



Full wwPDB NMR Structure Validation Report ⓘ

May 17, 2016 – 02:54 PM EDT

PDB ID : 5ID3
Title : Solution structure of the pore-forming region of *C. elegans* Mitochondrial Calcium Uniporter (MCU)
Authors : Oxenoid, K.; Dong, Y.; Cao, C.; Cui, T.; Sancak, Y.; Markhard, A.L.; Grabarek, Z.; Kong, L.; Liu, Z.; Ouyang, B.; Cong, Y.; Mootha, V.K.; Chou, J.J.; Membrane Protein Structures by Solution NMR (MPSbyNMR)
Deposited on : 2016-02-23

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

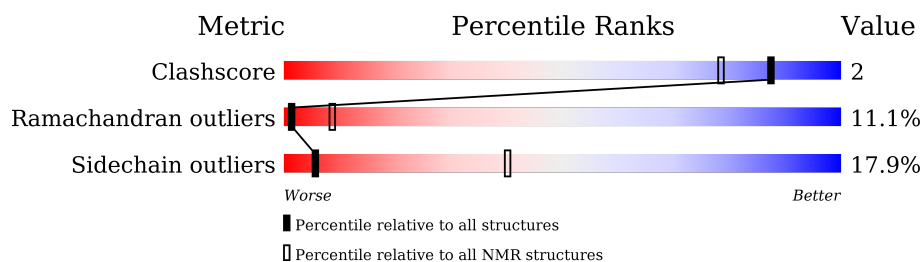
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 7%.

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	159	<div> <div>50%</div> <div>21%</div> <div>6%</div> <div>19%</div> <div>.</div> </div>
1	B	159	<div> <div>56%</div> <div>16%</div> <div>.</div> <div>19%</div> <div>.</div> </div>
1	C	159	<div> <div>51%</div> <div>19%</div> <div>5%</div> <div>21%</div> <div>.</div> </div>
1	D	159	<div> <div>50%</div> <div>21%</div> <div>.</div> <div>21%</div> <div>.</div> </div>
1	E	159	<div> <div>53%</div> <div>18%</div> <div>.</div> <div>19%</div> <div>.</div> </div>

2 Ensemble composition and analysis

This entry contains 15 models. Model 1 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:179-A:271, A:289-A:318, B:178-B:271, B:290-B:318, C:179-C:269, C:290-C:317, D:178-D:269, D:291-D:317, E:177-E:269, E:290-E:318 (606)	0.59	1

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 1 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 14, 15
Single-model clusters	12; 13

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12675 atoms, of which 6270 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mitochondrial Calcium Uniporter.

Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	
1	B	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	
1	C	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	
1	D	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	
1	E	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	MET	-	initiating methionine	UNP Q21121
A	170	SER	CYS	engineered mutation	UNP Q21121
A	207	ALA	CYS	engineered mutation	UNP Q21121
A	215	ALA	MET	engineered mutation	UNP Q21121
A	222	SER	MET	engineered mutation	UNP Q21121
A	242	VAL	MET	engineered mutation	UNP Q21121
A	255	ALA	CYS	engineered mutation	UNP Q21121
A	313	LEU	MET	engineered mutation	UNP Q21121
A	318	GLU	PHE	engineered mutation	UNP Q21121
A	319	HIS	-	expression tag	UNP Q21121
A	320	HIS	-	expression tag	UNP Q21121
A	321	HIS	-	expression tag	UNP Q21121
A	322	HIS	-	expression tag	UNP Q21121
A	323	HIS	-	expression tag	UNP Q21121
A	324	HIS	-	expression tag	UNP Q21121
B	166	MET	-	initiating methionine	UNP Q21121
B	170	SER	CYS	engineered mutation	UNP Q21121
B	207	ALA	CYS	engineered mutation	UNP Q21121
B	215	ALA	MET	engineered mutation	UNP Q21121
B	222	SER	MET	engineered mutation	UNP Q21121
B	242	VAL	MET	engineered mutation	UNP Q21121
B	255	ALA	CYS	engineered mutation	UNP Q21121
B	313	LEU	MET	engineered mutation	UNP Q21121

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Chain	Residue	Modelled	Actual	Comment	Reference
B	318	GLU	PHE	engineered mutation	UNP Q21121
B	319	HIS	-	expression tag	UNP Q21121
B	320	HIS	-	expression tag	UNP Q21121
B	321	HIS	-	expression tag	UNP Q21121
B	322	HIS	-	expression tag	UNP Q21121
B	323	HIS	-	expression tag	UNP Q21121
B	324	HIS	-	expression tag	UNP Q21121
C	166	MET	-	initiating methionine	UNP Q21121
C	170	SER	CYS	engineered mutation	UNP Q21121
C	207	ALA	CYS	engineered mutation	UNP Q21121
C	215	ALA	MET	engineered mutation	UNP Q21121
C	222	SER	MET	engineered mutation	UNP Q21121
C	242	VAL	MET	engineered mutation	UNP Q21121
C	255	ALA	CYS	engineered mutation	UNP Q21121
C	313	LEU	MET	engineered mutation	UNP Q21121
C	318	GLU	PHE	engineered mutation	UNP Q21121
C	319	HIS	-	expression tag	UNP Q21121
C	320	HIS	-	expression tag	UNP Q21121
C	321	HIS	-	expression tag	UNP Q21121
C	322	HIS	-	expression tag	UNP Q21121
C	323	HIS	-	expression tag	UNP Q21121
C	324	HIS	-	expression tag	UNP Q21121
D	166	MET	-	initiating methionine	UNP Q21121
D	170	SER	CYS	engineered mutation	UNP Q21121
D	207	ALA	CYS	engineered mutation	UNP Q21121
D	215	ALA	MET	engineered mutation	UNP Q21121
D	222	SER	MET	engineered mutation	UNP Q21121
D	242	VAL	MET	engineered mutation	UNP Q21121
D	255	ALA	CYS	engineered mutation	UNP Q21121
D	313	LEU	MET	engineered mutation	UNP Q21121
D	318	GLU	PHE	engineered mutation	UNP Q21121
D	319	HIS	-	expression tag	UNP Q21121
D	320	HIS	-	expression tag	UNP Q21121
D	321	HIS	-	expression tag	UNP Q21121
D	322	HIS	-	expression tag	UNP Q21121
D	323	HIS	-	expression tag	UNP Q21121
D	324	HIS	-	expression tag	UNP Q21121
E	166	MET	-	initiating methionine	UNP Q21121
E	170	SER	CYS	engineered mutation	UNP Q21121
E	207	ALA	CYS	engineered mutation	UNP Q21121
E	215	ALA	MET	engineered mutation	UNP Q21121
E	222	SER	MET	engineered mutation	UNP Q21121

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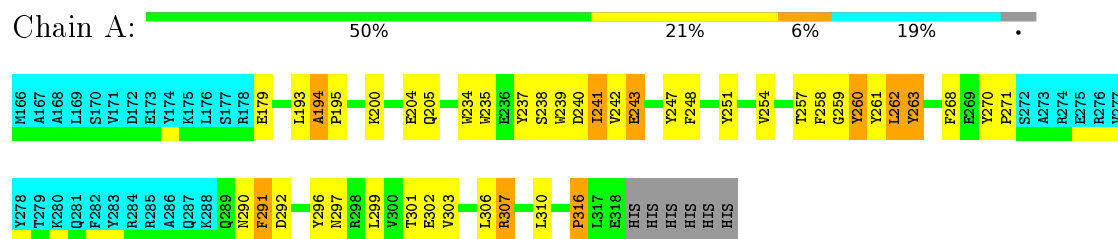
Chain	Residue	Modelled	Actual	Comment	Reference
E	242	VAL	MET	engineered mutation	UNP Q21121
E	255	ALA	CYS	engineered mutation	UNP Q21121
E	313	LEU	MET	engineered mutation	UNP Q21121
E	318	GLU	PHE	engineered mutation	UNP Q21121
E	319	HIS	-	expression tag	UNP Q21121
E	320	HIS	-	expression tag	UNP Q21121
E	321	HIS	-	expression tag	UNP Q21121
E	322	HIS	-	expression tag	UNP Q21121
E	323	HIS	-	expression tag	UNP Q21121
E	324	HIS	-	expression tag	UNP Q21121

4 Residue-property plots

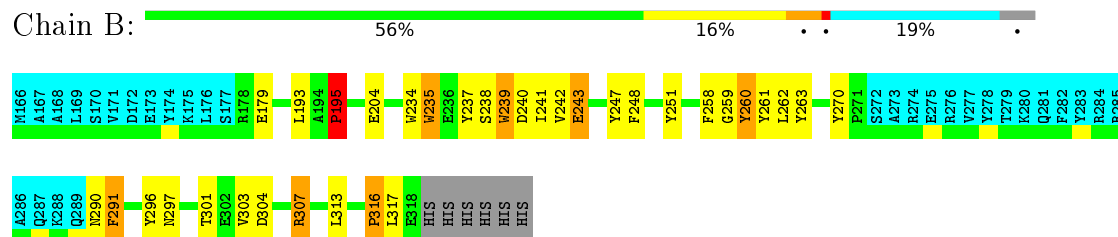
4.1 Average score per residue in the NMR ensemble

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.

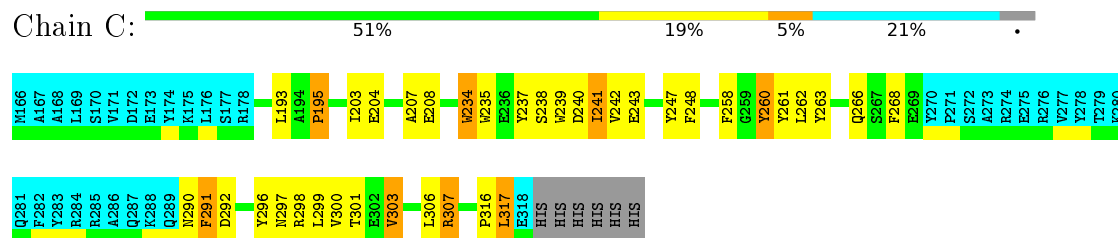
• Molecule 1: Mitochondrial Calcium Uniporter



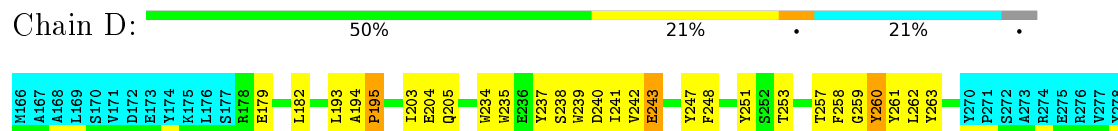
• Molecule 1: Mitochondrial Calcium Uniporter



• Molecule 1: Mitochondrial Calcium Uniporter



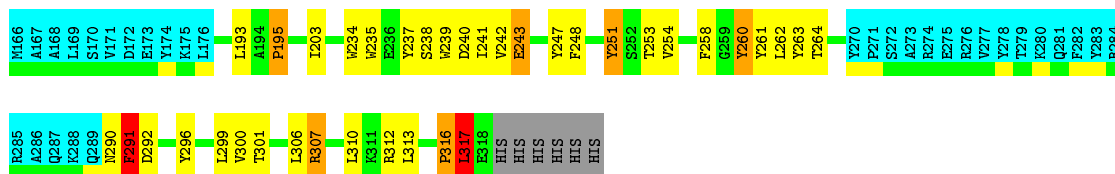
• Molecule 1: Mitochondrial Calcium Uniporter





• Molecule 1: Mitochondrial Calcium Uniporter

Chain E: 53% 18% 19%



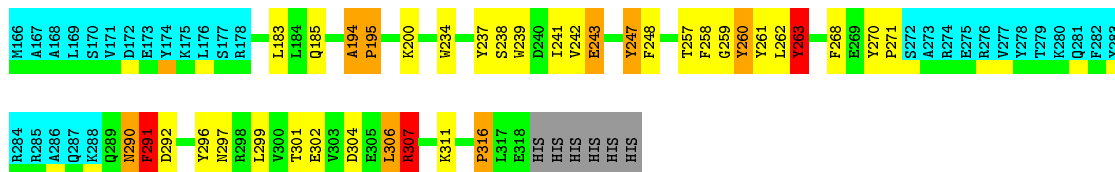
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

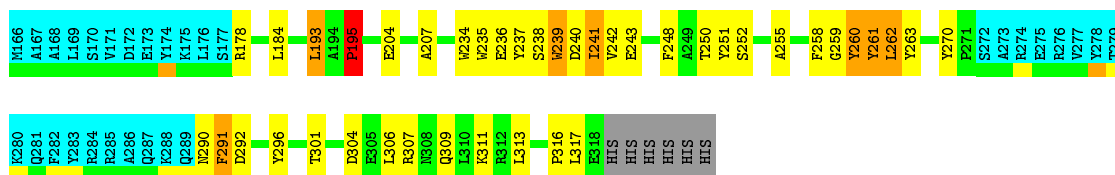
• Molecule 1: Mitochondrial Calcium Uniporter

Chain A: 54% 16% 5% 19%



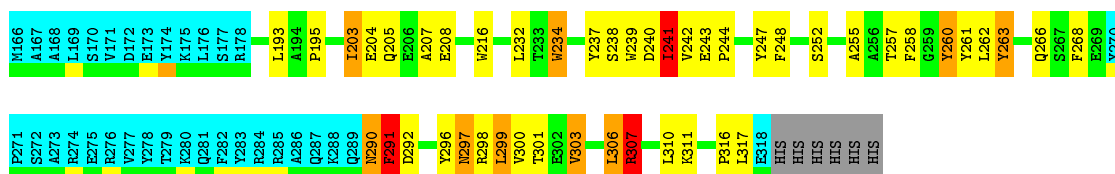
• Molecule 1: Mitochondrial Calcium Uniporter

Chain B: 52% 21% 19%

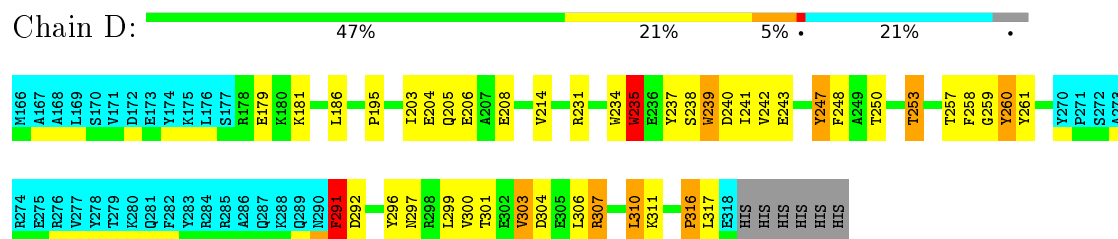


• Molecule 1: Mitochondrial Calcium Uniporter

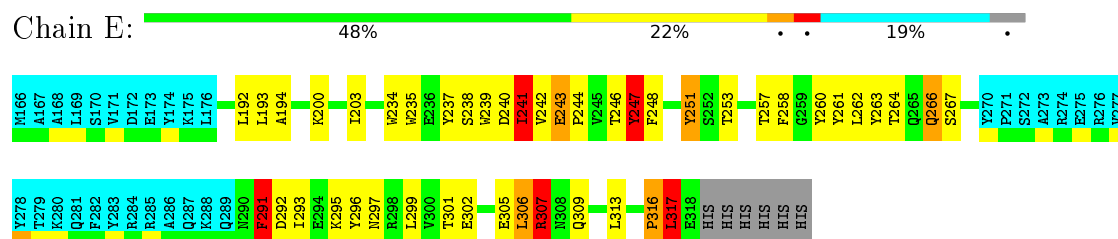
Chain C: 46% 21% 6% 21%



- Molecule 1: Mitochondrial Calcium Uniporter

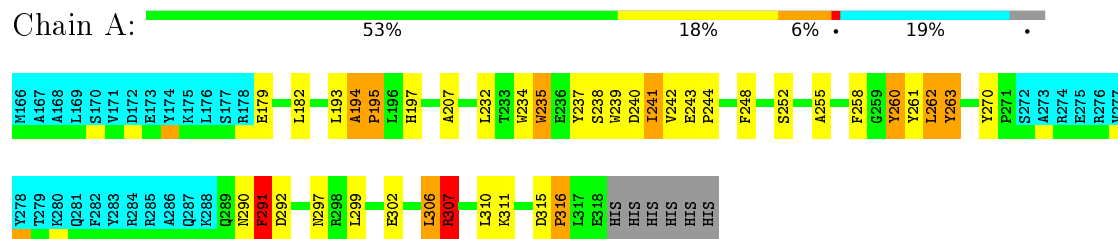


- Molecule 1: Mitochondrial Calcium Uniporter

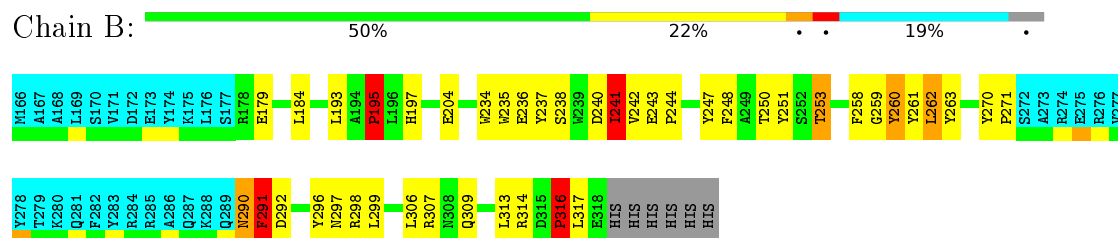


4.2.2 Score per residue for model 2

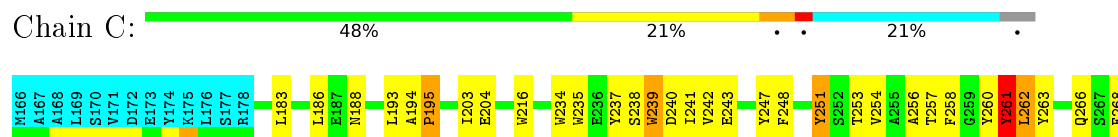
- Molecule 1: Mitochondrial Calcium Uniporter

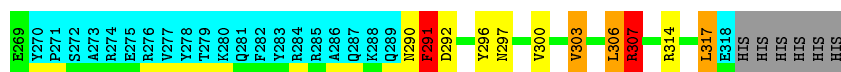


- Molecule 1: Mitochondrial Calcium Uniporter



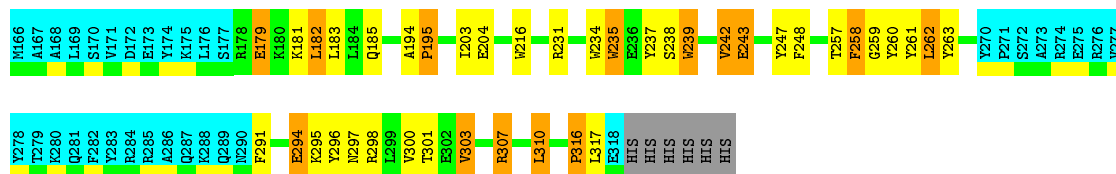
- Molecule 1: Mitochondrial Calcium Uniporter





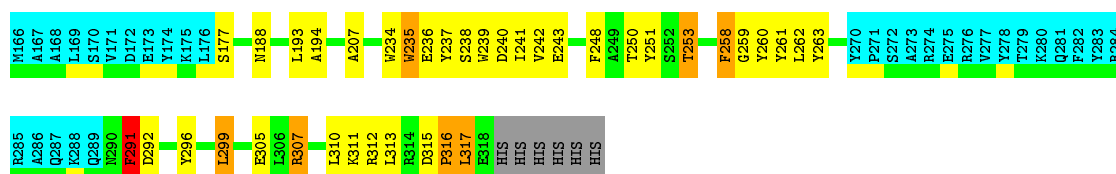
• Molecule 1: Mitochondrial Calcium Uniporter

Chain D: 50% 16% 9% 21% .



• Molecule 1: Mitochondrial Calcium Uniporter

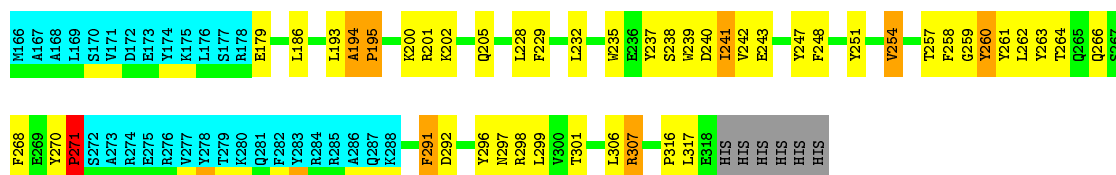
Chain E: 53% 19% . 19% .



4.2.3 Score per residue for model 3

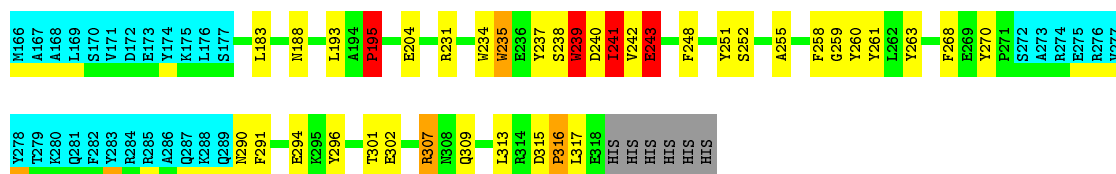
• Molecule 1: Mitochondrial Calcium Uniporter

Chain A: 48% 25% . 19% .



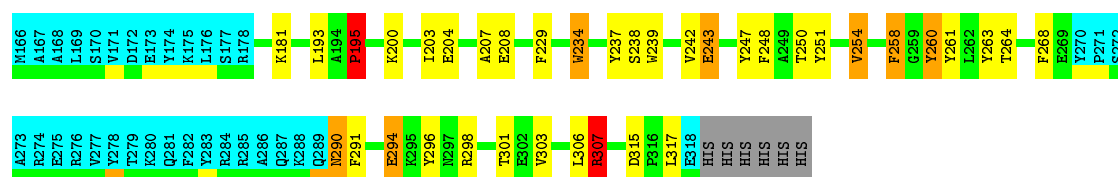
• Molecule 1: Mitochondrial Calcium Uniporter

Chain B: 53% 19% . 19% .



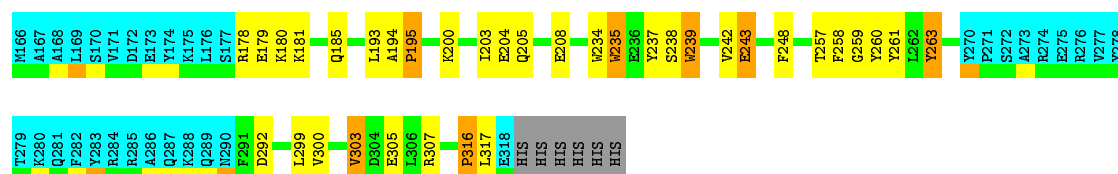
• Molecule 1: Mitochondrial Calcium Uniporter

Chain C: 52% 18% . 21% .



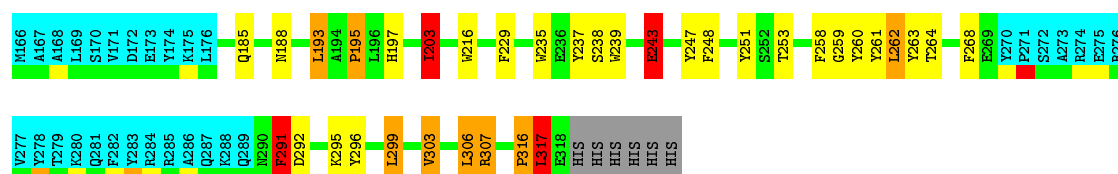
• Molecule 1: Mitochondrial Calcium Uniporter

Chain D: 53% 18% 21%



• Molecule 1: Mitochondrial Calcium Uniporter

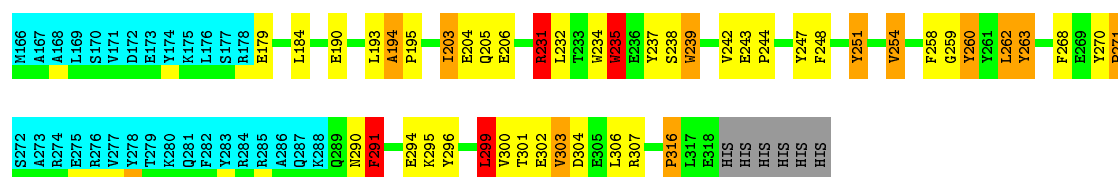
Chain E: 55% 14% 5% 19%



4.2.4 Score per residue for model 4

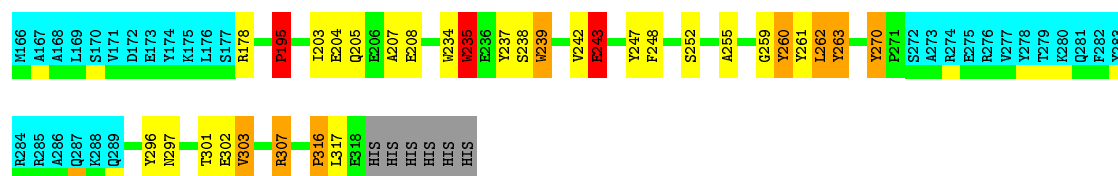
• Molecule 1: Mitochondrial Calcium Uniporter

Chain A: 48% 19% 7% 19%

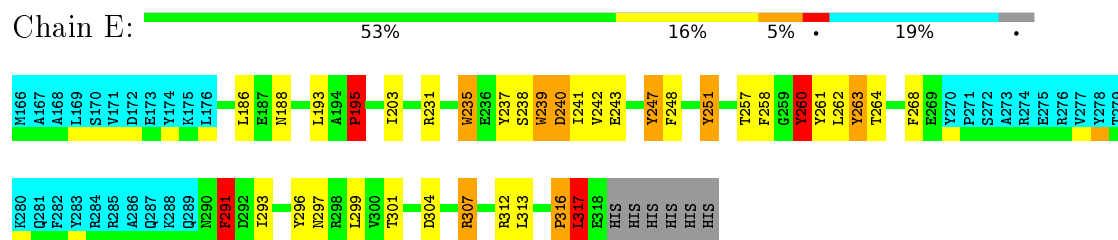


• Molecule 1: Mitochondrial Calcium Uniporter

Chain B: 57% 13% 5% 19%

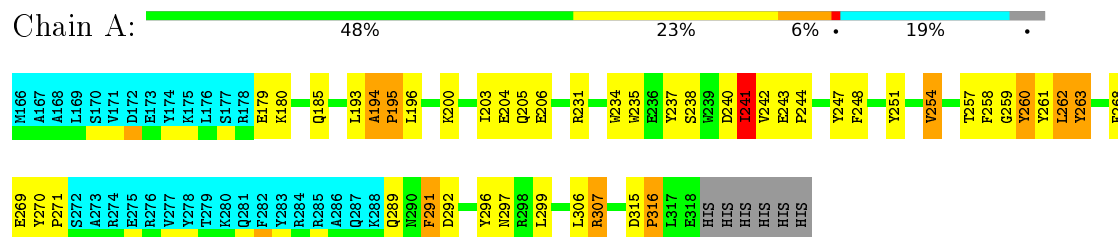


• Molecule 1: Mitochondrial Calcium Uniporter



4.2.5 Score per residue for model 5

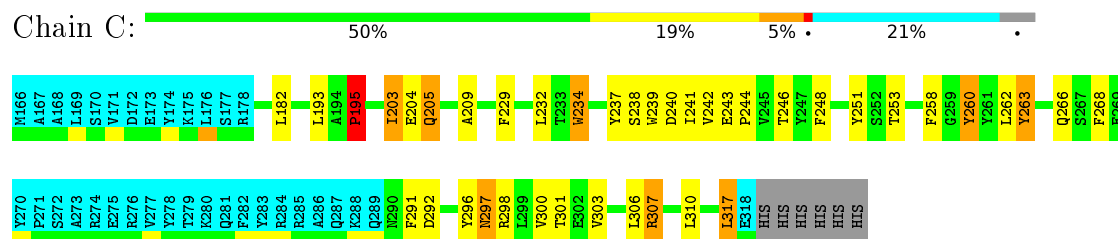
- Molecule 1: Mitochondrial Calcium Uniporter



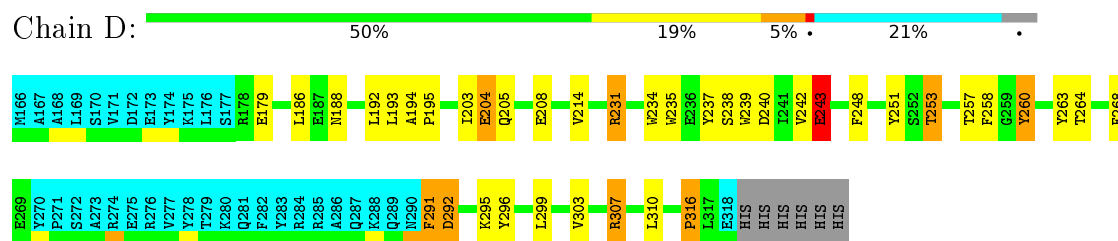
- Molecule 1: Mitochondrial Calcium Uniporter



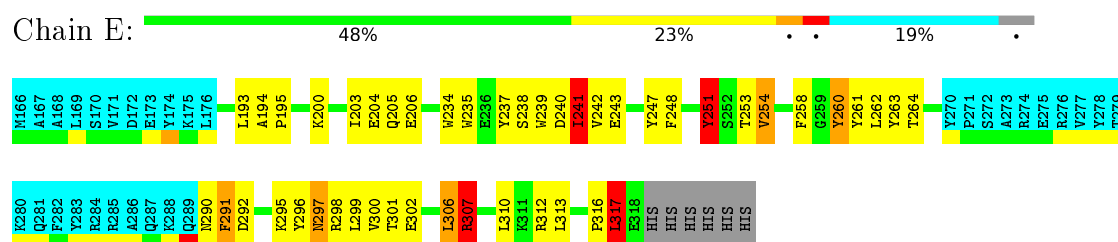
- Molecule 1: Mitochondrial Calcium Uniporter



- Molecule 1: Mitochondrial Calcium Uniporter

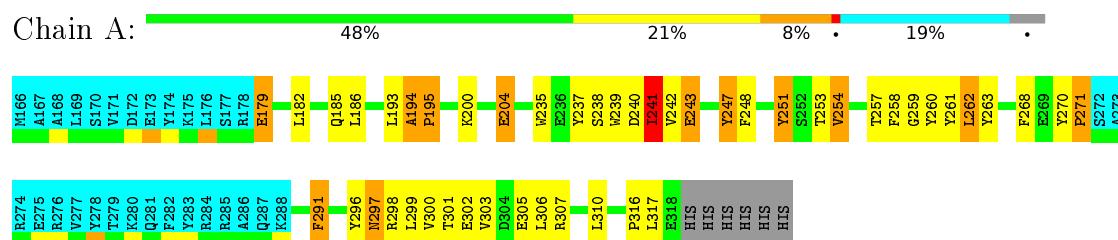


- Molecule 1: Mitochondrial Calcium Uniporter

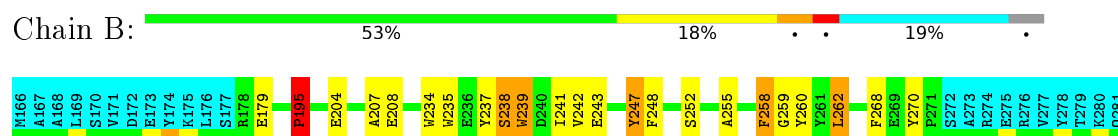


4.2.6 Score per residue for model 6

- Molecule 1: Mitochondrial Calcium Uniporter



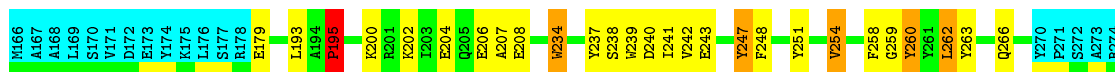
- Molecule 1: Mitochondrial Calcium Uniporter





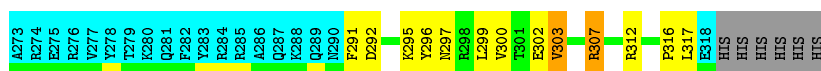
• Molecule 1: Mitochondrial Calcium Uniporter

Chain C: 50% 19% 6% 21%



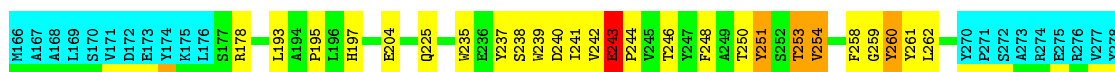
• Molecule 1: Mitochondrial Calcium Uniporter

Chain D: 48% 23% 21%



• Molecule 1: Mitochondrial Calcium Uniporter

Chain E: 52% 17% 5% 19%



4.2.7 Score per residue for model 7

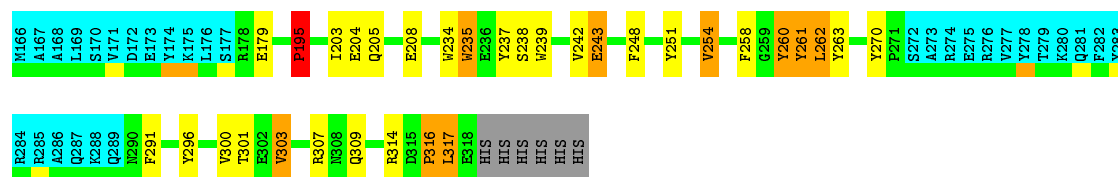
• Molecule 1: Mitochondrial Calcium Uniporter

Chain A: 52% 18% 6% 19%



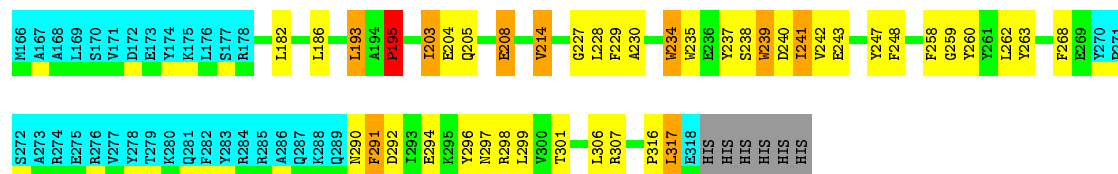
• Molecule 1: Mitochondrial Calcium Uniporter

Chain B: 57% 14% 6% 19%



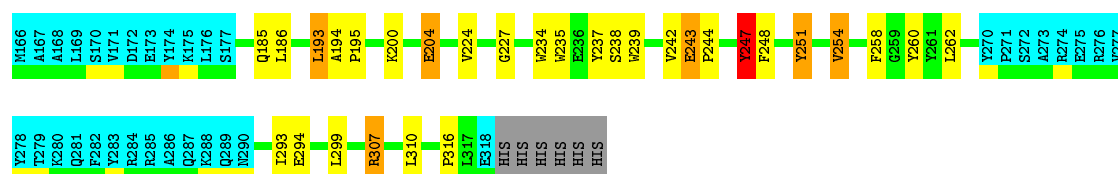
• Molecule 1: Mitochondrial Calcium Uniporter

Chain C: 48% 21% 6% 21%



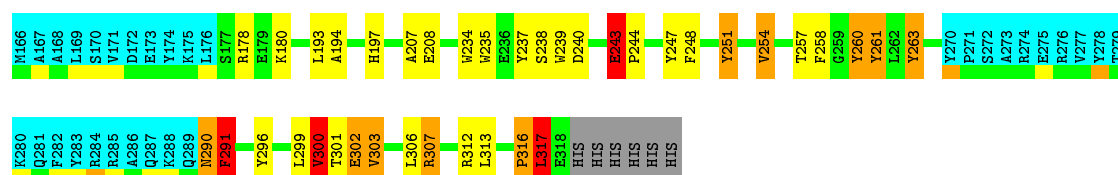
• Molecule 1: Mitochondrial Calcium Uniporter

Chain D: 56% 14% 6% 21%



• Molecule 1: Mitochondrial Calcium Uniporter

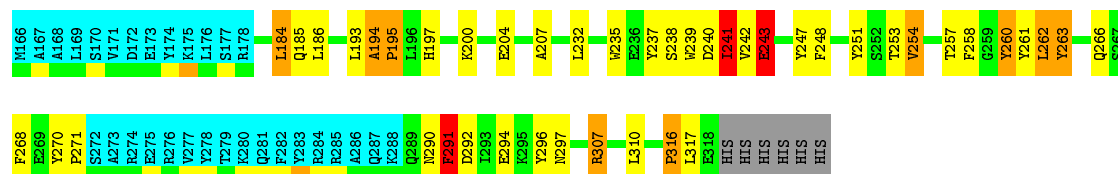
Chain E: 53% 15% 6% 19%



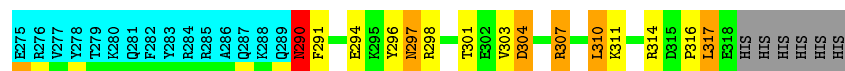
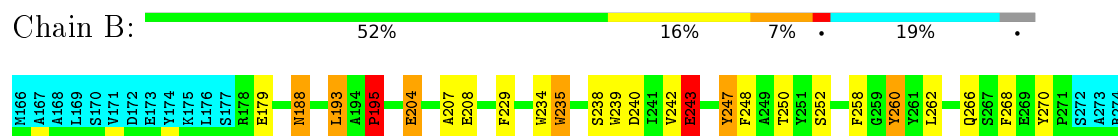
4.2.8 Score per residue for model 8

• Molecule 1: Mitochondrial Calcium Uniporter

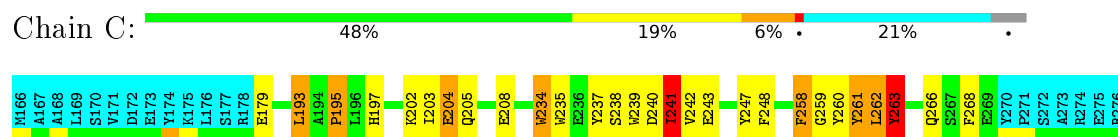
Chain A: 50% 20% 6% 19%



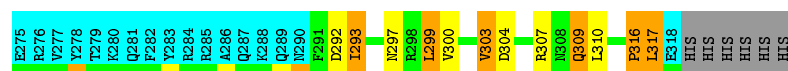
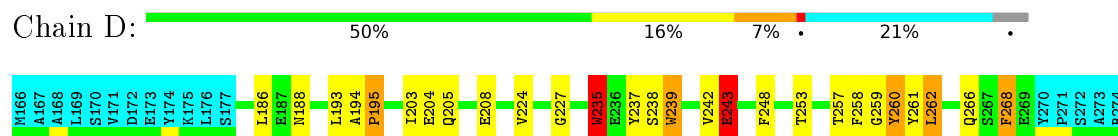
• Molecule 1: Mitochondrial Calcium Uniporter



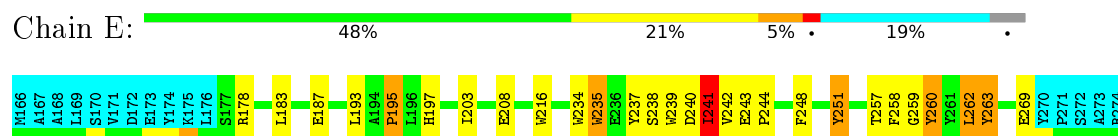
• Molecule 1: Mitochondrial Calcium Uniporter



• Molecule 1: Mitochondrial Calcium Uniporter

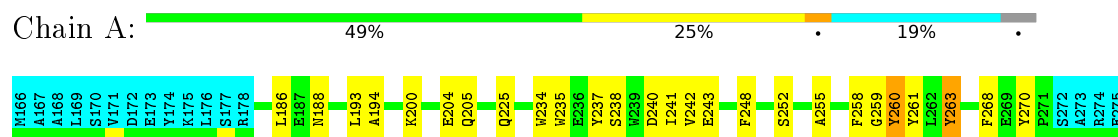


• Molecule 1: Mitochondrial Calcium Uniporter

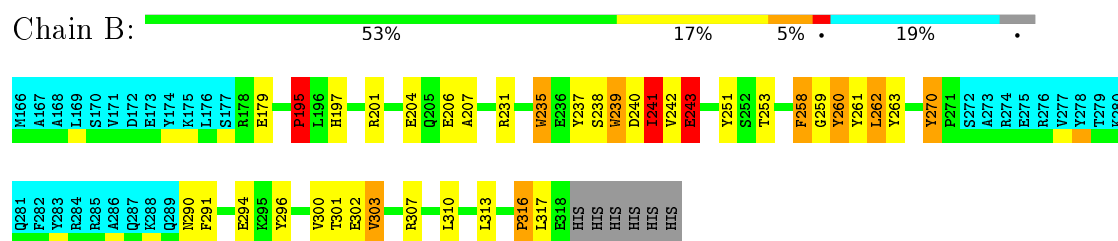


4.2.9 Score per residue for model 9

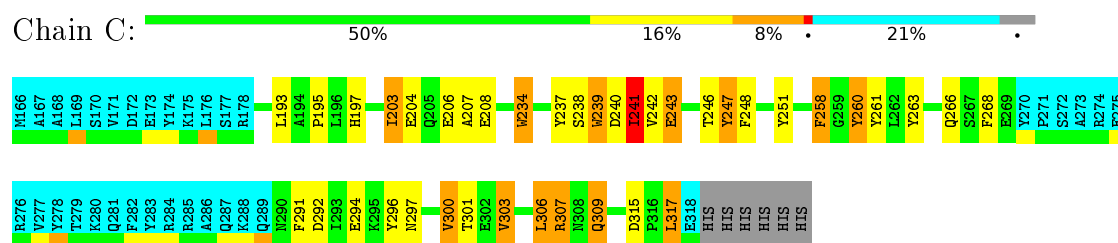
• Molecule 1: Mitochondrial Calcium Uniporter



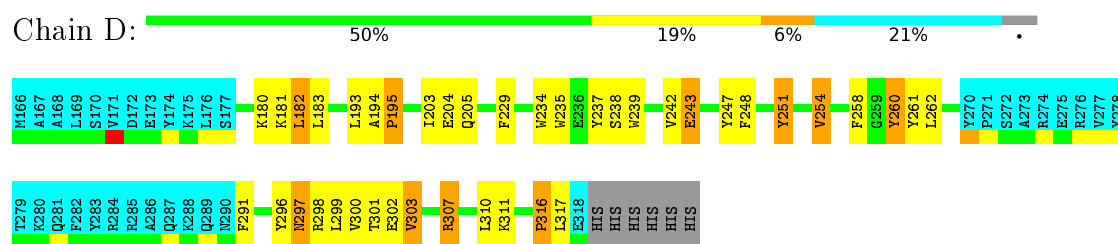
- Molecule 1: Mitochondrial Calcium Uniporter



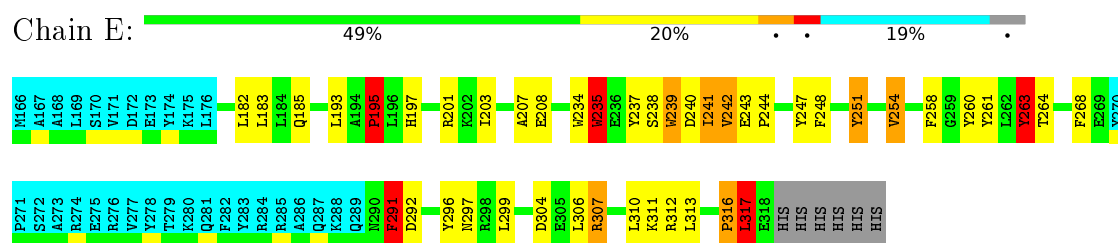
- Molecule 1: Mitochondrial Calcium Uniporter



- Molecule 1: Mitochondrial Calcium Uniporter

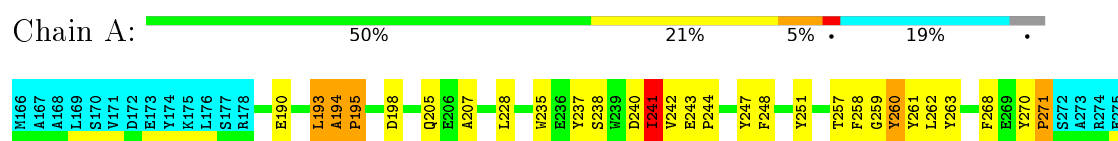


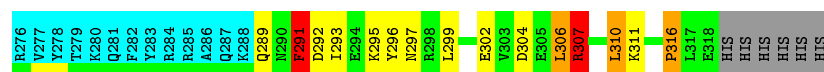
- Molecule 1: Mitochondrial Calcium Uniporter



4.2.10 Score per residue for model 10

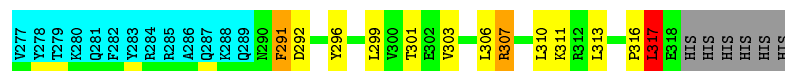
- Molecule 1: Mitochondrial Calcium Uniporter





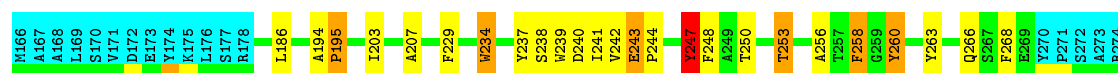
• Molecule 1: Mitochondrial Calcium Uniporter

Chain B: 52% 19% 5% 19%



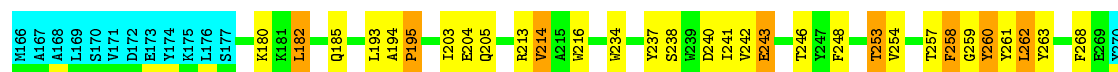
• Molecule 1: Mitochondrial Calcium Uniporter

Chain C: 49% 20% 5% 21%



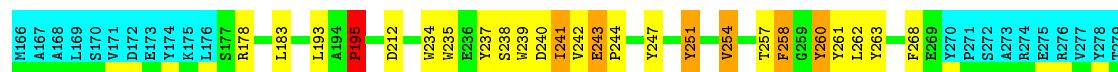
• Molecule 1: Mitochondrial Calcium Uniporter

Chain D: 48% 21% 6% 21%



• Molecule 1: Mitochondrial Calcium Uniporter

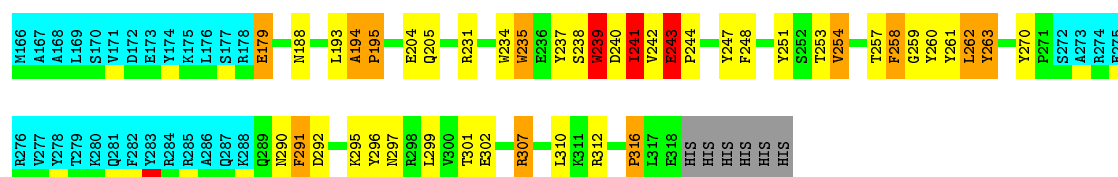
Chain E: 53% 16% 6% 19%



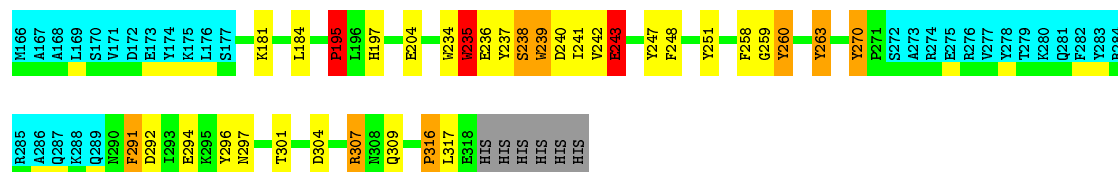
4.2.11 Score per residue for model 11

• Molecule 1: Mitochondrial Calcium Uniporter

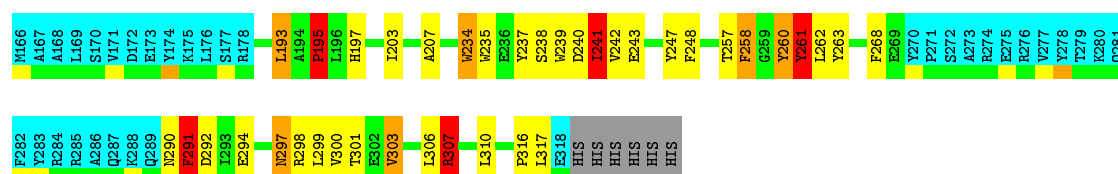
Chain A: 50% 19% 7% 19%



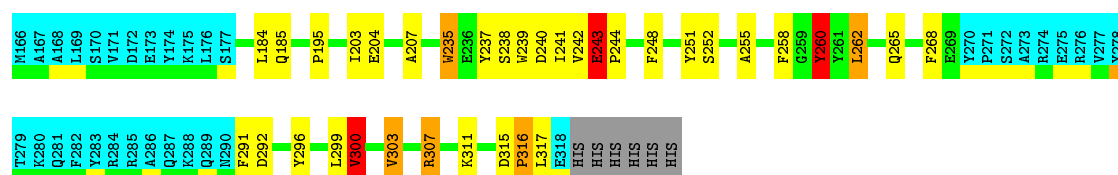
- Molecule 1: Mitochondrial Calcium Uniporter



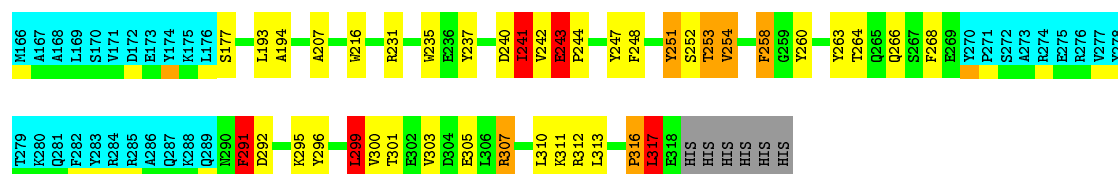
- Molecule 1: Mitochondrial Calcium Uniporter



- Molecule 1: Mitochondrial Calcium Uniporter

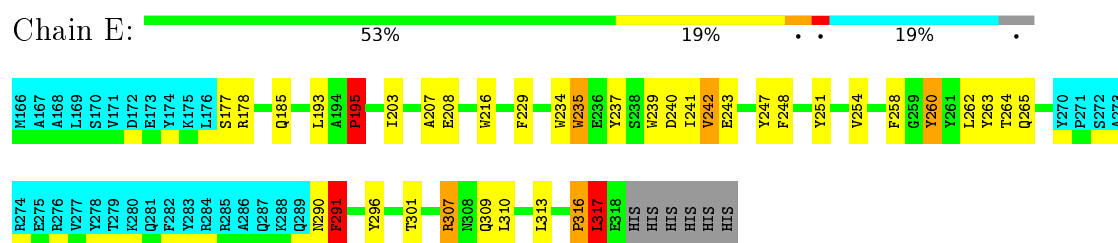


- Molecule 1: Mitochondrial Calcium Uniporter



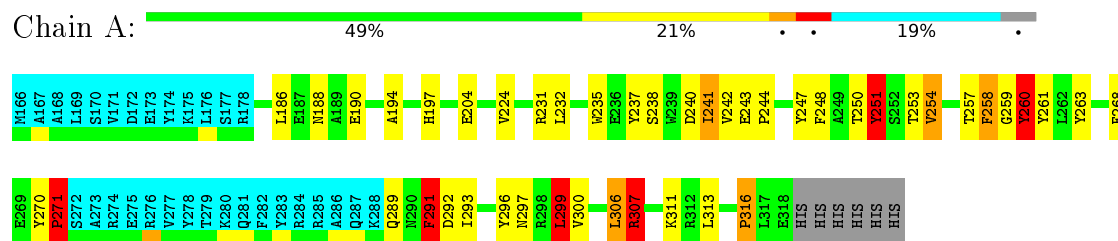
4.2.12 Score per residue for model 12

- Molecule 1: Mitochondrial Calcium Uniporter

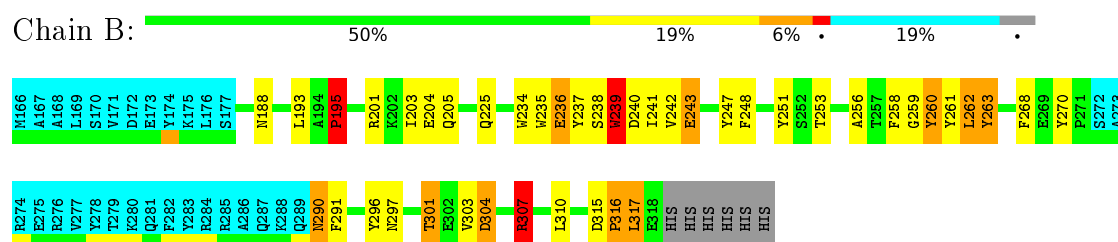


4.2.13 Score per residue for model 13

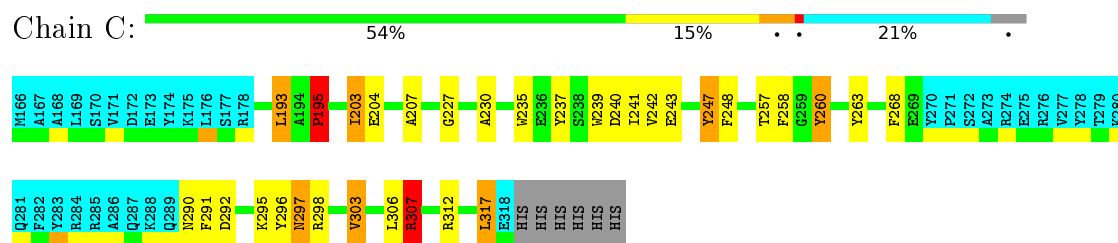
• Molecule 1: Mitochondrial Calcium Uniporter



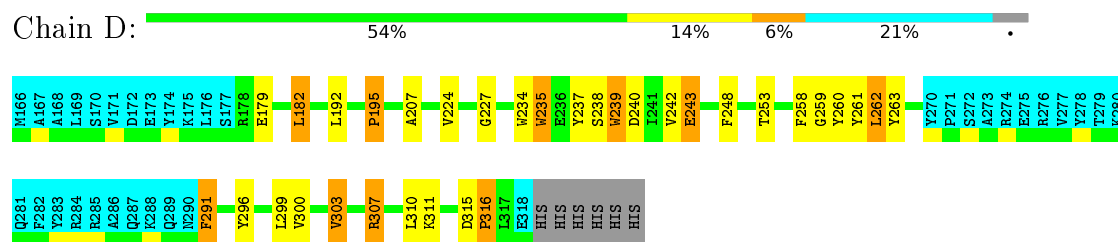
• Molecule 1: Mitochondrial Calcium Uniporter



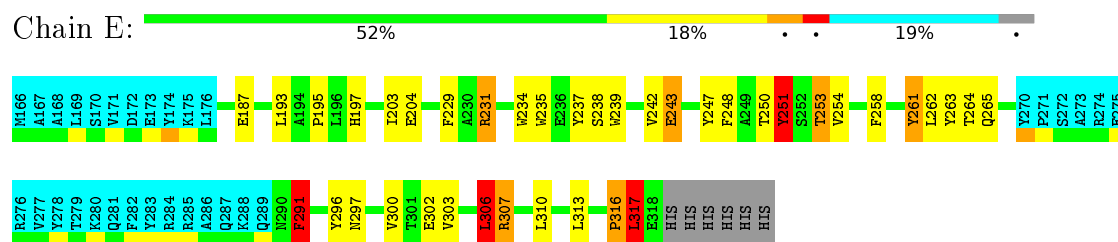
• Molecule 1: Mitochondrial Calcium Uniporter



• Molecule 1: Mitochondrial Calcium Uniporter

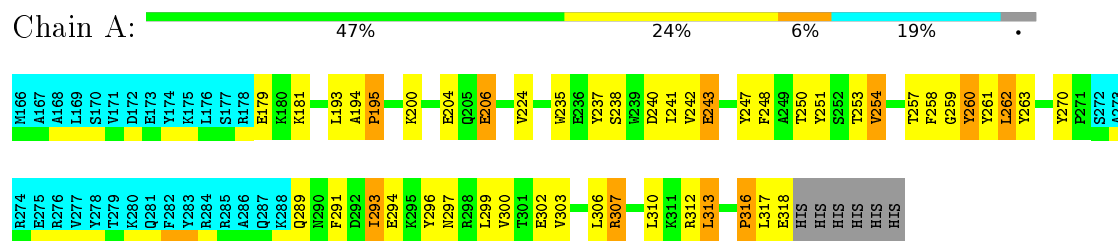


• Molecule 1: Mitochondrial Calcium Uniporter

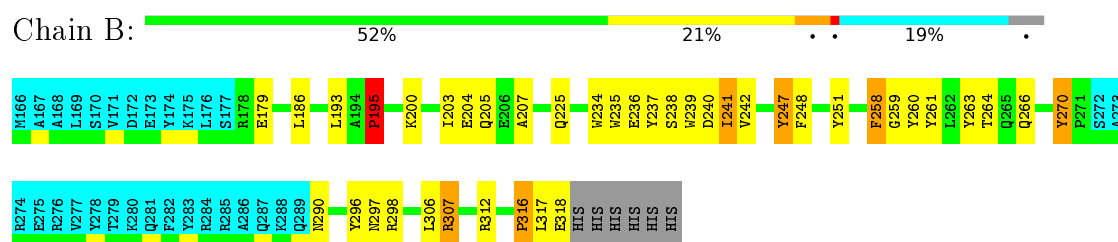


4.2.14 Score per residue for model 14

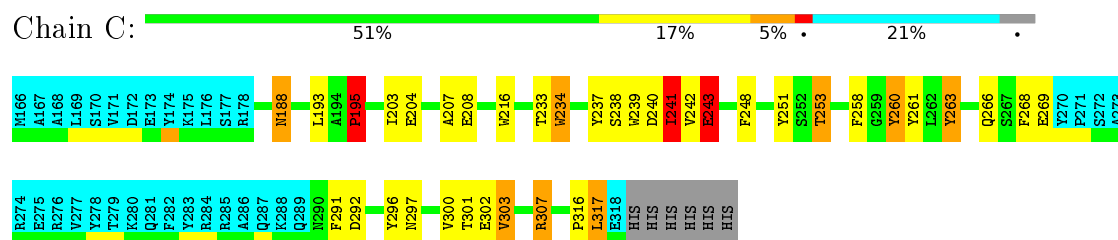
• Molecule 1: Mitochondrial Calcium Uniporter



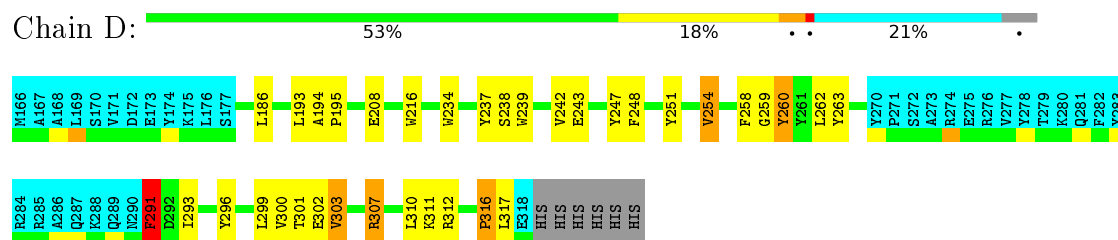
• Molecule 1: Mitochondrial Calcium Uniporter



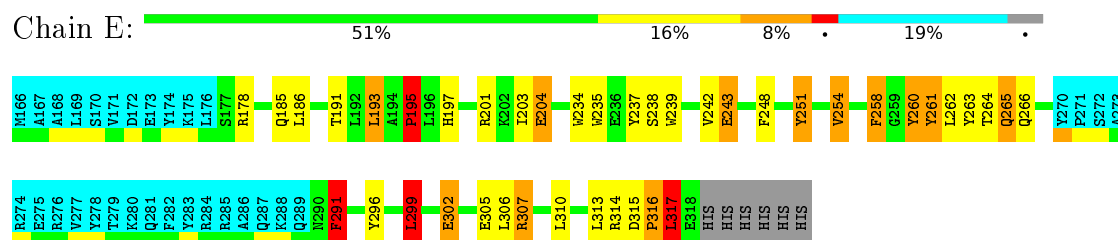
• Molecule 1: Mitochondrial Calcium Uniporter



• Molecule 1: Mitochondrial Calcium Uniporter



• Molecule 1: Mitochondrial Calcium Uniporter



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 15 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
XPLOR-NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	5id3_cs.cif
Number of chemical shift lists	1
Total number of shifts	657
Number of shifts mapped to atoms	657
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	7%

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

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	2.27±0.01	15±2/1052 (1.4±0.2%)	0.99±0.02	2±1/1432 (0.1±0.1%)
1	B	2.27±0.01	14±2/1054 (1.3±0.2%)	0.99±0.02	2±1/1434 (0.1±0.1%)
1	C	2.27±0.02	14±2/1014 (1.4±0.2%)	1.02±0.03	3±2/1381 (0.2±0.1%)
1	D	2.27±0.01	12±2/1017 (1.2±0.2%)	1.01±0.02	1±1/1384 (0.1±0.1%)
1	E	2.28±0.01	14±2/1039 (1.3±0.2%)	1.02±0.02	2±1/1412 (0.1±0.1%)
All	All	2.27	1031/77640 (1.3%)	1.01	151/105645 (0.1%)

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	D	0.0±0.0	0.2±0.4
1	C	0.0±0.0	0.2±0.4
1	E	0.0±0.0	0.1±0.2
All	All	0	7

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	E	296	TYR	CB-CG	6.90	1.62	1.51	12	15
1	C	248	PHE	CB-CG	6.84	1.62	1.51	10	15
1	B	237	TYR	CB-CG	6.80	1.61	1.51	12	14
1	C	296	TYR	CB-CG	6.78	1.61	1.51	12	13
1	D	243	GLU	CB-CG	6.76	1.65	1.52	8	6
1	E	237	TYR	CB-CG	6.74	1.61	1.51	8	15
1	D	260	TYR	CB-CG	6.66	1.61	1.51	4	8
1	D	248	PHE	CB-CG	6.62	1.62	1.51	7	15
1	A	237	TYR	CB-CG	6.60	1.61	1.51	12	15
1	D	316	PRO	N-CA	6.58	1.58	1.47	4	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	296	TYR	CB-CG	6.56	1.61	1.51	3	13
1	C	247	TYR	CB-CG	6.52	1.61	1.51	12	9
1	B	307	ARG	CA-CB	6.50	1.68	1.53	5	14
1	B	296	TYR	CB-CG	6.46	1.61	1.51	14	14
1	C	303	VAL	CB-CG2	6.45	1.66	1.52	8	11
1	E	263	TYR	CB-CG	6.41	1.61	1.51	5	13
1	D	258	PHE	CB-CG	6.39	1.62	1.51	2	15
1	B	247	TYR	CB-CG	6.39	1.61	1.51	2	5
1	C	237	TYR	CB-CG	6.38	1.61	1.51	6	15
1	D	237	TYR	CB-CG	6.37	1.61	1.51	3	15
1	D	307	ARG	CA-CB	6.37	1.68	1.53	1	14
1	D	296	TYR	CB-CG	6.34	1.61	1.51	9	9
1	C	254	VAL	CB-CG2	6.34	1.66	1.52	12	3
1	A	260	TYR	CB-CG	6.32	1.61	1.51	8	12
1	C	260	TYR	CB-CG	6.29	1.61	1.51	15	11
1	E	260	TYR	CB-CG	6.29	1.61	1.51	5	9
1	A	244	PRO	N-CA	6.27	1.57	1.47	13	7
1	A	248	PHE	CB-CG	6.25	1.61	1.51	14	15
1	D	247	TYR	CB-CG	6.18	1.60	1.51	15	5
1	B	243	GLU	CA-CB	6.18	1.67	1.53	11	5
1	B	243	GLU	CB-CG	6.17	1.63	1.52	4	2
1	A	307	ARG	CA-CB	6.12	1.67	1.53	13	12
1	D	254	VAL	CB-CG2	6.11	1.65	1.52	14	3
1	A	307	ARG	CB-CG	6.11	1.69	1.52	2	11
1	C	243	GLU	CB-CG	6.11	1.63	1.52	14	4
1	E	248	PHE	CB-CG	6.08	1.61	1.51	1	14
1	B	261	TYR	CB-CG	6.08	1.60	1.51	14	9
1	B	260	TYR	CB-CG	6.06	1.60	1.51	13	12
1	A	254	VAL	CB-CG2	6.06	1.65	1.52	7	11
1	D	263	TYR	CB-CG	6.05	1.60	1.51	10	5
1	A	261	TYR	CB-CG	6.05	1.60	1.51	3	10
1	D	307	ARG	CB-CG	6.01	1.68	1.52	1	6
1	B	254	VAL	CB-CG2	6.00	1.65	1.52	7	1
1	A	263	TYR	CB-CG	5.97	1.60	1.51	14	13
1	E	244	PRO	N-CA	5.97	1.57	1.47	9	6
1	B	270	TYR	CB-CG	5.97	1.60	1.51	2	15
1	B	316	PRO	N-CA	5.95	1.57	1.47	3	14
1	E	254	VAL	CB-CG2	5.93	1.65	1.52	5	7
1	E	307	ARG	CA-CB	5.92	1.67	1.53	2	15
1	B	248	PHE	CB-CG	5.92	1.61	1.51	6	14
1	E	307	ARG	CB-CG	5.90	1.68	1.52	2	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	D	261	TYR	CB-CG	5.90	1.60	1.51	6	7
1	C	307	ARG	CA-CB	5.89	1.67	1.53	1	13
1	E	243	GLU	CA-CB	5.87	1.66	1.53	7	5
1	B	241	ILE	CA-CB	5.87	1.68	1.54	3	3
1	C	261	TYR	CB-CG	5.87	1.60	1.51	8	6
1	E	316	PRO	N-CA	5.86	1.57	1.47	2	2
1	C	307	ARG	CB-CG	5.85	1.68	1.52	14	8
1	D	302	GLU	CB-CG	5.84	1.63	1.52	9	2
1	E	291	PHE	CB-CG	5.84	1.61	1.51	14	15
1	A	258	PHE	CB-CG	5.84	1.61	1.51	10	15
1	C	258	PHE	CB-CG	5.84	1.61	1.51	8	15
1	D	303	VAL	CB-CG2	5.82	1.65	1.52	11	10
1	B	258	PHE	CB-CG	5.82	1.61	1.51	6	13
1	C	316	PRO	N-CA	5.82	1.57	1.47	11	8
1	E	300	VAL	CA-CB	5.82	1.67	1.54	7	2
1	E	261	TYR	CB-CG	5.81	1.60	1.51	2	7
1	B	263	TYR	CB-CG	5.78	1.60	1.51	9	6
1	E	251	TYR	CB-CG	5.77	1.60	1.51	3	14
1	A	316	PRO	N-CA	5.76	1.57	1.47	5	12
1	D	291	PHE	CB-CG	5.74	1.61	1.51	5	9
1	E	258	PHE	CB-CG	5.72	1.61	1.51	15	15
1	B	195	PRO	N-CD	5.71	1.55	1.47	1	15
1	C	263	TYR	CB-CG	5.70	1.60	1.51	1	15
1	B	307	ARG	CB-CG	5.68	1.67	1.52	4	14
1	D	251	TYR	CB-CG	5.67	1.60	1.51	7	4
1	A	270	TYR	CB-CG	5.67	1.60	1.51	4	15
1	A	303	VAL	CA-CB	5.62	1.66	1.54	7	1
1	C	247	TYR	CG-CD2	5.61	1.46	1.39	15	2
1	E	317	LEU	CA-CB	5.61	1.66	1.53	14	8
1	A	241	ILE	CA-CB	5.57	1.67	1.54	11	9
1	A	303	VAL	CB-CG2	5.54	1.64	1.52	4	2
1	A	243	GLU	CB-CG	5.54	1.62	1.52	8	4
1	E	302	GLU	CB-CG	5.53	1.62	1.52	1	2
1	E	195	PRO	N-CD	5.53	1.55	1.47	3	7
1	D	224	VAL	CB-CG1	5.52	1.64	1.52	6	1
1	E	303	VAL	CB-CG2	5.50	1.64	1.52	7	1
1	B	294	GLU	CB-CG	5.49	1.62	1.52	11	4
1	B	291	PHE	CB-CG	5.49	1.60	1.51	5	7
1	C	306	LEU	CA-CB	5.48	1.66	1.53	9	3
1	B	303	VAL	CB-CG2	5.46	1.64	1.52	9	2
1	C	241	ILE	CA-CB	5.45	1.67	1.54	11	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	251	TYR	CB-CG	5.45	1.59	1.51	9	4
1	E	242	VAL	CB-CG2	5.44	1.64	1.52	9	2
1	D	268	PHE	CB-CG	5.44	1.60	1.51	8	5
1	A	251	TYR	CB-CG	5.43	1.59	1.51	13	4
1	A	184	LEU	CB-CG	5.43	1.68	1.52	8	1
1	D	241	ILE	CA-CB	5.42	1.67	1.54	15	2
1	D	243	GLU	CA-CB	5.40	1.65	1.53	9	3
1	A	291	PHE	CB-CG	5.40	1.60	1.51	15	8
1	E	241	ILE	CA-CB	5.40	1.67	1.54	11	4
1	C	291	PHE	CB-CG	5.39	1.60	1.51	5	11
1	B	251	TYR	CB-CG	5.36	1.59	1.51	1	8
1	C	195	PRO	N-CD	5.35	1.55	1.47	5	9
1	C	300	VAL	CA-CB	5.34	1.66	1.54	9	1
1	D	293	ILE	CA-CB	5.34	1.67	1.54	7	2
1	A	306	LEU	CB-CG	5.34	1.68	1.52	7	1
1	A	271	PRO	N-CA	5.33	1.56	1.47	10	5
1	A	313	LEU	N-CA	5.32	1.56	1.46	14	1
1	A	268	PHE	CB-CG	5.30	1.60	1.51	13	10
1	B	247	TYR	CG-CD2	5.29	1.46	1.39	8	2
1	B	268	PHE	CB-CG	5.29	1.60	1.51	10	7
1	C	294	GLU	CB-CG	5.29	1.62	1.52	3	2
1	B	242	VAL	N-CA	5.29	1.56	1.46	14	1
1	D	294	GLU	CA-CB	5.29	1.65	1.53	7	2
1	D	231	ARG	CA-CB	5.28	1.65	1.53	5	1
1	C	244	PRO	N-CA	5.27	1.56	1.47	5	3
1	D	247	TYR	CG-CD2	5.27	1.46	1.39	4	1
1	B	238	SER	CA-CB	5.27	1.60	1.52	6	1
1	C	229	PHE	CB-CG	5.27	1.60	1.51	4	6
1	A	243	GLU	CA-CB	5.26	1.65	1.53	12	3
1	E	236	GLU	CB-CG	5.25	1.62	1.52	2	1
1	D	203	ILE	CA-CB	5.25	1.67	1.54	6	1
1	C	236	GLU	CB-CG	5.25	1.62	1.52	15	1
1	E	306	LEU	CA-CB	5.25	1.65	1.53	3	2
1	C	268	PHE	CB-CG	5.25	1.60	1.51	1	13
1	E	296	TYR	CG-CD2	5.22	1.46	1.39	13	2
1	B	303	VAL	CA-CB	5.20	1.65	1.54	4	1
1	E	247	TYR	CB-CG	5.19	1.59	1.51	1	1
1	E	268	PHE	CB-CG	5.19	1.60	1.51	3	5
1	A	247	TYR	CB-CG	5.19	1.59	1.51	7	2
1	B	206	GLU	CB-CG	5.19	1.62	1.52	10	1
1	E	293	ILE	CA-CB	5.17	1.66	1.54	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	311	LYS	CA-CB	5.17	1.65	1.53	6	1
1	A	260	TYR	N-CA	5.17	1.56	1.46	13	1
1	B	317	LEU	CA-CB	5.16	1.65	1.53	10	1
1	D	244	PRO	N-CA	5.16	1.56	1.47	11	1
1	B	244	PRO	N-CA	5.15	1.56	1.47	2	1
1	D	214	VAL	CA-CB	5.14	1.65	1.54	10	1
1	E	299	LEU	N-CA	5.14	1.56	1.46	11	2
1	D	260	TYR	CG-CD2	5.12	1.45	1.39	4	1
1	A	269	GLU	CB-CG	5.12	1.61	1.52	5	1
1	D	242	VAL	CB-CG2	5.10	1.63	1.52	2	1
1	D	229	PHE	CB-CG	5.10	1.60	1.51	12	3
1	B	313	LEU	N-CA	5.10	1.56	1.46	5	1
1	C	241	ILE	CB-CG1	5.10	1.68	1.54	12	2
1	E	229	PHE	CB-CG	5.09	1.59	1.51	15	4
1	A	310	LEU	CB-CG	5.09	1.67	1.52	14	1
1	E	204	GLU	CB-CG	5.09	1.61	1.52	14	1
1	A	229	PHE	CB-CG	5.08	1.59	1.51	3	1
1	C	202	LYS	CA-CB	5.08	1.65	1.53	6	1
1	E	231	ARG	CA-CB	5.07	1.65	1.53	13	1
1	C	214	VAL	CA-CB	5.07	1.65	1.54	7	1
1	A	179	GLU	CB-CG	5.06	1.61	1.52	5	1
1	B	236	GLU	CB-CG	5.06	1.61	1.52	13	1
1	E	245	VAL	CB-CG1	5.06	1.63	1.52	15	1
1	A	231	ARG	CA-CB	5.06	1.65	1.53	4	1
1	D	204	GLU	CB-CG	5.06	1.61	1.52	5	1
1	B	302	GLU	CB-CG	5.04	1.61	1.52	4	2
1	C	262	LEU	CB-CG	5.04	1.67	1.52	8	1
1	E	309	GLN	CA-CB	5.04	1.65	1.53	6	1
1	A	206	GLU	CB-CG	5.03	1.61	1.52	14	1
1	D	300	VAL	CA-CB	5.03	1.65	1.54	11	1
1	B	229	PHE	CB-CG	5.03	1.59	1.51	8	2
1	B	271	PRO	N-CA	5.02	1.55	1.47	12	1
1	E	303	VAL	CA-CB	5.01	1.65	1.54	3	1
1	E	243	GLU	CB-CG	5.00	1.61	1.52	14	1
1	D	195	PRO	N-CD	5.00	1.54	1.47	15	1

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
1	B	263	TYR	CB-CG-CD1	7.42	125.45	121.00	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	263	TYR	CB-CG-CD2	6.84	125.10	121.00	15	2
1	B	195	PRO	N-CA-CB	-6.79	95.14	102.60	1	8
1	E	251	TYR	CB-CG-CD1	6.74	125.05	121.00	15	1
1	D	237	TYR	CB-CG-CD2	6.56	124.93	121.00	11	11
1	D	296	TYR	CB-CG-CD2	6.53	124.92	121.00	10	3
1	E	237	TYR	CB-CG-CD1	6.46	124.88	121.00	4	1
1	B	263	TYR	N-CA-CB	-6.34	99.19	110.60	11	1
1	C	296	TYR	CB-CG-CD1	6.31	124.79	121.00	14	7
1	B	296	TYR	CB-CG-CD1	6.30	124.78	121.00	1	2
1	C	237	TYR	CB-CG-CD1	6.30	124.78	121.00	6	10
1	E	237	TYR	CB-CG-CD2	6.25	124.75	121.00	1	11
1	A	237	TYR	CB-CG-CD1	6.22	124.73	121.00	10	5
1	E	251	TYR	CB-CG-CD2	-6.22	117.27	121.00	15	1
1	B	296	TYR	CB-CG-CD2	6.22	124.73	121.00	3	8
1	C	247	TYR	CB-CG-CD1	6.16	124.70	121.00	10	2
1	B	237	TYR	CB-CG-CD2	6.16	124.69	121.00	15	6
1	B	263	TYR	CB-CG-CD2	-6.16	117.31	121.00	15	1
1	C	296	TYR	CB-CG-CD2	-6.11	117.33	121.00	14	2
1	E	296	TYR	CB-CG-CD2	6.10	124.66	121.00	6	10
1	E	299	LEU	CB-CA-C	6.08	121.75	110.20	2	1
1	A	296	TYR	CB-CG-CD1	6.05	124.63	121.00	12	3
1	A	237	TYR	CB-CG-CD2	6.03	124.62	121.00	6	7
1	B	237	TYR	CB-CG-CD1	5.96	124.58	121.00	3	2
1	C	234	TRP	CB-CG-CD2	5.77	134.11	126.60	3	13
1	C	263	TYR	CB-CG-CD1	-5.70	117.58	121.00	15	2
1	C	307	ARG	NE-CZ-NH2	5.65	123.13	120.30	6	1
1	D	251	TYR	CB-CG-CD1	5.59	124.36	121.00	6	1
1	E	299	LEU	N-CA-CB	5.55	121.50	110.40	14	1
1	C	260	TYR	CB-CG-CD1	5.51	124.31	121.00	9	1
1	B	258	PHE	CB-CG-CD2	5.51	124.66	120.80	11	2
1	A	258	PHE	CB-CG-CD2	5.46	124.62	120.80	13	3
1	A	307	ARG	NE-CZ-NH1	-5.45	117.58	120.30	10	1
1	D	296	TYR	CB-CG-CD1	5.40	124.24	121.00	13	2
1	C	237	TYR	CB-CG-CD2	-5.37	117.78	121.00	3	1
1	E	260	TYR	CB-CG-CD1	5.37	124.22	121.00	4	1
1	C	258	PHE	CB-CG-CD2	5.36	124.55	120.80	9	2
1	D	299	LEU	CB-CA-C	5.35	120.37	110.20	11	1
1	D	251	TYR	CB-CG-CD2	-5.31	117.81	121.00	6	1
1	A	299	LEU	CB-CA-C	5.29	120.25	110.20	13	2
1	E	247	TYR	CB-CG-CD2	5.28	124.17	121.00	1	1
1	C	261	TYR	CB-CG-CD1	5.25	124.15	121.00	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	307	ARG	NE-CZ-NH2	5.21	122.90	120.30	7	2
1	A	247	TYR	CB-CG-CD2	5.20	124.12	121.00	15	1
1	D	307	ARG	NE-CZ-NH2	5.16	122.88	120.30	9	1
1	D	247	TYR	CB-CG-CD2	5.15	124.09	121.00	7	1
1	C	261	TYR	CB-CG-CD2	-5.12	117.93	121.00	11	1
1	E	296	TYR	CB-CG-CD1	-5.04	117.97	121.00	5	2

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	C	307	ARG	Sidechain	2
1	D	247	TYR	Sidechain	2
1	E	307	ARG	Sidechain	1
1	D	261	TYR	Sidechain	1
1	C	261	TYR	Sidechain	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	1025	989	987	6±2
1	B	1027	994	992	5±2
1	C	988	959	957	5±2
1	D	991	966	964	6±2
1	E	1014	983	981	6±2
All	All	75675	73365	73215	367

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:299:LEU:HD12	1:B:300:VAL:N	0.78	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:262:LEU:HD23	1:D:262:LEU:H	0.73	1.44	13	3
1:D:262:LEU:H	1:D:262:LEU:HD23	0.73	1.44	12	1
1:B:262:LEU:HD23	1:B:262:LEU:H	0.72	1.43	12	1
1:B:317:LEU:HD13	1:B:317:LEU:H	0.70	1.46	10	1
1:A:262:LEU:HD23	1:A:262:LEU:H	0.69	1.48	15	2
1:E:299:LEU:H	1:E:299:LEU:HD22	0.69	1.47	14	1
1:D:299:LEU:HD23	1:E:300:VAL:HG13	0.68	1.63	5	2
1:B:310:LEU:HD13	1:B:311:LYS:N	0.67	2.05	8	1
1:E:262:LEU:H	1:E:262:LEU:HD23	0.66	1.51	3	1
1:A:250:THR:O	1:A:253:THR:HG22	0.65	1.92	13	2
1:B:250:THR:O	1:B:253:THR:HG22	0.64	1.93	10	3
1:C:300:VAL:O	1:C:303:VAL:HG22	0.63	1.94	12	12
1:E:257:THR:O	1:E:260:TYR:CE1	0.63	2.52	1	2
1:A:262:LEU:HD13	1:A:262:LEU:H	0.61	1.55	6	5
1:E:306:LEU:HD13	1:E:307:ARG:N	0.61	2.10	1	2
1:A:254:VAL:HG21	1:E:253:THR:OG1	0.61	1.96	11	3
1:D:203:ILE:O	1:D:205:GLN:N	0.60	2.34	8	7
1:A:310:LEU:HD13	1:A:311:LYS:N	0.60	2.12	10	1
1:E:317:LEU:HD23	1:E:317:LEU:O	0.60	1.97	12	7
1:D:182:LEU:H	1:D:182:LEU:HD13	0.59	1.57	10	1
1:A:262:LEU:HD12	1:A:262:LEU:H	0.59	1.57	12	1
1:E:299:LEU:HD22	1:E:299:LEU:H	0.59	1.57	10	2
1:C:299:LEU:HD23	1:C:300:VAL:N	0.59	2.12	1	1
1:A:194:ALA:H	1:A:195:PRO:CD	0.58	2.11	3	11
1:D:253:THR:OG1	1:E:254:VAL:HG21	0.58	1.98	10	2
1:D:251:TYR:O	1:D:254:VAL:HG22	0.58	1.98	14	3
1:A:251:TYR:O	1:A:254:VAL:HG22	0.58	1.99	7	11
1:E:317:LEU:O	1:E:317:LEU:HD23	0.58	1.99	9	7
1:D:300:VAL:O	1:D:303:VAL:HG22	0.57	1.99	9	11
1:A:247:TYR:CD1	1:E:246:THR:HG21	0.57	2.34	6	2
1:E:262:LEU:HD12	1:E:262:LEU:H	0.57	1.59	12	1
1:D:257:THR:O	1:D:260:TYR:CE1	0.57	2.58	15	1
1:B:299:LEU:HD12	1:B:300:VAL:H	0.57	1.60	6	1
1:E:311:LYS:HZ2	1:E:314:ARG:HH22	0.56	1.43	15	1
1:A:300:VAL:O	1:A:303:VAL:HG22	0.56	2.00	6	5
1:E:251:TYR:O	1:E:254:VAL:HG22	0.56	2.00	6	8
1:E:265:GLN:NE2	1:E:265:GLN:H	0.56	1.99	14	1
1:D:224:VAL:HG11	1:D:248:PHE:CD1	0.55	2.36	6	1
1:E:300:VAL:O	1:E:303:VAL:HG22	0.55	2.02	7	1
1:D:250:THR:O	1:D:253:THR:HG22	0.55	2.02	1	3
1:D:262:LEU:H	1:D:262:LEU:HD13	0.54	1.61	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:ILE:O	1:A:205:GLN:N	0.54	2.40	4	3
1:D:246:THR:HG21	1:E:247:TYR:CD1	0.54	2.38	4	2
1:D:244:PRO:O	1:D:247:TYR:CD2	0.53	2.61	7	1
1:E:262:LEU:H	1:E:262:LEU:HD12	0.53	1.62	8	1
1:D:262:LEU:HD13	1:D:262:LEU:H	0.53	1.63	10	2
1:A:261:TYR:CE1	1:E:263:TYR:CD1	0.53	2.97	9	2
1:E:262:LEU:HD13	1:E:262:LEU:H	0.53	1.63	15	1
1:E:299:LEU:HD22	1:E:299:LEU:N	0.53	2.18	14	3
1:B:251:TYR:O	1:B:254:VAL:HG22	0.52	2.04	7	1
1:B:184:LEU:HD12	1:B:309:GLN:HE21	0.52	1.63	11	1
1:C:262:LEU:HD12	1:C:262:LEU:H	0.52	1.63	2	1
1:C:303:VAL:HG12	1:D:303:VAL:HG21	0.52	1.81	15	4
1:B:188:ASN:HD21	1:C:307:ARG:HH21	0.52	1.47	13	3
1:B:203:ILE:O	1:B:205:GLN:N	0.52	2.43	13	6
1:C:297:ASN:ND2	1:C:298:ARG:N	0.52	2.58	11	7
1:B:262:LEU:HD13	1:B:262:LEU:H	0.52	1.65	15	3
1:A:295:LYS:O	1:A:299:LEU:HD22	0.52	2.05	10	3
1:B:300:VAL:O	1:B:303:VAL:HG22	0.51	2.04	9	2
1:A:306:LEU:HD23	1:A:307:ARG:N	0.51	2.20	2	1
1:D:299:LEU:HD11	1:E:300:VAL:HG13	0.51	1.81	8	1
1:B:262:LEU:H	1:B:262:LEU:HD13	0.51	1.65	2	5
1:B:184:LEU:HD12	1:C:307:ARG:HH22	0.51	1.64	1	1
1:E:203:ILE:HD13	1:E:203:ILE:O	0.51	2.06	3	1
1:B:290:ASN:HD22	1:B:290:ASN:N	0.50	2.05	6	2
1:C:309:GLN:HE22	1:D:307:ARG:HE	0.50	1.49	10	1
1:B:297:ASN:ND2	1:B:298:ARG:N	0.49	2.60	8	5
1:A:299:LEU:HD23	1:A:300:VAL:N	0.49	2.21	4	2
1:A:308:ASN:HD22	1:E:185:GLN:HE22	0.49	1.50	9	2
1:A:262:LEU:H	1:A:262:LEU:HD13	0.49	1.67	14	2
1:D:265:GLN:H	1:D:265:GLN:NE2	0.49	2.05	11	1
1:D:297:ASN:ND2	1:D:298:ARG:N	0.49	2.60	9	1
1:D:231:ARG:HH21	1:D:239:TRP:HE1	0.49	1.51	6	3
1:D:182:LEU:HD22	1:D:183:LEU:N	0.48	2.23	2	2
1:E:264:THR:HG23	1:E:290:ASN:H	0.48	1.69	12	1
1:D:263:TYR:CD1	1:E:261:TYR:CE1	0.48	3.02	14	5
1:E:244:PRO:O	1:E:247:TYR:CD2	0.48	2.66	1	1
1:C:253:THR:O	1:C:256:ALA:HB3	0.48	2.09	2	2
1:C:188:ASN:N	1:C:188:ASN:HD22	0.48	2.07	14	1
1:C:251:TYR:O	1:C:254:VAL:HG22	0.48	2.09	3	2
1:B:184:LEU:HD12	1:C:307:ARG:NH2	0.47	2.23	2	3
1:A:188:ASN:HD22	1:B:307:ARG:NH1	0.47	2.07	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:262:LEU:H	1:D:262:LEU:CD2	0.47	2.19	13	2
1:E:203:ILE:O	1:E:205:GLN:N	0.47	2.47	5	1
1:C:188:ASN:HD22	1:C:188:ASN:N	0.47	2.07	15	1
1:D:316:PRO:O	1:D:317:LEU:HD23	0.47	2.09	12	1
1:A:306:LEU:HD22	1:B:306:LEU:HD21	0.47	1.85	12	1
1:B:309:GLN:HE22	1:C:307:ARG:NE	0.47	2.07	11	1
1:E:250:THR:O	1:E:253:THR:HG22	0.47	2.09	2	3
1:C:202:LYS:O	1:C:204:GLU:N	0.47	2.47	8	1
1:E:306:LEU:O	1:E:306:LEU:HD22	0.47	2.10	6	1
1:A:231:ARG:HE	1:A:239:TRP:HE1	0.47	1.53	4	1
1:E:235:TRP:NE1	1:E:239:TRP:NE1	0.47	2.61	12	2
1:E:307:ARG:O	1:E:307:ARG:CZ	0.46	2.64	6	1
1:E:231:ARG:HH11	1:E:240:ASP:N	0.46	2.08	4	1
1:C:252:SER:O	1:C:255:ALA:HB3	0.46	2.11	1	1
1:D:182:LEU:HD12	1:D:183:LEU:N	0.46	2.25	12	1
1:B:303:VAL:HG22	1:C:303:VAL:HG21	0.46	1.86	8	1
1:E:306:LEU:HD12	1:E:307:ARG:N	0.46	2.25	5	1
1:E:295:LYS:O	1:E:299:LEU:HD22	0.46	2.11	3	2
1:B:235:TRP:NE1	1:B:239:TRP:NE1	0.46	2.63	9	4
1:E:266:GLN:HE21	1:E:267:SER:H	0.46	1.53	1	1
1:D:303:VAL:O	1:D:306:LEU:HB3	0.46	2.11	12	2
1:C:290:ASN:ND2	1:C:294:GLU:H	0.46	2.09	3	1
1:E:191:THR:HG21	1:E:302:GLU:OE1	0.46	2.11	14	1
1:D:297:ASN:HD21	1:D:298:ARG:HH21	0.46	1.54	12	1
1:B:263:TYR:CE1	1:C:261:TYR:CZ	0.45	3.05	11	1
1:D:252:SER:O	1:D:255:ALA:HB3	0.45	2.12	11	1
1:D:257:THR:O	1:D:260:TYR:CE2	0.45	2.69	2	2
1:C:253:THR:OG1	1:D:254:VAL:HG21	0.45	2.11	14	1
1:A:205:GLN:NE2	1:A:205:GLN:H	0.45	2.10	11	1
1:C:293:ILE:N	1:C:293:ILE:HD12	0.45	2.27	8	1
1:D:262:LEU:CD2	1:D:262:LEU:H	0.45	2.23	8	1
1:A:235:TRP:NE1	1:A:239:TRP:NE1	0.45	2.65	11	2
1:A:309:GLN:HE22	1:B:314:ARG:HH22	0.45	1.53	7	1
1:B:263:TYR:CD2	1:C:261:TYR:CE2	0.45	3.05	15	1
1:C:309:GLN:NE2	1:C:309:GLN:O	0.45	2.50	9	1
1:A:303:VAL:O	1:A:306:LEU:HG	0.44	2.11	15	1
1:B:263:TYR:CE1	1:B:291:PHE:CZ	0.44	3.04	11	1
1:A:263:TYR:CD1	1:B:261:TYR:CE1	0.44	3.05	2	3
1:A:306:LEU:HD12	1:A:307:ARG:N	0.44	2.27	10	3
1:D:182:LEU:HD13	1:D:182:LEU:H	0.44	1.72	13	1
1:C:244:PRO:O	1:C:247:TYR:CD1	0.44	2.70	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:263:TYR:OH	1:C:261:TYR:CZ	0.44	2.68	4	1
1:A:194:ALA:N	1:A:195:PRO:CD	0.44	2.80	5	4
1:B:262:LEU:CD2	1:B:262:LEU:H	0.44	2.21	12	1
1:B:241:ILE:HG22	1:B:241:ILE:O	0.44	2.13	14	1
1:C:303:VAL:HG22	1:D:303:VAL:HG21	0.44	1.90	3	1
1:A:252:SER:O	1:A:255:ALA:HB3	0.44	2.12	9	2
1:A:262:LEU:CD2	1:A:262:LEU:H	0.43	2.22	15	2
1:C:225:GLN:NE2	1:C:225:GLN:H	0.43	2.11	4	1
1:D:235:TRP:NE1	1:D:239:TRP:NE1	0.43	2.67	13	8
1:A:306:LEU:C	1:A:306:LEU:HD12	0.43	2.34	12	1
1:C:263:TYR:CD1	1:D:261:TYR:CE1	0.43	3.06	8	1
1:C:227:GLY:O	1:C:230:ALA:HB3	0.43	2.13	7	2
1:C:290:ASN:HD21	1:C:294:GLU:H	0.43	1.57	3	1
1:A:307:ARG:NH1	1:A:311:LYS:HZ1	0.43	2.12	2	1
1:E:302:GLU:N	1:E:302:GLU:OE1	0.43	2.51	13	1
1:B:252:SER:O	1:B:255:ALA:HB3	0.43	2.14	6	4
1:A:299:LEU:HD23	1:A:300:VAL:H	0.43	1.74	4	1
1:C:205:GLN:H	1:C:205:GLN:NE2	0.43	2.11	8	1
1:C:235:TRP:NE1	1:C:239:TRP:NE1	0.43	2.67	2	1
1:B:263:TYR:CZ	1:C:261:TYR:OH	0.42	2.68	2	1
1:D:224:VAL:O	1:D:227:GLY:N	0.42	2.52	7	3
1:B:188:ASN:HD21	1:C:307:ARG:NH2	0.42	2.12	3	1
1:C:262:LEU:H	1:C:262:LEU:HD13	0.42	1.74	6	1
1:E:297:ASN:ND2	1:E:298:ARG:N	0.42	2.67	5	1
1:A:307:ARG:CZ	1:E:309:GLN:HE22	0.42	2.28	12	1
1:E:306:LEU:HD22	1:E:306:LEU:C	0.42	2.35	13	1
1:C:299:LEU:HD23	1:C:300:VAL:H	0.42	1.74	1	1
1:B:303:VAL:O	1:B:306:LEU:HB3	0.42	2.15	15	2
1:B:263:TYR:CZ	1:C:261:TYR:CZ	0.42	3.08	15	1
1:D:310:LEU:HD12	1:D:311:LYS:N	0.42	2.30	15	2
1:A:293:ILE:HD12	1:A:293:ILE:N	0.42	2.30	14	5
1:A:310:LEU:HD13	1:E:306:LEU:HD23	0.42	1.90	6	1
1:B:301:THR:O	1:B:304:ASP:N	0.42	2.53	8	3
1:C:257:THR:O	1:C:260:TYR:CE1	0.41	2.73	2	1
1:A:257:THR:O	1:A:260:TYR:CE2	0.41	2.73	13	1
1:C:206:GLU:O	1:C:208:GLU:N	0.41	2.53	9	1
1:C:300:VAL:O	1:C:303:VAL:HG13	0.41	2.15	9	1
1:D:310:LEU:HD22	1:D:310:LEU:C	0.41	2.36	2	1
1:B:262:LEU:H	1:B:262:LEU:HD12	0.41	1.74	6	1
1:B:309:GLN:HE21	1:C:307:ARG:HH12	0.41	1.56	1	1
1:B:253:THR:O	1:B:256:ALA:HB3	0.41	2.15	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:293:ILE:N	1:D:293:ILE:HD12	0.41	2.30	8	1
1:A:205:GLN:O	1:A:207:ALA:N	0.41	2.54	12	1
1:D:309:GLN:HE21	1:E:314:ARG:NH1	0.41	2.13	8	1
1:B:262:LEU:N	1:B:262:LEU:HD13	0.41	2.30	13	1
1:A:297:ASN:ND2	1:A:298:ARG:N	0.41	2.68	6	1
1:A:185:GLN:N	1:B:311:LYS:NZ	0.41	2.69	1	1
1:B:188:ASN:N	1:B:188:ASN:HD22	0.41	2.14	15	1
1:C:299:LEU:HD23	1:D:300:VAL:HG13	0.40	1.92	12	1
1:A:263:TYR:CZ	1:B:261:TYR:OH	0.40	2.71	7	1
1:D:257:THR:O	1:D:260:TYR:CD1	0.40	2.74	15	1
1:B:188:ASN:HD22	1:B:188:ASN:N	0.40	2.13	8	1
1:B:262:LEU:HD12	1:B:262:LEU:N	0.40	2.31	6	1
1:B:263:TYR:CD1	1:C:261:TYR:CE1	0.40	3.09	3	1
1:B:309:GLN:HE21	1:C:307:ARG:NH1	0.40	2.15	1	1
1:E:311:LYS:HZ2	1:E:314:ARG:NH2	0.40	2.11	15	1
1:C:301:THR:O	1:C:304:ASP:N	0.40	2.54	10	1
1:A:307:ARG:NH1	1:A:311:LYS:NZ	0.40	2.69	2	1
1:B:235:TRP:CZ2	1:B:239:TRP:CE2	0.40	3.10	13	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	122/159 (77%)	99±2 (81±1%)	8±2 (7±1%)	15±2 (12±1%)	1	7
1	B	122/159 (77%)	100±2 (82±2%)	8±3 (7±2%)	14±2 (11±2%)	1	8
1	C	119/159 (75%)	95±2 (80±2%)	10±2 (8±2%)	14±2 (12±2%)	1	7
1	D	119/159 (75%)	97±2 (81±2%)	12±3 (10±2%)	11±2 (9±1%)	2	13
1	E	121/159 (76%)	99±3 (82±2%)	9±2 (7±2%)	13±2 (11±2%)	1	9
All	All	9045/11925 (76%)	7352 (81%)	692 (8%)	1001 (11%)	1	9

All 114 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	E	316	PRO	15
1	E	243	GLU	15
1	E	291	PHE	15
1	A	194	ALA	15
1	A	291	PHE	15
1	A	238	SER	15
1	C	242	VAL	15
1	E	193	LEU	15
1	C	239	TRP	15
1	C	243	GLU	15
1	B	238	SER	15
1	B	204	GLU	15
1	A	242	VAL	15
1	E	317	LEU	15
1	D	242	VAL	15
1	A	316	PRO	15
1	B	195	PRO	15
1	D	243	GLU	15
1	A	243	GLU	15
1	A	241	ILE	14
1	B	317	LEU	14
1	C	317	LEU	14
1	B	243	GLU	14
1	B	242	VAL	14
1	B	239	TRP	14
1	C	238	SER	14
1	C	240	ASP	14
1	D	204	GLU	13
1	D	238	SER	13
1	C	203	ILE	13
1	E	239	TRP	13
1	C	241	ILE	13
1	E	238	SER	13
1	A	235	TRP	13
1	A	259	GLY	13
1	E	242	VAL	12
1	E	240	ASP	12
1	B	240	ASP	12
1	D	239	TRP	12
1	A	292	ASP	12
1	C	204	GLU	12
1	A	240	ASP	12
1	E	235	TRP	12

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Mol	Chain	Res	Type	Models (Total)
1	D	316	PRO	11
1	C	195	PRO	11
1	A	193	LEU	11
1	C	193	LEU	11
1	B	259	GLY	11
1	C	292	ASP	11
1	B	241	ILE	11
1	E	241	ILE	11
1	B	316	PRO	11
1	C	207	ALA	11
1	B	235	TRP	10
1	B	290	ASN	10
1	D	194	ALA	10
1	A	204	GLU	10
1	A	239	TRP	10
1	D	259	GLY	10
1	D	240	ASP	9
1	B	179	GLU	9
1	C	290	ASN	9
1	A	195	PRO	9
1	A	271	PRO	8
1	D	179	GLU	8
1	D	195	PRO	8
1	E	195	PRO	7
1	D	292	ASP	7
1	B	291	PHE	7
1	B	193	LEU	7
1	C	291	PHE	6
1	D	241	ILE	6
1	E	292	ASP	6
1	D	235	TRP	6
1	A	179	GLU	6
1	B	207	ALA	6
1	C	208	GLU	6
1	E	259	GLY	5
1	A	290	ASN	5
1	E	194	ALA	5
1	C	259	GLY	5
1	E	207	ALA	5
1	B	292	ASP	5
1	C	235	TRP	5
1	E	290	ASN	5

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Mol	Chain	Res	Type	Models (Total)
1	D	317	LEU	4
1	E	178	ARG	4
1	D	207	ALA	4
1	C	205	GLN	4
1	C	262	LEU	4
1	A	289	GLN	4
1	E	204	GLU	4
1	C	194	ALA	3
1	E	177	SER	3
1	A	207	ALA	3
1	E	203	ILE	2
1	B	236	GLU	2
1	D	291	PHE	2
1	A	206	GLU	2
1	C	179	GLU	2
1	D	193	LEU	2
1	D	203	ILE	2
1	B	208	GLU	2
1	A	203	ILE	1
1	A	209	ALA	1
1	D	260	TYR	1
1	C	316	PRO	1
1	A	208	GLU	1
1	E	208	GLU	1
1	B	237	TYR	1
1	B	178	ARG	1
1	B	271	PRO	1
1	C	237	TYR	1
1	C	209	ALA	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	106/138 (77%)	86±2 (81±2%)	20±2 (19±2%)	5	38
1	B	106/138 (77%)	90±3 (85±3%)	16±3 (15±3%)	7	46
1	C	102/138 (74%)	84±2 (82±2%)	18±2 (18±2%)	6	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	102/138 (74%)	85±3 (83±3%)	17±3 (17±3%)	6	43
1	E	105/138 (76%)	83±4 (79±4%)	22±4 (21±4%)	4	33
All	All	7815/10350 (76%)	6416 (82%)	1399 (18%)	5	40

All 318 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	307	ARG	15
1	C	195	PRO	15
1	C	307	ARG	15
1	D	195	PRO	15
1	E	317	LEU	15
1	B	195	PRO	15
1	E	307	ARG	15
1	B	234	TRP	14
1	D	307	ARG	14
1	A	297	ASN	14
1	A	291	PHE	14
1	C	260	TYR	14
1	A	260	TYR	14
1	E	291	PHE	14
1	E	260	TYR	13
1	A	262	LEU	13
1	C	297	ASN	13
1	C	234	TRP	13
1	D	234	TRP	13
1	B	260	TYR	13
1	C	306	LEU	13
1	A	247	TYR	13
1	E	299	LEU	13
1	E	313	LEU	13
1	B	307	ARG	12
1	A	306	LEU	12
1	D	262	LEU	12
1	B	235	TRP	11
1	E	195	PRO	11
1	E	234	TRP	11
1	D	260	TYR	11
1	A	302	GLU	11
1	E	262	LEU	11

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Mol	Chain	Res	Type	Models (Total)
1	B	262	LEU	11
1	B	301	THR	10
1	A	299	LEU	10
1	E	316	PRO	10
1	D	310	LEU	10
1	E	306	LEU	10
1	E	247	TYR	10
1	C	266	GLN	10
1	E	310	LEU	10
1	C	301	THR	10
1	B	313	LEU	9
1	D	299	LEU	9
1	A	257	THR	9
1	C	317	LEU	9
1	E	312	ARG	9
1	C	247	TYR	9
1	A	200	LYS	8
1	E	203	ILE	8
1	E	301	THR	8
1	D	235	TRP	8
1	E	253	THR	8
1	E	264	THR	8
1	C	193	LEU	8
1	D	253	THR	8
1	A	263	TYR	8
1	A	234	TRP	8
1	D	297	ASN	8
1	A	301	THR	8
1	B	291	PHE	8
1	B	297	ASN	7
1	C	299	LEU	7
1	D	193	LEU	7
1	D	247	TYR	7
1	D	317	LEU	7
1	A	186	LEU	7
1	C	241	ILE	7
1	E	197	HIS	7
1	B	243	GLU	7
1	D	243	GLU	7
1	C	291	PHE	6
1	A	241	ILE	6
1	C	263	TYR	6

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Mol	Chain	Res	Type	Models (Total)
1	C	203	ILE	6
1	B	317	LEU	6
1	E	243	GLU	6
1	C	258	PHE	6
1	D	186	LEU	6
1	E	235	TRP	6
1	E	241	ILE	6
1	C	262	LEU	6
1	D	311	LYS	6
1	D	301	THR	6
1	B	304	ASP	6
1	A	232	LEU	6
1	E	297	ASN	6
1	C	310	LEU	6
1	D	257	THR	6
1	B	197	HIS	5
1	A	193	LEU	5
1	A	310	LEU	5
1	D	180	LYS	5
1	D	208	GLU	5
1	E	263	TYR	5
1	B	310	LEU	5
1	A	290	ASN	5
1	D	185	GLN	5
1	E	251	TYR	5
1	A	231	ARG	5
1	B	247	TYR	5
1	C	253	THR	4
1	D	304	ASP	4
1	B	290	ASN	4
1	A	294	GLU	4
1	E	305	GLU	4
1	C	188	ASN	4
1	D	181	LYS	4
1	E	300	VAL	4
1	B	263	TYR	4
1	A	311	LYS	4
1	C	216	TRP	4
1	A	197	HIS	4
1	C	182	LEU	4
1	C	250	THR	4
1	A	271	PRO	4

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Mol	Chain	Res	Type	Models (Total)
1	E	216	TRP	4
1	A	258	PHE	4
1	B	241	ILE	4
1	B	270	TYR	4
1	E	315	ASP	4
1	C	315	ASP	4
1	C	197	HIS	4
1	B	306	LEU	4
1	A	205	GLN	4
1	B	250	THR	4
1	B	239	TRP	4
1	A	317	LEU	4
1	E	295	LYS	4
1	D	182	LEU	4
1	B	193	LEU	4
1	A	318	GLU	4
1	E	258	PHE	4
1	E	183	LEU	3
1	E	302	GLU	3
1	B	201	ARG	3
1	D	216	TRP	3
1	B	299	LEU	3
1	B	236	GLU	3
1	E	261	TYR	3
1	D	188	ASN	3
1	E	257	THR	3
1	A	253	THR	3
1	D	291	PHE	3
1	C	261	TYR	3
1	D	315	ASP	3
1	A	304	ASP	3
1	B	303	VAL	3
1	D	214	VAL	3
1	A	185	GLN	3
1	E	304	ASP	3
1	E	208	GLU	3
1	B	314	ARG	3
1	A	190	GLU	3
1	E	188	ASN	3
1	C	312	ARG	3
1	B	316	PRO	3
1	D	295	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	B	204	GLU	3
1	A	235	TRP	3
1	E	303	VAL	3
1	D	203	ILE	3
1	A	182	LEU	3
1	E	314	ARG	3
1	A	312	ARG	3
1	C	186	LEU	3
1	E	311	LYS	3
1	C	290	ASN	3
1	A	289	GLN	3
1	B	258	PHE	3
1	B	208	GLU	3
1	D	303	VAL	3
1	C	257	THR	3
1	D	258	PHE	3
1	B	315	ASP	3
1	B	309	GLN	3
1	E	265	GLN	3
1	C	294	GLU	3
1	E	266	GLN	3
1	B	188	ASN	3
1	A	243	GLU	3
1	E	290	ASN	3
1	E	292	ASP	2
1	D	178	ARG	2
1	C	181	LYS	2
1	D	305	GLU	2
1	C	302	GLU	2
1	B	312	ARG	2
1	E	309	GLN	2
1	A	250	THR	2
1	C	311	LYS	2
1	D	184	LEU	2
1	C	200	LYS	2
1	D	294	GLU	2
1	C	246	THR	2
1	D	312	ARG	2
1	B	186	LEU	2
1	A	206	GLU	2
1	B	257	THR	2
1	A	203	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	B	231	ARG	2
1	B	266	GLN	2
1	A	266	GLN	2
1	B	252	SER	2
1	B	225	GLN	2
1	A	305	GLU	2
1	B	200	LYS	2
1	A	313	LEU	2
1	C	239	TRP	2
1	C	232	LEU	2
1	C	206	GLU	2
1	E	186	LEU	2
1	C	314	ARG	2
1	E	185	GLN	2
1	C	305	GLU	2
1	E	178	ARG	2
1	A	181	LYS	2
1	E	200	LYS	2
1	E	231	ARG	2
1	A	264	THR	2
1	C	309	GLN	2
1	E	193	LEU	2
1	A	184	LEU	2
1	D	192	LEU	2
1	A	188	ASN	2
1	B	178	ARG	2
1	C	235	TRP	2
1	B	206	GLU	2
1	D	292	ASP	2
1	A	179	GLU	2
1	C	208	GLU	2
1	A	224	VAL	2
1	A	228	LEU	2
1	A	315	ASP	2
1	D	302	GLU	2
1	B	253	THR	2
1	D	306	LEU	2
1	E	187	GLU	2
1	E	201	ARG	2
1	A	198	ASP	1
1	C	251	TYR	1
1	B	294	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	196	LEU	1
1	D	250	THR	1
1	D	179	GLU	1
1	C	313	LEU	1
1	E	180	LYS	1
1	C	214	VAL	1
1	A	236	GLU	1
1	E	269	GLU	1
1	A	239	TRP	1
1	A	195	PRO	1
1	A	204	GLU	1
1	A	293	ILE	1
1	A	180	LYS	1
1	B	311	LYS	1
1	A	251	TYR	1
1	D	200	LYS	1
1	E	239	TRP	1
1	A	216	TRP	1
1	A	192	LEU	1
1	B	181	LYS	1
1	E	252	SER	1
1	D	268	PHE	1
1	C	264	THR	1
1	A	183	LEU	1
1	A	202	LYS	1
1	C	184	LEU	1
1	B	302	GLU	1
1	C	183	LEU	1
1	A	201	ARG	1
1	C	269	GLU	1
1	C	296	TYR	1
1	D	205	GLN	1
1	E	224	VAL	1
1	B	318	GLU	1
1	A	269	GLU	1
1	C	254	VAL	1
1	D	202	LYS	1
1	C	179	GLU	1
1	E	192	LEU	1
1	D	263	TYR	1
1	D	206	GLU	1
1	D	293	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	225	GLN	1
1	B	238	SER	1
1	E	254	VAL	1
1	D	213	ARG	1
1	C	205	GLN	1
1	D	246	THR	1
1	D	254	VAL	1
1	D	300	VAL	1
1	D	231	ARG	1
1	E	182	LEU	1
1	A	208	GLU	1
1	C	198	ASP	1
1	D	309	GLN	1
1	E	212	ASP	1
1	C	202	LYS	1
1	C	243	GLU	1
1	D	264	THR	1
1	C	293	ILE	1
1	B	264	THR	1
1	C	233	THR	1
1	D	241	ILE	1
1	E	206	GLU	1
1	D	298	ARG	1
1	E	225	GLN	1
1	B	183	LEU	1
1	A	303	VAL	1
1	D	252	SER	1
1	D	266	GLN	1
1	D	187	GLU	1
1	C	295	LYS	1
1	C	228	LEU	1
1	D	204	GLU	1
1	C	298	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 7% for the well-defined parts and 7% for the entire structure.

7.1 Chemical shift list 1

File name: 5id3_cs.cif

Chemical shift list name: *CS.bmrB*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	657
Number of shifts mapped to atoms	657
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	143	-0.43 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	103	-1.96 ± 0.07	Should be applied
$^{13}\text{C}'$	139	-0.46 ± 0.14	None needed (< 0.5 ppm)
^{15}N	136	0.27 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 7%, i.e. 545 atoms were assigned a chemical shift out of a possible 7817. 0 out of 110 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	460/2996 (15%)	113/1195 (9%)	234/1212 (19%)	113/589 (19%)
Sidechain	85/3935 (2%)	0/2290 (0%)	85/1451 (6%)	0/194 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/886 (0%)	0/458 (0%)	0/388 (0%)	0/40 (0%)
Overall	545/7817 (7%)	113/3943 (3%)	319/3051 (10%)	113/823 (14%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 657 atoms were assigned a chemical shift out of a possible 10025. 0 out of 130 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	554/3785 (15%)	136/1510 (9%)	282/1530 (18%)	136/745 (18%)
Sidechain	103/5165 (2%)	0/3025 (0%)	103/1850 (6%)	0/290 (0%)
Aromatic	0/1075 (0%)	0/555 (0%)	0/480 (0%)	0/40 (0%)
Overall	657/10025 (7%)	136/5090 (3%)	385/3860 (10%)	136/1075 (13%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

