



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:51 pm GMT

PDB ID : 1S4Z
Title : HP1 chromo shadow domain in complex with PXVXL motif of CAF-1
Authors : Thiru, A.; Nietlispach, D.; Mott, H.R.; Okuwaki, M.; Lyon, D.; Nielsen, P.R.;
Hirshberg, M.; Verreault, A.; Murzina, N.V.; Laue, E.D.
Deposited on : 2004-01-19

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

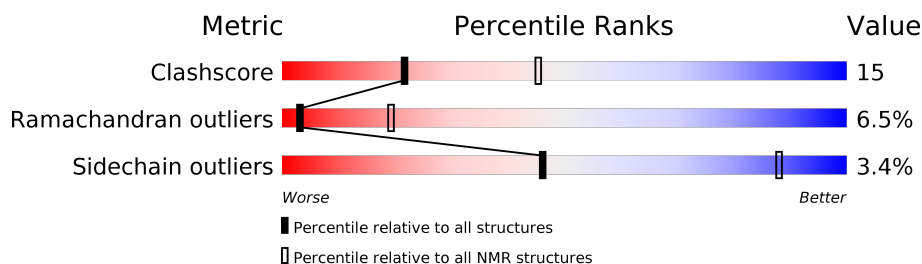
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	75	
1	B	75	
2	C	30	

2 Ensemble composition and analysis

This entry contains 25 models. Model 14 is the overall representative, medoid model (most similar to other models).

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:113-A:140, A:144-A:172, B:112-B:140, B:144-B:171, C:218-C:230 (127)	0.38	14

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25
2	6, 15

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2841 atoms, of which 1412 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chromobox protein homolog 1.

Mol	Chain	Residues	Atoms						Trace
1	A	75	Total	C	H	N	O	S	0
			1191	381	586	102	118	4	
1	B	75	Total	C	H	N	O	S	0
			1191	381	586	102	118	4	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	HIS	-	CLONING ARTIFACT	UNP P23197
A	103	MET	-	CLONING ARTIFACT	UNP P23197
A	176	ASP	GLU	ENGINEERED	UNP P23197
B	102	HIS	-	CLONING ARTIFACT	UNP P23197
B	103	MET	-	CLONING ARTIFACT	UNP P23197
B	176	ASP	GLU	ENGINEERED	UNP P23197

- Molecule 2 is a protein called Chromatin assembly factor 1 subunit A.

Mol	Chain	Residues	Atoms					Trace
2	C	30	Total	C	H	N	O	0
			459	143	240	33	43	

There is a discrepancy between the modelled and reference sequences:

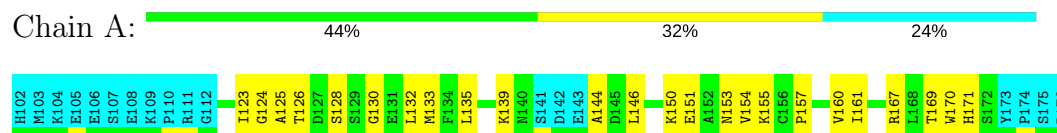
Chain	Residue	Modelled	Actual	Comment	Reference
C	209	GLY	-	CLONING ARTIFACT	UNP Q9QWF0

4 Residue-property plots

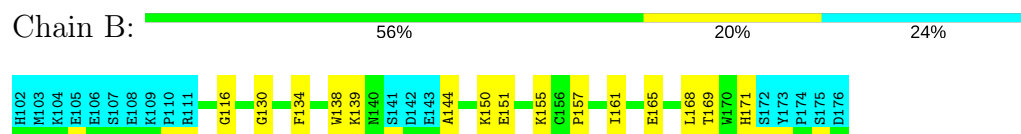
4.1 Average score per residue in the NMR ensemble

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

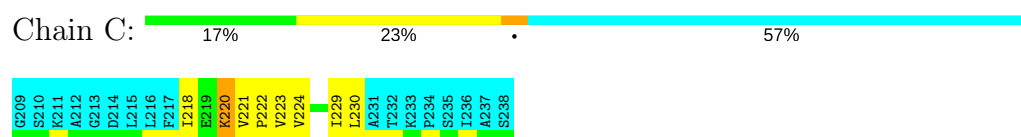
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1



- Molecule 2: Chromatin assembly factor 1 subunit A

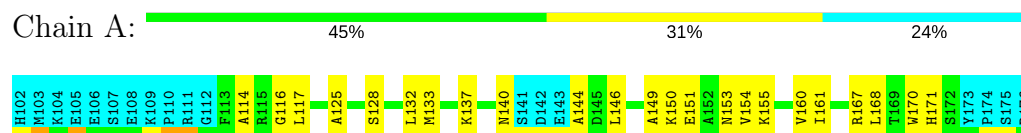


4.2 Scores per residue for each member of the ensemble

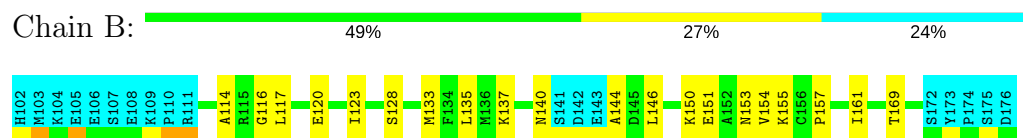
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

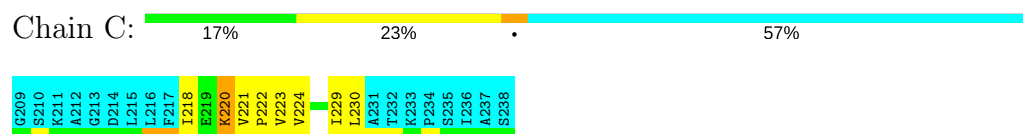
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

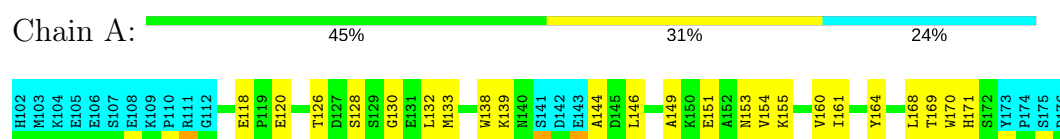


- Molecule 2: Chromatin assembly factor 1 subunit A

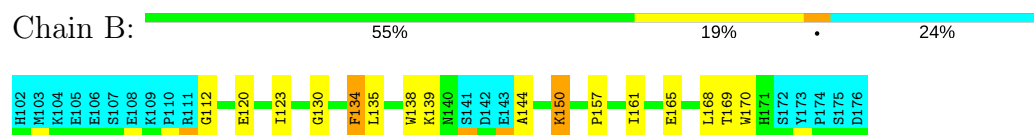


4.2.2 Score per residue for model 2

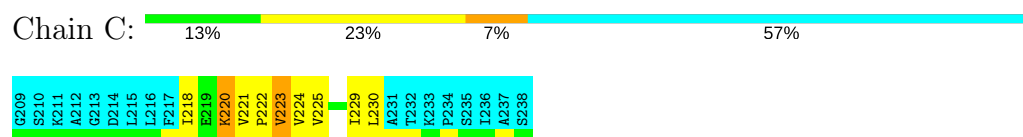
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

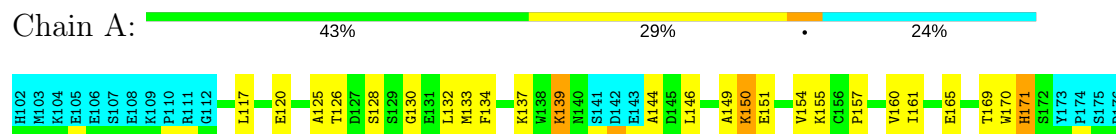


- Molecule 2: Chromatin assembly factor 1 subunit A

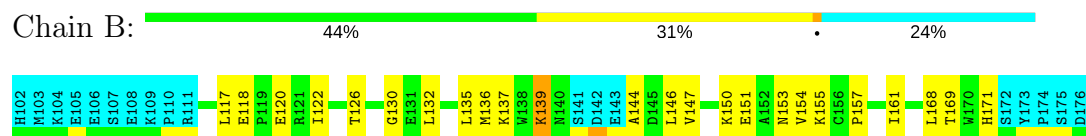


4.2.3 Score per residue for model 3

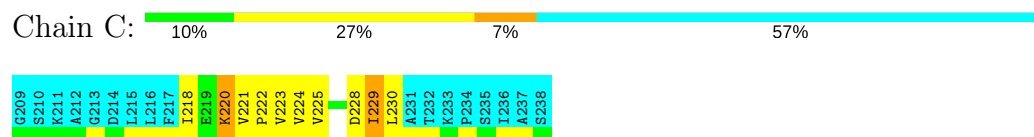
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

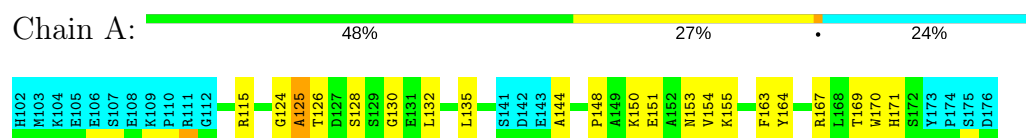


- Molecule 2: Chromatin assembly factor 1 subunit A

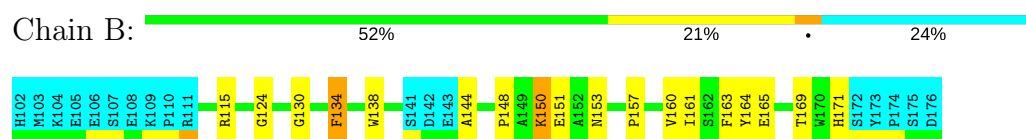


4.2.4 Score per residue for model 4

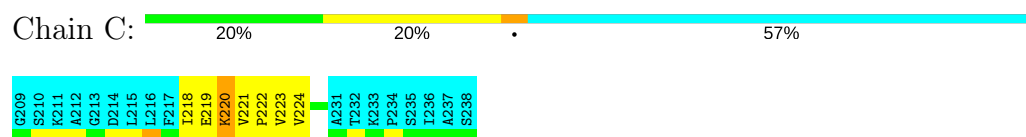
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

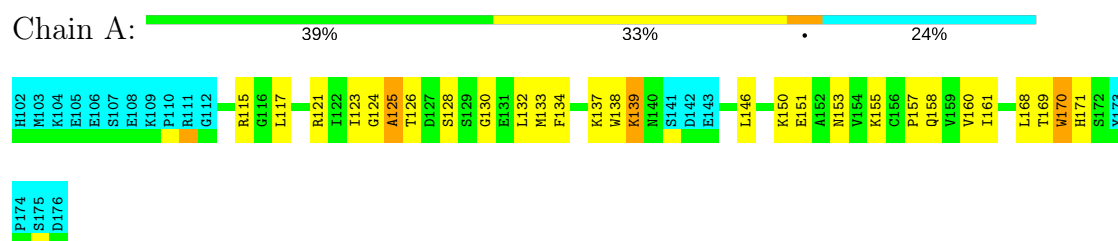


- Molecule 2: Chromatin assembly factor 1 subunit A

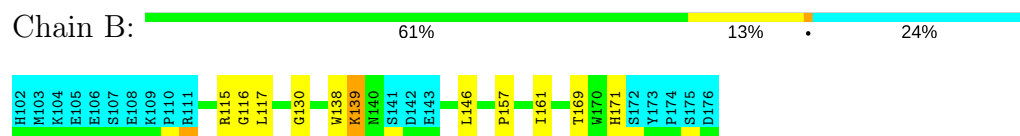


4.2.5 Score per residue for model 5

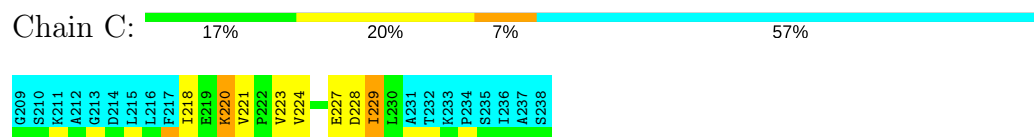
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

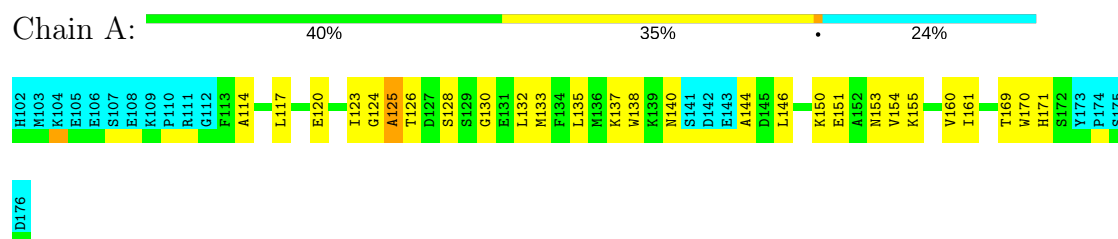


- Molecule 2: Chromatin assembly factor 1 subunit A

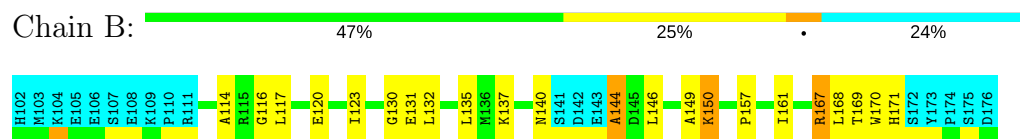


4.2.6 Score per residue for model 6

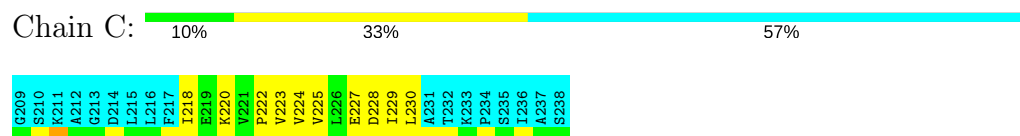
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

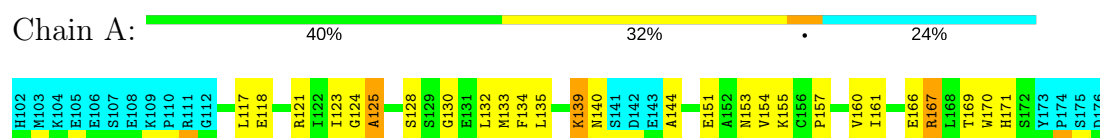


- Molecule 2: Chromatin assembly factor 1 subunit A

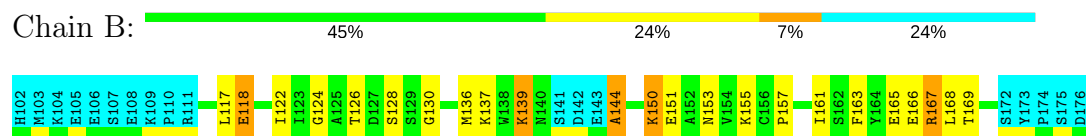


4.2.7 Score per residue for model 7

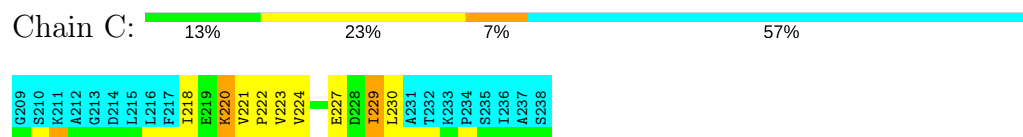
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

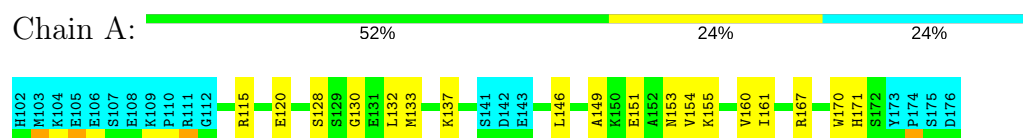


- Molecule 2: Chromatin assembly factor 1 subunit A

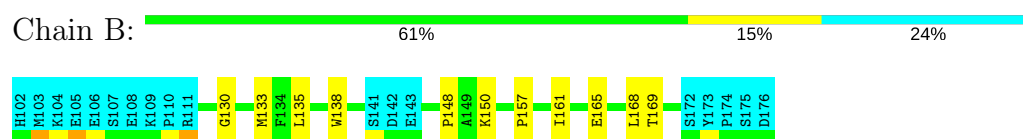


4.2.8 Score per residue for model 8

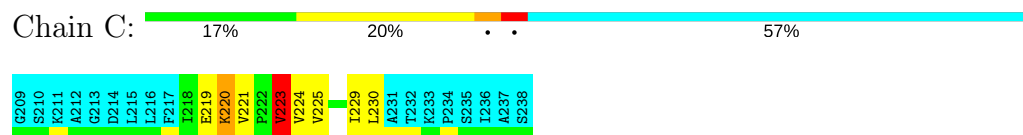
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

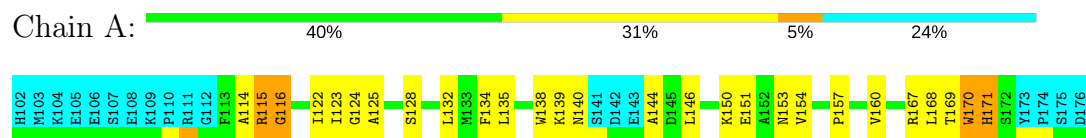


- Molecule 2: Chromatin assembly factor 1 subunit A



4.2.9 Score per residue for model 9

- Molecule 1: Chromobox protein homolog 1

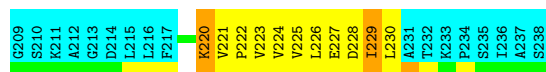
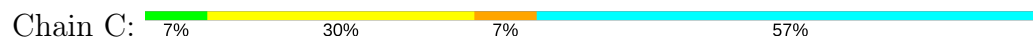


- Molecule 1: Chromobox protein homolog 1



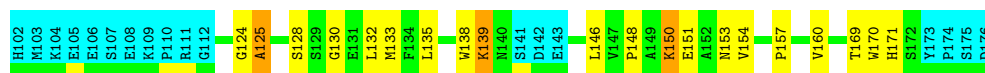


- Molecule 2: Chromatin assembly factor 1 subunit A

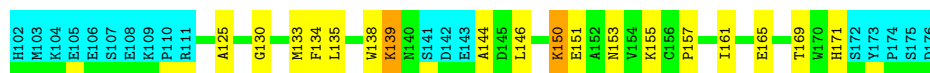


4.2.10 Score per residue for model 10

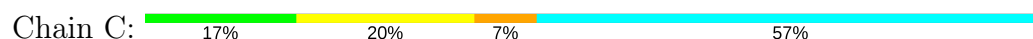
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

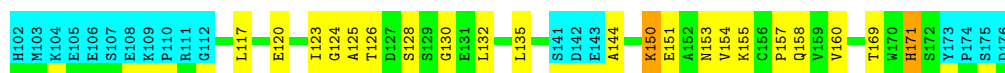


- Molecule 2: Chromatin assembly factor 1 subunit A



4.2.11 Score per residue for model 11

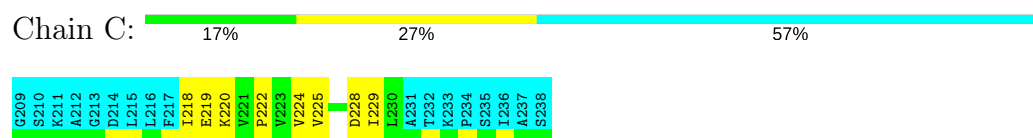
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

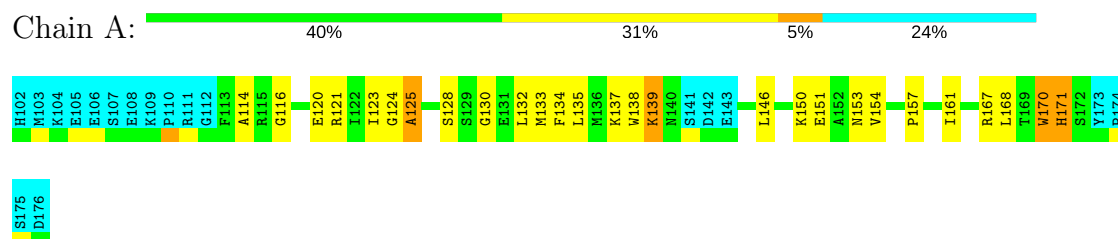


- Molecule 2: Chromatin assembly factor 1 subunit A

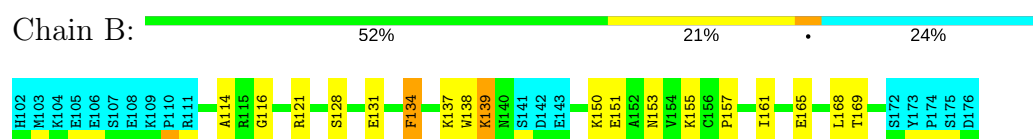


4.2.12 Score per residue for model 12

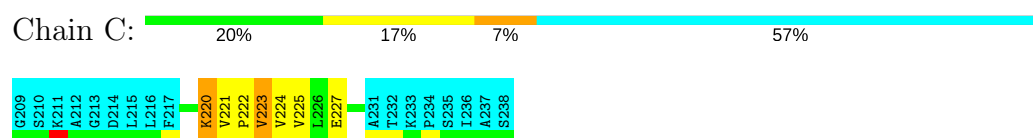
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

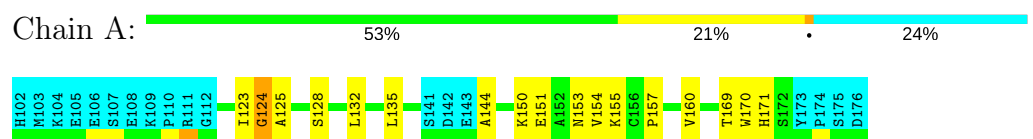


- Molecule 2: Chromatin assembly factor 1 subunit A

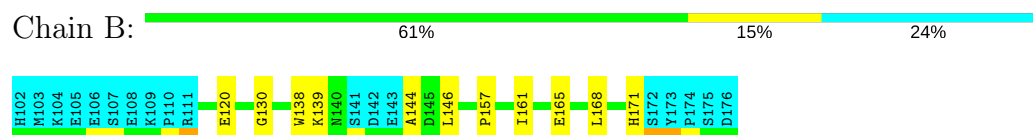


4.2.13 Score per residue for model 13

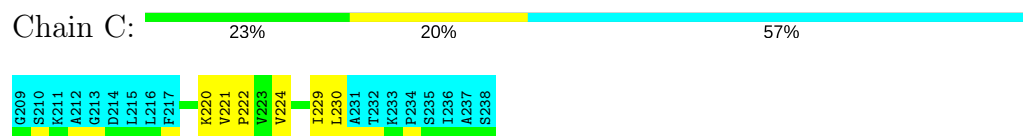
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

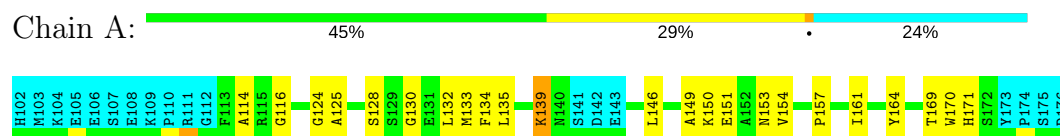


- Molecule 2: Chromatin assembly factor 1 subunit A

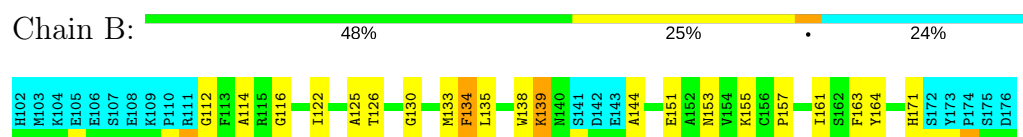


4.2.14 Score per residue for model 14 (medoid)

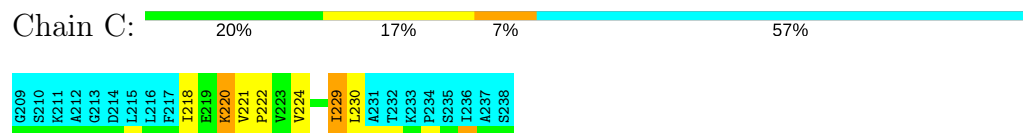
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

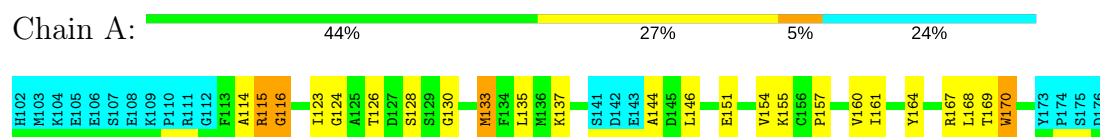


- Molecule 2: Chromatin assembly factor 1 subunit A

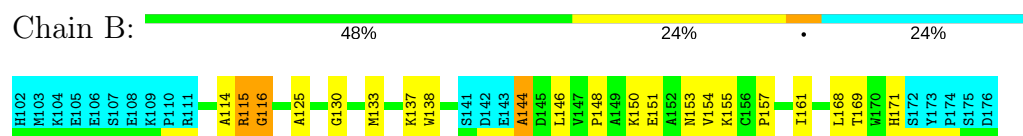


4.2.15 Score per residue for model 15

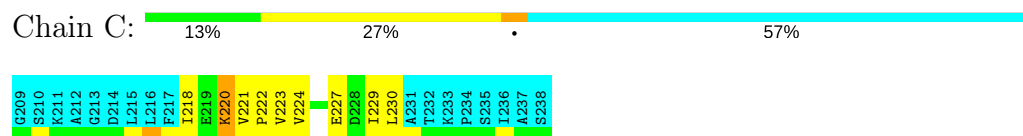
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

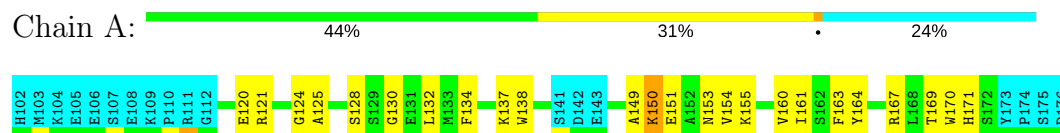


- Molecule 2: Chromatin assembly factor 1 subunit A

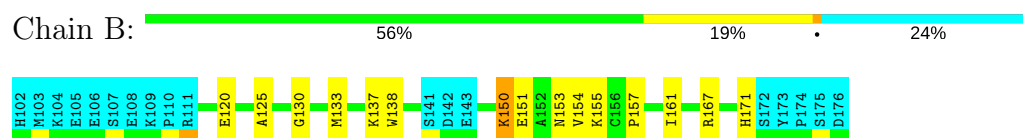


4.2.16 Score per residue for model 16

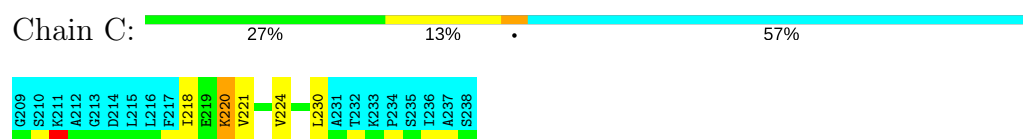
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

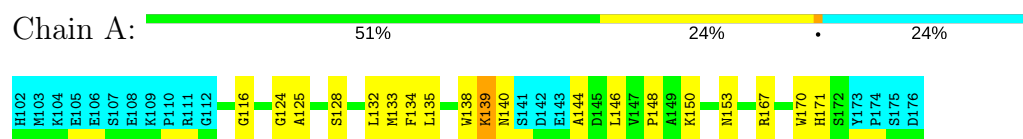


- Molecule 2: Chromatin assembly factor 1 subunit A

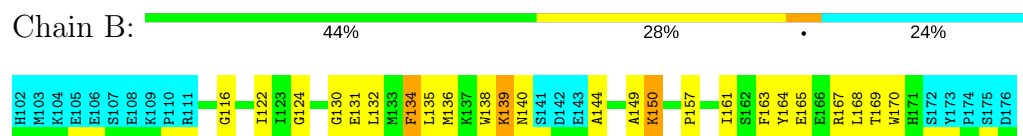


4.2.17 Score per residue for model 17

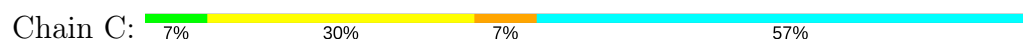
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1



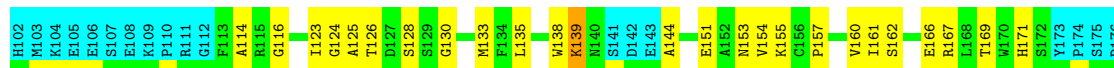
- Molecule 2: Chromatin assembly factor 1 subunit A





4.2.18 Score per residue for model 18

- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1



- Molecule 2: Chromatin assembly factor 1 subunit A



4.2.19 Score per residue for model 19

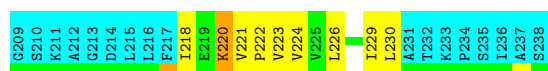
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

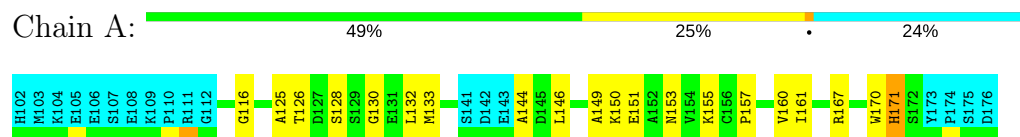


- Molecule 2: Chromatin assembly factor 1 subunit A

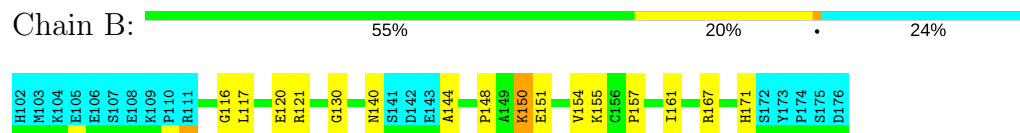


4.2.20 Score per residue for model 20

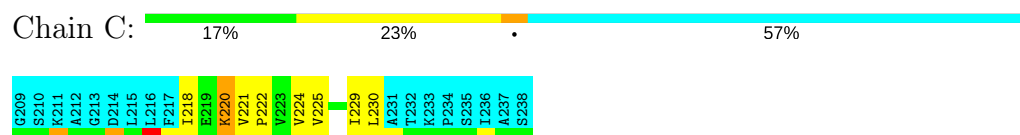
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

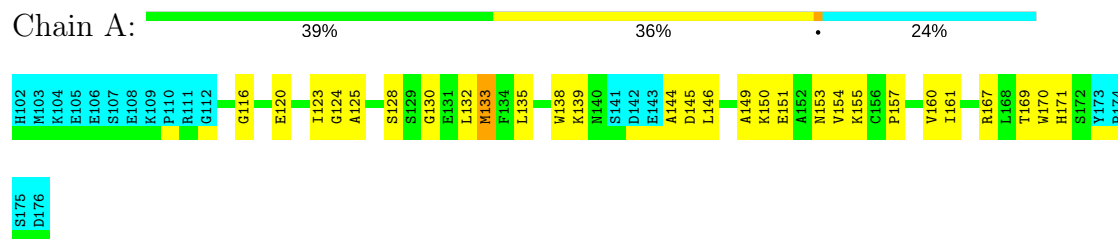


- Molecule 2: Chromatin assembly factor 1 subunit A

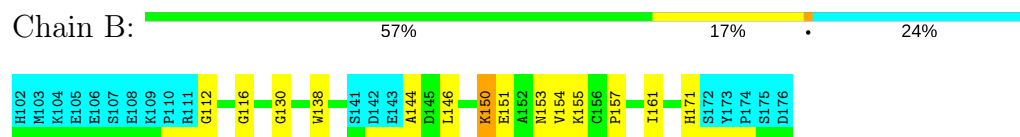


4.2.21 Score per residue for model 21

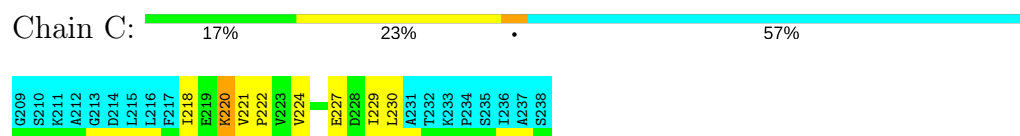
- Molecule 1: Chromobox protein homolog 1



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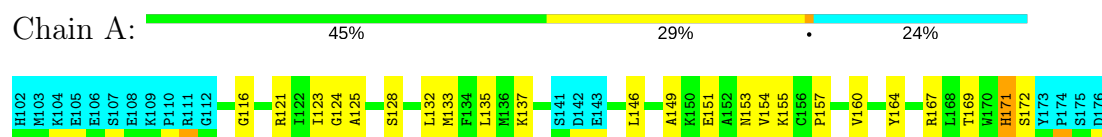


- Molecule 2: Chromatin assembly factor 1 subunit A

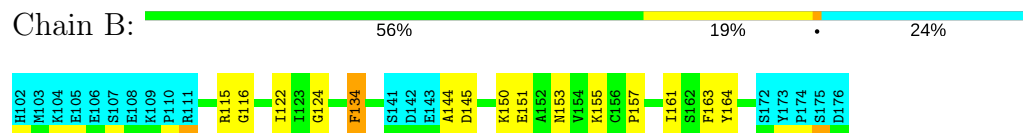


4.2.22 Score per residue for model 22

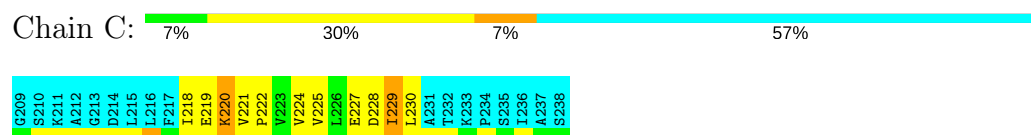
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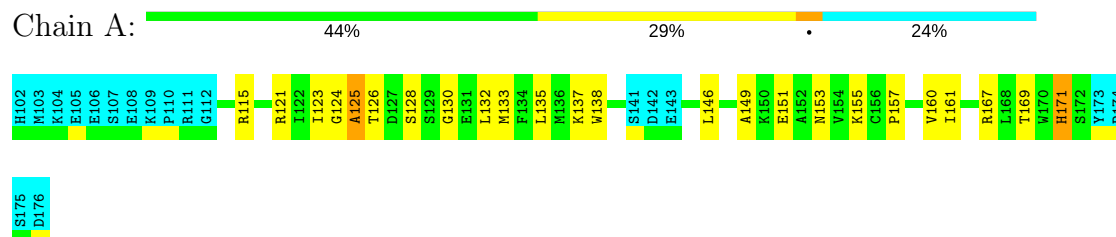


- Molecule 2: Chromatin assembly factor 1 subunit A

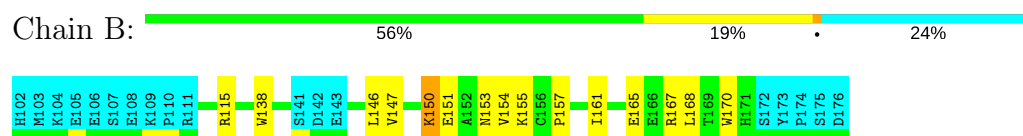


4.2.23 Score per residue for model 23

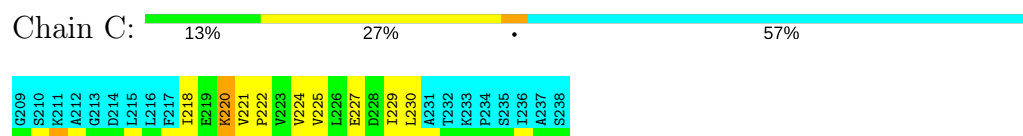
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

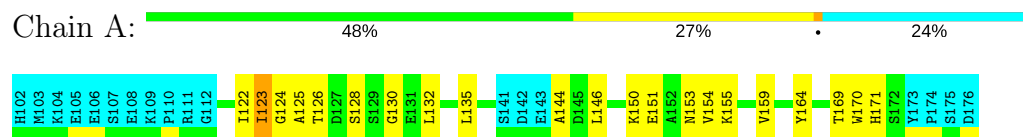


- Molecule 2: Chromatin assembly factor 1 subunit A

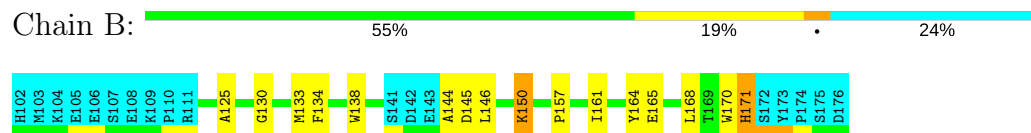


4.2.24 Score per residue for model 24

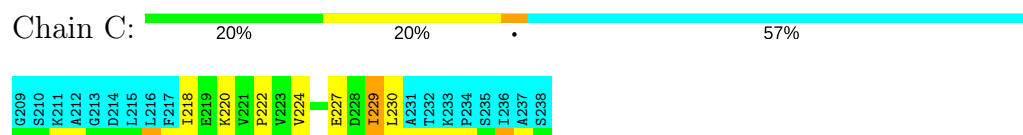
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1

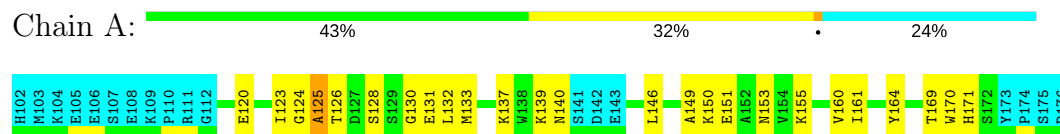


- Molecule 2: Chromatin assembly factor 1 subunit A

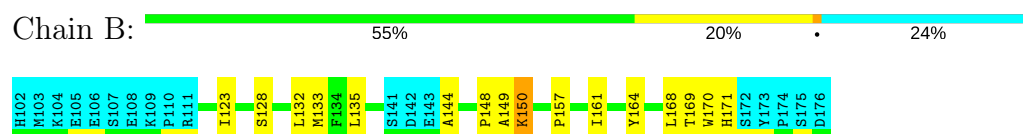


4.2.25 Score per residue for model 25

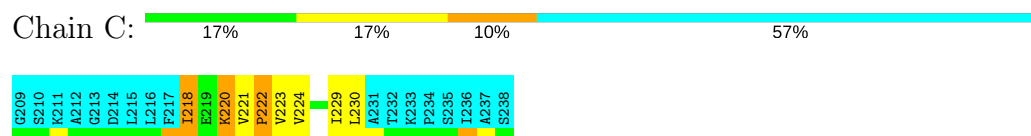
- Molecule 1: Chromobox protein homolog 1



- Molecule 1: Chromobox protein homolog 1



- Molecule 2: Chromatin assembly factor 1 subunit A



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *CNS/ARIA1.1*.

Of the 100 calculated structures, 25 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
CNS	structure solution	1.0
CNS	refinement	1.0

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	457	455	454	14±2
1	B	455	453	452	12±4
2	C	102	116	116	11±3
All	All	25350	25600	25550	746

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:LEU:HB2	1:A:149:ALA:HB2	0.88	1.46	20	10
1:B:169:THR:HG23	2:C:223:VAL:HG23	0.81	1.49	2	11
1:B:168:LEU:HD11	2:C:222:PRO:HB2	0.79	1.53	23	10
1:B:169:THR:HG23	2:C:223:VAL:HB	0.77	1.55	17	3
1:A:166:GLU:HG3	1:A:167:ARG:HD2	0.77	1.54	7	1
1:A:171:HIS:HB2	2:C:225:VAL:HG13	0.77	1.56	2	9
1:A:132:LEU:HD12	1:B:165:GLU:HG2	0.76	1.57	4	1
1:A:126:THR:HB	2:C:218:ILE:HG12	0.73	1.60	5	5
1:A:133:MET:HG2	1:A:148:PRO:HA	0.69	1.62	10	2
2:C:220:LYS:HG2	2:C:221:VAL:N	0.69	2.03	15	13
1:A:167:ARG:HB3	2:C:223:VAL:HA	0.68	1.65	17	1
1:B:170:TRP:HB3	2:C:220:LYS:HE3	0.67	1.66	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:170:TRP:HB3	2:C:220:LYS:NZ	0.66	2.05	2	2
1:A:124:GLY:HA3	1:A:135:LEU:HB3	0.66	1.66	11	15
1:A:132:LEU:HD12	1:B:165:GLU:HG3	0.66	1.68	19	10
2:C:229:ILE:H	2:C:229:ILE:HD13	0.65	1.52	24	6
1:B:120:GLU:HB2	1:B:139:LYS:HG2	0.65	1.68	13	2
1:A:133:MET:HB3	1:A:146:LEU:HG	0.65	1.67	3	9
1:A:123:ILE:HD12	1:A:124:GLY:N	0.64	2.06	13	3
1:A:150:LYS:HA	1:A:153:ASN:ND2	0.64	2.06	24	12
1:B:166:GLU:HG3	1:B:167:ARG:HD2	0.64	1.69	7	1
1:B:171:HIS:O	2:C:220:LYS:HG3	0.64	1.93	18	7
2:C:220:LYS:HE2	2:C:222:PRO:HG3	0.64	1.67	22	1
1:B:115:ARG:HD3	1:B:116:GLY:N	0.63	2.08	15	2
1:A:167:ARG:NE	2:C:221:VAL:HG11	0.63	2.08	8	1
2:C:218:ILE:HB	2:C:220:LYS:HE3	0.63	1.69	16	7
1:A:115:ARG:HD3	1:A:116:GLY:N	0.62	2.09	15	2
2:C:229:ILE:HD13	2:C:229:ILE:H	0.62	1.54	14	2
2:C:229:ILE:C	2:C:230:LEU:HD22	0.62	2.13	3	16
1:A:167:ARG:NE	2:C:221:VAL:HG21	0.61	2.10	23	1
1:B:115:ARG:HH21	1:B:117:LEU:HD11	0.61	1.55	5	1
1:B:135:LEU:HD11	1:B:144:ALA:HB1	0.60	1.72	17	4
1:A:135:LEU:HD22	1:A:146:LEU:HD13	0.60	1.72	22	1
1:A:120:GLU:O	1:A:121:ARG:HG2	0.59	1.97	19	1
1:A:125:ALA:O	2:C:218:ILE:HD11	0.59	1.98	3	6
1:B:135:LEU:HD22	2:C:229:ILE:HB	0.59	1.72	18	4
1:A:135:LEU:HD11	1:A:144:ALA:HB1	0.59	1.73	17	1
1:B:122:ILE:HD12	1:B:163:PHE:HB2	0.59	1.75	14	4
2:C:218:ILE:HB	2:C:220:LYS:HE2	0.59	1.74	2	4
1:A:115:ARG:HH21	1:A:117:LEU:HD11	0.58	1.58	5	1
1:B:171:HIS:O	2:C:220:LYS:HD3	0.58	1.98	6	2
1:B:150:LYS:HA	1:B:153:ASN:ND2	0.58	2.14	3	4
1:B:168:LEU:HD12	2:C:223:VAL:O	0.57	1.99	8	2
1:A:122:ILE:HD11	1:A:159:VAL:HG12	0.57	1.76	24	1
1:B:139:LYS:HB3	1:B:139:LYS:NZ	0.57	2.15	14	4
1:A:139:LYS:NZ	1:A:139:LYS:HB3	0.57	2.14	12	5
1:A:151:GLU:O	1:A:154:VAL:HG22	0.56	1.99	7	15
1:B:123:ILE:HD12	1:B:135:LEU:HD23	0.56	1.75	2	5
1:B:168:LEU:HD11	2:C:222:PRO:CB	0.56	2.30	9	2
1:B:171:HIS:O	2:C:221:VAL:HB	0.56	2.01	9	1
1:A:151:GLU:O	1:A:155:LYS:HG2	0.56	2.00	25	19
1:B:153:ASN:OD1	1:B:154:VAL:HG13	0.56	2.00	21	4
1:B:139:LYS:NZ	1:B:139:LYS:HB3	0.56	2.16	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:ARG:HG3	2:C:222:PRO:HG2	0.56	1.76	20	2
1:A:139:LYS:HB3	1:A:139:LYS:NZ	0.56	2.16	14	3
2:C:218:ILE:O	2:C:218:ILE:HD12	0.56	2.01	16	1
2:C:220:LYS:HD2	2:C:221:VAL:N	0.55	2.15	21	4
1:A:133:MET:O	1:A:146:LEU:HD11	0.55	2.01	14	7
1:A:153:ASN:OD1	1:A:154:VAL:HG13	0.55	2.01	18	10
1:A:169:THR:HG22	2:C:224:VAL:O	0.55	2.02	10	20
2:C:226:LEU:O	2:C:226:LEU:HD12	0.55	2.02	9	1
1:A:132:LEU:HD12	1:B:165:GLU:CG	0.55	2.32	10	4
2:C:228:ASP:OD1	2:C:229:ILE:HG12	0.54	2.02	6	1
1:B:167:ARG:N	1:B:167:ARG:HD2	0.54	2.18	6	1
2:C:220:LYS:HG2	2:C:221:VAL:H	0.54	1.62	10	3
2:C:229:ILE:HD13	2:C:229:ILE:N	0.54	2.18	14	2
1:B:154:VAL:HG23	1:B:155:LYS:HD2	0.53	1.79	23	2
1:B:168:LEU:HD12	1:B:169:THR:H	0.53	1.62	17	2
2:C:220:LYS:CG	2:C:221:VAL:N	0.53	2.71	10	6
2:C:220:LYS:NZ	2:C:220:LYS:HB3	0.53	2.18	14	3
1:A:164:TYR:HD2	2:C:224:VAL:HG21	0.53	1.64	2	4
1:A:152:ALA:HB1	1:A:160:VAL:HG11	0.53	1.81	19	1
1:A:125:ALA:HA	1:A:133:MET:O	0.53	2.03	7	7
1:B:151:GLU:O	1:B:155:LYS:HD3	0.53	2.04	20	2
1:A:126:THR:OG1	2:C:218:ILE:HD11	0.52	2.04	25	1
1:B:169:THR:O	2:C:223:VAL:N	0.52	2.42	17	2
2:C:229:ILE:HG13	2:C:230:LEU:HG	0.52	1.81	17	2
1:B:132:LEU:O	1:B:149:ALA:HB2	0.52	2.04	11	3
1:A:124:GLY:HA3	1:A:135:LEU:CB	0.52	2.35	23	7
2:C:218:ILE:HB	2:C:220:LYS:CE	0.52	2.35	10	5
2:C:229:ILE:O	2:C:230:LEU:HD13	0.52	2.05	9	3
2:C:220:LYS:HD2	2:C:220:LYS:C	0.52	2.25	22	2
1:B:151:GLU:O	1:B:155:LYS:HG2	0.52	2.05	16	11
1:B:157:PRO:O	1:B:161:ILE:HG13	0.51	2.05	4	25
1:B:163:PHE:O	1:B:167:ARG:HG2	0.51	2.05	19	1
1:B:125:ALA:HA	1:B:133:MET:O	0.51	2.06	10	6
1:A:139:LYS:HG3	1:A:140:ASN:OD1	0.51	2.05	25	3
2:C:220:LYS:HZ2	2:C:220:LYS:HB3	0.51	1.65	15	1
1:B:169:THR:HG21	2:C:225:VAL:HG23	0.51	1.83	8	1
1:A:134:PHE:HE2	1:A:160:VAL:HB	0.50	1.65	3	2
1:A:120:GLU:OE1	1:A:137:LYS:HE3	0.50	2.05	16	1
2:C:228:ASP:OD2	2:C:229:ILE:HD13	0.50	2.05	5	1
1:B:153:ASN:O	1:B:157:PRO:HD3	0.50	2.06	15	12
1:A:124:GLY:HA3	1:A:135:LEU:HD23	0.50	1.84	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:223:VAL:HG12	2:C:224:VAL:H	0.50	1.65	17	3
1:A:167:ARG:HE	2:C:221:VAL:HG21	0.50	1.66	23	1
1:A:167:ARG:O	2:C:223:VAL:HA	0.50	2.07	9	2
1:A:171:HIS:HB2	2:C:225:VAL:CG2	0.50	2.37	6	2
1:A:164:TYR:CD2	1:B:164:TYR:HB3	0.50	2.41	24	5
2:C:229:ILE:HG12	2:C:230:LEU:N	0.50	2.22	9	4
1:B:122:ILE:HD12	1:B:163:PHE:CE1	0.49	2.42	11	1
1:B:150:LYS:N	1:B:150:LYS:HD2	0.49	2.22	10	10
1:A:134:PHE:CD1	1:A:134:PHE:N	0.49	2.80	12	3
1:A:151:GLU:O	1:A:155:LYS:HD3	0.49	2.06	7	1
1:A:157:PRO:HA	1:A:160:VAL:HG22	0.49	1.85	19	11
1:A:157:PRO:HB3	1:B:161:ILE:HD11	0.49	1.84	23	1
1:A:124:GLY:HA3	1:A:135:LEU:H	0.49	1.67	19	3
1:A:133:MET:HE3	1:A:146:LEU:HD21	0.49	1.84	10	1
1:B:160:VAL:HA	1:B:163:PHE:HE1	0.49	1.67	11	1
1:A:131:GLU:HG3	1:A:133:MET:SD	0.49	2.48	25	1
1:A:124:GLY:O	1:A:134:PHE:HA	0.49	2.08	16	2
2:C:218:ILE:HD12	2:C:220:LYS:HD3	0.49	1.84	20	1
1:A:131:GLU:HG3	1:A:150:LYS:NZ	0.49	2.23	19	1
2:C:226:LEU:C	2:C:226:LEU:HD12	0.49	2.28	9	1
1:A:165:GLU:HG3	1:B:132:LEU:HD12	0.49	1.85	3	1
1:A:167:ARG:HA	1:A:167:ARG:NE	0.48	2.23	17	2
1:B:137:LYS:HA	1:B:144:ALA:H	0.48	1.68	15	3
2:C:229:ILE:N	2:C:229:ILE:HD13	0.48	2.23	7	3
1:B:132:LEU:HB2	1:B:149:ALA:HB2	0.48	1.86	25	1
2:C:220:LYS:C	2:C:220:LYS:HD2	0.48	2.29	1	1
1:A:121:ARG:O	1:A:137:LYS:HB3	0.48	2.08	16	4
1:B:170:TRP:HB3	2:C:220:LYS:HZ2	0.48	1.68	19	1
2:C:228:ASP:CG	2:C:229:ILE:HD13	0.48	2.29	5	1
1:A:167:ARG:HB3	2:C:222:PRO:O	0.48	2.09	4	4
1:A:117:LEU:HD13	1:A:140:ASN:HB2	0.47	1.86	7	1
1:A:167:ARG:HD2	2:C:221:VAL:HG13	0.47	1.86	9	2
2:C:218:ILE:HD12	2:C:220:LYS:HE3	0.47	1.86	1	2
1:B:124:GLY:HA3	2:C:228:ASP:O	0.47	2.09	9	2
1:B:115:ARG:NH2	1:B:117:LEU:HD11	0.47	2.22	5	1
1:B:133:MET:HG2	1:B:148:PRO:HA	0.47	1.87	15	1
1:A:148:PRO:HG2	1:A:151:GLU:HB3	0.47	1.86	4	1
1:B:133:MET:SD	1:B:148:PRO:HA	0.47	2.49	25	2
2:C:229:ILE:O	2:C:230:LEU:HD22	0.47	2.10	3	1
1:B:126:THR:HB	2:C:228:ASP:OD1	0.47	2.10	3	2
1:B:150:LYS:H	1:B:150:LYS:HD2	0.47	1.70	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:218:ILE:N	2:C:218:ILE:HD13	0.47	2.25	25	1
2:C:220:LYS:CG	2:C:221:VAL:H	0.47	2.23	10	1
1:B:150:LYS:N	1:B:150:LYS:HD3	0.47	2.25	24	1
1:A:132:LEU:HB2	1:A:149:ALA:CB	0.47	2.39	21	1
1:A:150:LYS:NZ	1:A:150:LYS:HB3	0.46	2.25	13	2
1:A:153:ASN:HB3	1:B:158:GLN:HE22	0.46	1.69	9	1
2:C:220:LYS:H	2:C:220:LYS:HD2	0.46	1.69	7	3
1:A:150:LYS:HE2	1:A:150:LYS:N	0.46	2.25	10	1
1:B:118:GLU:HB2	1:B:139:LYS:HD2	0.46	1.88	7	1
1:B:168:LEU:HD11	2:C:222:PRO:HB3	0.46	1.87	9	2
1:B:148:PRO:HG2	1:B:151:GLU:HB2	0.46	1.87	4	1
2:C:229:ILE:HG13	2:C:230:LEU:N	0.46	2.25	15	7
1:B:122:ILE:HG12	1:B:136:MET:SD	0.46	2.51	7	3
1:A:168:LEU:HG	1:A:170:TRP:CD1	0.46	2.46	2	5
1:B:148:PRO:HD2	1:B:151:GLU:OE1	0.46	2.11	20	1
1:B:124:GLY:HA2	1:B:163:PHE:CZ	0.46	2.46	9	5
1:B:147:VAL:HG13	1:B:151:GLU:OE1	0.46	2.10	23	2
1:B:150:LYS:HD2	1:B:150:LYS:N	0.46	2.26	16	6
2:C:220:LYS:HB3	2:C:220:LYS:NZ	0.46	2.26	20	1
1:B:168:LEU:HD12	1:B:169:THR:N	0.46	2.26	18	2
1:B:167:ARG:HA	1:B:167:ARG:NE	0.45	2.26	18	3
1:A:132:LEU:O	1:A:149:ALA:HB2	0.45	2.11	23	1
1:B:117:LEU:HD22	1:B:140:ASN:HB2	0.45	1.88	20	1
1:A:170:TRP:O	2:C:225:VAL:HG13	0.45	2.11	20	2
1:A:115:ARG:NH2	1:A:117:LEU:HD11	0.45	2.27	5	1
1:B:146:LEU:N	1:B:146:LEU:HD22	0.45	2.26	5	7
1:B:134:PHE:N	1:B:134:PHE:CD1	0.45	2.84	4	7
2:C:218:ILE:C	2:C:218:ILE:HD12	0.45	2.31	16	1
1:B:125:ALA:O	2:C:228:ASP:HA	0.45	2.11	9	1
1:B:167:ARG:O	2:C:224:VAL:HG13	0.45	2.11	20	2
1:B:170:TRP:HD1	2:C:222:PRO:HB3	0.45	1.72	24	1
1:B:134:PHE:CD1	1:B:134:PHE:N	0.45	2.85	17	3
1:A:124:GLY:O	1:A:125:ALA:HB3	0.45	2.12	13	3
2:C:218:ILE:HD13	2:C:220:LYS:HD2	0.45	1.89	19	1
2:C:220:LYS:HE3	2:C:220:LYS:H	0.45	1.72	21	1
1:B:170:TRP:CZ3	2:C:218:ILE:HD13	0.45	2.47	23	1
2:C:221:VAL:HG23	2:C:221:VAL:O	0.45	2.11	25	2
1:A:132:LEU:HG	1:B:165:GLU:HG3	0.45	1.88	8	1
1:A:140:ASN:HD22	1:A:140:ASN:N	0.45	2.09	1	1
1:B:126:THR:HG21	2:C:229:ILE:HD13	0.45	1.88	11	1
1:A:120:GLU:OE1	1:A:137:LYS:HE2	0.45	2.12	25	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:167:ARG:HB3	2:C:225:VAL:O	0.45	2.12	9	1
1:B:121:ARG:O	1:B:137:LYS:HB3	0.44	2.12	12	1
2:C:218:ILE:H	2:C:218:ILE:HD13	0.44	1.72	25	1
1:A:125:ALA:HB3	1:B:170:TRP:HE1	0.44	1.71	11	1
1:A:167:ARG:NH1	2:C:221:VAL:HG13	0.44	2.28	22	1
1:A:157:PRO:HG2	1:A:158:GLN:NE2	0.44	2.27	11	1
1:B:146:LEU:HD22	1:B:146:LEU:N	0.44	2.28	21	4
1:B:153:ASN:OD1	1:B:154:VAL:N	0.44	2.51	1	1
1:A:133:MET:C	1:A:146:LEU:HD11	0.44	2.32	22	1
2:C:220:LYS:HD2	2:C:220:LYS:H	0.44	1.72	3	4
1:B:120:GLU:OE1	1:B:137:LYS:HE2	0.44	2.12	6	2
1:B:150:LYS:HD2	1:B:150:LYS:H	0.44	1.73	16	1
1:A:125:ALA:O	1:A:132:LEU:HD22	0.44	2.11	6	2
1:B:151:GLU:O	1:B:154:VAL:HG22	0.44	2.13	16	1
1:A:123:ILE:HD11	1:A:135:LEU:HD23	0.44	1.89	13	1
1:A:150:LYS:N	1:A:150:LYS:HD2	0.44	2.28	4	4
2:C:220:LYS:HG3	2:C:221:VAL:N	0.43	2.28	13	1
1:A:160:VAL:HG23	1:A:161:ILE:N	0.43	2.29	21	11
1:A:168:LEU:HD11	2:C:226:LEU:HG	0.43	1.91	19	1
2:C:218:ILE:HB	2:C:220:LYS:NZ	0.43	2.28	11	1
1:B:157:PRO:O	1:B:160:VAL:HB	0.43	2.12	4	1
1:A:120:GLU:OE2	1:A:139:LYS:HE2	0.43	2.14	21	1
1:B:139:LYS:HG3	1:B:140:ASN:OD1	0.43	2.14	17	1
1:B:128:SER:HB3	1:B:133:MET:SD	0.43	2.53	1	1
1:A:118:GLU:OE2	1:A:139:LYS:HD2	0.43	2.13	2	1
1:A:163:PHE:O	1:A:167:ARG:HG2	0.43	2.13	16	1
1:B:119:PRO:HB3	1:B:136:MET:SD	0.43	2.54	18	1
1:B:120:GLU:OE1	1:B:121:ARG:HG2	0.43	2.13	20	1
1:A:126:THR:HB	2:C:218:ILE:HG13	0.43	1.91	2	1
1:A:120:GLU:OE1	1:A:137:LYS:HG2	0.43	2.14	3	1
1:A:134:PHE:C	1:A:146:LEU:HD12	0.43	2.35	17	3
1:B:146:LEU:HD11	2:C:229:ILE:HD12	0.43	1.90	23	1
1:A:140:ASN:N	1:A:140:ASN:HD22	0.43	2.11	6	1
1:A:151:GLU:OE2	1:A:155:LYS:HE3	0.42	2.14	11	1
1:A:122:ILE:HD12	1:A:160:VAL:HA	0.42	1.91	9	1
1:B:171:HIS:C	2:C:220:LYS:HD3	0.42	2.35	13	1
1:B:167:ARG:HD3	2:C:225:VAL:O	0.42	2.14	9	1
1:A:157:PRO:O	1:A:161:ILE:HG13	0.42	2.14	5	5
1:B:140:ASN:HD22	1:B:140:ASN:N	0.42	2.12	1	1
1:B:123:ILE:HD12	1:B:135:LEU:CD2	0.42	2.45	2	1
1:B:164:TYR:CE2	2:C:226:LEU:HD11	0.42	2.50	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:PRO:HB2	1:B:157:PRO:HB2	0.42	1.92	9	2
1:B:126:THR:CG2	2:C:229:ILE:HD12	0.42	2.45	14	1
1:A:125:ALA:O	2:C:218:ILE:HG13	0.42	2.15	7	1
1:B:166:GLU:HG3	1:B:167:ARG:CD	0.42	2.44	7	1
1:B:126:THR:HG23	1:B:128:SER:OG	0.42	2.15	9	2
2:C:219:GLU:OE1	2:C:219:GLU:N	0.42	2.53	8	1
1:A:135:LEU:HD13	1:A:146:LEU:HD12	0.42	1.92	6	1
2:C:220:LYS:HE3	2:C:220:LYS:N	0.42	2.29	21	1
1:B:128:SER:O	1:B:131:GLU:HG2	0.42	2.15	12	1
1:B:120:GLU:OE1	1:B:137:LYS:HE3	0.42	2.15	16	1
1:A:133:MET:O	1:A:146:LEU:HG	0.42	2.15	2	1
1:A:135:LEU:HD12	1:A:145:ASP:C	0.42	2.35	21	1
2:C:220:LYS:CE	2:C:220:LYS:H	0.41	2.28	10	1
1:B:124:GLY:HA2	1:B:163:PHE:CE2	0.41	2.50	19	1
2:C:221:VAL:HG13	2:C:221:VAL:O	0.41	2.15	10	1
1:B:146:LEU:HD11	2:C:229:ILE:HD13	0.41	1.91	21	1
1:A:134:PHE:CE2	1:A:160:VAL:HB	0.41	2.51	5	1
1:B:151:GLU:OE2	1:B:155:LYS:HE2	0.41	2.14	7	1
1:B:170:TRP:CD1	2:C:222:PRO:HB3	0.41	2.51	24	1
1:A:126:THR:HG22	1:A:133:MET:HB2	0.41	1.93	23	1
2:C:218:ILE:HG13	2:C:220:LYS:NZ	0.41	2.30	22	1
1:B:120:GLU:HG2	1:B:121:ARG:NH1	0.41	2.29	19	1
1:A:123:ILE:CD1	1:A:135:LEU:HD23	0.41	2.45	13	1
1:A:132:LEU:CD1	1:B:165:GLU:HG3	0.41	2.45	2	1
1:A:153:ASN:HB3	1:B:158:GLN:NE2	0.41	2.30	9	1
1:A:126:THR:O	1:A:133:MET:HG2	0.41	2.15	3	1
1:B:118:GLU:CD	1:B:118:GLU:H	0.41	2.19	3	1
1:B:140:ASN:N	1:B:140:ASN:HD22	0.41	2.14	6	1
1:A:123:ILE:HD12	1:A:123:ILE:C	0.41	2.36	21	1
1:B:169:THR:CG2	2:C:223:VAL:HB	0.41	2.39	17	1
1:A:133:MET:HB3	1:A:146:LEU:CG	0.41	2.45	21	2
2:C:220:LYS:H	2:C:220:LYS:HE3	0.41	1.75	10	1
1:B:171:HIS:HB2	2:C:221:VAL:O	0.41	2.16	10	1
1:A:121:ARG:HG2	1:A:137:LYS:HD3	0.41	1.91	22	1
1:A:163:PHE:CZ	2:C:222:PRO:HG3	0.41	2.51	4	1
1:B:146:LEU:HD11	2:C:229:ILE:CD1	0.41	2.46	6	1
1:A:153:ASN:O	1:A:157:PRO:HD3	0.41	2.15	21	1
1:A:171:HIS:HB2	2:C:225:VAL:CG1	0.40	2.46	17	1
1:A:150:LYS:O	1:A:153:ASN:ND2	0.40	2.53	25	1
1:B:113:PHE:HZ	1:B:156:CYS:HG	0.40	1.59	11	1
1:A:153:ASN:O	1:A:157:PRO:HG3	0.40	2.16	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:229:ILE:N	2:C:229:ILE:CD1	0.40	2.84	14	1
1:B:128:SER:HB3	1:B:133:MET:HG3	0.40	1.92	25	1
1:A:118:GLU:CD	1:A:139:LYS:HD2	0.40	2.37	2	1
1:A:157:PRO:O	1:A:160:VAL:HG22	0.40	2.17	9	1
1:A:168:LEU:HD12	2:C:224:VAL:HB	0.40	1.92	1	1
1:A:162:SER:O	1:A:166:GLU:HG3	0.40	2.17	18	1
1:A:125:ALA:HB3	2:C:218:ILE:HD11	0.40	1.92	18	1
1:A:153:ASN:OD1	1:B:161:ILE:HG21	0.40	2.17	24	1
1:B:169:THR:CG2	2:C:223:VAL:HG23	0.40	2.35	2	1
1:B:170:TRP:HB3	2:C:220:LYS:HD2	0.40	1.92	6	1
1:A:124:GLY:O	1:A:125:ALA:HB2	0.40	2.17	19	1
2:C:221:VAL:O	2:C:221:VAL:HG23	0.40	2.17	21	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	57/75 (76%)	43±1 (76±2%)	8±2 (14±3%)	6±1 (10±3%)	1	10
1	B	57/75 (76%)	47±2 (83±4%)	8±2 (13±4%)	2±1 (4±2%)	6	32
2	C	13/30 (43%)	8±1 (58±8%)	5±1 (39±6%)	0±1 (2±4%)	12	51
All	All	3175/4500 (71%)	2448 (77%)	521 (16%)	206 (6%)	3	19

All 21 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	128	SER	25
1	A	130	GLY	20
1	A	171	HIS	19
1	B	130	GLY	19
1	A	170	TRP	18
1	B	144	ALA	15
1	A	144	ALA	14

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Mol	Chain	Res	Type	Models (Total)
1	B	116	GLY	13
1	A	125	ALA	13
1	A	123	ILE	11
1	A	116	GLY	10
1	B	114	ALA	6
1	A	114	ALA	6
1	B	112	GLY	4
2	C	223	VAL	4
2	C	222	PRO	3
1	A	121	ARG	2
1	A	172	SER	1
1	A	124	GLY	1
1	A	118	GLU	1
1	B	118	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	49/66 (74%)	48±1 (98±2%)	1±1 (2±2%)	70	95
1	B	48/66 (73%)	46±1 (97±2%)	2±1 (3±2%)	47	88
2	C	13/25 (52%)	12±1 (90±5%)	1±1 (10±5%)	12	56
All	All	2750/3925 (70%)	2657 (97%)	93 (3%)	46	88

All 22 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	C	220	LYS	21
1	B	150	LYS	14
2	C	229	ILE	8
1	B	139	LYS	8
1	A	139	LYS	8
1	B	134	PHE	6
1	A	150	LYS	4
2	C	223	VAL	3
1	A	133	MET	2

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Mol	Chain	Res	Type	Models (Total)
1	B	131	GLU	2
1	A	120	GLU	2
1	A	115	ARG	2
1	B	170	TRP	2
1	B	115	ARG	2
1	B	167	ARG	2
2	C	218	ILE	1
1	B	120	GLU	1
1	B	163	PHE	1
1	A	167	ARG	1
1	A	158	GLN	1
2	C	230	LEU	1
1	B	171	HIS	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided