



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:36 PM BST

PDB ID : 1PD6
Title : The NMR structure of domain C2 of human cardiac Myosin Binding Protein C
Authors : Ababou, A.; Gautel, M.; Pfuhl, M.
Deposited on : 2003-05-19

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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

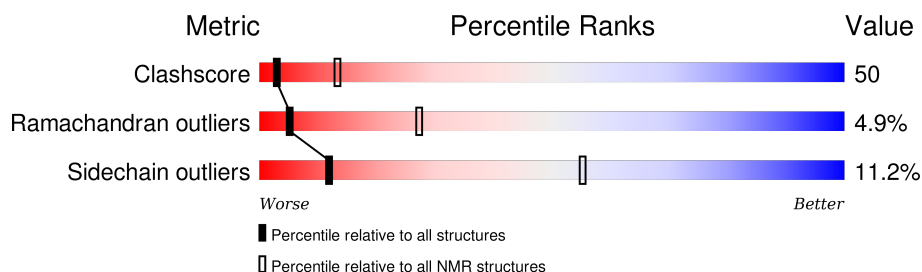
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	104	

2 Ensemble composition and analysis

This entry contains 28 models. Model 5 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:214-A:301 (88)	0.23	5

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

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

The models can be grouped into 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 5, 6, 7, 8, 13, 15, 16, 19, 22
2	3, 9, 11, 12, 18, 21, 27, 28
3	2, 4, 14
4	10, 17, 23
5	24, 26
Single-model clusters	20; 25

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1475 atoms, of which 740 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Myosin-binding protein C, cardiac-type, Domain C2.

Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1475	461	740	124	146	4	

There are 10 discrepancies between the modelled and reference sequences:

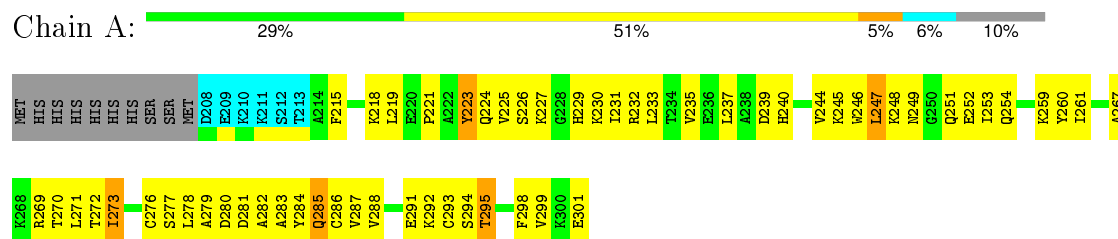
Chain	Residue	Modelled	Actual	Comment	Reference
A	198	MET	-	EXPRESSION TAG	UNP Q14896
A	199	HIS	-	EXPRESSION TAG	UNP Q14896
A	200	HIS	-	EXPRESSION TAG	UNP Q14896
A	201	HIS	-	EXPRESSION TAG	UNP Q14896
A	202	HIS	-	EXPRESSION TAG	UNP Q14896
A	203	HIS	-	EXPRESSION TAG	UNP Q14896
A	204	HIS	-	EXPRESSION TAG	UNP Q14896
A	205	SER	-	EXPRESSION TAG	UNP Q14896
A	206	SER	-	EXPRESSION TAG	UNP Q14896
A	207	MET	-	EXPRESSION TAG	UNP Q14896

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: Myosin-binding protein C, cardiac-type, Domain C2

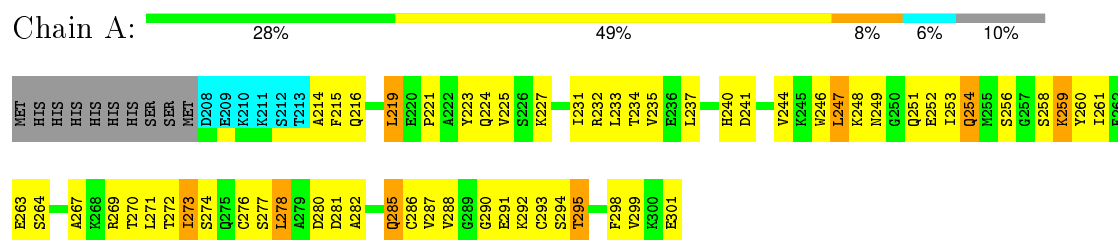


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

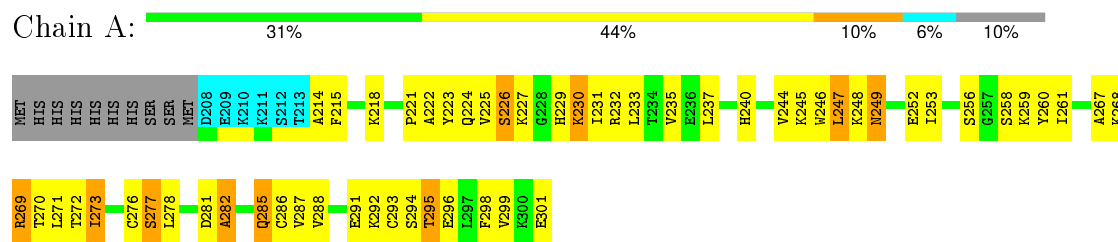
- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



4.2.2 Score per residue for model 2

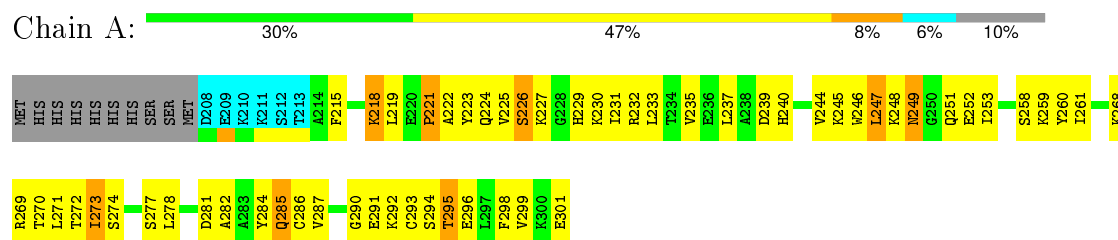
- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2





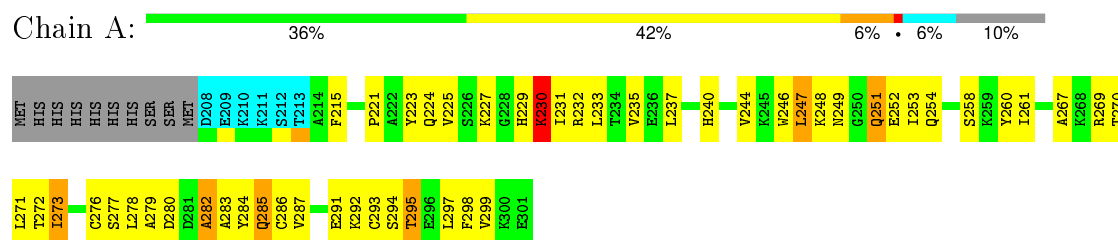
4.2.7 Score per residue for model 7

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



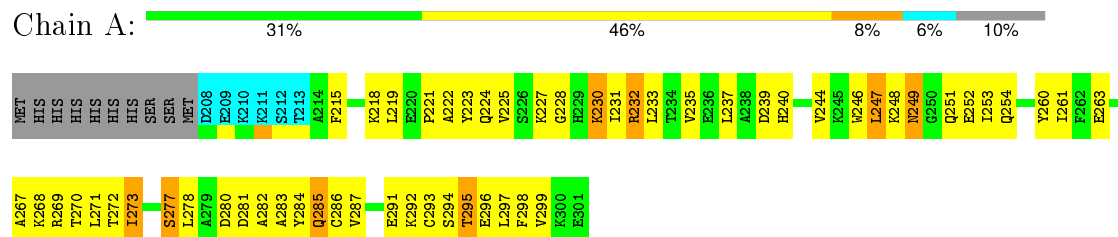
4.2.8 Score per residue for model 8

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



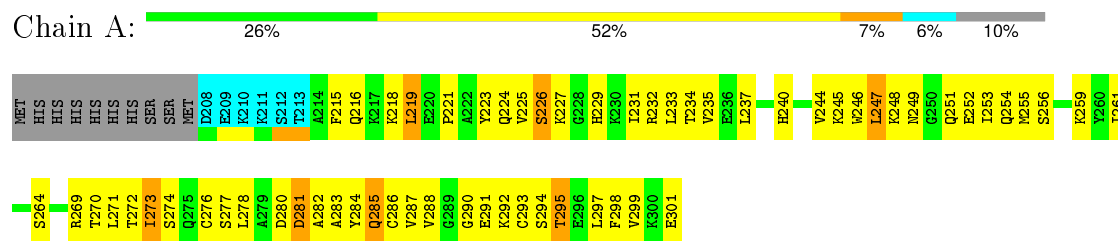
4.2.9 Score per residue for model 9

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



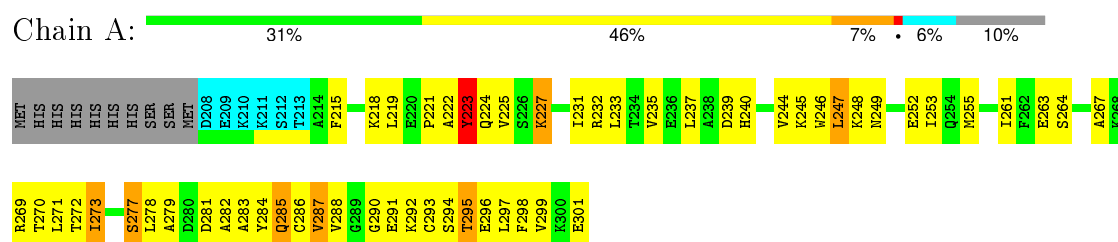
4.2.10 Score per residue for model 10

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



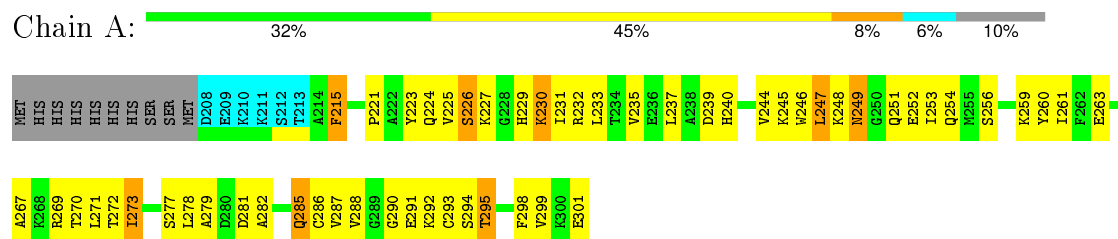
4.2.11 Score per residue for model 11

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



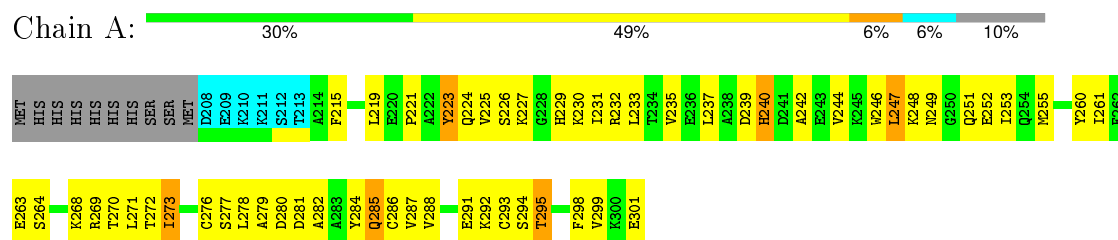
4.2.12 Score per residue for model 12

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



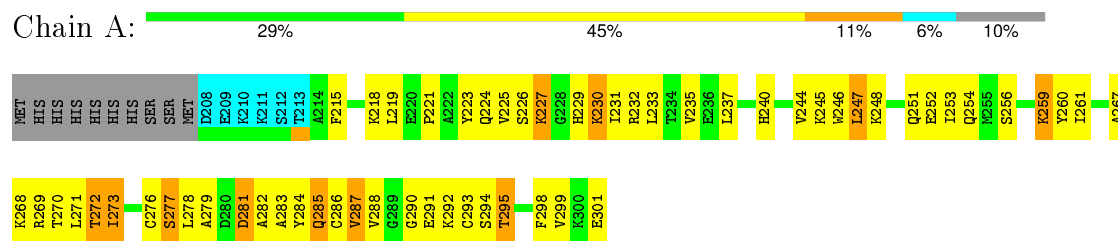
4.2.13 Score per residue for model 13

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



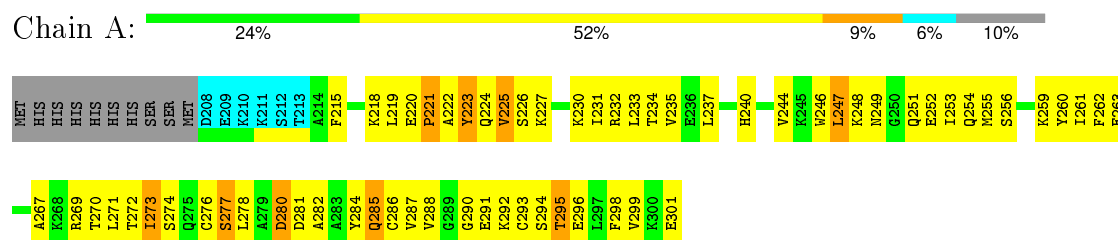
4.2.14 Score per residue for model 14

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



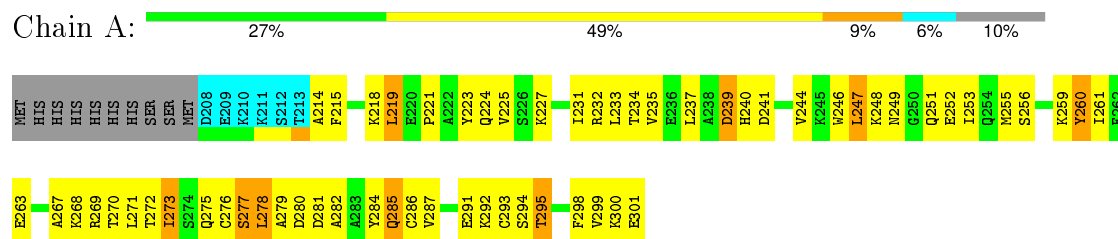
4.2.15 Score per residue for model 15

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



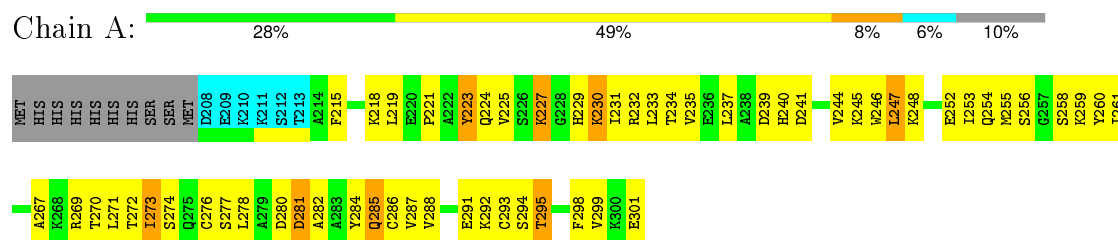
4.2.16 Score per residue for model 16

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



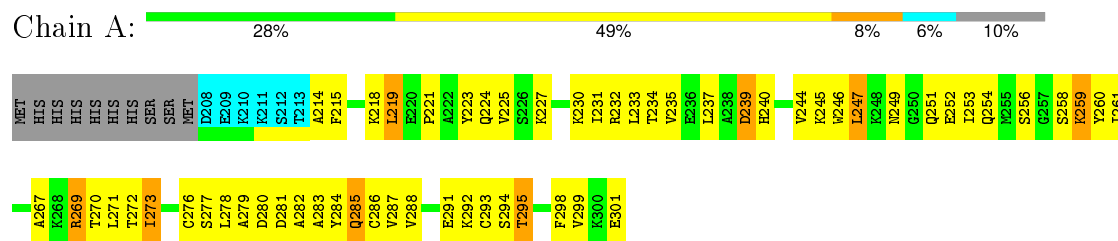
4.2.17 Score per residue for model 17

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



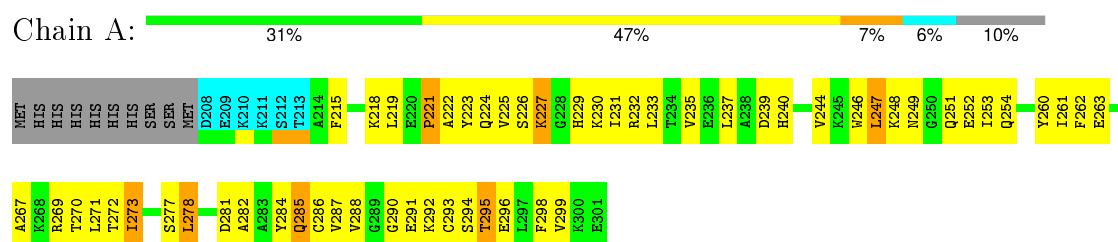
4.2.18 Score per residue for model 18

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



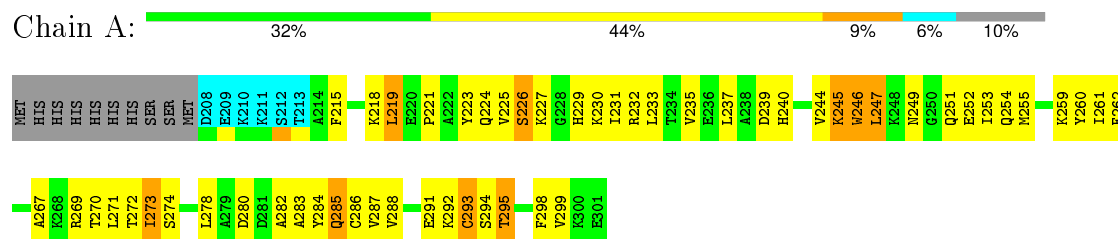
4.2.19 Score per residue for model 19

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



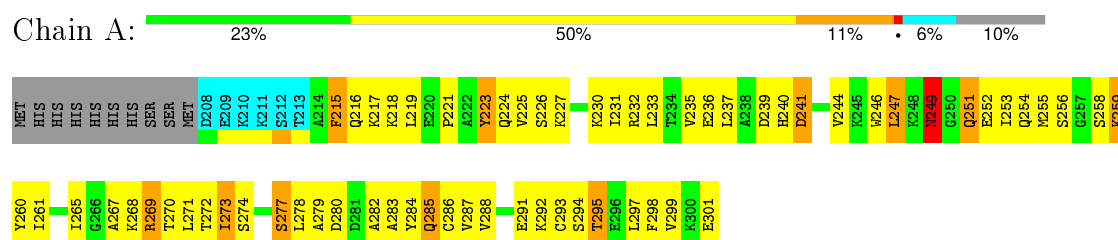
4.2.20 Score per residue for model 20

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



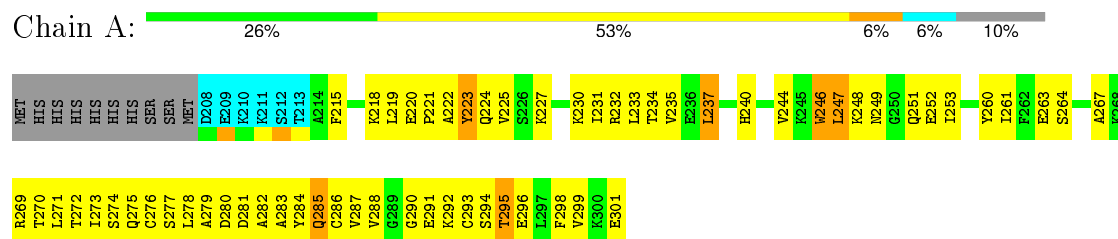
4.2.21 Score per residue for model 21

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



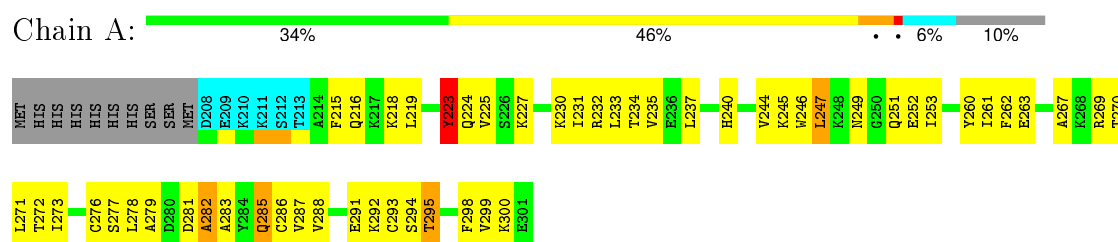
4.2.22 Score per residue for model 22

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



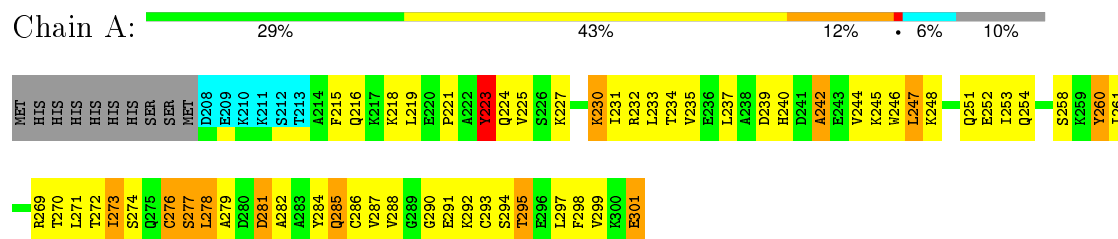
4.2.23 Score per residue for model 23

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



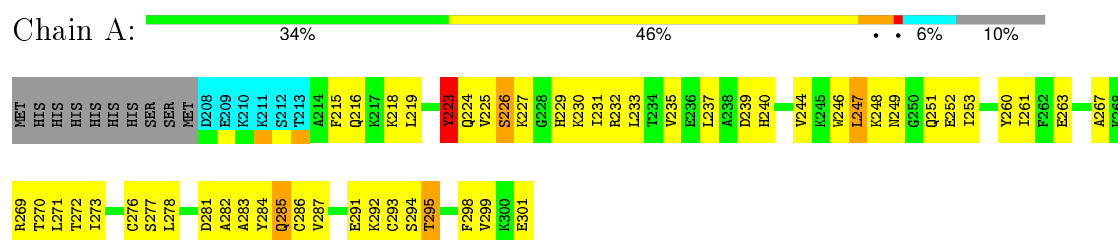
4.2.24 Score per residue for model 24

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



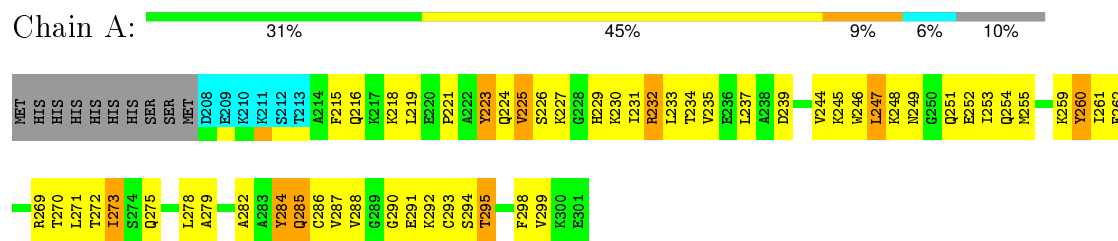
4.2.25 Score per residue for model 25

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



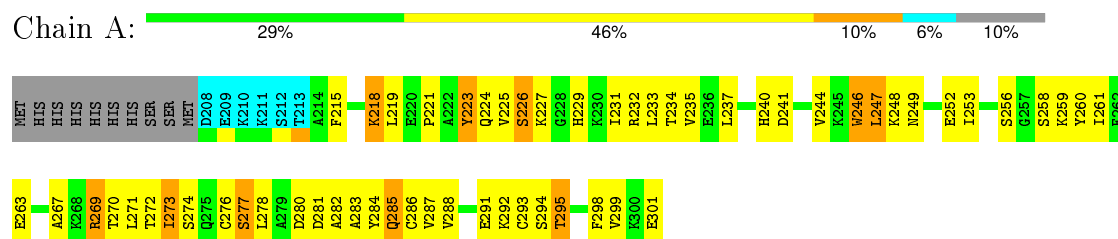
4.2.26 Score per residue for model 26

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



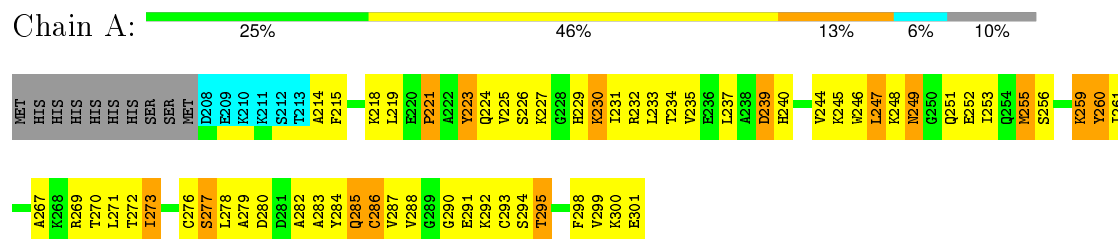
4.2.27 Score per residue for model 27

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



4.2.28 Score per residue for model 28

- Molecule 1: Myosin-binding protein C, cardiac-type, Domain C2



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *we have used ARIA protocols.*

Of the 200 calculated structures, 28 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
ARIA	structure solution	1.1
ARIA	refinement	1.1

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

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	0.53±0.07	1±1/697 (0.2±0.2%)	0.54±0.02	0±0/933 (0.0±0.0%)
All	All	0.53	30/19516 (0.2%)	0.54	0/26124 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.8
All	All	0	23

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	223	TYR	CE1-CZ	8.29	1.49	1.38	11	12
1	A	223	TYR	CE2-CZ	-8.20	1.27	1.38	28	14
1	A	284	TYR	CE1-CZ	-6.31	1.30	1.38	26	1
1	A	260	TYR	CE2-CZ	-6.13	1.30	1.38	16	1
1	A	260	TYR	CE1-CZ	5.92	1.46	1.38	16	1
1	A	284	TYR	CE2-CZ	5.61	1.45	1.38	26	1

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	226	SER	Mainchain	11
1	A	223	TYR	Sidechain	5

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	246	TRP	Mainchain	3
1	A	225	VAL	Mainchain	1
1	A	245	LYS	Mainchain	1
1	A	260	TYR	Sidechain	1
1	A	276	CYS	Mainchain	1

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	687	692	690	69±6
All	All	19236	19376	19320	1931

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 50.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:247:LEU:HB3	1:A:285:GLN:HE21	1.04	1.12	26	28
1:A:218:LYS:HE3	1:A:295:THR:HB	1.01	1.32	3	5
1:A:285:GLN:HG3	1:A:294:SER:HA	0.94	1.38	25	27
1:A:227:LYS:HD2	1:A:301:GLU:HA	0.90	1.44	15	5
1:A:247:LEU:HD22	1:A:252:GLU:HA	0.88	1.45	18	28
1:A:246:TRP:HB2	1:A:260:TYR:HE2	0.87	1.28	25	1
1:A:233:LEU:HB2	1:A:271:LEU:HB3	0.87	1.47	5	28
1:A:246:TRP:HB2	1:A:260:TYR:CE2	0.86	2.06	25	1
1:A:247:LEU:HB3	1:A:285:GLN:NE2	0.85	1.86	22	28
1:A:247:LEU:HD23	1:A:287:VAL:HG11	0.84	1.48	3	28
1:A:244:VAL:HG23	1:A:246:TRP:HE1	0.80	1.35	6	28
1:A:219:LEU:HB3	1:A:223:TYR:CE1	0.77	2.14	11	9
1:A:278:LEU:HD23	1:A:301:GLU:HB3	0.77	1.56	24	2
1:A:287:VAL:HA	1:A:291:GLU:O	0.76	1.78	1	28
1:A:261:ILE:HB	1:A:272:THR:HB	0.76	1.57	13	28
1:A:273:ILE:HG23	1:A:276:CYS:HB3	0.76	1.55	23	1
1:A:246:TRP:CD1	1:A:271:LEU:HG	0.76	2.16	23	5
1:A:248:LYS:HB3	1:A:251:GLN:HB2	0.75	1.58	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:218:LYS:HD2	1:A:286:CYS:SG	0.75	2.21	23	7
1:A:225:VAL:HG22	1:A:231:ILE:HG21	0.74	1.59	25	25
1:A:227:LYS:HE3	1:A:301:GLU:HB2	0.74	1.57	24	2
1:A:227:LYS:HD3	1:A:278:LEU:HD23	0.74	1.60	23	7
1:A:237:LEU:HD12	1:A:269:ARG:HB2	0.74	1.60	22	4
1:A:227:LYS:HD3	1:A:278:LEU:HG	0.74	1.59	28	1
1:A:218:LYS:HE3	1:A:295:THR:CB	0.73	2.13	23	5
1:A:223:TYR:HB3	1:A:231:ILE:HD11	0.73	1.60	21	27
1:A:244:VAL:HG23	1:A:246:TRP:NE1	0.73	1.99	28	6
1:A:215:PHE:HE1	1:A:288:VAL:HG23	0.72	1.44	22	2
1:A:225:VAL:HB	1:A:299:VAL:HG23	0.72	1.62	12	21
1:A:227:LYS:HG2	1:A:301:GLU:HA	0.72	1.60	22	10
1:A:225:VAL:HB	1:A:231:ILE:HB	0.71	1.62	26	3
1:A:249:ASN:HB3	1:A:283:ALA:HB3	0.71	1.60	18	14
1:A:286:CYS:O	1:A:292:LYS:HA	0.70	1.85	2	28
1:A:247:LEU:HB2	1:A:285:GLN:HB2	0.70	1.63	16	25
1:A:286:CYS:HB2	1:A:293:CYS:SG	0.70	2.26	20	3
1:A:219:LEU:HB2	1:A:223:TYR:OH	0.70	1.86	13	7
1:A:227:LYS:HD3	1:A:278:LEU:HB2	0.70	1.62	24	1
1:A:286:CYS:SG	1:A:293:CYS:SG	0.70	2.89	14	1
1:A:227:LYS:HB2	1:A:277:SER:HB2	0.70	1.64	21	16
1:A:282:ALA:O	1:A:297:LEU:HB3	0.70	1.87	10	1
1:A:286:CYS:SG	1:A:293:CYS:HB2	0.70	2.26	9	11
1:A:248:LYS:HB3	1:A:251:GLN:HB3	0.70	1.63	16	6
1:A:241:ASP:HA	1:A:269:ARG:NH2	0.69	2.01	17	4
1:A:233:LEU:O	1:A:270:THR:HA	0.69	1.88	17	28
1:A:218:LYS:HE2	1:A:295:THR:HB	0.69	1.64	20	1
1:A:286:CYS:SG	1:A:293:CYS:HB3	0.69	2.27	5	10
1:A:225:VAL:CB	1:A:231:ILE:HB	0.69	2.18	26	3
1:A:237:LEU:HD22	1:A:269:ARG:HB2	0.69	1.65	26	1
1:A:245:LYS:HB3	1:A:287:VAL:HG22	0.68	1.65	11	4
1:A:247:LEU:CB	1:A:285:GLN:HB2	0.68	2.18	27	28
1:A:224:GLN:HA	1:A:298:PHE:O	0.68	1.88	7	28
1:A:247:LEU:CB	1:A:285:GLN:HE21	0.68	2.01	16	11
1:A:232:ARG:HB3	1:A:270:THR:CG2	0.67	2.18	18	28
1:A:244:VAL:HG22	1:A:269:ARG:HG2	0.66	1.64	28	3
1:A:225:VAL:HA	1:A:231:ILE:HB	0.66	1.65	5	23
1:A:265:ILE:HG23	1:A:268:LYS:HB2	0.66	1.67	21	1
1:A:246:TRP:CE2	1:A:271:LEU:HB2	0.66	2.26	15	27
1:A:221:PRO:HA	1:A:295:THR:OG1	0.66	1.90	2	26
1:A:227:LYS:CE	1:A:301:GLU:HB2	0.66	2.21	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:215:PHE:CD2	1:A:235:VAL:HG21	0.66	2.26	26	27
1:A:244:VAL:CG2	1:A:246:TRP:HE1	0.65	2.04	20	26
1:A:223:TYR:CD2	1:A:233:LEU:HG	0.65	2.25	27	27
1:A:259:LYS:HE2	1:A:275:GLN:HB2	0.65	1.66	16	2
1:A:225:VAL:HB	1:A:231:ILE:CB	0.65	2.21	26	3
1:A:253:ILE:HG21	1:A:260:TYR:CZ	0.65	2.27	25	1
1:A:230:LYS:HD2	1:A:274:SER:HA	0.64	1.69	4	1
1:A:278:LEU:HD11	1:A:301:GLU:HG2	0.64	1.68	5	2
1:A:229:HIS:O	1:A:230:LYS:HG2	0.63	1.93	6	4
1:A:284:TYR:O	1:A:295:THR:HG22	0.63	1.93	7	19
1:A:227:LYS:HE2	1:A:278:LEU:HD23	0.63	1.71	9	3
1:A:215:PHE:HD2	1:A:235:VAL:HG21	0.63	1.54	16	18
1:A:218:LYS:HD2	1:A:219:LEU:O	0.63	1.93	9	7
1:A:237:LEU:HB3	1:A:240:HIS:H	0.63	1.54	17	26
1:A:285:GLN:HG3	1:A:294:SER:CA	0.62	2.21	25	18
1:A:237:LEU:HB2	1:A:267:ALA:O	0.62	1.95	25	23
1:A:227:LYS:HB3	1:A:301:GLU:HA	0.62	1.72	16	1
1:A:278:LEU:HD22	1:A:299:VAL:HG13	0.61	1.73	19	4
1:A:218:LYS:HD2	1:A:295:THR:HB	0.61	1.72	16	2
1:A:218:LYS:CE	1:A:295:THR:HB	0.61	2.19	3	6
1:A:273:ILE:HG13	1:A:284:TYR:HE2	0.61	1.56	2	7
1:A:246:TRP:O	1:A:253:ILE:HB	0.61	1.96	16	22
1:A:278:LEU:HA	1:A:299:VAL:HG11	0.60	1.73	11	28
1:A:231:ILE:HG22	1:A:273:ILE:HG22	0.60	1.71	24	22
1:A:227:LYS:HD2	1:A:301:GLU:CA	0.60	2.26	21	5
1:A:260:TYR:HA	1:A:271:LEU:HD11	0.60	1.73	18	20
1:A:245:LYS:HB2	1:A:287:VAL:HG22	0.60	1.73	12	9
1:A:230:LYS:HA	1:A:276:CYS:SG	0.60	2.37	25	1
1:A:219:LEU:HB3	1:A:223:TYR:CZ	0.59	2.32	22	7
1:A:253:ILE:HG21	1:A:260:TYR:CE2	0.59	2.31	25	1
1:A:215:PHE:CE1	1:A:288:VAL:HG23	0.59	2.32	21	18
1:A:232:ARG:HG2	1:A:272:THR:HG23	0.59	1.73	19	8
1:A:255:MET:SD	1:A:262:PHE:HB3	0.59	2.37	26	2
1:A:244:VAL:CG2	1:A:269:ARG:HG2	0.59	2.28	28	15
1:A:227:LYS:HE3	1:A:301:GLU:HG2	0.59	1.74	22	1
1:A:281:ASP:HB2	1:A:299:VAL:HG12	0.58	1.76	23	17
1:A:247:LEU:HD13	1:A:251:GLN:O	0.58	1.98	21	8
1:A:278:LEU:HD21	1:A:301:GLU:HG2	0.58	1.75	18	2
1:A:278:LEU:HD13	1:A:299:VAL:HG13	0.58	1.75	3	1
1:A:219:LEU:HB2	1:A:234:THR:O	0.57	1.99	17	10
1:A:227:LYS:HE3	1:A:278:LEU:HD23	0.57	1.76	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:276:CYS:SG	1:A:280:ASP:HB3	0.57	2.38	27	3
1:A:244:VAL:HG11	1:A:269:ARG:HG2	0.57	1.75	8	7
1:A:278:LEU:HD21	1:A:301:GLU:CG	0.57	2.29	10	1
1:A:249:ASN:HA	1:A:285:GLN:OE1	0.57	2.00	27	8
1:A:225:VAL:N	1:A:231:ILE:HD12	0.57	2.15	26	24
1:A:223:TYR:CE2	1:A:233:LEU:HG	0.56	2.36	7	16
1:A:225:VAL:HG13	1:A:299:VAL:HA	0.56	1.77	18	2
1:A:244:VAL:HG21	1:A:269:ARG:HG2	0.56	1.76	25	12
1:A:281:ASP:CB	1:A:299:VAL:HG12	0.56	2.30	24	1
1:A:225:VAL:HG13	1:A:231:ILE:HB	0.56	1.77	9	25
1:A:246:TRP:C	1:A:253:ILE:HB	0.56	2.20	28	26
1:A:225:VAL:HG22	1:A:231:ILE:CG2	0.56	2.31	25	20
1:A:233:LEU:HB3	1:A:246:TRP:CZ3	0.55	2.36	22	21
1:A:248:LYS:HG2	1:A:284:TYR:CE1	0.55	2.35	4	1
1:A:247:LEU:HB3	1:A:285:GLN:HB2	0.55	1.77	27	14
1:A:281:ASP:OD1	1:A:298:PHE:HA	0.55	2.01	18	8
1:A:273:ILE:HG23	1:A:276:CYS:HB2	0.55	1.78	24	1
1:A:285:GLN:HA	1:A:293:CYS:O	0.55	2.02	27	19
1:A:225:VAL:HB	1:A:231:ILE:CG2	0.55	2.32	26	3
1:A:247:LEU:CD2	1:A:287:VAL:HG11	0.55	2.30	6	8
1:A:256:SER:HB2	1:A:259:LYS:O	0.55	2.01	16	7
1:A:277:SER:O	1:A:299:VAL:HG11	0.54	2.03	25	7
1:A:235:VAL:O	1:A:268:LYS:HA	0.54	2.02	3	8
1:A:263:GLU:O	1:A:269:ARG:HD3	0.54	2.02	16	8
1:A:237:LEU:HD11	1:A:244:VAL:CG1	0.54	2.32	22	6
1:A:259:LYS:HD3	1:A:259:LYS:H	0.54	1.61	14	1
1:A:248:LYS:HD3	1:A:284:TYR:CE1	0.54	2.38	27	1
1:A:248:LYS:HG3	1:A:284:TYR:CE1	0.54	2.38	2	3
1:A:231:ILE:CG2	1:A:273:ILE:HG22	0.54	2.33	11	14
1:A:277:SER:C	1:A:299:VAL:HG21	0.54	2.23	22	15
1:A:219:LEU:HB3	1:A:223:TYR:OH	0.54	2.03	24	4
1:A:215:PHE:CD2	1:A:235:VAL:HG11	0.53	2.39	27	1
1:A:215:PHE:CE2	1:A:286:CYS:HB2	0.53	2.38	22	6
1:A:244:VAL:HG21	1:A:269:ARG:CG	0.53	2.34	16	18
1:A:237:LEU:HD11	1:A:244:VAL:HG13	0.53	1.78	12	4
1:A:246:TRP:CZ3	1:A:286:CYS:HB3	0.53	2.39	20	3
1:A:227:LYS:HG3	1:A:277:SER:HB2	0.53	1.79	28	3
1:A:217:LYS:HB3	1:A:236:GLU:HB3	0.53	1.79	21	1
1:A:273:ILE:HD12	1:A:276:CYS:SG	0.53	2.43	18	7
1:A:218:LYS:HE2	1:A:286:CYS:HB3	0.53	1.79	6	1
1:A:241:ASP:HA	1:A:269:ARG:NH1	0.53	2.19	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:248:LYS:HB2	1:A:253:ILE:HD11	0.53	1.80	17	13
1:A:223:TYR:CE2	1:A:233:LEU:HA	0.52	2.39	20	22
1:A:222:ALA:HA	1:A:296:GLU:O	0.52	2.03	3	10
1:A:215:PHE:CZ	1:A:286:CYS:HB2	0.52	2.38	8	13
1:A:276:CYS:HA	1:A:280:ASP:HB2	0.52	1.80	28	2
1:A:256:SER:HB3	1:A:259:LYS:O	0.52	2.05	15	7
1:A:277:SER:C	1:A:299:VAL:HG11	0.52	2.24	23	2
1:A:253:ILE:HD13	1:A:260:TYR:CE1	0.52	2.40	25	1
1:A:246:TRP:HA	1:A:287:VAL:HG13	0.51	1.81	25	3
1:A:232:ARG:HA	1:A:272:THR:HA	0.51	1.82	22	2
1:A:218:LYS:HE3	1:A:219:LEU:O	0.51	2.05	16	2
1:A:227:LYS:HG2	1:A:301:GLU:O	0.51	2.06	10	1
1:A:255:MET:HG3	1:A:262:PHE:CD2	0.51	2.40	5	1
1:A:249:ASN:HD22	1:A:283:ALA:HB3	0.51	1.65	28	1
1:A:258:SER:O	1:A:274:SER:HB2	0.51	2.05	7	3
1:A:260:TYR:CD1	1:A:273:ILE:HD11	0.51	2.41	18	2
1:A:218:LYS:HA	1:A:235:VAL:HG12	0.51	1.83	15	5
1:A:227:LYS:HA	1:A:277:SER:HB2	0.51	1.81	24	1
1:A:237:LEU:HD13	1:A:239:ASP:HB2	0.51	1.82	12	2
1:A:247:LEU:CD2	1:A:252:GLU:HA	0.50	2.36	25	9
1:A:227:LYS:HG3	1:A:227:LYS:O	0.50	2.05	10	5
1:A:245:LYS:HG3	1:A:287:VAL:HG22	0.50	1.83	20	1
1:A:218:LYS:NZ	1:A:295:THR:HB	0.50	2.22	17	1
1:A:226:SER:HB2	1:A:229:HIS:HB3	0.50	1.84	14	9
1:A:226:SER:HB3	1:A:229:HIS:HB3	0.50	1.82	19	4
1:A:249:ASN:ND2	1:A:282:ALA:HB1	0.50	2.21	10	4
1:A:215:PHE:HE2	1:A:246:TRP:CH2	0.50	2.24	22	2
1:A:249:ASN:N	1:A:249:ASN:HD22	0.50	2.05	21	1
1:A:230:LYS:HE3	1:A:274:SER:OG	0.50	2.06	5	2
1:A:285:GLN:CG	1:A:294:SER:HA	0.50	2.26	25	3
1:A:277:SER:HA	1:A:299:VAL:HG21	0.49	1.82	2	7
1:A:249:ASN:ND2	1:A:283:ALA:HB3	0.49	2.22	28	1
1:A:218:LYS:HD2	1:A:293:CYS:SG	0.49	2.47	27	2
1:A:231:ILE:HD13	1:A:297:LEU:HD11	0.49	1.82	9	5
1:A:276:CYS:HA	1:A:280:ASP:OD2	0.49	2.06	13	1
1:A:281:ASP:OD2	1:A:298:PHE:HA	0.49	2.07	13	2
1:A:247:LEU:O	1:A:284:TYR:HA	0.49	2.08	24	6
1:A:263:GLU:HB3	1:A:270:THR:HB	0.49	1.85	27	5
1:A:258:SER:O	1:A:274:SER:HB3	0.49	2.07	21	3
1:A:260:TYR:CE1	1:A:273:ILE:HD11	0.48	2.43	13	6
1:A:246:TRP:CG	1:A:271:LEU:HG	0.48	2.43	11	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:230:LYS:HA	1:A:273:ILE:O	0.48	2.07	13	1
1:A:227:LYS:O	1:A:227:LYS:HG3	0.48	2.08	12	4
1:A:225:VAL:HG13	1:A:299:VAL:CB	0.48	2.37	26	2
1:A:227:LYS:HA	1:A:277:SER:CB	0.48	2.38	24	1
1:A:281:ASP:HB3	1:A:299:VAL:HG12	0.48	1.85	24	1
1:A:246:TRP:CG	1:A:271:LEU:HD22	0.48	2.43	10	1
1:A:233:LEU:HB2	1:A:271:LEU:CB	0.48	2.32	5	6
1:A:227:LYS:CD	1:A:301:GLU:HA	0.48	2.31	21	1
1:A:246:TRP:CD1	1:A:271:LEU:HD13	0.48	2.43	10	1
1:A:230:LYS:HD2	1:A:274:SER:CA	0.48	2.39	4	1
1:A:276:CYS:HB3	1:A:280:ASP:CG	0.48	2.29	10	1
1:A:219:LEU:HB2	1:A:223:TYR:CZ	0.48	2.44	2	6
1:A:227:LYS:CG	1:A:301:GLU:HA	0.48	2.38	7	3
1:A:239:ASP:HB3	1:A:242:ALA:HB3	0.47	1.85	2	1
1:A:247:LEU:O	1:A:285:GLN:N	0.47	2.47	1	26
1:A:246:TRP:CB	1:A:260:TYR:HE2	0.47	2.12	25	1
1:A:248:LYS:HD2	1:A:249:ASN:N	0.47	2.24	4	1
1:A:232:ARG:HB3	1:A:270:THR:HG23	0.47	1.83	17	3
1:A:225:VAL:HG11	1:A:276:CYS:O	0.47	2.09	22	2
1:A:248:LYS:HB2	1:A:253:ILE:CD1	0.47	2.40	17	4
1:A:224:GLN:HG2	1:A:298:PHE:HB2	0.47	1.86	13	1
1:A:214:ALA:HB1	1:A:239:ASP:OD1	0.47	2.10	18	3
1:A:225:VAL:HB	1:A:299:VAL:CG2	0.47	2.38	25	2
1:A:227:LYS:HG2	1:A:301:GLU:CA	0.47	2.34	11	3
1:A:237:LEU:CD1	1:A:269:ARG:HB2	0.46	2.40	23	8
1:A:244:VAL:CG1	1:A:269:ARG:HG2	0.46	2.40	1	7
1:A:216:GLN:HB3	1:A:236:GLU:HG3	0.46	1.86	21	1
1:A:235:VAL:HG22	1:A:269:ARG:O	0.46	2.11	26	9
1:A:239:ASP:CG	1:A:242:ALA:HB2	0.46	2.30	24	2
1:A:260:TYR:HA	1:A:271:LEU:CD1	0.46	2.40	23	1
1:A:276:CYS:HB3	1:A:280:ASP:CB	0.45	2.41	17	1
1:A:215:PHE:HA	1:A:237:LEU:HD23	0.45	1.86	16	1
1:A:276:CYS:CA	1:A:280:ASP:HB2	0.45	2.41	28	1
1:A:233:LEU:HD23	1:A:246:TRP:CE3	0.45	2.46	10	8
1:A:218:LYS:HE2	1:A:295:THR:OG1	0.45	2.11	2	1
1:A:230:LYS:HB2	1:A:230:LYS:NZ	0.45	2.27	18	1
1:A:246:TRP:CE3	1:A:286:CYS:HB3	0.45	2.46	14	2
1:A:241:ASP:HA	1:A:269:ARG:HH21	0.45	1.70	17	1
1:A:260:TYR:H	1:A:273:ILE:HG13	0.45	1.71	12	1
1:A:215:PHE:HE1	1:A:288:VAL:CG2	0.45	2.23	27	1
1:A:235:VAL:CG1	1:A:246:TRP:HH2	0.45	2.25	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:239:ASP:OD2	1:A:288:VAL:HG11	0.45	2.11	12	1
1:A:248:LYS:HB2	1:A:253:ILE:HG13	0.45	1.87	15	1
1:A:230:LYS:HG2	1:A:274:SER:HA	0.45	1.86	22	2
1:A:215:PHE:N	1:A:215:PHE:CD1	0.45	2.85	22	10
1:A:218:LYS:HG3	1:A:286:CYS:SG	0.44	2.52	28	2
1:A:227:LYS:HE2	1:A:301:GLU:HB3	0.44	1.90	6	1
1:A:223:TYR:HB3	1:A:231:ILE:CD1	0.44	2.41	18	2
1:A:230:LYS:NZ	1:A:230:LYS:HB2	0.44	2.28	14	1
1:A:215:PHE:HD2	1:A:235:VAL:HG11	0.44	1.72	27	1
1:A:227:LYS:HB2	1:A:277:SER:CB	0.44	2.42	10	2
1:A:247:LEU:HG	1:A:292:LYS:HD3	0.44	1.89	11	1
1:A:218:LYS:HE3	1:A:293:CYS:SG	0.44	2.52	24	1
1:A:273:ILE:HG23	1:A:276:CYS:CB	0.44	2.35	23	1
1:A:218:LYS:HZ3	1:A:295:THR:HB	0.44	1.71	17	1
1:A:244:VAL:CG2	1:A:246:TRP:NE1	0.44	2.81	6	2
1:A:276:CYS:SG	1:A:280:ASP:HB2	0.44	2.53	1	2
1:A:232:ARG:HD2	1:A:270:THR:HG21	0.44	1.89	23	1
1:A:219:LEU:HG	1:A:234:THR:O	0.43	2.13	27	2
1:A:225:VAL:HG21	1:A:276:CYS:O	0.43	2.12	16	1
1:A:278:LEU:HD22	1:A:299:VAL:CG1	0.43	2.43	19	1
1:A:227:LYS:HE2	1:A:278:LEU:HG	0.43	1.89	5	1
1:A:285:GLN:H	1:A:285:GLN:NE2	0.43	2.11	28	1
1:A:227:LYS:HG3	1:A:277:SER:CB	0.43	2.44	8	1
1:A:246:TRP:CZ3	1:A:286:CYS:SG	0.43	3.11	11	1
1:A:248:LYS:HD3	1:A:284:TYR:HE1	0.43	1.73	27	1
1:A:277:SER:CA	1:A:299:VAL:HG21	0.43	2.43	25	4
1:A:248:LYS:HG3	1:A:251:GLN:HB2	0.43	1.91	28	1
1:A:248:LYS:N	1:A:251:GLN:O	0.43	2.52	10	5
1:A:259:LYS:N	1:A:259:LYS:HD3	0.43	2.29	28	1
1:A:248:LYS:HE2	1:A:251:GLN:HB3	0.43	1.91	10	1
1:A:237:LEU:HG	1:A:269:ARG:CB	0.43	2.44	8	2
1:A:227:LYS:HE3	1:A:301:GLU:HB3	0.43	1.89	7	1
1:A:273:ILE:HG13	1:A:284:TYR:CE2	0.43	2.44	7	4
1:A:215:PHE:CE2	1:A:235:VAL:HG21	0.43	2.49	21	1
1:A:283:ALA:C	1:A:284:TYR:HD1	0.43	2.17	25	2
1:A:218:LYS:HG3	1:A:235:VAL:HG12	0.43	1.91	19	1
1:A:223:TYR:HE2	1:A:233:LEU:HA	0.43	1.73	17	2
1:A:231:ILE:HG23	1:A:273:ILE:HG22	0.43	1.89	20	2
1:A:215:PHE:CD1	1:A:215:PHE:N	0.42	2.87	2	2
1:A:276:CYS:HA	1:A:280:ASP:CB	0.42	2.45	28	1
1:A:255:MET:HA	1:A:260:TYR:O	0.42	2.14	28	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:227:LYS:HG2	1:A:227:LYS:O	0.42	2.13	19	1
1:A:218:LYS:HG3	1:A:293:CYS:SG	0.42	2.55	14	1
1:A:227:LYS:HE3	1:A:301:GLU:CB	0.42	2.37	24	1
1:A:260:TYR:CD2	1:A:271:LEU:HD11	0.42	2.49	25	1
1:A:224:GLN:HB3	1:A:300:LYS:HG3	0.42	1.91	28	1
1:A:230:LYS:HG3	1:A:274:SER:HA	0.42	1.92	24	1
1:A:231:ILE:HG22	1:A:276:CYS:SG	0.42	2.55	2	1
1:A:226:SER:HB3	1:A:229:HIS:HB2	0.42	1.89	26	1
1:A:261:ILE:O	1:A:272:THR:N	0.42	2.51	5	2
1:A:264:SER:HB3	1:A:269:ARG:CZ	0.42	2.44	22	1
1:A:219:LEU:CB	1:A:223:TYR:OH	0.42	2.68	24	1
1:A:280:ASP:OD2	1:A:284:TYR:OH	0.42	2.33	21	1
1:A:285:GLN:NE2	1:A:285:GLN:H	0.42	2.13	15	1
1:A:230:LYS:HG2	1:A:274:SER:CB	0.42	2.45	20	1
1:A:258:SER:HB2	1:A:259:LYS:HD3	0.42	1.92	18	1
1:A:225:VAL:HG13	1:A:299:VAL:HB	0.41	1.92	26	1
1:A:223:TYR:O	1:A:297:LEU:HD12	0.41	2.14	24	1
1:A:244:VAL:HG22	1:A:269:ARG:CG	0.41	2.41	28	1
1:A:231:ILE:HD13	1:A:297:LEU:CD1	0.41	2.44	9	1
1:A:227:LYS:HE3	1:A:301:GLU:HA	0.41	1.92	14	1
1:A:244:VAL:HG12	1:A:288:VAL:HG22	0.41	1.92	20	1
1:A:273:ILE:CG2	1:A:276:CYS:HB3	0.41	2.37	23	1
1:A:246:TRP:HB2	1:A:253:ILE:CG2	0.41	2.45	28	2
1:A:259:LYS:HG2	1:A:274:SER:O	0.41	2.15	10	1
1:A:245:LYS:HZ1	1:A:252:GLU:HB3	0.41	1.74	11	1
1:A:264:SER:HB2	1:A:269:ARG:CZ	0.41	2.45	1	1
1:A:244:VAL:CG2	1:A:269:ARG:CG	0.41	2.98	11	1
1:A:244:VAL:HG12	1:A:288:VAL:CG2	0.41	2.46	20	1
1:A:285:GLN:HG3	1:A:294:SER:CB	0.41	2.45	20	1
1:A:225:VAL:O	1:A:300:LYS:N	0.41	2.52	28	2
1:A:269:ARG:HD3	1:A:270:THR:H	0.41	1.76	26	1
1:A:253:ILE:HG12	1:A:260:TYR:CE1	0.41	2.51	13	1
1:A:227:LYS:HE2	1:A:301:GLU:HA	0.41	1.92	28	1
1:A:232:ARG:HB3	1:A:270:THR:HG21	0.41	1.93	27	1
1:A:228:GLY:N	1:A:277:SER:HB3	0.41	2.31	9	1
1:A:232:ARG:NH2	1:A:263:GLU:HG2	0.40	2.31	19	1
1:A:248:LYS:HE3	1:A:251:GLN:HB2	0.40	1.94	26	1
1:A:259:LYS:HG3	1:A:274:SER:O	0.40	2.16	3	1
1:A:219:LEU:HG	1:A:220:GLU:HG2	0.40	1.94	22	1
1:A:253:ILE:HG23	1:A:260:TYR:CG	0.40	2.50	2	1
1:A:262:PHE:HD1	1:A:262:PHE:O	0.40	2.00	5	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	87/104 (84%)	70±2 (81±2%)	13±2 (15±3%)	4±2 (5±2%)	5	27
All	All	2436/2912 (84%)	1963 (81%)	354 (15%)	119 (5%)	5	27

All 14 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	282	ALA	27
1	A	279	ALA	16
1	A	277	SER	13
1	A	290	GLY	13
1	A	254	GLN	13
1	A	249	ASN	11
1	A	230	LYS	11
1	A	221	PRO	5
1	A	281	ASP	3
1	A	214	ALA	2
1	A	258	SER	2
1	A	255	MET	1
1	A	242	ALA	1
1	A	240	HIS	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	74/90 (82%)	66±2 (89±3%)	8±2 (11±3%)	12	55
All	All	2072/2520 (82%)	1840 (89%)	232 (11%)	12	55

All 37 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	285	GLN	28
1	A	247	LEU	28
1	A	295	THR	28
1	A	273	ILE	27
1	A	239	ASP	13
1	A	255	MET	9
1	A	269	ARG	8
1	A	219	LEU	8
1	A	259	LYS	8
1	A	227	LYS	6
1	A	216	GLN	6
1	A	230	LYS	6
1	A	260	TYR	5
1	A	249	ASN	5
1	A	251	GLN	4
1	A	254	GLN	4
1	A	278	LEU	4
1	A	262	PHE	4
1	A	280	ASP	4
1	A	215	PHE	3
1	A	264	SER	3
1	A	281	ASP	3
1	A	287	VAL	2
1	A	218	LYS	2
1	A	232	ARG	2
1	A	237	LEU	1
1	A	275	GLN	1
1	A	220	GLU	1
1	A	301	GLU	1
1	A	241	ASP	1
1	A	293	CYS	1
1	A	225	VAL	1
1	A	300	LYS	1
1	A	248	LYS	1
1	A	245	LYS	1
1	A	286	CYS	1
1	A	272	THR	1

6.3.3 RNA ⓘ

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