Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 01:52 PM BST

PDB ID	:	1AJW
Title	:	STRUCTURE OF RHOGDI: A C-TERMINAL BINDING DOMAIN TARGETS AN N-TERMINAL INHIBITORY PEPTIDE TO GTPASES, NMR, 20 STRUCTURES
Authors	:	Rosen, M.K.; Gosser, Y.Q.
Deposited on	:	1997-05-11

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:

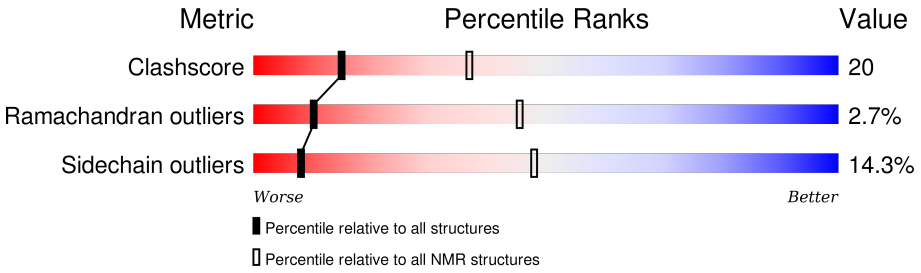
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	145	52% 36% · 8%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models).

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:69-A:183, A:187-A:204 (133)	0.47	4

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 5 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2346 atoms, of which 1171 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RHOGDI.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	145	2346	747	1171	199	224	5	0

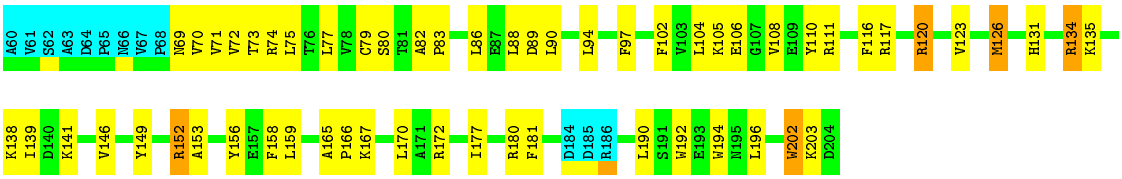
4 Residue-property plots (i)

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: RHOGDI

Chain A: 



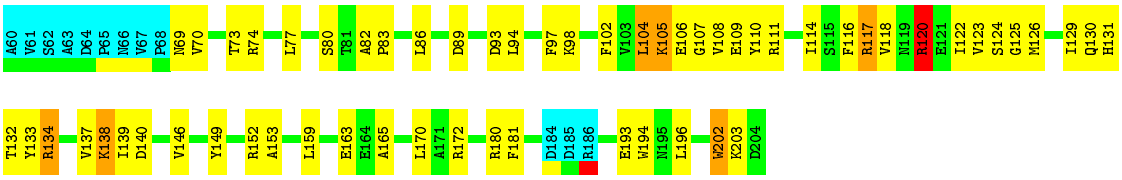
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: RHOGDI

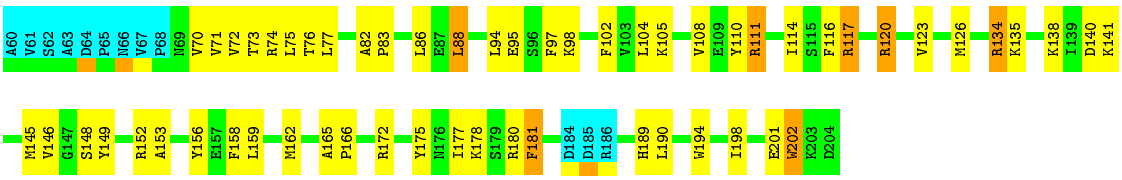
Chain A: 



4.2.2 Score per residue for model 2

- Molecule 1: RHOGDI

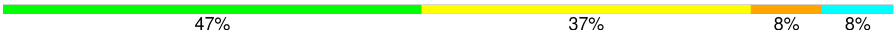
Chain A: 

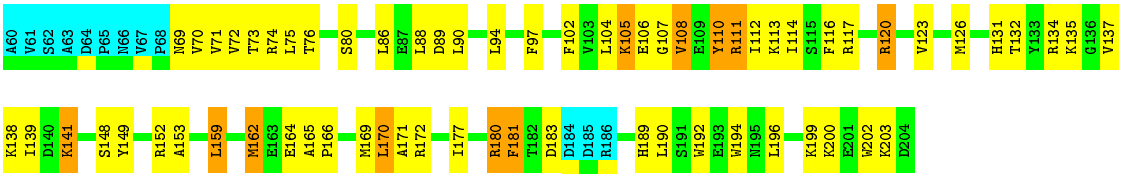


4.2.3 Score per residue for model 3

- Molecule 1: RHOGDI

Chain A:

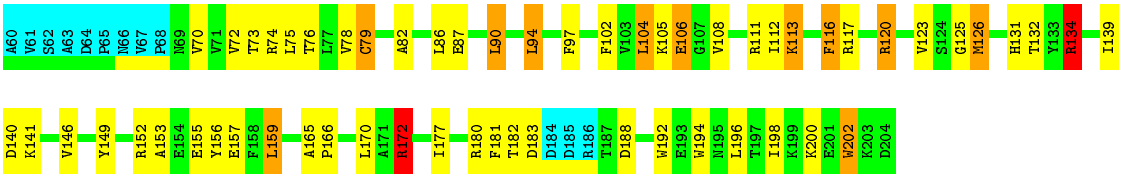




4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: RHOGDI

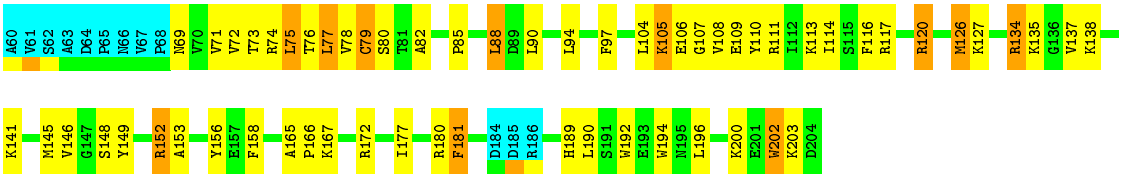
Chain A:



4.2.5 Score per residue for model 5

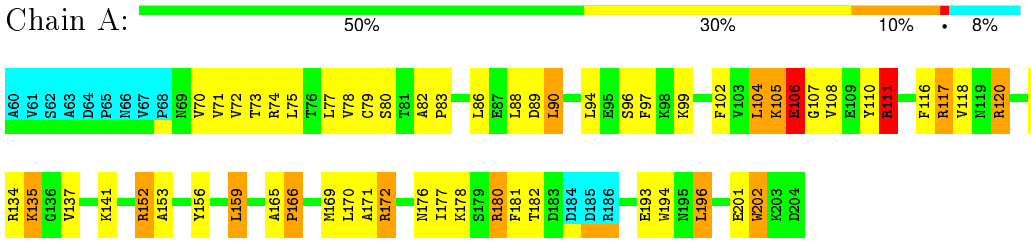
- Molecule 1: RHOGDI

Chain A:



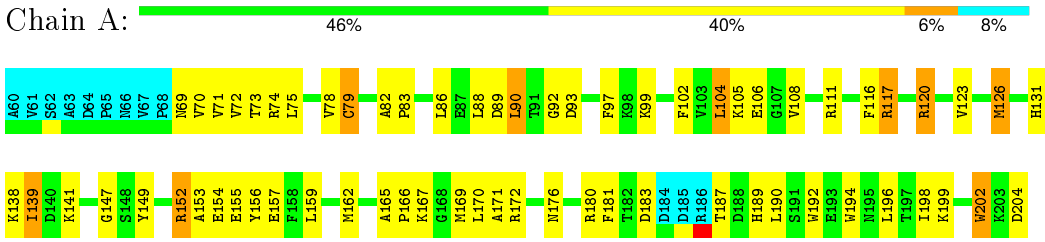
4.2.6 Score per residue for model 6

- Molecule 1: RHOGDI



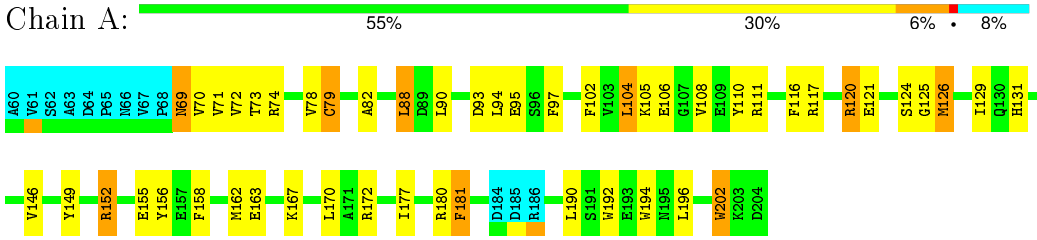
4.2.7 Score per residue for model 7

- Molecule 1: RHOGDI



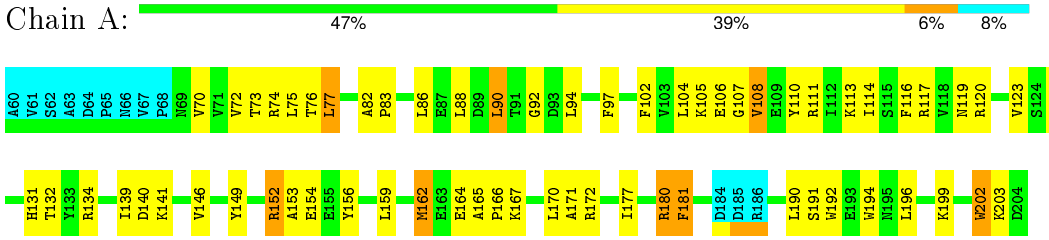
4.2.8 Score per residue for model 8

- Molecule 1: RHOGDI



4.2.9 Score per residue for model 9

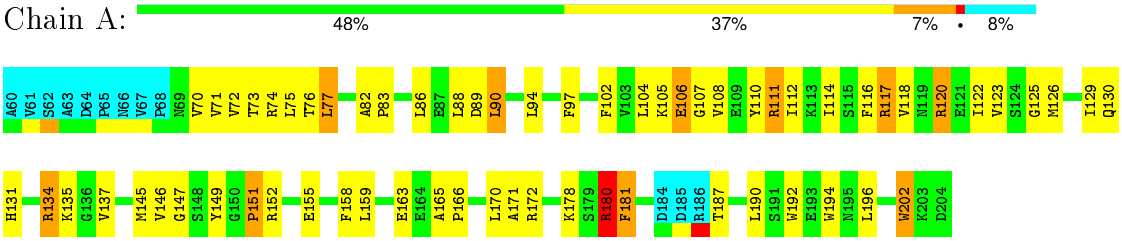
- Molecule 1: RHOGDI



4.2.10 Score per residue for model 10

- Molecule 1: RHOGDI

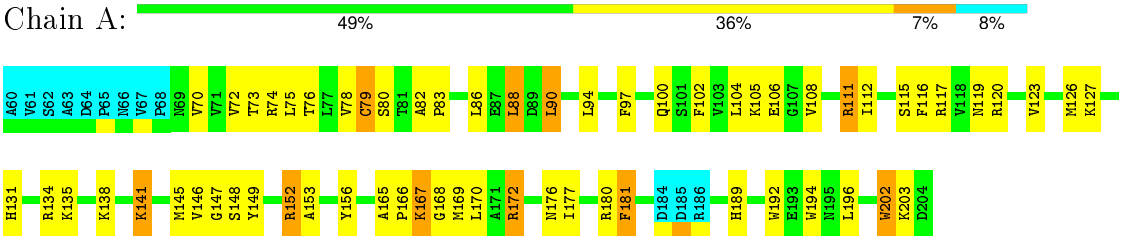
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: RHOGDI

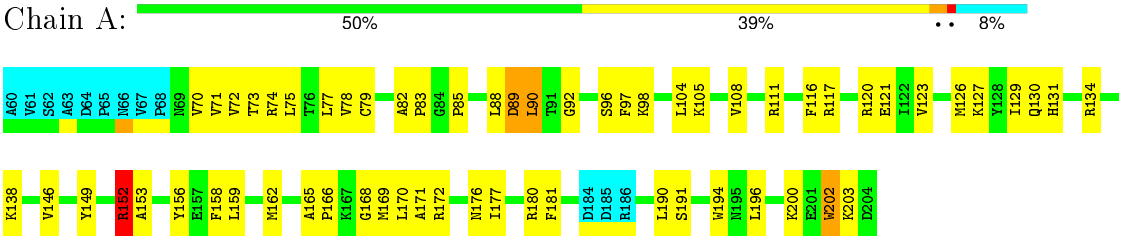
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: RHOGDI

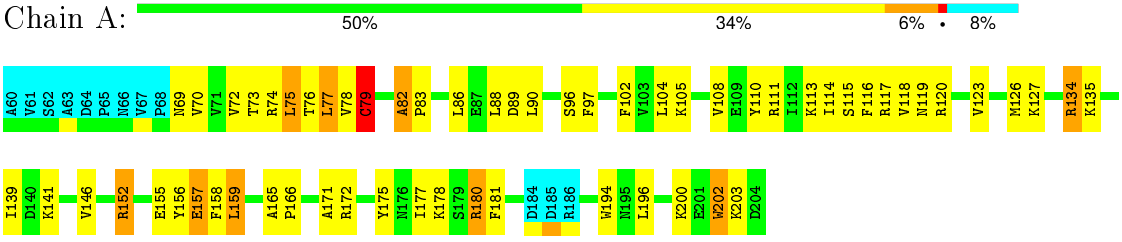
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: RHOGDI

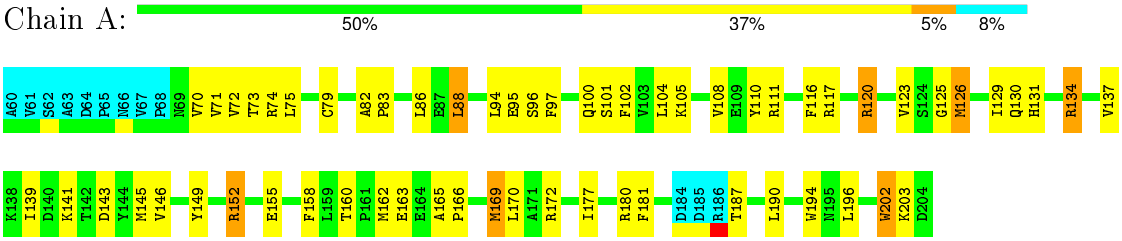
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: RHOGDI

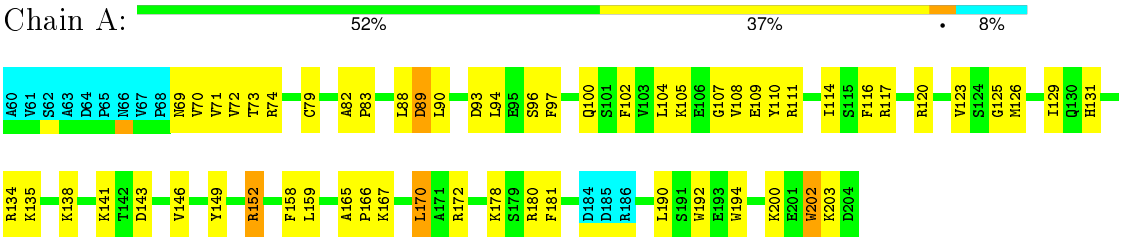
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: RHOGDI

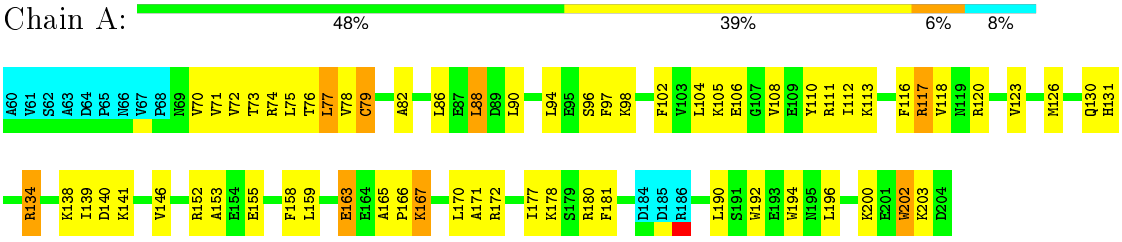
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: RHOGDI

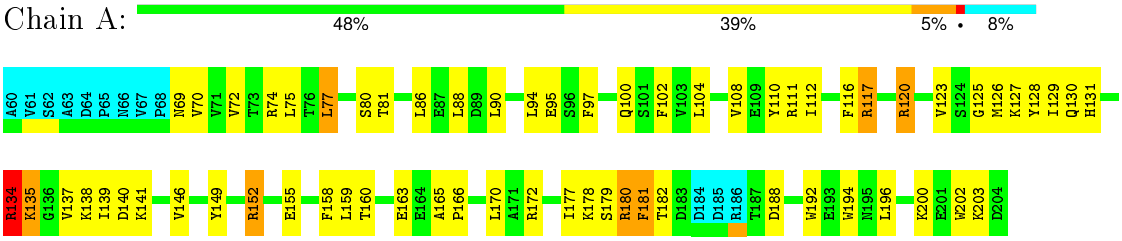
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: RHOGDI

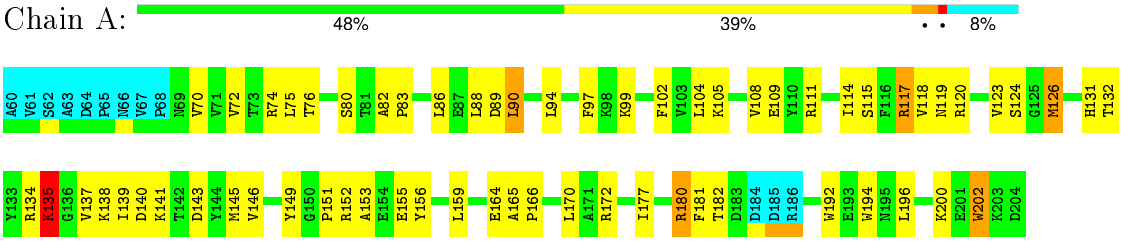
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: RHOGDI

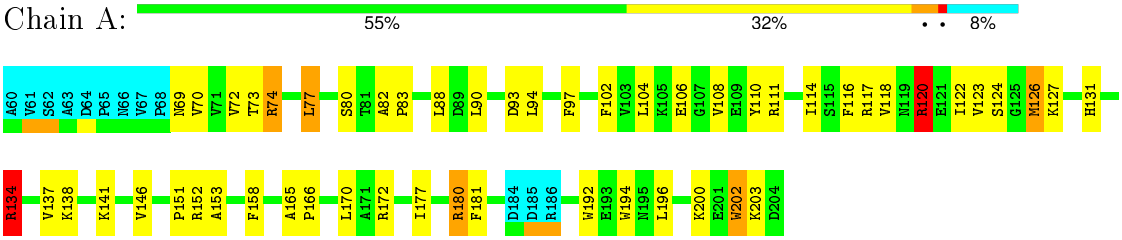
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: RHOGDI

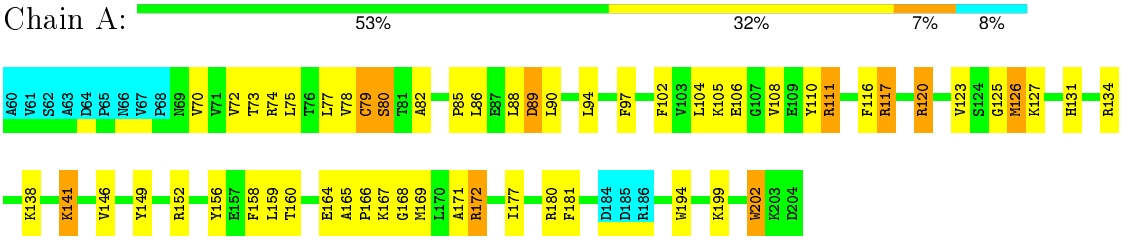
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: RHOGDI

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *HYBRID DISTANCE GEOMETRY/ SIMULATED ANNEALING*.

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *NO DISTANCE VIOLATIONS*.

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

Software name	Classification	Version
X-PLOR	refinement	3.0
NMRPIPE	structure solution	
NMRVIEW	structure solution	
X-PLOR	structure solution	

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.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	8.0±0.0
All	All	0	160

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	74	ARG	Sidechain	20
1	A	180	ARG	Sidechain	20
1	A	111	ARG	Sidechain	20
1	A	117	ARG	Sidechain	20
1	A	120	ARG	Sidechain	20
1	A	134	ARG	Sidechain	20
1	A	172	ARG	Sidechain	20
1	A	152	ARG	Sidechain	20

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	1088	1091	1091	43±6
All	All	21760	21820	21820	856

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:LEU:HD12	1:A:196:LEU:HD11	0.94	1.35	13	6
1:A:104:LEU:HD21	1:A:108:VAL:HG22	0.94	1.37	9	4
1:A:70:VAL:HG21	1:A:123:VAL:HG21	0.93	1.40	9	17
1:A:114:ILE:HG21	1:A:181:PHE:CE2	0.87	2.03	9	3
1:A:88:LEU:HD22	1:A:97:PHE:CZ	0.86	2.06	9	8
1:A:82:ALA:HB2	1:A:202:TRP:CZ2	0.83	2.08	1	5
1:A:82:ALA:HB2	1:A:202:TRP:CH2	0.83	2.08	1	15
1:A:86:LEU:HD22	1:A:102:PHE:CD1	0.82	2.08	9	9
1:A:177:ILE:HG21	1:A:194:TRP:CZ2	0.82	2.10	2	7
1:A:104:LEU:HD22	1:A:108:VAL:HG21	0.80	1.51	13	7
1:A:190:LEU:HD13	1:A:191:SER:N	0.80	1.91	9	2
1:A:146:VAL:HG21	1:A:181:PHE:CZ	0.80	2.11	11	3
1:A:70:VAL:HG22	1:A:118:VAL:HG22	0.78	1.54	6	4
1:A:104:LEU:HD23	1:A:202:TRP:CZ3	0.78	2.13	13	5
1:A:104:LEU:CD1	1:A:196:LEU:HD11	0.78	2.09	13	6
1:A:71:VAL:HG13	1:A:190:LEU:HD22	0.76	1.57	8	7
1:A:104:LEU:CD2	1:A:196:LEU:HD11	0.76	2.11	1	1
1:A:146:VAL:HG12	1:A:149:TYR:CE1	0.75	2.16	15	4
1:A:82:ALA:HB1	1:A:83:PRO:HD2	0.74	1.59	13	13
1:A:88:LEU:HD21	1:A:97:PHE:CE1	0.72	2.18	15	3
1:A:131:HIS:O	1:A:177:ILE:HG23	0.71	1.85	8	5
1:A:104:LEU:HD12	1:A:196:LEU:CD1	0.71	2.14	13	2
1:A:105:LYS:O	1:A:108:VAL:HG13	0.70	1.87	12	6
1:A:73:THR:HG23	1:A:116:PHE:HA	0.70	1.62	19	16
1:A:165:ALA:HB1	1:A:166:PRO:HD2	0.69	1.63	13	17
1:A:166:PRO:HB2	1:A:171:ALA:HB1	0.69	1.63	13	3
1:A:104:LEU:HD11	1:A:196:LEU:HD11	0.69	1.65	19	2
1:A:104:LEU:HD23	1:A:196:LEU:HD11	0.69	1.63	1	1
1:A:88:LEU:HD22	1:A:97:PHE:CE1	0.69	2.23	7	10
1:A:104:LEU:HD22	1:A:165:ALA:HB2	0.68	1.65	10	1
1:A:114:ILE:HG21	1:A:181:PHE:CZ	0.68	2.23	3	2
1:A:146:VAL:HG13	1:A:158:PHE:CD1	0.68	2.23	12	3
1:A:88:LEU:HD12	1:A:102:PHE:CZ	0.68	2.24	15	1
1:A:104:LEU:HD21	1:A:108:VAL:CG2	0.68	2.18	10	4
1:A:153:ALA:HB3	1:A:156:TYR:CE2	0.67	2.24	7	2
1:A:70:VAL:CG2	1:A:123:VAL:HG21	0.67	2.17	9	12
1:A:146:VAL:HG13	1:A:158:PHE:CG	0.66	2.25	16	4
1:A:153:ALA:HB3	1:A:156:TYR:CZ	0.66	2.24	9	3
1:A:72:VAL:HG22	1:A:181:PHE:CD2	0.66	2.25	5	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:TRP:CZ3	1:A:196:LEU:HD21	0.66	2.24	6	1
1:A:146:VAL:HG12	1:A:149:TYR:OH	0.66	1.91	5	2
1:A:71:VAL:CG1	1:A:190:LEU:HD22	0.65	2.22	8	2
1:A:70:VAL:HG21	1:A:123:VAL:CG2	0.65	2.22	1	3
1:A:72:VAL:HG11	1:A:90:LEU:HD22	0.64	1.68	18	3
1:A:170:LEU:O	1:A:170:LEU:HD23	0.64	1.91	7	3
1:A:108:VAL:HG11	1:A:202:TRP:CZ2	0.64	2.27	10	1
1:A:75:LEU:HD23	1:A:76:THR:N	0.64	2.07	18	6
1:A:102:PHE:HB2	1:A:196:LEU:HD12	0.63	1.70	19	1
1:A:104:LEU:CD2	1:A:108:VAL:HG21	0.63	2.23	7	5
1:A:170:LEU:O	1:A:170:LEU:HD13	0.63	1.93	15	3
1:A:104:LEU:HD22	1:A:165:ALA:CB	0.62	2.23	10	1
1:A:88:LEU:HD22	1:A:97:PHE:CE2	0.62	2.30	10	6
1:A:107:GLY:HA2	1:A:165:ALA:HB3	0.62	1.72	3	7
1:A:104:LEU:HD12	1:A:196:LEU:HD21	0.62	1.70	4	3
1:A:157:GLU:OE1	1:A:159:LEU:HD12	0.62	1.94	13	1
1:A:77:LEU:HD12	1:A:86:LEU:HB2	0.62	1.72	2	2
1:A:153:ALA:HB3	1:A:156:TYR:OH	0.61	1.95	6	2
1:A:108:VAL:HG21	1:A:202:TRP:CH2	0.61	2.30	10	2
1:A:114:ILE:HG21	1:A:181:PHE:CE1	0.61	2.30	3	4
1:A:167:LYS:O	1:A:171:ALA:HB3	0.61	1.95	16	2
1:A:86:LEU:HD13	1:A:102:PHE:HB3	0.60	1.74	9	3
1:A:134:ARG:O	1:A:137:VAL:HG22	0.60	1.96	14	5
1:A:177:ILE:HG21	1:A:194:TRP:CE2	0.60	2.31	11	7
1:A:104:LEU:HD23	1:A:105:LYS:O	0.59	1.97	10	3
1:A:76:THR:O	1:A:112:ILE:HG23	0.58	1.97	3	3
1:A:72:VAL:HG23	1:A:181:PHE:CD2	0.58	2.33	20	5
1:A:77:LEU:HD13	1:A:102:PHE:CE2	0.58	2.33	16	1
1:A:94:LEU:HD23	1:A:97:PHE:CE1	0.57	2.33	9	2
1:A:116:PHE:CD2	1:A:126:MET:HE1	0.57	2.34	11	9
1:A:69:ASN:ND2	1:A:70:VAL:HG23	0.57	2.13	1	3
1:A:76:THR:HG23	1:A:87:GLU:HG3	0.57	1.76	4	1
1:A:182:THR:HG22	1:A:188:ASP:CB	0.57	2.28	17	1
1:A:106:GLU:OE1	1:A:198:ILE:HG21	0.56	2.00	7	1
1:A:146:VAL:HG12	1:A:149:TYR:CE2	0.56	2.35	17	5
1:A:82:ALA:HB1	1:A:83:PRO:CD	0.56	2.31	12	7
1:A:113:LYS:CG	1:A:159:LEU:HD11	0.56	2.31	4	1
1:A:104:LEU:HD23	1:A:105:LYS:N	0.56	2.16	9	4
1:A:118:VAL:HG12	1:A:151:PRO:HA	0.56	1.77	19	3
1:A:132:THR:CG2	1:A:139:ILE:HD11	0.55	2.31	3	2
1:A:129:ILE:HD12	1:A:129:ILE:N	0.55	2.16	10	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:ARG:HG2	1:A:139:ILE:HD12	0.55	1.76	17	1
1:A:77:LEU:HD23	1:A:110:TYR:CD1	0.55	2.36	13	5
1:A:71:VAL:HG13	1:A:190:LEU:HD13	0.55	1.77	14	1
1:A:146:VAL:HG21	1:A:181:PHE:CE1	0.55	2.36	17	1
1:A:134:ARG:O	1:A:137:VAL:HG12	0.55	2.01	1	1
1:A:129:ILE:N	1:A:129:ILE:HD12	0.55	2.16	15	1
1:A:126:MET:SD	1:A:146:VAL:HG11	0.55	2.42	2	2
1:A:104:LEU:CG	1:A:196:LEU:HD11	0.55	2.31	1	1
1:A:170:LEU:C	1:A:170:LEU:HD13	0.54	2.22	10	1
1:A:72:VAL:CG1	1:A:90:LEU:HD12	0.54	2.32	20	1
1:A:122:ILE:HG23	1:A:149:TYR:O	0.54	2.03	1	2
1:A:70:VAL:HG12	1:A:70:VAL:O	0.54	2.02	8	2
1:A:104:LEU:CD2	1:A:108:VAL:HG22	0.54	2.23	10	1
1:A:104:LEU:HD22	1:A:202:TRP:CZ3	0.54	2.37	12	2
1:A:70:VAL:O	1:A:70:VAL:HG12	0.54	2.02	2	1
1:A:72:VAL:CG1	1:A:90:LEU:HD22	0.53	2.33	7	3
1:A:72:VAL:HG11	1:A:90:LEU:HD13	0.53	1.78	19	1
1:A:159:LEU:C	1:A:159:LEU:HD13	0.53	2.24	15	2
1:A:104:LEU:HD13	1:A:196:LEU:HD21	0.53	1.79	9	1
1:A:73:THR:HG21	1:A:155:GLU:OE1	0.53	2.03	16	1
1:A:72:VAL:CG1	1:A:90:LEU:HD13	0.53	2.33	10	10
1:A:135:LYS:O	1:A:137:VAL:HG23	0.53	2.04	18	2
1:A:78:VAL:HG22	1:A:85:PRO:HB3	0.52	1.81	12	2
1:A:170:LEU:N	1:A:170:LEU:HD22	0.52	2.19	1	1
1:A:132:THR:HG21	1:A:139:ILE:HD11	0.52	1.81	3	2
1:A:182:THR:HG22	1:A:188:ASP:HA	0.52	1.82	4	2
1:A:126:MET:HE2	1:A:181:PHE:CE2	0.52	2.40	14	2
1:A:72:VAL:HG12	1:A:90:LEU:HD13	0.52	1.80	10	3
1:A:90:LEU:HD21	1:A:192:TRP:CD2	0.52	2.40	9	4
1:A:123:VAL:HG13	1:A:183:ASP:HB2	0.52	1.81	4	1
1:A:134:ARG:HH11	1:A:139:ILE:HD12	0.52	1.65	4	1
1:A:146:VAL:HG13	1:A:158:PHE:HB2	0.52	1.82	10	3
1:A:177:ILE:CD1	1:A:196:LEU:HD23	0.52	2.35	6	1
1:A:86:LEU:HD13	1:A:102:PHE:CG	0.52	2.40	17	2
1:A:111:ARG:HD3	1:A:159:LEU:HD11	0.51	1.82	6	1
1:A:104:LEU:CD2	1:A:165:ALA:HB2	0.51	2.35	10	1
1:A:72:VAL:HG22	1:A:181:PHE:HD2	0.51	1.66	17	1
1:A:168:GLY:O	1:A:171:ALA:HB3	0.51	2.05	12	1
1:A:90:LEU:HD21	1:A:192:TRP:CE2	0.51	2.41	18	5
1:A:88:LEU:HD12	1:A:102:PHE:CE1	0.51	2.40	15	1
1:A:166:PRO:O	1:A:171:ALA:HB1	0.51	2.06	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:HG	1:A:114:ILE:HD13	0.51	1.81	13	4
1:A:153:ALA:HB1	1:A:156:TYR:OH	0.51	2.06	2	1
1:A:104:LEU:HD22	1:A:108:VAL:CG2	0.51	2.33	18	6
1:A:182:THR:HG22	1:A:188:ASP:CA	0.50	2.37	17	1
1:A:106:GLU:OE2	1:A:171:ALA:HB3	0.50	2.06	7	1
1:A:72:VAL:HG21	1:A:192:TRP:CZ3	0.50	2.40	8	2
1:A:128:TYR:CD1	1:A:181:PHE:CD2	0.50	2.98	9	1
1:A:72:VAL:HB	1:A:190:LEU:HD23	0.50	1.82	16	1
1:A:194:TRP:N	1:A:194:TRP:CD1	0.50	2.79	6	16
1:A:108:VAL:HG23	1:A:110:TYR:HD2	0.50	1.67	20	1
1:A:104:LEU:HD23	1:A:196:LEU:CD1	0.50	2.34	1	1
1:A:165:ALA:HB1	1:A:166:PRO:CD	0.50	2.36	13	4
1:A:159:LEU:O	1:A:159:LEU:HD13	0.50	2.06	15	1
1:A:116:PHE:CD2	1:A:181:PHE:CE2	0.50	3.00	8	1
1:A:190:LEU:HD13	1:A:191:SER:H	0.49	1.63	12	2
1:A:116:PHE:CD2	1:A:181:PHE:CZ	0.49	3.00	4	1
1:A:159:LEU:HD13	1:A:159:LEU:C	0.49	2.27	20	1
1:A:129:ILE:HG23	1:A:143:ASP:OD1	0.49	2.06	14	2
1:A:149:TYR:CD1	1:A:156:TYR:CE2	0.49	2.99	9	1
1:A:110:TYR:OH	1:A:196:LEU:HD21	0.49	2.08	3	1
1:A:114:ILE:HG21	1:A:181:PHE:CD2	0.49	2.43	1	1
1:A:104:LEU:CD1	1:A:196:LEU:HD21	0.49	2.38	17	2
1:A:75:LEU:C	1:A:75:LEU:HD23	0.49	2.29	7	7
1:A:105:LYS:HB3	1:A:108:VAL:HG11	0.49	1.84	15	5
1:A:149:TYR:CD1	1:A:156:TYR:CD1	0.49	3.01	2	1
1:A:76:THR:HG23	1:A:85:PRO:HB2	0.48	1.85	5	1
1:A:149:TYR:CE1	1:A:156:TYR:CD1	0.48	3.01	2	1
1:A:177:ILE:HD12	1:A:196:LEU:HD23	0.48	1.84	6	1
1:A:170:LEU:HD22	1:A:170:LEU:N	0.48	2.22	16	1
1:A:127:LYS:HE2	1:A:182:THR:HG23	0.48	1.84	6	1
1:A:170:LEU:HD23	1:A:170:LEU:O	0.48	2.08	12	2
1:A:102:PHE:HB3	1:A:196:LEU:HD12	0.48	1.84	10	2
1:A:88:LEU:HD21	1:A:97:PHE:CD1	0.48	2.44	3	2
1:A:132:THR:HG22	1:A:139:ILE:HD11	0.48	1.85	7	1
1:A:75:LEU:HD23	1:A:75:LEU:C	0.48	2.29	6	4
1:A:73:THR:HG21	1:A:155:GLU:HG2	0.48	1.84	7	1
1:A:70:VAL:CG2	1:A:118:VAL:HG22	0.48	2.34	16	2
1:A:156:TYR:N	1:A:156:TYR:CD1	0.48	2.82	5	4
1:A:146:VAL:HG22	1:A:158:PHE:CE2	0.48	2.44	12	1
1:A:149:TYR:CD1	1:A:156:TYR:CD2	0.48	3.01	9	2
1:A:139:ILE:HD12	1:A:140:ASP:OD2	0.48	2.08	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:VAL:HG11	1:A:126:MET:SD	0.47	2.48	9	1
1:A:104:LEU:HD23	1:A:105:LYS:H	0.47	1.68	6	1
1:A:116:PHE:CD1	1:A:116:PHE:N	0.47	2.82	10	4
1:A:104:LEU:HG	1:A:196:LEU:HD11	0.47	1.87	1	1
1:A:182:THR:HG22	1:A:188:ASP:HB3	0.47	1.86	17	1
1:A:139:ILE:HG22	1:A:140:ASP:OD2	0.47	2.10	17	2
1:A:116:PHE:CD2	1:A:126:MET:CE	0.47	2.98	2	13
1:A:146:VAL:HG12	1:A:149:TYR:CZ	0.47	2.44	15	2
1:A:88:LEU:HD23	1:A:89:ASP:N	0.47	2.24	15	2
1:A:131:HIS:CD2	1:A:131:HIS:N	0.47	2.83	16	6
1:A:88:LEU:CD2	1:A:97:PHE:CE1	0.47	2.98	19	7
1:A:104:LEU:CD2	1:A:202:TRP:CZ3	0.46	2.99	14	5
1:A:116:PHE:CZ	1:A:156:TYR:CB	0.46	2.99	7	2
1:A:82:ALA:CB	1:A:202:TRP:CH2	0.46	2.99	16	11
1:A:126:MET:CE	1:A:181:PHE:CE2	0.46	2.99	10	8
1:A:108:VAL:O	1:A:108:VAL:HG23	0.46	2.09	13	3
1:A:70:VAL:HG11	1:A:126:MET:CE	0.46	2.39	18	1
1:A:90:LEU:HA	1:A:94:LEU:HD21	0.46	1.85	20	2
1:A:72:VAL:HG11	1:A:90:LEU:HD12	0.46	1.87	20	1
1:A:105:LYS:CG	1:A:202:TRP:CE2	0.46	2.98	1	1
1:A:153:ALA:CB	1:A:156:TYR:CZ	0.46	2.99	11	2
1:A:72:VAL:CG2	1:A:181:PHE:CG	0.46	2.99	6	8
1:A:104:LEU:HB3	1:A:108:VAL:HG21	0.46	1.87	12	1
1:A:104:LEU:HB2	1:A:198:ILE:HD13	0.46	1.86	2	1
1:A:116:PHE:CD1	1:A:126:MET:CE	0.46	2.99	4	2
1:A:72:VAL:CG2	1:A:181:PHE:CD2	0.46	2.99	14	10
1:A:134:ARG:NH1	1:A:139:ILE:HD12	0.46	2.24	4	1
1:A:105:LYS:CB	1:A:108:VAL:HG13	0.46	2.40	1	1
1:A:170:LEU:N	1:A:170:LEU:CD2	0.46	2.79	1	1
1:A:77:LEU:HD21	1:A:112:ILE:CD1	0.46	2.41	17	1
1:A:132:THR:O	1:A:139:ILE:HD13	0.46	2.11	7	1
1:A:131:HIS:CE1	1:A:141:LYS:CD	0.46	2.99	16	1
1:A:194:TRP:CD1	1:A:194:TRP:N	0.46	2.84	16	2
1:A:131:HIS:N	1:A:131:HIS:CD2	0.45	2.84	10	7
1:A:134:ARG:NE	1:A:175:TYR:CE2	0.45	2.84	2	1
1:A:116:PHE:N	1:A:116:PHE:CD1	0.45	2.85	9	5
1:A:134:ARG:NH2	1:A:139:ILE:HD11	0.45	2.26	17	1
1:A:86:LEU:CD2	1:A:102:PHE:CD1	0.45	2.99	11	1
1:A:113:LYS:HG3	1:A:159:LEU:HD11	0.45	1.88	4	1
1:A:133:TYR:CZ	1:A:138:LYS:CG	0.45	3.00	1	1
1:A:88:LEU:CD1	1:A:102:PHE:CE1	0.45	3.00	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:TYR:HE1	1:A:112:ILE:HD11	0.45	1.71	17	1
1:A:158:PHE:CE2	1:A:160:THR:CG2	0.45	3.00	20	1
1:A:86:LEU:HD13	1:A:102:PHE:CB	0.45	2.42	7	3
1:A:116:PHE:CE1	1:A:126:MET:CE	0.45	2.99	8	2
1:A:116:PHE:CG	1:A:126:MET:HE1	0.45	2.47	16	5
1:A:123:VAL:HG12	1:A:123:VAL:O	0.45	2.12	19	1
1:A:86:LEU:CB	1:A:102:PHE:CE2	0.45	3.00	10	2
1:A:94:LEU:HD13	1:A:97:PHE:CE2	0.45	2.47	4	1
1:A:108:VAL:H	1:A:165:ALA:HB3	0.45	1.71	2	1
1:A:73:THR:HG23	1:A:116:PHE:CA	0.44	2.38	19	1
1:A:73:THR:HG21	1:A:117:ARG:HG3	0.44	1.89	20	1
1:A:158:PHE:CE2	1:A:160:THR:HG22	0.44	2.47	17	3
1:A:110:TYR:CE1	1:A:112:ILE:HD11	0.44	2.47	17	1
1:A:72:VAL:HG23	1:A:181:PHE:CG	0.44	2.48	20	1
1:A:75:LEU:HD12	1:A:114:ILE:CD1	0.44	2.43	18	1
1:A:105:LYS:CB	1:A:108:VAL:CG1	0.44	2.96	14	4
1:A:126:MET:CE	1:A:181:PHE:CZ	0.44	3.00	20	3
1:A:170:LEU:CD2	1:A:170:LEU:N	0.44	2.79	16	1
1:A:169:MET:O	1:A:171:ALA:N	0.44	2.51	20	2
1:A:113:LYS:NZ	1:A:159:LEU:HD21	0.44	2.27	3	1
1:A:86:LEU:HD13	1:A:102:PHE:CD1	0.44	2.48	14	2
1:A:94:LEU:HD11	1:A:192:TRP:CB	0.44	2.43	4	1
1:A:90:LEU:CD2	1:A:192:TRP:CD2	0.44	3.01	17	4
1:A:132:THR:O	1:A:139:ILE:HD12	0.44	2.13	18	1
1:A:126:MET:HE3	1:A:181:PHE:CE2	0.44	2.48	10	1
1:A:110:TYR:CE1	1:A:165:ALA:HB2	0.43	2.48	15	1
1:A:75:LEU:HD21	1:A:112:ILE:HG23	0.43	1.90	16	1
1:A:146:VAL:HG21	1:A:181:PHE:HZ	0.43	1.64	11	1
1:A:110:TYR:HE1	1:A:165:ALA:HB2	0.43	1.73	15	1
1:A:90:LEU:HD21	1:A:192:TRP:CD1	0.43	2.49	5	1
1:A:134:ARG:HB3	1:A:139:ILE:HD11	0.43	1.88	14	1
1:A:131:HIS:CE1	1:A:141:LYS:CE	0.43	3.01	20	1
1:A:110:TYR:CD1	1:A:110:TYR:N	0.43	2.86	2	1
1:A:110:TYR:CD1	1:A:110:TYR:C	0.43	2.91	9	3
1:A:102:PHE:CB	1:A:196:LEU:HD12	0.43	2.44	13	4
1:A:194:TRP:CZ3	1:A:196:LEU:HD13	0.43	2.48	13	2
1:A:104:LEU:HD21	1:A:202:TRP:CH2	0.43	2.49	8	1
1:A:104:LEU:HD12	1:A:110:TYR:OH	0.43	2.14	3	1
1:A:123:VAL:HG11	1:A:189:HIS:NE2	0.43	2.28	2	1
1:A:73:THR:HG21	1:A:117:ARG:CG	0.43	2.43	10	1
1:A:94:LEU:O	1:A:97:PHE:CD2	0.43	2.72	17	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:VAL:CG1	1:A:126:MET:CE	0.43	2.97	9	1
1:A:105:LYS:O	1:A:106:GLU:C	0.42	2.58	6	2
1:A:89:ASP:O	1:A:97:PHE:CZ	0.42	2.72	20	4
1:A:88:LEU:HD23	1:A:97:PHE:CZ	0.42	2.48	20	1
1:A:105:LYS:HB2	1:A:202:TRP:CD1	0.42	2.49	12	3
1:A:148:SER:O	1:A:149:TYR:CD1	0.42	2.72	5	4
1:A:129:ILE:HD13	1:A:180:ARG:NE	0.42	2.29	10	1
1:A:129:ILE:HG22	1:A:130:GLN:N	0.42	2.28	12	4
1:A:116:PHE:CE2	1:A:181:PHE:CZ	0.42	3.07	8	1
1:A:134:ARG:CG	1:A:139:ILE:HD12	0.42	2.45	17	1
1:A:146:VAL:CG1	1:A:149:TYR:CE1	0.42	2.99	8	2
1:A:90:LEU:CD2	1:A:192:TRP:CE2	0.42	3.03	19	1
1:A:78:VAL:HG12	1:A:79:CYS:N	0.42	2.29	13	10
1:A:105:LYS:HB3	1:A:108:VAL:HG13	0.42	1.91	5	1
1:A:104:LEU:CB	1:A:198:ILE:HD13	0.42	2.45	4	1
1:A:89:ASP:O	1:A:97:PHE:CE1	0.42	2.73	13	5
1:A:146:VAL:CG1	1:A:149:TYR:CZ	0.42	3.03	8	1
1:A:112:ILE:HG22	1:A:113:LYS:N	0.42	2.30	4	1
1:A:177:ILE:HD12	1:A:194:TRP:CZ2	0.42	2.50	9	1
1:A:153:ALA:CB	1:A:156:TYR:CE2	0.42	3.01	7	1
1:A:128:TYR:CE1	1:A:179:SER:OG	0.42	2.72	17	1
1:A:69:ASN:CB	1:A:120:ARG:CB	0.42	2.98	1	2
1:A:70:VAL:HG11	1:A:126:MET:HE2	0.42	1.92	6	1
1:A:194:TRP:CZ3	1:A:196:LEU:CD2	0.42	2.99	6	1
1:A:79:CYS:HB2	1:A:82:ALA:HB3	0.42	1.92	15	1
1:A:104:LEU:CD1	1:A:110:TYR:CZ	0.42	3.03	3	1
1:A:137:VAL:HG12	1:A:138:LYS:N	0.42	2.30	3	1
1:A:170:LEU:O	1:A:170:LEU:HD22	0.41	2.14	10	1
1:A:171:ALA:O	1:A:175:TYR:CE1	0.41	2.74	13	1
1:A:110:TYR:CE2	1:A:163:GLU:O	0.41	2.74	16	6
1:A:110:TYR:CD1	1:A:110:TYR:O	0.41	2.74	14	5
1:A:130:GLN:CG	1:A:177:ILE:CG2	0.41	2.99	16	2
1:A:79:CYS:HB3	1:A:82:ALA:HB2	0.41	1.92	4	1
1:A:77:LEU:CD2	1:A:110:TYR:CD1	0.41	3.04	19	1
1:A:122:ILE:HG22	1:A:123:VAL:N	0.41	2.31	19	1
1:A:170:LEU:C	1:A:170:LEU:HD23	0.41	2.36	12	1
1:A:129:ILE:HD13	1:A:180:ARG:CD	0.41	2.46	10	1
1:A:110:TYR:HE2	1:A:165:ALA:HB2	0.41	1.76	6	1
1:A:94:LEU:CD2	1:A:97:PHE:CE1	0.41	3.02	9	1
1:A:146:VAL:HG13	1:A:158:PHE:CB	0.41	2.45	14	1
1:A:134:ARG:CG	1:A:139:ILE:HD11	0.41	2.46	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:PHE:CD1	1:A:126:MET:HE1	0.41	2.51	6	1
1:A:139:ILE:HG22	1:A:140:ASP:CG	0.41	2.36	17	1
1:A:116:PHE:CE1	1:A:126:MET:HE3	0.41	2.51	15	1
1:A:183:ASP:OD1	1:A:189:HIS:CD2	0.41	2.74	3	2
1:A:72:VAL:CG2	1:A:181:PHE:CB	0.41	2.99	12	3
1:A:167:LYS:O	1:A:171:ALA:HB2	0.41	2.14	9	1
1:A:181:PHE:O	1:A:189:HIS:CD2	0.41	2.74	11	2
1:A:116:PHE:O	1:A:156:TYR:N	0.41	2.54	6	1
1:A:146:VAL:O	1:A:158:PHE:CE1	0.41	2.74	17	2
1:A:202:TRP:N	1:A:202:TRP:CD1	0.41	2.89	13	2
1:A:116:PHE:CE1	1:A:156:TYR:O	0.41	2.74	12	1
1:A:97:PHE:CE2	1:A:192:TRP:CD1	0.41	3.08	15	1
1:A:145:MET:O	1:A:158:PHE:CZ	0.41	2.74	10	1
1:A:127:LYS:HA	1:A:146:VAL:HG23	0.41	1.91	11	1
1:A:147:GLY:O	1:A:149:TYR:CE2	0.41	2.74	11	3
1:A:86:LEU:HB3	1:A:102:PHE:CE2	0.41	2.51	16	3
1:A:69:ASN:HD22	1:A:70:VAL:HG23	0.41	1.75	8	1
1:A:104:LEU:CD2	1:A:165:ALA:CB	0.41	2.99	10	1
1:A:133:TYR:CE1	1:A:138:LYS:CG	0.41	3.03	1	1
1:A:181:PHE:C	1:A:182:THR:HG23	0.40	2.37	18	1
1:A:133:TYR:CE1	1:A:138:LYS:HG2	0.40	2.52	1	1
1:A:97:PHE:CD1	1:A:97:PHE:N	0.40	2.87	19	1
1:A:116:PHE:O	1:A:116:PHE:CD1	0.40	2.74	6	1
1:A:114:ILE:HG21	1:A:181:PHE:HE2	0.40	1.67	15	2
1:A:154:GLU:O	1:A:156:TYR:CE1	0.40	2.74	9	1
1:A:131:HIS:ND1	1:A:141:LYS:CB	0.40	2.84	11	1
1:A:131:HIS:CG	1:A:141:LYS:HB2	0.40	2.51	3	1
1:A:88:LEU:HD12	1:A:102:PHE:HE2	0.40	1.76	20	1
1:A:149:TYR:CD1	1:A:156:TYR:CG	0.40	3.10	2	1
1:A:116:PHE:CE1	1:A:149:TYR:CE2	0.40	3.09	1	1
1:A:146:VAL:HG22	1:A:158:PHE:CZ	0.40	2.51	12	1
1:A:106:GLU:CB	1:A:168:GLY:N	0.40	2.84	20	1
1:A:106:GLU:CG	1:A:172:ARG:NH1	0.40	2.84	4	1
1:A:116:PHE:CD1	1:A:116:PHE:O	0.40	2.74	16	1
1:A:72:VAL:HG22	1:A:181:PHE:CG	0.40	2.51	19	1
1:A:177:ILE:HD12	1:A:194:TRP:CH2	0.40	2.51	17	1
1:A:97:PHE:N	1:A:97:PHE:CD1	0.40	2.87	3	1
1:A:86:LEU:HD22	1:A:102:PHE:CE1	0.40	2.51	14	1
1:A:90:LEU:HD21	1:A:192:TRP:NE1	0.40	2.32	19	1
1:A:80:SER:OG	1:A:81:THR:N	0.40	2.55	17	1
1:A:104:LEU:CD2	1:A:202:TRP:CH2	0.40	3.04	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:LYS:CG	1:A:159:LEU:CD1	0.40	3.00	4	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	132/145 (91%)	102±3 (77±3%)	27±3 (20±3%)	4±2 (3±1%)	10	45
All	All	2640/2900 (91%)	2031 (77%)	538 (20%)	71 (3%)	10	45

All 23 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	106	GLU	11
1	A	125	GLY	9
1	A	153	ALA	8
1	A	152	ARG	6
1	A	80	SER	4
1	A	135	LYS	3
1	A	93	ASP	3
1	A	203	LYS	3
1	A	92	GLY	3
1	A	124	SER	2
1	A	162	MET	2
1	A	108	VAL	2
1	A	169	MET	2
1	A	69	ASN	2
1	A	156	TYR	2
1	A	79	CYS	2
1	A	154	GLU	1
1	A	151	PRO	1
1	A	82	ALA	1
1	A	137	VAL	1
1	A	166	PRO	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	167	LYS	1
1	A	168	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	120/130 (92%)	103±3 (86±3%)	17±3 (14±3%)	8 48
All	All	2400/2600 (92%)	2056 (86%)	344 (14%)	8 48

All 65 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	202	TRP	20
1	A	141	LYS	15
1	A	120	ARG	13
1	A	138	LYS	13
1	A	159	LEU	12
1	A	126	MET	11
1	A	77	LEU	10
1	A	200	LYS	10
1	A	135	LYS	9
1	A	203	LYS	9
1	A	180	ARG	8
1	A	90	LEU	8
1	A	181	PHE	8
1	A	79	CYS	8
1	A	170	LEU	8
1	A	155	GLU	7
1	A	178	LYS	7
1	A	162	MET	7
1	A	117	ARG	7
1	A	127	LYS	6
1	A	152	ARG	6
1	A	96	SER	6
1	A	111	ARG	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	88	LEU	6
1	A	167	LYS	6
1	A	104	LEU	5
1	A	80	SER	5
1	A	145	MET	5
1	A	134	ARG	5
1	A	105	LYS	5
1	A	113	LYS	5
1	A	94	LEU	5
1	A	98	LYS	4
1	A	119	ASN	4
1	A	140	ASP	4
1	A	164	GLU	4
1	A	169	MET	4
1	A	199	LYS	4
1	A	176	ASN	4
1	A	89	ASP	4
1	A	100	GLN	4
1	A	109	GLU	4
1	A	95	GLU	4
1	A	172	ARG	4
1	A	115	SER	3
1	A	69	ASN	3
1	A	99	LYS	3
1	A	157	GLU	3
1	A	124	SER	2
1	A	201	GLU	2
1	A	193	GLU	2
1	A	93	ASP	2
1	A	121	GLU	2
1	A	75	LEU	2
1	A	196	LEU	1
1	A	143	ASP	1
1	A	116	PHE	1
1	A	106	GLU	1
1	A	110	TYR	1
1	A	101	SER	1
1	A	204	ASP	1
1	A	74	ARG	1
1	A	132	THR	1
1	A	139	ILE	1
1	A	163	GLU	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

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