Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 05:17 AM BST

PDB ID	:	2ROD
Title	:	Solution Structure of MCL-1 Complexed with NoxaA
Authors	:	Day, C.L.; Smits, C.; Fan, F.C.; Lee, E.F.; Fairlie, W.D.; Hinds, M.G.
Deposited on	:	2008-03-17

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

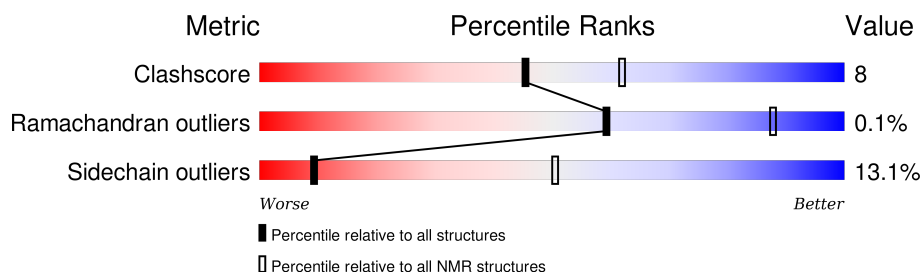|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457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

1　Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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

Metric	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0.1%
Sidechain outliers		13.1%

Worse .... *Better*

▮ Percentile relative to all structures
❑ Percentile relative to all NMR structures

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

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

Mol	Chain	Length	Quality of chain
1	A	162	60%　　24%　　15%
2	B	27	56%　　11%　　33%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:153-A:171, A:183-A:300, B:22-B:39 (155)	0.40	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2999 atoms, of which 1498 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Induced myeloid leukemia cell differentiation protein Mcl-1 homolog.

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

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Noxa.

Mol	Chain	Residues	Atoms						Trace
2	B	27	Total 422	C 137	H 209	N 34	O 40	S 2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	43	MET	-	EXPRESSION TAG	UNP Q9JM54

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog
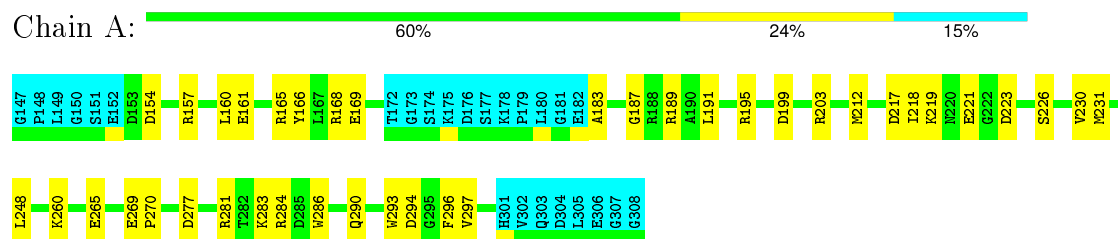
• Molecule 2: Noxa
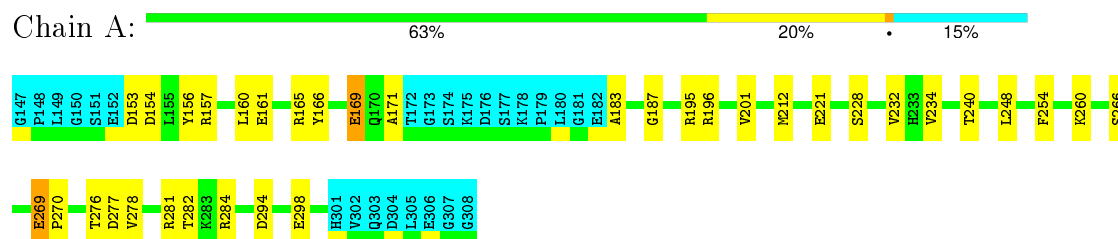

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

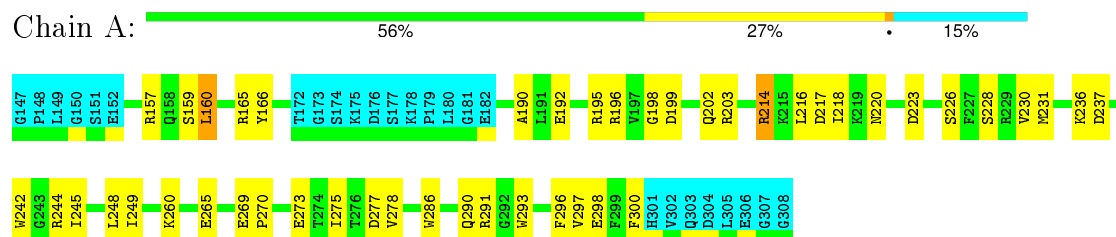• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

• Molecule 2: Noxa

Chain B: 52% 11% • 33%

A17 E18 L19 P20 P21 E22 F23 R28 V34 Y35 A40 P41 D42 M43

4.2.2 Score per residue for model 2

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A: 56% 27% • 15%

G147 P148 L149 G150 S151 E152 R157 Q158 S159 L160 R165 Y166 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A190 L191 E192 R195 R196 V197 G198 D199 Q202 R203 R214 K215 L216 D217 I218 K219 N220 D223 S226 F227 S228 R229 V230 M231 K236 D237

W242 G243 R244 I245 L248 I249 K260 E265 E269 P270 E273 T274 I275 T276 D277 V278 W286 Q290 R291 G292 W293 F296 V297 E298 F299 F300 H301 V302 Q303 D304 L305 E306 G307 G308

• Molecule 2: Noxa

Chain B: 48% 15% • 33%

A17 E18 L19 P20 P21 E22 F23 A24 Q25 Q26 G31 Y35 A40 P41 D42 M43

4.2.3 Score per residue for model 3

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A: 56% 27% • 15%

G147 P148 L149 G150 S151 E152 D153 D154 L455 Y156 R157 Q158 S159 L160 Y166 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 A186 G187 R188 R189 E192 R195 Q202 R203 E206 F209 M212 L213 R214 K215 L216 D217 E221 V224 K225 S226 R229

V230 V234 F235 T240 S250 F251 G252 A253 F254 V255 A256 K257 H258 E265 I268 E269 P270 E273 D277 R281 R284 Q290 D294 H301 V302 Q303 D304 L305 E306 G307 G308

• Molecule 2: Noxa

Chain B: 52% 11% • 33%

A17 E18 L19 P20 P21 E22 F23 Q26 K33 V34 Y35 A40 P41 D42 M43

4.2.4 Score per residue for model 4

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A:　　61%　　20%　•　15%
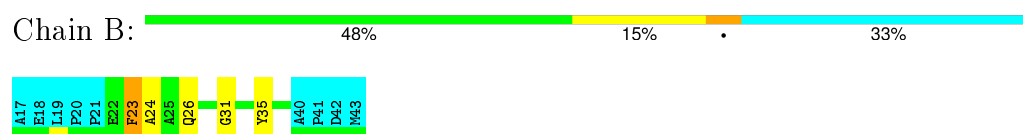
G147 P148 L149 G150 S151 E152 D153 D154 L155 Y156 R157 E161 I162 I163 S164 R165 Y166 L167 R168 E169 Q170 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G187 R188 R189 T193 L194 R195 G198 D199 Q202 R203 M212 L213 I218 D223 V232 K236

W242 F254 K257 E269 P270 R284 D285 M293 G295 F296 V297 F300 H301 V302 Q303 D304 L305 E306 G307 G308

● Molecule 2: Noxa

Chain B:　　56%　•　7%　　33%

A17 E18 L19 P20 P21 E22 F23 A24 R28 A40 P41 D42 M43
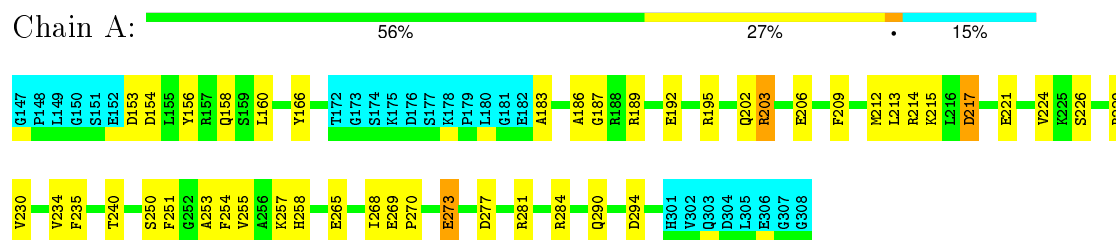
4.2.5 Score per residue for model 5

● Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A:　　49%　　31%　•　15%

G147 P148 L149 G150 S151 E152 D153 D154 R157 Q158 S159 L160 E161 I162 I163 S164 R165 Y166 L167 R168 E169 Q170 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G187 R188 R189 R195 G198 D199 Q202 R203 F209 M212 L213 L216 D217 I218 E221

V224 R229 V230 M231 K236 V239 I245 I248 I249 S250 F251 G252 A253 F254 V255 A256 K257 K260 F267 I268 E269 P270 E273 T276 D277 V278 L279 V280 R281 R284 D285 W286 K289 M293 F296 V297 E298 H301 V302 Q303 D304 L305 E306 G307 G308

● Molecule 2: Noxa

Chain B:　　52%　　11%　•　33%

A17 E18 L19 P20 P21 E22 F23 A24 A25 K29 A40 P41 D42 M43
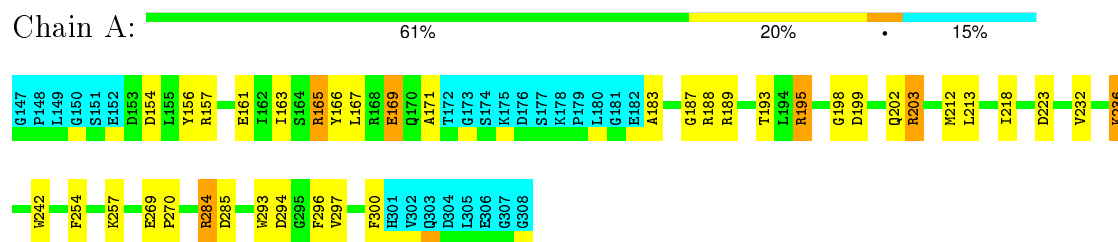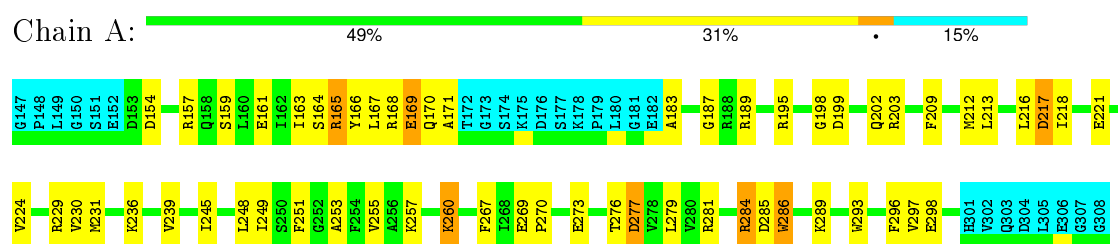
4.2.6 Score per residue for model 6

● Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A:　　66%　　19%　　15%

G147 P148 L149 G150 S151 E152 L155 L160 I163 L167 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G187 L191 R196 R203 Q210 R214 D217 I218 E221 G222 D223 S228 M231 I245 I249 S266 E269 P270 L271

T276 R284 D285 K289 W293 F296 V297 H301 V302 Q303 D304 L305 E306 G307 G308

● Molecule 2: Noxa

Chain B:　　56%　•　7%　　33%

A17 E18 L19 P20 P21 E22 F23 K29 Y35 A40 P41 D42 M43
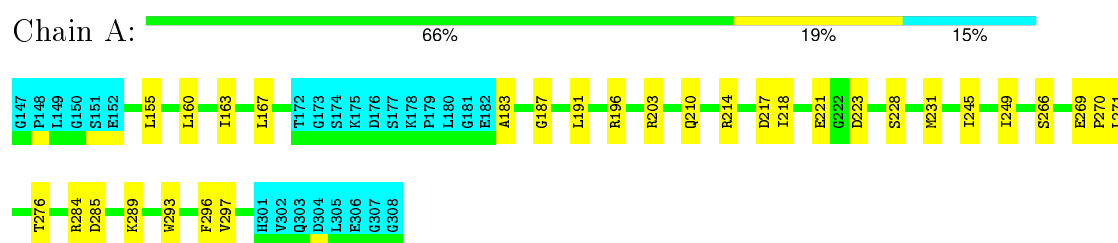
4.2.7 Score per residue for model 7

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A:

G147 P148 L149 G150 S151 E152 D153 Y156 R157 L160 E161 I162 I163 Y166 L167 R168 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 R189 E192 R195 R196 V197 V201 T207 M212 L216 D217 E221 V224 K225 S226 V230 K236 D237

T240 N241 W242 G243 R244 I245 L248 F251 F254 V255 A256 K257 K260 S261 V262 N263 Q264 E265 I268 E269 P270 E273 T282 K283 R284 D285 W286 Q290 W293 F296 V297 H301 V302 Q303 D304 L305 E306 G307 G308

• Molecule 2: Noxa
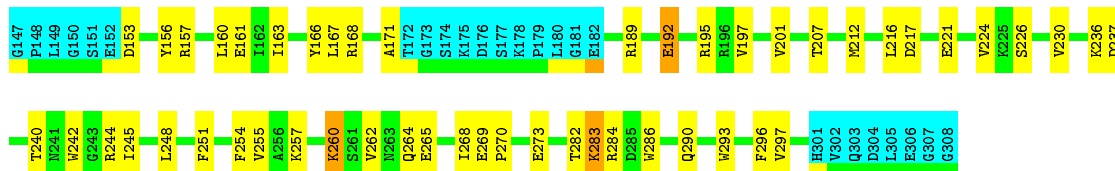
Chain B:

A17 E18 L19 P20 P21 E22 F23 Q26 L27 R28 K33 A40 P41 D42 M43
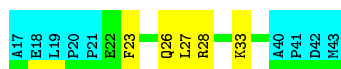
4.2.8 Score per residue for model 8

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A:

G147 P148 L149 G150 S151 E152 D153 D154 L155 Y156 L160 E161 R165 Y166 L167 R168 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A190 L191 E192 R195 R196 E206 M212 L216 D217 I218 K219 D223 S226 F227 S228 R229 V230 M231 V234 D237

W242 H258 L259 K260 Q264 E265 S266 F267 I268 E269 P270 I275 T276 D277 V278 L279 T282 K283 R284 Q290 W293 F296 V297 F300 H301 V302 Q303 D304 L305 E306 G307 G308

• Molecule 2: Noxa

Chain B:

A17 E18 L19 P20 P21 E22 F23 R28 K29 K33 A40 P41 D42 M43
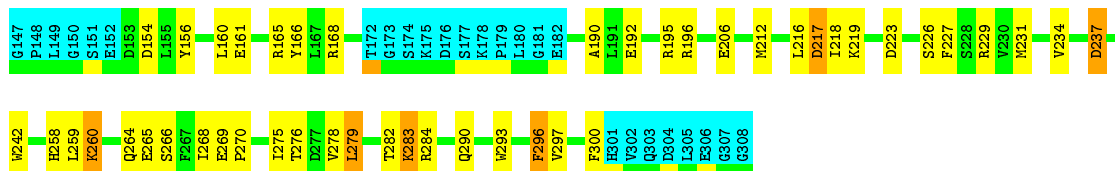
4.2.9 Score per residue for model 9

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A:

G147 P148 L149 G150 S151 E152 D153 D154 L155 Y156 R157 L160 Y166 L167 R168 E169 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 G187 R188 R189 A190 L191 E192 R195 G198 M212 L216 D217 I218 K219 N220 E221 S226 F227 V230 M231 V234 T240

I245 I249 H258 L259 Q264 E265 S266 F267 I268 E269 P270 E273 D277 V278 L279 V280 R281 W286 Q290 H301 V302 Q303 D304 L305 E306 G307 G308

● Molecule 2: Noxa

Chain B:　　48%　　19%　　33%

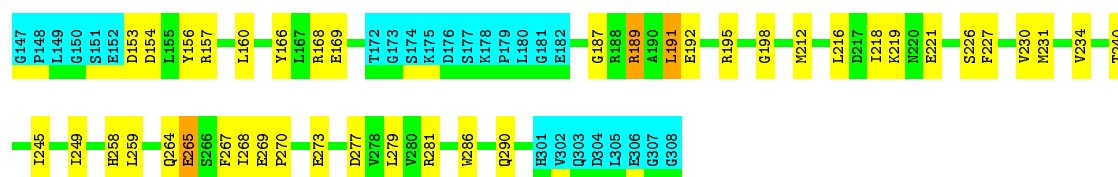A17 E18 L19 P20 P21 E22 F23 R28 K29 I30 V34 Y35 A40 P41 D42 M43

4.2.10　Score per residue for model 10

● Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A:　　60%　　19%　　5%　　15%

G147 P148 L149 G150 S151 E152 D153 D154 R157 E161 R165 Y166 L167 R168 E169 Q170 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G187 R188 R189 E192 R195 R196 V197 G198 D199 G200 V201 Q202 R203 E206 K219 S226 V230 M231 F235

V239 R244 L248 E269 P270 D277 R281 W286 K289 Q290 W293 D294 G295 F296 V297 H301 V302 Q303 D304 L305 E306 G307 G308

● Molecule 2: Noxa

Chain B:　　41%　　26%　　33%

A17 E18 L19 P20 P21 E22 F23 A24 A25 Q26 K29 K33 V34 Y35 A40 P41 D42 M43

4.2.11　Score per residue for model 11

● Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog
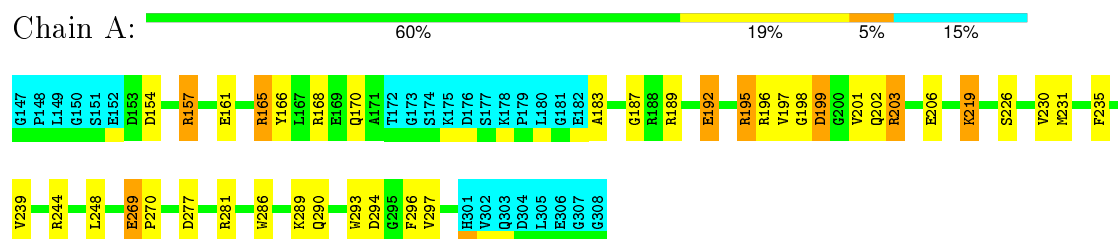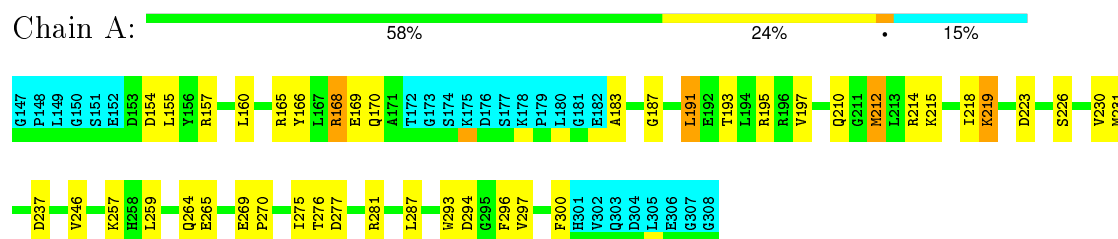
Chain A:　　58%　　24%　　·　　15%

G147 P148 L149 G150 S151 E152 D153 D154 L155 Y156 R157 L160 R165 Y166 L167 R168 E169 Q170 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G187 L191 E192 T193 L194 R195 R196 V197 Q210 G211 M212 I213 R214 K215 I218 K219 D223 S226 V230 M231

D237 V246 K257 H258 L259 Q264 E265 E269 P270 I275 T276 D277 R281 L287 W293 D294 G295 F296 V297 F300 H301 V302 Q303 D304 L305 E306 G307 G308

● Molecule 2: Noxa

Chain B:　　59%　　7%　　33%

A17 E18 L19 P20 P21 E22 F23 Y35 A40 P41 D42 M43
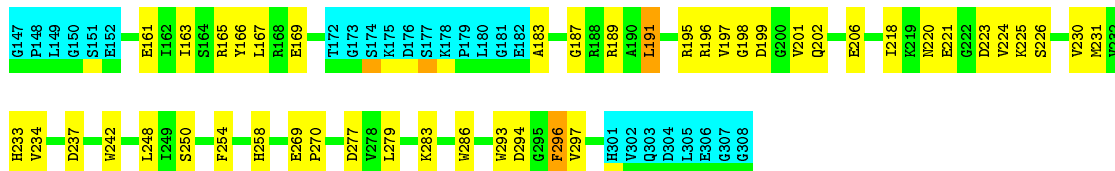
4.2.12 Score per residue for model 12

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A: 57% 27% • 15%

G147 P148 L149 G150 S151 E152 E161 I162 I163 S164 R165 Y166 L167 R168 E169 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G187 R188 R189 A190 L191 R195 R196 V197 G198 D199 G200 V201 Q202 E206 I218 K219 N220 E221 G222 D223 V224 K225 S226 V230 N231 V232

H233 V234 D237 W242 L248 I249 S250 F254 H258 E269 P270 D277 V278 L279 K283 W286 W293 D294 G295 F296 V297 H301 V302 Q303 D304 L305 E306 G307 G308

• Molecule 2: Noxa

Chain B: 59% 7% 33%

A17 E18 L19 P20 P21 A24 A25 Q26 A40 P41 D42 M43
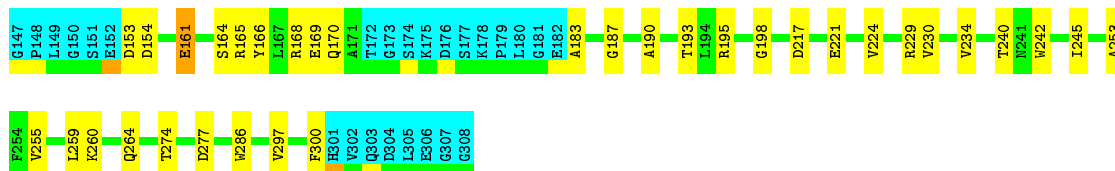
4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A: 64% 20% • 15%

G147 P148 L149 G150 S151 E152 D153 D154 E161 S164 R165 Y166 L167 R168 E169 Q170 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G187 A190 T193 L194 R195 G198 D217 E221 V224 R229 V230 V234 T240 N241 W242 I245 A253

F254 V255 L259 K260 Q264 T274 D277 W286 V297 F300 H301 V302 Q303 D304 L305 E306 G307 G308

• Molecule 2: Noxa

Chain B: 63% • 33%

A17 E18 L19 P20 P21 Y35 A40 P41 D42 M43
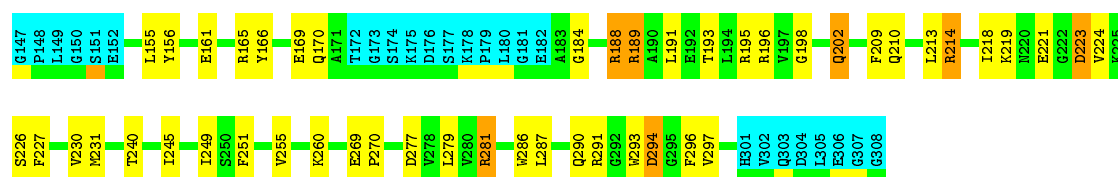
4.2.14 Score per residue for model 14

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog
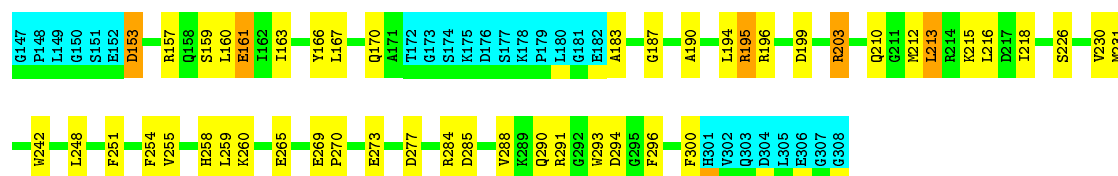
Chain A: 55% 25% • 15%

G147 P148 L149 G150 S151 E152 L155 Y156 E161 R165 Y166 E169 Q170 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G184 R188 R189 A190 L191 E192 T193 L194 R195 R196 V197 G198 Q202 F209 Q210 L213 R214 I218 K219 N220 E221 G222 D223 V224 K225

S226 F227 V230 M231 T240 I245 I249 S250 F251 V255 K260 E269 P270 D277 V278 L279 V280 R281 W286 L287 Q290 R291 G292 W293 D294 G295 F296 V297 H301 V302 Q303 D304 L305 E306 G307 G308

• Molecule 2: Noxa

Chain B:　　　　　　　　　56%　　　　　　　　11%　　　　　33%

A17 E18 L19 P20 P21 E22 F23 Q26 A40 P41 D42 M43

4.2.15　Score per residue for model 15

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A:　　　　　　　55%　　　　　　　27%　　　·　15%

G147 P148 L149 G150 S151 E152 D153 R157 Q158 S159 L160 E161 I162 I163 Y166 L167 Q170 A171 T172 G173 S174 D176 S177 K178 P179 L180 G181 E182 A183 G187 A190 L194 R195 R196 D199 R203 Q210 G211 M212 L213 R214 K215 L216 D217 I218 S226 V230 M231

W242 L248 F251 F254 V255 H258 L259 K260 E265 E269 P270 E273 D277 R284 D285 V288 K289 Q290 R291 G292 W293 D294 G295 F296 F300 H301 V302 Q303 D304 L305 E306 G307 G308

• Molecule 2: Noxa

Chain B:　　　　　　　　　56%　　　　　　　11%　　　　　33%

A17 E18 L19 P20 P21 E22 F23 Y35 A40 P41 D42 M43

4.2.16　Score per residue for model 16

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A:　　　　　　　59%　　　　　　23%　　　·　15%

G147 P148 L149 G150 S151 E152 D153 D154 L155 Q170 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G187 R188 R189 T207 A208 F209 Q210 G211 M212 L213 R214 D217 I218 E221 G222 D223 V224 K225 S226 F227 S228 R229 V230 M231 K236 L248 A253 F254

L259 Q264 E269 P270 T274 D277 V278 R281 R284 D285 W286 L287 R291 G292 W293 D294 V297 E298 H301 V302 Q303 D304 L305 E306 G307 G308

• Molecule 2: Noxa

Chain B:　　　　　　　　　56%　　　　　·　7%　　　　33%

4.2.17 Score per residue for model 17

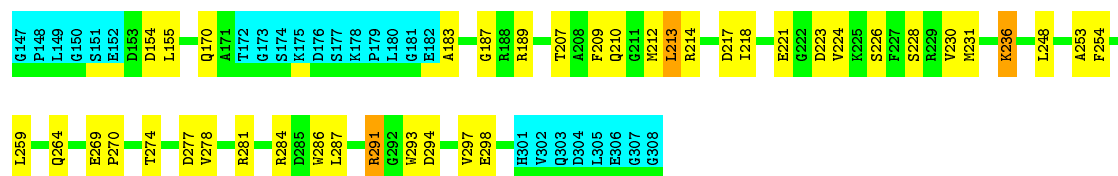• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

• Molecule 2: Noxa

4.2.18 Score per residue for model 18

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog
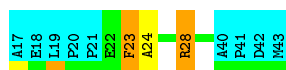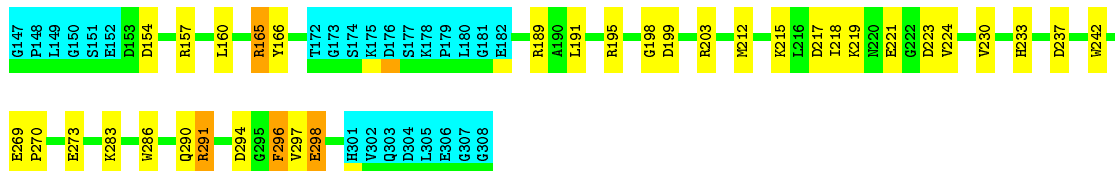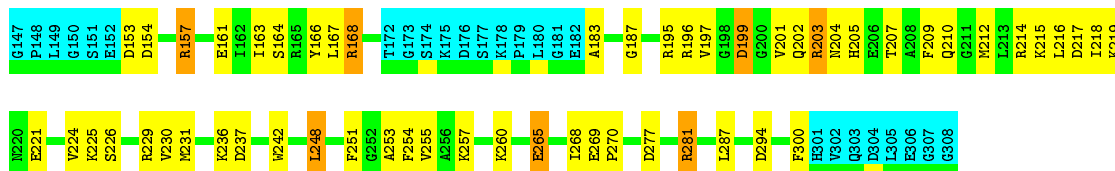

• Molecule 2: Noxa

4.2.19 Score per residue for model 19

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

G147 P148 L149 G150 S151 E152 D153 D154 L155 Y156 I163 S164 R165 Y166 L167 R168 E169 Q170 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 G187 R188 L191 E192 T193 L194 R195 R196 N220 S226 V230 M231 K236 D237 W242 L248 V255 A256 K257 H258

L259 E269 P270 K283 W286 K289 Q290 V297 H301 V302 Q303 D304 L305 E306 G307 G308

● Molecule 2: Noxa

Chain B: 56% 11% 33%

A17 E18 L19 P20 P21 E22 F23 R28 K33 A40 P41 D42 M43

4.2.20 Score per residue for model 20

● Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog

Chain A: 52% 29% • 15%
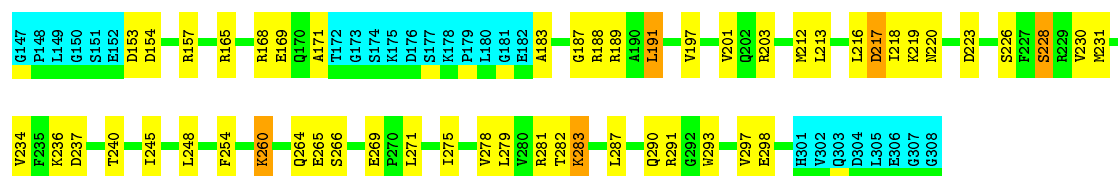
G147 P148 L149 G150 S151 E152 D153 D154 R157 R165 R168 E169 Q170 A171 T172 G173 S174 K175 D176 S177 K178 P179 L180 G181 E182 A183 G187 R188 R189 A190 L191 V197 V201 Q202 R203 M212 L213 L216 D217 I218 K219 N220 D223 S226 F227 S228 R229 V230 M231

V234 F235 K236 D237 T240 I245 L248 F254 K260 Q264 E265 S266 E269 P270 L271 I275 V278 L279 V280 R281 T282 K283 L287 Q290 R291 G292 W293 V297 E298 H301 V302 Q303 D304 L305 E306 G307 G308

● Molecule 2: Noxa

Chain B: 44% 22% 33%

A17 E18 L19 P20 P21 E22 F23 A24 A25 Q26 L27 R28 K29 I30 A40 P41 D42 M43

5 Refinement protocol and experimental data overview (i)

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: *structures with the least restraint violations.*

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

Software name	Classification	Version
CYANA	structure solution	2.1
X-PLOR NIH	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality (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	1113	1123	1120	20±4
2	B	148	146	146	2±1
All	All	25220	25380	25320	411

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 8.

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:218:ILE:HA	1:A:223:ASP:HB3	0.75	1.58	11	1
1:A:166:TYR:HE1	1:A:195:ARG:HA	0.75	1.42	11	15
1:A:228:SER:HB2	1:A:278:VAL:HG21	0.74	1.58	2	1
1:A:166:TYR:CE1	1:A:195:ARG:HA	0.73	2.17	1	16
1:A:231:MET:HG3	1:A:248:LEU:HG	0.73	1.59	18	3
1:A:189:ARG:HD3	1:A:297:VAL:HG11	0.73	1.61	14	1
1:A:265:GLU:HA	1:A:268:ILE:HG22	0.71	1.63	7	1
1:A:230:VAL:HG13	2:B:24:ALA:HA	0.70	1.60	12	3
1:A:269:GLU:HB2	1:A:270:PRO:HD3	0.67	1.66	9	14
1:A:171:ALA:HA	1:A:257:LYS:HG2	0.67	1.67	7	3
1:A:282:THR:HG23	1:A:283:LYS:HD2	0.66	1.65	7	2
1:A:218:ILE:HG12	1:A:259:LEU:HD11	0.65	1.68	11	1
1:A:212:MET:HG2	2:B:23:PHE:HA	0.64	1.67	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:291:ARG:HB3	1:A:294:ASP:HB2	0.64	1.69	16	2
2:B:26:GLN:O	2:B:30:ILE:HG12	0.63	1.92	20	1
1:A:269:GLU:HB3	1:A:270:PRO:HD3	0.63	1.71	18	4
1:A:212:MET:SD	2:B:23:PHE:HA	0.62	2.33	20	3
1:A:216:LEU:HG	1:A:218:ILE:HG12	0.61	1.73	18	1
1:A:161:GLU:O	1:A:165:ARG:HG2	0.61	1.95	13	1
1:A:165:ARG:O	1:A:169:GLU:HG2	0.61	1.96	12	1
1:A:235:PHE:HE2	1:A:248:LEU:HD11	0.60	1.56	10	1
1:A:234:VAL:HB	2:B:28:ARG:HB3	0.59	1.72	8	1
1:A:210:GLN:O	1:A:214:ARG:HG2	0.59	1.97	6	3
1:A:231:MET:HG3	1:A:248:LEU:HD13	0.58	1.73	2	2
1:A:184:GLY:HA2	1:A:188:ARG:NH2	0.58	2.13	14	1
1:A:160:LEU:HA	1:A:276:THR:HG21	0.58	1.75	11	4
1:A:163:ILE:O	1:A:167:LEU:HG	0.58	1.99	7	8
1:A:192:GLU:O	1:A:196:ARG:HG2	0.58	1.99	8	1
1:A:233:HIS:CD2	2:B:24:ALA:HB1	0.57	2.34	17	2
1:A:183:ALA:O	1:A:187:GLY:HA3	0.57	1.99	4	13
1:A:170:GLN:HB2	1:A:253:ALA:HB1	0.57	1.76	16	1
1:A:216:LEU:HB3	1:A:218:ILE:HG12	0.57	1.76	8	2
1:A:293:TRP:O	1:A:297:VAL:HG23	0.57	2.00	16	10
1:A:226:SER:O	1:A:230:VAL:HG23	0.56	1.99	20	12
1:A:259:LEU:HG	1:A:264:GLN:HB3	0.56	1.78	8	3
2:B:24:ALA:O	2:B:28:ARG:HB2	0.55	2.00	4	2
1:A:218:ILE:HG12	1:A:223:ASP:HB3	0.55	1.78	4	5
1:A:189:ARG:HB3	1:A:297:VAL:HG11	0.55	1.79	17	7
1:A:240:THR:HG22	1:A:245:ILE:HD11	0.55	1.79	7	2
1:A:286:TRP:HA	1:A:289:LYS:HD2	0.55	1.79	5	1
1:A:213:LEU:HD12	1:A:216:LEU:HD12	0.55	1.78	20	1
1:A:231:MET:HE1	1:A:275:ILE:HG13	0.54	1.78	2	1
1:A:170:GLN:HB3	1:A:257:LYS:HE3	0.54	1.79	11	2
1:A:277:ASP:O	1:A:281:ARG:HB2	0.54	2.03	16	6
1:A:242:TRP:HB3	1:A:300:PHE:CZ	0.54	2.38	4	3
1:A:201:VAL:HG13	2:B:34:VAL:HG21	0.53	1.80	1	2
1:A:171:ALA:HB1	1:A:260:LYS:HG3	0.53	1.79	5	1
1:A:198:GLY:O	1:A:202:GLN:HB2	0.53	2.03	5	2
1:A:170:GLN:HG2	1:A:253:ALA:HB1	0.53	1.81	5	1
1:A:160:LEU:HD11	1:A:273:GLU:HG3	0.52	1.81	3	1
1:A:265:GLU:HA	1:A:268:ILE:CG2	0.52	2.33	7	1
1:A:231:MET:HE3	1:A:275:ILE:HG13	0.52	1.80	11	1
1:A:218:ILE:HG23	1:A:223:ASP:HB2	0.52	1.82	8	1
1:A:224:VAL:HB	1:A:274:THR:HG21	0.52	1.81	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:227:PHE:O	1:A:231:MET:HG3	0.52	2.05	14	3
1:A:277:ASP:OD1	1:A:281:ARG:HD2	0.52	2.05	9	4
1:A:166:TYR:CE1	1:A:195:ARG:HG2	0.52	2.40	10	1
1:A:278:VAL:O	1:A:282:THR:HG22	0.51	2.05	20	2
1:A:161:GLU:O	1:A:165:ARG:HB2	0.51	2.05	4	1
1:A:187:GLY:O	1:A:191:LEU:HB2	0.51	2.05	9	5
1:A:209:PHE:O	1:A:213:LEU:HB2	0.51	2.06	16	1
1:A:255:VAL:O	1:A:259:LEU:HG	0.50	2.05	15	3
1:A:245:ILE:HG23	1:A:279:LEU:HD21	0.50	1.82	9	2
1:A:221:GLU:O	1:A:224:VAL:HG22	0.50	2.07	7	7
1:A:190:ALA:O	1:A:194:LEU:HB2	0.50	2.07	15	1
1:A:244:ARG:O	1:A:248:LEU:HG	0.50	2.06	7	1
1:A:209:PHE:O	1:A:213:LEU:HG	0.50	2.06	14	2
1:A:228:SER:HB3	1:A:278:VAL:HG21	0.50	1.83	20	1
1:A:166:TYR:OH	1:A:198:GLY:HA3	0.50	2.07	14	7
1:A:192:GLU:OE2	1:A:196:ARG:HD3	0.50	2.06	2	1
1:A:230:VAL:HG22	2:B:23:PHE:HE1	0.50	1.67	9	1
1:A:234:VAL:HG21	1:A:248:LEU:HD21	0.49	1.84	1	1
2:B:23:PHE:HD1	2:B:24:ALA:N	0.49	2.05	16	5
1:A:253:ALA:O	1:A:257:LYS:HG3	0.49	2.06	18	2
1:A:160:LEU:HD11	1:A:273:GLU:HG2	0.49	1.84	15	1
1:A:228:SER:HB2	1:A:278:VAL:HG11	0.49	1.84	1	1
1:A:259:LEU:HB3	1:A:264:GLN:HB2	0.49	1.84	13	1
1:A:190:ALA:HA	1:A:297:VAL:HG22	0.49	1.84	8	1
1:A:235:PHE:CE1	1:A:240:THR:HA	0.48	2.43	3	1
1:A:260:LYS:HE3	1:A:265:GLU:HG3	0.48	1.84	8	1
1:A:154:ASP:HA	1:A:157:ARG:CZ	0.48	2.39	20	1
1:A:202:GLN:HG3	1:A:250:SER:HB3	0.48	1.82	3	1
1:A:153:ASP:O	1:A:157:ARG:HG3	0.48	2.09	20	2
1:A:283:LYS:HB2	1:A:283:LYS:NZ	0.47	2.24	19	1
1:A:249:ILE:HD11	1:A:279:LEU:HD22	0.47	1.85	14	1
1:A:212:MET:HA	1:A:215:LYS:HE2	0.47	1.85	3	1
1:A:270:PRO:HA	1:A:273:GLU:OE1	0.47	2.09	7	2
1:A:242:TRP:HB3	1:A:300:PHE:CE2	0.47	2.45	15	4
1:A:230:VAL:HG22	2:B:23:PHE:CE1	0.47	2.44	9	5
1:A:159:SER:HA	1:A:293:TRP:CZ2	0.47	2.45	5	3
1:A:170:GLN:HB3	1:A:253:ALA:HB1	0.47	1.86	13	1
2:B:23:PHE:O	2:B:27:LEU:HG	0.46	2.10	18	2
1:A:155:LEU:HD21	1:A:287:LEU:HB3	0.46	1.88	11	2
1:A:231:MET:HA	1:A:248:LEU:HD11	0.46	1.87	18	1
1:A:265:GLU:HA	1:A:268:ILE:HD12	0.46	1.87	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:293:TRP:O	1:A:297:VAL:HG22	0.46	2.11	2	2
1:A:275:ILE:O	1:A:279:LEU:HB2	0.46	2.11	8	1
1:A:202:GLN:HB3	1:A:203:ARG:NH2	0.46	2.26	4	1
1:A:232:VAL:HG12	1:A:282:THR:HG21	0.46	1.87	1	1
1:A:259:LEU:HG	1:A:264:GLN:CB	0.46	2.40	9	1
1:A:202:GLN:HG3	1:A:250:SER:OG	0.46	2.10	12	1
1:A:171:ALA:O	1:A:260:LYS:HG2	0.46	2.10	1	2
1:A:273:GLU:O	1:A:277:ASP:HB2	0.46	2.11	2	1
1:A:197:VAL:O	1:A:201:VAL:HG23	0.45	2.10	7	5
1:A:218:ILE:HA	1:A:223:ASP:HB2	0.45	1.88	14	2
1:A:271:LEU:O	1:A:275:ILE:HG22	0.45	2.11	20	1
1:A:197:VAL:HG12	1:A:246:VAL:HG21	0.45	1.87	11	1
1:A:216:LEU:HB3	1:A:218:ILE:HG22	0.45	1.87	2	1
1:A:160:LEU:HD21	1:A:273:GLU:HA	0.45	1.88	17	2
1:A:189:ARG:O	1:A:192:GLU:HG3	0.45	2.11	7	1
1:A:216:LEU:HG	1:A:218:ILE:HG13	0.45	1.88	15	1
1:A:283:LYS:HB2	1:A:283:LYS:HZ3	0.45	1.70	8	1
1:A:216:LEU:HD22	1:A:218:ILE:HG13	0.45	1.87	20	1
1:A:286:TRP:O	1:A:290:GLN:HG2	0.45	2.12	19	1
1:A:245:ILE:O	1:A:249:ILE:HG12	0.45	2.11	5	4
1:A:221:GLU:O	1:A:225:LYS:HG2	0.45	2.11	12	1
1:A:242:TRP:CZ3	1:A:296:PHE:HB2	0.45	2.47	7	3
1:A:202:GLN:HA	1:A:209:PHE:CE2	0.44	2.46	5	1
1:A:193:THR:HG21	1:A:297:VAL:HA	0.44	1.88	19	3
1:A:291:ARG:HD2	1:A:294:ASP:OD2	0.44	2.13	17	1
1:A:189:ARG:HA	1:A:192:GLU:OE1	0.44	2.12	9	1
1:A:231:MET:CE	1:A:275:ILE:HG13	0.44	2.43	2	1
1:A:212:MET:HB3	2:B:23:PHE:HB3	0.44	1.90	8	1
1:A:195:ARG:O	1:A:199:ASP:HB2	0.44	2.13	10	2
1:A:212:MET:O	1:A:216:LEU:HB2	0.44	2.13	15	1
1:A:226:SER:HA	1:A:229:ARG:HE	0.44	1.71	3	1
1:A:231:MET:HG2	1:A:248:LEU:HD22	0.44	1.90	15	1
2:B:25:ALA:O	2:B:29:LYS:HG2	0.44	2.13	10	1
1:A:218:ILE:HA	1:A:223:ASP:CG	0.44	2.34	4	1
1:A:168:ARG:HD3	1:A:269:GLU:OE2	0.44	2.13	7	1
1:A:239:VAL:HB	1:A:244:ARG:NH2	0.44	2.28	10	1
1:A:157:ARG:HD2	1:A:161:GLU:OE2	0.43	2.12	18	1
1:A:277:ASP:OD1	1:A:281:ARG:HD3	0.43	2.13	16	1
1:A:236:LYS:HG2	1:A:236:LYS:O	0.43	2.13	16	1
2:B:23:PHE:CD1	2:B:24:ALA:N	0.43	2.86	5	3
1:A:202:GLN:HG3	1:A:203:ARG:CZ	0.43	2.44	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:ALA:HA	1:A:297:VAL:CG1	0.43	2.43	2	2
1:A:213:LEU:HD13	1:A:258:HIS:HB2	0.43	1.89	3	1
1:A:225:LYS:O	1:A:229:ARG:HG2	0.43	2.13	18	1
1:A:228:SER:HA	1:A:231:MET:HG2	0.43	1.91	6	1
1:A:212:MET:O	1:A:216:LEU:HG	0.43	2.13	5	2
1:A:231:MET:HG2	1:A:248:LEU:HD13	0.43	1.89	19	1
1:A:284:ARG:HG2	1:A:285:ASP:N	0.43	2.27	5	1
1:A:165:ARG:O	1:A:169:GLU:HB2	0.43	2.14	1	2
1:A:230:VAL:O	1:A:234:VAL:HG23	0.43	2.13	12	4
1:A:165:ARG:HD2	1:A:169:GLU:OE2	0.43	2.13	20	2
1:A:164:SER:O	1:A:168:ARG:HB2	0.42	2.14	13	2
1:A:168:ARG:HD2	1:A:269:GLU:OE1	0.42	2.13	11	1
1:A:193:THR:OG1	1:A:297:VAL:HG13	0.42	2.14	14	2
1:A:214:ARG:O	1:A:214:ARG:HD3	0.42	2.14	2	2
1:A:251:PHE:O	1:A:255:VAL:HG23	0.42	2.14	18	6
1:A:199:ASP:O	1:A:203:ARG:HB2	0.42	2.13	10	2
1:A:197:VAL:HG21	1:A:300:PHE:HB3	0.42	1.91	18	1
1:A:245:ILE:HG23	1:A:279:LEU:HD11	0.42	1.91	14	1
1:A:158:GLN:OE1	1:A:186:ALA:HB3	0.42	2.15	3	1
1:A:232:VAL:O	1:A:236:LYS:HB2	0.42	2.14	4	1
2:B:29:LYS:HA	2:B:29:LYS:HE3	0.42	1.91	8	1
2:B:25:ALA:O	2:B:29:LYS:HG3	0.42	2.14	5	1
1:A:218:ILE:CG1	1:A:259:LEU:HD11	0.42	2.44	11	1
1:A:237:ASP:N	1:A:237:ASP:OD1	0.42	2.52	8	1
1:A:262:VAL:HG23	1:A:264:GLN:HG3	0.42	1.92	7	1
1:A:189:ARG:HB3	1:A:297:VAL:HG21	0.42	1.90	4	1
1:A:213:LEU:HD21	1:A:258:HIS:HB2	0.42	1.92	15	1
1:A:166:TYR:HE1	1:A:195:ARG:HG2	0.42	1.75	15	1
1:A:218:ILE:HA	1:A:223:ASP:CB	0.42	2.45	6	1
1:A:216:LEU:HD11	1:A:251:PHE:CZ	0.42	2.50	7	1
1:A:231:MET:HE1	1:A:278:VAL:HB	0.41	1.90	16	1
1:A:168:ARG:HD2	1:A:269:GLU:OE2	0.41	2.14	9	1
1:A:259:LEU:HD22	1:A:264:GLN:NE2	0.41	2.30	16	1
1:A:285:ASP:O	1:A:289:LYS:HB2	0.41	2.15	6	1
1:A:198:GLY:O	1:A:202:GLN:HG2	0.41	2.15	10	1
1:A:206:GLU:HG3	1:A:254:PHE:CZ	0.41	2.50	3	1
1:A:296:PHE:CE1	1:A:300:PHE:HE2	0.41	2.33	11	1
2:B:29:LYS:HA	2:B:29:LYS:CE	0.41	2.45	6	1
2:B:30:ILE:O	2:B:34:VAL:HG23	0.41	2.15	9	1
1:A:265:GLU:HA	1:A:268:ILE:HG12	0.41	1.92	9	1
1:A:210:GLN:HB3	1:A:214:ARG:NH2	0.41	2.31	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:226:SER:O	1:A:229:ARG:HB3	0.41	2.15	8	1
1:A:218:ILE:HG22	1:A:267:PHE:HE2	0.41	1.75	5	1
1:A:242:TRP:CH2	1:A:296:PHE:HB2	0.41	2.51	8	1
1:A:203:ARG:HA	1:A:206:GLU:OE1	0.41	2.16	10	1
1:A:283:LYS:HB3	1:A:287:LEU:HD23	0.41	1.91	20	1
1:A:217:ASP:OD1	1:A:219:LYS:NZ	0.41	2.51	20	1
1:A:169:GLU:CD	1:A:195:ARG:HH21	0.41	2.18	13	1
1:A:231:MET:SD	1:A:248:LEU:HD13	0.41	2.56	5	1
1:A:286:TRP:CZ2	1:A:290:GLN:HG2	0.41	2.50	14	1
1:A:291:ARG:HG2	1:A:294:ASP:HB2	0.41	1.93	14	1
1:A:234:VAL:HG13	2:B:28:ARG:HA	0.41	1.91	20	1
1:A:267:PHE:O	1:A:270:PRO:HD2	0.40	2.16	9	1
1:A:203:ARG:HD3	1:A:206:GLU:OE1	0.40	2.16	3	1
1:A:188:ARG:HE	1:A:192:GLU:HG2	0.40	1.76	19	1
1:A:202:GLN:HA	1:A:209:PHE:CD2	0.40	2.52	18	1
1:A:163:ILE:HD12	1:A:276:THR:HG23	0.40	1.93	5	1
1:A:244:ARG:HA	2:B:31:GLY:HA3	0.40	1.91	2	1
1:A:242:TRP:CE3	1:A:242:TRP:HA	0.40	2.51	19	1
1:A:205:HIS:ND1	2:B:30:ILE:HG12	0.40	2.32	18	1
1:A:160:LEU:CA	1:A:276:THR:HG21	0.40	2.45	8	1
1:A:251:PHE:CD2	2:B:27:LEU:HD11	0.40	2.52	7	1
1:A:240:THR:HG21	1:A:283:LYS:HG2	0.40	1.92	20	1
1:A:189:ARG:O	1:A:192:GLU:HG2	0.40	2.17	3	1
1:A:269:GLU:CB	1:A:270:PRO:HD3	0.40	2.47	19	1
1:A:228:SER:HA	1:A:231:MET:HE3	0.40	1.93	16	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	137/162 (85%)	131±1 (96±1%)	6±1 (4±1%)	0±0 (0±0%)	59	88
2	B	18/27 (67%)	18±0 (99±2%)	0±0 (1±2%)	0±0 (0±0%)	100	100
All	All	3100/3780 (82%)	2983 (96%)	114 (4%)	3 (0%)	59	88

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	219	LYS	3

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	117/136 (86%)	102±4 (87±4%)	15±4 (13±4%)	10	52
2	B	15/22 (68%)	12±1 (82±9%)	3±1 (18±9%)	6	41
All	All	2640/3160 (84%)	2294 (87%)	346 (13%)	9	50

All 73 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	23	PHE	13
1	A	154	ASP	11
2	B	35	TYR	11
1	A	203	ARG	10
1	A	217	ASP	10
1	A	296	PHE	10
1	A	286	TRP	9
1	A	237	ASP	9
1	A	260	LYS	9
1	A	290	GLN	9
2	B	26	GLN	8
2	B	28	ARG	8
1	A	196	ARG	8
1	A	236	LYS	8
1	A	254	PHE	8
1	A	191	LEU	8
1	A	294	ASP	8
1	A	156	TYR	8
2	B	33	LYS	7
1	A	199	ASP	7
1	A	165	ARG	7
1	A	169	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	284	ARG	6
1	A	283	LYS	6
1	A	298	GLU	6
1	A	265	GLU	6
1	A	219	LYS	6
1	A	161	GLU	5
1	A	277	ASP	5
1	A	168	ARG	5
1	A	281	ARG	4
1	A	212	MET	4
1	A	291	ARG	4
1	A	221	GLU	4
1	A	220	ASN	4
2	B	22	GLU	4
1	A	213	LEU	4
1	A	266	SER	4
1	A	215	LYS	4
1	A	155	LEU	3
1	A	195	ARG	3
1	A	188	ARG	3
1	A	207	THR	3
1	A	170	GLN	3
1	A	269	GLU	3
1	A	157	ARG	3
1	A	160	LEU	3
1	A	153	ASP	3
1	A	258	HIS	3
1	A	240	THR	3
1	A	214	ARG	3
1	A	279	LEU	3
2	B	29	LYS	2
1	A	229	ARG	2
1	A	273	GLU	2
1	A	202	GLN	2
1	A	192	GLU	2
1	A	210	GLN	2
1	A	289	LYS	2
1	A	206	GLU	2
1	A	285	ASP	2
1	A	287	LEU	2
1	A	248	LEU	2
1	A	223	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	189	ARG	2
1	A	228	SER	1
1	A	264	GLN	1
1	A	239	VAL	1
1	A	271	LEU	1
1	A	204	ASN	1
1	A	164	SER	1
1	A	224	VAL	1
1	A	288	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided