WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Dec 13, 2023 – 11:26 PM EST

PDB ID	:	2JPB
Title	:	Solution Structure of OMPR-C DNA Binding Protein
Authors	:	Liao, X.; Kenney, L.; Liao, W.; Integrated Center for Structure and Function Innovation (ISFI)
Deposited on	:	2007-05-03

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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

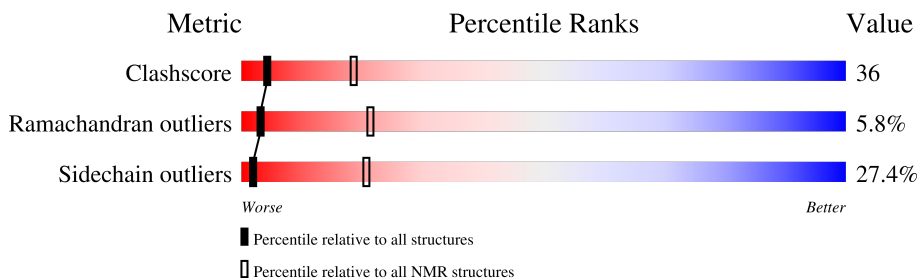|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Clashscore		36
Ramachandran outliers		5.8%
Sidechain outliers		27.4%

Worse ... *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	104	19% 56% 5% 20%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 12 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:137-A:188, A:200-A:214, A:219-A:234 (83)	0.84	12

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 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1530 atoms, of which 696 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcriptional regulatory protein ompR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	104	1530	529	696	151	149	5	0

4 Residue-property plots ⓘ

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.

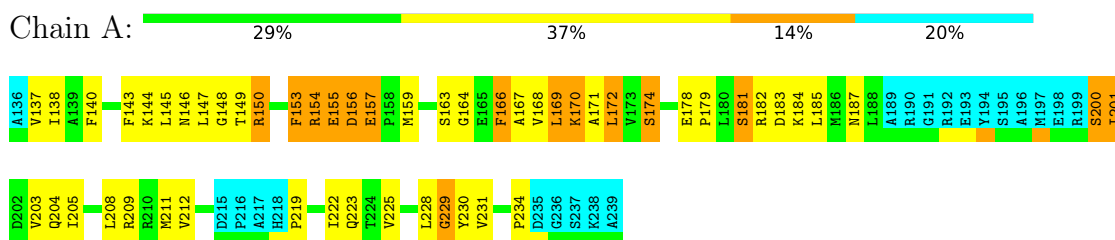• Molecule 1: Transcriptional regulatory protein ompR
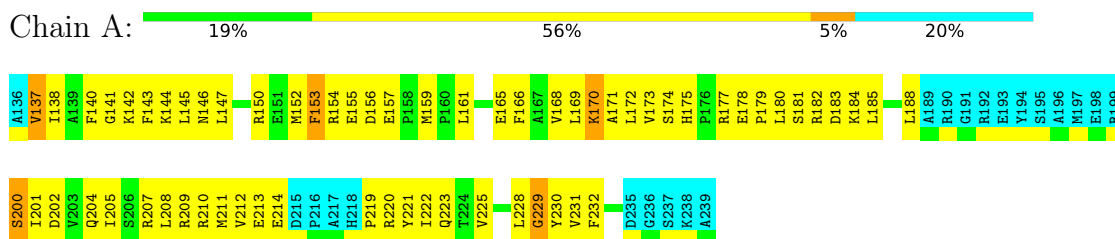
4.2 Scores per residue for each member of the ensemble
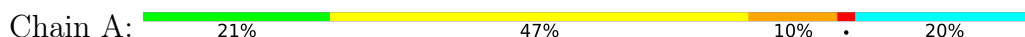
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Transcriptional regulatory protein ompR

4.2.2 Score per residue for model 2

• Molecule 1: Transcriptional regulatory protein ompR

4.2.3 Score per residue for model 3

• Molecule 1: Transcriptional regulatory protein ompR

4.2.4 Score per residue for model 4

• Molecule 1: Transcriptional regulatory protein ompR

4.2.5 Score per residue for model 5

• Molecule 1: Transcriptional regulatory protein ompR

4.2.6 Score per residue for model 6

• Molecule 1: Transcriptional regulatory protein ompR

Chain A:

4.2.7　Score per residue for model 7

• Molecule 1: Transcriptional regulatory protein ompR

Chain A:

4.2.8　Score per residue for model 8

• Molecule 1: Transcriptional regulatory protein ompR

Chain A:
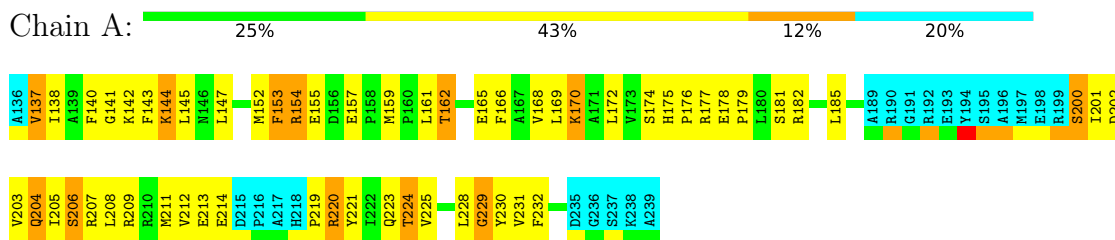
4.2.9　Score per residue for model 9

• Molecule 1: Transcriptional regulatory protein ompR

Chain A:
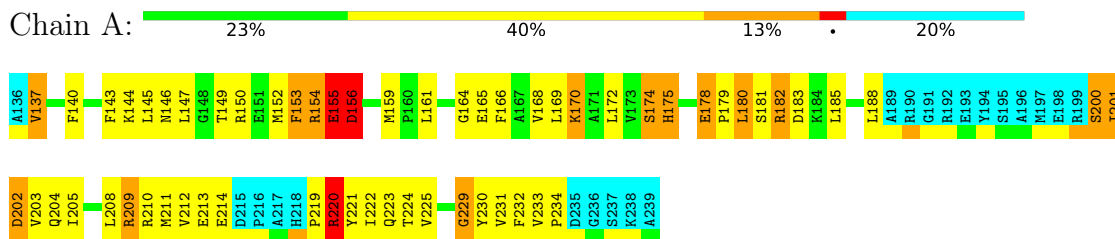
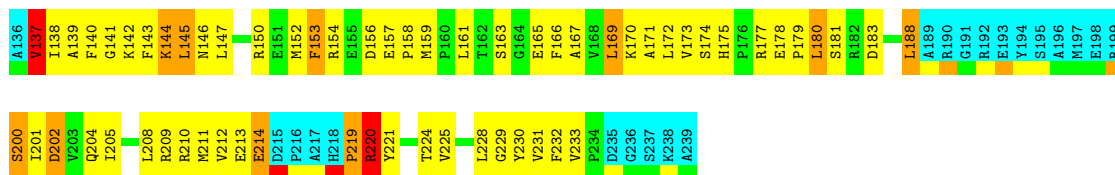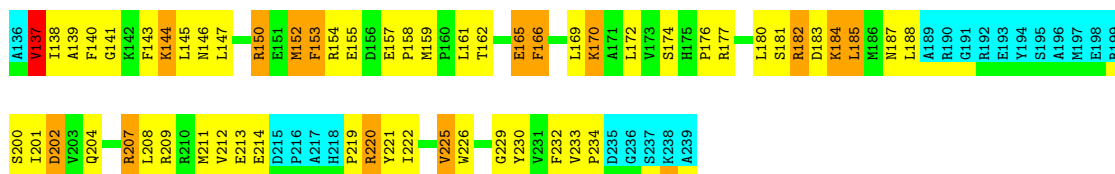### 4.2.10 Score per residue for model 10

• Molecule 1: Transcriptional regulatory protein ompR
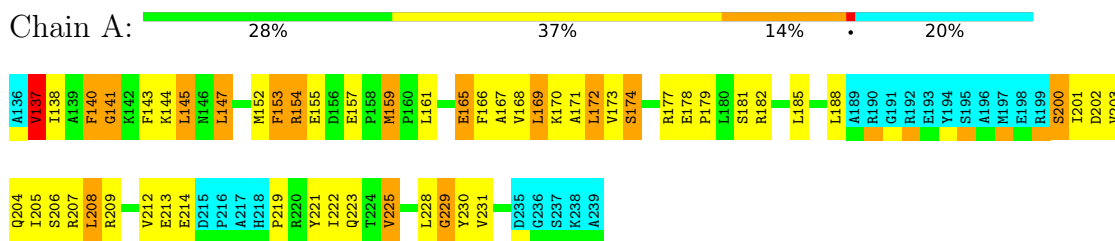
4.2.11 Score per residue for model 11

• Molecule 1: Transcriptional regulatory protein ompR
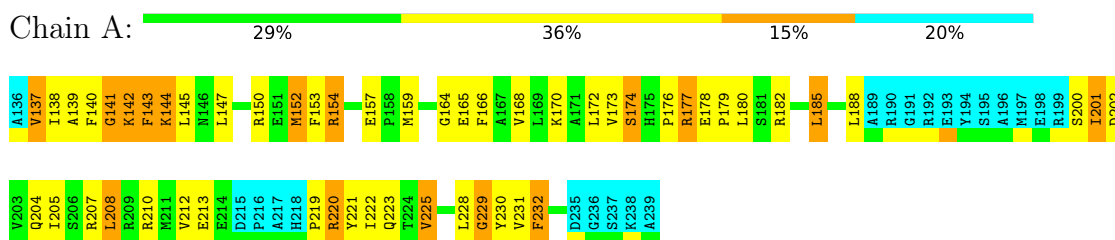
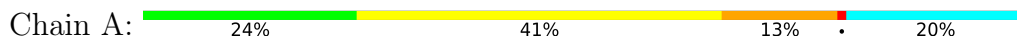### 4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: Transcriptional regulatory protein ompR
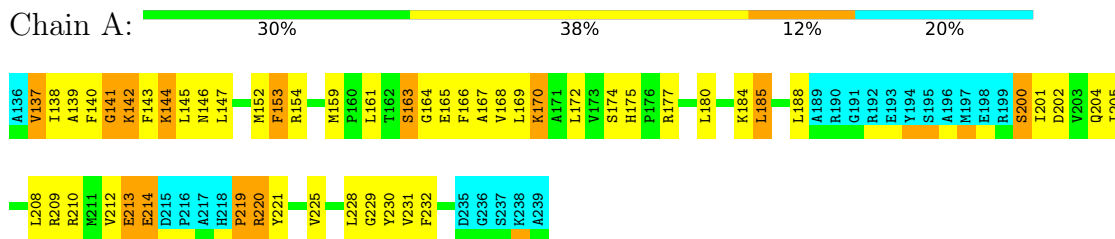
4.2.13 Score per residue for model 13

• Molecule 1: Transcriptional regulatory protein ompR
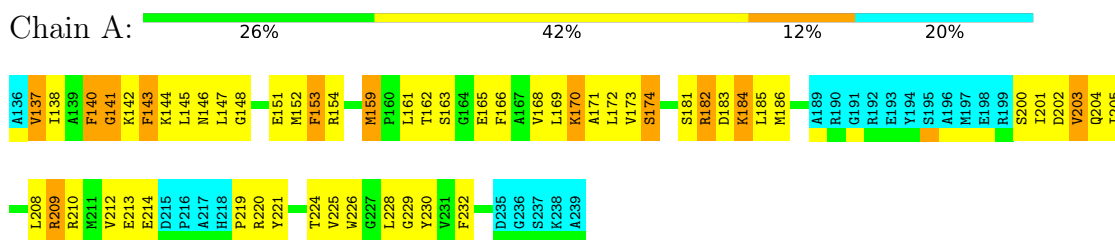
4.2.14 Score per residue for model 14

• Molecule 1: Transcriptional regulatory protein ompR
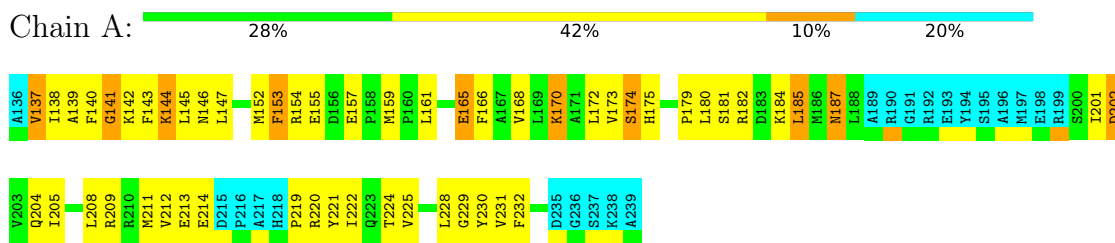
4.2.15 Score per residue for model 15
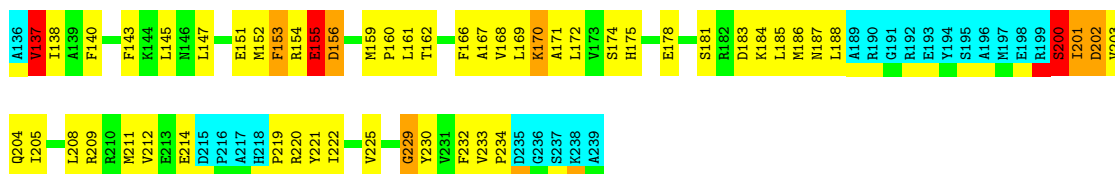
• Molecule 1: Transcriptional regulatory protein ompR
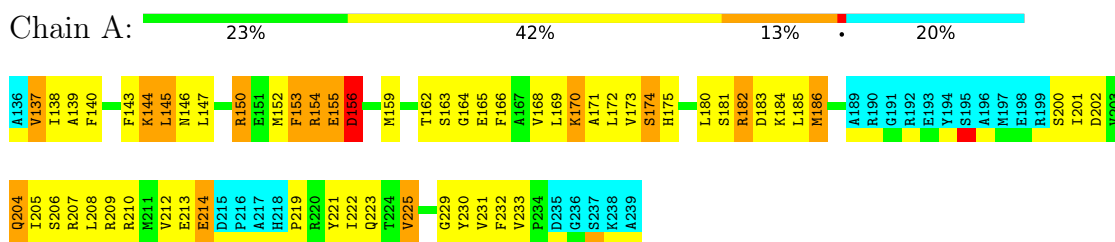
4.2.16 Score per residue for model 16

• Molecule 1: Transcriptional regulatory protein ompR
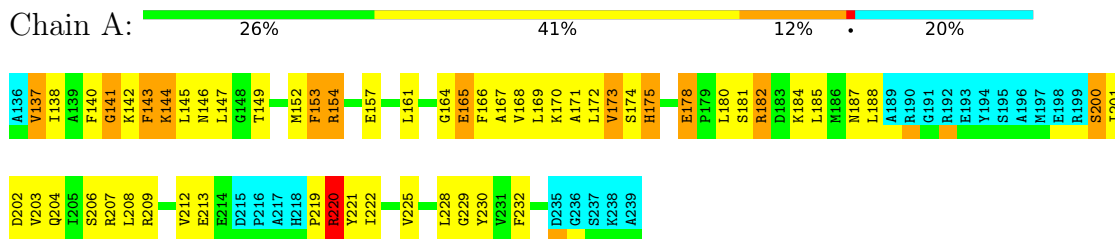
4.2.17 Score per residue for model 17

• Molecule 1: Transcriptional regulatory protein ompR
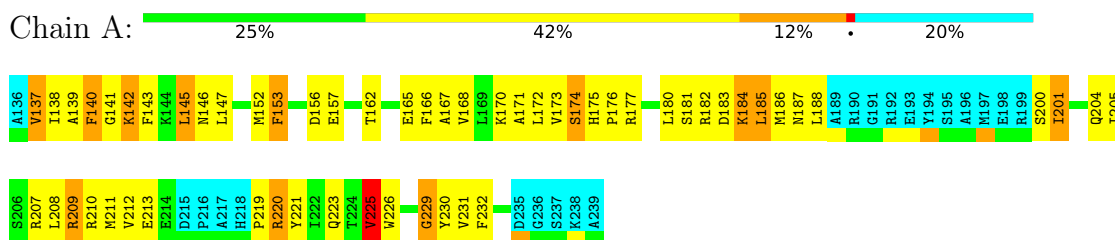
4.2.18　Score per residue for model 18

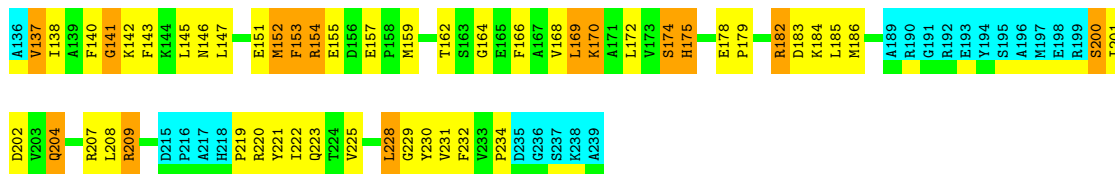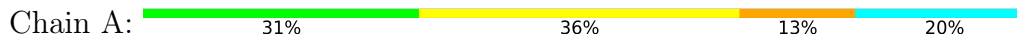• Molecule 1: Transcriptional regulatory protein ompR
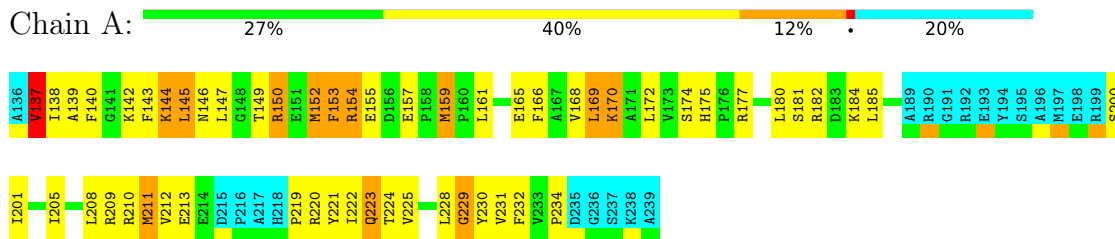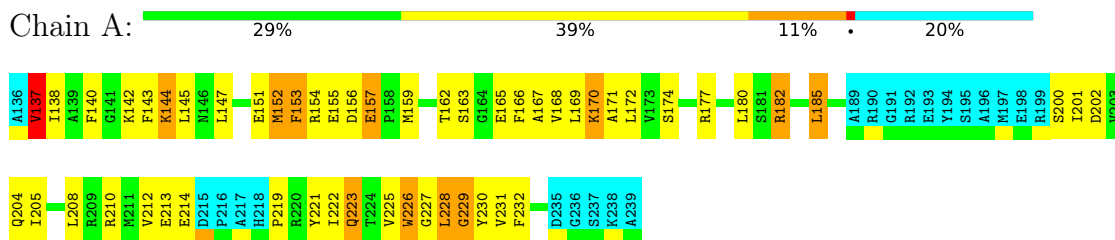
Chain A:
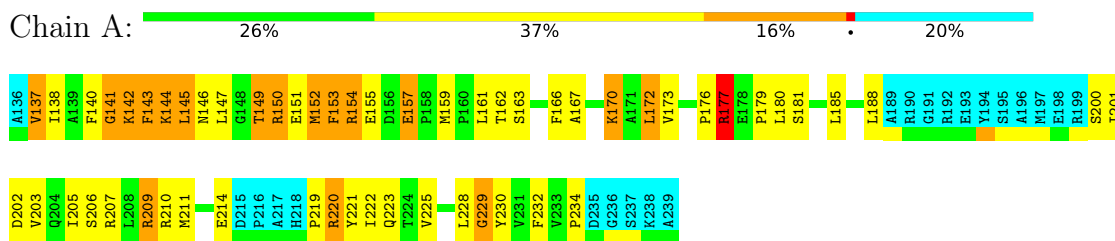
4.2.19　Score per residue for model 19

• Molecule 1: Transcriptional regulatory protein ompR

Chain A:
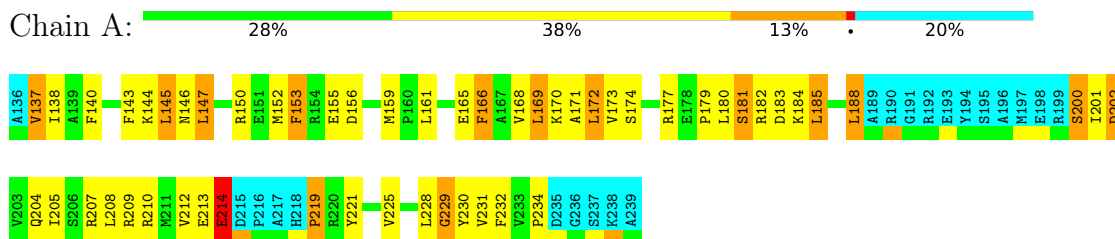
4.2.20　Score per residue for model 20

• Molecule 1: Transcriptional regulatory protein ompR

Chain A:
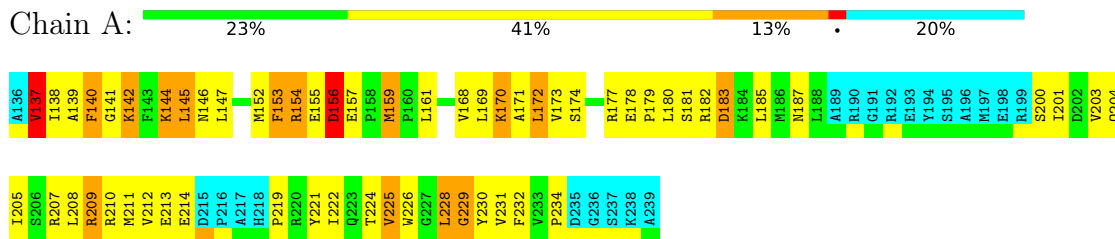
5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
DYANA	structure solution	
DYANA	refinement	

No chemical shift data was provided.

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	676	579	698	49±8
All	All	13520	11580	13960	985

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:145:LEU:HD21	1:A:147:LEU:CD1	0.97	1.90	6	3
1:A:147:LEU:HD22	1:A:166:PHE:CE1	0.94	1.96	1	1
1:A:147:LEU:HD22	1:A:166:PHE:CD1	0.90	2.02	1	1
1:A:169:LEU:HD22	1:A:169:LEU:O	0.89	1.65	10	1
1:A:140:PHE:CZ	1:A:143:PHE:CD1	0.84	2.66	19	1
1:A:169:LEU:HD12	1:A:208:LEU:HD22	0.83	1.49	20	1
1:A:147:LEU:HD13	1:A:170:LYS:HG3	0.82	1.49	8	6
1:A:169:LEU:HD23	1:A:208:LEU:HD22	0.82	1.50	5	1
1:A:164:GLY:O	1:A:168:VAL:HG23	0.82	1.74	16	7
1:A:137:VAL:O	1:A:138:ILE:HD13	0.81	1.75	17	1
1:A:179:PRO:CG	1:A:228:LEU:HD13	0.80	2.07	14	3
1:A:179:PRO:CB	1:A:228:LEU:HD13	0.79	2.07	8	4
1:A:140:PHE:CE2	1:A:143:PHE:CD1	0.79	2.70	19	1
1:A:147:LEU:HD13	1:A:170:LYS:CG	0.78	2.09	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:140:PHE:CZ	1:A:143:PHE:CG	0.76	2.73	19	1
1:A:205:ILE:HD12	1:A:222:ILE:CG2	0.76	2.11	14	1
1:A:147:LEU:HD13	1:A:170:LYS:HG2	0.76	1.58	12	5
1:A:212:VAL:HG23	1:A:213:GLU:HG2	0.76	1.56	9	9
1:A:140:PHE:CE2	1:A:143:PHE:CG	0.73	2.75	8	2
1:A:137:VAL:C	1:A:138:ILE:HD12	0.72	2.05	4	4
1:A:185:LEU:HD23	1:A:201:ILE:HD12	0.71	1.59	12	1
1:A:145:LEU:C	1:A:145:LEU:HD23	0.71	2.06	6	2
1:A:168:VAL:HG22	1:A:201:ILE:HD13	0.71	1.61	15	2
1:A:140:PHE:CD2	1:A:221:TYR:CE2	0.71	2.77	5	2
1:A:145:LEU:HD12	1:A:146:ASN:N	0.71	2.00	17	2
1:A:223:GLN:O	1:A:231:VAL:HG12	0.70	1.85	1	9
1:A:145:LEU:HD12	1:A:146:ASN:H	0.70	1.46	17	3
1:A:138:ILE:HG13	1:A:173:VAL:HG21	0.70	1.63	18	1
1:A:153:PHE:CD1	1:A:153:PHE:N	0.70	2.60	10	9
1:A:165:GLU:HG2	1:A:208:LEU:HD21	0.69	1.64	2	2
1:A:145:LEU:HD12	1:A:152:MET:HG3	0.69	1.63	9	2
1:A:205:ILE:HD12	1:A:222:ILE:HG21	0.69	1.64	14	1
1:A:208:LEU:O	1:A:212:VAL:HG22	0.69	1.88	3	10
1:A:140:PHE:N	1:A:140:PHE:CD1	0.68	2.62	10	9
1:A:204:GLN:O	1:A:208:LEU:HD23	0.68	1.87	11	2
1:A:152:MET:HE1	1:A:212:VAL:HG12	0.67	1.66	10	1
1:A:140:PHE:CE2	1:A:143:PHE:CD2	0.67	2.83	5	2
1:A:169:LEU:C	1:A:169:LEU:HD13	0.67	2.10	7	1
1:A:179:PRO:C	1:A:180:LEU:HD22	0.67	2.10	18	1
1:A:224:THR:HG23	1:A:230:TYR:CD1	0.67	2.25	9	3
1:A:172:LEU:HD11	1:A:205:ILE:HD11	0.67	1.66	10	1
1:A:221:TYR:O	1:A:222:ILE:HD13	0.66	1.90	16	6
1:A:165:GLU:HB3	1:A:208:LEU:HD21	0.66	1.67	6	4
1:A:145:LEU:HD12	1:A:152:MET:SD	0.66	2.31	14	5
1:A:137:VAL:HG12	1:A:146:ASN:CG	0.66	2.11	16	9
1:A:137:VAL:HG23	1:A:138:ILE:N	0.66	2.06	19	11
1:A:152:MET:SD	1:A:161:LEU:HD11	0.66	2.30	2	2
1:A:145:LEU:HD21	1:A:147:LEU:HD12	0.66	1.67	6	2
1:A:145:LEU:HD21	1:A:147:LEU:CD2	0.65	2.21	13	2
1:A:145:LEU:HD23	1:A:146:ASN:N	0.65	2.06	6	3
1:A:201:ILE:CG2	1:A:230:TYR:CE2	0.65	2.79	10	7
1:A:181:SER:O	1:A:185:LEU:HD23	0.65	1.90	1	1
1:A:138:ILE:HG12	1:A:173:VAL:HG21	0.65	1.68	16	1
1:A:161:LEU:HD22	1:A:208:LEU:HD22	0.64	1.68	4	1
1:A:172:LEU:HD11	1:A:205:ILE:CD1	0.64	2.23	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:HD12	1:A:138:ILE:N	0.63	2.08	16	2
1:A:145:LEU:HD21	1:A:147:LEU:HD11	0.63	1.70	19	2
1:A:224:THR:HG23	1:A:230:TYR:CE1	0.63	2.28	20	3
1:A:209:ARG:HH21	1:A:212:VAL:HG21	0.63	1.53	14	1
1:A:142:LYS:C	1:A:143:PHE:CD1	0.63	2.72	13	4
1:A:172:LEU:HD22	1:A:232:PHE:HB2	0.62	1.70	16	3
1:A:180:LEU:O	1:A:185:LEU:HD13	0.62	1.95	12	1
1:A:179:PRO:HG3	1:A:228:LEU:HD13	0.62	1.72	14	1
1:A:201:ILE:HG21	1:A:230:TYR:CE2	0.62	2.29	10	3
1:A:208:LEU:C	1:A:208:LEU:HD12	0.62	2.14	10	1
1:A:179:PRO:HB2	1:A:228:LEU:HD13	0.62	1.72	8	1
1:A:169:LEU:O	1:A:173:VAL:HG23	0.62	1.95	15	1
1:A:168:VAL:HG11	1:A:204:GLN:HB3	0.61	1.72	8	1
1:A:229:GLY:C	1:A:230:TYR:CD1	0.61	2.74	12	8
1:A:143:PHE:CD1	1:A:143:PHE:N	0.61	2.68	18	6
1:A:165:GLU:CG	1:A:208:LEU:HD21	0.61	2.25	3	4
1:A:180:LEU:HD22	1:A:184:LYS:HG3	0.60	1.73	16	1
1:A:201:ILE:HG22	1:A:230:TYR:CE2	0.60	2.32	6	9
1:A:145:LEU:HD13	1:A:152:MET:CE	0.60	2.26	10	1
1:A:168:VAL:HG13	1:A:185:LEU:CD2	0.60	2.25	5	2
1:A:181:SER:O	1:A:185:LEU:HD12	0.60	1.97	6	5
1:A:143:PHE:CE1	1:A:212:VAL:O	0.60	2.54	8	2
1:A:221:TYR:O	1:A:232:PHE:CE2	0.60	2.55	2	1
1:A:221:TYR:O	1:A:232:PHE:CE1	0.60	2.55	20	2
1:A:143:PHE:CE2	1:A:212:VAL:O	0.60	2.55	12	4
1:A:138:ILE:HG22	1:A:140:PHE:CE1	0.59	2.32	18	9
1:A:229:GLY:O	1:A:230:TYR:CD1	0.59	2.55	8	2
1:A:185:LEU:HD22	1:A:201:ILE:HD12	0.59	1.75	16	3
1:A:221:TYR:O	1:A:232:PHE:CD1	0.59	2.55	20	4
1:A:143:PHE:CE2	1:A:152:MET:CE	0.59	2.85	19	1
1:A:169:LEU:HD22	1:A:169:LEU:C	0.59	2.17	10	1
1:A:139:ALA:C	1:A:140:PHE:CD1	0.58	2.77	20	3
1:A:138:ILE:HB	1:A:145:LEU:HD23	0.58	1.74	10	1
1:A:139:ALA:HB2	1:A:144:LYS:HB2	0.58	1.74	15	1
1:A:140:PHE:O	1:A:141:GLY:C	0.58	2.42	14	9
1:A:145:LEU:HD13	1:A:169:LEU:HD13	0.58	1.74	15	1
1:A:166:PHE:CD1	1:A:166:PHE:C	0.57	2.78	19	13
1:A:145:LEU:HD12	1:A:152:MET:CG	0.57	2.29	11	1
1:A:152:MET:HG2	1:A:161:LEU:HD11	0.57	1.76	6	2
1:A:169:LEU:HD13	1:A:208:LEU:HD12	0.57	1.75	8	1
1:A:209:ARG:HB3	1:A:222:ILE:HG21	0.57	1.75	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:208:LEU:HD11	1:A:222:ILE:HD11	0.57	1.76	10	1
1:A:170:LYS:HA	1:A:173:VAL:HG12	0.57	1.75	18	2
1:A:152:MET:C	1:A:153:PHE:CD1	0.57	2.78	19	10
1:A:140:PHE:CD1	1:A:221:TYR:CE2	0.57	2.93	12	1
1:A:209:ARG:HG3	1:A:222:ILE:HG21	0.56	1.76	1	1
1:A:200:SER:OG	1:A:203:VAL:HG21	0.56	2.00	8	1
1:A:166:PHE:CE1	1:A:170:LYS:CD	0.56	2.89	14	1
1:A:143:PHE:CZ	1:A:152:MET:HE1	0.56	2.34	19	1
1:A:147:LEU:HD21	1:A:169:LEU:HD22	0.56	1.77	20	1
1:A:139:ALA:HB2	1:A:144:LYS:HG2	0.56	1.77	11	6
1:A:182:ARG:HG2	1:A:201:ILE:HD12	0.56	1.78	9	2
1:A:140:PHE:CE2	1:A:143:PHE:CB	0.55	2.89	8	2
1:A:205:ILE:HG22	1:A:209:ARG:NE	0.55	2.16	12	1
1:A:143:PHE:CZ	1:A:212:VAL:O	0.55	2.59	17	3
1:A:143:PHE:CZ	1:A:152:MET:CE	0.55	2.90	19	1
1:A:154:ARG:O	1:A:155:GLU:CB	0.55	2.55	20	5
1:A:147:LEU:CD1	1:A:147:LEU:N	0.55	2.70	10	5
1:A:145:LEU:HD13	1:A:152:MET:HE2	0.55	1.77	10	1
1:A:173:VAL:HG22	1:A:232:PHE:CE2	0.55	2.37	13	1
1:A:179:PRO:O	1:A:180:LEU:HD22	0.55	2.01	18	2
1:A:169:LEU:CD2	1:A:208:LEU:HD22	0.55	2.29	5	1
1:A:179:PRO:CG	1:A:228:LEU:CD1	0.55	2.84	14	1
1:A:180:LEU:HD21	1:A:188:LEU:HD13	0.55	1.79	2	1
1:A:168:VAL:O	1:A:171:ALA:HB3	0.55	2.01	13	5
1:A:145:LEU:HD23	1:A:145:LEU:C	0.55	2.22	13	2
1:A:201:ILE:HG21	1:A:230:TYR:CD2	0.54	2.37	8	1
1:A:161:LEU:HD22	1:A:208:LEU:CD2	0.54	2.30	4	1
1:A:168:VAL:HG11	1:A:208:LEU:CD1	0.54	2.31	17	1
1:A:168:VAL:HG22	1:A:201:ILE:HD11	0.54	1.80	17	2
1:A:138:ILE:HB	1:A:145:LEU:HD22	0.54	1.80	6	5
1:A:152:MET:O	1:A:153:PHE:CD1	0.54	2.61	16	1
1:A:144:LYS:CD	1:A:153:PHE:CZ	0.54	2.91	20	1
1:A:140:PHE:CE2	1:A:143:PHE:CE1	0.53	2.95	19	1
1:A:223:GLN:HB2	1:A:231:VAL:HG13	0.53	1.80	5	1
1:A:140:PHE:CZ	1:A:143:PHE:CB	0.53	2.91	8	2
1:A:147:LEU:N	1:A:147:LEU:HD12	0.53	2.19	16	4
1:A:139:ALA:O	1:A:140:PHE:CD1	0.53	2.62	12	1
1:A:182:ARG:CD	1:A:183:ASP:N	0.53	2.72	13	1
1:A:201:ILE:HG22	1:A:205:ILE:HG12	0.52	1.79	19	1
1:A:145:LEU:HD11	1:A:161:LEU:CD1	0.52	2.34	3	1
1:A:182:ARG:HA	1:A:185:LEU:HD13	0.52	1.80	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:140:PHE:CD2	1:A:143:PHE:HB3	0.52	2.39	3	3
1:A:160:PRO:O	1:A:161:LEU:HD23	0.52	2.05	4	1
1:A:137:VAL:C	1:A:138:ILE:HD13	0.52	2.24	17	1
1:A:180:LEU:HD13	1:A:188:LEU:CD1	0.52	2.35	17	1
1:A:172:LEU:HD23	1:A:232:PHE:CD2	0.52	2.40	6	1
1:A:165:GLU:HB3	1:A:208:LEU:HD11	0.52	1.82	14	1
1:A:147:LEU:HD23	1:A:166:PHE:CE1	0.52	2.39	18	2
1:A:143:PHE:CD2	1:A:154:ARG:HG3	0.52	2.40	14	4
1:A:185:LEU:CD2	1:A:201:ILE:HD12	0.52	2.35	12	3
1:A:185:LEU:HB2	1:A:201:ILE:HD13	0.52	1.82	8	2
1:A:169:LEU:HD13	1:A:208:LEU:HD22	0.52	1.81	6	2
1:A:138:ILE:CG2	1:A:140:PHE:CE1	0.52	2.93	14	1
1:A:205:ILE:HD11	1:A:224:THR:OG1	0.52	2.05	14	1
1:A:145:LEU:HD11	1:A:169:LEU:CD2	0.51	2.35	2	3
1:A:154:ARG:O	1:A:154:ARG:CG	0.51	2.59	4	4
1:A:166:PHE:CE1	1:A:170:LYS:HG3	0.51	2.41	14	4
1:A:168:VAL:HG13	1:A:201:ILE:CD1	0.51	2.35	17	1
1:A:223:GLN:CB	1:A:231:VAL:HG13	0.51	2.36	5	1
1:A:209:ARG:HG2	1:A:222:ILE:HG21	0.51	1.83	6	1
1:A:205:ILE:HG22	1:A:209:ARG:HE	0.51	1.65	12	1
1:A:182:ARG:O	1:A:201:ILE:CD1	0.51	2.59	8	1
1:A:138:ILE:HG22	1:A:140:PHE:CZ	0.51	2.40	20	3
1:A:170:LYS:O	1:A:174:SER:CB	0.51	2.59	10	7
1:A:137:VAL:CG1	1:A:146:ASN:CG	0.51	2.79	16	5
1:A:209:ARG:CG	1:A:222:ILE:HG21	0.51	2.35	1	2
1:A:137:VAL:CG2	1:A:138:ILE:N	0.51	2.74	19	5
1:A:147:LEU:HA	1:A:166:PHE:CE2	0.51	2.41	17	4
1:A:173:VAL:HG22	1:A:232:PHE:CZ	0.51	2.40	13	1
1:A:168:VAL:CG1	1:A:208:LEU:CD1	0.51	2.89	17	1
1:A:179:PRO:HB2	1:A:228:LEU:HD12	0.51	1.81	2	3
1:A:137:VAL:HG12	1:A:146:ASN:OD1	0.51	2.04	12	5
1:A:140:PHE:CE1	1:A:143:PHE:CG	0.51	2.99	19	1
1:A:185:LEU:HG	1:A:230:TYR:CD2	0.50	2.42	14	2
1:A:200:SER:O	1:A:204:GLN:CG	0.50	2.59	16	2
1:A:145:LEU:CD1	1:A:161:LEU:HD11	0.50	2.36	3	3
1:A:201:ILE:HG22	1:A:230:TYR:CZ	0.50	2.41	9	2
1:A:163:SER:O	1:A:167:ALA:CB	0.50	2.60	2	4
1:A:200:SER:OG	1:A:203:VAL:CG1	0.50	2.60	1	1
1:A:169:LEU:O	1:A:173:VAL:CG2	0.50	2.60	15	1
1:A:202:ASP:CA	1:A:230:TYR:OH	0.50	2.58	19	1
1:A:175:HIS:CD2	1:A:178:GLU:CB	0.50	2.94	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:LEU:HD12	1:A:201:ILE:HG12	0.50	1.83	14	1
1:A:140:PHE:CE1	1:A:143:PHE:HB3	0.50	2.41	19	1
1:A:143:PHE:CD1	1:A:143:PHE:C	0.50	2.84	19	1
1:A:169:LEU:CD1	1:A:208:LEU:HD22	0.50	2.33	20	1
1:A:155:GLU:O	1:A:156:ASP:CB	0.50	2.60	1	5
1:A:138:ILE:CD1	1:A:147:LEU:HD13	0.50	2.37	16	1
1:A:143:PHE:CE2	1:A:152:MET:HE1	0.50	2.41	19	1
1:A:147:LEU:HB3	1:A:166:PHE:CE1	0.50	2.42	3	2
1:A:143:PHE:CE2	1:A:154:ARG:HB3	0.50	2.41	6	1
1:A:166:PHE:CD1	1:A:166:PHE:O	0.50	2.65	3	1
1:A:144:LYS:HG3	1:A:153:PHE:CD2	0.50	2.41	8	1
1:A:170:LYS:O	1:A:174:SER:N	0.49	2.45	14	16
1:A:137:VAL:HG12	1:A:146:ASN:ND2	0.49	2.22	17	2
1:A:138:ILE:HD11	1:A:173:VAL:HG11	0.49	1.84	20	1
1:A:149:THR:O	1:A:150:ARG:CB	0.49	2.61	18	2
1:A:142:LYS:HG2	1:A:143:PHE:CE1	0.49	2.43	12	1
1:A:172:LEU:HD13	1:A:185:LEU:HD21	0.49	1.85	6	1
1:A:166:PHE:CZ	1:A:170:LYS:HD2	0.49	2.43	14	1
1:A:166:PHE:O	1:A:170:LYS:CB	0.49	2.61	11	5
1:A:178:GLU:O	1:A:180:LEU:CD1	0.49	2.61	20	1
1:A:153:PHE:CB	1:A:157:GLU:O	0.49	2.61	14	3
1:A:185:LEU:HD21	1:A:230:TYR:HB2	0.49	1.85	1	4
1:A:222:ILE:HG12	1:A:232:PHE:CE1	0.49	2.43	11	1
1:A:225:VAL:O	1:A:229:GLY:N	0.49	2.46	10	20
1:A:182:ARG:HB3	1:A:230:TYR:CE1	0.49	2.43	13	5
1:A:180:LEU:O	1:A:185:LEU:CD1	0.49	2.61	7	4
1:A:145:LEU:CD2	1:A:147:LEU:CD1	0.48	2.90	11	2
1:A:182:ARG:HB2	1:A:201:ILE:HD12	0.48	1.85	5	1
1:A:172:LEU:CD2	1:A:231:VAL:C	0.48	2.81	20	3
1:A:179:PRO:HG2	1:A:228:LEU:HD22	0.48	1.84	11	1
1:A:221:TYR:O	1:A:232:PHE:CD2	0.48	2.66	16	2
1:A:179:PRO:O	1:A:180:LEU:HD12	0.48	2.08	9	1
1:A:145:LEU:HD11	1:A:147:LEU:HD12	0.48	1.84	17	1
1:A:144:LYS:HD3	1:A:153:PHE:CZ	0.48	2.44	20	2
1:A:205:ILE:HG13	1:A:230:TYR:CE1	0.48	2.43	1	2
1:A:152:MET:CE	1:A:212:VAL:HG11	0.48	2.38	4	1
1:A:147:LEU:HB3	1:A:166:PHE:CZ	0.48	2.43	12	6
1:A:164:GLY:O	1:A:168:VAL:CG2	0.48	2.61	11	2
1:A:222:ILE:HD11	1:A:232:PHE:CD2	0.48	2.43	4	2
1:A:175:HIS:CD2	1:A:178:GLU:HG3	0.48	2.43	5	1
1:A:140:PHE:O	1:A:142:LYS:N	0.48	2.47	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:144:LYS:HB3	1:A:153:PHE:CE2	0.48	2.44	20	2
1:A:140:PHE:CD1	1:A:143:PHE:HB2	0.48	2.44	7	4
1:A:143:PHE:CE2	1:A:154:ARG:HB2	0.48	2.44	10	3
1:A:143:PHE:CZ	1:A:212:VAL:HG12	0.48	2.44	3	2
1:A:229:GLY:O	1:A:230:TYR:CG	0.48	2.67	8	3
1:A:147:LEU:HB3	1:A:166:PHE:CE2	0.48	2.43	9	3
1:A:231:VAL:HG22	1:A:232:PHE:H	0.48	1.69	11	2
1:A:201:ILE:CG2	1:A:230:TYR:CD2	0.47	2.97	8	1
1:A:145:LEU:HD11	1:A:169:LEU:HD22	0.47	1.84	1	2
1:A:233:VAL:HG13	1:A:234:PRO:HD2	0.47	1.86	4	1
1:A:168:VAL:HG13	1:A:185:LEU:HD23	0.47	1.85	5	1
1:A:221:TYR:CD2	1:A:234:PRO:HB3	0.47	2.44	5	2
1:A:205:ILE:HG21	1:A:230:TYR:CD1	0.47	2.44	11	2
1:A:166:PHE:CE1	1:A:170:LYS:HB2	0.47	2.45	3	2
1:A:180:LEU:HD22	1:A:184:LYS:HB3	0.47	1.84	12	1
1:A:152:MET:O	1:A:159:MET:N	0.47	2.47	15	5
1:A:159:MET:CE	1:A:211:MET:SD	0.47	3.02	4	1
1:A:175:HIS:CD2	1:A:178:GLU:HG2	0.47	2.44	9	1
1:A:145:LEU:CD1	1:A:169:LEU:HD11	0.47	2.40	4	1
1:A:151:GLU:HB3	1:A:153:PHE:CZ	0.47	2.45	4	2
1:A:154:ARG:CD	1:A:154:ARG:O	0.47	2.62	5	2
1:A:165:GLU:HA	1:A:208:LEU:HD21	0.47	1.85	17	2
1:A:165:GLU:CB	1:A:208:LEU:HD11	0.47	2.39	14	1
1:A:138:ILE:O	1:A:145:LEU:N	0.47	2.48	3	10
1:A:209:ARG:O	1:A:213:GLU:N	0.47	2.48	8	8
1:A:176:PRO:O	1:A:177:ARG:CB	0.47	2.63	3	5
1:A:205:ILE:O	1:A:209:ARG:CB	0.47	2.63	10	1
1:A:143:PHE:C	1:A:144:LYS:CD	0.47	2.83	16	1
1:A:208:LEU:HD11	1:A:222:ILE:CD1	0.47	2.40	10	1
1:A:220:ARG:HG2	1:A:221:TYR:CE1	0.47	2.45	16	2
1:A:144:LYS:HD2	1:A:153:PHE:CE2	0.47	2.45	19	3
1:A:205:ILE:HG13	1:A:230:TYR:CD2	0.47	2.45	12	2
1:A:145:LEU:HD21	1:A:147:LEU:HD21	0.47	1.87	13	1
1:A:138:ILE:N	1:A:145:LEU:O	0.47	2.46	15	1
1:A:152:MET:SD	1:A:159:MET:CG	0.47	3.03	6	1
1:A:154:ARG:O	1:A:157:GLU:CB	0.47	2.63	16	2
1:A:208:LEU:CB	1:A:209:ARG:NH2	0.46	2.78	4	1
1:A:140:PHE:HB2	1:A:143:PHE:CD1	0.46	2.45	16	4
1:A:152:MET:C	1:A:153:PHE:CG	0.46	2.88	16	1
1:A:140:PHE:CE1	1:A:143:PHE:CB	0.46	2.99	19	1
1:A:140:PHE:CD2	1:A:143:PHE:CB	0.46	2.98	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:205:ILE:HG13	1:A:230:TYR:CD1	0.46	2.46	8	1
1:A:168:VAL:CG1	1:A:205:ILE:CD1	0.46	2.94	9	1
1:A:173:VAL:O	1:A:173:VAL:HG12	0.46	2.10	20	3
1:A:162:THR:HG22	1:A:163:SER:N	0.46	2.26	15	1
1:A:140:PHE:CZ	1:A:212:VAL:HB	0.46	2.45	20	1
1:A:166:PHE:CZ	1:A:170:LYS:HE2	0.46	2.46	2	1
1:A:140:PHE:CD2	1:A:143:PHE:HB2	0.46	2.46	8	1
1:A:146:ASN:ND2	1:A:149:THR:OG1	0.46	2.49	16	2
1:A:181:SER:O	1:A:184:LYS:N	0.46	2.49	3	7
1:A:143:PHE:CE1	1:A:154:ARG:HG3	0.46	2.45	8	2
1:A:147:LEU:CD2	1:A:170:LYS:CB	0.46	2.94	18	1
1:A:221:TYR:HB3	1:A:232:PHE:CZ	0.46	2.46	2	5
1:A:221:TYR:HB3	1:A:232:PHE:CE1	0.46	2.46	4	8
1:A:201:ILE:O	1:A:203:VAL:N	0.46	2.48	4	2
1:A:150:ARG:O	1:A:150:ARG:CG	0.46	2.62	15	1
1:A:205:ILE:HG13	1:A:230:TYR:CE2	0.46	2.46	19	1
1:A:178:GLU:N	1:A:231:VAL:HG23	0.46	2.26	5	1
1:A:140:PHE:O	1:A:140:PHE:CD1	0.46	2.69	19	1
1:A:161:LEU:HD23	1:A:211:MET:HE1	0.46	1.86	8	1
1:A:172:LEU:CD1	1:A:205:ILE:HD11	0.46	2.40	10	1
1:A:201:ILE:O	1:A:205:ILE:N	0.46	2.49	11	2
1:A:206:SER:O	1:A:210:ARG:CB	0.46	2.65	18	1
1:A:205:ILE:HG22	1:A:209:ARG:HD2	0.46	1.87	19	1
1:A:211:MET:HG3	1:A:212:VAL:HG13	0.45	1.88	1	1
1:A:185:LEU:CB	1:A:201:ILE:CD1	0.45	2.94	3	1
1:A:229:GLY:C	1:A:230:TYR:CG	0.45	2.89	8	4
1:A:145:LEU:HD21	1:A:147:LEU:HD23	0.45	1.88	13	1
1:A:223:GLN:O	1:A:225:VAL:HG23	0.45	2.11	18	1
1:A:201:ILE:O	1:A:204:GLN:N	0.45	2.50	8	6
1:A:162:THR:O	1:A:165:GLU:N	0.45	2.49	3	3
1:A:204:GLN:O	1:A:207:ARG:N	0.45	2.49	10	5
1:A:226:TRP:O	1:A:228:LEU:N	0.45	2.50	7	1
1:A:200:SER:O	1:A:202:ASP:N	0.45	2.49	9	1
1:A:172:LEU:CD1	1:A:205:ILE:CD1	0.45	2.94	11	1
1:A:146:ASN:O	1:A:150:ARG:N	0.45	2.48	3	5
1:A:145:LEU:CD1	1:A:169:LEU:CD2	0.45	2.94	2	1
1:A:145:LEU:HD11	1:A:161:LEU:HD11	0.45	1.88	3	1
1:A:181:SER:O	1:A:185:LEU:CD1	0.45	2.63	6	2
1:A:168:VAL:O	1:A:171:ALA:N	0.45	2.49	7	2
1:A:169:LEU:HD22	1:A:208:LEU:CD1	0.45	2.41	8	1
1:A:165:GLU:HG3	1:A:208:LEU:HD21	0.45	1.88	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:N	1:A:138:ILE:CD1	0.45	2.78	16	1
1:A:146:ASN:ND2	1:A:149:THR:CB	0.45	2.80	16	2
1:A:147:LEU:HD13	1:A:170:LYS:CD	0.45	2.42	5	2
1:A:137:VAL:CG1	1:A:146:ASN:ND2	0.45	2.79	17	2
1:A:204:GLN:O	1:A:208:LEU:N	0.45	2.50	20	3
1:A:213:GLU:OE1	1:A:220:ARG:N	0.45	2.50	12	1
1:A:205:ILE:O	1:A:208:LEU:N	0.45	2.50	1	2
1:A:138:ILE:CD1	1:A:173:VAL:HG11	0.45	2.42	2	1
1:A:165:GLU:N	1:A:204:GLN:OE1	0.45	2.50	16	1
1:A:220:ARG:HG2	1:A:221:TYR:CD1	0.45	2.47	16	1
1:A:165:GLU:O	1:A:168:VAL:N	0.45	2.49	14	2
1:A:219:PRO:O	1:A:220:ARG:NH1	0.45	2.50	2	1
1:A:140:PHE:N	1:A:143:PHE:O	0.45	2.49	8	1
1:A:144:LYS:HD2	1:A:153:PHE:CD2	0.45	2.47	19	1
1:A:201:ILE:HG22	1:A:205:ILE:CG1	0.45	2.41	19	1
1:A:201:ILE:C	1:A:203:VAL:N	0.45	2.69	10	5
1:A:185:LEU:CB	1:A:201:ILE:HD12	0.45	2.42	10	2
1:A:152:MET:SD	1:A:161:LEU:CD1	0.45	3.03	2	1
1:A:147:LEU:CD2	1:A:166:PHE:CE1	0.44	2.99	12	2
1:A:202:ASP:N	1:A:230:TYR:OH	0.44	2.49	14	4
1:A:202:ASP:OD2	1:A:226:TRP:CZ2	0.44	2.70	3	1
1:A:221:TYR:CD2	1:A:234:PRO:HA	0.44	2.47	19	4
1:A:168:VAL:HG11	1:A:204:GLN:CB	0.44	2.42	8	1
1:A:171:ALA:HB2	1:A:188:LEU:HD22	0.44	1.89	19	1
1:A:183:ASP:O	1:A:187:ASN:N	0.44	2.50	20	1
1:A:144:LYS:N	1:A:153:PHE:O	0.44	2.51	1	1
1:A:147:LEU:HD23	1:A:170:LYS:HG3	0.44	1.88	19	3
1:A:145:LEU:C	1:A:145:LEU:CD2	0.44	2.80	6	1
1:A:221:TYR:O	1:A:222:ILE:CD1	0.44	2.64	16	2
1:A:147:LEU:CD1	1:A:170:LYS:CG	0.44	2.94	7	1
1:A:182:ARG:HG3	1:A:230:TYR:CE1	0.44	2.47	16	1
1:A:145:LEU:CD1	1:A:152:MET:SD	0.44	3.05	19	1
1:A:221:TYR:O	1:A:232:PHE:CZ	0.44	2.71	5	1
1:A:172:LEU:HD11	1:A:205:ILE:HD12	0.44	1.89	11	1
1:A:223:GLN:O	1:A:231:VAL:CG1	0.44	2.66	15	1
1:A:201:ILE:O	1:A:202:ASP:C	0.44	2.55	4	4
1:A:182:ARG:CG	1:A:230:TYR:CE2	0.44	3.00	8	1
1:A:140:PHE:CD1	1:A:143:PHE:HB3	0.44	2.47	10	2
1:A:143:PHE:CE2	1:A:154:ARG:HG3	0.44	2.48	18	2
1:A:169:LEU:O	1:A:172:LEU:N	0.44	2.50	1	2
1:A:154:ARG:O	1:A:154:ARG:NE	0.44	2.50	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:PHE:CD2	1:A:143:PHE:CD2	0.44	3.06	8	1
1:A:224:THR:C	1:A:225:VAL:CG2	0.44	2.86	8	1
1:A:225:VAL:HG11	1:A:228:LEU:HD12	0.44	1.88	8	1
1:A:179:PRO:HB2	1:A:228:LEU:HD22	0.44	1.90	20	1
1:A:140:PHE:CG	1:A:221:TYR:CE2	0.44	3.05	5	1
1:A:180:LEU:HD23	1:A:184:LYS:HB3	0.44	1.89	6	1
1:A:146:ASN:OD1	1:A:148:GLY:N	0.44	2.51	1	2
1:A:152:MET:CE	1:A:212:VAL:CG1	0.44	2.95	16	1
1:A:165:GLU:HG3	1:A:208:LEU:HD11	0.44	1.88	3	1
1:A:140:PHE:CZ	1:A:143:PHE:HB3	0.44	2.48	8	2
1:A:168:VAL:HG12	1:A:172:LEU:HD12	0.43	1.90	10	1
1:A:147:LEU:CD2	1:A:170:LYS:HB2	0.43	2.43	18	1
1:A:180:LEU:HD12	1:A:184:LYS:HB3	0.43	1.90	19	1
1:A:143:PHE:CD1	1:A:154:ARG:HG3	0.43	2.47	1	1
1:A:153:PHE:CD1	1:A:158:PRO:HB3	0.43	2.48	3	2
1:A:146:ASN:OD1	1:A:146:ASN:C	0.43	2.55	15	2
1:A:168:VAL:HG22	1:A:201:ILE:CD1	0.43	2.42	17	1
1:A:179:PRO:HA	1:A:231:VAL:HG23	0.43	1.90	19	1
1:A:144:LYS:HD2	1:A:153:PHE:CZ	0.43	2.48	20	1
1:A:166:PHE:CE1	1:A:170:LYS:HE2	0.43	2.49	2	1
1:A:172:LEU:HD11	1:A:230:TYR:HB3	0.43	1.89	3	2
1:A:144:LYS:HB3	1:A:153:PHE:CD2	0.43	2.48	7	1
1:A:205:ILE:O	1:A:209:ARG:N	0.43	2.49	10	1
1:A:185:LEU:HB3	1:A:201:ILE:HD13	0.43	1.89	14	1
1:A:184:LYS:O	1:A:188:LEU:N	0.43	2.50	16	1
1:A:138:ILE:HG22	1:A:140:PHE:HE1	0.43	1.73	17	2
1:A:200:SER:CB	1:A:203:VAL:CG2	0.43	2.97	8	1
1:A:208:LEU:CD1	1:A:222:ILE:HD11	0.43	2.43	10	1
1:A:145:LEU:HD23	1:A:147:LEU:CD1	0.43	2.43	11	1
1:A:185:LEU:HB2	1:A:201:ILE:CD1	0.43	2.43	3	1
1:A:142:LYS:HG3	1:A:143:PHE:CD1	0.43	2.49	7	1
1:A:169:LEU:HB2	1:A:208:LEU:HD13	0.43	1.90	16	1
1:A:183:ASP:O	1:A:187:ASN:ND2	0.43	2.52	17	1
1:A:138:ILE:HD13	1:A:173:VAL:HG11	0.43	1.90	2	2
1:A:231:VAL:HG22	1:A:232:PHE:N	0.43	2.29	11	2
1:A:230:TYR:CD1	1:A:230:TYR:N	0.43	2.87	3	2
1:A:221:TYR:O	1:A:222:ILE:CG1	0.43	2.66	10	2
1:A:165:GLU:CB	1:A:208:LEU:HD21	0.43	2.44	19	3
1:A:171:ALA:HA	1:A:188:LEU:HD22	0.43	1.89	16	1
1:A:229:GLY:C	1:A:230:TYR:CD2	0.43	2.92	18	1
1:A:202:ASP:OD2	1:A:226:TRP:CH2	0.43	2.71	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:LEU:O	1:A:185:LEU:HD12	0.43	2.14	3	1
1:A:220:ARG:HG3	1:A:221:TYR:CD2	0.43	2.49	4	1
1:A:226:TRP:C	1:A:228:LEU:N	0.43	2.72	7	1
1:A:140:PHE:CD2	1:A:140:PHE:O	0.42	2.72	5	1
1:A:171:ALA:CB	1:A:185:LEU:O	0.42	2.67	17	1
1:A:222:ILE:CD1	1:A:232:PHE:CE2	0.42	3.02	9	1
1:A:155:GLU:C	1:A:157:GLU:N	0.42	2.72	10	2
1:A:203:VAL:CG1	1:A:204:GLN:N	0.42	2.82	13	1
1:A:205:ILE:O	1:A:209:ARG:CG	0.42	2.68	13	1
1:A:147:LEU:HD21	1:A:169:LEU:HD12	0.42	1.91	7	1
1:A:171:ALA:O	1:A:175:HIS:N	0.42	2.53	15	1
1:A:219:PRO:O	1:A:220:ARG:CB	0.42	2.66	2	1
1:A:207:ARG:O	1:A:211:MET:CG	0.42	2.68	8	1
1:A:137:VAL:CG1	1:A:146:ASN:HB2	0.42	2.44	15	1
1:A:174:SER:O	1:A:175:HIS:CD2	0.42	2.72	14	1
1:A:178:GLU:O	1:A:180:LEU:HD12	0.42	2.15	20	1
1:A:145:LEU:HD13	1:A:169:LEU:CD2	0.42	2.44	8	1
1:A:147:LEU:HA	1:A:166:PHE:CZ	0.42	2.50	12	1
1:A:142:LYS:C	1:A:143:PHE:CG	0.42	2.93	13	1
1:A:205:ILE:HG21	1:A:224:THR:OG1	0.42	2.15	2	1
1:A:153:PHE:HA	1:A:157:GLU:O	0.42	2.15	5	2
1:A:175:HIS:NE2	1:A:178:GLU:OE2	0.42	2.53	16	1
1:A:209:ARG:O	1:A:213:GLU:CB	0.42	2.67	8	1
1:A:169:LEU:O	1:A:173:VAL:N	0.42	2.50	15	1
1:A:173:VAL:O	1:A:173:VAL:CG1	0.42	2.67	20	1
1:A:183:ASP:O	1:A:187:ASN:CB	0.42	2.67	4	1
1:A:169:LEU:C	1:A:169:LEU:CD1	0.42	2.83	7	1
1:A:144:LYS:O	1:A:153:PHE:CD1	0.42	2.72	18	1
1:A:145:LEU:CD1	1:A:169:LEU:HD23	0.42	2.45	8	1
1:A:225:VAL:HG22	1:A:228:LEU:N	0.42	2.30	10	1
1:A:185:LEU:HD23	1:A:201:ILE:CD1	0.42	2.41	12	1
1:A:212:VAL:HG23	1:A:213:GLU:N	0.42	2.29	17	1
1:A:140:PHE:O	1:A:141:GLY:O	0.41	2.38	5	1
1:A:204:GLN:C	1:A:206:SER:N	0.41	2.72	8	1
1:A:145:LEU:CD1	1:A:146:ASN:N	0.41	2.79	17	2
1:A:208:LEU:O	1:A:211:MET:N	0.41	2.53	6	1
1:A:138:ILE:HD13	1:A:147:LEU:CD1	0.41	2.45	16	1
1:A:178:GLU:C	1:A:231:VAL:HG23	0.41	2.36	20	1
1:A:205:ILE:CD1	1:A:224:THR:OG1	0.41	2.68	13	1
1:A:152:MET:SD	1:A:152:MET:C	0.41	2.99	5	1
1:A:207:ARG:NH1	1:A:210:ARG:NH1	0.41	2.68	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:SER:C	1:A:183:ASP:N	0.41	2.74	3	1
1:A:143:PHE:CE2	1:A:154:ARG:HD2	0.41	2.50	14	1
1:A:169:LEU:O	1:A:170:LYS:C	0.41	2.59	12	1
1:A:203:VAL:O	1:A:207:ARG:N	0.41	2.49	20	1
1:A:137:VAL:HB	1:A:146:ASN:CB	0.41	2.46	6	2
1:A:152:MET:SD	1:A:153:PHE:N	0.41	2.93	9	1
1:A:175:HIS:CD2	1:A:178:GLU:CG	0.41	3.03	9	1
1:A:152:MET:O	1:A:159:MET:O	0.41	2.39	10	3
1:A:145:LEU:HD12	1:A:161:LEU:HD11	0.41	1.93	16	1
1:A:142:LYS:N	1:A:143:PHE:CD1	0.41	2.89	18	1
1:A:140:PHE:CD2	1:A:221:TYR:CZ	0.41	3.09	5	1
1:A:140:PHE:CD1	1:A:140:PHE:N	0.41	2.88	6	1
1:A:166:PHE:O	1:A:170:LYS:N	0.41	2.52	11	1
1:A:209:ARG:O	1:A:213:GLU:O	0.40	2.39	9	3
1:A:165:GLU:O	1:A:167:ALA:N	0.40	2.54	10	1
1:A:220:ARG:O	1:A:233:VAL:O	0.40	2.39	9	2
1:A:225:VAL:O	1:A:225:VAL:HG23	0.40	2.16	5	1
1:A:150:ARG:HG3	1:A:166:PHE:CD2	0.40	2.51	6	1
1:A:161:LEU:O	1:A:162:THR:C	0.40	2.59	8	1
1:A:175:HIS:CD2	1:A:178:GLU:HB3	0.40	2.51	9	1
1:A:213:GLU:O	1:A:214:GLU:CG	0.40	2.69	10	1
1:A:165:GLU:OE1	1:A:211:MET:CE	0.40	2.70	17	1
1:A:185:LEU:HD11	1:A:230:TYR:HB2	0.40	1.92	17	1
1:A:186:MET:SD	1:A:186:MET:C	0.40	3.00	4	1
1:A:172:LEU:HD23	1:A:232:PHE:HD2	0.40	1.75	6	1
1:A:142:LYS:HG3	1:A:143:PHE:CE1	0.40	2.51	7	1
1:A:204:GLN:O	1:A:205:ILE:C	0.40	2.59	8	1
1:A:166:PHE:CD1	1:A:170:LYS:HG3	0.40	2.51	14	1
1:A:143:PHE:CE2	1:A:152:MET:HE3	0.40	2.51	19	1
1:A:152:MET:SD	1:A:161:LEU:HD21	0.40	2.56	2	1
1:A:152:MET:SD	1:A:159:MET:SD	0.40	3.20	5	1
1:A:163:SER:O	1:A:167:ALA:HB3	0.40	2.16	7	1
1:A:179:PRO:CA	1:A:231:VAL:HG23	0.40	2.47	19	1
1:A:207:ARG:CZ	1:A:207:ARG:CB	0.40	2.99	11	1
1:A:145:LEU:CD1	1:A:169:LEU:HD13	0.40	2.46	15	1
1:A:162:THR:OG1	1:A:163:SER:N	0.40	2.55	18	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	83/104 (80%)	64±3 (77±3%)	14±3 (17±4%)	5±2 (6±2%)	3	21
All	All	1660/2080 (80%)	1274 (77%)	290 (17%)	96 (6%)	3	21

All 15 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	219	PRO	20
1	A	137	VAL	13
1	A	229	GLY	12
1	A	141	GLY	11
1	A	200	SER	8
1	A	220	ARG	8
1	A	214	GLU	6
1	A	156	ASP	5
1	A	155	GLU	3
1	A	162	THR	3
1	A	177	ARG	3
1	A	227	GLY	1
1	A	201	ILE	1
1	A	225	VAL	1
1	A	150	ARG	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	75/89 (84%)	54±2 (73±3%)	21±2 (27±3%)	2	21
All	All	1500/1780 (84%)	1089 (73%)	411 (27%)	2	21

All 61 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	153	PHE	20
1	A	200	SER	16
1	A	144	LYS	15
1	A	170	LYS	14
1	A	182	ARG	14
1	A	202	ASP	14
1	A	154	ARG	13
1	A	159	MET	13
1	A	172	LEU	13
1	A	137	VAL	13
1	A	220	ARG	12
1	A	210	ARG	11
1	A	155	GLU	10
1	A	174	SER	10
1	A	142	LYS	10
1	A	175	HIS	9
1	A	188	LEU	9
1	A	185	LEU	9
1	A	157	GLU	8
1	A	178	GLU	8
1	A	145	LEU	8
1	A	228	LEU	8
1	A	169	LEU	7
1	A	183	ASP	7
1	A	156	ASP	7
1	A	211	MET	7
1	A	209	ARG	7
1	A	150	ARG	6
1	A	204	GLN	6
1	A	177	ARG	6
1	A	152	MET	6
1	A	165	GLU	6
1	A	225	VAL	6
1	A	161	LEU	6
1	A	181	SER	5
1	A	184	LYS	5
1	A	214	GLU	5
1	A	143	PHE	5
1	A	187	ASN	4
1	A	201	ILE	4
1	A	226	TRP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	206	SER	4
1	A	140	PHE	4
1	A	173	VAL	4
1	A	166	PHE	3
1	A	180	LEU	3
1	A	207	ARG	3
1	A	151	GLU	3
1	A	186	MET	3
1	A	231	VAL	2
1	A	205	ILE	2
1	A	223	GLN	2
1	A	147	LEU	2
1	A	208	LEU	2
1	A	213	GLU	2
1	A	162	THR	1
1	A	224	THR	1
1	A	232	PHE	1
1	A	163	SER	1
1	A	203	VAL	1
1	A	149	THR	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 monosaccharides 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