL:CG1	0.45	2.95	11	4
1:A:35:GLY:O	1:A:36:GLY:C	0.45	2.55	13	2
1:A:138:ALA:HB1	1:A:141:ARG:CG	0.45	2.41	10	2
1:A:35:GLY:C	1:A:143:ASP:OD2	0.45	2.55	11	1
1:A:111:LEU:HD12	1:A:113:ILE:CD1	0.45	2.41	2	2
1:A:56:PHE:CD1	1:A:56:PHE:N	0.45	2.84	1	5
1:A:124:ALA:HB2	1:A:129:LEU:HD13	0.45	1.88	20	1
1:A:128:HIS:CE1	1:A:131:ASP:OD1	0.45	2.69	6	1
1:A:38:THR:O	1:A:40:ARG:N	0.44	2.50	1	1
1:A:101:ASN:OD1	1:A:101:ASN:C	0.44	2.55	7	3
1:A:39:ALA:HB2	1:A:117:LEU:CD2	0.44	2.42	10	1
1:A:100:HIS:CG	1:A:100:HIS:O	0.44	2.70	11	2
1:A:101:ASN:C	1:A:101:ASN:OD1	0.44	2.55	4	3
1:A:109:PHE:CD2	1:A:109:PHE:O	0.44	2.70	13	1
1:A:88:ASN:HD22	1:A:88:ASN:N	0.44	2.09	11	3
1:A:88:ASN:N	1:A:88:ASN:HD22	0.44	2.09	3	5
1:A:74:PRO:CB	1:A:103:PHE:CD2	0.44	3.01	8	2
1:A:117:LEU:O	1:A:134:HIS:CD2	0.44	2.71	1	2
1:A:70:LEU:HB2	1:A:132:PHE:CE2	0.44	2.47	19	1
1:A:94:GLU:C	1:A:95:GLU:OE2	0.43	2.56	8	1
1:A:69:ALA:O	1:A:85:SER:CB	0.43	2.66	20	2
1:A:59:ASN:OD1	1:A:71:HIS:ND1	0.43	2.50	16	1
1:A:141:ARG:O	1:A:143:ASP:CG	0.43	2.56	7	1
1:A:38:THR:OG1	1:A:39:ALA:N	0.43	2.51	10	1
1:A:59:ASN:ND2	1:A:71:HIS:CG	0.43	2.86	9	1
1:A:32:ARG:CG	1:A:32:ARG:O	0.43	2.65	15	2
1:A:30:PHE:CD2	1:A:146:GLU:HB3	0.43	2.48	14	2
1:A:38:THR:C	1:A:40:ARG:N	0.43	2.72	1	1
1:A:58:ILE:HG13	1:A:147:ILE:HG23	0.43	1.90	5	1
1:A:120:PHE:CD1	1:A:132:PHE:CD2	0.43	3.07	4	1
1:A:114:ARG:O	1:A:120:PHE:CG	0.43	2.72	9	1
1:A:118:ASP:OD1	1:A:119:ARG:N	0.43	2.51	9	1
1:A:63:GLY:N	1:A:144:THR:OG1	0.42	2.53	14	1
1:A:128:HIS:NE2	1:A:131:ASP:OD1	0.42	2.52	6	1
1:A:23:PHE:O	1:A:24:ASN:C	0.42	2.56	16	1
1:A:111:LEU:CD2	1:A:129:LEU:HD22	0.42	2.44	15	1
1:A:111:LEU:CD1	1:A:112:SER:N	0.42	2.78	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:TYR:CE1	1:A:157:GLN:HB2	0.42	2.49	20	1
1:A:98:ILE:HG12	1:A:99:THR:N	0.42	2.29	14	3
1:A:124:ALA:O	1:A:127:GLN:N	0.42	2.53	15	1
1:A:100:HIS:ND1	1:A:100:HIS:O	0.42	2.52	17	1
1:A:22:THR:HG22	1:A:23:PHE:N	0.42	2.30	20	2
1:A:118:ASP:OD2	1:A:119:ARG:NH1	0.42	2.52	9	1
1:A:71:HIS:O	1:A:71:HIS:CG	0.42	2.72	3	2
1:A:54:LYS:O	1:A:76:MET:SD	0.42	2.78	8	3
1:A:61:LYS:HG2	1:A:62:VAL:N	0.42	2.30	8	3
1:A:32:ARG:HG3	1:A:32:ARG:O	0.42	2.15	15	1
1:A:60:PHE:N	1:A:60:PHE:CD1	0.41	2.88	19	1
1:A:83:ARG:NH1	1:A:95:GLU:O	0.41	2.53	11	1
1:A:67:ASP:OD1	1:A:88:ASN:OD1	0.41	2.39	16	10
1:A:83:ARG:HD3	1:A:83:ARG:N	0.41	2.31	16	1
1:A:43:ILE:N	1:A:43:ILE:HD12	0.41	2.30	3	1
1:A:34:GLN:O	1:A:41:ARG:NH2	0.41	2.53	6	2
1:A:100:HIS:O	1:A:100:HIS:ND1	0.41	2.52	19	1
1:A:155:TYR:CD1	1:A:155:TYR:C	0.41	2.94	4	1
1:A:33:LEU:HD13	1:A:41:ARG:NH2	0.41	2.30	8	1
1:A:60:PHE:HB3	1:A:142:VAL:HG11	0.41	1.92	8	1
1:A:88:ASN:CG	1:A:88:ASN:O	0.41	2.59	14	7
1:A:27:VAL:CG1	1:A:28:PRO:HA	0.41	2.44	6	7
1:A:35:GLY:O	1:A:36:GLY:O	0.41	2.39	17	2
1:A:151:VAL:CG2	1:A:152:THR:N	0.41	2.84	6	1
1:A:36:GLY:CA	1:A:143:ASP:CG	0.41	2.89	13	1
1:A:76:MET:N	1:A:76:MET:SD	0.41	2.94	7	1
1:A:113:ILE:HG23	1:A:122:VAL:HG22	0.41	1.92	20	1
1:A:86:LEU:CD1	1:A:91:TRP:CD1	0.41	3.03	9	1
1:A:88:ASN:O	1:A:88:ASN:CG	0.41	2.60	3	1
1:A:72:ILE:HD13	1:A:130:PHE:HZ	0.41	1.74	16	1
1:A:48:TYR:CD1	1:A:48:TYR:O	0.41	2.74	8	1
1:A:48:TYR:CD1	1:A:48:TYR:C	0.40	2.94	20	1
1:A:151:VAL:HG22	1:A:152:THR:N	0.40	2.30	6	1
1:A:124:ALA:C	1:A:125:ASN:ND2	0.40	2.75	14	1
1:A:87:LEU:O	1:A:88:ASN:C	0.40	2.59	8	1
1:A:113:ILE:HG22	1:A:120:PHE:HD2	0.40	1.76	10	1
1:A:38:THR:O	1:A:115:CYS:SG	0.40	2.79	13	2
1:A:119:ARG:C	1:A:119:ARG:CD	0.40	2.90	15	1
1:A:101:ASN:OD1	1:A:103:PHE:CD2	0.40	2.74	16	1
1:A:111:LEU:CD1	1:A:113:ILE:CD1	0.40	2.99	2	1
1:A:85:SER:OG	1:A:135:ARG:CD	0.40	2.70	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:ASP:C	1:A:118:ASP:OD1	0.40	2.59	8	1
1:A:43:ILE:HD12	1:A:43:ILE:N	0.40	2.31	4	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	134/164 (82%)	114±2 (85±1%)	18±2 (13±1%)	3±1 (2±1%)	13	52
All	All	2680/3280 (82%)	2272 (85%)	350 (13%)	58 (2%)	13	52

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	88	ASN	20
1	A	142	VAL	18
1	A	103	PHE	8
1	A	128	HIS	4
1	A	37	LEU	3
1	A	36	GLY	2
1	A	134	HIS	1
1	A	76	MET	1
1	A	39	ALA	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	114/136 (84%)	101±2 (88±2%)	13±2 (12±2%)	11	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2280/2720 (84%)	2016 (88%)	264 (12%)	11 54

All 27 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	90	SER	20
1	A	76	MET	20
1	A	132	PHE	20
1	A	111	LEU	19
1	A	110	ASP	19
1	A	73	ASN	19
1	A	83	ARG	18
1	A	148	GLN	17
1	A	71	HIS	16
1	A	48	TYR	15
1	A	32	ARG	10
1	A	88	ASN	9
1	A	84	ASN	9
1	A	97	LYS	8
1	A	143	ASP	7
1	A	67	ASP	6
1	A	125	ASN	6
1	A	150	ASP	5
1	A	144	THR	5
1	A	131	ASP	4
1	A	119	ARG	3
1	A	40	ARG	3
1	A	118	ASP	2
1	A	140	GLN	1
1	A	38	THR	1
1	A	135	ARG	1
1	A	114	ARG	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

No chemical shift data were provided