Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 12:20 AM EDT

PDB ID	:	2M9M
BMRB ID	:	19302
Title	:	Solution Structure of ERCC4 domain of human FAAP24
Authors	:	Wu, F.; Han, X.; Shi, C.; Gong, W.; Tian, C.
Deposited on	:	2013-06-18

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

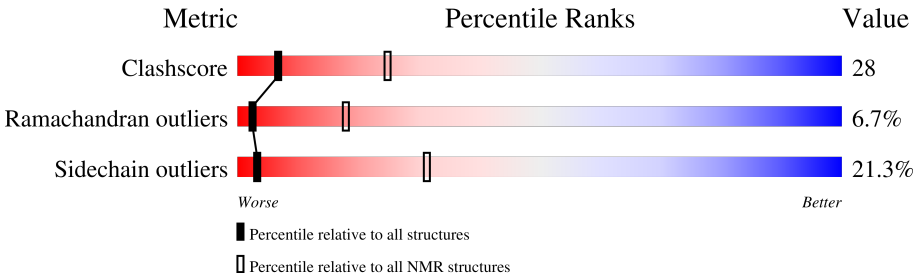
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 81%.

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	147	42% 32% 7% 14% 5%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:17-A:135 (119)	0.82	4

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 6, 7, 9, 10
2	3, 8
Single-model clusters	2

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2220 atoms, of which 1124 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fanconi anemia-associated protein of 24 kDa.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	139	2220	695	1124	190	203	8	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	LEU	-	expression tag	UNP Q9BTP7
A	141	GLU	-	expression tag	UNP Q9BTP7
A	142	HIS	-	expression tag	UNP Q9BTP7
A	143	HIS	-	expression tag	UNP Q9BTP7
A	144	HIS	-	expression tag	UNP Q9BTP7
A	145	HIS	-	expression tag	UNP Q9BTP7
A	146	HIS	-	expression tag	UNP Q9BTP7
A	147	HIS	-	expression tag	UNP Q9BTP7

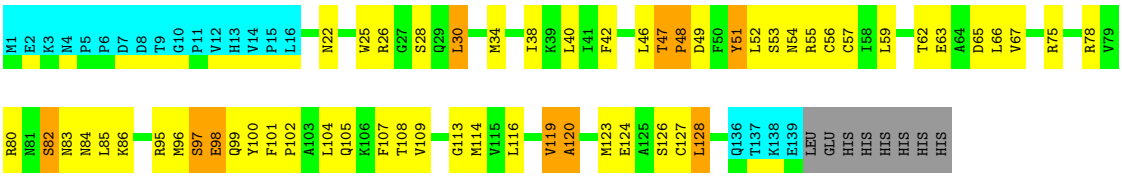
4 Residue-property plots (i)

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: Fanconi anemia-associated protein of 24 kDa

Chain A: 42% 32% 7% 14% 5%



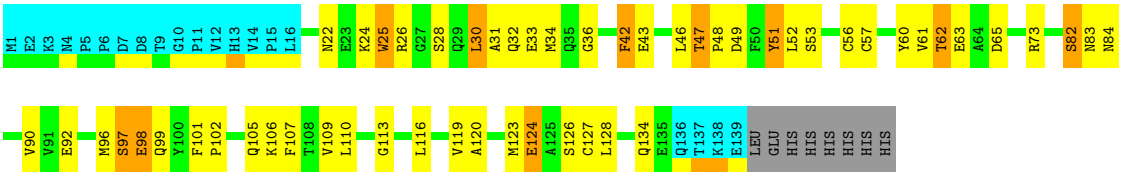
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Fanconi anemia-associated protein of 24 kDa

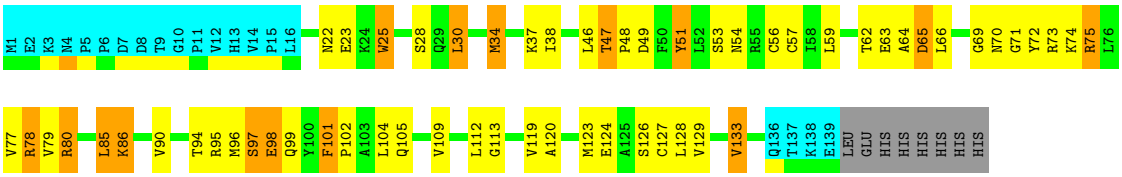
Chain A: 44% 30% 7% 14% 5%



4.2.2 Score per residue for model 2

• Molecule 1: Fanconi anemia-associated protein of 24 kDa

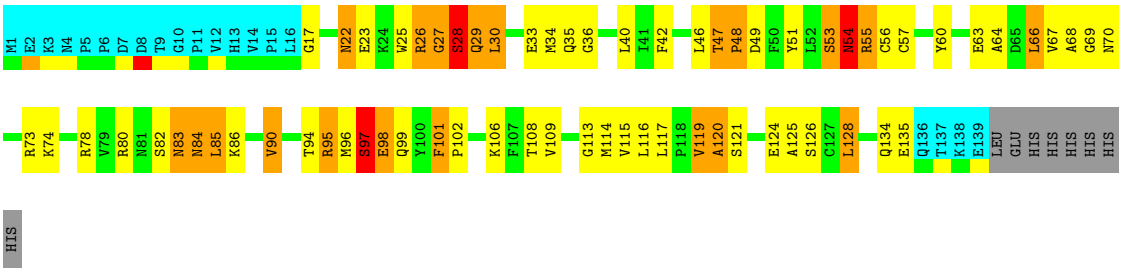
Chain A: 41% 30% 10% 14% 5%



4.2.3 Score per residue for model 3

- Molecule 1: Fanconi anemia-associated protein of 24 kDa

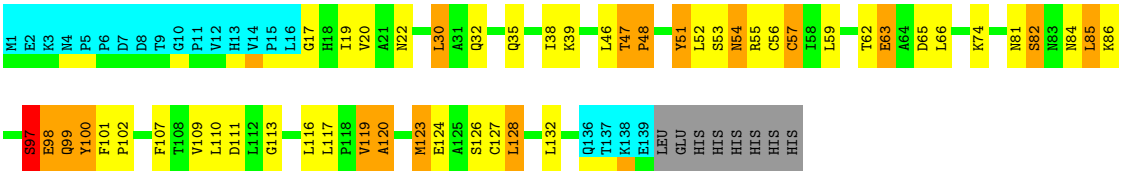
Chain A: 35% 31% 14% • 14% 5%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Fanconi anemia-associated protein of 24 kDa

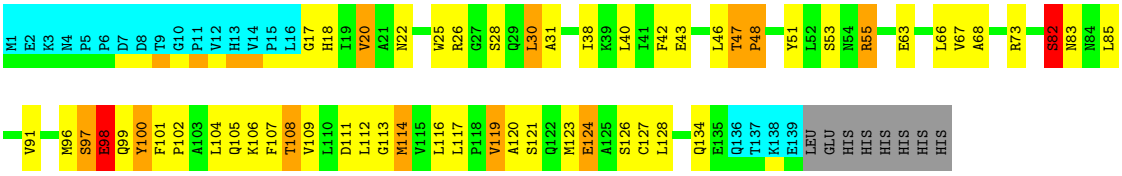
Chain A: 46% 23% 11% • 14% 5%



4.2.5 Score per residue for model 5

- Molecule 1: Fanconi anemia-associated protein of 24 kDa

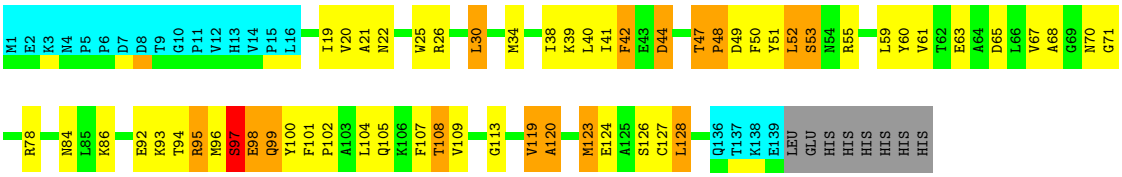
Chain A: 43% 29% 7% • 14% 5%



4.2.6 Score per residue for model 6

- Molecule 1: Fanconi anemia-associated protein of 24 kDa

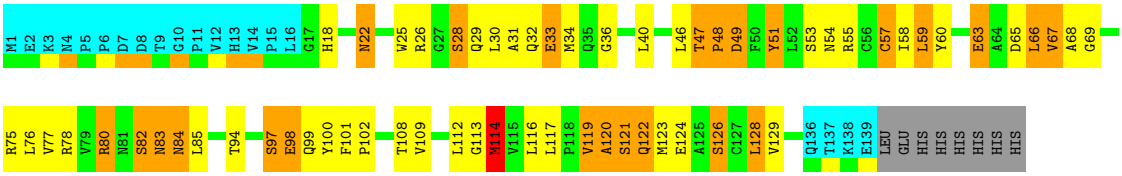
Chain A: 41% 29% 10% • 14% 5%



4.2.7 Score per residue for model 7

- Molecule 1: Fanconi anemia-associated protein of 24 kDa

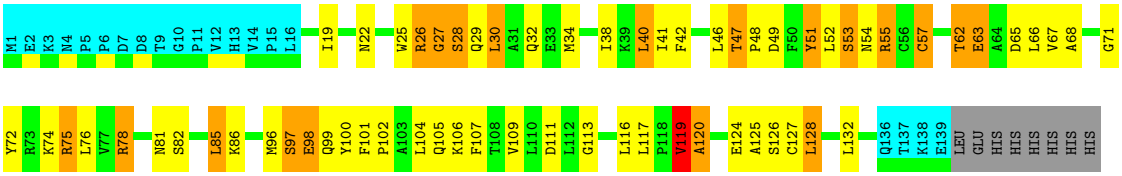
Chain A: 38% 26% 16% • 14% 5%



4.2.8 Score per residue for model 8

- Molecule 1: Fanconi anemia-associated protein of 24 kDa

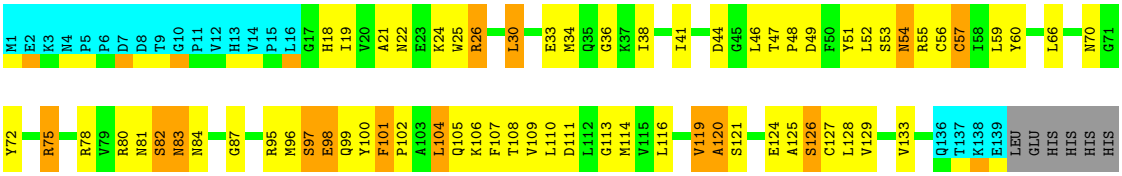
Chain A: 37% 30% 13% • 14% 5%



4.2.9 Score per residue for model 9

- Molecule 1: Fanconi anemia-associated protein of 24 kDa

Chain A: 35% 36% 10% 14% 5%



HIS
HIS

4.2.10 Score per residue for model 10

- Molecule 1: Fanconi anemia-associated protein of 24 kDa

Chain A: 41% 28% 12% 14% 5%

M1 E2 K3 N4 P5 P6 D7 D8 T9 G10 P11 V12 H13 V14 P15 L16 E23 K24 W25 R26 G27 S28 Q29 L30 A31 Q32 I38 K39 L40 I41 F42 L46 T47 P48 D49 F50 Y51 L52 S53 N54 R55 C56 V61 T62 E63 A64 D65 L66 V67 A68 G69 N70 G71 Y72 S82

N83 N84 V90 K93 M96 S97 E98 Q99 Y100 F101 P102 Q105 K106 F107 T108 V109 G113 M114 V115 L116 V119 A120 S121 Q122 M123 E124 A125 S126 C127 L128 V129 V133 Q134 E135 Q136 T137 K138 E139 LEU GLU HIS HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	**Classification**	**Version**
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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	1540
Number of shifts mapped to atoms	1540
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	941	972	972	53±8
All	All	9410	9720	9720	529

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:HD13	1:A:126:SER:OG	0.91	1.65	3	5
1:A:105:GLN:O	1:A:109:VAL:HG23	0.84	1.71	6	4
1:A:30:LEU:O	1:A:30:LEU:HD12	0.83	1.74	3	7
1:A:110:LEU:HD23	1:A:110:LEU:O	0.80	1.77	4	1
1:A:128:LEU:HD12	1:A:128:LEU:O	0.77	1.79	5	2
1:A:114:MET:SD	1:A:114:MET:N	0.77	2.58	7	1
1:A:30:LEU:HD12	1:A:30:LEU:C	0.76	2.01	5	7
1:A:85:LEU:O	1:A:85:LEU:HD12	0.75	1.81	8	1
1:A:96:MET:SD	1:A:96:MET:N	0.73	2.61	10	1
1:A:116:LEU:C	1:A:117:LEU:HD12	0.73	2.03	5	1
1:A:101:PHE:N	1:A:102:PRO:CD	0.73	2.52	6	7
1:A:40:LEU:HD13	1:A:41:ILE:N	0.73	1.98	8	1
1:A:30:LEU:HD13	1:A:31:ALA:N	0.72	1.99	7	1
1:A:25:TRP:O	1:A:27:GLY:N	0.70	2.25	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:VAL:O	1:A:113:GLY:N	0.70	2.25	2	9
1:A:99:GLN:OE1	1:A:100:TYR:CD2	0.69	2.45	6	1
1:A:34:MET:N	1:A:34:MET:SD	0.69	2.64	2	1
1:A:51:TYR:CE2	1:A:53:SER:O	0.69	2.45	5	1
1:A:123:MET:SD	1:A:123:MET:N	0.68	2.67	4	2
1:A:57:CYS:SG	1:A:58:ILE:N	0.68	2.66	7	1
1:A:82:SER:OG	1:A:83:ASN:N	0.68	2.26	5	3
1:A:97:SER:O	1:A:99:GLN:N	0.68	2.27	10	10
1:A:26:ARG:O	1:A:28:SER:N	0.68	2.26	8	4
1:A:30:LEU:HD13	1:A:126:SER:CB	0.68	2.19	1	6
1:A:30:LEU:HD13	1:A:30:LEU:C	0.68	2.08	7	1
1:A:47:THR:N	1:A:48:PRO:CD	0.67	2.57	4	6
1:A:124:GLU:O	1:A:128:LEU:N	0.67	2.27	5	10
1:A:65:ASP:O	1:A:69:GLY:N	0.67	2.27	2	1
1:A:63:GLU:OE2	1:A:67:VAL:HG23	0.67	1.89	6	1
1:A:22:ASN:ND2	1:A:46:LEU:O	0.67	2.28	8	5
1:A:25:TRP:NE1	1:A:49:ASP:OD2	0.66	2.28	6	3
1:A:25:TRP:CE2	1:A:49:ASP:OD2	0.66	2.48	9	5
1:A:85:LEU:H	1:A:85:LEU:HD12	0.66	1.51	3	2
1:A:47:THR:H	1:A:48:PRO:CD	0.66	2.04	3	5
1:A:97:SER:O	1:A:101:PHE:N	0.65	2.28	6	9
1:A:94:THR:HG23	1:A:95:ARG:H	0.65	1.51	2	1
1:A:33:GLU:O	1:A:36:GLY:N	0.65	2.29	3	4
1:A:33:GLU:N	1:A:33:GLU:OE1	0.65	2.30	7	1
1:A:66:LEU:HD23	1:A:67:VAL:N	0.64	2.08	7	2
1:A:26:ARG:O	1:A:26:ARG:CG	0.64	2.44	8	2
1:A:30:LEU:HD13	1:A:126:SER:HB3	0.64	1.69	1	3
1:A:119:VAL:O	1:A:120:ALA:HB2	0.63	1.91	9	5
1:A:65:ASP:N	1:A:65:ASP:OD1	0.63	2.30	2	2
1:A:97:SER:OG	1:A:98:GLU:N	0.63	2.30	4	3
1:A:69:GLY:O	1:A:73:ARG:NH2	0.62	2.33	3	1
1:A:66:LEU:HD11	1:A:100:TYR:C	0.62	2.15	9	5
1:A:104:LEU:HD23	1:A:108:THR:HG1	0.61	1.55	9	1
1:A:28:SER:O	1:A:30:LEU:N	0.61	2.34	3	2
1:A:29:GLN:HE21	1:A:122:GLN:NE2	0.61	1.93	10	1
1:A:114:MET:SD	1:A:114:MET:C	0.61	2.79	7	1
1:A:53:SER:O	1:A:55:ARG:N	0.60	2.35	8	3
1:A:51:TYR:CD1	1:A:53:SER:O	0.60	2.53	2	3
1:A:49:ASP:OD2	1:A:60:TYR:CD1	0.60	2.54	1	1
1:A:101:PHE:C	1:A:101:PHE:CD1	0.60	2.72	10	3
1:A:99:GLN:O	1:A:99:GLN:NE2	0.60	2.34	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:VAL:O	1:A:113:GLY:CA	0.59	2.50	4	10
1:A:29:GLN:NE2	1:A:122:GLN:HE22	0.59	1.95	10	1
1:A:94:THR:HG23	1:A:95:ARG:N	0.59	2.13	2	1
1:A:26:ARG:O	1:A:27:GLY:C	0.59	2.41	8	1
1:A:34:MET:SD	1:A:40:LEU:HD13	0.59	2.38	6	2
1:A:101:PHE:O	1:A:101:PHE:CD1	0.58	2.56	8	1
1:A:30:LEU:HD13	1:A:126:SER:HB2	0.58	1.74	4	2
1:A:22:ASN:O	1:A:25:TRP:N	0.58	2.36	5	4
1:A:116:LEU:O	1:A:117:LEU:HD12	0.58	1.97	5	2
1:A:27:GLY:O	1:A:28:SER:O	0.58	2.21	8	1
1:A:26:ARG:C	1:A:28:SER:N	0.58	2.58	3	1
1:A:46:LEU:CD2	1:A:46:LEU:N	0.57	2.67	4	2
1:A:29:GLN:NE2	1:A:122:GLN:NE2	0.57	2.53	10	1
1:A:116:LEU:HD12	1:A:116:LEU:N	0.57	2.15	3	3
1:A:55:ARG:O	1:A:85:LEU:CB	0.57	2.52	8	1
1:A:25:TRP:NE1	1:A:49:ASP:CG	0.57	2.58	3	2
1:A:104:LEU:O	1:A:108:THR:OG1	0.57	2.22	5	3
1:A:121:SER:OG	1:A:122:GLN:N	0.57	2.38	7	1
1:A:63:GLU:CB	1:A:94:THR:OG1	0.57	2.52	3	2
1:A:25:TRP:CG	1:A:25:TRP:O	0.56	2.58	7	1
1:A:84:ASN:O	1:A:84:ASN:ND2	0.56	2.38	9	1
1:A:30:LEU:C	1:A:30:LEU:CD1	0.56	2.69	5	8
1:A:30:LEU:CD1	1:A:30:LEU:C	0.56	2.74	10	2
1:A:65:ASP:OD2	1:A:72:TYR:CE1	0.56	2.59	10	1
1:A:26:ARG:C	1:A:28:SER:H	0.56	2.04	3	4
1:A:116:LEU:HD23	1:A:117:LEU:N	0.56	2.14	8	2
1:A:29:GLN:O	1:A:33:GLU:OE2	0.56	2.24	7	1
1:A:93:LYS:NZ	1:A:119:VAL:O	0.56	2.31	10	1
1:A:64:ALA:O	1:A:67:VAL:HG12	0.56	1.99	3	1
1:A:25:TRP:O	1:A:26:ARG:C	0.56	2.45	8	2
1:A:63:GLU:HB2	1:A:94:THR:HG21	0.56	1.76	2	1
1:A:55:ARG:C	1:A:56:CYS:SG	0.56	2.84	10	1
1:A:46:LEU:N	1:A:46:LEU:HD22	0.55	2.16	4	2
1:A:63:GLU:OE1	1:A:96:MET:N	0.55	2.39	5	1
1:A:25:TRP:CD1	1:A:49:ASP:CG	0.55	2.80	8	1
1:A:90:VAL:HG13	1:A:117:LEU:O	0.55	2.01	3	1
1:A:42:PHE:CD1	1:A:42:PHE:N	0.54	2.73	6	4
1:A:53:SER:C	1:A:55:ARG:H	0.54	2.06	3	3
1:A:119:VAL:HG23	1:A:120:ALA:N	0.54	2.17	4	5
1:A:84:ASN:O	1:A:84:ASN:OD1	0.54	2.26	10	1
1:A:125:ALA:O	1:A:129:VAL:HG23	0.54	2.03	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:SER:C	1:A:30:LEU:N	0.54	2.62	3	2
1:A:85:LEU:HD12	1:A:85:LEU:N	0.54	2.18	3	1
1:A:34:MET:O	1:A:38:ILE:O	0.54	2.25	6	2
1:A:47:THR:CB	1:A:48:PRO:CD	0.54	2.86	6	3
1:A:54:ASN:OD1	1:A:54:ASN:N	0.53	2.40	3	1
1:A:83:ASN:O	1:A:84:ASN:CG	0.53	2.47	7	1
1:A:49:ASP:OD1	1:A:49:ASP:C	0.53	2.46	6	1
1:A:25:TRP:CD1	1:A:49:ASP:OD1	0.53	2.61	6	1
1:A:119:VAL:O	1:A:120:ALA:CB	0.53	2.57	9	1
1:A:51:TYR:CD1	1:A:56:CYS:O	0.53	2.62	4	1
1:A:22:ASN:OD1	1:A:46:LEU:O	0.53	2.26	3	2
1:A:29:GLN:HE21	1:A:122:GLN:HE22	0.53	1.47	10	1
1:A:29:GLN:O	1:A:33:GLU:CD	0.52	2.48	7	1
1:A:56:CYS:SG	1:A:86:LYS:O	0.52	2.67	2	2
1:A:22:ASN:HD22	1:A:23:GLU:N	0.52	2.03	3	1
1:A:119:VAL:HG23	1:A:120:ALA:H	0.52	1.63	3	4
1:A:97:SER:C	1:A:99:GLN:N	0.52	2.60	10	10
1:A:30:LEU:CD1	1:A:31:ALA:N	0.52	2.72	7	1
1:A:47:THR:OG1	1:A:48:PRO:CD	0.52	2.58	6	2
1:A:95:ARG:CG	1:A:96:MET:N	0.52	2.72	9	1
1:A:66:LEU:HD13	1:A:97:SER:HA	0.51	1.82	9	3
1:A:83:ASN:OD1	1:A:83:ASN:C	0.51	2.49	1	1
1:A:69:GLY:O	1:A:70:ASN:CB	0.51	2.58	10	1
1:A:98:GLU:H	1:A:98:GLU:CD	0.51	2.08	3	1
1:A:101:PHE:N	1:A:102:PRO:HD2	0.51	2.20	4	4
1:A:81:ASN:O	1:A:82:SER:C	0.51	2.48	9	2
1:A:107:PHE:O	1:A:111:ASP:CG	0.51	2.49	9	1
1:A:52:LEU:CD1	1:A:133:VAL:HG22	0.51	2.35	9	1
1:A:66:LEU:O	1:A:68:ALA:N	0.51	2.44	8	1
1:A:77:VAL:O	1:A:80:ARG:N	0.51	2.40	2	2
1:A:86:LYS:O	1:A:86:LYS:CG	0.51	2.58	3	1
1:A:22:ASN:CG	1:A:46:LEU:O	0.51	2.49	4	1
1:A:30:LEU:C	1:A:30:LEU:HD13	0.51	2.26	10	2
1:A:84:ASN:O	1:A:84:ASN:CG	0.50	2.49	9	1
1:A:56:CYS:SG	1:A:57:CYS:N	0.50	2.84	9	1
1:A:63:GLU:CG	1:A:64:ALA:N	0.50	2.74	2	1
1:A:47:THR:N	1:A:48:PRO:HD2	0.50	2.22	9	5
1:A:124:GLU:O	1:A:128:LEU:CD1	0.50	2.59	1	1
1:A:34:MET:SD	1:A:129:VAL:HG11	0.50	2.47	7	1
1:A:53:SER:C	1:A:55:ARG:N	0.50	2.65	3	3
1:A:38:ILE:CG2	1:A:39:LYS:N	0.50	2.75	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:GLU:O	1:A:128:LEU:HD13	0.50	2.07	1	1
1:A:104:LEU:CD2	1:A:108:THR:OG1	0.49	2.60	9	1
1:A:75:ARG:HH21	1:A:78:ARG:HE	0.49	1.48	8	1
1:A:94:THR:CG2	1:A:95:ARG:H	0.49	2.17	2	1
1:A:25:TRP:CD1	1:A:49:ASP:OD2	0.49	2.65	8	1
1:A:83:ASN:CG	1:A:84:ASN:N	0.49	2.63	1	3
1:A:115:VAL:C	1:A:116:LEU:HD12	0.49	2.27	3	1
1:A:52:LEU:O	1:A:53:SER:OG	0.49	2.24	9	1
1:A:57:CYS:SG	1:A:85:LEU:HD13	0.49	2.47	8	1
1:A:116:LEU:HD23	1:A:116:LEU:C	0.49	2.28	8	1
1:A:104:LEU:HD23	1:A:108:THR:OG1	0.49	2.07	9	1
1:A:66:LEU:C	1:A:68:ALA:N	0.49	2.65	8	2
1:A:18:HIS:ND1	1:A:18:HIS:C	0.49	2.65	5	1
1:A:122:GLN:O	1:A:126:SER:OG	0.48	2.31	7	1
1:A:125:ALA:O	1:A:129:VAL:N	0.48	2.40	9	2
1:A:25:TRP:CH2	1:A:60:TYR:CZ	0.48	3.01	1	1
1:A:63:GLU:O	1:A:66:LEU:N	0.48	2.46	10	1
1:A:25:TRP:CH2	1:A:60:TYR:CE2	0.48	3.01	1	1
1:A:51:TYR:CE1	1:A:53:SER:O	0.48	2.67	4	2
1:A:124:GLU:N	1:A:124:GLU:OE1	0.48	2.47	1	1
1:A:123:MET:O	1:A:127:CYS:N	0.48	2.44	5	2
1:A:128:LEU:HD12	1:A:128:LEU:C	0.48	2.28	2	2
1:A:46:LEU:HD22	1:A:51:TYR:CD2	0.48	2.44	10	1
1:A:72:TYR:O	1:A:75:ARG:N	0.48	2.43	8	3
1:A:77:VAL:O	1:A:79:VAL:N	0.48	2.46	2	1
1:A:24:LYS:C	1:A:26:ARG:H	0.48	2.10	1	2
1:A:34:MET:C	1:A:36:GLY:H	0.48	2.12	9	2
1:A:101:PHE:N	1:A:102:PRO:HD3	0.47	2.24	2	6
1:A:56:CYS:C	1:A:57:CYS:SG	0.47	2.92	4	1
1:A:83:ASN:C	1:A:84:ASN:HD22	0.47	2.12	1	1
1:A:96:MET:SD	1:A:99:GLN:OE1	0.47	2.72	2	1
1:A:18:HIS:CD2	1:A:41:ILE:HD12	0.47	2.45	9	1
1:A:25:TRP:CE2	1:A:49:ASP:OD1	0.47	2.68	2	1
1:A:105:GLN:O	1:A:109:VAL:CG2	0.47	2.56	6	2
1:A:96:MET:O	1:A:97:SER:O	0.47	2.32	10	1
1:A:83:ASN:OD1	1:A:84:ASN:N	0.47	2.48	3	1
1:A:52:LEU:O	1:A:52:LEU:HD23	0.47	2.10	10	1
1:A:20:VAL:HG11	1:A:43:GLU:OE2	0.47	2.10	5	1
1:A:97:SER:O	1:A:98:GLU:C	0.46	2.53	6	8
1:A:77:VAL:C	1:A:79:VAL:N	0.46	2.68	2	1
1:A:63:GLU:CD	1:A:63:GLU:C	0.46	2.74	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:LEU:O	1:A:85:LEU:CD1	0.46	2.61	8	1
1:A:85:LEU:N	1:A:85:LEU:CD1	0.46	2.77	3	1
1:A:83:ASN:OD1	1:A:85:LEU:CD1	0.46	2.64	7	1
1:A:30:LEU:O	1:A:32:GLN:N	0.46	2.48	1	1
1:A:82:SER:O	1:A:83:ASN:CB	0.46	2.64	10	1
1:A:60:TYR:O	1:A:60:TYR:CG	0.46	2.67	1	1
1:A:51:TYR:CE1	1:A:56:CYS:O	0.46	2.69	4	1
1:A:25:TRP:C	1:A:27:GLY:N	0.46	2.69	8	1
1:A:83:ASN:OD1	1:A:84:ASN:OD1	0.46	2.34	9	1
1:A:25:TRP:CD1	1:A:50:PHE:CZ	0.46	3.04	10	1
1:A:68:ALA:C	1:A:70:ASN:H	0.46	2.14	6	1
1:A:49:ASP:CG	1:A:60:TYR:H	0.46	2.14	7	1
1:A:67:VAL:HG22	1:A:96:MET:SD	0.46	2.51	5	1
1:A:21:ALA:N	1:A:41:ILE:O	0.46	2.49	6	2
1:A:31:ALA:HB1	1:A:40:LEU:CD2	0.46	2.41	7	1
1:A:101:PHE:CZ	1:A:105:GLN:NE2	0.46	2.83	2	1
1:A:74:LYS:CD	1:A:74:LYS:O	0.46	2.64	3	1
1:A:125:ALA:O	1:A:128:LEU:N	0.46	2.49	8	3
1:A:112:LEU:O	1:A:113:GLY:C	0.45	2.52	5	1
1:A:104:LEU:HD23	1:A:104:LEU:O	0.45	2.10	9	1
1:A:61:VAL:O	1:A:92:GLU:N	0.45	2.48	6	2
1:A:54:ASN:ND2	1:A:54:ASN:H	0.45	2.09	4	1
1:A:84:ASN:OD1	1:A:84:ASN:C	0.45	2.55	10	1
1:A:101:PHE:CB	1:A:102:PRO:CD	0.45	2.95	9	2
1:A:68:ALA:C	1:A:70:ASN:N	0.45	2.69	6	1
1:A:85:LEU:HD23	1:A:85:LEU:N	0.45	2.27	2	1
1:A:102:PRO:O	1:A:105:GLN:N	0.45	2.50	10	2
1:A:66:LEU:CD2	1:A:96:MET:O	0.45	2.65	3	1
1:A:107:PHE:O	1:A:111:ASP:N	0.45	2.50	9	3
1:A:31:ALA:O	1:A:40:LEU:HD22	0.45	2.12	5	1
1:A:19:ILE:HD11	1:A:133:VAL:HG21	0.45	1.89	9	1
1:A:25:TRP:NE1	1:A:50:PHE:CZ	0.45	2.85	10	1
1:A:81:ASN:C	1:A:81:ASN:OD1	0.44	2.55	8	1
1:A:61:VAL:N	1:A:90:VAL:O	0.44	2.50	1	2
1:A:29:GLN:O	1:A:33:GLU:OE1	0.44	2.34	7	1
1:A:52:LEU:HD11	1:A:133:VAL:HG22	0.44	1.88	9	1
1:A:25:TRP:CD2	1:A:49:ASP:OD1	0.44	2.70	2	1
1:A:94:THR:CG2	1:A:95:ARG:N	0.44	2.77	2	1
1:A:95:ARG:C	1:A:97:SER:N	0.44	2.70	2	1
1:A:99:GLN:OE1	1:A:100:TYR:CE2	0.44	2.71	6	1
1:A:119:VAL:CG2	1:A:120:ALA:N	0.44	2.80	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:CD1	1:A:126:SER:OG	0.44	2.66	4	1
1:A:63:GLU:CD	1:A:63:GLU:O	0.44	2.56	6	1
1:A:99:GLN:CD	1:A:99:GLN:C	0.44	2.76	6	1
1:A:66:LEU:HD23	1:A:66:LEU:C	0.44	2.32	7	1
1:A:68:ALA:O	1:A:69:GLY:C	0.44	2.56	7	1
1:A:51:TYR:OH	1:A:85:LEU:CD2	0.44	2.66	8	1
1:A:57:CYS:O	1:A:87:GLY:CA	0.44	2.66	9	1
1:A:101:PHE:CD1	1:A:101:PHE:C	0.44	2.92	2	2
1:A:33:GLU:O	1:A:34:MET:C	0.44	2.56	3	1
1:A:94:THR:HG22	1:A:95:ARG:HG2	0.43	1.89	6	1
1:A:97:SER:C	1:A:99:GLN:H	0.43	2.16	10	1
1:A:25:TRP:CD2	1:A:49:ASP:OD2	0.43	2.70	10	1
1:A:49:ASP:CG	1:A:50:PHE:CE2	0.43	2.92	6	1
1:A:49:ASP:OD2	1:A:60:TYR:CB	0.43	2.67	7	1
1:A:26:ARG:NH2	1:A:42:PHE:CE2	0.43	2.84	3	1
1:A:30:LEU:C	1:A:32:GLN:N	0.43	2.70	1	1
1:A:49:ASP:OD2	1:A:60:TYR:N	0.43	2.45	3	1
1:A:119:VAL:CG2	1:A:120:ALA:H	0.43	2.24	3	2
1:A:72:TYR:O	1:A:73:ARG:C	0.43	2.55	2	1
1:A:47:THR:H	1:A:48:PRO:HD2	0.43	1.71	3	1
1:A:53:SER:OG	1:A:54:ASN:N	0.43	2.52	7	1
1:A:49:ASP:OD1	1:A:59:LEU:HD23	0.42	2.14	7	1
1:A:19:ILE:HG22	1:A:20:VAL:N	0.42	2.29	6	2
1:A:60:TYR:C	1:A:60:TYR:CD1	0.42	2.92	6	1
1:A:44:ASP:OD1	1:A:44:ASP:N	0.42	2.46	6	1
1:A:29:GLN:NE2	1:A:122:GLN:OE1	0.42	2.51	10	1
1:A:33:GLU:O	1:A:35:GLN:N	0.42	2.52	3	1
1:A:63:GLU:OE1	1:A:97:SER:N	0.42	2.49	5	1
1:A:124:GLU:N	1:A:124:GLU:CD	0.42	2.72	5	1
1:A:22:ASN:O	1:A:26:ARG:N	0.42	2.51	8	1
1:A:30:LEU:HD13	1:A:30:LEU:O	0.42	2.15	10	1
1:A:123:MET:CG	1:A:124:GLU:N	0.42	2.83	7	1
1:A:62:THR:O	1:A:63:GLU:C	0.42	2.58	1	4
1:A:49:ASP:OD2	1:A:50:PHE:CE2	0.42	2.73	6	1
1:A:46:LEU:HD12	1:A:51:TYR:CD2	0.42	2.49	7	1
1:A:97:SER:O	1:A:100:TYR:N	0.42	2.52	7	1
1:A:34:MET:O	1:A:38:ILE:N	0.42	2.53	6	1
1:A:83:ASN:O	1:A:84:ASN:ND2	0.42	2.53	1	2
1:A:30:LEU:CD1	1:A:34:MET:SD	0.42	3.08	2	1
1:A:28:SER:C	1:A:30:LEU:H	0.42	2.18	3	1
1:A:46:LEU:N	1:A:46:LEU:HD23	0.42	2.28	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:TRP:CZ2	1:A:60:TYR:HB3	0.42	2.49	9	1
1:A:30:LEU:HD21	1:A:126:SER:N	0.42	2.29	10	2
1:A:62:THR:O	1:A:65:ASP:N	0.41	2.47	1	2
1:A:19:ILE:CG2	1:A:20:VAL:N	0.41	2.83	4	2
1:A:94:THR:OG1	1:A:95:ARG:N	0.41	2.54	2	1
1:A:51:TYR:CZ	1:A:53:SER:O	0.41	2.74	5	1
1:A:112:LEU:O	1:A:114:MET:N	0.41	2.53	5	1
1:A:30:LEU:HD12	1:A:34:MET:SD	0.41	2.55	2	1
1:A:129:VAL:O	1:A:133:VAL:HG23	0.41	2.15	2	1
1:A:17:GLY:O	1:A:38:ILE:HD11	0.41	2.15	5	1
1:A:52:LEU:C	1:A:53:SER:OG	0.41	2.59	6	1
1:A:128:LEU:O	1:A:128:LEU:HD23	0.41	2.16	8	1
1:A:95:ARG:O	1:A:98:GLU:OE1	0.41	2.39	3	1
1:A:63:GLU:OE2	1:A:63:GLU:O	0.41	2.38	6	1
1:A:98:GLU:CD	1:A:98:GLU:N	0.41	2.74	3	1
1:A:76:LEU:O	1:A:112:LEU:HD21	0.41	2.15	7	1
1:A:22:ASN:OD1	1:A:23:GLU:N	0.41	2.54	2	1
1:A:46:LEU:N	1:A:46:LEU:HD12	0.41	2.30	2	1
1:A:27:GLY:O	1:A:28:SER:CB	0.41	2.68	3	1
1:A:28:SER:O	1:A:29:GLN:C	0.41	2.59	3	1
1:A:110:LEU:O	1:A:110:LEU:CD2	0.41	2.60	4	1
1:A:95:ARG:C	1:A:97:SER:H	0.41	2.19	2	1
1:A:81:ASN:O	1:A:81:ASN:CG	0.41	2.60	4	1
1:A:46:LEU:N	1:A:46:LEU:CD1	0.40	2.83	2	1
1:A:70:ASN:OD1	1:A:71:GLY:N	0.40	2.53	2	1
1:A:72:TYR:O	1:A:74:LYS:N	0.40	2.54	2	1
1:A:63:GLU:HG2	1:A:94:THR:HG21	0.40	1.93	3	1
1:A:34:MET:C	1:A:36:GLY:N	0.40	2.74	9	1
1:A:91:VAL:O	1:A:119:VAL:HG22	0.40	2.17	5	1
1:A:18:HIS:ND1	1:A:18:HIS:O	0.40	2.55	5	1
1:A:116:LEU:N	1:A:116:LEU:CD1	0.40	2.84	3	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	119/147 (81%)	94±3 (79±2%)	17±3 (14±2%)	8±2 (7±2%)	2 18
All	All	1190/1470 (81%)	940 (79%)	170 (14%)	80 (7%)	2 18

All 23 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	98	GLU	10
1	A	119	VAL	10
1	A	97	SER	9
1	A	120	ALA	9
1	A	48	PRO	6
1	A	82	SER	5
1	A	54	ASN	4
1	A	83	ASN	3
1	A	84	ASN	3
1	A	55	ARG	3
1	A	26	ARG	2
1	A	27	GLY	2
1	A	28	SER	2
1	A	29	GLN	2
1	A	71	GLY	2
1	A	25	TRP	1
1	A	31	ALA	1
1	A	78	ARG	1
1	A	17	GLY	1
1	A	68	ALA	1
1	A	114	MET	1
1	A	67	VAL	1
1	A	69	GLY	1

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	104/131 (79%)	82±3 (79±3%)	22±3 (21±3%)	3 31
All	All	1040/1310 (79%)	818 (79%)	222 (21%)	3 31

All 77 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	30	LEU	9
1	A	47	THR	9
1	A	51	TYR	9
1	A	57	CYS	7
1	A	78	ARG	6
1	A	128	LEU	6
1	A	52	LEU	5
1	A	106	LYS	5
1	A	127	CYS	5
1	A	59	LEU	5
1	A	85	LEU	5
1	A	114	MET	5
1	A	42	PHE	4
1	A	96	MET	4
1	A	107	PHE	4
1	A	123	MET	4
1	A	134	GLN	4
1	A	54	ASN	4
1	A	75	ARG	4
1	A	80	ARG	4
1	A	86	LYS	4
1	A	101	PHE	4
1	A	55	ARG	4
1	A	82	SER	4
1	A	97	SER	4
1	A	108	THR	4
1	A	121	SER	4
1	A	32	GLN	4
1	A	62	THR	3
1	A	28	SER	3
1	A	38	ILE	3
1	A	65	ASP	3
1	A	104	LEU	3
1	A	53	SER	3
1	A	63	GLU	3
1	A	126	SER	3
1	A	56	CYS	2
1	A	73	ARG	2
1	A	110	LEU	2
1	A	124	GLU	2
1	A	90	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	22	ASN	2
1	A	66	LEU	2
1	A	70	ASN	2
1	A	95	ARG	2
1	A	74	LYS	2
1	A	99	GLN	2
1	A	100	TYR	2
1	A	132	LEU	2
1	A	98	GLU	2
1	A	26	ARG	2
1	A	44	ASP	2
1	A	40	LEU	2
1	A	43	GLU	1
1	A	25	TRP	1
1	A	34	MET	1
1	A	37	LYS	1
1	A	112	LEU	1
1	A	133	VAL	1
1	A	84	ASN	1
1	A	35	GLN	1
1	A	20	VAL	1
1	A	111	ASP	1
1	A	39	LYS	1
1	A	93	LYS	1
1	A	18	HIS	1
1	A	33	GLU	1
1	A	49	ASP	1
1	A	67	VAL	1
1	A	83	ASN	1
1	A	122	GLN	1
1	A	19	ILE	1
1	A	76	LEU	1
1	A	105	GLN	1
1	A	119	VAL	1
1	A	23	GLU	1
1	A	116	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 79% 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	1540
Number of shifts mapped to atoms	1540
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	138	-0.11 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	128	-0.10 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	136	0.27 ± 0.13	None needed (< 0.5 ppm)
^{15}N	130	-0.18 ± 0.37	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 81%, i.e. 1363 atoms were assigned a chemical shift out of a possible 1682. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	595/597 (100%)	243/243 (100%)	236/238 (99%)	116/116 (100%)
Sidechain	747/990 (75%)	515/646 (80%)	232/302 (77%)	0/42 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	21/95 (22%)	20/46 (43%)	0/47 (0%)	1/2 (50%)
Overall	1363/1682 (81%)	778/935 (83%)	468/587 (80%)	117/160 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1540 atoms were assigned a chemical shift out of a possible 1941. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	678/690 (98%)	274/280 (98%)	274/278 (99%)	130/132 (98%)
Sidechain	841/1149 (73%)	573/748 (77%)	268/355 (75%)	0/46 (0%)
Aromatic	21/102 (21%)	20/50 (40%)	0/49 (0%)	1/3 (33%)
Overall	1540/1941 (79%)	867/1078 (80%)	542/682 (79%)	131/181 (72%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	58	ILE	CG2	46.91	10.93 – 24.12	22.3
1	A	78	ARG	HE	2.99	4.52 – 10.19	-7.7
1	A	88	ILE	CG2	27.47	10.93 – 24.12	7.5
1	A	57	CYS	C	160.64	164.77 – 184.97	-7.0
1	A	88	ILE	CG1	17.03	19.24 – 36.26	-6.3
1	A	3	LYS	CE	36.87	37.57 – 46.21	-5.8
1	A	93	LYS	HD2	0.46	0.58 – 2.64	-5.5
1	A	24	LYS	HG2	0.02	0.13 – 2.61	-5.5
1	A	99	GLN	HG2	0.92	1.01 – 3.62	-5.4
1	A	124	GLU	HG2	1.23	1.24 – 3.30	-5.0

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:

RCI
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
1:MET
7:ASP
12:VAL
17:GLY
22:ASN
27:GLY
32:GLN
37:LYS
42:PHE
47:THR
52:LEU
57:CYS
62:THR
67:VAL
72:TYR
77:VAL
82:SER
87:GLY
92:GLU
97:SER
102:PRO
107:PHE
112:LEU
117:LEU
122:GLN
127:CYS
132:LEU
137:THR
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1714
Intra-residue (|i-j|=0)	428
Sequential (|i-j|=1)	572
Medium range (|i-j|>1 and |i-j|<5)	342
Long range (|i-j|≥5)	372
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.7
Number of long range restraints per residue[1]	2.5

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	1.1	0.18
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

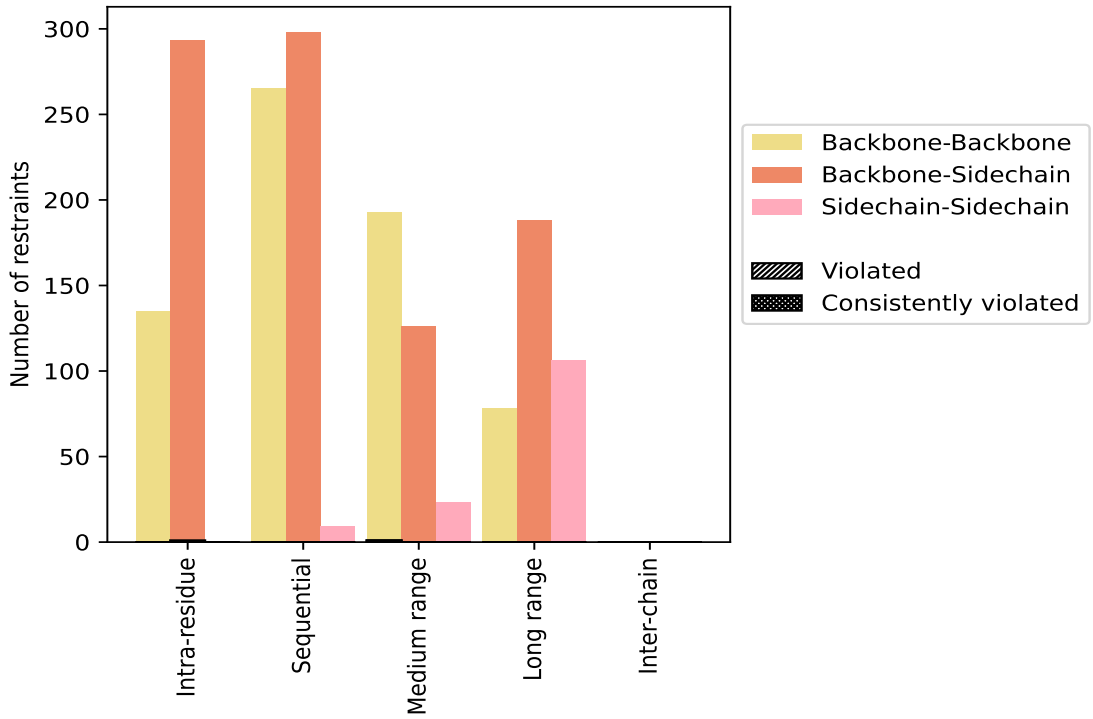
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	428	25.0	1	0.2	0.1	0	0.0	0.0
Backbone-Backbone	135	7.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	293	17.1	1	0.3	0.1	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	572	33.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	265	15.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	298	17.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	9	0.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	342	20.0	1	0.3	0.1	1	0.3	0.1
Backbone-Backbone	193	11.3	1	0.5	0.1	1	0.5	0.1
Backbone-Sidechain	126	7.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	23	1.3	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	372	21.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	78	4.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	188	11.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	106	6.2	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1714	100.0	2	0.1	0.1	1	0.1	0.1
Backbone-Backbone	671	39.1	1	0.1	0.1	1	0.1	0.1
Backbone-Sidechain	905	52.8	1	0.1	0.1	0	0.0	0.0
Sidechain-Sidechain	138	8.1	0	0.0	0.0	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

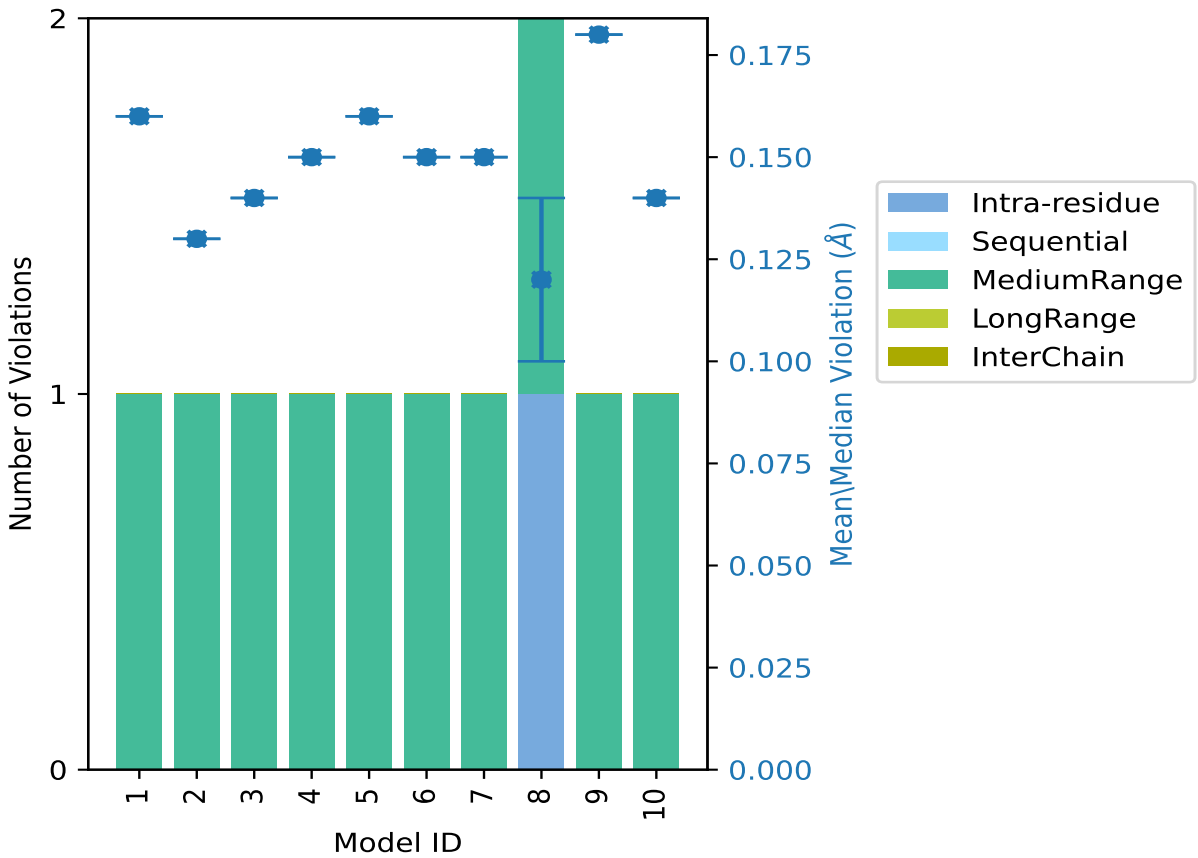
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	1	0	0	1	0.16	0.16	0.0	0.16
2	0	0	1	0	0	1	0.13	0.13	0.0	0.13
3	0	0	1	0	0	1	0.14	0.14	0.0	0.14
4	0	0	1	0	0	1	0.15	0.15	0.0	0.15
5	0	0	1	0	0	1	0.16	0.16	0.0	0.16
6	0	0	1	0	0	1	0.15	0.15	0.0	0.15
7	0	0	1	0	0	1	0.15	0.15	0.0	0.15
8	1	0	1	0	0	2	0.12	0.14	0.02	0.12
9	0	0	1	0	0	1	0.18	0.18	0.0	0.18
10	0	0	1	0	0	1	0.14	0.14	0.0	0.14

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints,

[5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model (i)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1712(IR:427, SQ:572, MR:341, LR:372, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	0	0	0	0	1	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0
0	0	0	0	0	0	4	40.0

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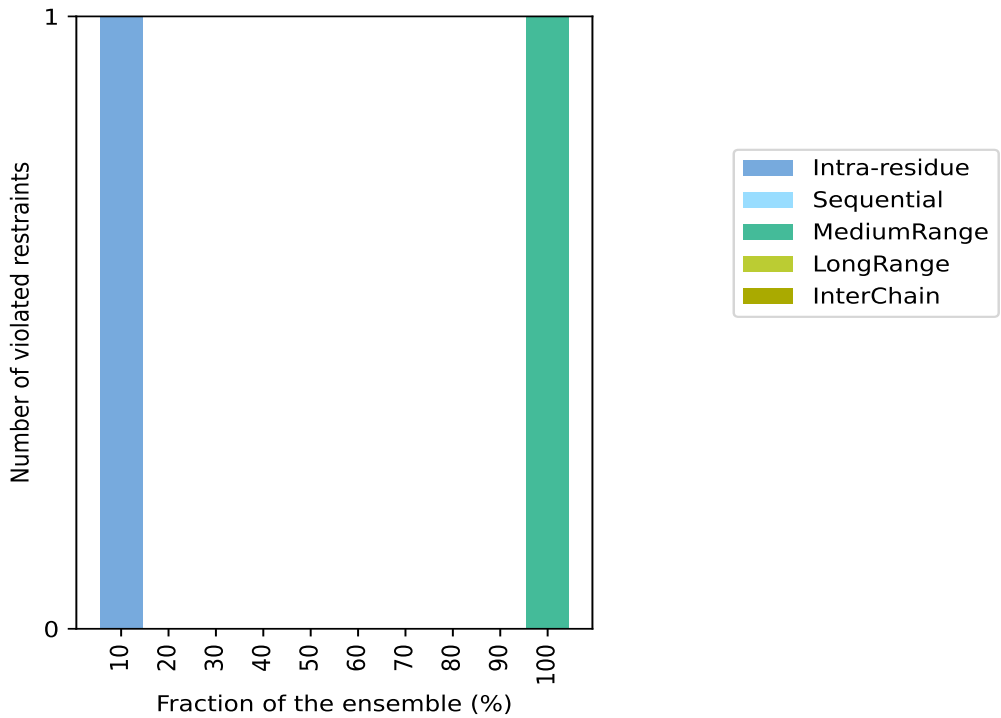
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	0	0	9	90.0
0	0	1	0	0	1	10	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

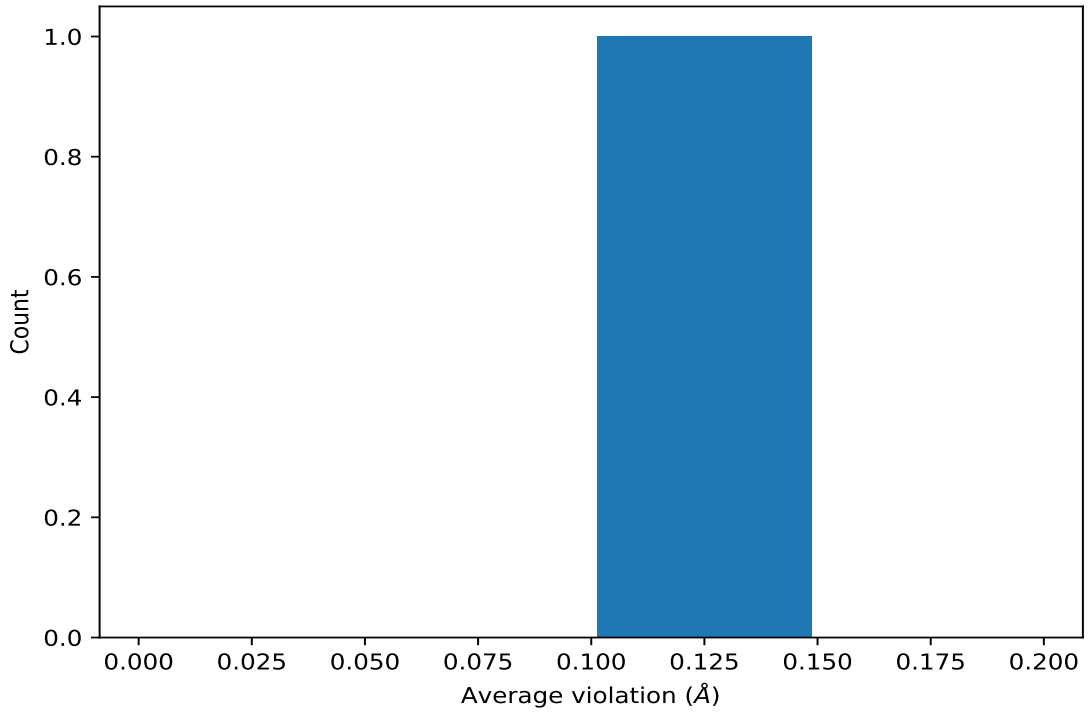
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

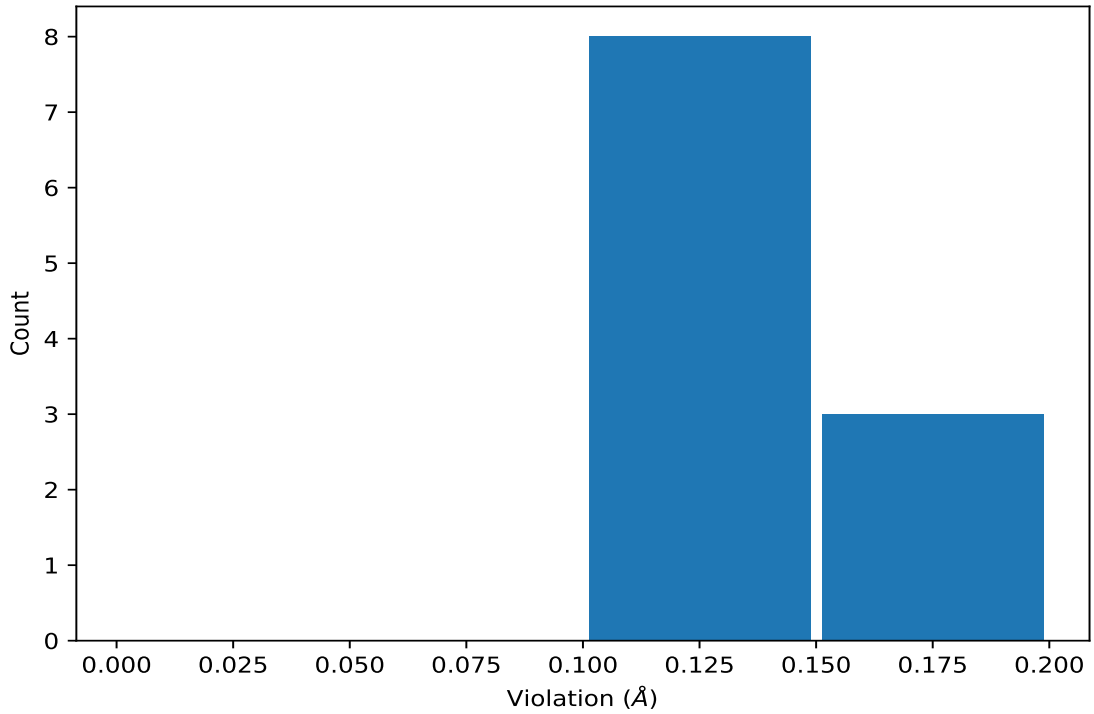
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	10	0.15	0.01	0.15

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	9	0.18
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	1	0.16
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	5	0.16
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	4	0.15
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	6	0.15
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	7	0.15
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	3	0.14
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	8	0.14
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	10	0.14
(1,1534)	1:A:125:ALA:H	1:A:128:LEU:H	2	0.13
(1,188)	1:A:26:ARG:H	1:A:26:ARG:HB3	8	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found