



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 10:15 AM UTC

PDB ID : 2KZ7 / pdb_00002kz7
Title : Solution structure of the CARMIL CAH3a/b domain bound to capping protein (CP)
Authors : Zwolak, A.; Tjandra, N.
Deposited on : 2010-06-12

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

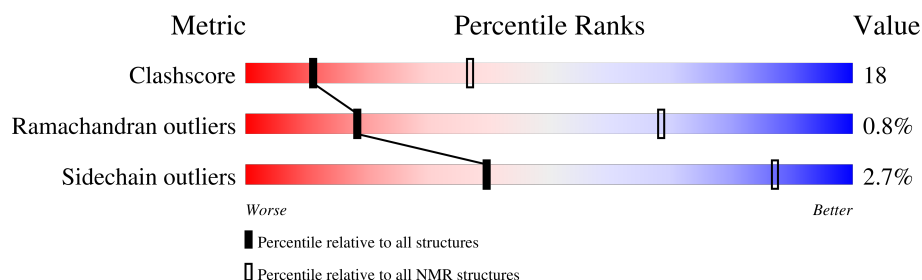
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	286	
2	B	277	
3	C	85	

2 Ensemble composition and analysis

This entry contains 10 models. Model 7 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:8-A:281, B:302-B:554 (527)	0.09	7

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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 4, 7, 10
2	3, 6
3	5, 9
4	2, 8

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9973 atoms, of which 4953 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms						Trace
1	A	275	Total	C	H	N	O	S	0
			4413	1413	2175	392	428	5	

- Molecule 2 is a protein called F-actin-capping protein subunit beta isoforms 1 and 2.

Mol	Chain	Residues	Atoms						Trace
2	B	270	Total	C	H	N	O	S	0
			4273	1334	2133	374	422	10	

- Molecule 3 is a protein called Leucine-rich repeat-containing protein 16A.

Mol	Chain	Residues	Atoms						Trace
3	C	82	Total	C	H	N	O	S	0
			1287	393	645	121	124	4	

There are 10 discrepancies between the modelled and reference sequences:

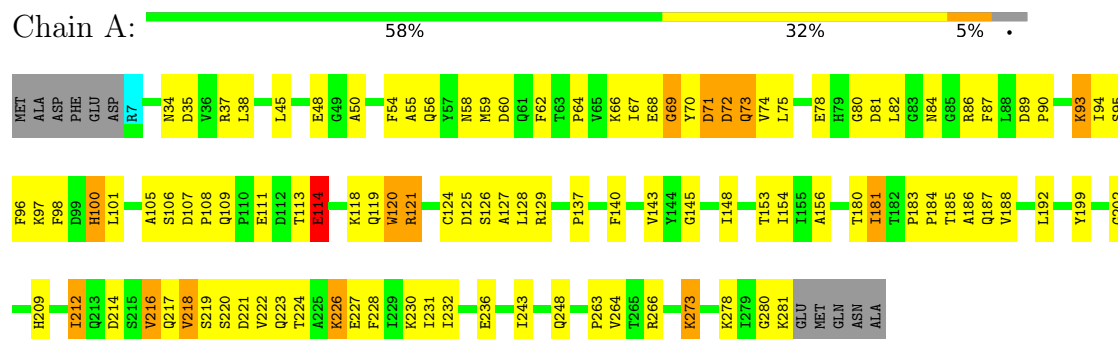
Chain	Residue	Modelled	Actual	Comment	Reference
C	598	GLY	-	expression tag	UNP Q6EDY6
C	599	ALA	-	expression tag	UNP Q6EDY6
C	600	MET	-	expression tag	UNP Q6EDY6
C	601	GLY	-	expression tag	UNP Q6EDY6
C	602	SER	-	expression tag	UNP Q6EDY6
C	603	TRP	-	expression tag	UNP Q6EDY6
C	604	GLY	-	expression tag	UNP Q6EDY6
C	605	CYS	-	expression tag	UNP Q6EDY6
C	681	GLY	-	expression tag	UNP Q6EDY6
C	682	CYS	-	expression tag	UNP Q6EDY6

4 Residue-property plots

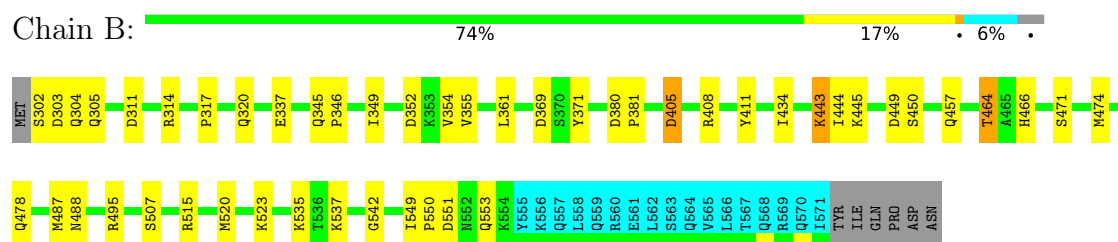
4.1 Average score per residue in the NMR ensemble

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: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

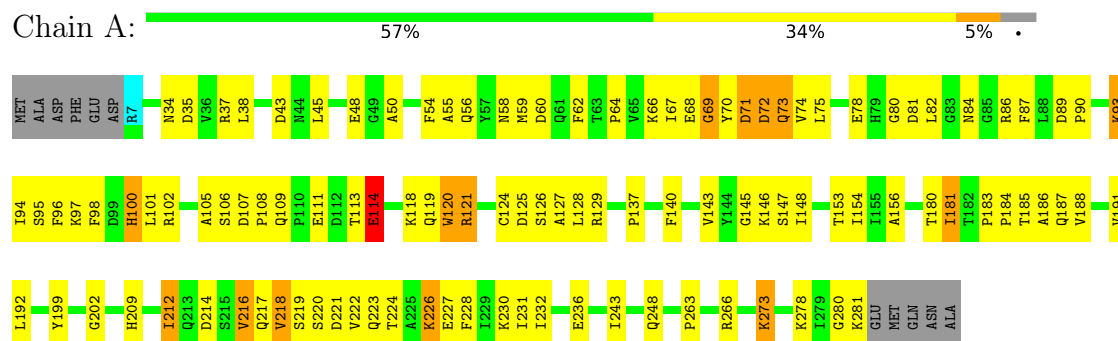


4.2 Scores per residue for each member of the ensemble

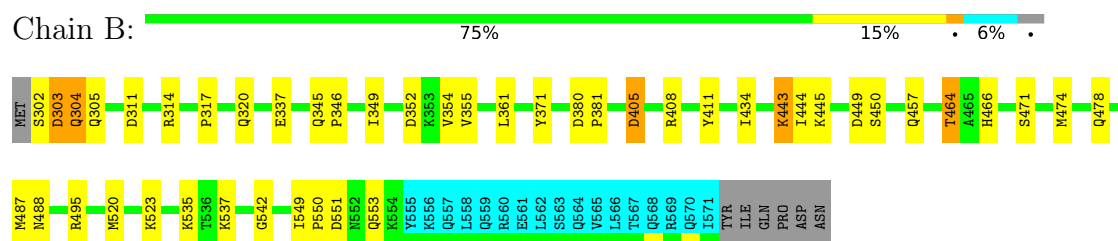
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

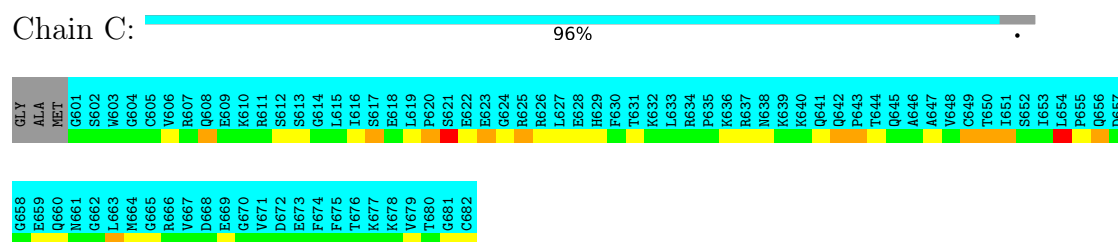
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

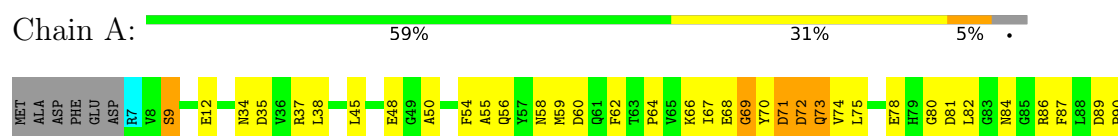


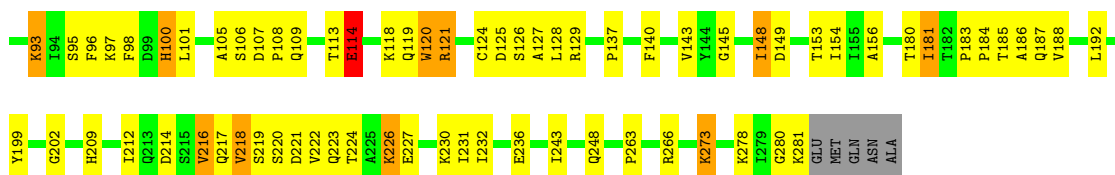
- Molecule 3: Leucine-rich repeat-containing protein 16A



4.2.2 Score per residue for model 2

- Molecule 1: F-actin-capping protein subunit alpha-1

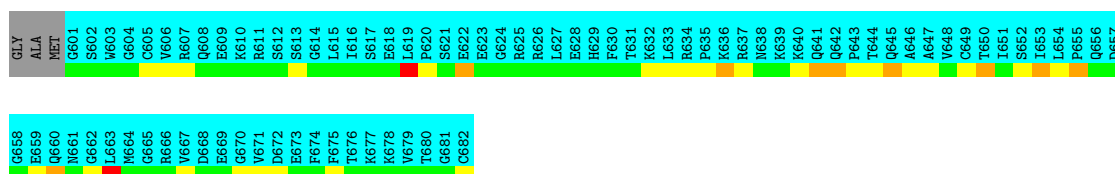




- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

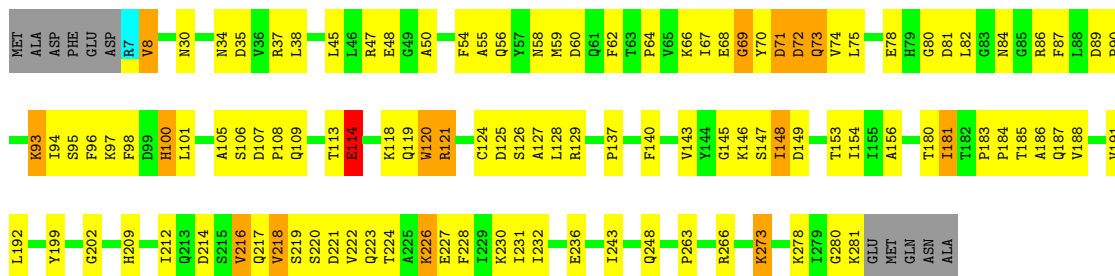


- Molecule 3: Leucine-rich repeat-containing protein 16A

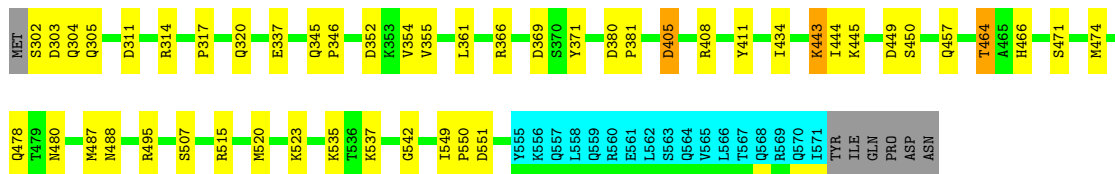


4.2.3 Score per residue for model 3

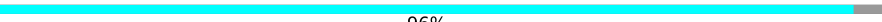
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



- Molecule 3: Leucine-rich repeat-containing protein 16A

Chain C:  96%



4.2.4 Score per residue for model 4

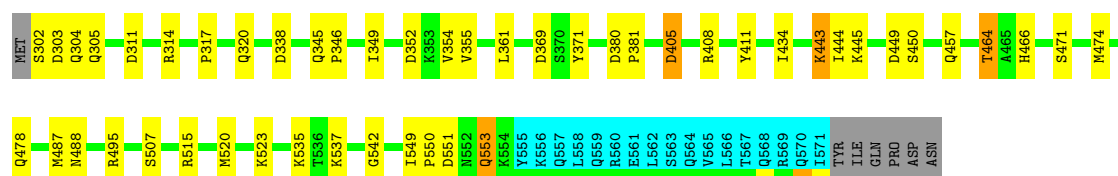
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain A:  58%  32%  5%

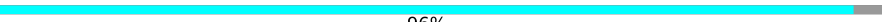


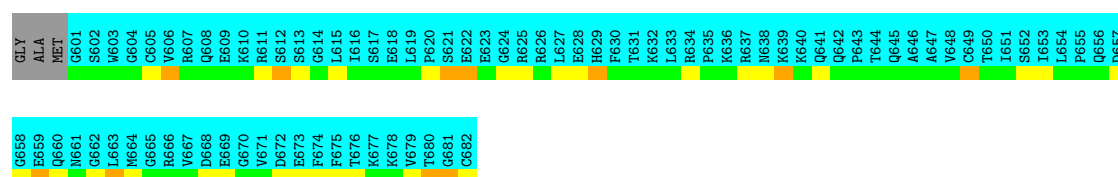
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain B:  74%  16%  6%



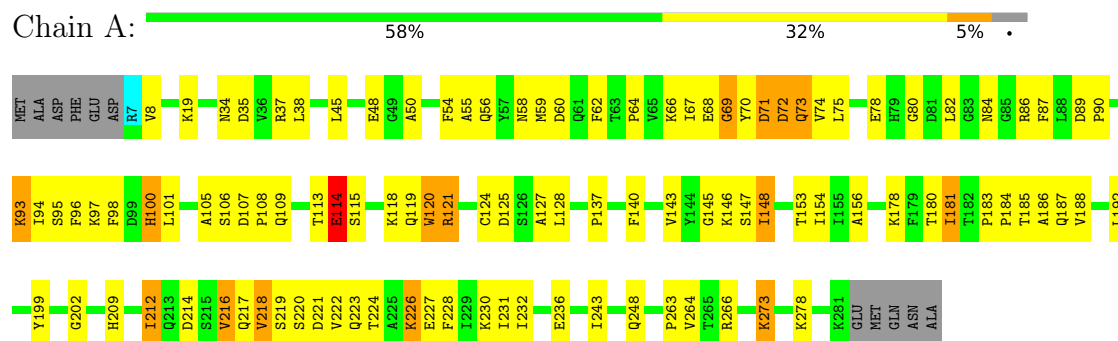
- Molecule 3: Leucine-rich repeat-containing protein 16A

Chain C:  96%

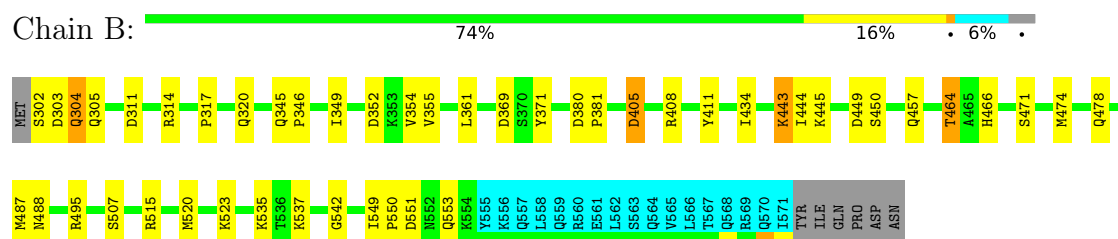


4.2.5 Score per residue for model 5

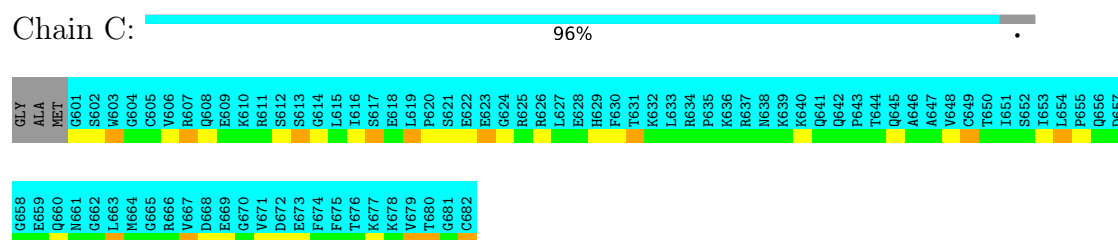
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

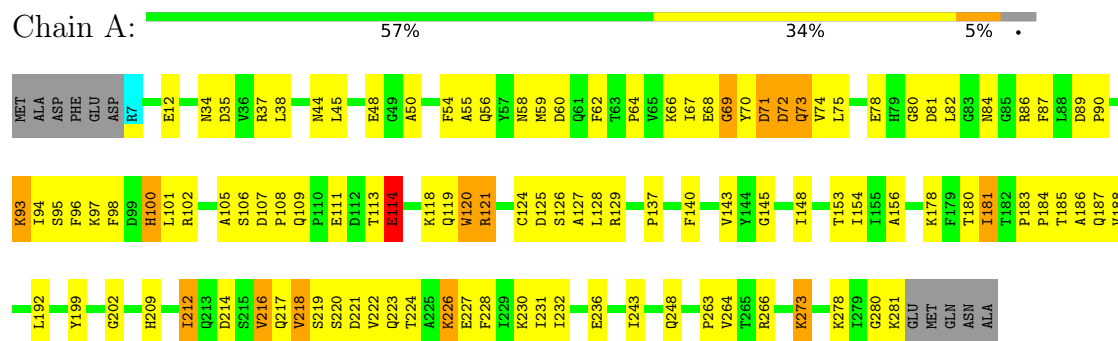


- Molecule 3: Leucine-rich repeat-containing protein 16A



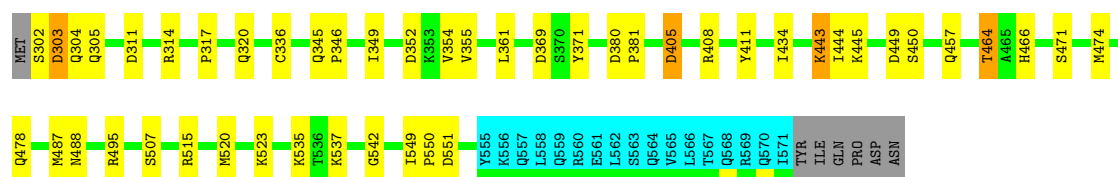
4.2.6 Score per residue for model 6

- Molecule 1: F-actin-capping protein subunit alpha-1



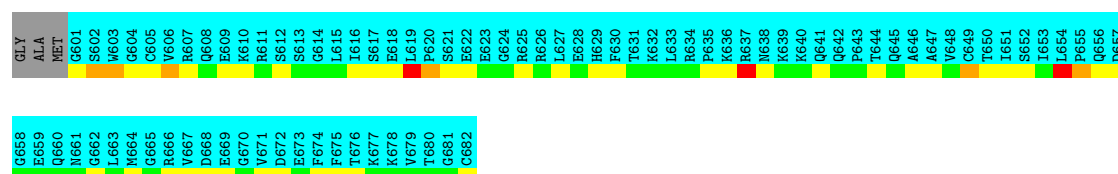
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2





- Molecule 3: Leucine-rich repeat-containing protein 16A

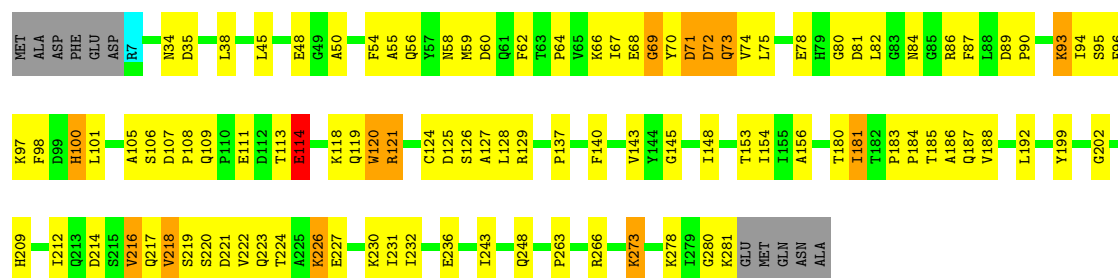
Chain C: 96%



4.2.7 Score per residue for model 7 (medoid)

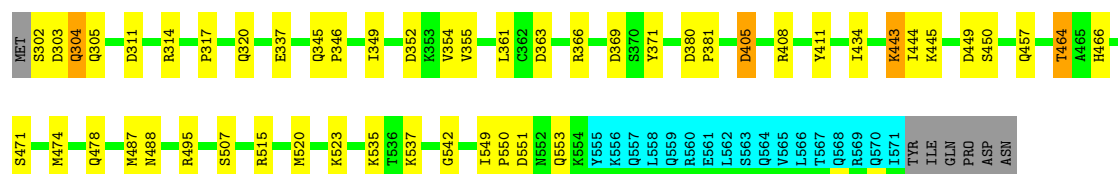
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain A: 59%



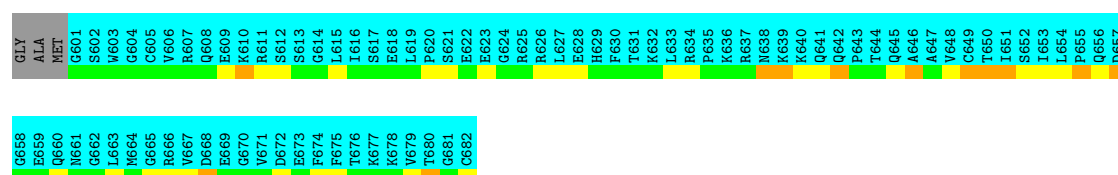
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain B: 73%



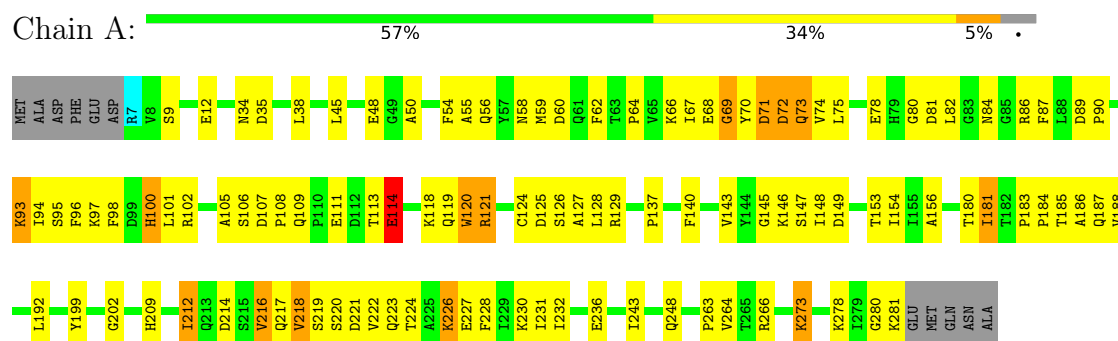
- Molecule 3: Leucine-rich repeat-containing protein 16A

Chain C: 96%

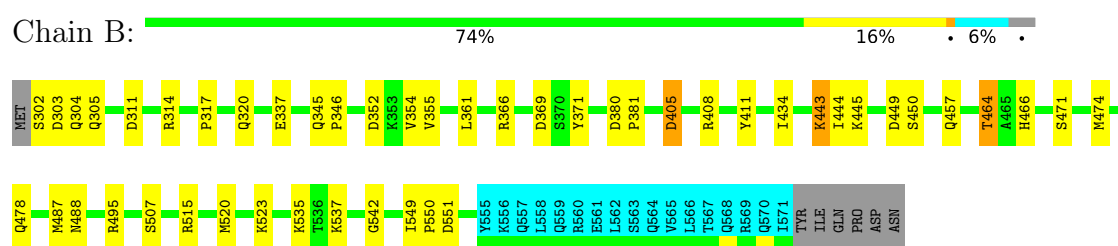


4.2.8 Score per residue for model 8

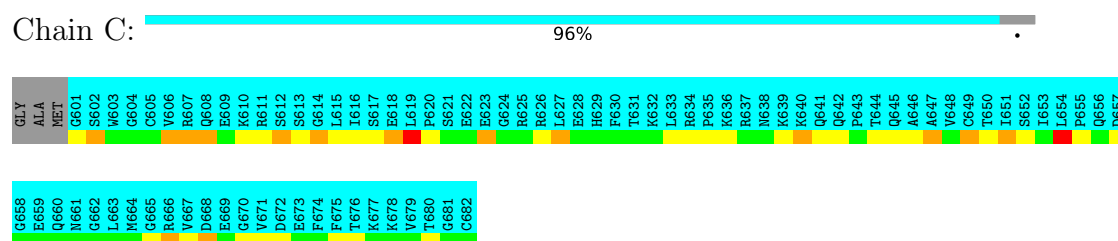
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



- Molecule 3: Leucine-rich repeat-containing protein 16A

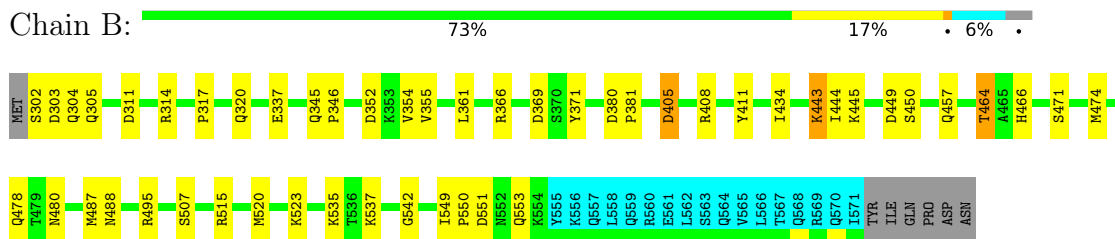


4.2.9 Score per residue for model 9

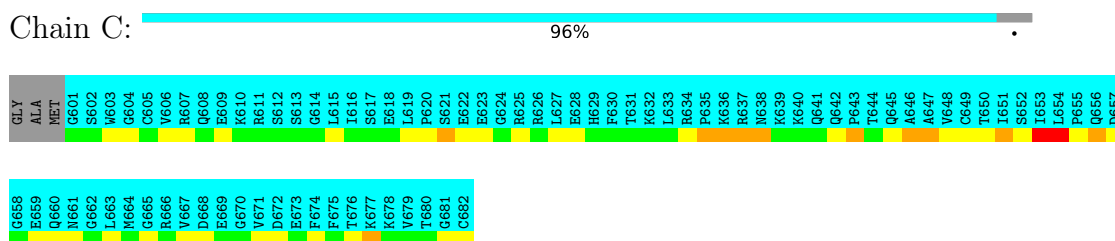
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

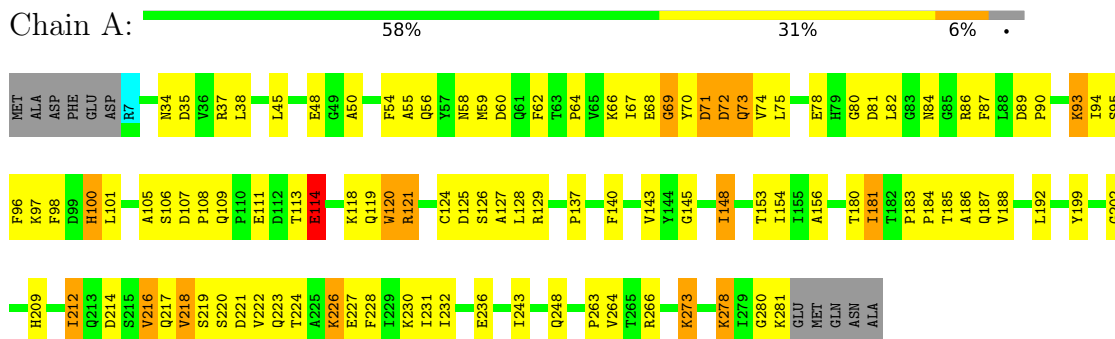


- Molecule 3: Leucine-rich repeat-containing protein 16A

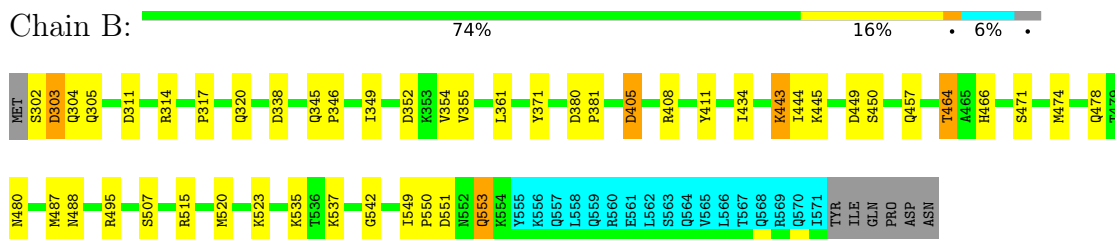


4.2.10 Score per residue for model 10

- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



- Molecule 3: Leucine-rich repeat-containing protein 16A



GLY	ALA	MET
G601	G602	G603
G604	G605	G606
G607	G608	G609
G610	G611	G612
G613	G614	G615
G616	G617	G618
G619	G620	G621
G622	G623	G624
G625	G626	G627
G628	G629	G630
G631	G632	G633
G634	G635	G636
G637	G638	G639
G640	G641	G642
G643	G644	G645
G646	G647	G648
G649	G650	G651
G652	G653	G654
G655	G656	G657

5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics, simulated annealing, torsion angle dynamics*.

Of the 200 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	2.23
X-PLOR NIH	refinement	2.23

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.42±0.00	0±0/2279 (0.0± 0.0%)	1.01±0.00	12±0/3088 (0.4± 0.0%)
2	B	0.44±0.00	0±0/2026 (0.0± 0.0%)	0.91±0.00	5±0/2738 (0.2± 0.0%)
All	All	0.43	0/43050 (0.0%)	0.96	170/58260 (0.3%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	464	THR	N-CA-C	-9.90	91.82	108.75	8	10
1	A	72	ASP	N-CA-C	9.67	126.72	113.37	1	10
1	A	113	THR	N-CA-C	9.65	123.66	110.35	7	10
1	A	71	ASP	N-CA-C	-8.21	103.21	113.23	8	10
1	A	100	HIS	N-CA-C	7.24	120.21	111.82	4	10
2	B	535	LYS	N-CA-C	6.84	118.38	111.07	6	10
2	B	304	GLN	N-CA-C	-6.42	104.38	111.82	9	10
1	A	127	ALA	N-CA-C	-6.17	104.10	111.69	7	10
1	A	181	ILE	N-CA-C	6.12	117.39	108.58	10	10
1	A	216	VAL	N-CA-C	6.00	117.23	108.53	6	10
1	A	114	GLU	N-CA-C	-5.86	104.84	112.23	8	10
1	A	199	TYR	N-CA-C	5.53	119.12	111.71	2	10
1	A	93	LYS	N-CA-C	5.49	119.27	112.58	1	10
2	B	405	ASP	N-CA-C	-5.48	105.39	111.36	7	10
1	A	218	VAL	N-CA-C	5.47	115.98	107.99	9	10
1	A	75	LEU	N-CA-C	5.30	117.39	108.96	4	10
2	B	303	ASP	N-CA-C	-5.29	105.57	112.23	8	10

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	2227	2162	2154	126±2
2	B	1991	1974	1969	34±1
3	C	0	0	0	0±0
All	All	42180	41360	41230	1522

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:MET:HE3	1:A:78:GLU:HA	0.98	1.34	4	10
1:A:67:ILE:HG22	1:A:72:ASP:CG	0.94	1.88	9	10
1:A:202:GLY:O	2:B:314:ARG:HD2	0.82	1.75	5	10
2:B:443:LYS:N	2:B:443:LYS:HD3	0.78	1.94	4	7
1:A:82:LEU:HD12	1:A:86:ARG:HB2	0.78	1.56	4	10
2:B:443:LYS:HD3	2:B:443:LYS:N	0.77	1.94	9	3
1:A:280:GLY:O	1:A:281:LYS:O	0.76	2.04	9	8
1:A:98:PHE:HD1	1:A:105:ALA:HB2	0.75	1.42	6	10
1:A:59:MET:HE3	1:A:78:GLU:CA	0.73	2.13	1	10
2:B:443:LYS:HG2	2:B:444:ILE:HG13	0.73	1.61	5	10
1:A:185:THR:HG23	1:A:216:VAL:C	0.70	2.11	1	10
1:A:219:SER:H	1:A:224:THR:HG22	0.70	1.46	7	10
1:A:120:TRP:CZ3	1:A:221:ASP:HA	0.69	2.23	6	10
1:A:72:ASP:O	1:A:73:GLN:C	0.68	2.37	3	10
1:A:70:TYR:CB	1:A:72:ASP:HB3	0.68	2.19	1	10
1:A:67:ILE:N	1:A:72:ASP:OD1	0.68	2.27	7	10
1:A:181:ILE:HG22	1:A:183:PRO:HD3	0.67	1.67	2	10
1:A:67:ILE:HD13	1:A:96:PHE:HB2	0.67	1.67	1	10
1:A:106:SER:O	1:A:107:ASP:OD1	0.67	2.13	7	10
2:B:495:ARG:NH1	2:B:523:LYS:HB3	0.66	2.06	3	10
1:A:114:GLU:CD	1:A:114:GLU:H	0.65	2.00	4	10
1:A:153:THR:CG2	1:A:180:THR:HG22	0.65	2.22	4	10
1:A:227:GLU:O	1:A:231:ILE:HG13	0.64	1.93	4	10
1:A:121:ARG:HG3	1:A:145:GLY:CA	0.64	2.23	2	10
1:A:58:ASN:HD22	1:A:100:HIS:HD2	0.64	1.36	7	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:457:GLN:HB2	2:B:466:HIS:HB3	0.64	1.70	9	10
1:A:58:ASN:HD22	1:A:100:HIS:CD2	0.63	2.12	4	10
1:A:90:PRO:O	1:A:121:ARG:NH1	0.63	2.32	1	10
1:A:82:LEU:HD12	1:A:86:ARG:CB	0.63	2.24	7	10
1:A:98:PHE:CD1	1:A:105:ALA:HB2	0.63	2.29	5	10
1:A:266:ARG:HG3	1:A:266:ARG:HH11	0.63	1.54	3	10
1:A:55:ALA:HA	1:A:100:HIS:NE2	0.62	2.10	1	10
1:A:34:ASN:O	1:A:38:LEU:HD23	0.62	1.95	9	10
1:A:185:THR:HG23	1:A:216:VAL:O	0.62	1.95	4	10
1:A:66:LYS:HA	1:A:72:ASP:OD1	0.61	1.96	5	10
1:A:95:SER:HB3	1:A:109:GLN:O	0.60	1.96	8	10
2:B:478:GLN:HG2	2:B:488:ASN:ND2	0.60	2.12	6	10
1:A:220:SER:HB3	1:A:223:GLN:HB2	0.60	1.74	1	10
1:A:243:ILE:HG23	2:B:487:MET:CE	0.60	2.27	5	10
1:A:188:VAL:N	1:A:214:ASP:O	0.60	2.29	1	10
1:A:125:ASP:HA	1:A:143:VAL:HG21	0.59	1.74	1	10
1:A:67:ILE:CG2	1:A:70:TYR:HB2	0.58	2.29	6	10
1:A:121:ARG:HG3	1:A:145:GLY:HA3	0.57	1.76	7	10
1:A:186:ALA:N	1:A:216:VAL:O	0.57	2.37	9	10
1:A:220:SER:OG	1:A:221:ASP:N	0.57	2.38	2	10
2:B:354:VAL:HG23	2:B:355:VAL:HG23	0.57	1.76	1	10
1:A:56:GLN:O	1:A:60:ASP:OD2	0.57	2.23	1	10
1:A:72:ASP:O	1:A:74:VAL:N	0.56	2.38	2	10
1:A:153:THR:HG22	1:A:180:THR:HG22	0.56	1.78	5	10
2:B:434:ILE:HB	2:B:450:SER:HB2	0.56	1.77	4	10
1:A:70:TYR:C	1:A:72:ASP:N	0.56	2.64	5	10
1:A:67:ILE:HD12	1:A:105:ALA:O	0.55	2.02	4	10
2:B:380:ASP:HA	2:B:381:PRO:C	0.55	2.26	1	10
1:A:70:TYR:HB2	1:A:72:ASP:HB3	0.55	1.79	7	10
1:A:120:TRP:CZ3	1:A:221:ASP:CA	0.55	2.90	7	10
2:B:443:LYS:N	2:B:443:LYS:CD	0.55	2.70	5	10
1:A:153:THR:HG22	1:A:180:THR:HA	0.55	1.79	4	10
1:A:70:TYR:O	1:A:71:ASP:HB3	0.55	2.02	2	10
2:B:495:ARG:CZ	2:B:523:LYS:HD3	0.54	2.33	3	10
1:A:219:SER:H	1:A:224:THR:CG2	0.54	2.16	7	10
2:B:495:ARG:NH1	2:B:523:LYS:HD3	0.54	2.18	2	10
1:A:101:LEU:C	1:A:101:LEU:HD23	0.54	2.28	1	10
1:A:67:ILE:O	1:A:69:GLY:N	0.54	2.41	2	10
1:A:137:PRO:HG2	2:B:542:GLY:O	0.53	2.04	2	10
1:A:266:ARG:HG3	1:A:266:ARG:NH1	0.53	2.19	3	10
2:B:352:ASP:OD1	2:B:354:VAL:HG22	0.53	2.04	5	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:TYR:HB3	1:A:72:ASP:HB3	0.52	1.81	3	10
1:A:232:ILE:O	1:A:236:GLU:HG3	0.52	2.05	2	10
1:A:230:LYS:O	1:A:230:LYS:HD2	0.52	2.05	5	7
1:A:90:PRO:O	1:A:93:LYS:HG2	0.52	2.05	6	10
1:A:67:ILE:HG22	1:A:72:ASP:CB	0.52	2.35	1	10
1:A:120:TRP:HB3	1:A:154:ILE:HD11	0.52	1.82	2	10
1:A:230:LYS:HD2	1:A:230:LYS:O	0.52	2.05	9	3
1:A:73:GLN:HG3	1:A:140:PHE:CE1	0.51	2.41	1	10
1:A:87:PHE:HB2	1:A:96:PHE:CZ	0.51	2.40	4	10
2:B:449:ASP:HB2	2:B:474:MET:HB2	0.51	1.83	1	10
1:A:119:GLN:OE1	1:A:221:ASP:HB2	0.51	2.05	3	10
1:A:89:ASP:O	1:A:93:LYS:HA	0.51	2.06	7	10
1:A:121:ARG:HG3	1:A:145:GLY:N	0.51	2.21	3	10
2:B:445:LYS:N	2:B:445:LYS:HD2	0.51	2.21	2	7
1:A:280:GLY:C	1:A:281:LYS:O	0.50	2.55	1	3
2:B:443:LYS:HD3	2:B:443:LYS:H	0.50	1.66	8	10
2:B:445:LYS:HD2	2:B:445:LYS:N	0.50	2.21	9	3
1:A:80:GLY:O	1:A:87:PHE:HA	0.50	2.07	3	10
1:A:120:TRP:CD1	1:A:181:ILE:HD13	0.50	2.42	7	10
2:B:495:ARG:NH2	2:B:523:LYS:HD3	0.49	2.22	1	10
2:B:405:ASP:OD1	2:B:408:ARG:NH1	0.49	2.45	9	10
1:A:248:GLN:HA	1:A:248:GLN:NE2	0.49	2.23	9	3
1:A:67:ILE:HD13	1:A:96:PHE:CB	0.49	2.36	3	10
1:A:55:ALA:HA	1:A:100:HIS:CD2	0.49	2.43	10	10
1:A:243:ILE:HG23	2:B:487:MET:HE1	0.49	1.85	4	10
1:A:248:GLN:NE2	1:A:248:GLN:HA	0.49	2.23	7	7
1:A:58:ASN:ND2	1:A:100:HIS:HD2	0.49	2.06	7	10
1:A:223:GLN:O	1:A:226:LYS:HG3	0.49	2.08	2	10
1:A:120:TRP:CD1	1:A:181:ILE:CD1	0.48	2.96	7	10
1:A:120:TRP:NE1	1:A:181:ILE:HD13	0.48	2.23	6	10
2:B:549:ILE:O	2:B:551:ASP:N	0.48	2.46	5	10
1:A:50:ALA:O	1:A:54:PHE:HD1	0.48	1.92	2	10
1:A:9:SER:CB	1:A:12:GLU:OE1	0.48	2.62	2	2
1:A:114:GLU:CD	1:A:114:GLU:N	0.48	2.72	6	10
1:A:86:ARG:NH1	1:A:97:LYS:HB2	0.48	2.24	5	10
1:A:192:LEU:O	1:A:209:HIS:HA	0.48	2.09	1	10
1:A:8:VAL:O	1:A:9:SER:CB	0.48	2.62	9	1
1:A:95:SER:O	1:A:108:PRO:HA	0.48	2.09	9	10
1:A:62:PHE:O	1:A:64:PRO:HD3	0.47	2.09	3	10
1:A:66:LYS:HE3	1:A:72:ASP:OD2	0.47	2.10	2	10
1:A:192:LEU:HD12	1:A:192:LEU:N	0.47	2.25	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:380:ASP:OD1	2:B:381:PRO:HA	0.47	2.10	7	10
1:A:124:CYS:SG	1:A:154:ILE:HD13	0.47	2.50	3	10
1:A:58:ASN:ND2	1:A:100:HIS:CD2	0.47	2.83	3	10
1:A:89:ASP:O	1:A:93:LYS:N	0.47	2.48	1	10
1:A:180:THR:O	1:A:186:ALA:HB1	0.47	2.10	3	10
1:A:95:SER:N	1:A:109:GLN:O	0.47	2.48	4	10
1:A:183:PRO:HA	1:A:184:PRO:C	0.46	2.36	2	10
1:A:221:ASP:OD2	1:A:222:VAL:HG23	0.46	2.11	4	10
1:A:101:LEU:C	1:A:101:LEU:CD2	0.46	2.89	5	10
2:B:553:GLN:N	2:B:553:GLN:CD	0.46	2.74	4	1
1:A:273:LYS:HB2	1:A:273:LYS:NZ	0.46	2.26	1	10
1:A:114:GLU:OE2	1:A:118:LYS:HG2	0.46	2.11	4	10
1:A:184:PRO:O	1:A:218:VAL:HB	0.45	2.12	2	10
1:A:107:ASP:OD1	1:A:107:ASP:O	0.45	2.35	7	10
1:A:125:ASP:HA	1:A:143:VAL:CG2	0.45	2.42	2	10
2:B:345:GLN:O	2:B:346:PRO:C	0.45	2.60	1	10
1:A:70:TYR:C	1:A:72:ASP:H	0.45	2.17	6	4
1:A:67:ILE:CD1	1:A:96:PHE:HB2	0.45	2.41	5	10
1:A:45:LEU:O	1:A:48:GLU:HB2	0.45	2.12	4	10
1:A:263:PRO:HG3	2:B:411:TYR:CE2	0.45	2.47	5	10
1:A:243:ILE:HD12	2:B:487:MET:HE3	0.44	1.89	1	10
1:A:84:ASN:O	1:A:84:ASN:CG	0.44	2.61	3	9
1:A:221:ASP:CG	1:A:222:VAL:N	0.44	2.76	1	10
1:A:84:ASN:CG	1:A:84:ASN:O	0.44	2.61	1	1
1:A:54:PHE:HB3	1:A:100:HIS:HB3	0.44	1.90	4	10
1:A:120:TRP:HZ3	1:A:221:ASP:CA	0.44	2.26	7	10
1:A:219:SER:N	1:A:224:THR:CG2	0.44	2.81	2	10
2:B:302:SER:HA	2:B:305:GLN:HG3	0.44	1.90	5	10
2:B:553:GLN:CD	2:B:553:GLN:N	0.44	2.75	10	1
1:A:86:ARG:CZ	1:A:97:LYS:HB2	0.44	2.43	9	10
1:A:202:GLY:C	2:B:314:ARG:HD2	0.43	2.38	4	5
1:A:97:LYS:HD2	1:A:97:LYS:C	0.43	2.39	1	10
1:A:8:VAL:O	1:A:12:GLU:OE1	0.43	2.37	9	1
1:A:153:THR:HG21	1:A:180:THR:HG22	0.43	1.91	1	4
1:A:219:SER:OG	1:A:220:SER:N	0.43	2.52	4	10
2:B:317:PRO:HB2	2:B:320:GLN:NE2	0.43	2.29	3	10
1:A:120:TRP:HZ3	1:A:221:ASP:CB	0.43	2.27	7	10
1:A:217:GLN:HG3	1:A:227:GLU:OE2	0.43	2.14	2	10
1:A:228:PHE:C	1:A:230:LYS:N	0.43	2.77	4	8
1:A:128:LEU:HD22	1:A:156:ALA:HB1	0.42	1.91	6	10
1:A:35:ASP:OD2	2:B:311:ASP:OD2	0.42	2.37	3	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LEU:CD2	1:A:156:ALA:HB1	0.42	2.45	9	10
1:A:121:ARG:HH21	1:A:125:ASP:CB	0.42	2.27	7	10
1:A:243:ILE:HG23	2:B:487:MET:HE3	0.42	1.92	9	9
1:A:82:LEU:HB2	1:A:86:ARG:O	0.42	2.15	8	10
1:A:119:GLN:OE1	1:A:221:ASP:CB	0.42	2.68	4	10
2:B:361:LEU:HD22	2:B:371:TYR:CG	0.42	2.50	1	10
1:A:126:SER:HA	1:A:129:ARG:HB2	0.41	1.92	7	9
1:A:192:LEU:N	1:A:192:LEU:CD1	0.41	2.84	7	10
1:A:192:LEU:HD11	1:A:212:ILE:HD11	0.41	1.93	1	7
2:B:507:SER:OG	2:B:515:ARG:NH2	0.41	2.54	5	9
2:B:471:SER:OG	2:B:520:MET:HG2	0.41	2.16	6	10
1:A:120:TRP:HE1	1:A:181:ILE:HD13	0.41	1.76	2	3
1:A:264:VAL:O	1:A:266:ARG:NH1	0.41	2.54	4	6
1:A:70:TYR:OH	1:A:94:ILE:HG21	0.41	2.16	4	9
1:A:186:ALA:O	1:A:216:VAL:N	0.41	2.53	7	4
1:A:191:VAL:HG13	1:A:191:VAL:O	0.41	2.16	1	1
2:B:443:LYS:CD	2:B:443:LYS:H	0.41	2.28	8	7
1:A:278:LYS:CD	1:A:278:LYS:H	0.41	2.28	4	1
1:A:81:ASP:HA	1:A:87:PHE:CD1	0.41	2.51	1	8
1:A:95:SER:HB2	1:A:111:GLU:CG	0.41	2.46	6	7
1:A:146:LYS:HG2	1:A:147:SER:N	0.40	2.32	3	4
1:A:191:VAL:O	1:A:191:VAL:HG13	0.40	2.16	3	1
1:A:114:GLU:OE2	1:A:115:SER:N	0.40	2.54	4	2
1:A:66:LYS:C	1:A:66:LYS:HD3	0.40	2.42	1	1
1:A:66:LYS:HD3	1:A:66:LYS:C	0.40	2.42	4	1
2:B:443:LYS:H	2:B:443:LYS:CD	0.40	2.28	7	1
1:A:148:ILE:O	1:A:149:ASP:OD1	0.40	2.40	3	2
1:A:278:LYS:H	1:A:278:LYS:CD	0.40	2.29	10	1
1:A:8:VAL:C	1:A:9:SER:OG	0.40	2.65	9	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	273/286 (95%)	248±1 (91±0%)	22±1 (8±0%)	3±0 (1±0%)	13	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	252/277 (91%)	244±0 (97±0%)	7±0 (3±0%)	1±0 (0±0%)	31	76
3	C	0	-	-	-	-	-
All	All	5250/6480 (81%)	4918 (94%)	289 (6%)	43 (1%)	18	68

All 6 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	68	GLU	10
1	A	69	GLY	10
1	A	73	GLN	10
2	B	550	PRO	10
1	A	8	VAL	2
1	A	9	SER	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	242/252 (96%)	233±0 (96±0%)	9±0 (4±0%)	30	81
2	B	224/248 (90%)	220±0 (98±0%)	4±0 (2±0%)	52	92
3	C	0	-	-	-	-
All	All	4660/5720 (81%)	4532 (97%)	128 (3%)	40	87

All 14 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	114	GLU	10
1	A	120	TRP	10
1	A	121	ARG	10
1	A	148	ILE	10
1	A	187	GLN	10
1	A	212	ILE	10
1	A	226	LYS	10
1	A	273	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	278	LYS	10
2	B	443	LYS	10
2	B	464	THR	10
2	B	537	LYS	10
2	B	553	GLN	7
1	A	9	SER	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 oligosaccharides 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