



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:00 pm BST

PDB ID : 2KZ7
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 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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

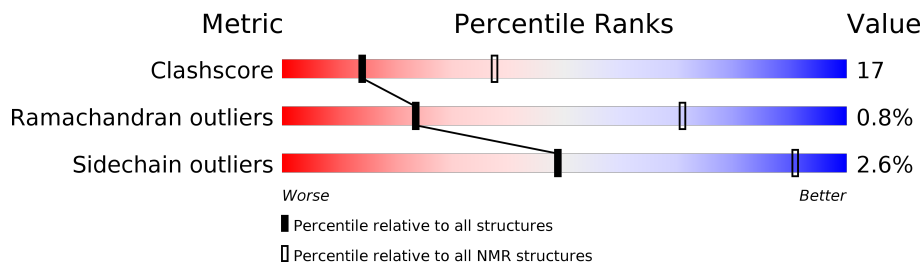
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	286	
2	B	277	
3	C	85	

2 Ensemble composition and analysis i

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)	0.05	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 [i](#)

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	
			Total	C	H	N	O		S
1	A	275	4413	1413	2175	392	428	5	0

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

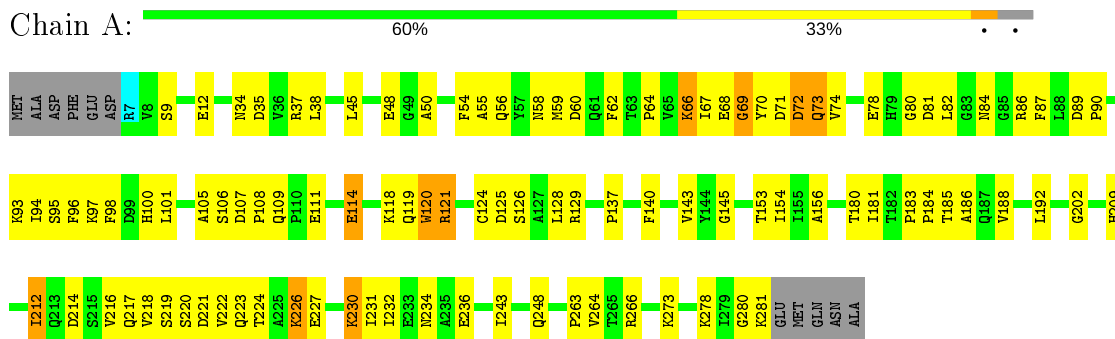
Chain	Residue	Modelled	Actual	Comment	Reference
C	598	GLY	-	EXPRESSION TAG	UNP Q6EDY6
C	599	ALA	-	EXPRESSION TAG	UNP Q6EDY6
C	600	MET	-	EXPRESSION TAG	UNP Q6EDY6
C	601	GLY	-	EXPRESSION TAG	UNP Q6EDY6
C	602	SER	-	EXPRESSION TAG	UNP Q6EDY6
C	603	TRP	-	EXPRESSION TAG	UNP Q6EDY6
C	604	GLY	-	EXPRESSION TAG	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 [i](#)

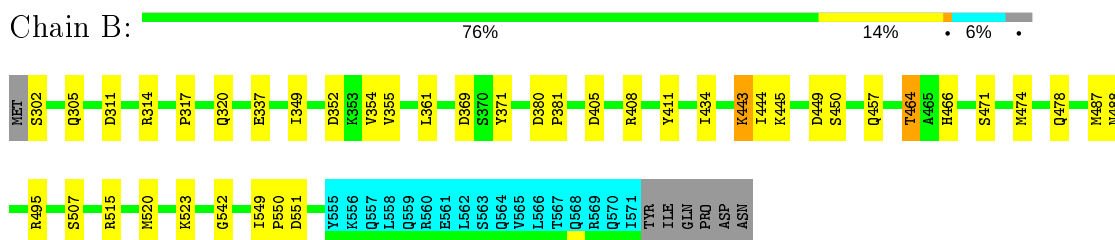
4.1 Average score per residue in the NMR ensemble

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.

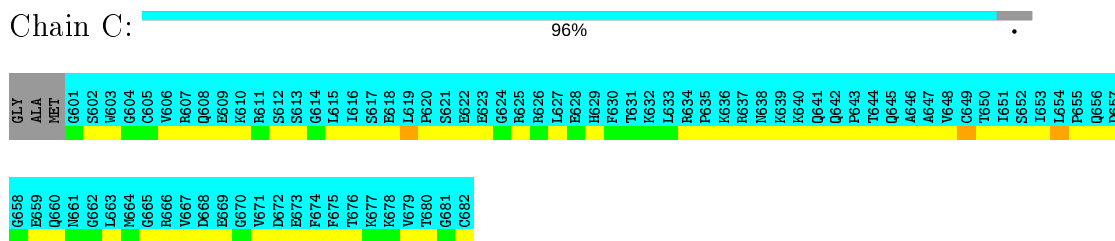
- Molecule 1: F-actin-capping protein subunit alpha-1



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



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

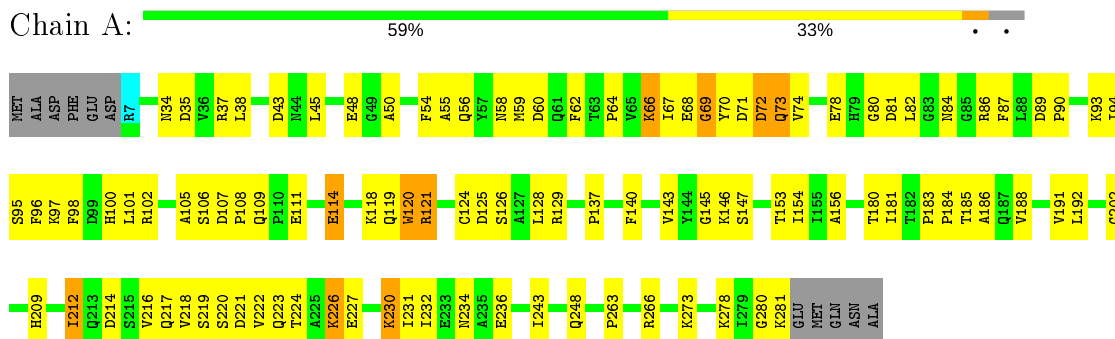


4.2 Scores per residue for each member of the ensemble

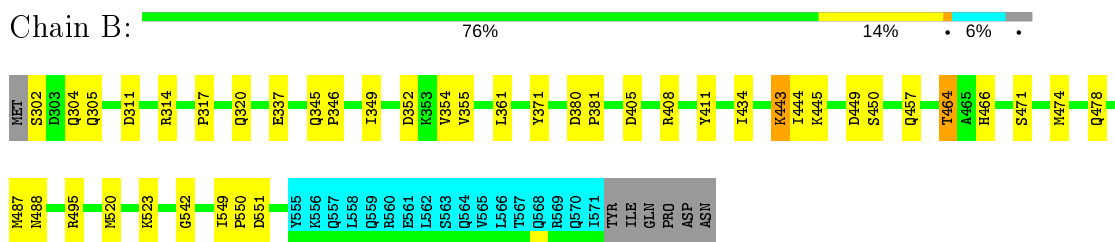
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

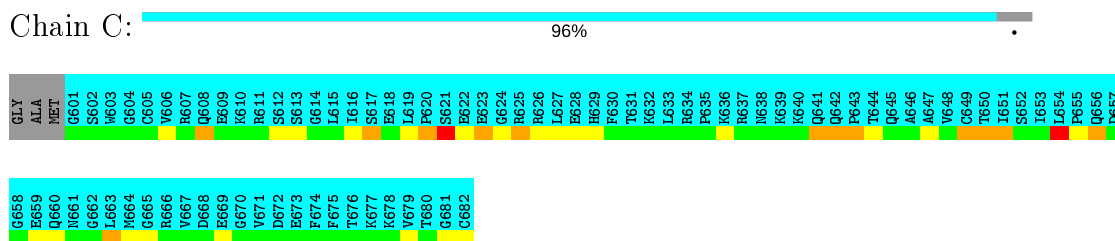
- Molecule 1: F-actin-capping protein subunit alpha-1



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

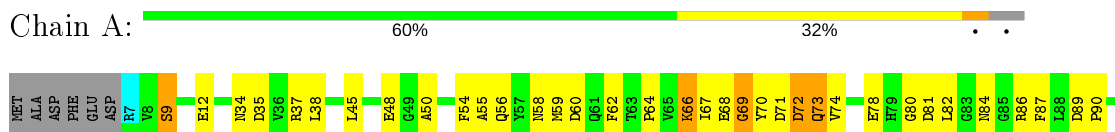


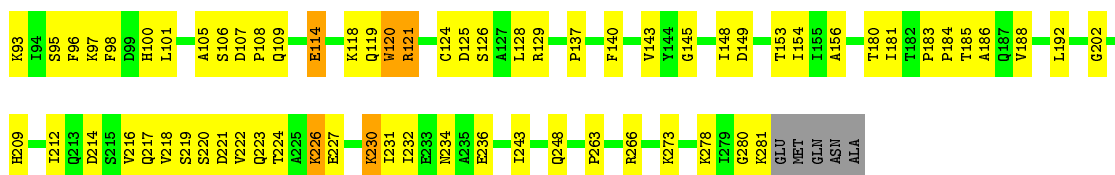
- Molecule 3: Leucine-rich repeat-containing protein 16A



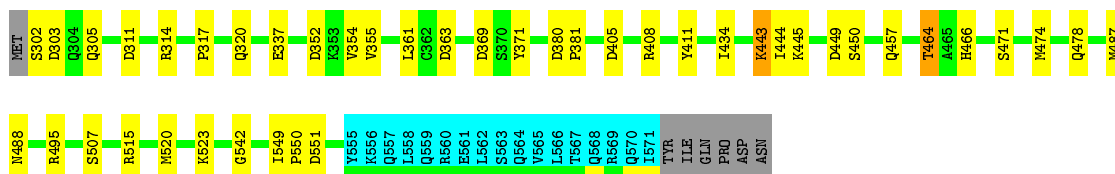
4.2.2 Score per residue for model 2

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

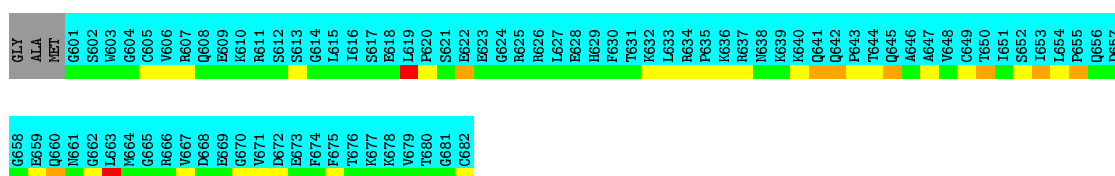




- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

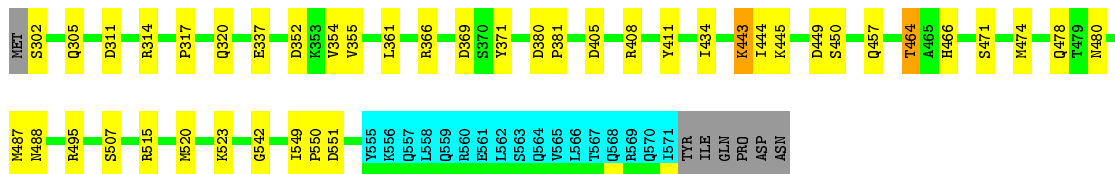
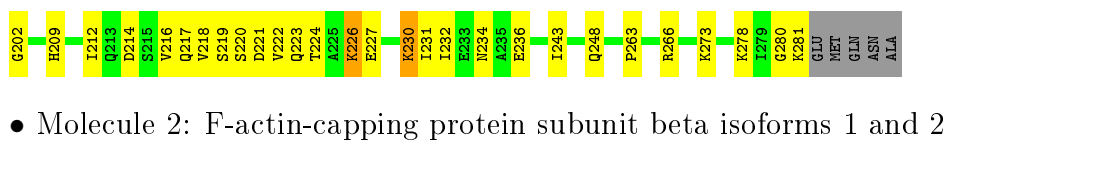
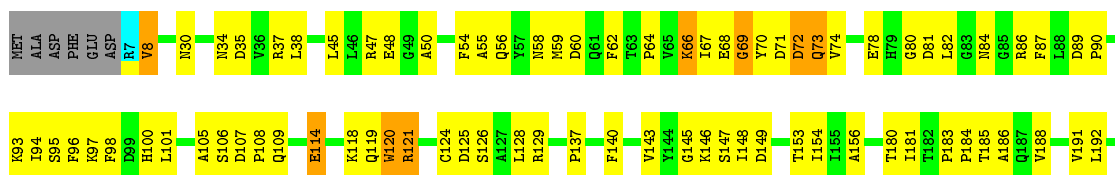


- Molecule 3: Leucine-rich repeat-containing protein 16A



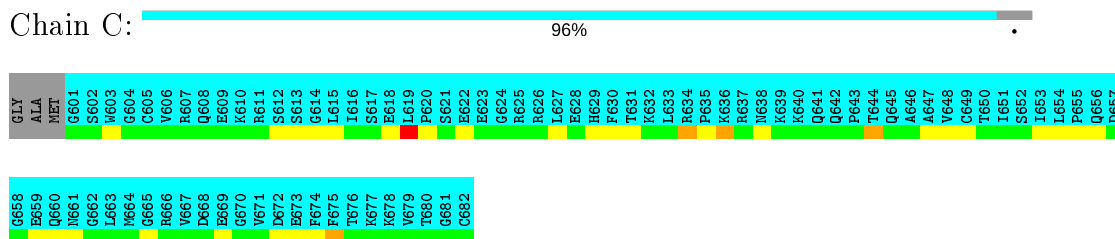
4.2.3 Score per residue for model 3

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



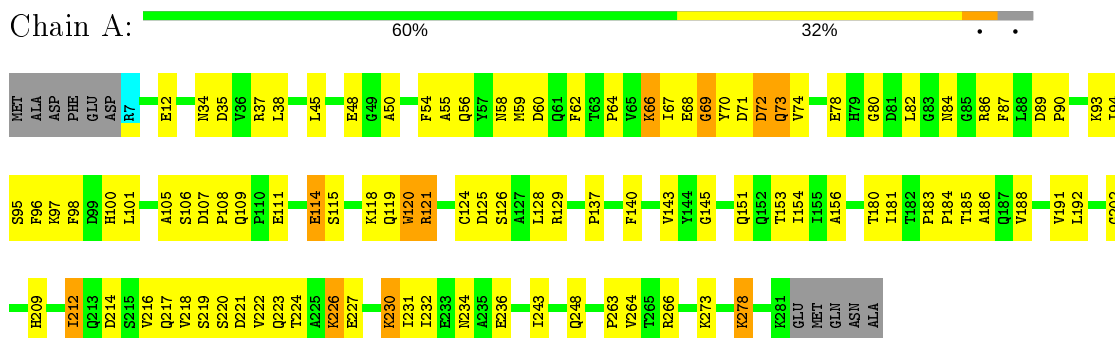
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

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

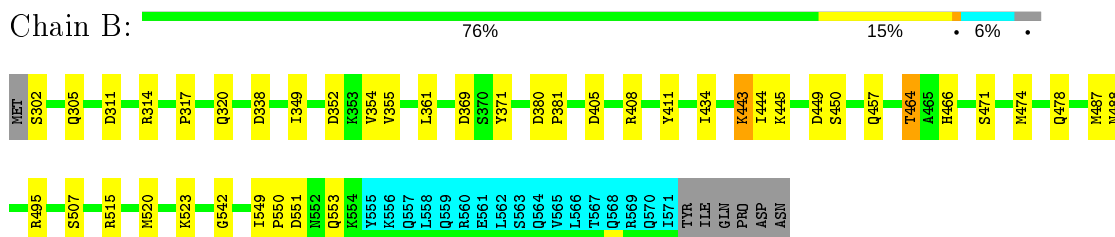


4.2.4 Score per residue for model 4

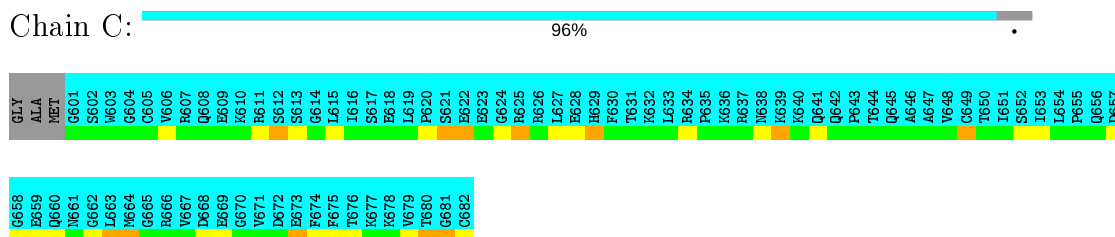
- Molecule 1: F-actin-capping protein subunit alpha-1



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

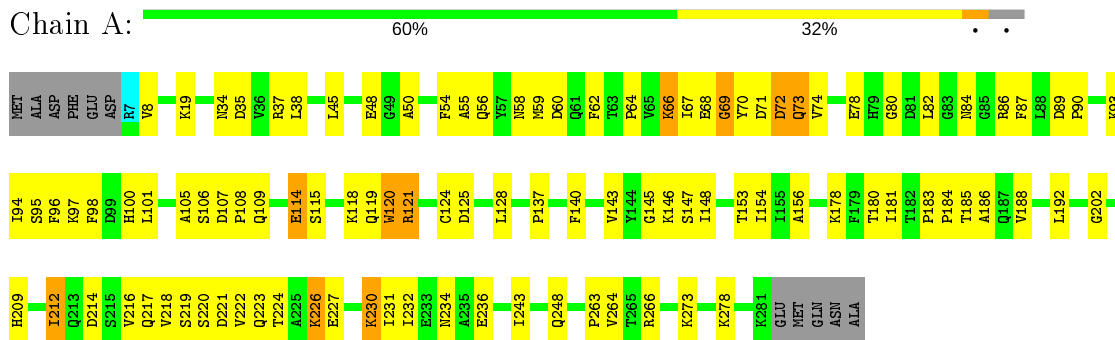


- Molecule 3: Leucine-rich repeat-containing protein 16A

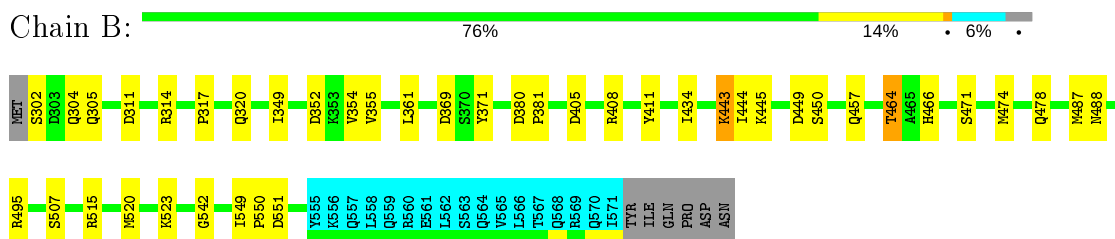


4.2.5 Score per residue for model 5

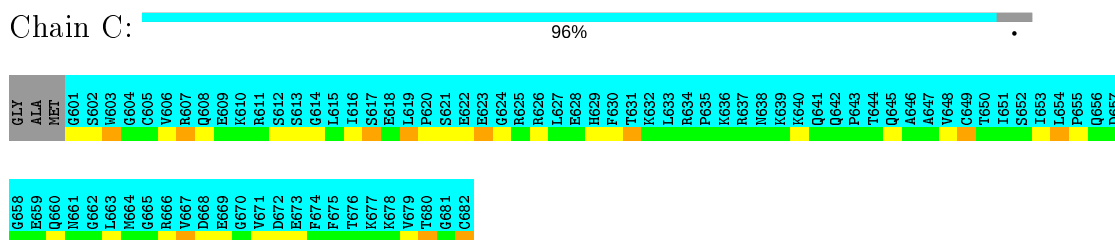
- Molecule 1: F-actin-capping protein subunit alpha-1



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

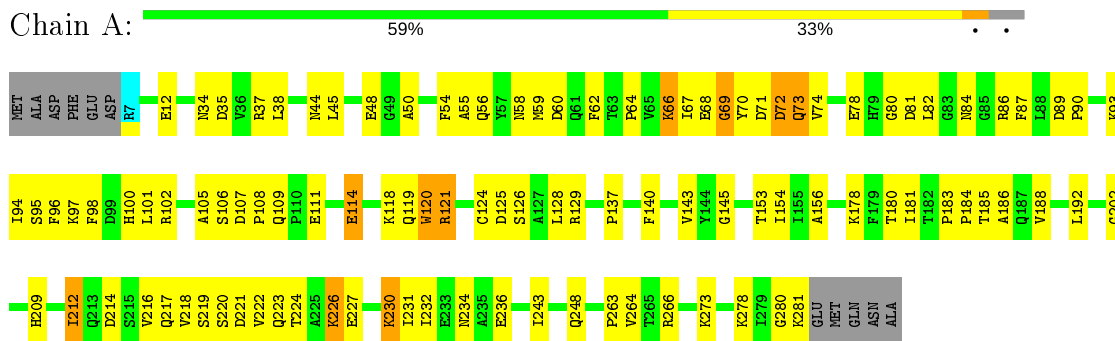


- Molecule 3: Leucine-rich repeat-containing protein 16A



4.2.6 Score per residue for model 6

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

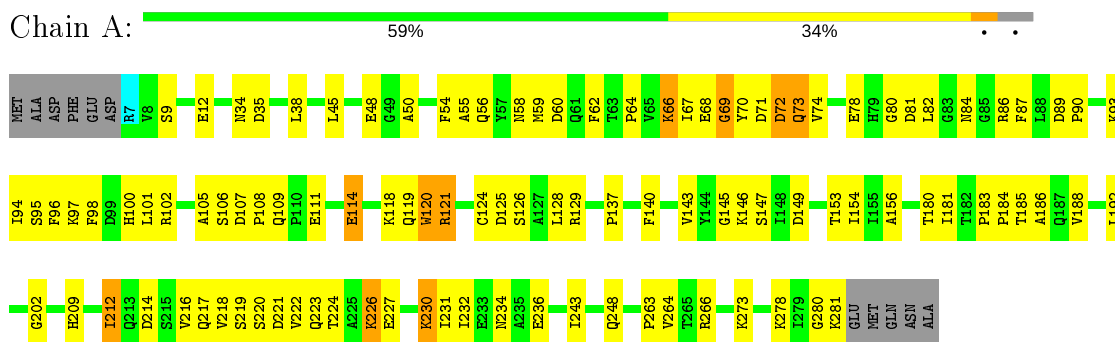


- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

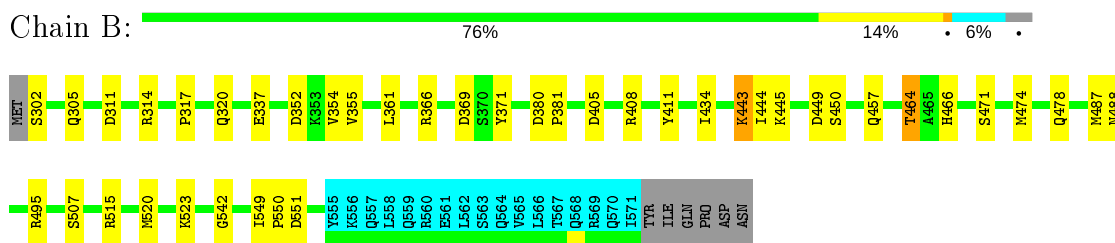


4.2.8 Score per residue for model 8

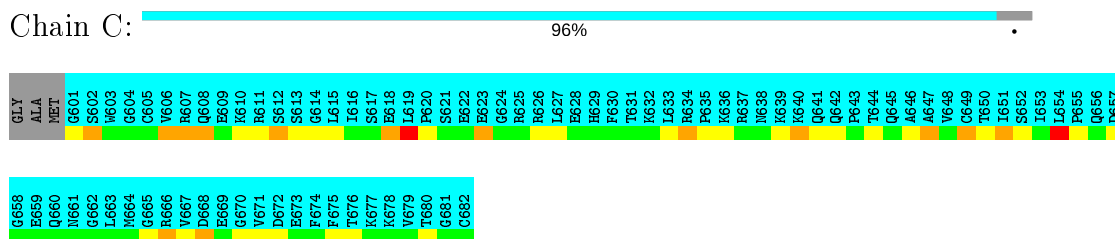
- Molecule 1: F-actin-capping protein subunit alpha-1



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

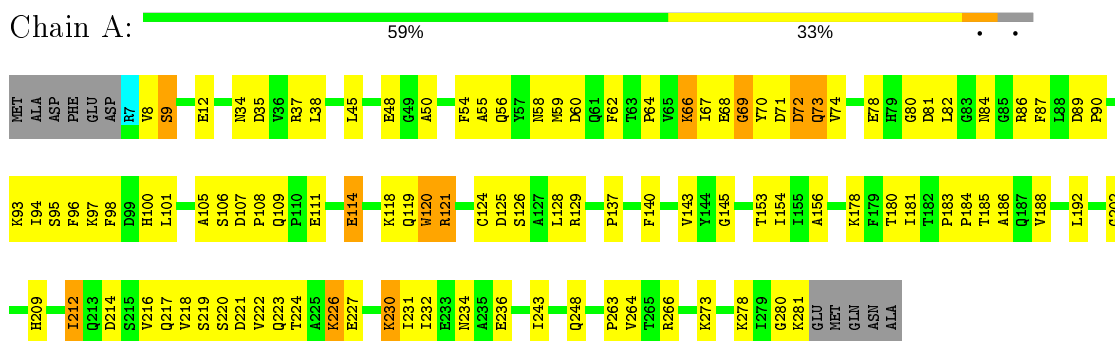


- Molecule 3: Leucine-rich repeat-containing protein 16A

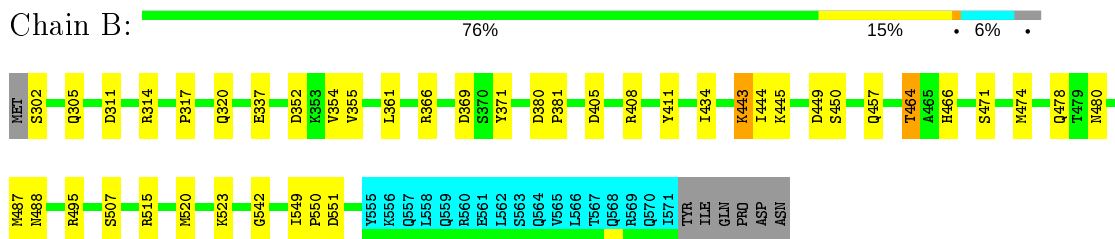


4.2.9 Score per residue for model 9

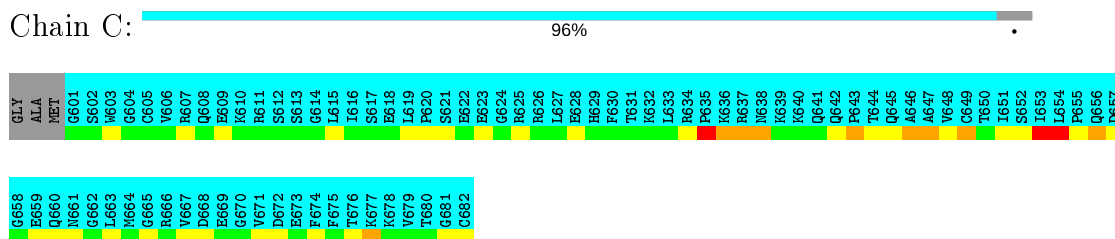
- Molecule 1: F-actin-capping protein subunit alpha-1



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

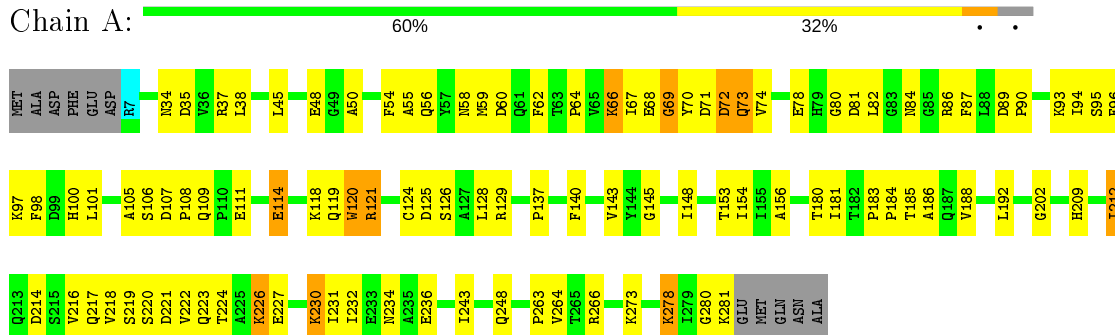


- Molecule 3: Leucine-rich repeat-containing protein 16A

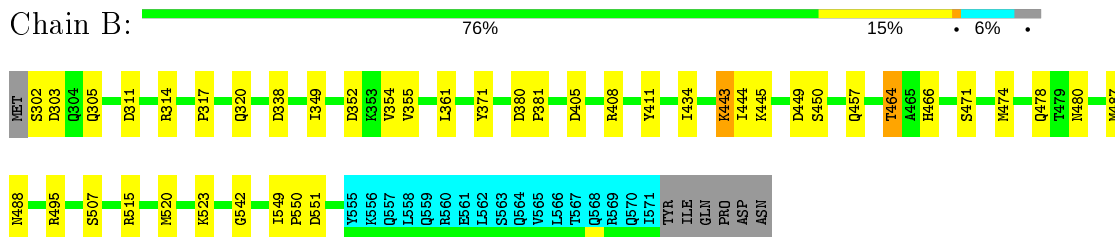


4.2.10 Score per residue for model 10

- 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



5 Refinement protocol and experimental data overview (i)

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	2227	2162	2154	120±3
2	B	1991	1974	1969	31±1
3	C	0	0	0	0±0
All	All	42180	41360	41230	1450

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ILE:HG22	1:A:72:ASP:CG	0.89	1.88	9	10
1:A:202:GLY:O	2:B:314:ARG:HD2	0.82	1.75	5	10
2:B:443:LYS:HD3	2:B:443:LYS:N	0.78	1.94	4	6
1:A:82:LEU:HD12	1:A:86:ARG:HB2	0.78	1.56	4	10
2:B:443:LYS:N	2:B:443:LYS:HD3	0.77	1.94	10	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:443:LYS:HG2	2:B:444:ILE:HG13	0.73	1.61	5	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:243:ILE:HG23	2:B:487:MET:HE1	0.68	1.66	2	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:185:THR:HG23	1:A:216:VAL:C	0.66	2.11	1	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
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:72:ASP:O	1:A:73:GLN:C	0.63	2.37	3	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:266:ARG:HH11	1:A:266:ARG:HG3	0.63	1.54	3	6
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	0.62	1.54	2	4
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
2:B:478:GLN:HG2	2:B:488:ASN:ND2	0.60	2.12	6	10
1:A:95:SER:HB3	1:A:109:GLN:O	0.60	1.96	8	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:114:GLU:H	1:A:114:GLU:CD	0.60	2.00	3	4
1:A:114:GLU:CD	1:A:114:GLU:H	0.60	2.00	5	6
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:59:MET:CE	1:A:78:GLU:HA	0.58	2.29	3	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
2:B:354:VAL:HG23	2:B:355:VAL:HG23	0.57	1.76	1	10
1:A:220:SER:OG	1:A:221:ASP:N	0.57	2.38	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:67:ILE:HD12	1:A:105:ALA:O	0.55	2.02	4	10
1:A:70:TYR:HB2	1:A:72:ASP:HB3	0.55	1.79	7	10
1:A:59:MET:HE3	1:A:78:GLU:HA	0.55	1.77	1	9
1:A:70:TYR:O	1:A:71:ASP:HB3	0.55	2.02	1	10
1:A:120:TRP:CZ3	1:A:221:ASP:CA	0.55	2.90	7	10
2:B:443:LYS:CD	2:B:443:LYS:N	0.55	2.70	5	5
2:B:443:LYS:N	2:B:443:LYS:CD	0.55	2.70	1	5
1:A:153:THR:HG22	1:A:180:THR:HA	0.55	1.79	4	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: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:NH1	1:A:266:ARG:HG3	0.53	2.19	3	8
2:B:352:ASP:OD1	2:B:354:VAL:HG22	0.53	2.04	5	10
1:A:70:TYR:HB3	1:A:72:ASP:HB3	0.52	1.81	3	10
1:A:266:ARG:HG3	1:A:266:ARG:NH1	0.52	2.19	6	2
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	6
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	1	4
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
1:A:70:TYR:C	1:A:72:ASP:N	0.51	2.64	1	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
2:B:380:ASP:HA	2:B:381:PRO:C	0.51	2.26	4	10
1:A:121:ARG:HG3	1:A:145:GLY:N	0.51	2.21	3	10
1:A:89:ASP:O	1:A:93:LYS:HA	0.51	2.06	7	10
2:B:445:LYS:HD2	2:B:445:LYS:N	0.51	2.21	2	6
2:B:445:LYS:N	2:B:445:LYS:HD2	0.51	2.21	1	4
2:B:443:LYS:H	2:B:443:LYS:HD3	0.50	1.66	8	4
2:B:443:LYS:HD3	2:B:443:LYS:H	0.50	1.66	7	6
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:495:ARG:NH2	2:B:523:LYS:HD3	0.49	2.22	1	10
1:A:248:GLN:HA	1:A:248:GLN:NE2	0.49	2.23	9	7
2:B:405:ASP:OD1	2:B:408:ARG:NH1	0.49	2.45	9	10
1:A:67:ILE:HD13	1:A:96:PHE:CB	0.49	2.36	3	10
1:A:248:GLN:NE2	1:A:248:GLN:HA	0.49	2.23	10	3
1:A:101:LEU:HD23	1:A:101:LEU:C	0.49	2.28	1	4
1:A:55:ALA:HA	1:A:100:HIS:CD2	0.49	2.43	10	10
1:A:223:GLN:O	1:A:226:LYS:HG3	0.49	2.08	2	10
1:A:58:ASN:ND2	1:A:100:HIS:HD2	0.49	2.06	7	10
1:A:101:LEU:C	1:A:101:LEU:HD23	0.49	2.28	7	6
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:120:TRP:CD1	1:A:181:ILE:CD1	0.48	2.96	7	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:192:LEU:O	1:A:209:HIS:HA	0.48	2.09	1	10
1:A:86:ARG:NH1	1:A:97:LYS:HB2	0.48	2.24	5	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
2:B:380:ASP:OD1	2:B:381:PRO:HA	0.47	2.10	7	10
1:A:66:LYS:HE3	1:A:72:ASP:OD2	0.47	2.10	2	10
1:A:192:LEU:N	1:A:192:LEU:HD12	0.47	2.25	5	7
1:A:192:LEU:HD12	1:A:192:LEU:N	0.47	2.25	2	3
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:221:ASP:OD2	1:A:222:VAL:HG23	0.46	2.11	4	10
1:A:273:LYS:HB2	1:A:273:LYS:NZ	0.46	2.26	1	9
1:A:280:GLY:C	1:A:281:LYS:O	0.46	2.55	1	3
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	6
1:A:125:ASP:HA	1:A:143:VAL:CG2	0.45	2.42	2	10
1:A:107:ASP:O	1:A:107:ASP:OD1	0.45	2.35	8	4
1:A:273:LYS:NZ	1:A:273:LYS:HB2	0.45	2.26	3	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:54:PHE:HB3	1:A:100:HIS:HB3	0.44	1.90	4	10
1:A:86:ARG:CZ	1:A:97:LYS:HB2	0.44	2.43	9	10
1:A:59:MET:HE2	1:A:78:GLU:HA	0.44	1.87	9	4
1:A:243:ILE:HD12	2:B:487:MET:HE3	0.44	1.89	7	2
1:A:114:GLU:CD	1:A:114:GLU:N	0.43	2.72	6	6
1:A:114:GLU:N	1:A:114:GLU:CD	0.43	2.72	9	2
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
2:B:317:PRO:HB2	2:B:320:GLN:NE2	0.43	2.29	3	10
1:A:219:SER:OG	1:A:220:SER:N	0.43	2.52	4	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: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
1:A:128:LEU:CD2	1:A:156:ALA:HB1	0.42	2.45	9	10
1:A:59:MET:HE2	1:A:78:GLU:CA	0.42	2.44	9	4
1:A:121:ARG:HH21	1:A:125:ASP:CB	0.42	2.27	7	10
1:A:119:GLN:OE1	1:A:221:ASP:CB	0.42	2.68	4	10
1:A:82:LEU:HB2	1:A:86:ARG:O	0.42	2.15	8	10
2:B:361:LEU:HD22	2:B:371:TYR:CG	0.42	2.50	1	10
1:A:243:ILE:HG23	2:B:487:MET:HE3	0.42	1.92	7	2
1:A:183:PRO:HA	1:A:184:PRO:C	0.41	2.36	2	7
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	6
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
1:A:192:LEU:CD1	1:A:192:LEU:N	0.41	2.84	10	4
2:B:553:GLN:CD	2:B:553:GLN:N	0.41	2.74	4	1
1:A:101:LEU:CD2	1:A:101:LEU:C	0.41	2.89	5	7
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:101:LEU:C	1:A:101:LEU:CD2	0.41	2.89	4	3
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	2
2:B:443:LYS:H	2:B:443:LYS:CD	0.41	2.28	8	4
1:A:278:LYS:CD	1:A:278:LYS:H	0.41	2.28	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:B:443:LYS:CD	2:B:443:LYS:H	0.41	2.28	5	4
1:A:146:LYS:HG2	1:A:147:SER:N	0.40	2.32	3	4
1:A:114:GLU:OE2	1:A:115:SER:N	0.40	2.54	4	2
1:A:191:VAL:O	1:A:191:VAL:HG13	0.40	2.16	4	1
2:B:345:GLN:O	2:B:346:PRO:C	0.40	2.60	1	1
1:A:148:ILE:O	1:A:149:ASP:OD1	0.40	2.40	3	2

5.2 Torsion angles [i](#)

5.2.1 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	273/286 (95%)	248±1 (91±0%)	22±1 (8±0%)	3±0 (1±0%)	17	64
2	B	252/277 (91%)	244±0 (97±0%)	7±0 (3±0%)	1±0 (0±0%)	38	78
3	C	0	-	-	-	-	-
All	All	5250/6480 (81%)	4918 (94%)	289 (6%)	43 (1%)	24	71

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)
2	B	550	PRO	10
1	A	73	GLN	10
1	A	69	GLY	10
1	A	68	GLU	10
1	A	8	VAL	2
1	A	9	SER	1

5.2.2 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	242/252 (96%)	232±0 (96±0%)	10±0 (4±0%)	33	82
2	B	224/248 (90%)	222±0 (99±0%)	2±0 (1±0%)	79	97
3	C	0	-	-	-	-
All	All	4660/5720 (81%)	4539 (97%)	121 (3%)	49	91

All 13 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	120	TRP	10
1	A	84	ASN	10
1	A	121	ARG	10
2	B	464	THR	10
1	A	278	LYS	10
2	B	443	LYS	10
1	A	230	LYS	10
1	A	212	ILE	10
1	A	66	LYS	10
1	A	114	GLU	10
1	A	226	LYS	10
1	A	234	ASN	10
1	A	9	SER	1

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided