



Full wwPDB NMR Structure Validation Report ⓘ

May 23, 2022 – 07:20 pm BST

PDB ID : 7OLG
Title : EB1 bound to MACF peptide
Authors : Almeida, T.B.; Barsukov, I.L.
Deposited on : 2021-05-20

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.28.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

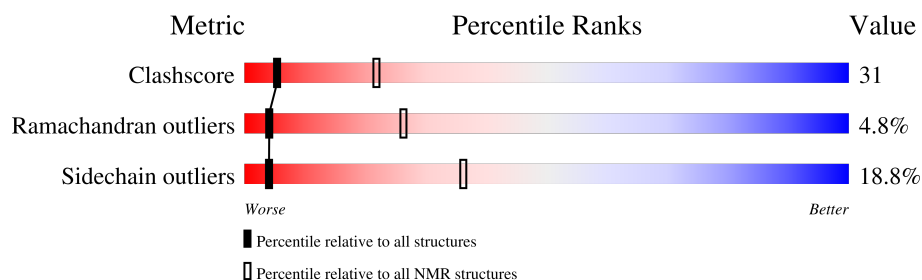
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 38%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	70	
1	B	70	
2	C	11	
2	D	11	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:192-A:258, B:192-B:258, C:5477-C:5482, D:5477- D:5482 (146)	0.39	6

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 6 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2624 atoms, of which 1314 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
1	A	70	Total	C	H	N	O	S	0
			1116	355	551	90	118	2	
1	B	70	Total	C	H	N	O	S	0
			1116	355	551	90	118	2	

- Molecule 2 is a protein called 11MACF.

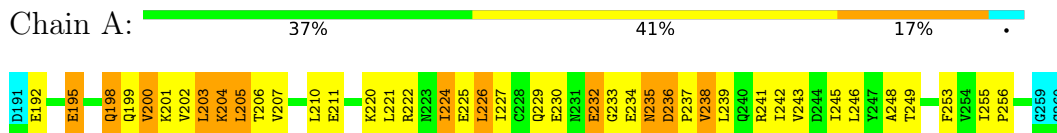
Mol	Chain	Residues	Atoms					Trace
2	C	11	Total	C	H	N	O	0
			196	57	106	18	15	
2	D	11	Total	C	H	N	O	0
			196	57	106	18	15	

4 Residue-property plots

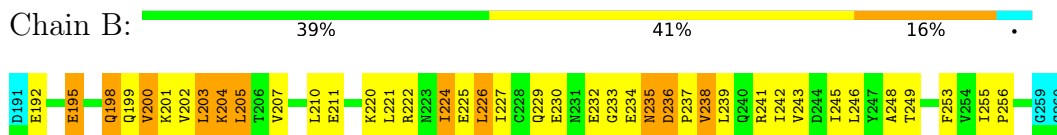
4.1 Average score per residue in the NMR ensemble

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.

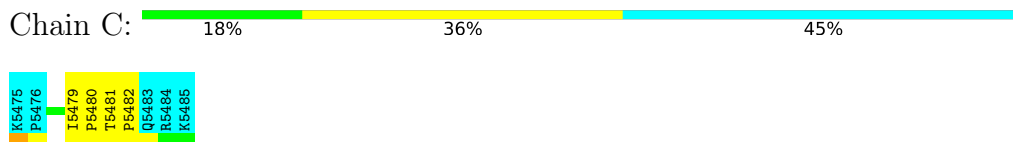
- Molecule 1: Microtubule-associated protein RP/EB family member 1



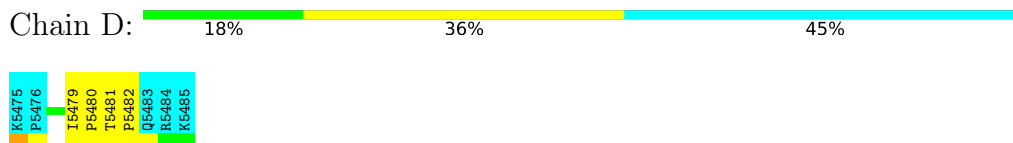
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF



- Molecule 2: 11MACF

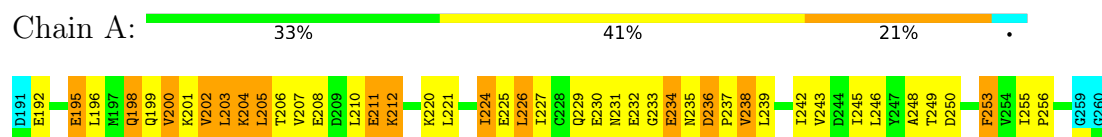


4.2 Scores per residue for each member of the ensemble

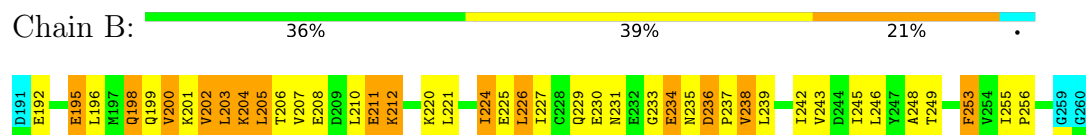
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

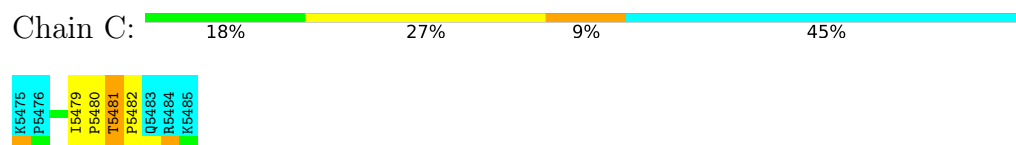
- Molecule 1: Microtubule-associated protein RP/EB family member 1



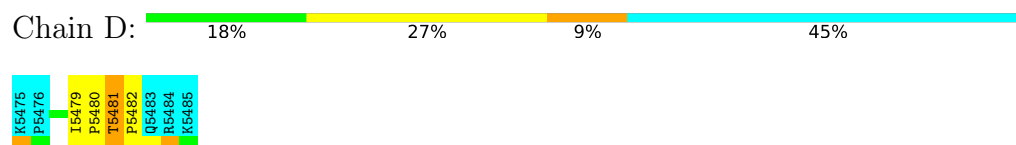
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF

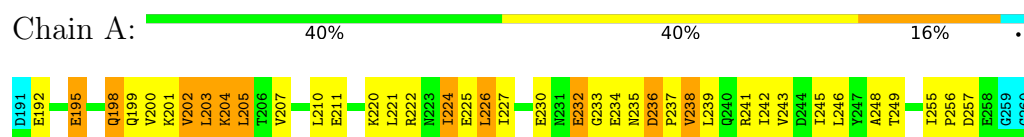


- Molecule 2: 11MACF

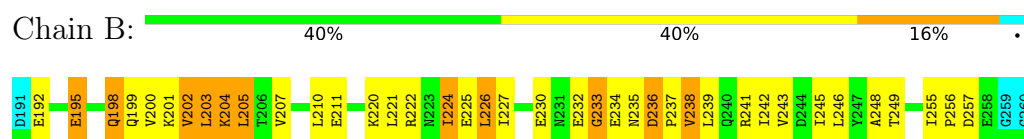


4.2.2 Score per residue for model 2

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



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

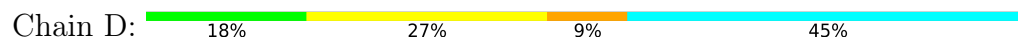


- Molecule 2: 11MACF



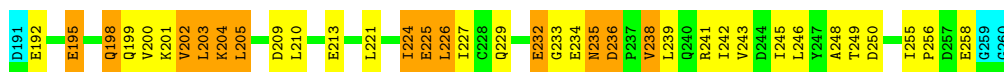


- Molecule 2: 11MACF



4.2.3 Score per residue for model 3

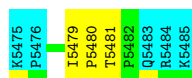
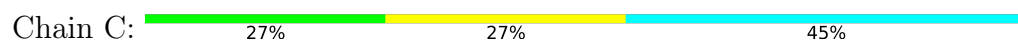
- Molecule 1: Microtubule-associated protein RP/EB family member 1



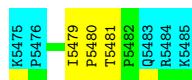
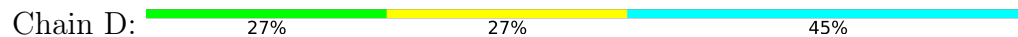
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF



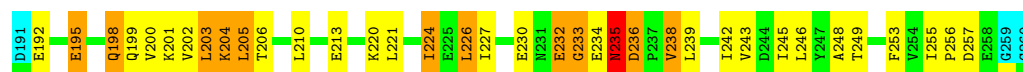
- Molecule 2: 11MACF



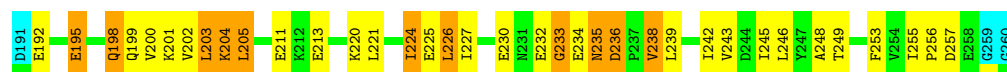
4.2.4 Score per residue for model 4

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

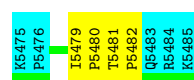




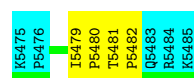
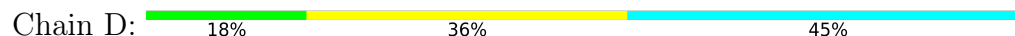
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF



- Molecule 2: 11MACF

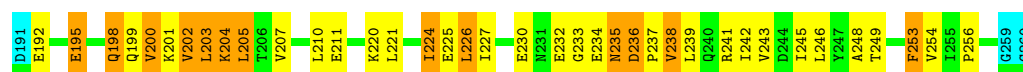


4.2.5 Score per residue for model 5

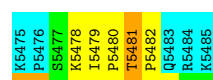
- Molecule 1: Microtubule-associated protein RP/EB family member 1



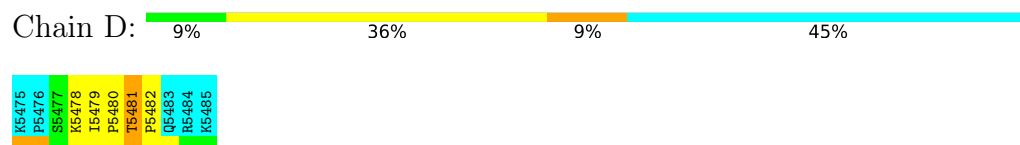
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF

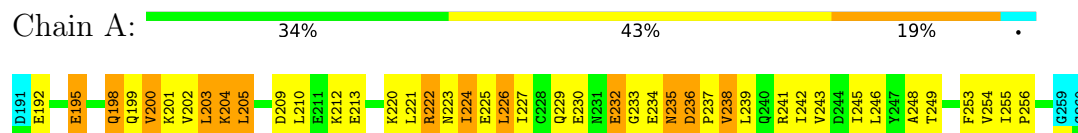


- Molecule 2: 11MACF

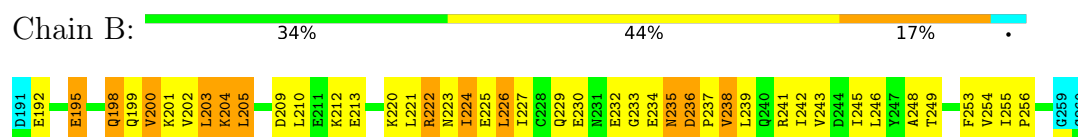


4.2.6 Score per residue for model 6 (medoid)

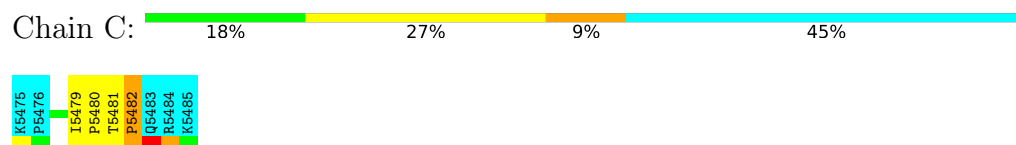
- Molecule 1: Microtubule-associated protein RP/EB family member 1



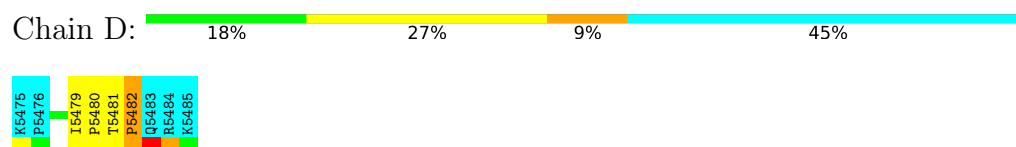
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF

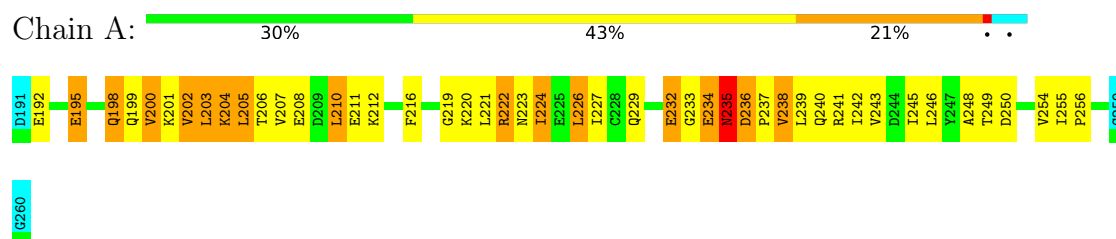


- Molecule 2: 11MACF



4.2.7 Score per residue for model 7

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



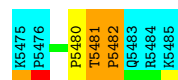
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 



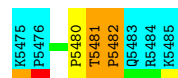
- Molecule 2: 11MACF

Chain C: 



- Molecule 2: 11MACF

Chain D: 



4.2.8 Score per residue for model 8

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

Chain A: 



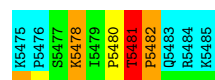
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 



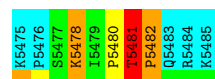
- Molecule 2: 11MACF

Chain C: 



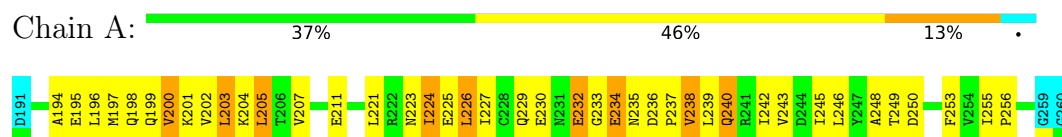
- Molecule 2: 11MACF

Chain D: 

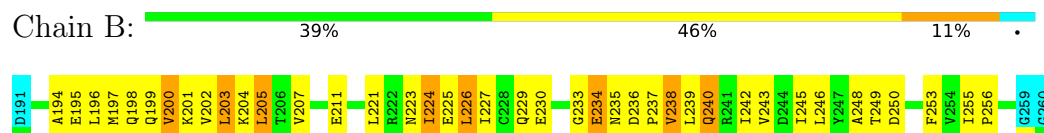


4.2.9 Score per residue for model 9

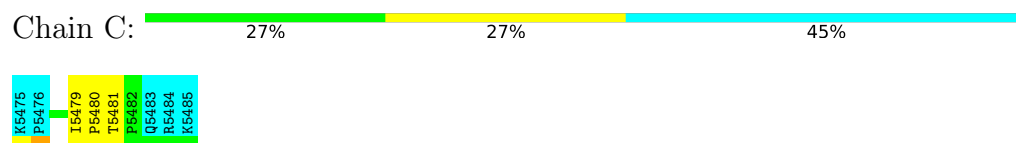
- Molecule 1: Microtubule-associated protein RP/EB family member 1



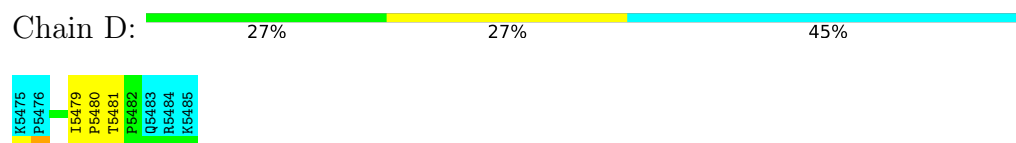
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF

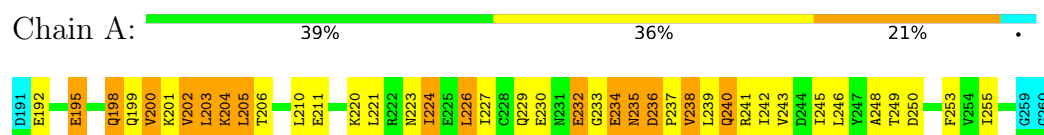


- Molecule 2: 11MACF

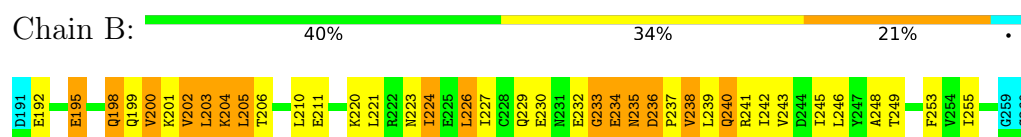


4.2.10 Score per residue for model 10

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

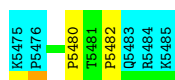


- Molecule 1: Microtubule-associated protein RP/EB family member 1

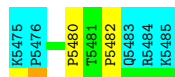


- Molecule 2: 11MACF



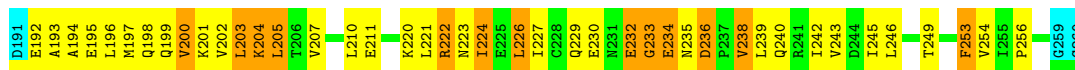


- Molecule 2: 11MACF

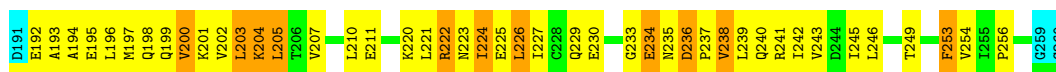


4.2.11 Score per residue for model 11

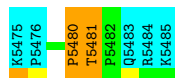
- Molecule 1: Microtubule-associated protein RP/EB family member 1



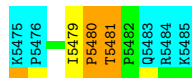
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF



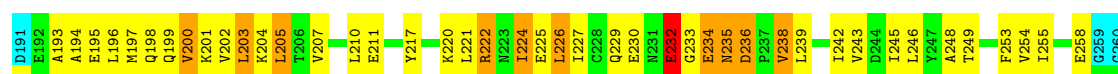
- Molecule 2: 11MACF



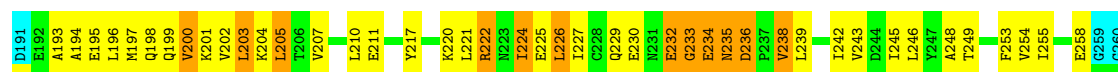
4.2.12 Score per residue for model 12

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

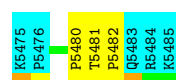
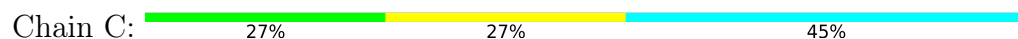




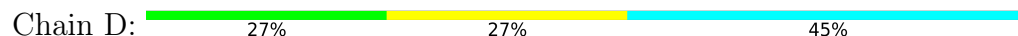
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF



- Molecule 2: 11MACF

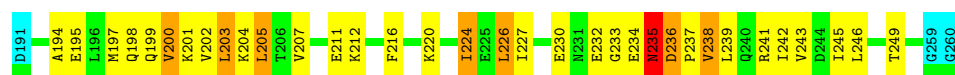


4.2.13 Score per residue for model 13

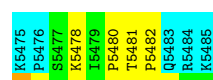
- Molecule 1: Microtubule-associated protein RP/EB family member 1



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

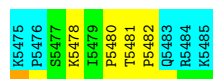


- Molecule 2: 11MACF



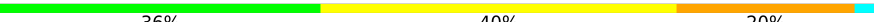
- Molecule 2: 11MACF

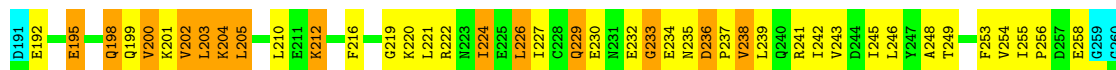
Chain D:  18% 36% 45%



4.2.14 Score per residue for model 14

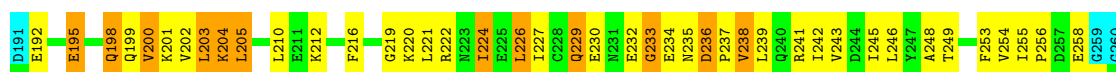
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A:  36% 40% 20% .



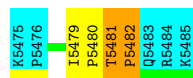
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B:  36% 43% 17% .



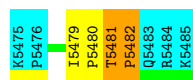
- Molecule 2: 11MACF

Chain C:  18% 18% 18% 45%



- Molecule 2: 11MACF

Chain D:  18% 18% 18% 45%



4.2.15 Score per residue for model 15

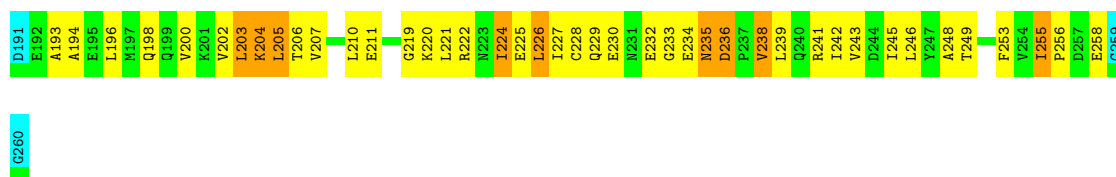
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A:  37% 44% 14% .



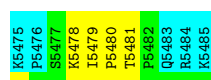
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B:  36% 47% 13% .



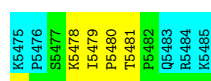
- Molecule 2: 11MACF

Chain C: 18% 36% 45%



- Molecule 2: 11MACF

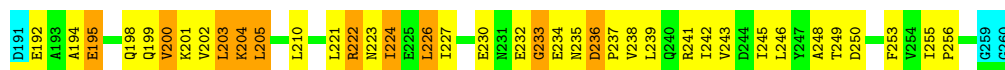
Chain D: 18% 36% 45%



4.2.16 Score per residue for model 16

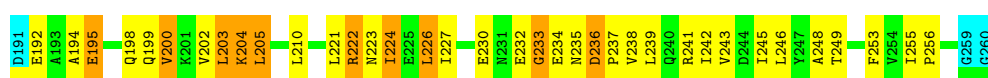
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 41% 40% 14%



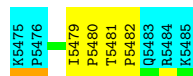
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 44% 37% 14%



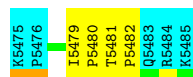
- Molecule 2: 11MACF

Chain C: 18% 36% 45%



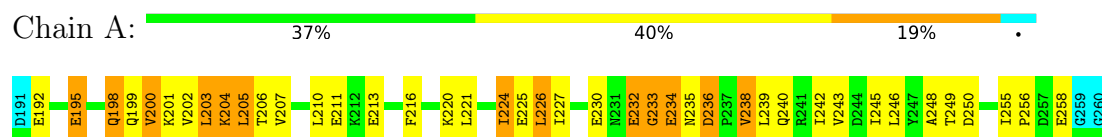
- Molecule 2: 11MACF

Chain D: 18% 36% 45%

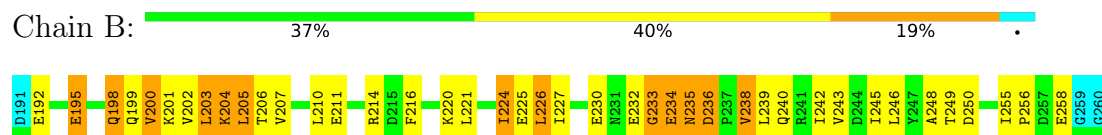


4.2.17 Score per residue for model 17

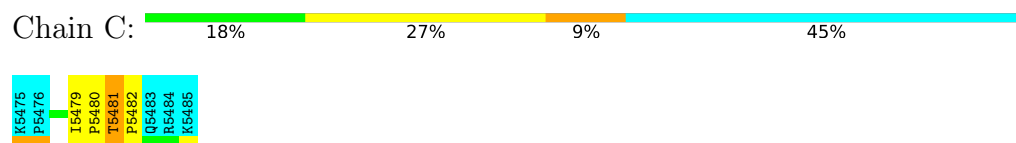
- Molecule 1: Microtubule-associated protein RP/EB family member 1



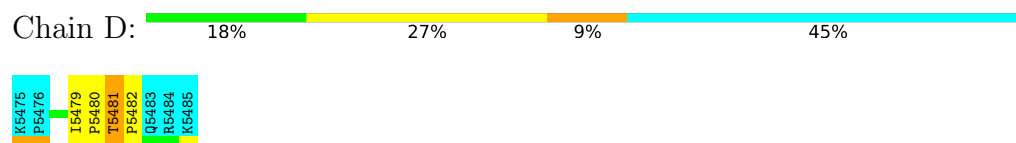
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF

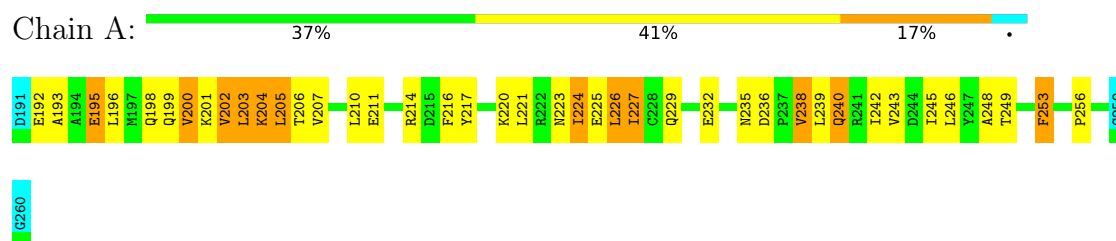


- Molecule 2: 11MACF

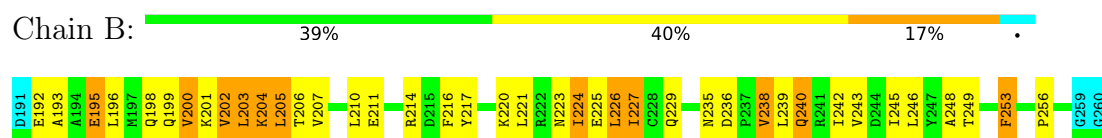


4.2.18 Score per residue for model 18

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

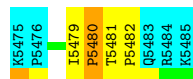


- Molecule 1: Microtubule-associated protein RP/EB family member 1



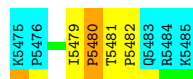
- Molecule 2: 11MACF

Chain C: 



- Molecule 2: 11MACF

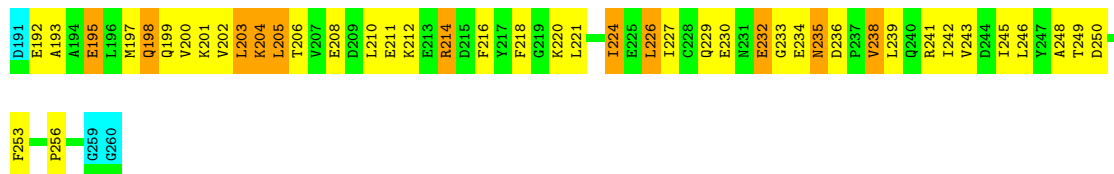
Chain D: 



4.2.19 Score per residue for model 19

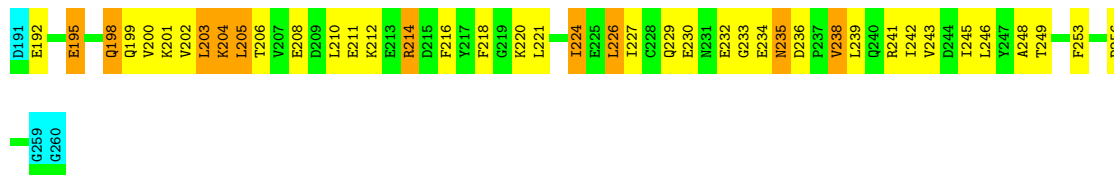
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain A: 



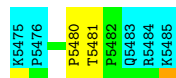
- Molecule 1: Microtubule-associated protein RP/EB family member 1

Chain B: 



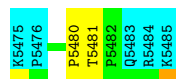
- Molecule 2: 11MACF

Chain C: 



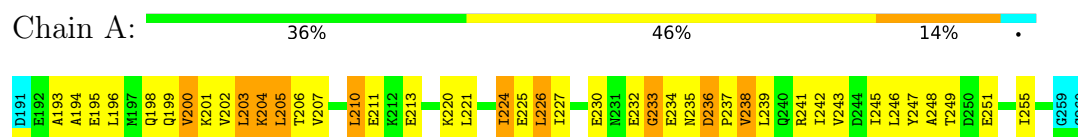
- Molecule 2: 11MACF

Chain D: 

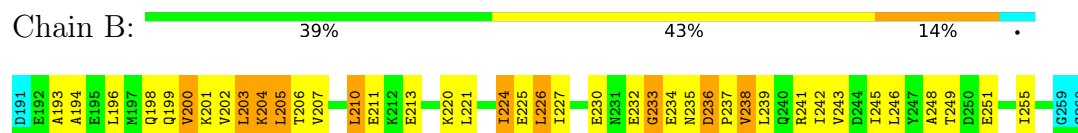


4.2.20 Score per residue for model 20

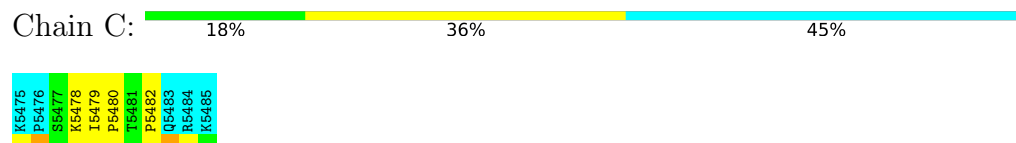
- Molecule 1: Microtubule-associated protein RP/EB family member 1



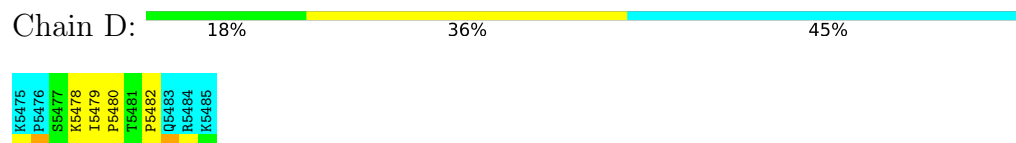
- Molecule 1: Microtubule-associated protein RP/EB family member 1



- Molecule 2: 11MACF



- Molecule 2: 11MACF



5 Refinement protocol and experimental data overview

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

Of the 160 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	1
Total number of shifts	849
Number of shifts mapped to atoms	849
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.4
2	C	0.0±0.0	0.3±0.5
2	D	0.0±0.0	0.3±0.5
All	All	0	30

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	232	GLU	Peptide	16
2	C	5481	THR	Peptide	7
2	D	5481	THR	Peptide	7

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	548	539	539	41±5
1	B	548	539	539	40±5
2	C	44	50	50	4±1
2	D	44	50	50	4±2
All	All	23680	23560	23560	1482

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:VAL:O	1:A:204:LYS:HG2	0.83	1.73	13	3
1:B:200:VAL:O	1:B:204:LYS:HG2	0.82	1.74	13	3
1:A:239:LEU:HD21	1:B:238:VAL:HG11	0.78	1.54	1	18
1:A:206:THR:O	1:A:210:LEU:HG	0.78	1.78	15	6
1:B:206:THR:O	1:B:210:LEU:HG	0.78	1.78	8	6
1:A:238:VAL:HG11	1:B:239:LEU:HD21	0.78	1.55	1	18
1:B:249:THR:HB	2:D:5480:PRO:CB	0.76	2.10	13	2
1:A:249:THR:HB	2:C:5480:PRO:CB	0.74	2.12	13	2
1:A:198:GLN:O	1:A:202:VAL:HG13	0.73	1.84	19	20
1:A:221:LEU:HD12	1:A:224:ILE:HD11	0.72	1.61	12	16
1:B:198:GLN:O	1:B:202:VAL:HG13	0.72	1.84	4	20
1:A:199:GLN:O	1:A:203:LEU:HD22	0.72	1.84	12	19
1:B:221:LEU:HD12	1:B:224:ILE:HD11	0.71	1.62	12	16
1:B:199:GLN:O	1:B:203:LEU:HD22	0.70	1.86	12	19
1:B:242:ILE:O	1:B:246:LEU:HG	0.70	1.87	8	20
1:A:249:THR:HG23	1:A:253:PHE:HB3	0.69	1.62	11	3
1:A:242:ILE:O	1:A:246:LEU:HG	0.69	1.87	8	20
1:B:256:PRO:HD3	2:D:5481:THR:OG1	0.69	1.88	11	16
1:B:249:THR:HG23	1:B:253:PHE:HB3	0.69	1.62	11	3
1:A:256:PRO:HD3	2:C:5481:THR:OG1	0.68	1.89	11	16
1:A:207:VAL:O	1:A:211:GLU:HG3	0.67	1.89	1	12
1:B:207:VAL:O	1:B:211:GLU:HG3	0.67	1.90	1	12
1:A:200:VAL:O	1:A:204:LYS:HB2	0.65	1.92	16	15
1:B:200:VAL:O	1:B:204:LYS:HB2	0.65	1.92	16	14
1:A:194:ALA:O	1:A:198:GLN:HG2	0.65	1.92	16	7
1:B:195:GLU:O	1:B:199:GLN:HG3	0.64	1.92	3	17
1:A:195:GLU:O	1:A:199:GLN:HG3	0.64	1.92	3	17
1:B:194:ALA:O	1:B:198:GLN:HG2	0.64	1.92	16	7
1:B:253:PHE:CE1	2:D:5480:PRO:HB2	0.64	2.27	4	6
1:B:249:THR:HB	2:D:5480:PRO:HB2	0.64	1.69	13	1
1:B:249:THR:OG1	2:D:5480:PRO:HG3	0.64	1.93	19	6
1:A:253:PHE:CE1	2:C:5480:PRO:HB2	0.63	2.28	4	6
1:A:204:LYS:NZ	1:B:203:LEU:HG	0.63	2.08	17	3
1:A:242:ILE:O	1:A:245:ILE:HB	0.63	1.94	6	20
1:B:208:GLU:O	1:B:212:LYS:HD3	0.63	1.94	7	2
1:B:249:THR:OG1	2:D:5480:PRO:HB3	0.63	1.93	11	8
1:B:242:ILE:O	1:B:245:ILE:HB	0.63	1.94	20	20
1:A:208:GLU:O	1:A:212:LYS:HD3	0.63	1.94	7	2
1:B:254:VAL:HB	2:D:5482:PRO:O	0.63	1.94	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:220:LYS:HE3	1:B:245:ILE:O	0.62	1.92	17	10
1:A:254:VAL:HB	2:C:5482:PRO:O	0.62	1.94	14	2
1:A:249:THR:OG1	2:C:5480:PRO:HG3	0.62	1.94	19	6
1:B:210:LEU:HD12	1:B:211:GLU:N	0.62	2.10	18	6
1:A:210:LEU:HD12	1:A:211:GLU:N	0.62	2.10	18	6
1:A:203:LEU:HG	1:B:204:LYS:NZ	0.61	2.10	5	3
1:A:245:ILE:O	1:B:220:LYS:HE3	0.61	1.95	17	10
1:A:239:LEU:O	1:A:243:VAL:HG22	0.61	1.95	3	20
1:B:249:THR:CB	2:D:5480:PRO:HB3	0.61	2.25	11	2
1:A:220:LYS:HE2	1:B:245:ILE:O	0.61	1.96	10	3
1:A:192:GLU:O	1:A:195:GLU:HG3	0.61	1.95	19	15
1:A:200:VAL:O	1:A:204:LYS:HD2	0.60	1.96	19	12
1:A:249:THR:HB	2:C:5480:PRO:HB2	0.60	1.72	13	1
1:B:192:GLU:O	1:B:195:GLU:HG3	0.59	1.96	19	15
1:B:239:LEU:O	1:B:243:VAL:HG22	0.59	1.96	3	20
1:A:249:THR:CB	2:C:5480:PRO:HB3	0.59	2.27	11	2
1:B:200:VAL:O	1:B:204:LYS:HD2	0.59	1.97	19	12
1:A:203:LEU:HB3	1:B:203:LEU:HB3	0.59	1.74	1	19
1:A:208:GLU:O	1:A:212:LYS:HB3	0.59	1.97	1	1
1:A:195:GLU:O	1:A:198:GLN:HG3	0.59	1.98	3	5
1:B:195:GLU:O	1:B:198:GLN:HG3	0.59	1.98	3	5
1:B:208:GLU:O	1:B:212:LYS:HB3	0.59	1.97	1	1
1:A:213:GLU:OE1	2:D:5482:PRO:HG3	0.58	1.98	4	1
1:A:249:THR:OG1	2:C:5480:PRO:HB3	0.58	1.98	11	8
1:A:245:ILE:O	1:B:220:LYS:HE2	0.57	1.99	10	3
1:A:198:GLN:O	1:A:201:LYS:HB2	0.57	2.00	6	17
1:A:220:LYS:HB3	1:B:245:ILE:HG23	0.57	1.74	19	2
1:A:221:LEU:HA	1:A:224:ILE:HD11	0.57	1.77	2	4
1:A:232:GLU:O	1:A:234:GLU:N	0.57	2.37	14	16
1:A:199:GLN:O	1:A:202:VAL:HG22	0.56	2.00	12	15
1:A:238:VAL:O	1:A:242:ILE:HG23	0.56	2.00	18	16
1:B:249:THR:HB	2:D:5480:PRO:HB3	0.56	1.78	12	2
1:A:226:LEU:O	1:A:230:GLU:HG3	0.56	2.00	20	17
1:B:210:LEU:O	1:B:214:ARG:HG2	0.56	1.99	18	1
1:B:221:LEU:HA	1:B:224:ILE:HD11	0.56	1.77	2	4
1:B:198:GLN:O	1:B:201:LYS:HB2	0.56	2.00	8	14
1:B:226:LEU:O	1:B:230:GLU:HG3	0.56	2.01	20	17
1:A:210:LEU:O	1:A:214:ARG:HG2	0.56	1.99	18	1
1:A:223:ASN:O	1:A:227:ILE:HG13	0.56	2.00	10	3
1:A:204:LYS:HA	1:A:204:LYS:HE2	0.55	1.78	13	15
1:A:198:GLN:O	1:A:201:LYS:HB3	0.55	2.00	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:238:VAL:O	1:B:242:ILE:HG23	0.55	2.01	18	16
1:B:232:GLU:O	1:B:234:GLU:N	0.55	2.39	14	10
1:B:199:GLN:O	1:B:202:VAL:HG22	0.55	2.01	12	14
1:A:237:PRO:O	1:A:241:ARG:HG2	0.55	2.01	14	9
1:A:203:LEU:CD2	1:B:204:LYS:HZ3	0.55	2.14	14	3
1:B:223:ASN:O	1:B:227:ILE:HG13	0.55	2.01	10	3
1:A:249:THR:HB	2:C:5480:PRO:HB3	0.55	1.79	12	2
1:B:225:GLU:HB2	2:D:5479:ILE:HD11	0.55	1.77	5	8
1:B:198:GLN:O	1:B:201:LYS:HB3	0.55	2.01	4	2
1:B:237:PRO:O	1:B:241:ARG:HG2	0.55	2.02	14	10
1:B:204:LYS:HE2	1:B:204:LYS:HA	0.54	1.79	13	15
1:A:234:GLU:O	1:A:236:ASP:N	0.54	2.41	6	19
1:A:225:GLU:HB2	2:C:5479:ILE:HD11	0.54	1.78	5	7
1:A:227:ILE:HD13	1:B:241:ARG:HG3	0.54	1.79	13	7
1:A:245:ILE:HG23	1:B:220:LYS:HB3	0.54	1.78	7	2
1:B:234:GLU:O	1:B:236:ASP:N	0.54	2.41	13	19
1:A:203:LEU:HG	1:B:204:LYS:HZ1	0.53	1.63	5	1
1:A:213:GLU:CD	2:D:5482:PRO:HG3	0.53	2.24	4	1
1:A:204:LYS:HZ1	1:B:203:LEU:HG	0.53	1.63	5	1
1:A:204:LYS:HZ3	1:B:203:LEU:CD2	0.53	2.15	17	3
1:A:205:LEU:HD22	1:A:205:LEU:O	0.53	2.04	10	20
1:A:239:LEU:HD12	1:A:239:LEU:N	0.53	2.19	20	20
1:B:236:ASP:OD2	1:B:237:PRO:HD2	0.53	2.04	1	1
1:A:236:ASP:OD2	1:A:237:PRO:HD2	0.53	2.05	1	1
1:B:253:PHE:CD1	2:D:5480:PRO:HB2	0.52	2.39	4	2
1:B:249:THR:HB	2:D:5480:PRO:CG	0.52	2.34	12	1
1:A:203:LEU:CG	1:B:204:LYS:HZ3	0.52	2.17	14	2
1:A:214:ARG:HE	1:A:218:PHE:HB2	0.52	1.64	19	1
1:B:254:VAL:HG12	2:D:5481:THR:O	0.52	2.05	12	1
1:B:214:ARG:HE	1:B:218:PHE:HB2	0.52	1.64	19	1
1:B:205:LEU:O	1:B:205:LEU:HD22	0.52	2.05	10	20
1:A:204:LYS:HZ3	1:B:203:LEU:CG	0.52	2.18	14	2
1:A:219:GLY:O	1:A:222:ARG:HG3	0.52	2.03	7	3
1:B:238:VAL:HG13	1:B:239:LEU:HD12	0.52	1.82	18	8
1:A:253:PHE:CD1	2:C:5480:PRO:HB2	0.52	2.39	4	2
1:B:239:LEU:N	1:B:239:LEU:HD12	0.51	2.21	20	16
1:A:195:GLU:O	1:A:198:GLN:HG2	0.51	2.05	19	7
1:A:204:LYS:NZ	1:B:203:LEU:HD21	0.51	2.21	16	2
1:B:219:GLY:O	1:B:222:ARG:HG3	0.51	2.04	7	3
1:A:237:PRO:HA	1:A:240:GLN:OE1	0.51	2.06	9	2
1:A:249:THR:HB	2:C:5480:PRO:CG	0.51	2.36	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:VAL:HG13	1:A:239:LEU:HD12	0.51	1.83	18	7
1:A:249:THR:HG21	1:A:255:ILE:HG13	0.51	1.82	16	14
1:B:217:TYR:O	1:B:221:LEU:HB2	0.51	2.06	12	1
1:B:237:PRO:HA	1:B:240:GLN:OE1	0.51	2.06	9	2
1:A:254:VAL:HG12	2:C:5481:THR:O	0.51	2.06	12	1
1:A:214:ARG:CZ	1:A:214:ARG:HA	0.51	2.36	19	1
1:B:214:ARG:CZ	1:B:214:ARG:HA	0.51	2.36	19	1
1:A:203:LEU:HD21	1:B:204:LYS:NZ	0.50	2.21	16	2
1:B:195:GLU:O	1:B:198:GLN:HG2	0.50	2.06	19	6
1:A:217:TYR:O	1:A:221:LEU:HB2	0.50	2.06	12	1
1:A:226:LEU:HD22	1:A:226:LEU:C	0.50	2.27	13	19
1:B:249:THR:HG21	1:B:255:ILE:HG13	0.49	1.83	3	14
1:A:204:LYS:HZ3	1:B:203:LEU:HG	0.49	1.68	14	2
1:A:236:ASP:CG	1:A:237:PRO:HD2	0.49	2.28	13	1
1:B:236:ASP:CG	1:B:237:PRO:HD2	0.49	2.28	13	1
1:A:200:VAL:O	1:A:204:LYS:HE3	0.49	2.08	16	2
1:B:253:PHE:CE2	2:D:5480:PRO:HB2	0.49	2.42	10	2
1:B:200:VAL:O	1:B:204:LYS:HE3	0.49	2.08	16	2
1:B:226:LEU:HD22	1:B:226:LEU:C	0.48	2.29	13	17
2:C:5481:THR:HB	2:C:5482:PRO:O	0.48	2.08	1	2
1:A:253:PHE:CE2	2:C:5480:PRO:HB2	0.48	2.43	10	2
1:B:213:GLU:HG2	2:C:5482:PRO:HG2	0.48	1.85	20	1
1:A:214:ARG:HA	1:A:217:TYR:CD1	0.48	2.44	18	1
1:A:228:CYS:SG	1:A:246:LEU:HD11	0.48	2.48	15	1
1:B:225:GLU:HB3	2:D:5479:ILE:HD11	0.48	1.84	1	2
2:D:5481:THR:HB	2:D:5482:PRO:O	0.48	2.08	1	2
1:A:239:LEU:HA	1:A:242:ILE:HG12	0.48	1.85	4	5
1:B:228:CYS:SG	1:B:246:LEU:HD11	0.48	2.49	15	1
1:B:214:ARG:HA	1:B:217:TYR:CD1	0.48	2.44	18	1
2:C:5479:ILE:HG23	2:C:5480:PRO:HD2	0.48	1.85	15	5
1:A:225:GLU:HB3	2:C:5479:ILE:HD11	0.48	1.84	1	2
1:B:213:GLU:OE1	2:C:5482:PRO:HG3	0.48	2.09	4	1
1:B:257:ASP:O	2:D:5478:LYS:HD3	0.48	2.08	8	1
1:A:221:LEU:HD11	1:B:221:LEU:HD11	0.48	1.83	18	1
2:D:5479:ILE:HG23	2:D:5480:PRO:HD2	0.48	1.85	15	4
1:A:198:GLN:HA	1:A:201:LYS:HD3	0.48	1.84	17	3
1:A:213:GLU:HG2	2:D:5482:PRO:HG2	0.48	1.85	20	1
1:A:210:LEU:HB3	1:B:210:LEU:HB3	0.47	1.86	1	9
1:B:239:LEU:HA	1:B:242:ILE:HG12	0.47	1.86	4	5
1:A:257:ASP:O	2:C:5478:LYS:HD3	0.47	2.08	8	1
1:B:217:TYR:OH	2:C:5482:PRO:HD3	0.47	2.09	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:204:LYS:HZ2	1:B:204:LYS:N	0.47	2.08	5	2
1:B:209:ASP:O	1:B:213:GLU:HG3	0.47	2.10	6	1
1:A:209:ASP:O	1:A:213:GLU:HG3	0.47	2.10	6	1
1:B:226:LEU:O	1:B:229:GLN:HG2	0.47	2.10	19	9
1:B:239:LEU:HD12	1:B:239:LEU:N	0.47	2.25	6	4
1:A:210:LEU:HD21	1:B:211:GLU:HG2	0.47	1.85	19	3
1:A:226:LEU:O	1:A:229:GLN:HG2	0.47	2.10	19	9
1:A:203:LEU:HG	1:B:204:LYS:HZ3	0.46	1.70	14	1
1:B:198:GLN:HA	1:B:201:LYS:HD3	0.46	1.85	17	3
1:A:196:LEU:HD22	1:B:197:MET:HA	0.46	1.86	8	1
1:B:216:PHE:CE2	1:B:220:LYS:HD2	0.46	2.45	14	2
1:A:221:LEU:HA	1:A:224:ILE:CD1	0.46	2.40	20	4
1:B:221:LEU:HA	1:B:224:ILE:CD1	0.46	2.40	20	4
1:A:239:LEU:HD12	1:A:239:LEU:H	0.46	1.70	7	4
1:A:216:PHE:CE2	1:A:220:LYS:HD2	0.46	2.45	14	2
1:A:240:GLN:NE2	1:A:240:GLN:N	0.46	2.64	10	5
1:A:204:LYS:HZ2	1:A:204:LYS:N	0.46	2.09	5	1
1:B:255:ILE:HG23	2:D:5478:LYS:O	0.46	2.10	15	1
1:B:208:GLU:O	1:B:212:LYS:HG3	0.46	2.11	19	1
1:A:208:GLU:O	1:A:212:LYS:HG3	0.46	2.11	19	1
2:C:5479:ILE:CG2	2:C:5480:PRO:HD2	0.46	2.41	14	5
1:B:239:LEU:HD12	1:B:239:LEU:H	0.46	1.70	7	4
1:A:206:THR:HG22	1:A:210:LEU:HD22	0.45	1.87	1	2
2:D:5479:ILE:CG2	2:D:5480:PRO:HD2	0.45	2.41	14	5
1:B:224:ILE:HD12	1:B:246:LEU:CD2	0.45	2.41	13	3
1:A:213:GLU:HG2	2:D:5482:PRO:CG	0.45	2.42	20	1
1:A:203:LEU:HD21	1:B:204:LYS:HZ3	0.45	1.70	14	2
1:A:255:ILE:HG23	2:C:5478:LYS:O	0.45	2.10	15	1
1:A:239:LEU:HD11	1:B:239:LEU:HD11	0.45	1.89	9	1
1:A:226:LEU:HD22	1:A:227:ILE:N	0.45	2.27	15	1
1:B:202:VAL:HG23	1:B:203:LEU:HD13	0.45	1.88	12	3
1:A:204:LYS:NZ	1:B:203:LEU:CG	0.45	2.80	17	2
1:A:206:THR:O	1:A:210:LEU:HB2	0.45	2.11	17	3
1:A:224:ILE:HD12	1:A:246:LEU:CD2	0.45	2.41	13	3
1:B:249:THR:HB	2:D:5480:PRO:HG3	0.45	1.89	12	1
1:A:238:VAL:HG22	1:A:239:LEU:HD12	0.45	1.88	17	1
1:B:206:THR:HG22	1:B:210:LEU:HD22	0.44	1.88	1	1
1:A:222:ARG:HD3	1:A:223:ASN:N	0.44	2.27	7	4
1:B:235:ASN:ND2	1:B:240:GLN:HE22	0.44	2.09	7	1
1:B:232:GLU:HG3	1:B:233:GLY:H	0.44	1.72	17	8
1:A:217:TYR:OH	2:D:5482:PRO:HD3	0.44	2.12	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:232:GLU:O	1:A:235:ASN:N	0.44	2.50	6	10
1:A:216:PHE:O	1:A:220:LYS:HG2	0.44	2.12	7	2
1:B:249:THR:OG1	2:D:5480:PRO:CB	0.44	2.63	11	2
1:A:205:LEU:O	1:A:208:GLU:HG2	0.44	2.12	1	1
1:B:225:GLU:CG	2:D:5479:ILE:HD11	0.44	2.42	3	1
1:B:232:GLU:O	1:B:235:ASN:N	0.44	2.50	5	11
1:A:241:ARG:HG3	1:B:227:ILE:HD13	0.44	1.89	16	5
1:A:235:ASN:ND2	1:A:240:GLN:HE22	0.44	2.10	7	1
1:B:216:PHE:O	1:B:220:LYS:HG2	0.44	2.13	7	2
1:B:212:LYS:O	1:B:216:PHE:HB2	0.44	2.13	13	1
1:B:226:LEU:HD22	1:B:227:ILE:N	0.44	2.27	15	1
1:B:213:GLU:HG2	2:C:5482:PRO:CG	0.44	2.43	20	1
1:A:197:MET:HA	1:B:196:LEU:HD22	0.44	1.87	8	1
1:B:206:THR:O	1:B:210:LEU:HB2	0.44	2.12	17	2
1:A:225:GLU:HG3	1:A:226:LEU:N	0.44	2.28	1	1
1:A:236:ASP:OD1	1:A:237:PRO:HD2	0.44	2.13	7	1
1:B:232:GLU:CD	1:B:233:GLY:H	0.44	2.15	12	1
1:A:212:LYS:O	1:A:216:PHE:HB2	0.44	2.13	13	1
1:A:203:LEU:CG	1:B:204:LYS:NZ	0.43	2.81	17	3
1:B:222:ARG:HD3	1:B:223:ASN:N	0.43	2.28	7	4
1:B:205:LEU:O	1:B:208:GLU:HG2	0.43	2.13	1	1
1:B:236:ASP:OD1	1:B:237:PRO:HD2	0.43	2.13	7	1
1:A:202:VAL:HG23	1:A:203:LEU:HD13	0.43	1.89	12	3
1:B:240:GLN:N	1:B:240:GLN:NE2	0.43	2.67	10	5
1:B:238:VAL:HG22	1:B:239:LEU:HD12	0.43	1.90	17	1
1:B:225:GLU:HG3	1:B:226:LEU:N	0.43	2.29	1	1
1:A:225:GLU:CG	2:C:5479:ILE:HD11	0.43	2.42	3	1
1:A:232:GLU:HG3	1:A:233:GLY:H	0.43	1.73	11	7
1:B:254:VAL:HG11	2:D:5482:PRO:C	0.43	2.33	12	1
1:A:205:LEU:HD22	1:A:205:LEU:C	0.43	2.34	14	4
1:A:203:LEU:HG	1:B:203:LEU:HB3	0.43	1.89	14	1
1:A:210:LEU:HD12	1:A:210:LEU:C	0.43	2.34	20	2
1:B:197:MET:O	1:B:201:LYS:HG3	0.43	2.13	11	4
1:B:246:LEU:O	2:D:5480:PRO:HD2	0.43	2.13	11	1
1:A:249:THR:HB	2:C:5480:PRO:HG3	0.43	1.90	12	1
1:A:211:GLU:HG2	1:B:210:LEU:HD21	0.43	1.89	19	1
1:A:221:LEU:HD12	1:A:224:ILE:CD1	0.43	2.42	15	4
1:B:214:ARG:NE	1:B:218:PHE:HB2	0.43	2.29	19	1
1:A:197:MET:O	1:A:201:LYS:HG3	0.43	2.13	12	4
1:B:255:ILE:O	1:B:258:GLU:HB2	0.43	2.14	12	2
1:B:205:LEU:HD22	1:B:205:LEU:C	0.43	2.35	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:ALA:HA	1:A:196:LEU:HB2	0.43	1.91	11	4
1:A:255:ILE:O	1:A:258:GLU:HB2	0.43	2.14	12	2
1:A:216:PHE:O	1:A:220:LYS:HG3	0.43	2.14	17	1
1:A:214:ARG:NE	1:A:218:PHE:HB2	0.43	2.28	19	1
1:B:204:LYS:NZ	1:B:204:LYS:N	0.42	2.67	5	3
1:B:226:LEU:HA	1:B:229:GLN:HB3	0.42	1.90	14	1
1:A:196:LEU:HB3	1:B:196:LEU:HB3	0.42	1.91	1	2
1:A:239:LEU:O	1:A:243:VAL:HG13	0.42	2.14	11	3
1:B:216:PHE:O	1:B:220:LYS:HG3	0.42	2.14	17	1
1:A:209:ASP:O	1:A:213:GLU:HG2	0.42	2.15	3	1
1:B:209:ASP:O	1:B:213:GLU:HG2	0.42	2.14	3	1
1:A:246:LEU:O	2:C:5480:PRO:HD2	0.42	2.14	11	1
1:A:226:LEU:HA	1:A:229:GLN:HB3	0.42	1.90	14	1
1:A:249:THR:HG22	1:A:250:ASP:N	0.42	2.30	3	7
1:B:221:LEU:HD12	1:B:224:ILE:CD1	0.42	2.43	15	4
1:A:221:LEU:HA	1:A:224:ILE:HG13	0.42	1.92	7	3
1:A:226:LEU:O	1:A:229:GLN:HB2	0.42	2.14	7	1
1:A:222:ARG:O	1:A:225:GLU:HB3	0.42	2.14	12	2
1:A:204:LYS:HA	1:A:204:LYS:CE	0.42	2.45	17	3
1:B:222:ARG:O	1:B:225:GLU:HB3	0.42	2.15	12	2
1:B:193:ALA:HA	1:B:196:LEU:HB2	0.42	1.90	15	4
1:A:226:LEU:O	1:A:229:GLN:HB3	0.42	2.14	14	1
1:A:223:ASN:O	1:A:227:ILE:HD12	0.42	2.15	8	2
1:B:221:LEU:HA	1:B:224:ILE:HG13	0.42	1.92	7	2
1:B:223:ASN:O	1:B:227:ILE:HD12	0.42	2.15	8	2
1:A:205:LEU:HD13	1:A:206:THR:N	0.42	2.30	19	1
1:B:205:LEU:HD13	1:B:206:THR:N	0.42	2.30	19	1
1:B:239:LEU:O	1:B:243:VAL:HG13	0.42	2.14	11	3
1:A:193:ALA:HB1	1:B:196:LEU:HD12	0.42	1.91	18	1
1:A:231:ASN:O	1:A:234:GLU:HG2	0.42	2.15	1	2
1:A:204:LYS:NZ	1:A:204:LYS:N	0.42	2.68	5	2
1:A:222:ARG:HD3	1:A:222:ARG:C	0.42	2.36	16	2
1:B:210:LEU:HD12	1:B:210:LEU:C	0.41	2.35	20	1
1:A:212:LYS:HD3	2:D:5482:PRO:HG3	0.41	1.93	14	1
1:B:226:LEU:O	1:B:229:GLN:HB2	0.41	2.15	7	1
1:A:236:ASP:HB3	1:A:239:LEU:HD13	0.41	1.91	9	1
1:A:213:GLU:CD	1:B:214:ARG:HD3	0.41	2.35	17	1
1:B:226:LEU:C	1:B:226:LEU:HD22	0.41	2.36	8	1
1:B:236:ASP:HB3	1:B:239:LEU:HD13	0.41	1.91	9	1
1:B:225:GLU:HB2	2:D:5479:ILE:CD1	0.41	2.46	11	1
1:A:193:ALA:O	1:A:197:MET:HG2	0.41	2.16	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:195:GLU:O	1:B:198:GLN:HB2	0.41	2.16	9	3
1:A:210:LEU:HD11	1:B:210:LEU:HD11	0.41	1.91	20	1
1:B:226:LEU:O	1:B:229:GLN:HB3	0.41	2.16	14	1
1:B:204:LYS:CE	1:B:204:LYS:HA	0.41	2.46	17	1
1:B:249:THR:HG22	1:B:250:ASP:N	0.40	2.31	3	2
1:A:207:VAL:O	1:A:211:GLU:HB2	0.40	2.16	7	1
1:A:204:LYS:HZ3	1:B:203:LEU:HD21	0.40	1.74	17	1
1:B:231:ASN:O	1:B:234:GLU:HG2	0.40	2.16	1	1
1:A:196:LEU:HD12	1:B:193:ALA:HB1	0.40	1.93	18	1
1:B:226:LEU:HA	1:B:229:GLN:CB	0.40	2.47	14	1
1:A:247:TYR:C	1:A:249:THR:H	0.40	2.20	20	1
1:B:207:VAL:O	1:B:211:GLU:HB2	0.40	2.16	7	1
1:B:208:GLU:HG3	1:B:209:ASP:N	0.40	2.31	7	1
1:A:254:VAL:HG11	2:C:5482:PRO:C	0.40	2.37	12	1
1:A:204:LYS:HE2	1:A:204:LYS:CA	0.40	2.43	13	1
1:A:198:GLN:HA	1:A:201:LYS:HE2	0.40	1.92	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	67/70 (96%)	62±1 (92±2%)	2±2 (3±2%)	3±0 (4±0%)	5	29
1	B	67/70 (96%)	62±1 (93±2%)	2±2 (3±2%)	3±0 (4±1%)	5	29
2	C	6/11 (55%)	4±1 (67±13%)	1±1 (23±11%)	1±1 (10±10%)	1	10
2	D	6/11 (55%)	4±1 (67±13%)	1±1 (23±11%)	1±1 (10±10%)	1	10
All	All	2920/3240 (90%)	2644 (91%)	137 (5%)	139 (5%)	4	26

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	235	ASN	20
1	B	235	ASN	20

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Mol	Chain	Res	Type	Models (Total)
1	A	233	GLY	19
1	B	233	GLY	19
1	A	248	ALA	18
1	B	248	ALA	18
2	C	5482	PRO	10
2	D	5482	PRO	10
2	C	5480	PRO	2
2	D	5480	PRO	2
1	A	232	GLU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	61/62 (98%)	49±2 (80±4%)	12±2 (20±4%)	3	33
1	B	61/62 (98%)	49±2 (80±4%)	12±2 (20±4%)	4	34
2	C	6/11 (55%)	6±1 (94±11%)	0±1 (6±11%)	24	73
2	D	6/11 (55%)	6±1 (94±11%)	0±1 (6±11%)	24	73
All	All	2680/2920 (92%)	2175 (81%)	505 (19%)	4	36

All 70 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	203	LEU	20
1	A	205	LEU	20
1	A	224	ILE	20
1	A	226	LEU	20
1	A	238	VAL	20
1	B	203	LEU	20
1	B	205	LEU	20
1	B	224	ILE	20
1	B	226	LEU	20
1	B	238	VAL	20
1	A	204	LYS	17
1	A	236	ASP	17

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Mol	Chain	Res	Type	Models (Total)
1	B	204	LYS	17
1	B	236	ASP	17
1	A	200	VAL	15
1	B	200	VAL	15
1	A	195	GLU	14
1	B	195	GLU	14
1	A	198	GLN	12
1	A	227	ILE	12
1	B	198	GLN	12
1	B	227	ILE	12
1	A	202	VAL	9
1	A	234	GLU	8
1	B	202	VAL	8
1	A	253	PHE	7
1	B	234	GLU	7
1	B	253	PHE	7
1	A	222	ARG	6
1	B	222	ARG	6
2	C	5478	LYS	4
2	D	5478	LYS	4
1	A	212	LYS	3
1	B	212	LYS	3
1	A	258	GLU	3
1	B	258	GLU	3
1	A	235	ASN	3
2	C	5481	THR	3
2	D	5481	THR	3
1	A	240	GLN	3
1	B	240	GLN	3
1	A	257	ASP	2
1	B	257	ASP	2
1	A	229	GLN	2
1	A	241	ARG	2
1	B	229	GLN	2
1	B	241	ARG	2
1	A	210	LEU	2
1	B	210	LEU	2
1	B	235	ASN	2
1	A	211	GLU	1
1	B	211	GLU	1
1	A	225	GLU	1
1	B	225	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	196	LEU	1
1	B	196	LEU	1
1	A	220	LYS	1
1	A	254	VAL	1
1	B	220	LYS	1
1	B	254	VAL	1
1	A	232	GLU	1
1	B	232	GLU	1
1	A	255	ILE	1
1	B	255	ILE	1
1	A	250	ASP	1
1	B	250	ASP	1
1	A	214	ARG	1
1	B	214	ARG	1
1	A	251	GLU	1
1	B	251	GLU	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 ⓘ

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 38% 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*

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	849
Number of shifts mapped to atoms	849
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 \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	66	-0.40 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	61	0.16 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	65	-0.29 ± 0.35	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 38%, i.e. 712 atoms were assigned a chemical shift out of a possible 1852. 14 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	262/714 (37%)	136/284 (48%)	63/292 (22%)	63/138 (46%)
Sidechain	407/1052 (39%)	253/610 (41%)	147/400 (37%)	7/42 (17%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	43/86 (50%)	23/46 (50%)	20/40 (50%)	0/0 (—%)
Overall	712/1852 (38%)	412/940 (44%)	230/732 (31%)	70/180 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 36%, i.e. 744 atoms were assigned a chemical shift out of a possible 2062. 14 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	274/790 (35%)	143/314 (46%)	66/324 (20%)	65/152 (43%)
Sidechain	427/1186 (36%)	272/692 (39%)	148/440 (34%)	7/54 (13%)
Aromatic	43/86 (50%)	23/46 (50%)	20/40 (50%)	0/0 (—%)
Overall	744/2062 (36%)	438/1052 (42%)	234/804 (29%)	72/206 (35%)

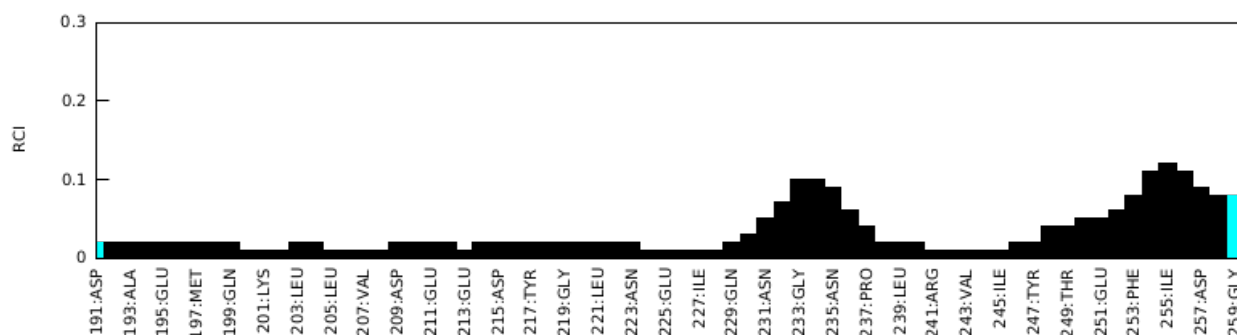
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain C:

