



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 13, 2023 – 06:45 PM EST

PDB ID : 2JM6  
Title : Solution structure of MCL-1 complexed with NOXAB  
Authors : Czabotar, P.E.; Lee, E.F.; van Delft, M.F.; Day, C.L.; Smith, B.J.; Huang, D.C.S.; Fairlie, W.D.; Hinds, M.G.; Colman, P.M.  
Deposited on : 2006-10-17

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

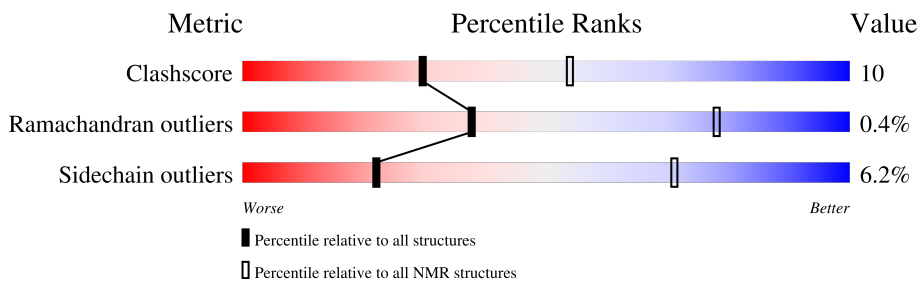
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	27	
2	B	162	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:74-A:90, B:154-B:172, B:183-B:301 (155)	0.68	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 4 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3030 atoms, of which 1524 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Noxa.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	27	453	133	235	43	40	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MET	-	expression tag	UNP Q9JM54

- Molecule 2 is a protein called Myeloid cell leukemia-1 protein Mcl-1 homolog.

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

There are 5 discrepancies between the modelled and reference sequences:

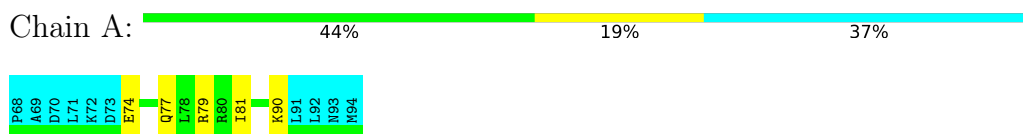
Chain	Residue	Modelled	Actual	Comment	Reference
B	147	GLY	-	expression tag	UNP P97287
B	148	PRO	-	expression tag	UNP P97287
B	149	LEU	-	expression tag	UNP P97287
B	150	GLY	-	expression tag	UNP P97287
B	151	SER	-	expression tag	UNP P97287

## 4 Residue-property plots

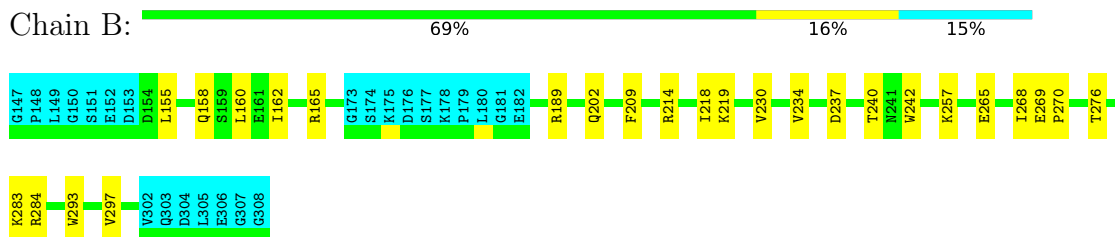
### 4.1 Average score per residue in the NMR ensemble

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: Noxa



- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog

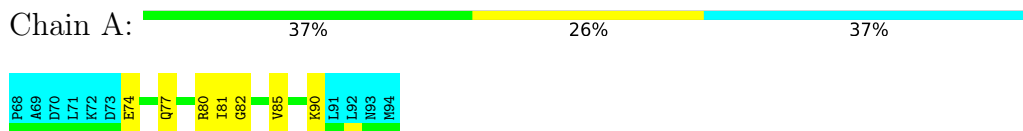


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

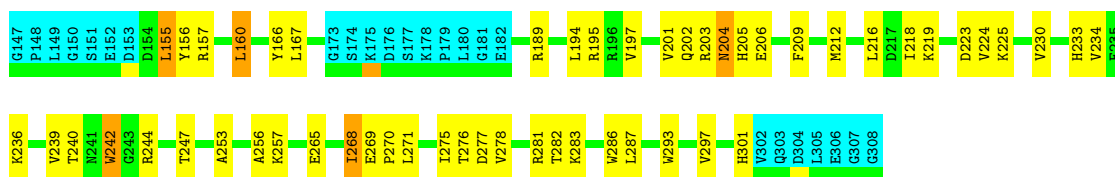
#### 4.2.1 Score per residue for model 1

- Molecule 1: Noxa



- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



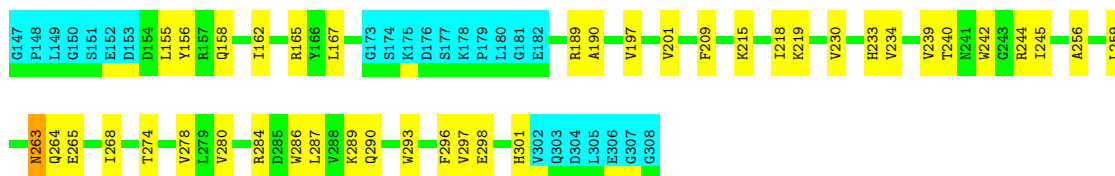


#### 4.2.2 Score per residue for model 2

- Molecule 1: Noxa

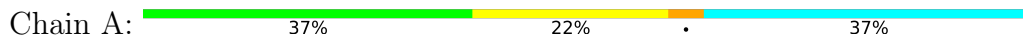


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog

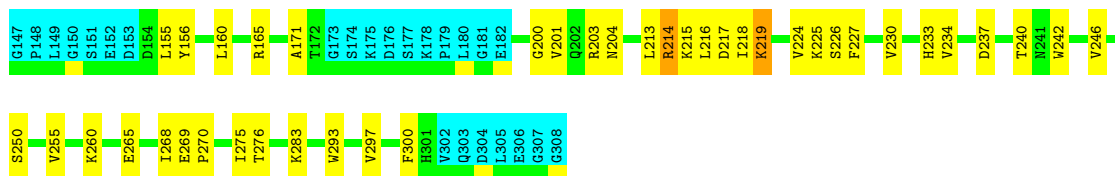


#### 4.2.3 Score per residue for model 3

- Molecule 1: Noxa

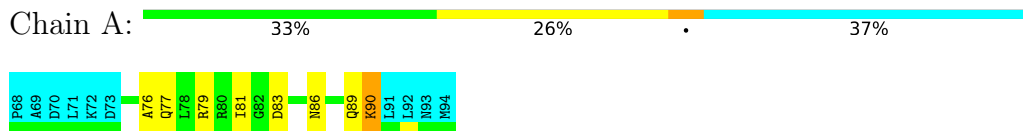


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



#### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Noxa



- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog

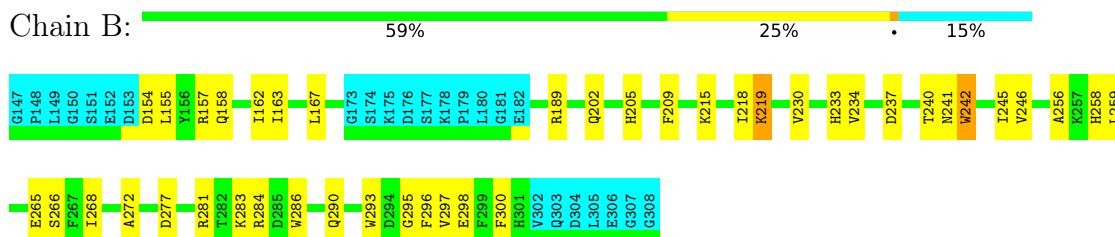


#### 4.2.5 Score per residue for model 5

- Molecule 1: Noxa



- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



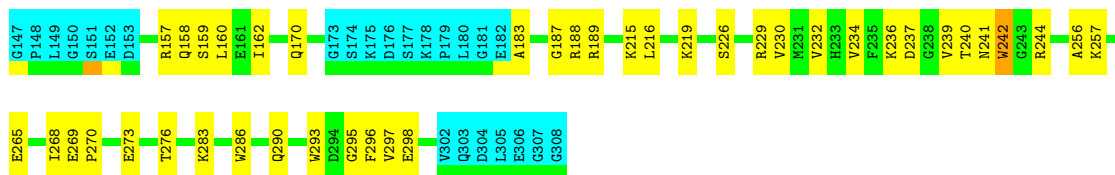
#### 4.2.6 Score per residue for model 6

- Molecule 1: Noxa



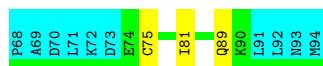
- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



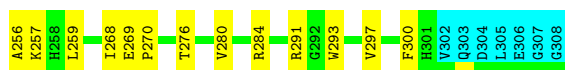
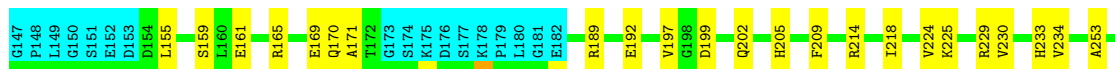


#### 4.2.7 Score per residue for model 7

- Molecule 1: Noxa

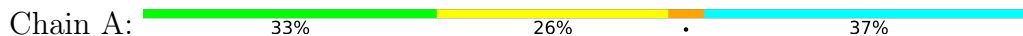


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



#### 4.2.8 Score per residue for model 8

- Molecule 1: Noxa



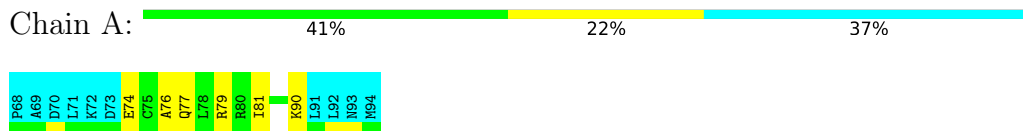
- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



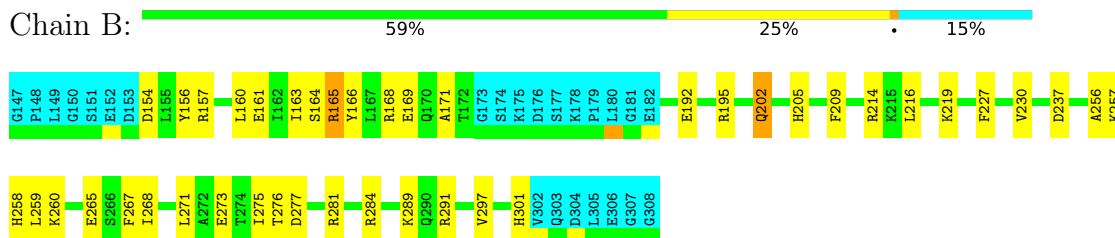
#### 4.2.9 Score per residue for model 9

- Molecule 1: Noxa



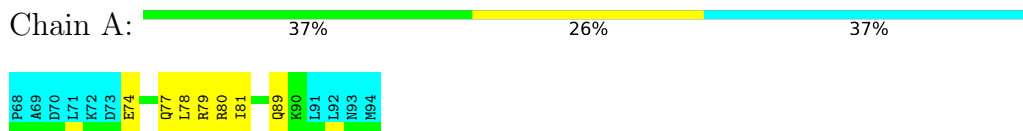


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog

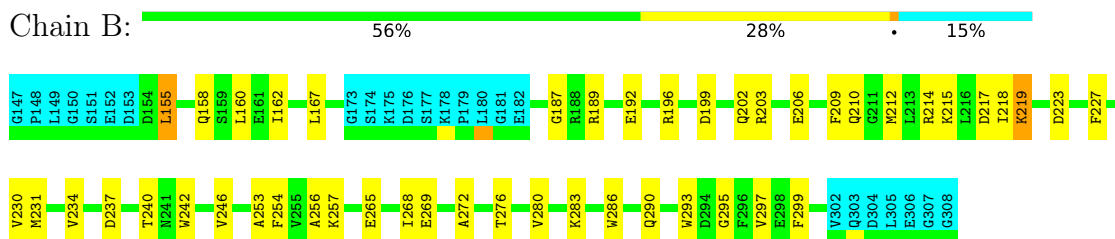


#### 4.2.10 Score per residue for model 10

- Molecule 1: Noxa

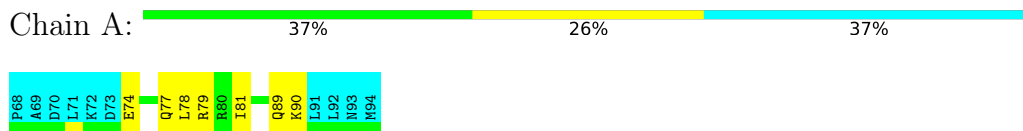


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



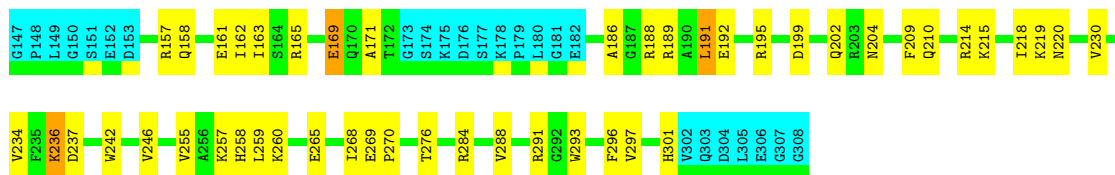
#### 4.2.11 Score per residue for model 11

- Molecule 1: Noxa



- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



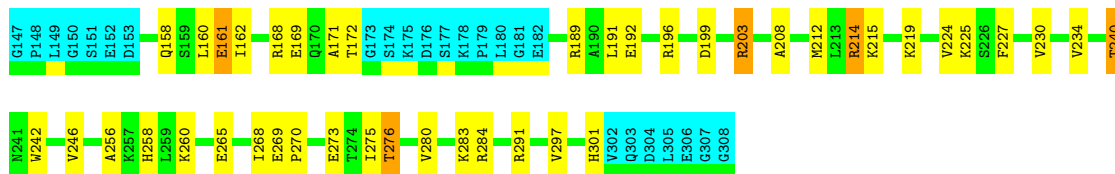


#### 4.2.12 Score per residue for model 12

- Molecule 1: Noxa

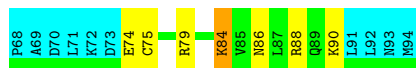
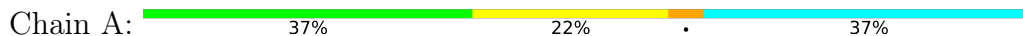


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog

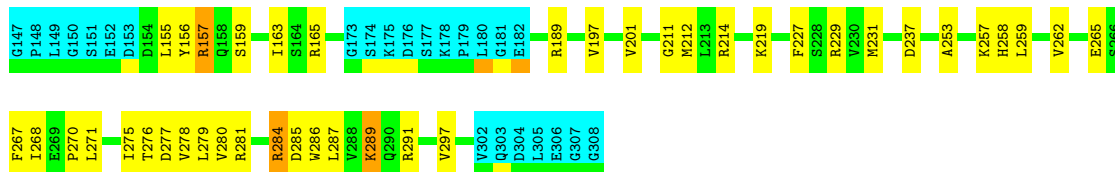


#### 4.2.13 Score per residue for model 13

- Molecule 1: Noxa

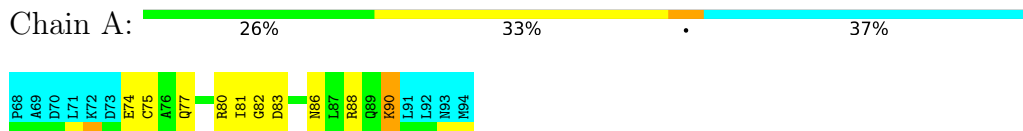


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



#### 4.2.14 Score per residue for model 14

- Molecule 1: Noxa

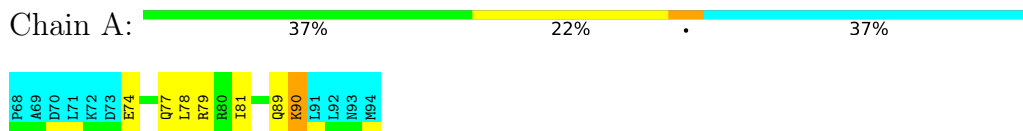


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog

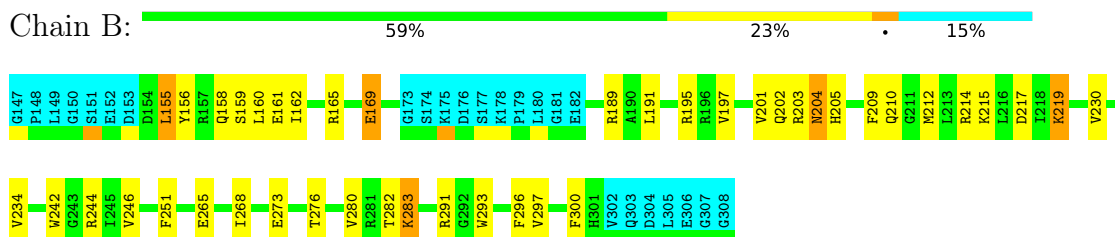


#### 4.2.15 Score per residue for model 15

- Molecule 1: Noxa



- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



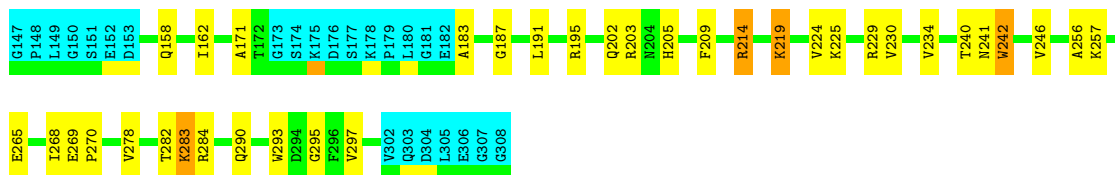
#### 4.2.16 Score per residue for model 16

- Molecule 1: Noxa



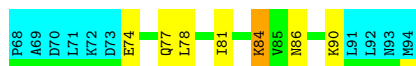
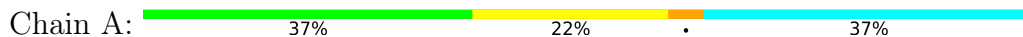
- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog





#### 4.2.17 Score per residue for model 17

- Molecule 1: Noxa

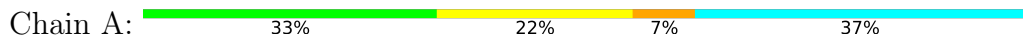


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog

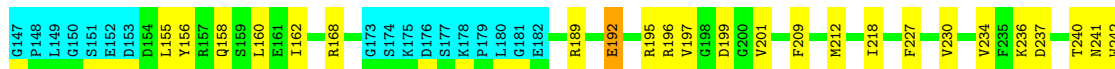


#### 4.2.18 Score per residue for model 18

- Molecule 1: Noxa

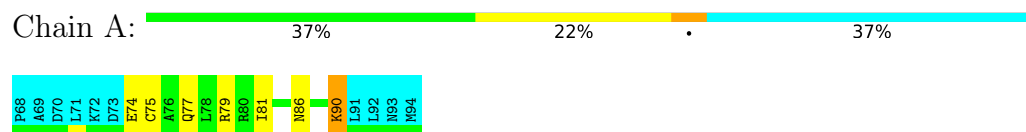


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog

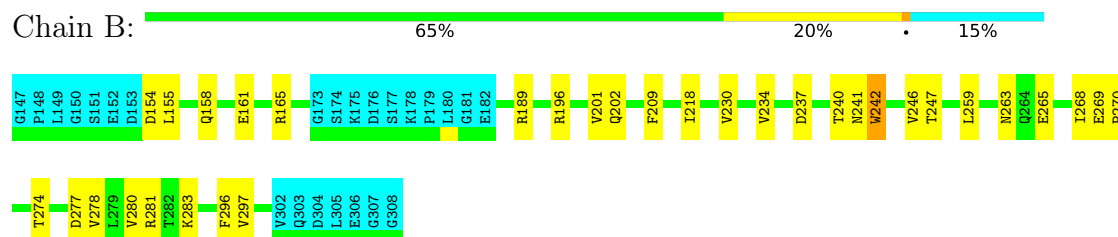


#### 4.2.19 Score per residue for model 19

- Molecule 1: Noxa

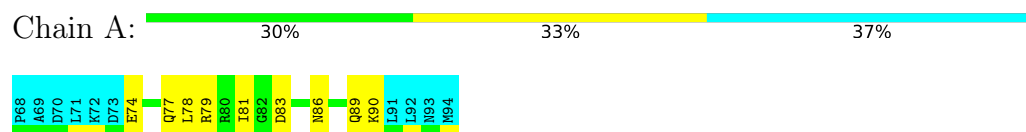


- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog

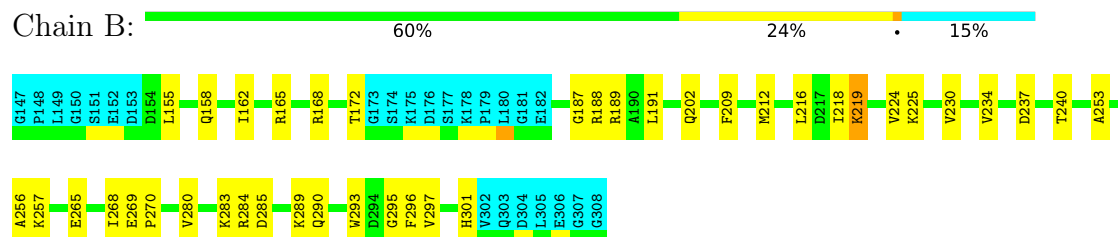


#### 4.2.20 Score per residue for model 20

- Molecule 1: Noxa



- Molecule 2: Myeloid cell leukemia-1 protein Mcl-1 homolog



## 5 Refinement protocol and experimental data overview

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

Of the 256 calculated structures, 20 were deposited, based on the following criterion: *lowest energy, 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
TopSpin	structure solution	1.3
XEASY	structure solution	1.3.13
CYANA	structure solution	2.1
X-PLOR NIH	refinement	2.14

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	140	152	152	5±2
2	B	1122	1134	1130	23±4
All	All	25240	25720	25640	512

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:GLU:HB3	2:B:212:MET:HG3	0.90	1.43	13	2
2:B:240:THR:HG21	2:B:283:LYS:HG2	0.83	1.50	8	10
2:B:282:THR:HG23	2:B:283:LYS:HD2	0.81	1.51	15	2
2:B:189:ARG:HG2	2:B:297:VAL:HG11	0.79	1.55	10	1
2:B:256:ALA:HB1	2:B:268:ILE:HG13	0.74	1.58	9	8
2:B:240:THR:HG22	2:B:245:ILE:HD11	0.74	1.59	8	4
2:B:260:LYS:HG3	2:B:265:GLU:HG2	0.73	1.59	12	1
2:B:189:ARG:HB3	2:B:297:VAL:HG11	0.72	1.62	2	14
2:B:163:ILE:HD12	2:B:276:THR:HB	0.72	1.61	11	4
2:B:156:TYR:HE1	2:B:277:ASP:HA	0.71	1.45	9	1
1:A:86:ASN:HA	1:A:89:GLN:HG2	0.69	1.65	4	1
2:B:259:LEU:HG	2:B:264:GLN:HB3	0.68	1.66	2	1
1:A:74:GLU:HB3	2:B:212:MET:HG2	0.67	1.66	1	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:LYS:HE3	1:A:88:ARG:HG3	0.67	1.65	13	1
2:B:269:GLU:HB2	2:B:270:PRO:HD3	0.66	1.67	16	8
1:A:74:GLU:HG3	2:B:212:MET:HG2	0.66	1.68	10	2
2:B:202:GLN:HA	2:B:209:PHE:HE2	0.66	1.51	19	10
2:B:160:LEU:HG	2:B:276:THR:HG21	0.65	1.69	9	1
1:A:75:CYS:O	1:A:79:ARG:HG3	0.65	1.92	19	4
2:B:269:GLU:HB3	2:B:270:PRO:HD3	0.64	1.67	3	3
2:B:200:GLY:HA2	2:B:203:ARG:HD3	0.64	1.69	3	1
2:B:213:LEU:HG	2:B:255:VAL:HG23	0.64	1.69	3	1
2:B:196:ARG:HA	2:B:196:ARG:HE	0.63	1.53	4	1
2:B:171:ALA:HA	2:B:257:LYS:HG2	0.63	1.69	16	3
1:A:77:GLN:O	1:A:81:ILE:HG12	0.61	1.95	1	17
2:B:201:VAL:HG11	2:B:247:THR:HA	0.61	1.70	4	2
2:B:265:GLU:O	2:B:268:ILE:HG22	0.61	1.96	10	9
2:B:159:SER:HB2	2:B:276:THR:HG22	0.61	1.73	15	2
2:B:277:ASP:O	2:B:281:ARG:HG2	0.60	1.97	1	1
2:B:202:GLN:HA	2:B:209:PHE:CE2	0.60	2.32	19	8
2:B:277:ASP:O	2:B:281:ARG:HD3	0.59	1.97	5	2
1:A:86:ASN:HB2	2:B:243:GLY:HA3	0.59	1.72	18	2
2:B:206:GLU:HG2	2:B:210:GLN:HE21	0.59	1.57	10	2
2:B:203:ARG:NE	2:B:203:ARG:HA	0.59	2.13	14	1
2:B:240:THR:CG2	2:B:283:LYS:HG2	0.58	2.27	8	7
2:B:242:TRP:HA	2:B:242:TRP:CE3	0.58	2.33	6	3
2:B:260:LYS:HE2	2:B:268:ILE:HD13	0.58	1.75	12	2
2:B:155:LEU:HD12	2:B:280:VAL:HG22	0.58	1.74	15	4
2:B:166:TYR:CE1	2:B:195:ARG:HA	0.57	2.34	9	5
1:A:90:LYS:O	1:A:90:LYS:HE2	0.57	1.99	12	4
2:B:231:MET:HG2	2:B:278:VAL:HG21	0.57	1.75	13	1
2:B:171:ALA:HA	2:B:257:LYS:HG3	0.57	1.75	9	1
2:B:217:ASP:HA	2:B:219:LYS:NZ	0.57	2.13	10	1
2:B:156:TYR:O	2:B:160:LEU:HG	0.57	2.00	15	1
2:B:160:LEU:HD23	2:B:276:THR:HG21	0.56	1.76	10	1
2:B:224:VAL:HG23	2:B:225:LYS:HD2	0.56	1.76	14	6
2:B:167:LEU:HD23	2:B:256:ALA:HB2	0.56	1.76	10	3
2:B:242:TRP:HB3	2:B:300:PHE:HE2	0.56	1.60	3	1
2:B:293:TRP:O	2:B:297:VAL:HG23	0.56	2.00	3	12
2:B:218:ILE:HG22	2:B:259:LEU:HD13	0.56	1.77	11	3
2:B:256:ALA:HA	2:B:259:LEU:HD12	0.56	1.78	9	1
2:B:227:PHE:CE2	2:B:275:ILE:HG12	0.55	2.35	3	7
2:B:160:LEU:HD11	2:B:273:GLU:HG3	0.55	1.78	4	1
2:B:195:ARG:O	2:B:199:ASP:HB2	0.55	2.01	18	2

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:230:VAL:O	2:B:234:VAL:HG23	0.55	2.02	20	16
2:B:170:GLN:HG3	2:B:257:LYS:HD2	0.54	1.77	7	1
2:B:160:LEU:HD12	2:B:276:THR:HG21	0.54	1.79	3	1
2:B:164:SER:O	2:B:168:ARG:HD3	0.54	2.03	9	2
2:B:227:PHE:HE2	2:B:275:ILE:HG12	0.54	1.63	18	2
1:A:83:ASP:HA	1:A:86:ASN:ND2	0.54	2.18	14	1
2:B:158:GLN:O	2:B:162:ILE:HG13	0.54	2.03	11	13
2:B:204:ASN:HD22	2:B:205:HIS:N	0.54	2.01	1	2
2:B:277:ASP:OD1	2:B:281:ARG:HD2	0.54	2.03	13	1
1:A:81:ILE:HG23	2:B:205:HIS:CD2	0.53	2.38	9	5
1:A:80:ARG:HA	1:A:80:ARG:HE	0.53	1.62	14	2
2:B:188:ARG:O	2:B:192:GLU:HG2	0.53	2.04	4	1
1:A:79:ARG:HD2	2:B:237:ASP:OD2	0.53	2.03	8	6
2:B:280:VAL:O	2:B:284:ARG:HB2	0.53	2.04	7	3
1:A:75:CYS:SG	2:B:233:HIS:HB3	0.53	2.43	7	3
2:B:290:GLN:O	2:B:295:GLY:HA3	0.53	2.04	20	5
2:B:169:GLU:HG2	2:B:195:ARG:HH12	0.53	1.63	15	1
2:B:270:PRO:HA	2:B:273:GLU:HG2	0.52	1.79	12	1
2:B:160:LEU:HD22	2:B:276:THR:HG21	0.52	1.81	8	2
2:B:239:VAL:HB	2:B:244:ARG:CZ	0.52	2.35	6	2
2:B:201:VAL:HB	2:B:250:SER:OG	0.52	2.04	3	1
1:A:82:GLY:HA2	2:B:247:THR:OG1	0.52	2.05	18	3
2:B:242:TRP:CE2	2:B:296:PHE:HB2	0.52	2.40	2	1
2:B:170:GLN:O	2:B:257:LYS:HE2	0.51	2.05	6	1
2:B:155:LEU:HD23	2:B:287:LEU:HD13	0.51	1.83	2	1
2:B:212:MET:HB2	2:B:251:PHE:CE1	0.51	2.41	4	2
1:A:76:ALA:HA	1:A:79:ARG:HH21	0.50	1.67	9	2
2:B:297:VAL:O	2:B:301:HIS:HB2	0.50	2.06	1	6
2:B:186:ALA:HA	2:B:189:ARG:HE	0.50	1.67	11	1
1:A:88:ARG:HA	1:A:88:ARG:HE	0.50	1.65	3	1
2:B:161:GLU:O	2:B:165:ARG:HG2	0.50	2.07	7	2
2:B:242:TRP:O	2:B:246:VAL:HG23	0.50	2.07	16	10
2:B:278:VAL:O	2:B:282:THR:HG22	0.50	2.06	16	2
1:A:90:LYS:HD3	1:A:90:LYS:C	0.49	2.26	3	2
2:B:260:LYS:HG2	2:B:265:GLU:OE2	0.49	2.07	9	1
2:B:242:TRP:HB3	2:B:300:PHE:CE2	0.49	2.40	3	1
2:B:226:SER:HA	2:B:229:ARG:HE	0.49	1.66	6	1
1:A:83:ASP:HA	1:A:86:ASN:HD21	0.49	1.67	14	1
2:B:191:LEU:O	2:B:195:ARG:HG3	0.49	2.07	17	2
2:B:270:PRO:HA	2:B:273:GLU:OE1	0.49	2.06	4	1
2:B:277:ASP:O	2:B:281:ARG:HB2	0.49	2.07	9	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ARG:HD3	2:B:237:ASP:OD2	0.49	2.07	3	3
1:A:90:LYS:HE2	1:A:90:LYS:C	0.49	2.28	4	6
2:B:271:LEU:O	2:B:275:ILE:HG13	0.49	2.07	14	5
2:B:212:MET:HB3	2:B:251:PHE:CZ	0.49	2.43	17	1
2:B:155:LEU:HD23	2:B:280:VAL:HG13	0.49	1.85	19	1
2:B:218:ILE:HG23	2:B:259:LEU:HD13	0.49	1.84	5	1
2:B:160:LEU:HA	2:B:276:THR:HG21	0.49	1.85	14	2
2:B:214:ARG:O	2:B:214:ARG:HD3	0.49	2.08	16	3
2:B:196:ARG:HA	2:B:196:ARG:NE	0.48	2.21	4	1
2:B:216:LEU:HB3	2:B:218:ILE:HG12	0.48	1.83	20	4
2:B:197:VAL:O	2:B:201:VAL:HG23	0.48	2.08	18	6
2:B:281:ARG:O	2:B:281:ARG:HD3	0.48	2.08	4	1
1:A:74:GLU:CD	2:B:215:LYS:HG2	0.48	2.28	10	1
2:B:167:LEU:HB3	2:B:268:ILE:HD11	0.48	1.85	1	1
2:B:156:TYR:CE2	2:B:160:LEU:HD11	0.48	2.44	15	1
1:A:83:ASP:HA	1:A:86:ASN:OD1	0.48	2.08	4	2
1:A:74:GLU:O	1:A:78:LEU:HB2	0.48	2.08	8	3
1:A:82:GLY:HA3	2:B:244:ARG:HA	0.48	1.86	18	2
2:B:201:VAL:HG12	2:B:209:PHE:HZ	0.48	1.69	18	2
2:B:225:LYS:O	2:B:229:ARG:HG3	0.47	2.08	7	1
1:A:74:GLU:OE2	2:B:215:LYS:HG3	0.47	2.09	11	2
2:B:280:VAL:O	2:B:284:ARG:HB3	0.47	2.08	14	1
2:B:219:LYS:HA	2:B:219:LYS:NZ	0.47	2.24	16	2
1:A:79:ARG:NH2	2:B:244:ARG:HB3	0.47	2.25	15	1
2:B:273:GLU:HA	2:B:276:THR:OG1	0.47	2.10	15	1
2:B:227:PHE:HA	2:B:230:VAL:HG12	0.47	1.85	9	1
2:B:284:ARG:H	2:B:284:ARG:HD3	0.47	1.70	13	1
2:B:218:ILE:HG23	2:B:223:ASP:HB2	0.47	1.87	10	2
2:B:227:PHE:O	2:B:231:MET:HG3	0.47	2.10	17	2
2:B:183:ALA:HB1	2:B:187:GLY:HA3	0.47	1.85	17	1
2:B:199:ASP:O	2:B:203:ARG:HG3	0.47	2.09	10	1
2:B:163:ILE:HG22	2:B:272:ALA:HB1	0.46	1.88	5	1
2:B:265:GLU:O	2:B:269:GLU:HG2	0.46	2.10	4	1
2:B:222:GLY:HA2	2:B:225:LYS:HD3	0.46	1.86	8	1
2:B:253:ALA:O	2:B:257:LYS:HG3	0.46	2.11	7	7
2:B:156:TYR:O	2:B:160:LEU:HB2	0.46	2.11	17	2
2:B:154:ASP:O	2:B:158:GLN:HG3	0.46	2.10	19	2
2:B:240:THR:HG21	2:B:283:LYS:HD2	0.46	1.85	14	1
1:A:78:LEU:HD13	2:B:234:VAL:HG21	0.46	1.86	15	1
2:B:218:ILE:HG13	2:B:255:VAL:HG11	0.46	1.86	18	1
1:A:81:ILE:O	1:A:85:VAL:HG23	0.46	2.11	2	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:240:THR:HG23	2:B:283:LYS:HD3	0.46	1.87	12	1
2:B:265:GLU:HA	2:B:268:ILE:HG22	0.46	1.88	20	8
2:B:274:THR:O	2:B:278:VAL:HG22	0.46	2.11	2	1
1:A:86:ASN:O	1:A:90:LYS:HB2	0.46	2.11	19	3
1:A:89:GLN:HG2	2:B:300:PHE:CD1	0.46	2.46	15	1
2:B:165:ARG:HD3	2:B:169:GLU:OE2	0.45	2.11	11	1
2:B:218:ILE:HA	2:B:223:ASP:CB	0.45	2.41	10	2
2:B:225:LYS:O	2:B:229:ARG:HG2	0.45	2.10	16	1
2:B:263:ASN:HA	2:B:265:GLU:OE1	0.45	2.12	2	1
2:B:159:SER:HB2	2:B:276:THR:OG1	0.45	2.10	7	1
2:B:259:LEU:HD13	2:B:267:PHE:CB	0.45	2.42	9	1
2:B:160:LEU:CA	2:B:276:THR:HG21	0.45	2.41	14	1
2:B:218:ILE:HG21	2:B:259:LEU:HD11	0.45	1.88	2	1
2:B:240:THR:CG2	2:B:283:LYS:HD3	0.45	2.42	5	1
2:B:208:ALA:O	2:B:212:MET:HG3	0.45	2.12	12	2
2:B:211:GLY:HA2	2:B:214:ARG:HH21	0.45	1.72	13	1
1:A:84:LYS:HA	1:A:84:LYS:HE2	0.45	1.87	17	1
2:B:239:VAL:HB	2:B:244:ARG:NH2	0.45	2.27	1	1
2:B:259:LEU:HA	2:B:262:VAL:HG12	0.45	1.89	13	1
2:B:189:ARG:NE	2:B:189:ARG:HA	0.45	2.26	14	1
2:B:285:ASP:O	2:B:289:LYS:HG3	0.45	2.12	20	1
1:A:78:LEU:HG	2:B:212:MET:CE	0.44	2.42	20	2
2:B:242:TRP:CZ2	2:B:296:PHE:HB2	0.44	2.47	5	1
2:B:160:LEU:CD1	2:B:273:GLU:HG3	0.44	2.42	4	1
2:B:224:VAL:HG11	2:B:270:PRO:HB2	0.44	1.89	16	1
1:A:86:ASN:OD1	2:B:241:ASN:HB3	0.44	2.12	17	1
2:B:286:TRP:CH2	2:B:290:GLN:HG3	0.44	2.48	10	1
2:B:210:GLN:O	2:B:214:ARG:HG3	0.44	2.13	15	2
2:B:232:VAL:O	2:B:236:LYS:HB2	0.44	2.13	6	1
2:B:199:ASP:O	2:B:202:GLN:HG2	0.43	2.13	10	1
2:B:162:ILE:CD1	2:B:187:GLY:HA2	0.43	2.43	6	4
2:B:215:LYS:HB3	2:B:215:LYS:NZ	0.43	2.27	12	1
2:B:267:PHE:C	2:B:270:PRO:HD2	0.43	2.34	13	1
2:B:161:GLU:O	2:B:165:ARG:HD3	0.43	2.14	15	1
2:B:183:ALA:CB	2:B:187:GLY:HA3	0.43	2.43	17	1
1:A:74:GLU:OE2	2:B:215:LYS:HD3	0.43	2.13	6	1
2:B:171:ALA:HB1	2:B:260:LYS:HB3	0.43	1.90	12	1
2:B:273:GLU:HA	2:B:276:THR:CG2	0.43	2.43	12	2
2:B:192:GLU:O	2:B:196:ARG:HG3	0.43	2.12	12	1
2:B:192:GLU:O	2:B:196:ARG:HG2	0.43	2.13	10	2
1:A:74:GLU:CD	2:B:215:LYS:HG3	0.43	2.34	15	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:265:GLU:HA	2:B:268:ILE:CG2	0.43	2.43	4	1
1:A:89:GLN:HG2	2:B:300:PHE:CE2	0.43	2.49	7	1
2:B:169:GLU:HB3	2:B:195:ARG:NH1	0.43	2.29	9	1
2:B:236:LYS:O	2:B:236:LYS:HG2	0.43	2.12	11	1
1:A:76:ALA:HA	1:A:79:ARG:NH2	0.42	2.29	9	1
2:B:154:ASP:O	2:B:157:ARG:HG2	0.42	2.14	9	1
2:B:297:VAL:O	2:B:301:HIS:HB3	0.42	2.14	11	1
1:A:81:ILE:HG23	2:B:205:HIS:CG	0.42	2.49	5	1
2:B:183:ALA:HB3	2:B:187:GLY:HA3	0.42	1.90	16	1
2:B:158:GLN:HA	2:B:183:ALA:HB2	0.42	1.92	6	1
2:B:206:GLU:HG3	2:B:254:PHE:CE1	0.42	2.50	10	1
2:B:216:LEU:HD23	2:B:218:ILE:HD11	0.42	1.90	17	1
2:B:165:ARG:O	2:B:169:GLU:HB2	0.42	2.14	11	1
2:B:187:GLY:O	2:B:191:LEU:HG	0.42	2.15	20	1
2:B:201:VAL:HG12	2:B:209:PHE:CZ	0.42	2.50	18	2
1:A:89:GLN:HG3	2:B:300:PHE:CE1	0.42	2.49	3	1
2:B:219:LYS:HG3	2:B:220:ASN:ND2	0.42	2.30	11	1
2:B:158:GLN:HG2	2:B:162:ILE:HD11	0.42	1.91	2	1
2:B:256:ALA:HB1	2:B:268:ILE:CD1	0.42	2.45	10	1
2:B:158:GLN:HG2	2:B:183:ALA:HA	0.42	1.92	6	1
2:B:233:HIS:HA	2:B:236:LYS:HG2	0.41	1.92	1	1
1:A:89:GLN:HE22	2:B:242:TRP:HB2	0.41	1.75	10	2
2:B:289:LYS:HD3	2:B:290:GLN:HG3	0.41	1.91	2	1
2:B:168:ARG:NH1	2:B:268:ILE:HD11	0.41	2.30	8	1
2:B:202:GLN:O	2:B:206:GLU:HB2	0.41	2.15	1	2
2:B:217:ASP:HB2	2:B:226:SER:HB2	0.41	1.92	3	1
2:B:274:THR:O	2:B:278:VAL:HG12	0.41	2.14	19	1
2:B:215:LYS:NZ	2:B:215:LYS:HB3	0.41	2.31	5	1
2:B:192:GLU:HA	2:B:195:ARG:NH1	0.41	2.30	14	1
2:B:171:ALA:HB1	2:B:260:LYS:HB2	0.41	1.92	8	1
2:B:168:ARG:O	2:B:172:THR:HG22	0.41	2.15	20	2
2:B:199:ASP:O	2:B:203:ARG:HB2	0.41	2.15	12	1
2:B:286:TRP:HE3	2:B:287:LEU:HD12	0.41	1.76	13	1
2:B:171:ALA:O	2:B:260:LYS:HG2	0.41	2.15	3	1
2:B:294:ASP:O	2:B:298:GLU:HG2	0.41	2.15	4	1
2:B:227:PHE:O	2:B:230:VAL:HG12	0.41	2.16	10	1
2:B:280:VAL:O	2:B:284:ARG:HG3	0.41	2.15	20	1
2:B:293:TRP:HE3	2:B:296:PHE:CD2	0.41	2.34	11	1
2:B:285:ASP:O	2:B:289:LYS:HB2	0.41	2.16	13	1
2:B:216:LEU:O	2:B:218:ILE:HD12	0.41	2.16	17	1
1:A:79:ARG:O	1:A:83:ASP:HB2	0.41	2.16	20	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:155:LEU:HD12	2:B:287:LEU:HD13	0.41	1.93	1	1
2:B:156:TYR:CE1	2:B:277:ASP:HA	0.41	2.51	1	1
2:B:283:LYS:HB3	2:B:286:TRP:HB3	0.41	1.91	1	1
2:B:226:SER:O	2:B:229:ARG:HB3	0.41	2.16	4	1
2:B:272:ALA:O	2:B:276:THR:HG22	0.41	2.16	10	1
2:B:156:TYR:HA	2:B:159:SER:OG	0.41	2.16	13	1
2:B:189:ARG:HA	2:B:189:ARG:HE	0.41	1.76	14	1
2:B:160:LEU:HG	2:B:276:THR:CG2	0.41	2.43	9	1
2:B:165:ARG:N	2:B:165:ARG:HD2	0.41	2.30	9	1
2:B:284:ARG:O	2:B:288:VAL:HG23	0.41	2.15	11	1
2:B:218:ILE:CG2	2:B:259:LEU:HD13	0.40	2.44	5	1
2:B:166:TYR:HB2	2:B:194:LEU:HD23	0.40	1.93	1	1
2:B:218:ILE:HG13	2:B:255:VAL:CG1	0.40	2.46	11	1
2:B:190:ALA:HA	2:B:297:VAL:HG22	0.40	1.92	2	1
1:A:75:CYS:HB3	2:B:230:VAL:HG23	0.40	1.93	3	1
2:B:160:LEU:HD11	2:B:273:GLU:HG2	0.40	1.94	6	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	17/27 (63%)	17±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	138/162 (85%)	132±2 (96±1%)	5±2 (4±1%)	1±1 (0±0%)	38	78
All	All	3100/3780 (82%)	2979 (96%)	109 (4%)	12 (0%)	38	78

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	219	LYS	7
2	B	241	ASN	5

### 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	15/24 (62%)	14±1 (92±4%)	1±1 (8±4%)	16	64
2	B	118/136 (87%)	111±2 (94±2%)	7±2 (6±2%)	22	71
All	All	2660/3200 (83%)	2494 (94%)	166 (6%)	22	71

All 56 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)
2	B	219	LYS	13
1	A	90	LYS	12
2	B	155	LEU	8
2	B	160	LEU	6
2	B	242	TRP	6
2	B	165	ARG	6
2	B	286	TRP	6
2	B	214	ARG	6
2	B	258	HIS	6
2	B	291	ARG	6
2	B	203	ARG	5
2	B	188	ARG	5
2	B	296	PHE	5
2	B	192	GLU	5
2	B	204	ASN	4
2	B	240	THR	4
2	B	298	GLU	4
1	A	88	ARG	3
2	B	169	GLU	3
2	B	268	ILE	2
2	B	263	ASN	2
2	B	196	ARG	2
2	B	266	SER	2
1	A	79	ARG	2
2	B	237	ASP	2
2	B	216	LEU	2
1	A	78	LEU	2
2	B	289	LYS	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
2	B	269	GLU	2
2	B	299	PHE	2
2	B	161	GLU	2
2	B	236	LYS	2
1	A	84	LYS	2
2	B	283	LYS	2
2	B	168	ARG	2
2	B	154	ASP	1
2	B	281	ARG	1
2	B	233	HIS	1
2	B	300	PHE	1
2	B	199	ASP	1
2	B	202	GLN	1
2	B	273	GLU	1
1	A	80	ARG	1
2	B	191	LEU	1
2	B	260	LYS	1
2	B	276	THR	1
2	B	157	ARG	1
2	B	229	ARG	1
2	B	279	LEU	1
2	B	284	ARG	1
2	B	221	GLU	1
2	B	217	ASP	1
2	B	265	GLU	1
2	B	259	LEU	1
2	B	301	HIS	1
1	A	89	GLN	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 7 Chemical shift validation

No chemical shift data were provided