Full wwPDB NMR Structure Validation Report (i)

Jun 23, 2024 – 06:55 AM EDT

PDB ID	:	6EVQ
BMRB ID	:	34192
Title	:	solution NMR structure of EB1 C terminus (191-260) with a small molecule bound into the SxIP binding site
Authors	:	Barsukov, I.L.; Almeida, T.B.
Deposited on	:	2017-11-02

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 (i) 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 (i)) were used in the production of this report:

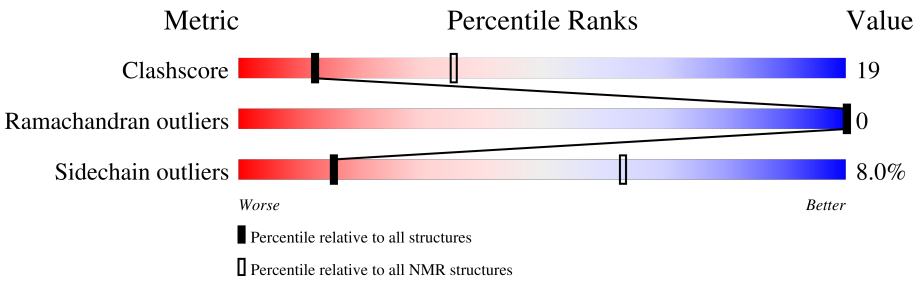
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 is 36%.

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 >=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	70	49% 31% • 17%
1	B	70	49% 31% • 17%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:192-A:249, B:192-B:249 (116)	0.37	11

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 3 clusters. No single-model clusters were found.

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

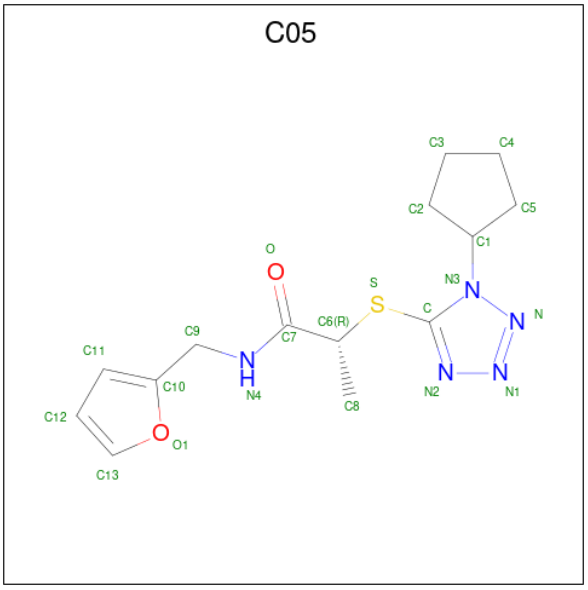
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2314 atoms, of which 1140 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Microtubule-associated protein RP/EB family member 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	70	1116	355	551	90	118	2	0
1	B	70	1116	355	551	90	118	2	0

- Molecule 2 is (2 {R})-2-[(1-cyclopentyl-1,2,3,4-tetrazol-5-yl)sulfanyl]- {N}-(furan-2-ylmethyl)propanamide (three-letter code: C05) (formula: $C_{14}H_{19}N_5O_2S$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	1	41	14	19	5	2	1
2	B	1	41	14	19	5	2	1

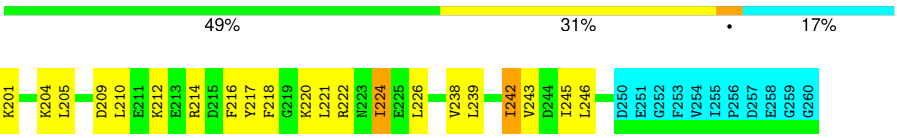
4 Residue-property plots (i)

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.

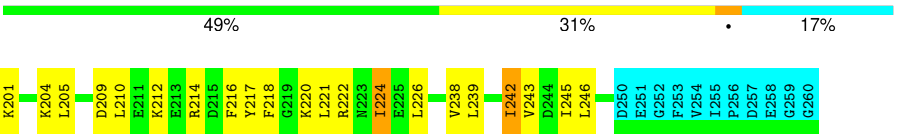
• Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A:



• Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B:



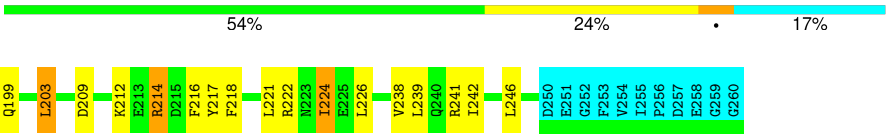
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

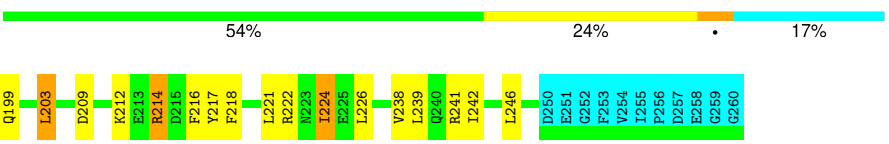
• Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A:



• Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B:



4.2.2 Score per residue for model 2

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 47% 31% • 17%

D191 E192 A193 L196 M197 K201 L205 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 Q229 D236 P237 V238 L239 I242 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 47% 31% • 17%

D191 E192 A193 L196 M197 K201 L205 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 Q229 D236 P237 V238 L239 I242 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.3 Score per residue for model 3

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 46% 34% • 17%

D191 E192 A193 L196 M197 K201 K204 L205 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 C228 Q229 E230 V238 L239 Q240 R241 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 47% 33% • 17%

D191 E192 A193 L196 M197 K201 K204 L205 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 E230 V238 L239 Q240 R241 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.4 Score per residue for model 4

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 47% 34% • 17%

D191 E192 A193 L196 M197 K201 L205 T206 V207 E211 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 C228 D236 P237 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

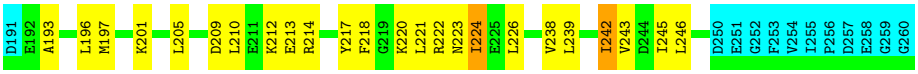
Chain B: 50% 31% • 17%

D191 E192 A193 L196 M197 K201 L205 T206 V207 E211 R214 Y217 F218 L221 R222 N223 I224 E225 L226 I227 C228 D236 P237 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.5 Score per residue for model 5

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 49% 31% • 17%



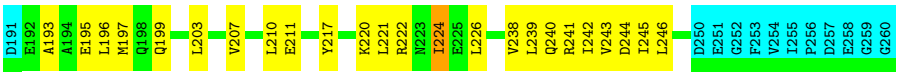
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 50% 30% • 17%

4.2.6 Score per residue for model 6

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 49% 33% • 17%



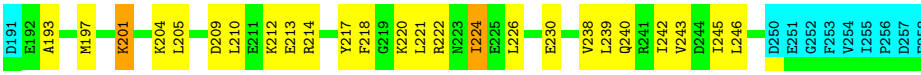
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 49% 33% • 17%

4.2.7 Score per residue for model 7

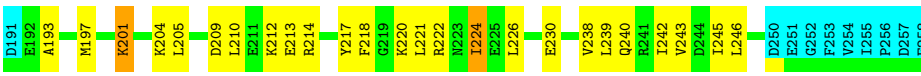
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 47% 33% • 17%



- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 47% 33% • 17%



4.2.8 Score per residue for model 8

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 53% 24% 6% 17%

D191 E192 A193 L196 M197 K201 K204 L205 L210 E211 K212 E213 R214 D215 F216 Y217 F218 L221 R222 N223 I224 E225 L226 V238 L239 I242 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 53% 24% 6% 17%

D191 E192 A193 L196 M197 K201 K204 L205 L210 E211 K212 E213 R214 D215 F216 Y217 F218 L221 R222 N223 I224 E225 L226 V238 L239 I242 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.9 Score per residue for model 9

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 47% 34% • 17%

D191 E192 A193 L196 M197 K201 V202 L203 K204 L205 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 C228 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 47% 34% • 17%

D191 E192 A193 L196 M197 K201 V202 L203 K204 L205 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 C228 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.10 Score per residue for model 10

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 50% 27% 6% 17%

D191 E192 A193 M197 Q198 Q199 V200 K201 V202 L203 K204 L205 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 L221 R222 N223 I224 E225 L226 V238 L239 I242 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 50% 27% 6% 17%

D191 E192 A193 M197 Q198 Q199 V200 K201 V202 L203 K204 L205 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 L221 R222 N223 I224 E225 L226 V238 L239 I242 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 51% 29% • 17%

D191 E192 A193 L196 M197 K201 L205 L210 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 D236 P237 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 51% 27% • 17%

D191 E192 A193 L196 M197 K201 L205 L210 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 D236 P237 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.12 Score per residue for model 12

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 46% 34% • 17%

D191 E192 A193 L196 M197 Q198 Q199 V200 K201 V202 L203 K204 V207 E208 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 L221 R222 N223 I224 E225 L226 V238 L239 Q240 R241 I242 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 44% 36% • 17%

D191 E192 A193 L196 M197 Q198 Q199 V200 K201 V202 L203 K204 V207 E208 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 L221 R222 N223 I224 E225 L226 V238 L239 Q240 R241 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.13 Score per residue for model 13

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 53% 27% • 17%

D191 E192 A193 L196 M197 K201 K204 L205 R214 Y217 F218 L221 R222 N223 I224 E225 L226 I227 C228 V238 L239 Q240 R241 I242 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 53% 27% • 17%

D191 E192 A193 L196 M197 K201 K204 L205 R214 Y217 F218 L221 R222 N223 I224 E225 L226 I227 C228 V238 L239 Q240 R241 I242 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.14 Score per residue for model 14

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 44% 36% • 17%

D191 E192 A193 A194 E195 L196 M197 K201 K204 L205 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 44% 36% • 17%

D191 E192 A193 A194 E195 L196 M197 K201 K204 L205 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.15 Score per residue for model 15

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 46% 34% • 17%

D191 E192 A193 A194 E195 L196 M197 K201 K204 L205 D209 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 C228 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 46% 34% • 17%

D191 E192 A193 A194 E195 L196 M197 K201 K204 L205 D209 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 C228 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.16 Score per residue for model 16

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 50% 29% • 17%

D191 E192 A193 L196 M197 Q198 Q199 V200 K201 K204 L205 T206 V207 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 47% 31% • 17%

D191 E192 A193 L196 M197 Q198 Q199 V200 K201 K204 L205 T206 V207 K212 E213 R214 D215 F216 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.17 Score per residue for model 17

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 49% 27% 7% 17%

D191 E192 A193 L196 M197 K201 K204 L205 D209 L210 E213 R214 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 46% 30% 7% 17%

D191 E192 A193 L196 M197 K201 K204 L205 D209 L210 E213 R214 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 V238 L239 Q240 R241 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.18 Score per residue for model 18

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 47% 34% • 17%

D191 E192 A193 L196 M197 K201 K204 L205 T206 V207 E208 D209 L210 E211 K212 E213 R214 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 C228 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 47% 34% • 17%

D191 E192 A193 L196 M197 K201 K204 L205 T206 V207 E208 D209 L210 E211 K212 E213 R214 Y217 F218 G219 K220 L221 R222 N223 I224 E225 L226 I227 C228 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.19 Score per residue for model 19

- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 54% 26% • 17%

D191 E192 A193 M197 E208 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 L221 R222 N223 I224 E225 L226 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

- Molecule 1: Microtubule-associated protein RP/EB family member 1

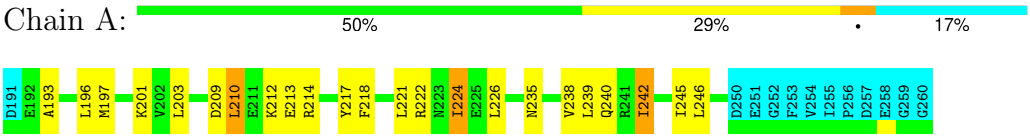
Chain B: 53% 27% • 17%

D191 E192 A193 L196 M197 E208 D209 L210 E211 K212 E213 R214 D215 F216 Y217 F218 L221 R222 N223 I224 E225 L226 V238 L239 I242 V243 D244 I245 L246 D250 E251 G252 F253 V254 I255 P256 D257 E258 G259 G260

4.2.20 Score per residue for model 20

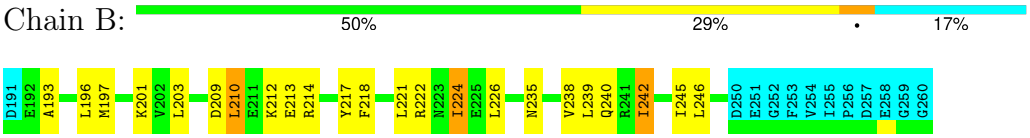
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A:



- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CNS	refinement	
ARIA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	1456
Number of shifts mapped to atoms	1456
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	36%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: C05

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	477	480	480	19±2
1	B	477	480	480	19±2
2	A	22	19	0	0±0
2	B	22	19	0	0±0
All	All	19960	19960	19200	738

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:224:ILE:HD13	1:A:246:LEU:HD21	0.76	1.56	17	20
1:B:224:ILE:HD13	1:B:246:LEU:HD21	0.75	1.57	17	20
1:A:239:LEU:HD13	1:A:242:ILE:HD12	0.74	1.60	9	20
1:B:239:LEU:HD13	1:B:242:ILE:HD12	0.73	1.61	9	20
1:A:217:TYR:O	1:A:221:LEU:HD22	0.65	1.91	11	20
1:B:217:TYR:O	1:B:221:LEU:HD22	0.65	1.92	11	20
1:B:214:ARG:O	1:B:218:PHE:HB2	0.64	1.93	18	19
1:A:224:ILE:CD1	1:A:246:LEU:HD21	0.63	2.23	7	19
1:A:214:ARG:O	1:A:218:PHE:HB2	0.63	1.93	18	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:VAL:HG23	1:A:239:LEU:HD22	0.63	1.70	20	20
1:B:238:VAL:HG23	1:B:239:LEU:HD22	0.63	1.71	20	20
1:B:224:ILE:CD1	1:B:246:LEU:HD21	0.61	2.25	7	18
1:A:238:VAL:HG21	1:B:238:VAL:HG21	0.58	1.73	18	16
1:A:212:LYS:HA	1:A:215:ASP:OD1	0.58	1.98	14	1
1:B:212:LYS:HA	1:B:215:ASP:OD1	0.58	1.98	14	1
1:A:193:ALA:O	1:A:197:MET:HG2	0.58	1.99	1	20
1:B:209:ASP:O	1:B:213:GLU:HG2	0.57	2.00	7	7
1:B:193:ALA:O	1:B:197:MET:HG2	0.57	2.00	1	20
1:A:209:ASP:O	1:A:213:GLU:HG2	0.57	2.00	7	7
1:B:201:LYS:O	1:B:205:LEU:HG	0.55	2.02	11	15
1:A:201:LYS:O	1:A:205:LEU:HG	0.55	2.02	11	15
1:A:242:ILE:O	1:A:245:ILE:HB	0.54	2.01	2	19
1:B:242:ILE:O	1:B:245:ILE:HB	0.54	2.02	20	19
1:A:222:ARG:O	1:A:226:LEU:HD13	0.53	2.04	4	20
1:B:222:ARG:O	1:B:226:LEU:HD13	0.53	2.03	4	20
2:B:301:C05:S	2:B:301:C05:C5	0.53	2.97	17	5
1:A:224:ILE:HG12	1:A:246:LEU:HD11	0.53	1.81	4	6
2:A:301:C05:S	2:A:301:C05:C5	0.53	2.97	17	5
1:A:221:LEU:HA	1:A:224:ILE:HG23	0.52	1.80	7	15
1:A:238:VAL:O	1:A:242:ILE:HG13	0.52	2.04	18	20
1:B:221:LEU:HA	1:B:224:ILE:HG23	0.52	1.81	7	11
1:A:212:LYS:O	1:A:216:PHE:HB2	0.52	2.04	1	9
1:B:224:ILE:HG12	1:B:246:LEU:HD11	0.52	1.82	4	6
1:B:212:LYS:O	1:B:216:PHE:HB2	0.52	2.04	1	10
1:B:239:LEU:O	1:B:243:VAL:HG23	0.52	2.04	6	14
1:B:238:VAL:O	1:B:242:ILE:HG13	0.52	2.04	18	20
1:A:239:LEU:O	1:A:243:VAL:HG23	0.51	2.04	6	13
1:A:209:ASP:O	1:A:212:LYS:HG2	0.51	2.05	2	7
1:A:221:LEU:HB3	1:A:246:LEU:HD22	0.51	1.82	7	6
1:A:239:LEU:CD1	1:A:242:ILE:HD12	0.51	2.32	2	4
1:B:239:LEU:CD1	1:B:242:ILE:HD12	0.51	2.33	2	4
1:B:209:ASP:O	1:B:212:LYS:HG2	0.51	2.05	2	7
1:B:221:LEU:HB3	1:B:246:LEU:HD22	0.51	1.82	7	6
1:A:220:LYS:HD2	1:B:245:ILE:HG23	0.51	1.83	17	1
1:A:201:LYS:O	1:A:204:LYS:HG2	0.49	2.07	15	8
1:B:201:LYS:O	1:B:204:LYS:HG2	0.49	2.07	15	8
1:A:226:LEU:O	1:A:230:GLU:HG2	0.49	2.07	7	1
1:A:238:VAL:O	1:A:241:ARG:HG2	0.49	2.06	1	1
1:B:226:LEU:O	1:B:230:GLU:HG2	0.49	2.08	7	1
1:B:238:VAL:O	1:B:241:ARG:HG2	0.49	2.06	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:TYR:O	1:A:220:LYS:HB2	0.48	2.08	9	10
1:A:236:ASP:HB3	1:A:238:VAL:HG22	0.48	1.86	2	3
1:A:239:LEU:HD13	1:A:242:ILE:CD1	0.48	2.35	2	15
1:A:226:LEU:O	1:A:230:GLU:HG3	0.48	2.09	3	1
1:B:236:ASP:HB3	1:B:238:VAL:HG22	0.48	1.86	2	3
1:B:239:LEU:HD13	1:B:242:ILE:CD1	0.48	2.35	2	15
1:B:217:TYR:O	1:B:220:LYS:HB2	0.47	2.09	9	9
1:B:226:LEU:O	1:B:230:GLU:HG3	0.47	2.10	3	1
1:B:199:GLN:O	1:B:203:LEU:HB2	0.47	2.10	1	4
1:B:228:CYS:SG	1:B:239:LEU:HB3	0.47	2.50	9	2
1:A:210:LEU:HB3	1:B:210:LEU:HB3	0.47	1.86	18	11
1:A:228:CYS:SG	1:A:239:LEU:HB3	0.47	2.50	9	2
1:A:199:GLN:O	1:A:203:LEU:HB2	0.46	2.10	1	4
1:A:245:ILE:HG23	1:B:220:LYS:HD2	0.46	1.87	17	1
1:A:207:VAL:O	1:A:211:GLU:HG3	0.46	2.09	12	3
1:A:216:PHE:O	1:A:220:LYS:HG2	0.46	2.11	11	3
1:B:207:VAL:O	1:B:211:GLU:HG3	0.46	2.10	12	3
1:B:216:PHE:O	1:B:220:LYS:HG2	0.46	2.11	11	2
1:A:208:GLU:HG3	1:A:209:ASP:N	0.45	2.27	19	1
1:B:208:GLU:HG3	1:B:209:ASP:N	0.45	2.27	19	1
1:A:192:GLU:O	1:A:195:GLU:HG2	0.44	2.12	15	1
1:B:241:ARG:HA	1:B:244:ASP:OD2	0.44	2.13	6	1
1:B:192:GLU:O	1:B:195:GLU:HG2	0.44	2.13	15	1
1:A:241:ARG:HA	1:A:244:ASP:OD2	0.43	2.14	6	1
1:A:208:GLU:O	1:A:212:LYS:HG2	0.43	2.13	18	1
1:A:228:CYS:HA	1:A:239:LEU:HG	0.43	1.90	4	4
1:B:208:GLU:O	1:B:212:LYS:HG2	0.43	2.13	18	1
1:B:216:PHE:O	1:B:220:LYS:HD3	0.43	2.14	14	1
1:A:216:PHE:O	1:A:220:LYS:HD3	0.43	2.14	14	1
1:A:224:ILE:HD11	1:A:242:ILE:HG22	0.43	1.90	16	2
1:B:228:CYS:HA	1:B:239:LEU:HG	0.42	1.91	13	3
1:A:221:LEU:HA	1:A:224:ILE:CG2	0.42	2.43	17	3
1:B:221:LEU:HA	1:B:224:ILE:CG2	0.42	2.43	17	3
1:B:224:ILE:HD11	1:B:242:ILE:HG22	0.42	1.90	16	2
1:A:204:LYS:O	1:A:207:VAL:HB	0.42	2.15	12	3
1:A:227:ILE:HG12	1:B:241:ARG:NH2	0.42	2.29	17	1
1:A:220:LYS:HG3	1:B:245:ILE:HG23	0.42	1.92	15	1
1:B:192:GLU:O	1:B:196:LEU:HD12	0.41	2.15	15	1
1:A:192:GLU:O	1:A:196:LEU:HD12	0.41	2.15	15	1
1:B:204:LYS:O	1:B:207:VAL:HB	0.41	2.16	12	3
1:A:223:ASN:O	1:A:227:ILE:HG13	0.41	2.15	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:223:ASN:O	1:B:227:ILE:HG13	0.41	2.15	9	2
1:A:197:MET:SD	1:B:196:LEU:HD21	0.41	2.55	19	1
1:B:221:LEU:O	1:B:224:ILE:HG23	0.40	2.16	15	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	58/70 (83%)	56±1 (97±1%)	2±1 (3±1%)	0±0 (0±0%)	100	100
1	B	58/70 (83%)	56±1 (97±1%)	2±1 (3±1%)	0±0 (0±0%)	100	100
All	All	2320/2800 (83%)	2255 (97%)	65 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	53/62 (85%)	49±2 (92±3%)	4±2 (8±3%)	16	63
1	B	53/62 (85%)	49±2 (92±3%)	4±2 (8±3%)	16	63
All	All	2120/2480 (85%)	1951 (92%)	169 (8%)	16	63

All 35 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	224	ILE	20
1	B	224	ILE	20

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Mol	Chain	Res	Type	Models (Total)
1	A	196	LEU	17
1	B	196	LEU	17
1	A	242	ILE	13
1	B	242	ILE	13
1	A	240	GLN	6
1	B	240	GLN	6
1	A	210	LEU	6
1	B	210	LEU	6
1	A	201	LYS	5
1	B	201	LYS	5
1	A	203	LEU	3
1	A	214	ARG	3
1	B	203	LEU	3
1	B	214	ARG	3
1	A	223	ASN	3
1	B	223	ASN	3
1	A	229	GLN	1
1	B	229	GLN	1
1	A	244	ASP	1
1	B	244	ASP	1
1	A	195	GLU	1
1	B	195	GLU	1
1	B	221	LEU	1
1	A	199	GLN	1
1	A	204	LYS	1
1	A	215	ASP	1
1	B	199	GLN	1
1	B	204	LYS	1
1	B	215	ASP	1
1	A	218	PHE	1
1	B	218	PHE	1
1	A	235	ASN	1
1	B	235	ASN	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	C05	B	301	-	18,24,24	1.53±0.05	3±0 (17±2%)
2	C05	A	301	-	18,24,24	1.53±0.05	3±0 (17±2%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	C05	B	301	-	17,32,32	1.21±0.08	1±0 (8±2%)
2	C05	A	301	-	17,32,32	1.21±0.08	2±0 (8±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C05	B	301	-	-	0±0,9,24,24	0±0,3,3,3
2	C05	A	301	-	-	0±0,9,24,24	0±0,3,3,3

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst

occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	301	C05	N2-N1	4.37	1.41	1.35	12	20
2	B	301	C05	N2-N1	4.34	1.41	1.35	12	20
2	B	301	C05	C11-C10	3.17	1.35	1.39	2	20
2	A	301	C05	C11-C10	3.16	1.35	1.39	2	20
2	B	301	C05	C1-N3	3.11	1.54	1.49	5	4
2	A	301	C05	C1-N3	3.11	1.54	1.49	16	4
2	A	301	C05	N-N1	3.02	1.37	1.30	17	20
2	B	301	C05	N-N1	3.01	1.37	1.30	17	20

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	301	C05	C5-C1-N3	3.39	116.72	112.11	14	4
2	A	301	C05	C5-C1-N3	3.38	116.70	112.11	14	4
2	B	301	C05	N1-N-N3	2.72	103.81	106.02	3	14
2	A	301	C05	N1-N-N3	2.71	103.82	106.02	3	15
2	A	301	C05	C-S-C6	2.64	100.19	103.37	16	11
2	B	301	C05	C-S-C6	2.64	100.20	103.37	16	11

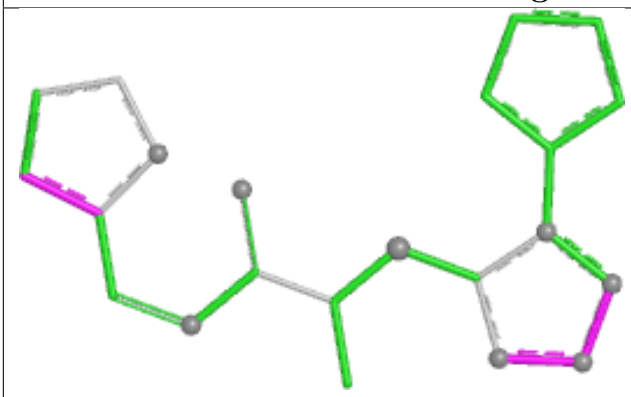
There are no chirality outliers.

There are no torsion outliers.

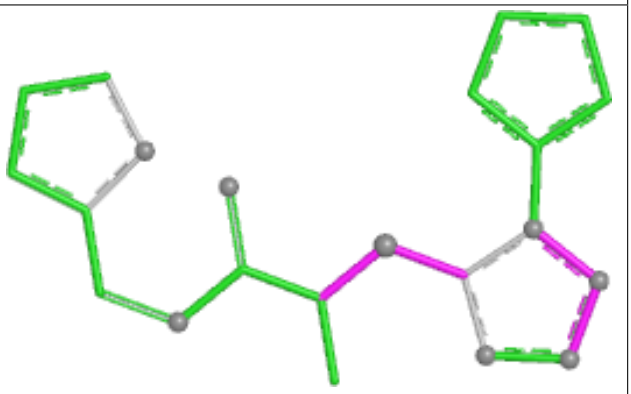
There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

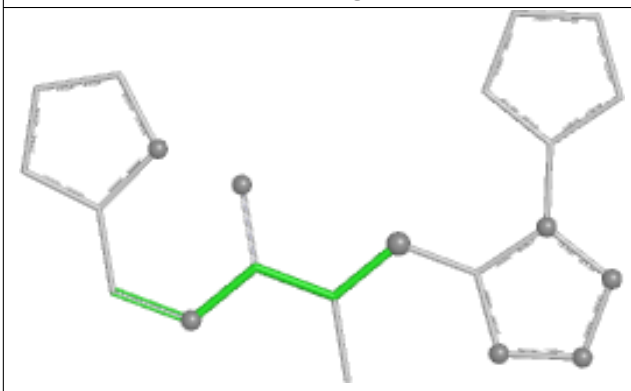
Ligand C05 B 301



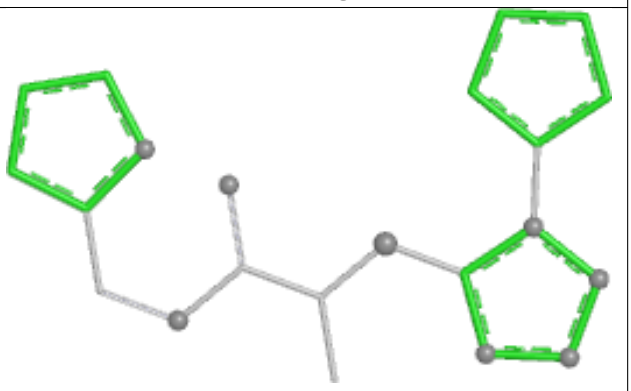
Bond lengths



Bond angles

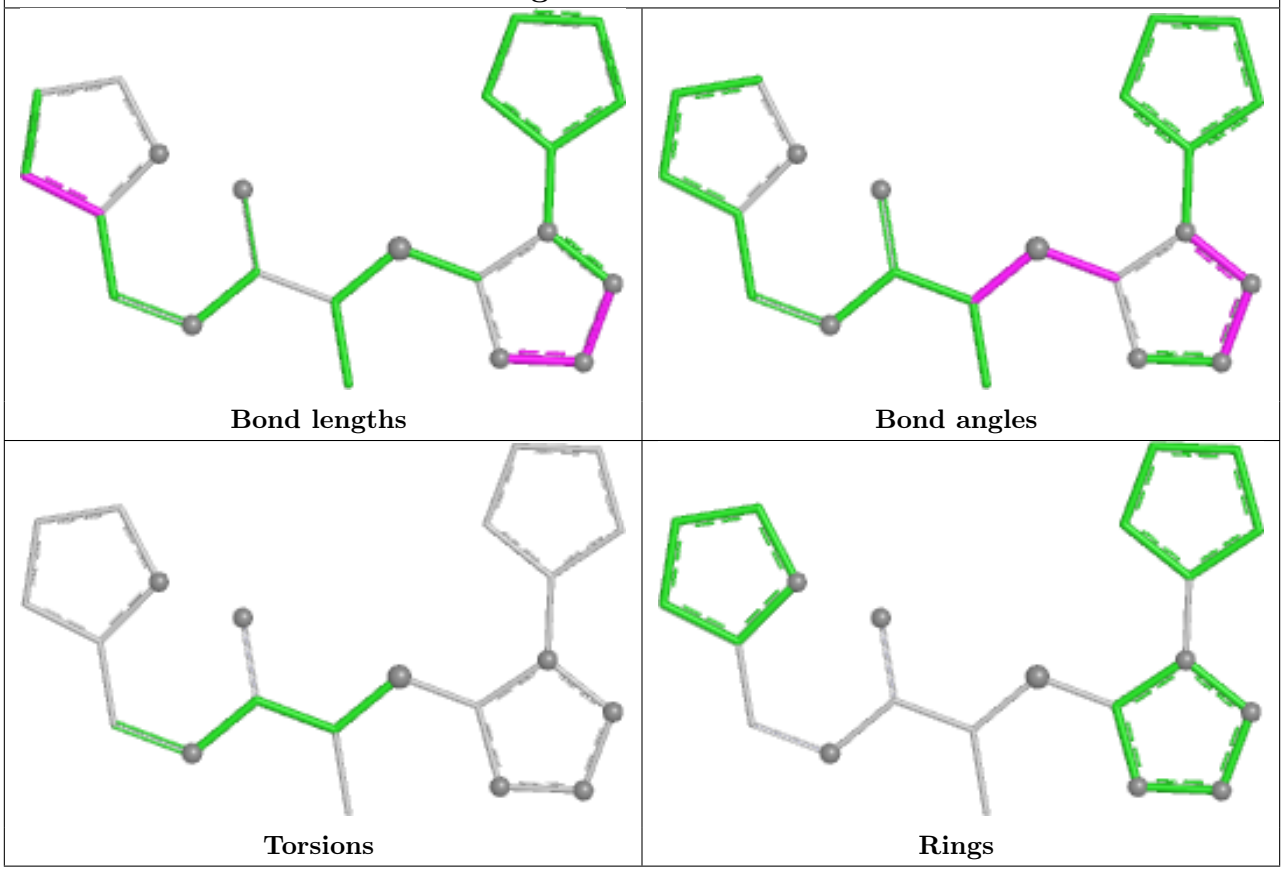


Torsions



Rings

Ligand C05 A 301



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 (i)

The completeness of assignment taking into account all chemical shift lists is 36% for the well-defined parts and 36% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	728
Number of shifts mapped to atoms	728
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	69	-0.43 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	64	0.29 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	67	-0.26 ± 0.19	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 36%, i.e. 601 atoms were assigned a chemical shift out of a possible 1676. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	231/580 (40%)	116/234 (50%)	58/232 (25%)	57/114 (50%)
Sidechain	334/1020 (33%)	216/656 (33%)	118/324 (36%)	0/40 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	36/76 (47%)	18/36 (50%)	18/40 (45%)	0/0 (—%)
Overall	601/1676 (36%)	350/926 (38%)	194/596 (33%)	57/154 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 36%, i.e. 707 atoms were assigned a chemical shift out of a possible 1940. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	273/702 (39%)	137/286 (48%)	69/280 (25%)	67/136 (49%)
Sidechain	389/1142 (34%)	253/732 (35%)	136/370 (37%)	0/40 (0%)
Aromatic	45/96 (47%)	23/46 (50%)	22/50 (44%)	0/0 (—%)
Overall	707/1940 (36%)	413/1064 (39%)	227/700 (32%)	67/176 (38%)

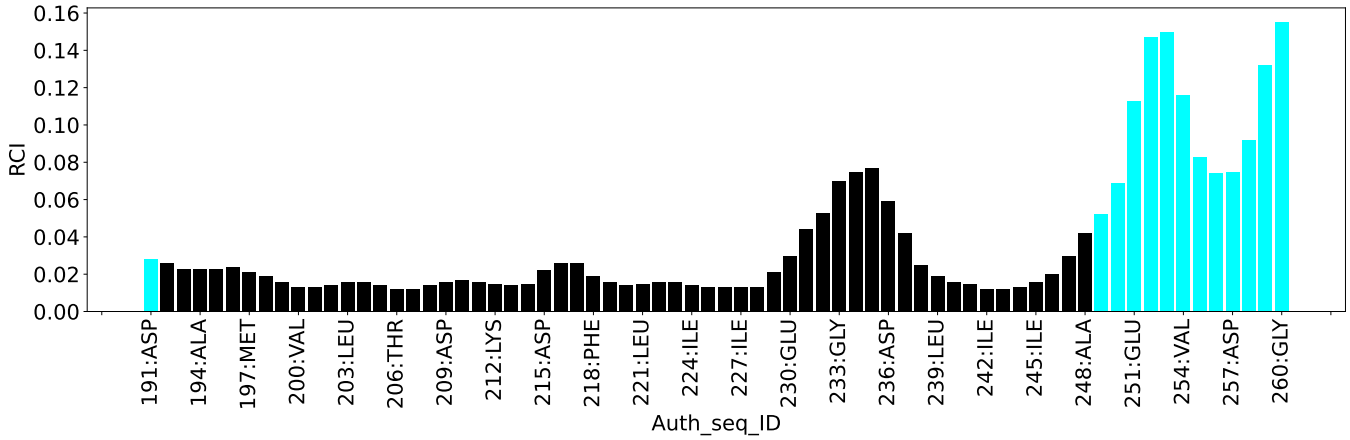
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_2*

7.2.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	728
Number of shifts mapped to atoms	728
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	69	-0.43 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	64	0.29 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	67	-0.26 ± 0.17	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 36%, i.e. 601 atoms were assigned a chemical shift out of a possible 1676. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	231/580 (40%)	116/234 (50%)	58/232 (25%)	57/114 (50%)
Sidechain	334/1020 (33%)	216/656 (33%)	118/324 (36%)	0/40 (0%)
Aromatic	36/76 (47%)	18/36 (50%)	18/40 (45%)	0/0 (—%)
Overall	601/1676 (36%)	350/926 (38%)	194/596 (33%)	57/154 (37%)

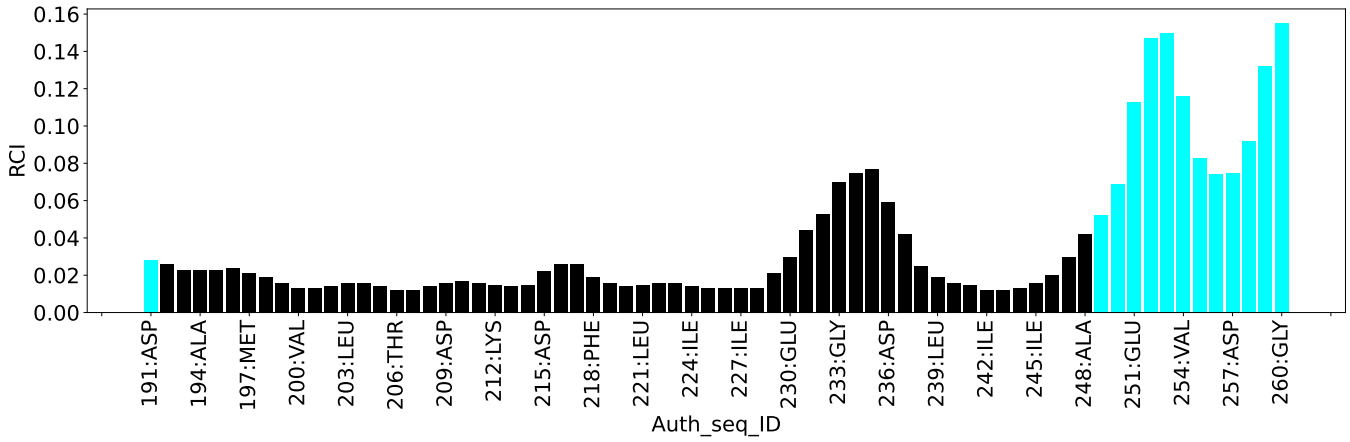
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 36%, i.e. 707 atoms were assigned a chemical shift out of a possible 1940. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	273/702 (39%)	137/286 (48%)	69/280 (25%)	67/136 (49%)
Sidechain	389/1142 (34%)	253/732 (35%)	136/370 (37%)	0/40 (0%)
Aromatic	45/96 (47%)	23/46 (50%)	22/50 (44%)	0/0 (—%)
Overall	707/1940 (36%)	413/1064 (39%)	227/700 (32%)	67/176 (38%)

7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: