



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 01:18 PM UTC

PDB ID : 1WSX / pdb_00001wsx
Title : Solution structure of MCL-1
Authors : Day, C.L.; Chen, L.; Richardson, S.J.; Harrison, P.J.; Huang, D.C.; Hinds, M.G.
Deposited on : 2004-11-12

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:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

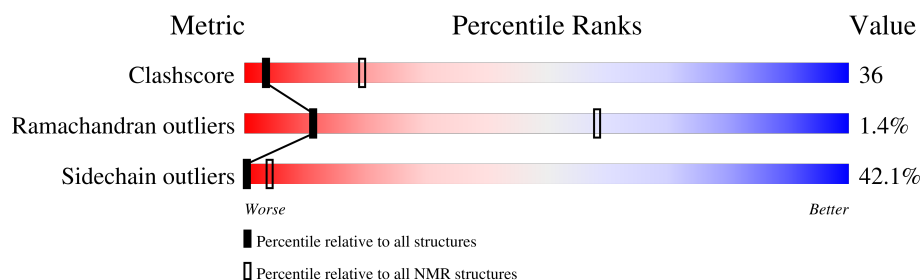
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	162	18% 47% 14% 21%

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: *closest to the average*.

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:155-A:172, A:185-A:234, A:241-A:300 (128)	0.33	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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2577 atoms, of which 1289 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called myeloid cell leukemia sequence 1.

Mol	Chain	Residues	Atoms						Trace
1	A	162	Total	C	H	N	O	S	0
			2577	810	1289	236	240	2	

There are 5 discrepancies between the modelled and reference sequences:

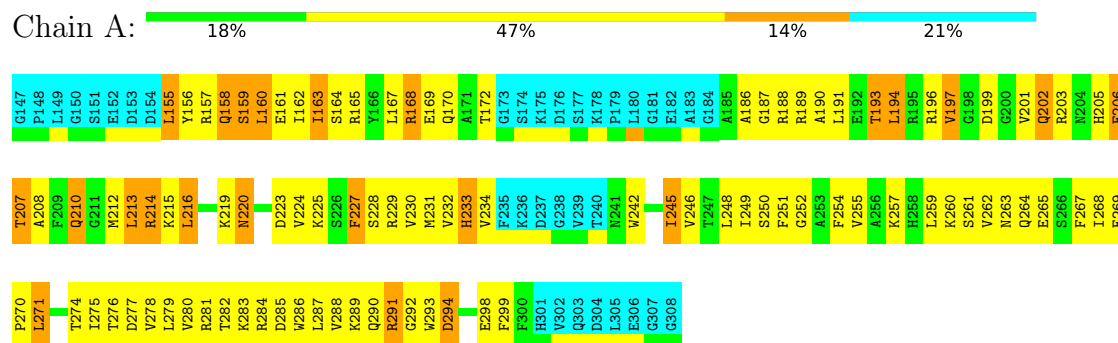
Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLY	-	cloning artifact	UNP P97287
A	148	PRO	-	cloning artifact	UNP P97287
A	149	LEU	-	cloning artifact	UNP P97287
A	150	GLY	-	cloning artifact	UNP P97287
A	151	SER	-	cloning artifact	UNP P97287

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: myeloid cell leukemia sequence 1



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

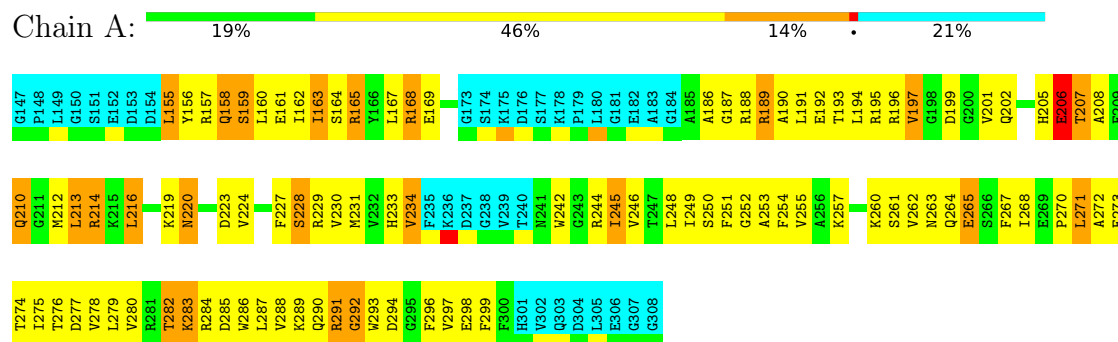
4.2.1 Score per residue for model 1

- Molecule 1: myeloid cell leukemia sequence 1



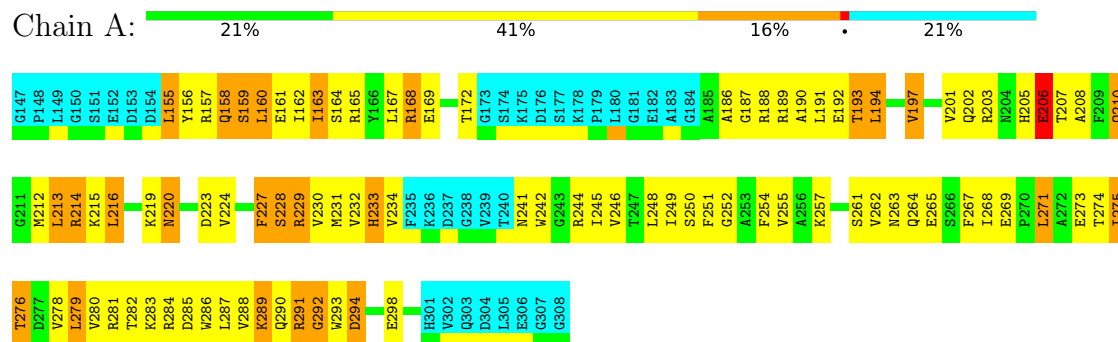
4.2.2 Score per residue for model 2

- Molecule 1: myeloid cell leukemia sequence 1



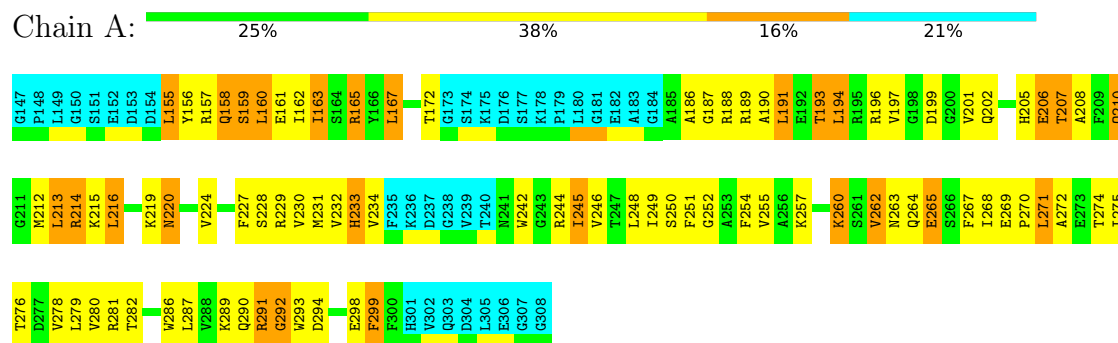
4.2.3 Score per residue for model 3

- Molecule 1: myeloid cell leukemia sequence 1



4.2.4 Score per residue for model 4

- Molecule 1: myeloid cell leukemia sequence 1



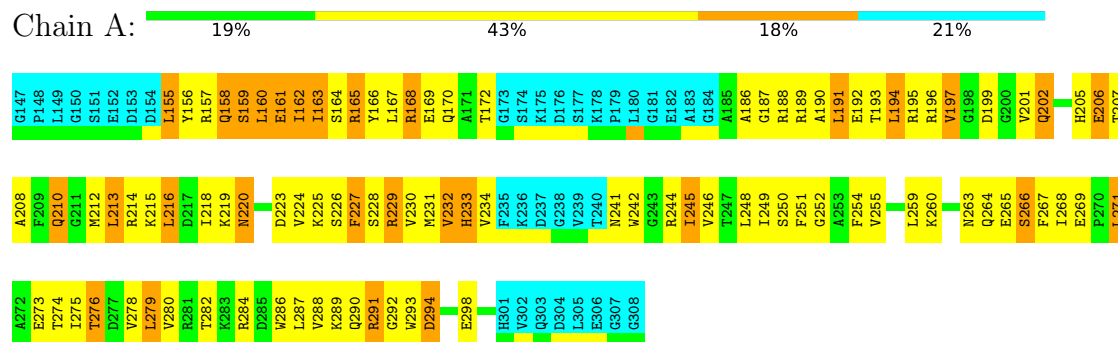
4.2.5 Score per residue for model 5

- Molecule 1: myeloid cell leukemia sequence 1



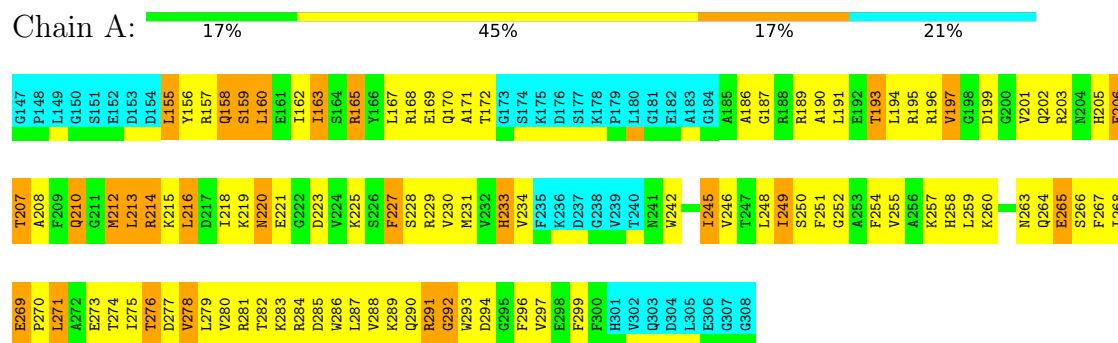
4.2.6 Score per residue for model 6

- Molecule 1: myeloid cell leukemia sequence 1



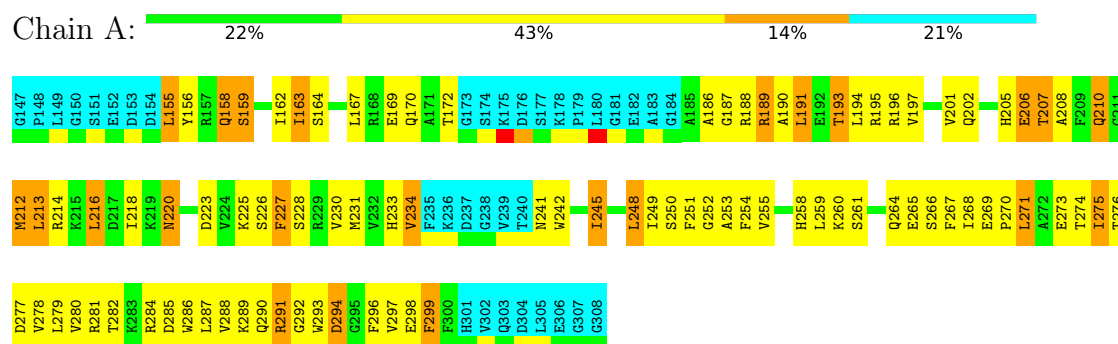
4.2.7 Score per residue for model 7

- Molecule 1: myeloid cell leukemia sequence 1



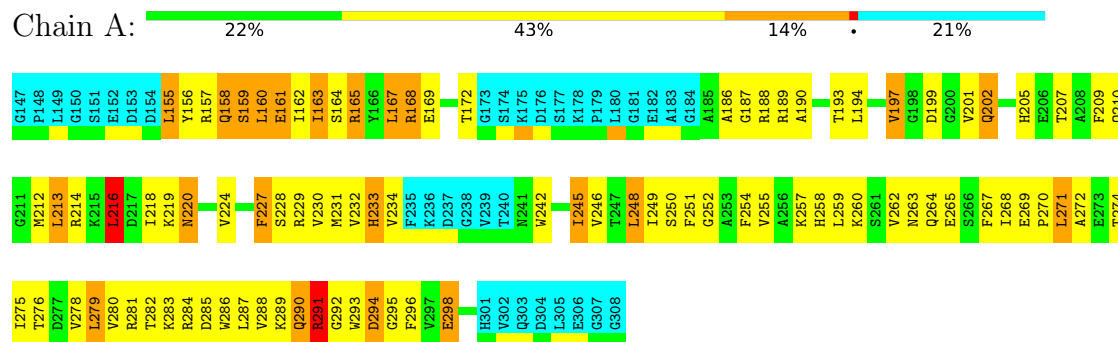
4.2.8 Score per residue for model 8

- Molecule 1: myeloid cell leukemia sequence 1



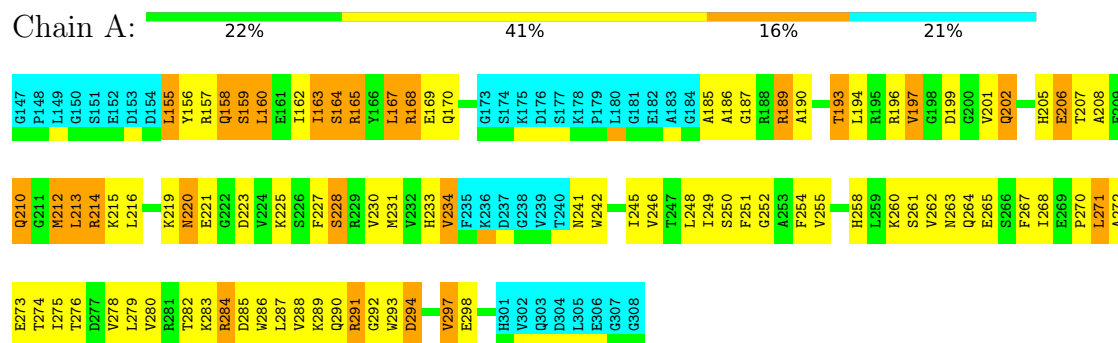
4.2.9 Score per residue for model 9

- Molecule 1: myeloid cell leukemia sequence 1



4.2.10 Score per residue for model 10

- Molecule 1: myeloid cell leukemia sequence 1



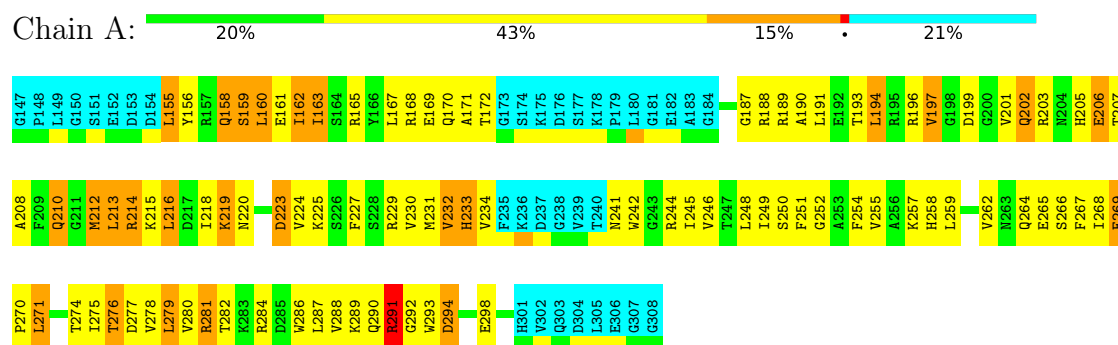
4.2.11 Score per residue for model 11

- Molecule 1: myeloid cell leukemia sequence 1



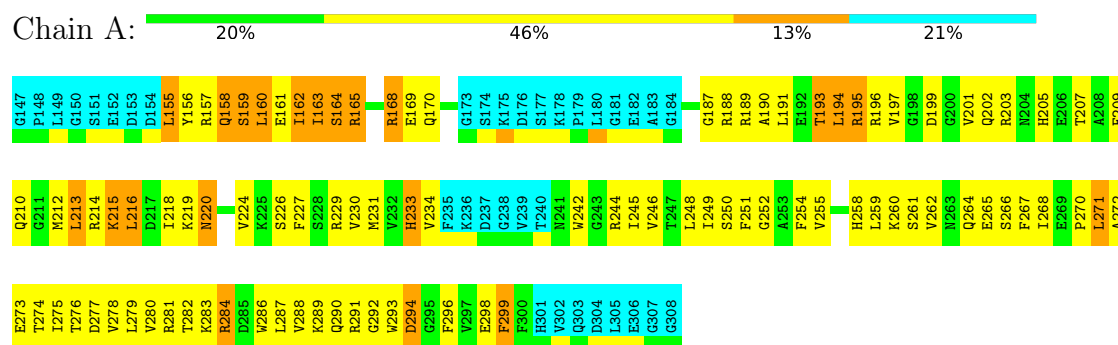
4.2.12 Score per residue for model 12

- Molecule 1: myeloid cell leukemia sequence 1



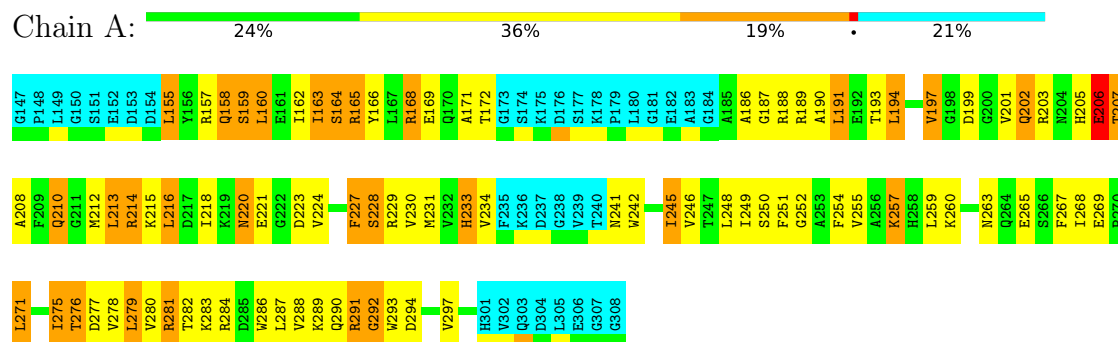
4.2.13 Score per residue for model 13

- Molecule 1: myeloid cell leukemia sequence 1



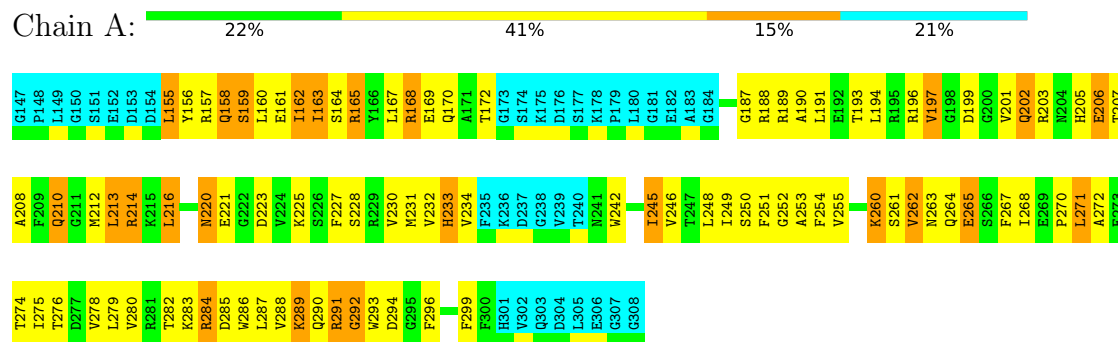
4.2.14 Score per residue for model 14

- Molecule 1: myeloid cell leukemia sequence 1



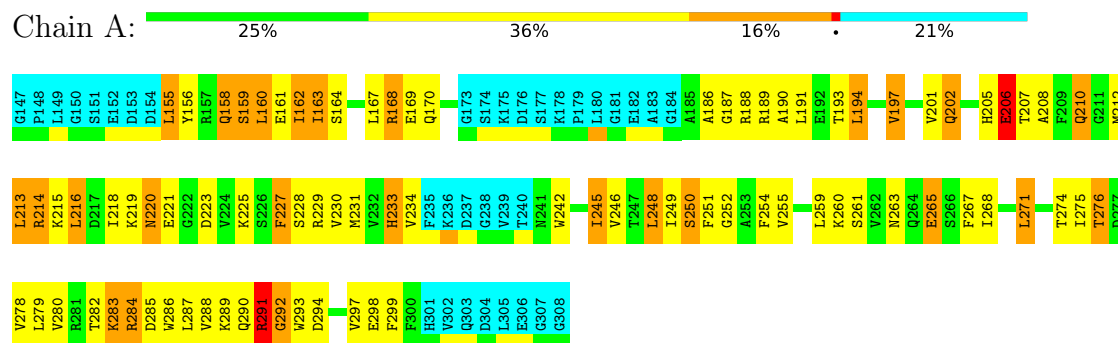
4.2.15 Score per residue for model 15

- Molecule 1: myeloid cell leukemia sequence 1



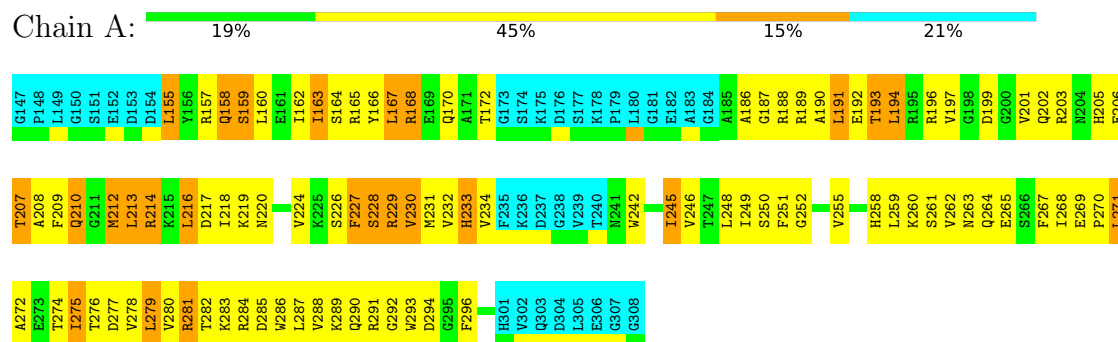
4.2.16 Score per residue for model 16

- Molecule 1: myeloid cell leukemia sequence 1



4.2.17 Score per residue for model 17

- Molecule 1: myeloid cell leukemia sequence 1



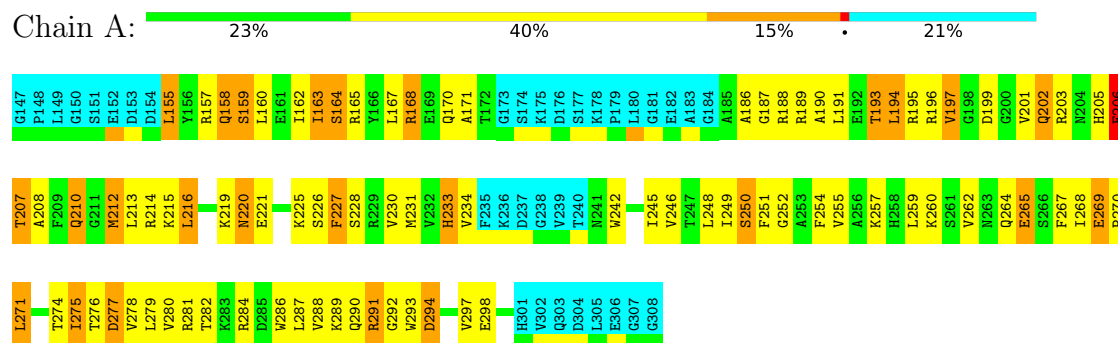
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: myeloid cell leukemia sequence 1



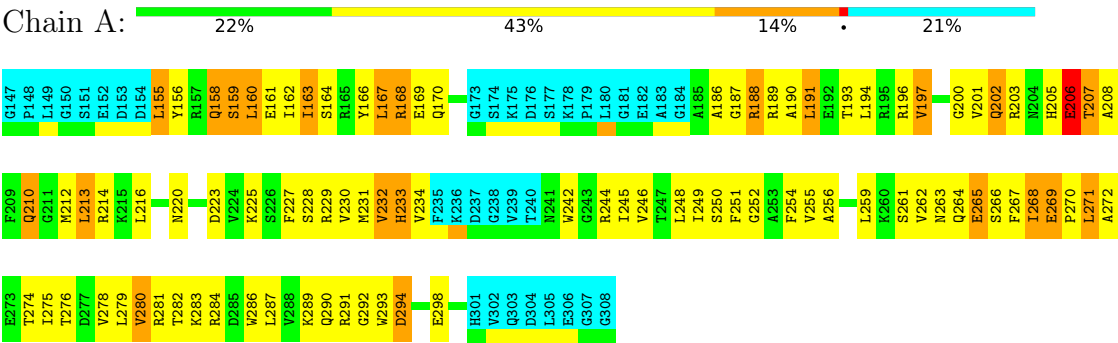
4.2.19 Score per residue for model 19

- Molecule 1: myeloid cell leukemia sequence 1



4.2.20 Score per residue for model 20

● Molecule 1: myeloid cell leukemia sequence 1



5 Refinement protocol and experimental data overview

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

Of the 256 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy, structures with the least restraint violations, structures with acceptable covalent geometry*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
XPLOR-NIH	refinement	2

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1049	1069	1066	75±5
All	All	20980	21380	21320	1502

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	Total
1:A:231:MET:HE2	1:A:248:LEU:HD11	0.91	1.41	3	2
1:A:163:ILE:HD13	1:A:276:THR:HG23	0.89	1.45	18	18
1:A:212:MET:O	1:A:216:LEU:HD13	0.87	1.69	18	6
1:A:248:LEU:HD12	1:A:279:LEU:HD23	0.85	1.47	18	10
1:A:163:ILE:HG21	1:A:276:THR:OG1	0.82	1.74	12	19
1:A:252:GLY:HA3	1:A:275:ILE:HD13	0.80	1.52	18	11
1:A:234:VAL:HG11	1:A:248:LEU:HB2	0.79	1.54	19	6
1:A:158:GLN:NE2	1:A:186:ALA:HB3	0.78	1.93	1	3
1:A:155:LEU:HD21	1:A:287:LEU:HD13	0.78	1.54	5	20
1:A:193:THR:O	1:A:197:VAL:HG22	0.77	1.78	17	16
1:A:248:LEU:HD13	1:A:279:LEU:HD12	0.76	1.57	17	2
1:A:245:ILE:HD11	1:A:283:LYS:HD2	0.76	1.55	17	1
1:A:231:MET:SD	1:A:248:LEU:HD21	0.76	2.20	19	11
1:A:248:LEU:HD12	1:A:279:LEU:HD13	0.74	1.59	2	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:231:MET:SD	1:A:248:LEU:HD11	0.72	2.24	13	15
1:A:274:THR:O	1:A:278:VAL:HG22	0.72	1.84	18	18
1:A:167:LEU:HD22	1:A:272:ALA:HB2	0.71	1.59	20	6
1:A:162:ILE:HG12	1:A:187:GLY:HA2	0.70	1.63	18	20
1:A:205:HIS:O	1:A:209:PHE:HB2	0.70	1.86	9	2
1:A:231:MET:HE2	1:A:278:VAL:HB	0.69	1.62	7	8
1:A:160:LEU:HA	1:A:276:THR:HG21	0.69	1.64	14	5
1:A:262:VAL:HG23	1:A:264:GLN:HG3	0.68	1.64	19	11
1:A:231:MET:HE2	1:A:278:VAL:HG22	0.67	1.66	1	2
1:A:248:LEU:HD22	1:A:279:LEU:HD23	0.67	1.66	19	1
1:A:197:VAL:O	1:A:201:VAL:HG23	0.66	1.90	13	13
1:A:234:VAL:HB	1:A:248:LEU:HD22	0.66	1.68	16	3
1:A:213:LEU:C	1:A:213:LEU:HD22	0.65	2.17	13	2
1:A:165:ARG:HB3	1:A:191:LEU:HD22	0.65	1.68	7	4
1:A:252:GLY:HA3	1:A:275:ILE:HD12	0.65	1.69	17	9
1:A:201:VAL:HG11	1:A:250:SER:HB3	0.64	1.68	3	13
1:A:231:MET:HA	1:A:248:LEU:HD21	0.64	1.69	5	12
1:A:231:MET:HA	1:A:248:LEU:HD11	0.64	1.68	19	1
1:A:278:VAL:O	1:A:282:THR:HB	0.64	1.92	17	19
1:A:201:VAL:HG11	1:A:250:SER:CB	0.63	2.22	17	20
1:A:230:VAL:O	1:A:234:VAL:HG23	0.63	1.93	9	20
1:A:259:LEU:HD12	1:A:271:LEU:HD22	0.62	1.70	7	4
1:A:201:VAL:HG13	1:A:205:HIS:CD2	0.62	2.28	17	1
1:A:230:VAL:HG12	1:A:233:HIS:CD2	0.62	2.30	20	2
1:A:231:MET:CE	1:A:278:VAL:HG13	0.62	2.25	14	2
1:A:234:VAL:HG21	1:A:248:LEU:HD23	0.62	1.72	20	6
1:A:230:VAL:HG21	1:A:251:PHE:HE2	0.61	1.55	9	12
1:A:283:LYS:HG2	1:A:286:TRP:HB3	0.61	1.71	17	1
1:A:159:SER:O	1:A:163:ILE:HB	0.61	1.94	19	16
1:A:166:TYR:N	1:A:191:LEU:HD11	0.61	2.09	17	3
1:A:286:TRP:HA	1:A:289:LYS:HG2	0.61	1.72	3	4
1:A:280:VAL:HG23	1:A:287:LEU:HD13	0.61	1.73	1	20
1:A:230:VAL:HA	1:A:233:HIS:CD2	0.60	2.31	20	16
1:A:291:ARG:HB3	1:A:294:ASP:HB3	0.60	1.71	16	2
1:A:231:MET:HE3	1:A:278:VAL:CG2	0.60	2.27	17	2
1:A:213:LEU:HG	1:A:255:VAL:HG22	0.60	1.72	13	2
1:A:211:GLY:HA2	1:A:214:ARG:HG2	0.60	1.73	1	1
1:A:230:VAL:HG21	1:A:251:PHE:CE2	0.60	2.32	5	17
1:A:229:ARG:O	1:A:233:HIS:HB3	0.60	1.96	17	2
1:A:158:GLN:OE1	1:A:162:ILE:HD11	0.60	1.96	7	4
1:A:267:PHE:O	1:A:271:LEU:HB2	0.59	1.97	20	17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:227:PHE:O	1:A:231:MET:HG2	0.59	1.96	6	16
1:A:218:ILE:CG2	1:A:259:LEU:HD21	0.59	2.28	12	3
1:A:218:ILE:HG21	1:A:259:LEU:HD21	0.59	1.75	12	9
1:A:212:MET:O	1:A:216:LEU:HG	0.58	1.97	5	12
1:A:287:LEU:HD23	1:A:292:GLY:HA2	0.58	1.73	1	20
1:A:213:LEU:HA	1:A:216:LEU:HD22	0.58	1.75	12	2
1:A:220:ASN:H	1:A:223:ASP:CG	0.58	2.06	12	1
1:A:230:VAL:HG11	1:A:251:PHE:CD2	0.58	2.33	12	1
1:A:265:GLU:HG2	1:A:268:ILE:HD12	0.58	1.76	2	2
1:A:155:LEU:CD2	1:A:287:LEU:HD13	0.58	2.29	2	20
1:A:233:HIS:C	1:A:233:HIS:ND1	0.57	2.61	12	3
1:A:194:LEU:HA	1:A:197:VAL:CG2	0.57	2.29	14	16
1:A:158:GLN:HA	1:A:158:GLN:OE1	0.57	1.99	10	1
1:A:283:LYS:HD3	1:A:287:LEU:HG	0.57	1.75	17	1
1:A:265:GLU:HA	1:A:268:ILE:HD12	0.57	1.77	17	20
1:A:287:LEU:O	1:A:292:GLY:N	0.57	2.38	16	20
1:A:164:SER:O	1:A:168:ARG:HB2	0.57	2.00	11	16
1:A:213:LEU:HA	1:A:216:LEU:HG	0.57	1.76	13	2
1:A:193:THR:O	1:A:197:VAL:HG12	0.57	2.00	5	4
1:A:278:VAL:O	1:A:282:THR:N	0.57	2.37	7	1
1:A:291:ARG:NE	1:A:294:ASP:HB3	0.57	2.15	20	2
1:A:194:LEU:HD11	1:A:249:ILE:HD13	0.56	1.76	7	1
1:A:231:MET:HE2	1:A:278:VAL:HG13	0.56	1.75	14	2
1:A:251:PHE:O	1:A:255:VAL:HG23	0.56	1.99	10	18
1:A:227:PHE:CE2	1:A:275:ILE:HD12	0.56	2.36	2	6
1:A:248:LEU:HD12	1:A:275:ILE:HD11	0.56	1.77	5	2
1:A:231:MET:HB2	1:A:248:LEU:HD11	0.56	1.78	17	2
1:A:189:ARG:HG2	1:A:297:VAL:HG11	0.55	1.79	10	1
1:A:159:SER:N	1:A:293:TRP:HE1	0.55	1.99	10	18
1:A:165:ARG:HA	1:A:165:ARG:HE	0.55	1.62	14	4
1:A:282:THR:HG22	1:A:283:LYS:HD3	0.55	1.79	9	1
1:A:231:MET:SD	1:A:232:VAL:HG23	0.55	2.42	3	1
1:A:202:GLN:NE2	1:A:254:PHE:HB2	0.55	2.17	16	17
1:A:205:HIS:O	1:A:208:ALA:N	0.54	2.41	2	18
1:A:227:PHE:CE2	1:A:271:LEU:HD11	0.54	2.37	3	9
1:A:231:MET:HE2	1:A:278:VAL:CG2	0.54	2.32	1	3
1:A:206:GLU:O	1:A:210:GLN:HB2	0.54	2.02	10	18
1:A:160:LEU:HD13	1:A:276:THR:HG21	0.54	1.79	7	1
1:A:213:LEU:HD21	1:A:258:HIS:NE2	0.54	2.17	9	2
1:A:282:THR:HG23	1:A:283:LYS:HD2	0.53	1.80	11	2
1:A:156:TYR:HE1	1:A:160:LEU:HD22	0.53	1.63	3	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:290:GLN:O	1:A:291:ARG:HG2	0.53	2.04	9	2
1:A:291:ARG:O	1:A:291:ARG:HD3	0.53	2.04	16	1
1:A:272:ALA:HA	1:A:275:ILE:HG22	0.53	1.81	20	9
1:A:248:LEU:HD13	1:A:279:LEU:CD1	0.53	2.31	17	1
1:A:220:ASN:O	1:A:223:ASP:OD2	0.53	2.27	12	1
1:A:163:ILE:HD13	1:A:276:THR:CG2	0.53	2.30	2	8
1:A:216:LEU:HD12	1:A:216:LEU:N	0.53	2.18	11	2
1:A:214:ARG:HG3	1:A:215:LYS:N	0.53	2.17	1	1
1:A:171:ALA:HA	1:A:257:LYS:HA	0.53	1.81	7	5
1:A:156:TYR:CE1	1:A:160:LEU:HD22	0.53	2.38	5	15
1:A:158:GLN:HE21	1:A:162:ILE:HD12	0.53	1.64	6	5
1:A:227:PHE:CE1	1:A:271:LEU:HD11	0.52	2.39	20	6
1:A:231:MET:HE3	1:A:278:VAL:HB	0.52	1.80	17	2
1:A:229:ARG:O	1:A:232:VAL:HG13	0.52	2.04	20	3
1:A:212:MET:HE2	1:A:251:PHE:CD1	0.52	2.39	15	11
1:A:245:ILE:HD12	1:A:286:TRP:CZ3	0.52	2.39	15	9
1:A:280:VAL:HA	1:A:287:LEU:HD11	0.52	1.81	17	4
1:A:210:GLN:O	1:A:214:ARG:HB2	0.52	2.04	2	17
1:A:283:LYS:HE3	1:A:286:TRP:CD2	0.52	2.40	17	1
1:A:227:PHE:HE2	1:A:275:ILE:HD12	0.52	1.64	2	3
1:A:189:ARG:O	1:A:193:THR:HB	0.52	2.05	5	2
1:A:227:PHE:HA	1:A:230:VAL:CG2	0.52	2.35	17	5
1:A:234:VAL:CB	1:A:248:LEU:HD22	0.52	2.34	16	2
1:A:227:PHE:CE1	1:A:275:ILE:HD12	0.52	2.39	15	2
1:A:256:ALA:O	1:A:268:ILE:HD11	0.52	2.05	20	1
1:A:282:THR:HG22	1:A:283:LYS:HE2	0.52	1.81	1	1
1:A:228:SER:O	1:A:231:MET:HG3	0.52	2.05	17	2
1:A:219:LYS:H	1:A:223:ASP:CG	0.52	2.13	12	1
1:A:230:VAL:HG11	1:A:251:PHE:HD2	0.52	1.65	12	1
1:A:155:LEU:CD1	1:A:293:TRP:CD1	0.51	2.93	17	19
1:A:188:ARG:HG3	1:A:189:ARG:N	0.51	2.20	2	1
1:A:280:VAL:HA	1:A:287:LEU:CD1	0.51	2.34	16	9
1:A:212:MET:HE3	1:A:251:PHE:CD1	0.51	2.40	18	5
1:A:216:LEU:HD22	1:A:226:SER:HB2	0.51	1.82	19	1
1:A:194:LEU:HA	1:A:197:VAL:HG12	0.51	1.82	8	4
1:A:201:VAL:HG11	1:A:250:SER:OG	0.51	2.06	12	4
1:A:205:HIS:O	1:A:206:GLU:C	0.51	2.52	3	18
1:A:277:ASP:O	1:A:281:ARG:HB2	0.51	2.05	8	8
1:A:227:PHE:CZ	1:A:271:LEU:HD11	0.51	2.40	20	1
1:A:186:ALA:O	1:A:190:ALA:N	0.51	2.43	8	15
1:A:163:ILE:HD13	1:A:276:THR:OG1	0.51	2.05	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:234:VAL:HG21	1:A:248:LEU:HD13	0.51	1.81	16	1
1:A:286:TRP:C	1:A:286:TRP:CD1	0.50	2.89	1	16
1:A:227:PHE:CE1	1:A:255:VAL:HG11	0.50	2.41	2	7
1:A:230:VAL:O	1:A:233:HIS:HB2	0.50	2.06	2	3
1:A:246:VAL:O	1:A:250:SER:HB3	0.50	2.06	12	3
1:A:218:ILE:HG21	1:A:259:LEU:HD11	0.50	1.84	8	1
1:A:158:GLN:NE2	1:A:162:ILE:HD11	0.50	2.22	10	1
1:A:234:VAL:HB	1:A:248:LEU:HD12	0.50	1.83	19	1
1:A:291:ARG:HD3	1:A:294:ASP:HB3	0.50	1.83	1	5
1:A:287:LEU:HD23	1:A:292:GLY:CA	0.50	2.37	17	8
1:A:227:PHE:CE2	1:A:255:VAL:HG11	0.50	2.41	15	2
1:A:227:PHE:O	1:A:230:VAL:HB	0.50	2.06	12	1
1:A:166:TYR:N	1:A:191:LEU:HD21	0.49	2.22	14	2
1:A:205:HIS:O	1:A:207:THR:N	0.49	2.46	12	18
1:A:202:GLN:HE22	1:A:254:PHE:HB2	0.49	1.67	2	2
1:A:162:ILE:HD13	1:A:293:TRP:CZ2	0.49	2.43	11	2
1:A:234:VAL:CG2	1:A:248:LEU:HD22	0.49	2.37	8	2
1:A:213:LEU:HD21	1:A:258:HIS:CE1	0.49	2.42	9	2
1:A:216:LEU:N	1:A:216:LEU:CD1	0.49	2.76	11	2
1:A:228:SER:O	1:A:231:MET:HB2	0.49	2.08	1	12
1:A:252:GLY:HA3	1:A:275:ILE:CD1	0.49	2.38	10	7
1:A:164:SER:HB3	1:A:165:ARG:NH2	0.49	2.23	15	2
1:A:191:LEU:O	1:A:195:ARG:HB2	0.49	2.08	7	5
1:A:230:VAL:HA	1:A:233:HIS:CG	0.49	2.43	2	3
1:A:282:THR:HG22	1:A:283:LYS:HD2	0.49	1.85	16	1
1:A:242:TRP:O	1:A:246:VAL:HG23	0.48	2.07	9	18
1:A:190:ALA:O	1:A:194:LEU:HB2	0.48	2.08	6	12
1:A:155:LEU:CD2	1:A:280:VAL:HG23	0.48	2.38	7	8
1:A:155:LEU:CD1	1:A:159:SER:OG	0.48	2.61	17	12
1:A:271:LEU:O	1:A:275:ILE:HG12	0.48	2.08	12	9
1:A:278:VAL:O	1:A:282:THR:CB	0.48	2.61	19	16
1:A:227:PHE:CZ	1:A:252:GLY:HA2	0.48	2.44	7	5
1:A:194:LEU:HA	1:A:197:VAL:HG23	0.48	1.85	17	16
1:A:168:ARG:O	1:A:172:THR:HG22	0.48	2.09	3	2
1:A:276:THR:HG22	1:A:277:ASP:N	0.48	2.23	7	1
1:A:158:GLN:HG2	1:A:162:ILE:CD1	0.48	2.39	1	1
1:A:209:PHE:HZ	1:A:250:SER:HB3	0.48	1.68	9	1
1:A:162:ILE:HG12	1:A:187:GLY:CA	0.48	2.39	15	8
1:A:213:LEU:HA	1:A:216:LEU:HB2	0.48	1.85	17	3
1:A:242:TRP:CE3	1:A:245:ILE:HG21	0.48	2.43	17	1
1:A:231:MET:HE2	1:A:278:VAL:CG1	0.47	2.38	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:LEU:HD11	1:A:253:ALA:HA	0.47	1.87	8	3
1:A:233:HIS:C	1:A:233:HIS:HD1	0.47	2.16	12	1
1:A:231:MET:HE3	1:A:278:VAL:CB	0.47	2.39	17	1
1:A:275:ILE:O	1:A:279:LEU:HB2	0.47	2.10	14	2
1:A:194:LEU:HA	1:A:197:VAL:CG1	0.47	2.39	13	3
1:A:160:LEU:HD13	1:A:276:THR:CG2	0.47	2.40	7	1
1:A:158:GLN:HB3	1:A:293:TRP:CD1	0.47	2.45	11	4
1:A:163:ILE:CD1	1:A:276:THR:HG23	0.47	2.35	6	2
1:A:163:ILE:HD11	1:A:249:ILE:HD11	0.47	1.85	7	1
1:A:213:LEU:HD12	1:A:255:VAL:HG22	0.47	1.86	3	10
1:A:165:ARG:NE	1:A:165:ARG:HA	0.47	2.25	12	3
1:A:284:ARG:O	1:A:288:VAL:HG23	0.47	2.10	19	15
1:A:186:ALA:O	1:A:190:ALA:CB	0.47	2.63	10	2
1:A:283:LYS:O	1:A:283:LYS:CG	0.47	2.63	17	1
1:A:167:LEU:HD22	1:A:272:ALA:CB	0.46	2.38	5	4
1:A:218:ILE:HD13	1:A:223:ASP:HB2	0.46	1.86	12	1
1:A:194:LEU:HD13	1:A:296:PHE:HZ	0.46	1.70	17	1
1:A:267:PHE:C	1:A:270:PRO:HD2	0.46	2.35	1	12
1:A:163:ILE:O	1:A:167:LEU:HB2	0.46	2.10	2	3
1:A:259:LEU:CD1	1:A:271:LEU:HD22	0.46	2.40	19	3
1:A:193:THR:O	1:A:196:ARG:HG2	0.46	2.11	18	1
1:A:230:VAL:O	1:A:233:HIS:HD2	0.46	1.93	3	9
1:A:286:TRP:CD1	1:A:286:TRP:C	0.46	2.94	15	3
1:A:291:ARG:HB3	1:A:294:ASP:HB2	0.46	1.87	5	2
1:A:291:ARG:HG3	1:A:294:ASP:HB3	0.46	1.87	9	2
1:A:158:GLN:NE2	1:A:158:GLN:HA	0.46	2.24	11	5
1:A:162:ILE:HD13	1:A:293:TRP:CE2	0.46	2.46	11	1
1:A:213:LEU:HD13	1:A:214:ARG:N	0.46	2.26	13	1
1:A:213:LEU:C	1:A:213:LEU:CD2	0.46	2.89	9	2
1:A:155:LEU:CD2	1:A:287:LEU:HD22	0.46	2.41	17	1
1:A:291:ARG:O	1:A:292:GLY:C	0.45	2.58	15	10
1:A:156:TYR:CD1	1:A:280:VAL:HG11	0.45	2.47	5	7
1:A:191:LEU:O	1:A:191:LEU:HD12	0.45	2.11	7	1
1:A:165:ARG:HH21	1:A:168:ARG:HD3	0.45	1.70	9	1
1:A:213:LEU:HD22	1:A:258:HIS:CE1	0.45	2.46	12	6
1:A:295:GLY:HA2	1:A:298:GLU:HG3	0.45	1.88	9	1
1:A:220:ASN:HA	1:A:267:PHE:CE1	0.45	2.46	8	18
1:A:279:LEU:O	1:A:283:LYS:HB3	0.45	2.12	17	1
1:A:162:ILE:CG1	1:A:187:GLY:HA2	0.45	2.40	6	2
1:A:227:PHE:O	1:A:230:VAL:HG23	0.45	2.11	8	3
1:A:259:LEU:O	1:A:262:VAL:HG22	0.45	2.12	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:GLU:O	1:A:165:ARG:HD2	0.45	2.12	9	2
1:A:212:MET:HB3	1:A:251:PHE:CE1	0.45	2.46	9	2
1:A:165:ARG:HA	1:A:165:ARG:NE	0.45	2.26	14	1
1:A:242:TRP:CZ3	1:A:296:PHE:HB2	0.44	2.47	15	5
1:A:167:LEU:HD23	1:A:256:ALA:CB	0.44	2.42	5	1
1:A:155:LEU:O	1:A:158:GLN:N	0.44	2.51	5	3
1:A:158:GLN:NE2	1:A:161:GLU:HB2	0.44	2.27	6	1
1:A:228:SER:O	1:A:232:VAL:HG12	0.44	2.12	20	2
1:A:227:PHE:HZ	1:A:255:VAL:HB	0.44	1.73	3	5
1:A:283:LYS:HD2	1:A:286:TRP:HE3	0.44	1.73	10	1
1:A:227:PHE:HE2	1:A:255:VAL:HG11	0.44	1.72	15	1
1:A:234:VAL:CG2	1:A:248:LEU:HD23	0.44	2.41	20	2
1:A:260:LYS:N	1:A:268:ILE:HD11	0.44	2.27	4	2
1:A:163:ILE:CG2	1:A:164:SER:N	0.44	2.80	19	2
1:A:163:ILE:HG22	1:A:164:SER:N	0.44	2.26	14	2
1:A:187:GLY:O	1:A:191:LEU:HB2	0.43	2.14	6	1
1:A:268:ILE:HG22	1:A:269:GLU:N	0.43	2.28	20	1
1:A:259:LEU:HD12	1:A:271:LEU:HG	0.43	1.91	14	5
1:A:201:VAL:HG11	1:A:250:SER:HB2	0.43	1.90	12	2
1:A:248:LEU:C	1:A:248:LEU:HD13	0.43	2.38	18	4
1:A:205:HIS:O	1:A:209:PHE:CB	0.43	2.62	9	2
1:A:262:VAL:HG12	1:A:264:GLN:HG3	0.43	1.91	15	2
1:A:158:GLN:HE22	1:A:186:ALA:HB3	0.43	1.74	8	1
1:A:219:LYS:N	1:A:223:ASP:OD2	0.43	2.51	12	1
1:A:155:LEU:HB3	1:A:284:ARG:NH2	0.43	2.28	20	1
1:A:242:TRP:CH2	1:A:296:PHE:HB2	0.43	2.49	9	1
1:A:291:ARG:O	1:A:293:TRP:N	0.43	2.52	16	1
1:A:227:PHE:HE1	1:A:255:VAL:HG11	0.43	1.74	20	3
1:A:242:TRP:HB2	1:A:299:PHE:CD2	0.43	2.49	13	4
1:A:269:GLU:N	1:A:270:PRO:HD2	0.43	2.29	19	8
1:A:290:GLN:HG3	1:A:291:ARG:HH21	0.43	1.72	9	1
1:A:292:GLY:O	1:A:293:TRP:C	0.43	2.62	13	2
1:A:227:PHE:HA	1:A:230:VAL:HG23	0.43	1.91	17	1
1:A:282:THR:HB	1:A:283:LYS:HZ3	0.42	1.73	5	1
1:A:252:GLY:CA	1:A:275:ILE:HD13	0.42	2.42	8	1
1:A:167:LEU:CD1	1:A:253:ALA:HA	0.42	2.44	8	2
1:A:213:LEU:HA	1:A:216:LEU:CD1	0.42	2.44	9	2
1:A:185:ALA:O	1:A:189:ARG:HB2	0.42	2.14	10	1
1:A:290:GLN:C	1:A:292:GLY:N	0.42	2.78	16	2
1:A:212:MET:HE2	1:A:251:PHE:CG	0.42	2.49	17	1
1:A:210:GLN:O	1:A:214:ARG:HB3	0.42	2.15	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:216:LEU:HD22	1:A:226:SER:HB3	0.42	1.92	8	1
1:A:226:SER:O	1:A:230:VAL:HG22	0.42	2.14	17	1
1:A:213:LEU:CD1	1:A:255:VAL:HG22	0.42	2.45	5	1
1:A:279:LEU:HA	1:A:283:LYS:NZ	0.42	2.29	9	1
1:A:218:ILE:HA	1:A:223:ASP:CB	0.42	2.45	12	1
1:A:205:HIS:C	1:A:207:THR:N	0.42	2.78	10	5
1:A:265:GLU:HA	1:A:268:ILE:HB	0.42	1.91	15	2
1:A:158:GLN:HE21	1:A:186:ALA:HB3	0.42	1.67	1	1
1:A:215:LYS:HG3	1:A:216:LEU:HD23	0.42	1.90	13	1
1:A:167:LEU:HD12	1:A:272:ALA:HB2	0.42	1.91	17	1
1:A:231:MET:HE2	1:A:248:LEU:CD1	0.42	2.35	17	1
1:A:283:LYS:HG2	1:A:283:LYS:O	0.42	2.15	17	1
1:A:155:LEU:HD12	1:A:155:LEU:O	0.41	2.15	4	2
1:A:190:ALA:O	1:A:194:LEU:N	0.41	2.51	9	1
1:A:212:MET:HE3	1:A:251:PHE:CE1	0.41	2.50	12	1
1:A:155:LEU:HD13	1:A:293:TRP:CD1	0.41	2.49	17	1
1:A:213:LEU:CG	1:A:255:VAL:HG22	0.41	2.45	13	1
1:A:231:MET:HG3	1:A:278:VAL:HG21	0.41	1.91	14	2
1:A:275:ILE:O	1:A:278:VAL:HG12	0.41	2.15	1	1
1:A:264:GLN:C	1:A:266:SER:N	0.41	2.78	5	6
1:A:213:LEU:HA	1:A:216:LEU:CG	0.41	2.45	13	1
1:A:165:ARG:HB3	1:A:191:LEU:HD12	0.41	1.92	18	1
1:A:207:THR:HG23	1:A:208:ALA:N	0.41	2.31	12	3
1:A:230:VAL:HA	1:A:233:HIS:HB2	0.41	1.92	8	2
1:A:165:ARG:HE	1:A:165:ARG:CA	0.41	2.29	15	1
1:A:283:LYS:CE	1:A:287:LEU:HG	0.41	2.46	17	1
1:A:155:LEU:O	1:A:156:TYR:C	0.41	2.64	1	2
1:A:191:LEU:HD12	1:A:191:LEU:O	0.41	2.15	1	1
1:A:186:ALA:O	1:A:190:ALA:HB3	0.41	2.16	10	1
1:A:283:LYS:CD	1:A:287:LEU:HG	0.41	2.42	17	1
1:A:200:GLY:O	1:A:203:ARG:HG2	0.41	2.16	20	1
1:A:228:SER:HA	1:A:231:MET:CG	0.41	2.46	3	1
1:A:231:MET:CE	1:A:278:VAL:HB	0.41	2.46	3	1
1:A:234:VAL:HG21	1:A:248:LEU:HD22	0.41	1.93	5	1
1:A:156:TYR:OH	1:A:277:ASP:HB2	0.41	2.15	2	1
1:A:194:LEU:CD1	1:A:249:ILE:HG21	0.41	2.45	5	1
1:A:293:TRP:O	1:A:297:VAL:HG23	0.41	2.16	8	1
1:A:269:GLU:CB	1:A:270:PRO:HD3	0.40	2.46	1	1
1:A:248:LEU:HD13	1:A:248:LEU:C	0.40	2.40	10	1
1:A:231:MET:HE2	1:A:278:VAL:CB	0.40	2.45	16	1
1:A:227:PHE:O	1:A:231:MET:N	0.40	2.54	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:SER:CA	1:A:293:TRP:HE1	0.40	2.29	10	1
1:A:160:LEU:HD13	1:A:276:THR:CB	0.40	2.46	1	1
1:A:248:LEU:HB3	1:A:279:LEU:HD11	0.40	1.94	5	1
1:A:290:GLN:O	1:A:292:GLY:N	0.40	2.54	9	1
1:A:196:ARG:HG3	1:A:197:VAL:N	0.40	2.31	5	1
1:A:277:ASP:O	1:A:281:ARG:CB	0.40	2.69	14	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	128/162 (79%)	118±2 (92±1%)	8±2 (6±1%)	2±1 (1±0%)	11	58
All	All	2560/3240 (79%)	2361 (92%)	163 (6%)	36 (1%)	11	58

All 4 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	206	GLU	17
1	A	291	ARG	9
1	A	292	GLY	8
1	A	216	LEU	2

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	111/136 (82%)	64±4 (58±3%)	47±4 (42±3%)	0	4
All	All	2220/2720 (82%)	1285 (58%)	935 (42%)	0	4

All 88 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	155	LEU	20
1	A	159	SER	20
1	A	163	ILE	20
1	A	189	ARG	20
1	A	210	GLN	20
1	A	213	LEU	20
1	A	245	ILE	20
1	A	249	ILE	20
1	A	271	LEU	20
1	A	294	ASP	19
1	A	220	ASN	18
1	A	290	GLN	18
1	A	158	GLN	18
1	A	160	LEU	17
1	A	168	ARG	17
1	A	233	HIS	17
1	A	298	GLU	16
1	A	197	VAL	15
1	A	216	LEU	15
1	A	260	LYS	15
1	A	289	LYS	15
1	A	165	ARG	14
1	A	169	GLU	14
1	A	199	ASP	14
1	A	207	THR	14
1	A	214	ARG	14
1	A	263	ASN	14
1	A	219	LYS	14
1	A	223	ASP	14
1	A	157	ARG	13
1	A	170	GLN	13
1	A	188	ARG	13
1	A	202	GLN	13
1	A	215	LYS	13
1	A	229	ARG	13
1	A	261	SER	13
1	A	196	ARG	13
1	A	291	ARG	13
1	A	203	ARG	12
1	A	224	VAL	12
1	A	225	LYS	12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	285	ASP	12
1	A	161	GLU	12
1	A	167	LEU	12
1	A	194	LEU	11
1	A	227	PHE	11
1	A	279	LEU	11
1	A	283	LYS	11
1	A	191	LEU	11
1	A	193	THR	11
1	A	228	SER	9
1	A	265	GLU	9
1	A	269	GLU	9
1	A	172	THR	9
1	A	206	GLU	8
1	A	276	THR	8
1	A	244	ARG	8
1	A	273	GLU	8
1	A	299	PHE	8
1	A	281	ARG	8
1	A	192	GLU	7
1	A	241	ASN	7
1	A	297	VAL	7
1	A	232	VAL	7
1	A	164	SER	7
1	A	212	MET	7
1	A	275	ILE	6
1	A	257	LYS	6
1	A	162	ILE	6
1	A	221	GLU	6
1	A	284	ARG	6
1	A	195	ARG	4
1	A	226	SER	4
1	A	248	LEU	4
1	A	234	VAL	3
1	A	282	THR	2
1	A	262	VAL	2
1	A	266	SER	2
1	A	250	SER	2
1	A	278	VAL	1
1	A	288	VAL	1
1	A	209	PHE	1
1	A	217	ASP	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	230	VAL	1
1	A	277	ASP	1
1	A	259	LEU	1
1	A	268	ILE	1
1	A	280	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided