WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 05:39 pm BST

PDB ID	:	6TVM
BMRB ID	:	34475
Title	:	LEDGF/p75 dimer (residues 345-467)
Authors	:	Lux, V.; Veverka, V.
Deposited on	:	2020-01-10

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 45%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
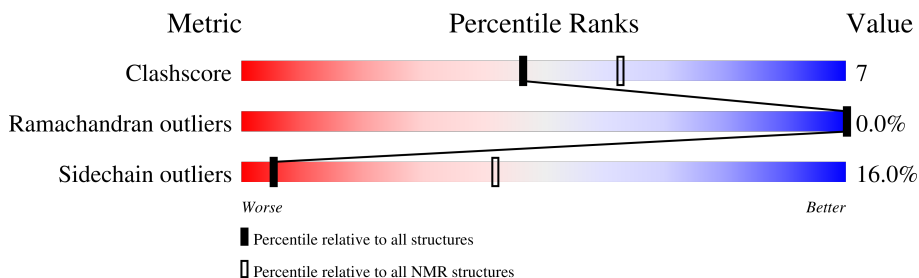
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	128	50% 13% 37%
1	B	128	49% 14% 37%

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. Model 22 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:347-A:427, B:347-B:427 (162)	0.27	22

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

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

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

Cluster number	Models
1	1, 3, 4, 5, 7, 8, 9, 10, 12, 14, 15, 16, 17, 18, 20, 21, 22, 23, 26, 27, 28
2	2, 6, 11, 13, 24, 25, 30
Single-model clusters	19; 29

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 4152 atoms, of which 2114 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms						Trace
1	A	128	Total 2076	C 627	H 1057	N 187	O 198	S 7	0
1	B	128	Total 2076	C 627	H 1057	N 187	O 198	S 7	0

There are 10 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	340	SER	-	expression tag	UNP O75475
A	341	ASN	-	expression tag	UNP O75475
A	342	ALA	-	expression tag	UNP O75475
A	343	ALA	-	expression tag	UNP O75475
A	344	SER	-	expression tag	UNP O75475
B	340	SER	-	expression tag	UNP O75475
B	341	ASN	-	expression tag	UNP O75475
B	342	ALA	-	expression tag	UNP O75475
B	343	ALA	-	expression tag	UNP O75475
B	344	SER	-	expression tag	UNP O75475

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

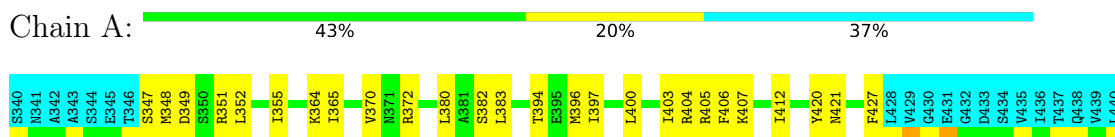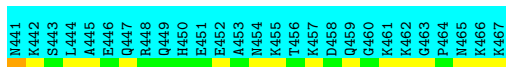• Molecule 1: PC4 and SFRS1-interacting protein
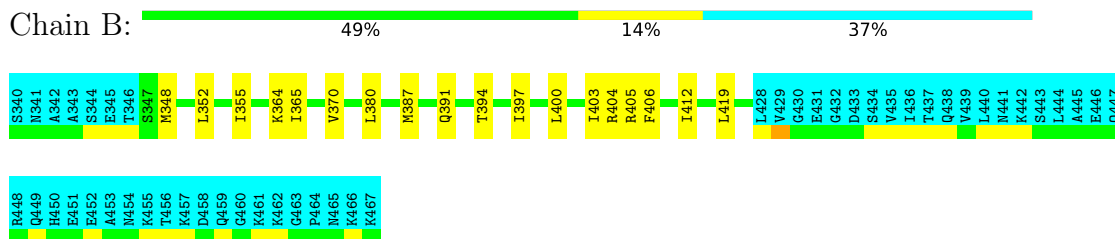
Chain B:

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: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.2 Score per residue for model 2

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.3 Score per residue for model 3

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.4 Score per residue for model 4
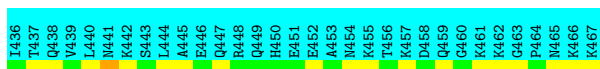
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.5 Score per residue for model 5
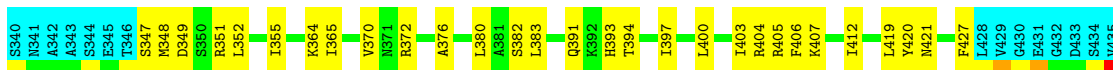
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.6 Score per residue for model 6

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.7 Score per residue for model 7

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.8 Score per residue for model 8

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.9 Score per residue for model 9

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.10 Score per residue for model 10

• Molecule 1: PC4 and SFRS1-interacting protein

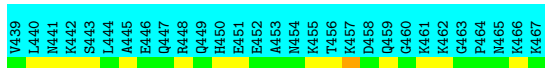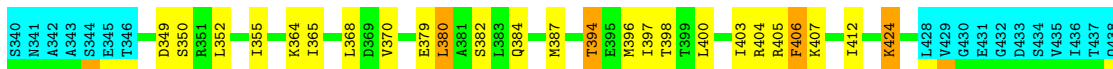Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.11 Score per residue for model 11

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
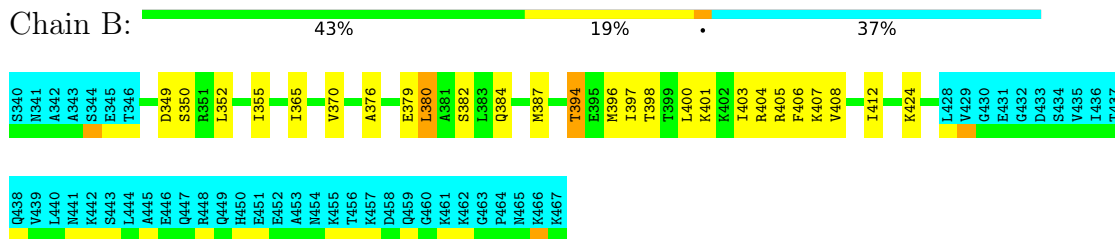

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.12 Score per residue for model 12

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

• Molecule 1: PC4 and SFRS1-interacting protein

4.2.13 Score per residue for model 13

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
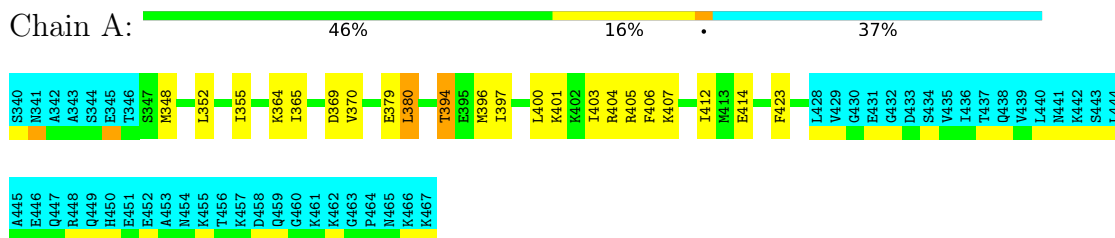
• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

4.2.14 Score per residue for model 14

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
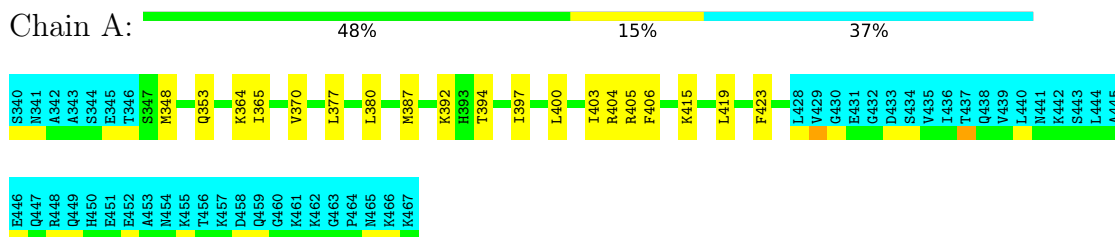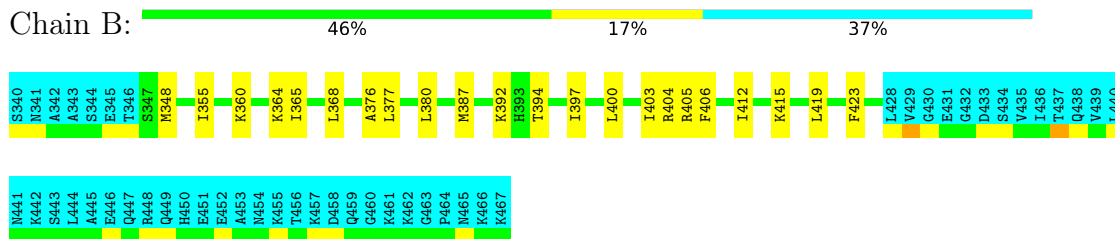
4.2.15 Score per residue for model 15

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

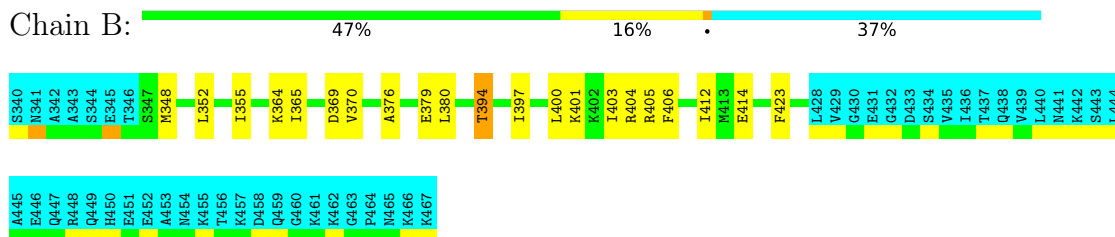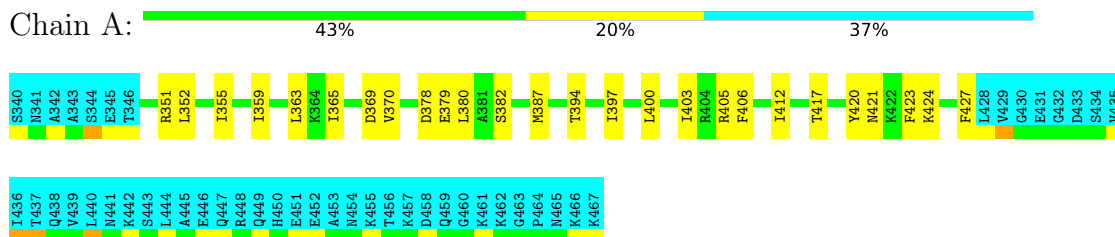Chain B:
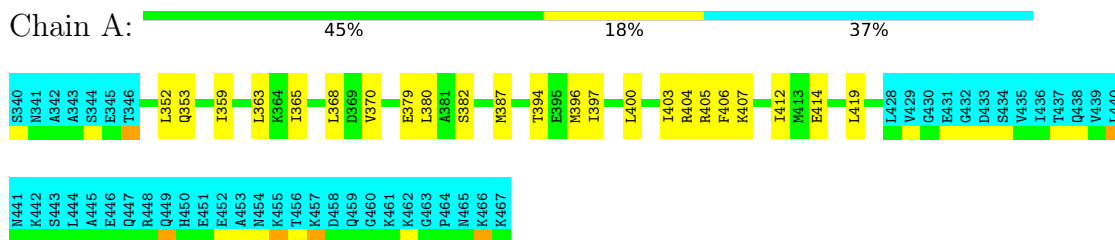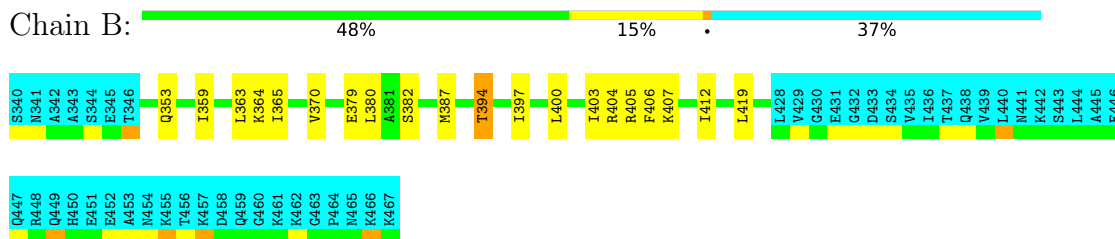
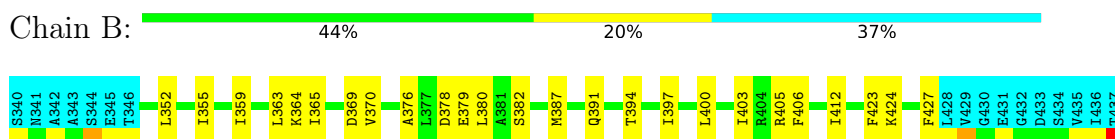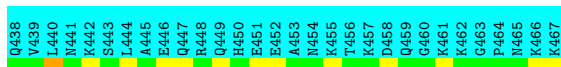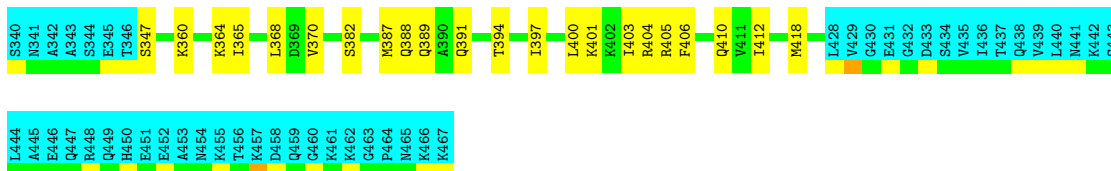### 4.2.16 Score per residue for model 16

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

N441 K442 S443 L444 A445 E446 Q447 R448 Q449 H450 E451 E452 A453 N454 T456 K457 D458 Q459 G460 K461 K462 G463 P464 N465 K466 K467
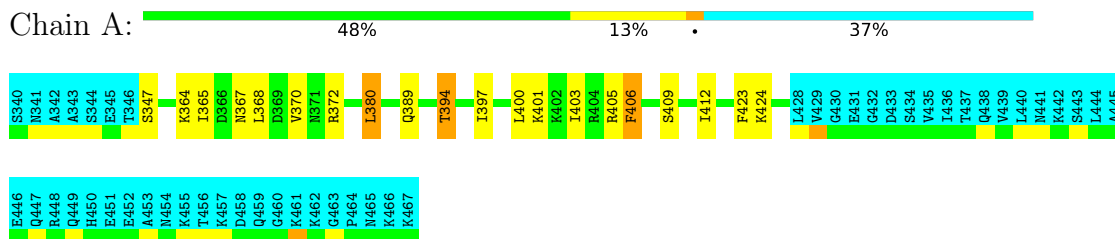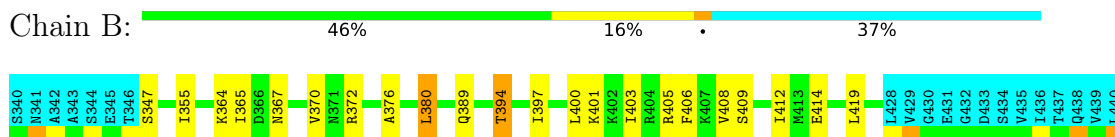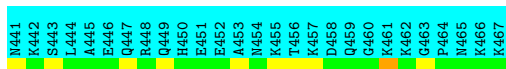
4.2.17   Score per residue for model 17

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

S340 N341 A342 A343 S344 E345 T346 R351 L352 Q353 R354 I355 I359 L363 K364 I365 L368 D369 V370 L377 L380 M387 T394 E395 M396 I397 L400 I403 R404 R405 F406 K407 I412 L419 F427 L428 V429 G430 E431 G432 D433 S434 V435 I436 T437 Q438 V439

L440 N441 K442 S443 L444 A445 E446 Q447 R448 Q449 H450 E451 E452 A453 N454 K455 T456 K457 D458 Q459 G460 K461 K462 G463 P464 N465 K466 K467

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

S340 N341 A342 A343 S344 E345 T346 R351 L352 Q353 R354 I355 I359 L363 K364 I365 V370 A376 L380 M387 T394 I397 I403 R404 R405 F406 K407 I412 M413 E414 L419 F423 F427 L428 V429 G430 E431 G432 D433 S434 V435 I436 T437 Q438 V439 L440

N441 K442 S443 L444 A445 E446 Q447 R448 Q449 H450 E451 E452 A453 N454 K455 T456 K457 D458 Q459 G460 K461 K462 G463 P464 N465 K466 K467

4.2.18   Score per residue for model 18

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

S340 N341 A342 A343 S344 E345 T346 S347 M348 D349 S350 I355 K364 I365 D369 V370 L380 L383 K392 H393 T394 I397 L400 I403 R404 R405 F406 I412 L419 K424 L428 V429 G430 E431 G432 D433 S434 V435 I436 T437 Q438 V439 L440 N441 K442 S443 L444

A445 E446 Q447 R448 Q449 H450 E451 E452 A453 N454 K455 T456 K457 D458 Q459 G460 K461 K462 G463 P464 N465 K466 K467

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

S340 N341 A342 A343 S344 E345 T346 S347 M348 D349 S350 R351 L352 I355 I359 K364 I365 D369 V370 C373 L380 K392 H393 T394 I397 L400 I403 R404 R405 F406 I412 K424 L428 V429 G430 E431 G432 D433 S434 V435 I436 T437 Q438 V439 L440 N441 K442

S443 L444 A445 E446 Q447 R448 Q449 H450 E451 E452 A453 N454 K455 T456 K457 D458 Q459 G460 K461 K462 G463 P464 N465 K466 K467

4.2.19 Score per residue for model 19

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

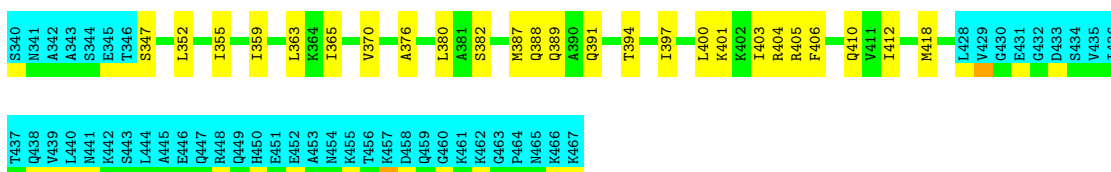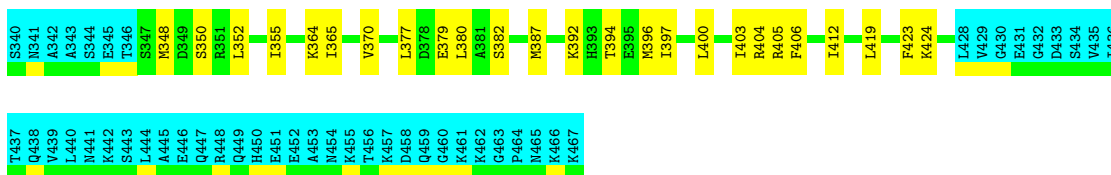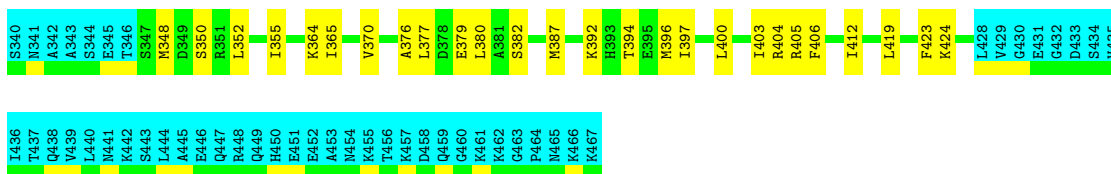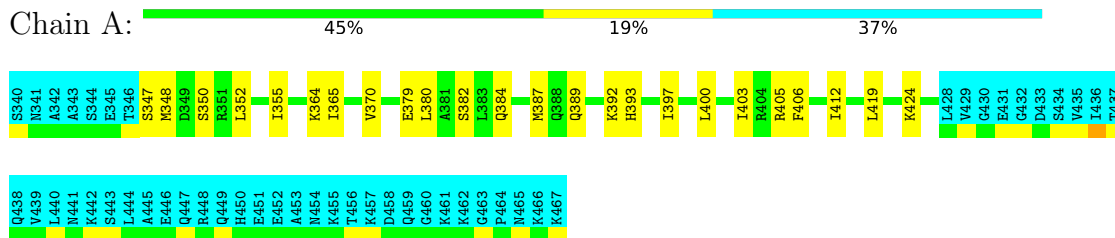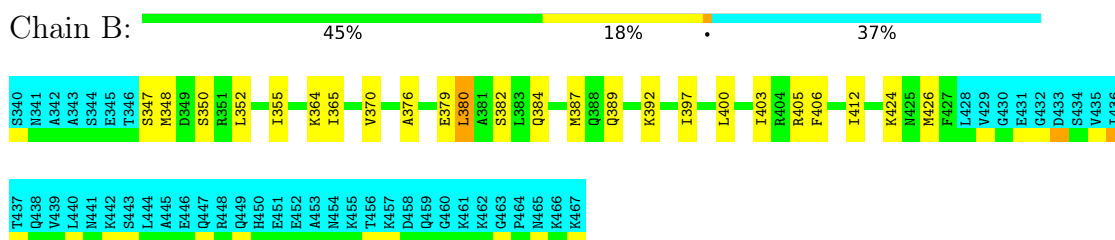• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
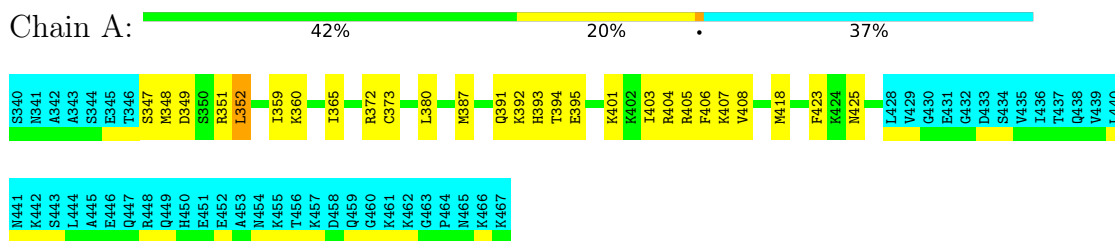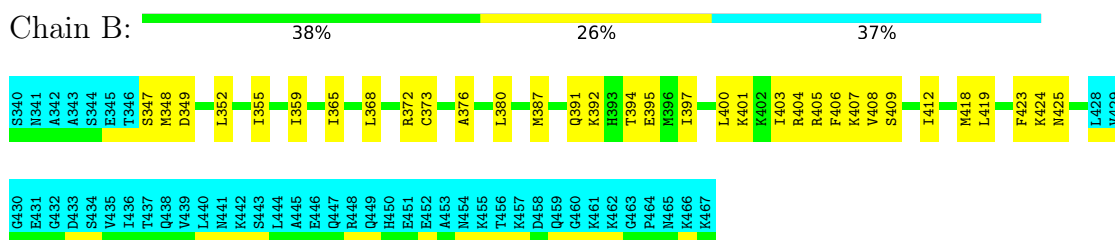
4.2.20 Score per residue for model 20

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:
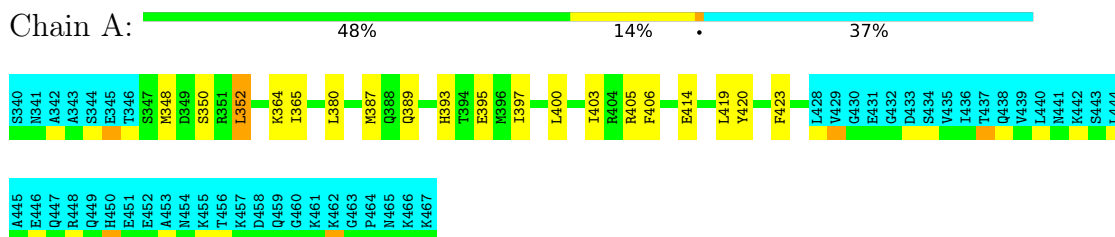
• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
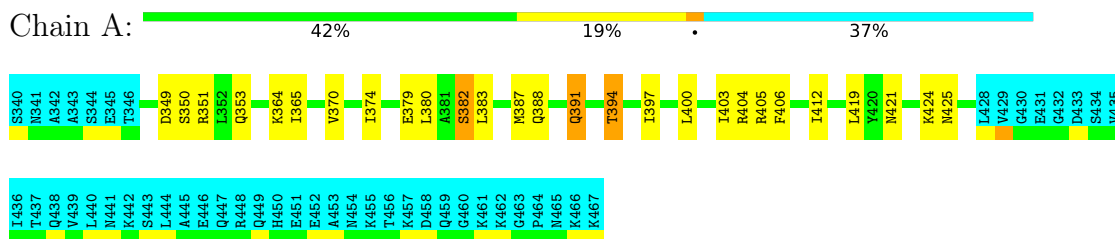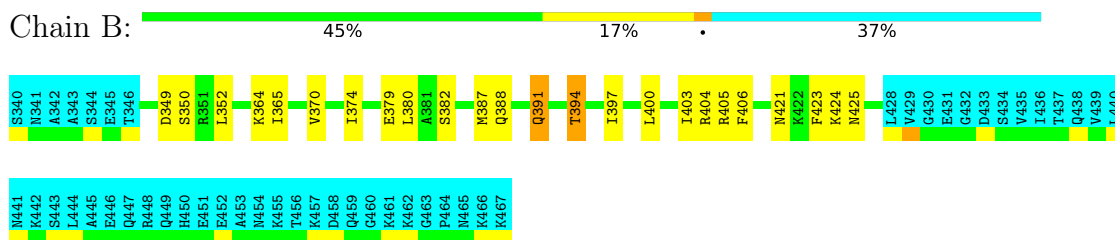
4.2.21 Score per residue for model 21

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
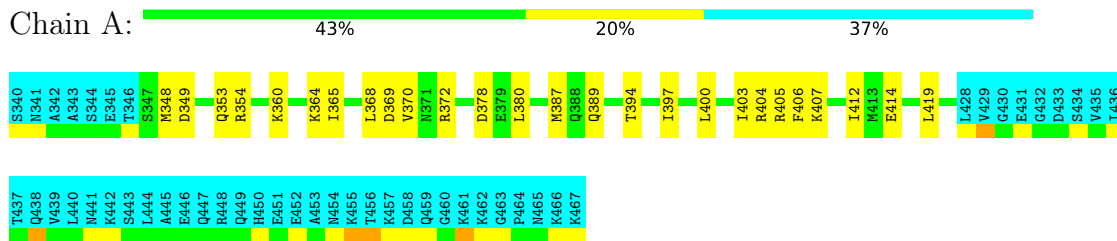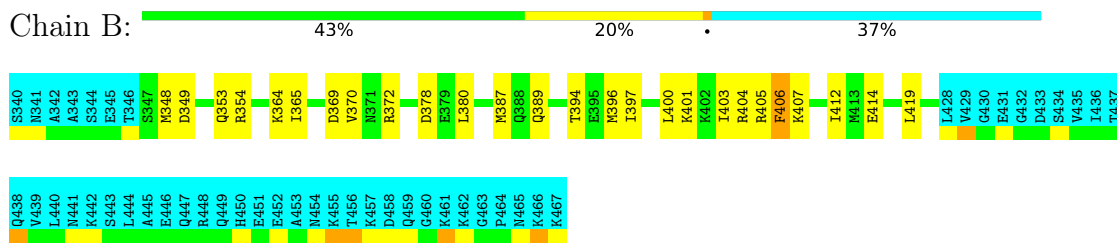
4.2.22 Score per residue for model 22 (medoid)

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

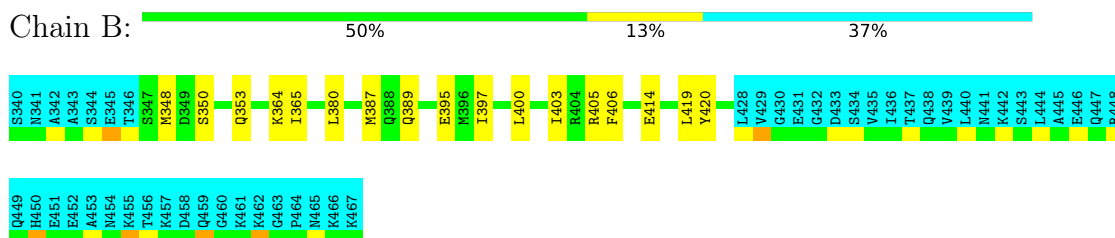• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
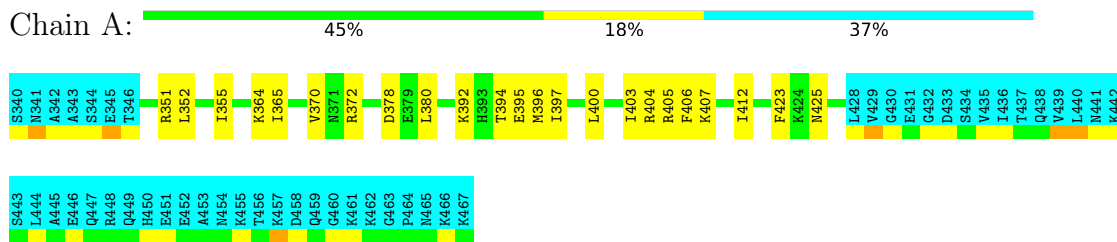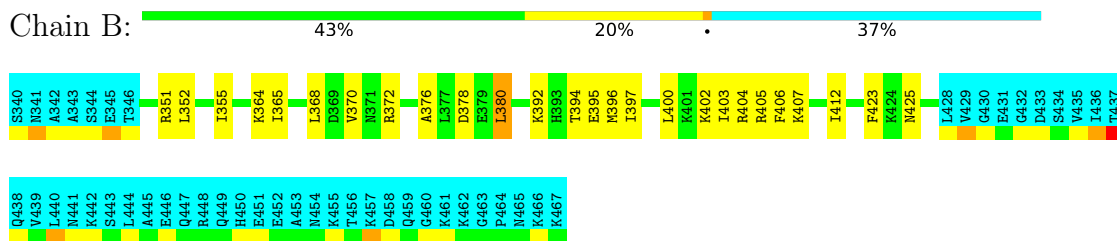
4.2.23 Score per residue for model 23

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
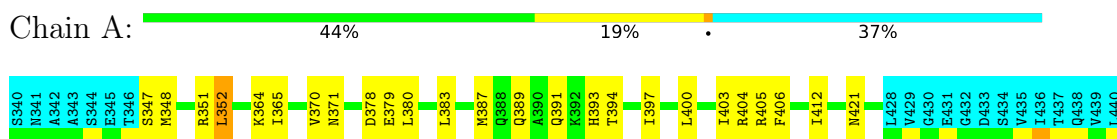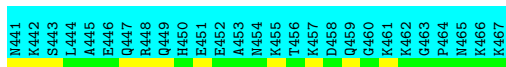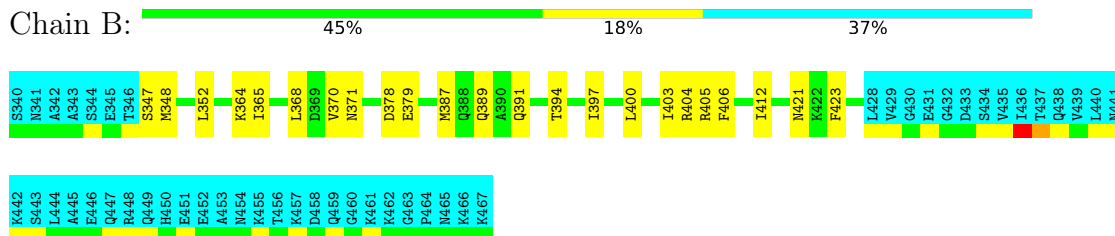
4.2.24 Score per residue for model 24

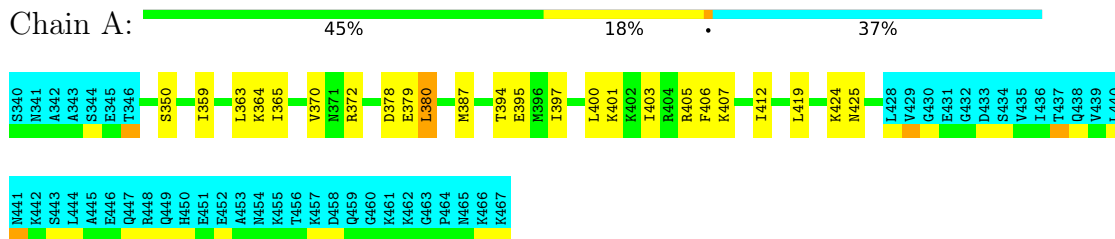• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

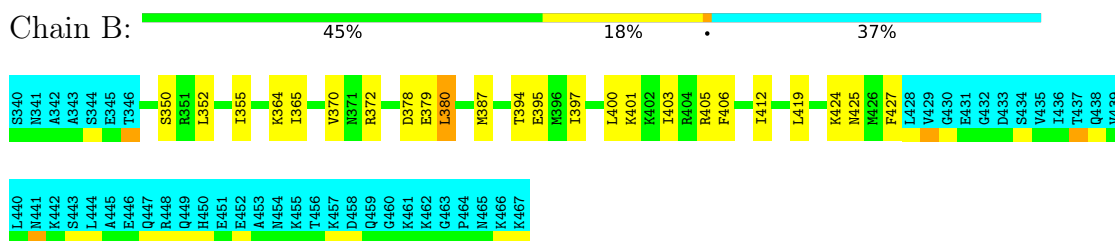• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
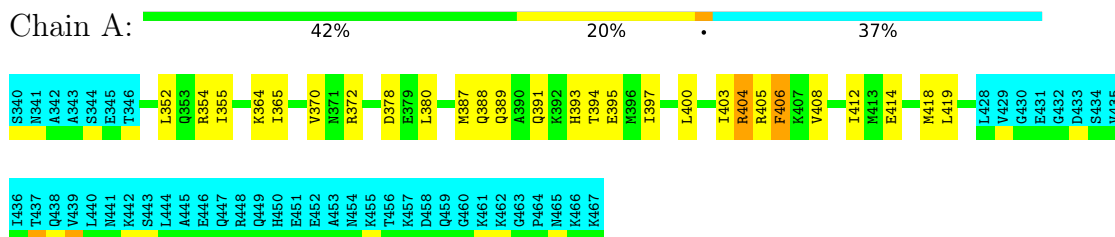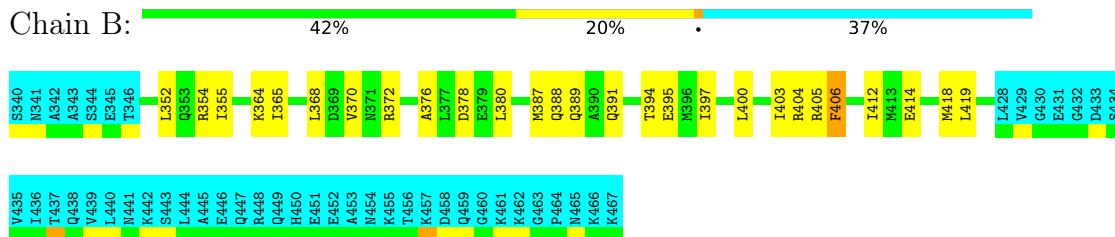
4.2.25 Score per residue for model 25

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B: 49% 13% • 37%
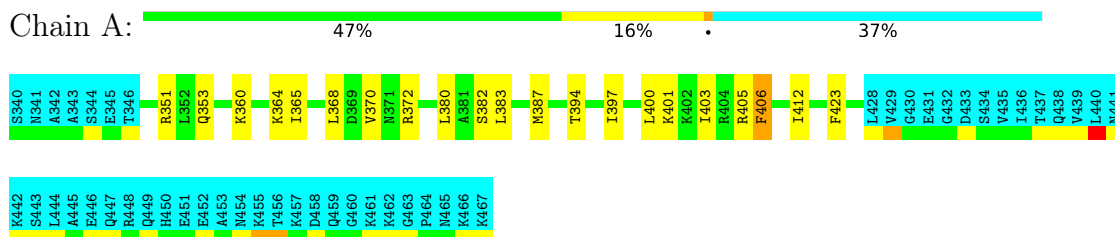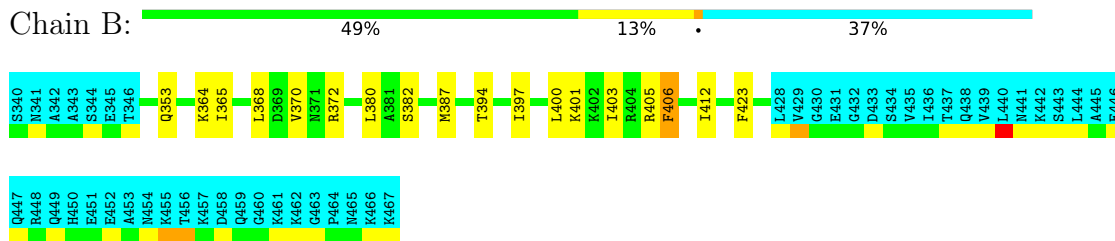
4.2.26 Score per residue for model 26

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 46% 16% • 37%

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B: 46% 16% • 37%
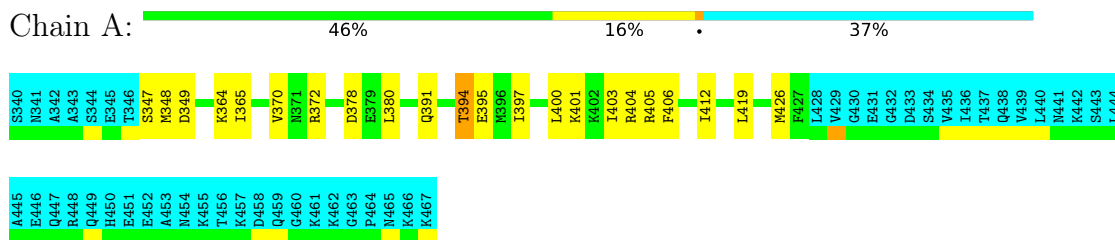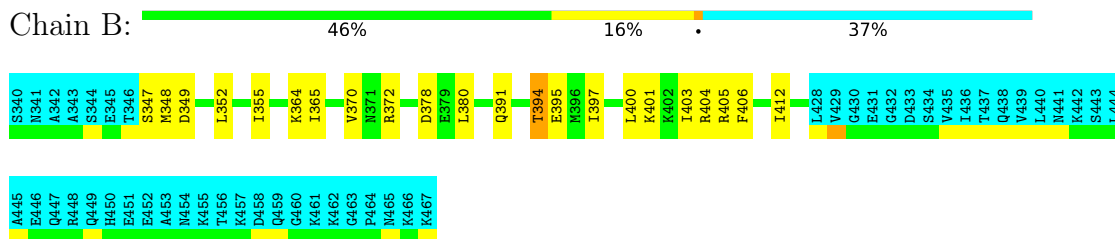
4.2.27 Score per residue for model 27

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 47% 16% 37%

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B: 44% 20% 37%
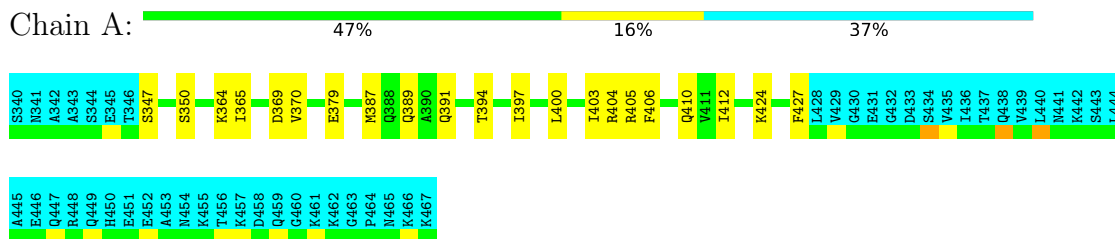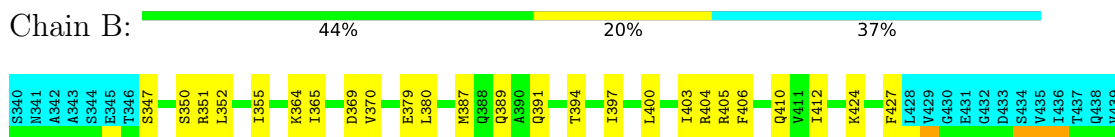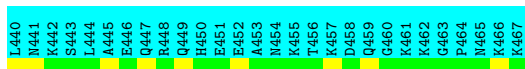
4.2.28 Score per residue for model 28

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
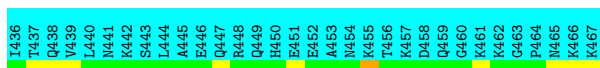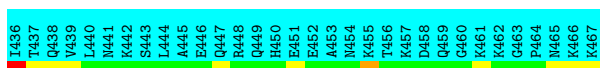
4.2.29 Score per residue for model 29

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
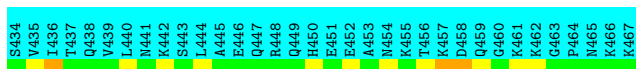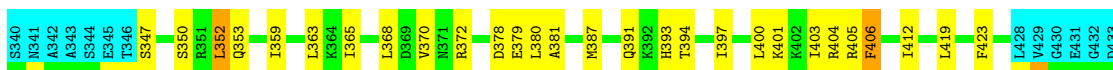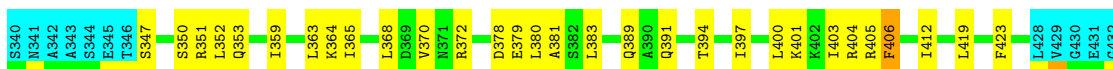
4.2.30 Score per residue for model 30
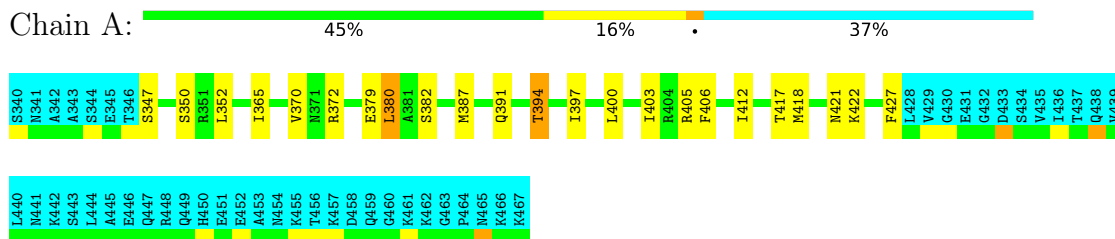
• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

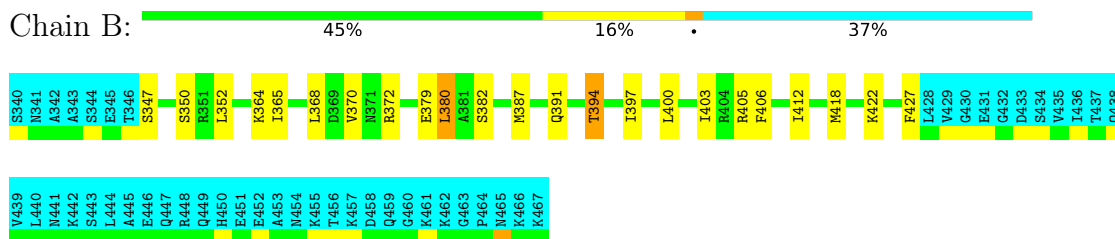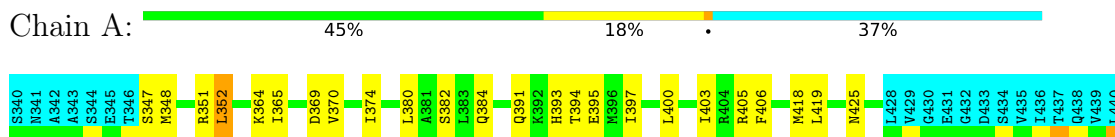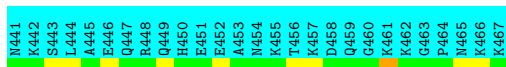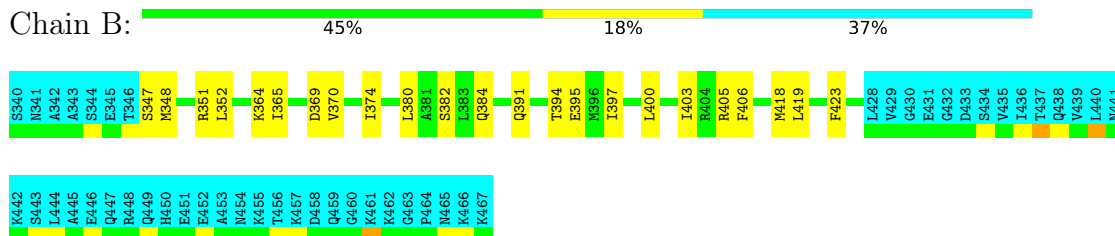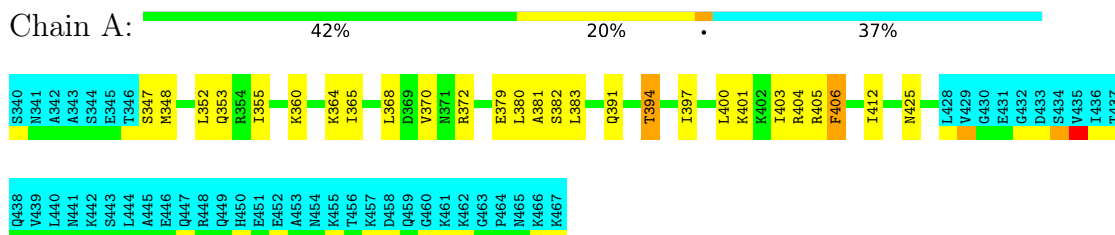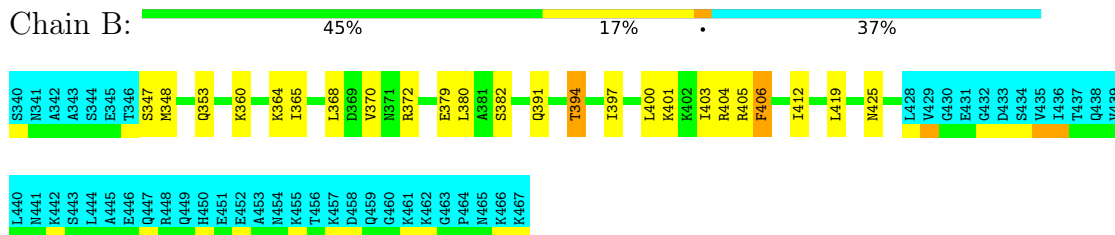• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:
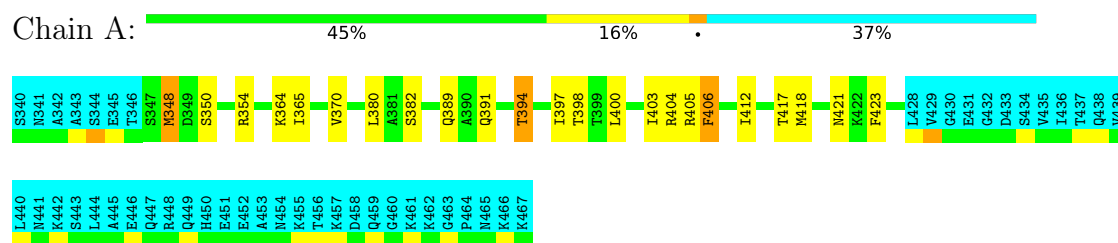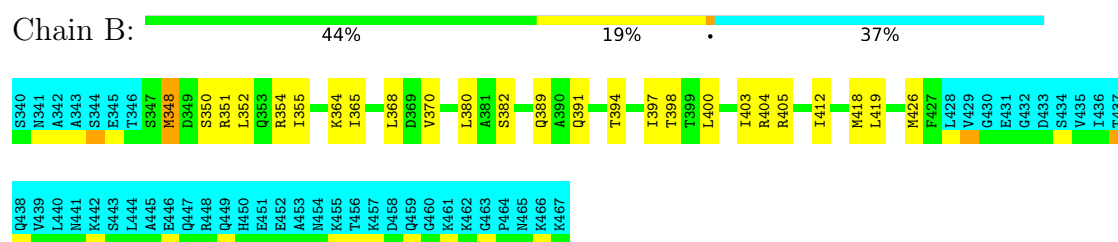
5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *torsion angle dynamics.*

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *structures with the least restraint violations.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1561
Number of shifts mapped to atoms	1561
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6   Model quality (i)

6.1   Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2   Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	665	701	701	14±2
1	B	665	701	701	14±2
All	All	39900	42060	42060	535

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:403:ILE:HG22	1:B:365:ILE:HD11	0.94	1.39	3	30
1:A:365:ILE:HD11	1:B:403:ILE:HG22	0.94	1.39	13	30
1:A:380:LEU:HD23	1:B:419:LEU:HD13	0.82	1.50	21	1
1:A:419:LEU:HD13	1:B:380:LEU:HD23	0.82	1.50	18	2
1:A:419:LEU:HD12	1:B:380:LEU:HD12	0.66	1.66	17	4
1:A:419:LEU:HD13	1:B:380:LEU:CD2	0.65	2.21	18	2
1:A:380:LEU:HD21	1:A:396:MET:HE1	0.64	1.69	3	2
1:A:406:PHE:CD2	1:B:368:LEU:HD13	0.63	2.28	19	8
1:A:380:LEU:HD12	1:B:419:LEU:HD12	0.63	1.70	28	3
1:A:412:ILE:HD11	1:B:370:VAL:HB	0.62	1.71	17	26
1:A:380:LEU:CD2	1:B:419:LEU:HD13	0.62	2.24	21	1
1:B:380:LEU:HD21	1:B:396:MET:HE1	0.61	1.72	3	1
1:A:368:LEU:HD13	1:B:406:PHE:CE1	0.61	2.31	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:380:LEU:HD12	1:B:419:LEU:HD22	0.61	1.72	12	4
1:A:397:ILE:HD13	1:B:427:PHE:CE2	0.60	2.32	27	3
1:A:406:PHE:CE2	1:B:368:LEU:HD13	0.60	2.32	19	5
1:A:370:VAL:HB	1:B:412:ILE:HD11	0.59	1.72	11	26
1:A:397:ILE:HA	1:A:400:LEU:HD12	0.59	1.74	20	29
1:B:397:ILE:HA	1:B:400:LEU:HD12	0.59	1.74	20	29
1:B:352:LEU:HA	1:B:355:ILE:HD12	0.59	1.74	8	17
1:A:427:PHE:CE2	1:B:397:ILE:HD13	0.59	2.33	27	3
1:B:394:THR:HA	1:B:397:ILE:HD12	0.58	1.74	12	12
1:A:380:LEU:O	1:A:380:LEU:HD13	0.58	1.99	20	6
1:A:380:LEU:HD13	1:A:380:LEU:O	0.57	2.00	25	7
1:A:394:THR:HA	1:A:397:ILE:HD12	0.57	1.74	12	12
1:B:380:LEU:O	1:B:380:LEU:HD13	0.57	2.00	1	7
1:A:365:ILE:CD1	1:B:403:ILE:HG22	0.57	2.26	11	29
1:A:415:LYS:CB	1:B:377:LEU:HD23	0.57	2.30	14	1
1:A:351:ARG:CZ	1:A:383:LEU:HD21	0.56	2.30	23	2
1:B:351:ARG:CZ	1:B:383:LEU:HD21	0.56	2.31	29	2
1:B:380:LEU:HD13	1:B:380:LEU:O	0.56	2.00	15	3
1:A:381:ALA:HB2	1:B:419:LEU:HD21	0.56	1.78	29	2
1:A:419:LEU:HG	1:B:380:LEU:HD12	0.56	1.77	20	1
1:A:377:LEU:HD23	1:B:419:LEU:HD12	0.56	1.77	17	1
1:A:403:ILE:HG22	1:B:365:ILE:CD1	0.55	2.28	6	29
1:A:352:LEU:HD23	1:A:393:HIS:CG	0.55	2.37	8	7
1:B:355:ILE:HG23	1:B:376:ALA:HB1	0.53	1.80	16	15
1:A:419:LEU:HD13	1:B:380:LEU:HD12	0.53	1.78	24	4
1:A:423:PHE:CZ	1:B:380:LEU:HD11	0.52	2.39	2	12
1:A:377:LEU:HD22	1:B:419:LEU:HD12	0.52	1.80	7	1
1:A:419:LEU:HD22	1:B:380:LEU:HD12	0.52	1.82	12	3
1:A:377:LEU:HD23	1:B:415:LYS:CB	0.52	2.34	14	1
1:A:380:LEU:HD11	1:B:423:PHE:CZ	0.52	2.39	29	13
1:A:391:GLN:O	1:A:394:THR:HG23	0.52	2.05	20	10
1:A:406:PHE:CD1	1:B:368:LEU:HD13	0.52	2.40	14	3
1:A:380:LEU:HD21	1:A:396:MET:HE3	0.52	1.82	7	2
1:A:380:LEU:HD12	1:B:419:LEU:HD13	0.51	1.82	19	5
1:A:352:LEU:HA	1:A:355:ILE:HD12	0.51	1.83	28	11
1:B:352:LEU:HD22	1:B:396:MET:HE1	0.50	1.82	22	1
1:A:417:THR:HG22	1:A:421:ASN:OD1	0.50	2.06	11	2
1:B:391:GLN:O	1:B:394:THR:HG23	0.50	2.07	6	12
1:B:380:LEU:HD21	1:B:396:MET:HE3	0.49	1.84	7	1
1:A:394:THR:HG22	1:B:427:PHE:CZ	0.49	2.42	1	1
1:A:419:LEU:CD1	1:B:380:LEU:HD12	0.49	2.36	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:419:LEU:HD21	1:B:381:ALA:HB2	0.49	1.83	29	1
1:A:427:PHE:CZ	1:B:394:THR:HG22	0.49	2.42	1	1
1:A:397:ILE:HD13	1:B:427:PHE:CZ	0.48	2.42	11	2
1:A:355:ILE:CD1	1:A:383:LEU:HD11	0.48	2.39	13	2
1:A:368:LEU:HD13	1:B:406:PHE:CD1	0.48	2.43	6	6
1:A:368:LEU:HD13	1:B:406:PHE:CD2	0.47	2.44	25	4
1:A:406:PHE:CE1	1:B:368:LEU:HD13	0.47	2.45	22	2
1:A:380:LEU:HD23	1:A:383:LEU:HD12	0.47	1.85	18	1
1:A:427:PHE:CZ	1:B:397:ILE:HD13	0.47	2.44	27	2
1:A:406:PHE:CE1	1:B:408:VAL:HG13	0.46	2.45	3	2
1:B:370:VAL:O	1:B:374:ILE:HD12	0.46	2.11	20	2
1:A:415:LYS:HB2	1:B:377:LEU:HD23	0.45	1.87	14	1
1:B:359:ILE:HG22	1:B:363:LEU:HD12	0.45	1.89	6	5
1:B:352:LEU:CD2	1:B:380:LEU:HD23	0.45	2.42	20	1
1:A:406:PHE:CD2	1:B:365:ILE:HD13	0.45	2.47	14	1
1:A:380:LEU:HD12	1:B:419:LEU:CD1	0.44	2.42	10	2
1:A:370:VAL:O	1:A:374:ILE:HD12	0.44	2.13	12	2
1:A:359:ILE:HG22	1:A:363:LEU:HD12	0.44	1.88	15	5
1:A:359:ILE:HG23	1:A:373:CYS:SG	0.44	2.52	19	1
1:A:419:LEU:HD12	1:B:377:LEU:HD22	0.43	1.89	7	1
1:A:408:VAL:O	1:A:408:VAL:HG13	0.43	2.13	19	1
1:A:423:PHE:HZ	1:B:380:LEU:HD11	0.43	1.74	9	1
1:A:408:VAL:HG13	1:B:406:PHE:CE2	0.43	2.48	24	1
1:A:352:LEU:HD22	1:A:396:MET:HE1	0.42	1.90	22	1
1:A:365:ILE:HD11	1:B:403:ILE:CG2	0.42	2.29	30	1
1:A:380:LEU:HD13	1:A:380:LEU:C	0.42	2.35	29	3
1:A:368:LEU:HD13	1:B:406:PHE:CE2	0.42	2.50	25	1
1:A:352:LEU:HD23	1:A:355:ILE:HD12	0.42	1.92	13	1
1:A:382:SER:O	1:A:383:LEU:HD23	0.42	2.14	20	1
1:A:380:LEU:C	1:A:380:LEU:HD13	0.42	2.34	30	4
1:A:351:ARG:NH2	1:A:383:LEU:HD22	0.41	2.30	20	1
1:B:408:VAL:HG22	1:B:412:ILE:HB	0.41	1.92	19	2
1:A:351:ARG:HH11	1:A:383:LEU:HD22	0.41	1.75	25	1
1:A:352:LEU:HD22	1:A:396:MET:CE	0.41	2.46	15	2
1:B:380:LEU:HD13	1:B:380:LEU:C	0.41	2.36	13	4
1:A:417:THR:HG22	1:A:421:ASN:ND2	0.41	2.30	5	1
1:A:380:LEU:HD11	1:B:423:PHE:HZ	0.41	1.76	17	2
1:A:408:VAL:HG22	1:A:412:ILE:HB	0.41	1.92	28	1
1:B:396:MET:HB3	1:B:396:MET:HE2	0.41	1.86	28	1
1:B:352:LEU:HD23	1:B:393:HIS:CG	0.41	2.51	1	1
1:A:370:VAL:CB	1:B:412:ILE:HD11	0.40	2.45	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:412:ILE:HD11	1:B:370:VAL:CB	0.40	2.45	17	1
1:B:359:ILE:HG23	1:B:373:CYS:SG	0.40	2.56	19	2
1:B:380:LEU:C	1:B:380:LEU:HD13	0.40	2.36	26	1
1:A:403:ILE:CG2	1:B:365:ILE:HD11	0.40	2.28	3	1
1:A:415:LYS:HB3	1:B:377:LEU:HD23	0.40	1.93	14	1

6.3   Torsion angles (i)

6.3.1   Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	81/128 (63%)	76±1 (93±1%)	5±1 (7±1%)	0±0 (0±0%)	100	100
1	B	81/128 (63%)	76±1 (93±1%)	5±1 (7±1%)	0±0 (0±0%)	100	100
All	All	4860/7680 (63%)	4538 (93%)	321 (7%)	1 (0%)	100	100

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	B	409	SER	1

6.3.2   Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	77/116 (66%)	65±2 (84±3%)	12±2 (16±3%)	5	42
1	B	77/116 (66%)	65±2 (84±3%)	12±2 (16±3%)	5	42
All	All	4620/6960 (66%)	3883 (84%)	737 (16%)	5	42

All 83 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	405	ARG	30
1	B	405	ARG	30
1	B	364	LYS	26
1	A	406	PHE	25
1	A	364	LYS	24
1	B	406	PHE	24
1	A	404	ARG	22
1	B	404	ARG	22
1	A	387	MET	19
1	A	394	THR	18
1	B	387	MET	18
1	B	394	THR	18
1	A	348	MET	15
1	A	382	SER	15
1	B	348	MET	15
1	B	382	SER	15
1	A	379	GLU	14
1	B	379	GLU	14
1	A	347	SER	13
1	A	372	ARG	13
1	B	347	SER	13
1	B	372	ARG	13
1	A	350	SER	12
1	B	350	SER	12
1	B	401	LYS	12
1	B	389	GLN	11
1	A	407	LYS	10
1	A	401	LYS	10
1	B	380	LEU	10
1	A	389	GLN	10
1	B	407	LYS	8
1	A	392	LYS	8
1	B	392	LYS	8
1	A	380	LEU	8
1	A	378	ASP	8
1	B	378	ASP	8
1	A	349	ASP	7
1	B	349	ASP	7
1	A	369	ASP	7
1	A	425	ASN	7
1	B	369	ASP	7
1	B	425	ASN	7

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Mol	Chain	Res	Type	Models (Total)
1	A	418	MET	7
1	B	418	MET	7
1	A	395	GLU	7
1	B	395	GLU	7
1	A	353	GLN	7
1	B	414	GLU	6
1	A	360	LYS	6
1	A	352	LEU	6
1	B	353	GLN	6
1	A	424	LYS	5
1	A	414	GLU	5
1	A	351	ARG	5
1	B	352	LEU	5
1	A	391	GLN	5
1	B	391	GLN	5
1	B	424	LYS	4
1	B	351	ARG	4
1	A	354	ARG	4
1	B	354	ARG	4
1	A	421	ASN	3
1	B	421	ASN	3
1	A	384	GLN	3
1	B	384	GLN	3
1	A	388	GLN	3
1	B	388	GLN	3
1	A	398	THR	2
1	B	398	THR	2
1	A	410	GLN	2
1	B	410	GLN	2
1	B	360	LYS	2
1	B	427	PHE	1
1	A	422	LYS	1
1	B	422	LYS	1
1	A	367	ASN	1
1	A	409	SER	1
1	B	367	ASN	1
1	B	409	SER	1
1	B	396	MET	1
1	B	402	LYS	1
1	A	371	ASN	1
1	B	371	ASN	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 ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

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 45% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	1561
Number of shifts mapped to atoms	1561
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	126	-0.67 ± 0.12	Should be checked
$^{13}C_\beta$	121	0.27 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	126	-0.47 ± 0.10	None needed (< 0.5 ppm)
^{15}N	122	-0.42 ± 0.24	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 45%, i.e. 1064 atoms were assigned a chemical shift out of a possible 2382. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	396/810 (49%)	158/324 (49%)	160/324 (49%)	78/162 (48%)
Sidechain	638/1466 (44%)	435/948 (46%)	195/448 (44%)	8/70 (11%)

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	Total	**^{1}H**	**^{13}C**	**^{15}N**
Aromatic	30/106 (28%)	20/54 (37%)	10/48 (21%)	0/4 (0%)
Overall	1064/2382 (45%)	613/1326 (46%)	365/820 (45%)	86/236 (36%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 1559 atoms were assigned a chemical shift out of a possible 3590. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	626/1284 (49%)	252/518 (49%)	252/512 (49%)	122/254 (48%)
Sidechain	903/2186 (41%)	608/1404 (43%)	287/676 (42%)	8/106 (8%)
Aromatic	30/120 (25%)	20/62 (32%)	10/52 (19%)	0/6 (0%)
Overall	1559/3590 (43%)	880/1984 (44%)	549/1240 (44%)	130/366 (36%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	**Chain**	**Res**	**Type**	**Atom**	**Shift, *ppm***	**Expected range, *ppm***	**Z-score**
1	A	417	THR	HG1	5.62	0.08 − 2.19	21.2
1	A	386	THR	HG1	5.57	0.08 − 2.19	21.0

7.1.5 Random Coil Index (RCI) plots ⓘ

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:
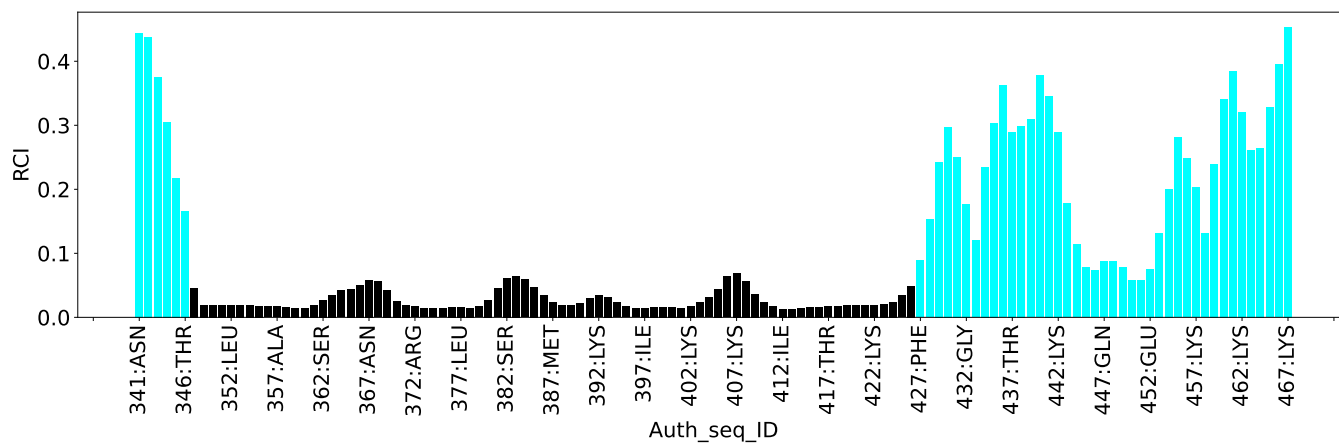
8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	4091
Intra-residue ($\lvert$i-j$\rvert$=0)	1140
Sequential ($\lvert$i-j$\rvert$=1)	925
Medium range ($\lvert$i-j$\rvert$>1 and $\lvert$i-j$\rvert$<5)	985
Long range ($\lvert$i-j$\rvert \geq$5)	346
Inter-chain	695
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.0
Number of long range restraints per residue[1]	1.4

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	16.7	0.2
0.2-0.5 (Medium)	6.9	0.41
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model ⓘ

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1140	27.9	9	0.8	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	943	23.1	9	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	197	4.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	925	22.6	14	1.5	0.3	0	0.0	0.0
Backbone-Backbone	204	5.0	3	1.5	0.1	0	0.0	0.0
Backbone-Sidechain	633	15.5	9	1.4	0.2	0	0.0	0.0
Sidechain-Sidechain	88	2.2	2	2.3	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	985	24.1	5	0.5	0.1	0	0.0	0.0
Backbone-Backbone	286	7.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	409	10.0	5	1.2	0.1	0	0.0	0.0
Sidechain-Sidechain	290	7.1	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	346	8.5	5	1.4	0.1	0	0.0	0.0
Backbone-Backbone	42	1.0	3	7.1	0.1	0	0.0	0.0
Backbone-Sidechain	100	2.4	2	2.0	0.0	0	0.0	0.0
Sidechain-Sidechain	204	5.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	695	17.0	39	5.6	1.0	8	1.2	0.2
Backbone-Backbone	238	5.8	38	16.0	0.9	8	3.4	0.2
Backbone-Sidechain	130	3.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	327	8.0	1	0.3	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4091	100.0	72	1.8	1.8	8	0.2	0.2
Backbone-Backbone	770	18.8	44	5.7	1.1	8	1.0	0.2
Backbone-Sidechain	2215	54.1	25	1.1	0.6	0	0.0	0.0
Sidechain-Sidechain	1106	27.0	3	0.3	0.1	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1　Bar chart : Distribution of distance restraints and violations ⓘ
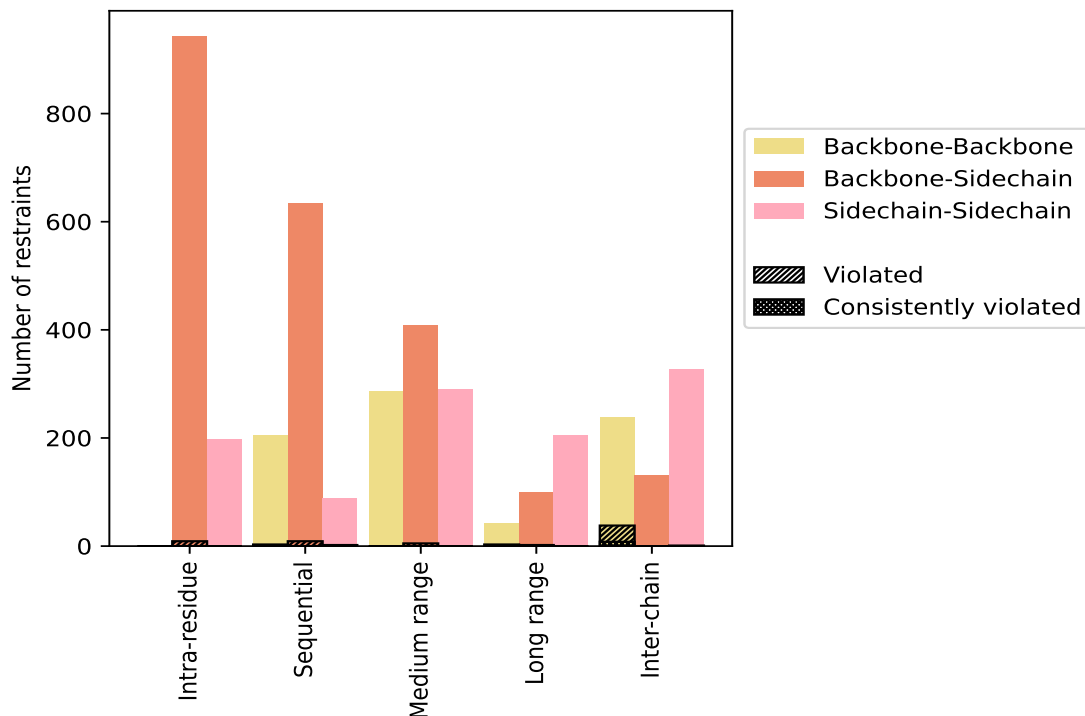
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2　Distance violation statistics for each model ⓘ

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	22	22	0.17	0.32	0.07	0.16
2	0	0	2	1	23	26	0.17	0.41	0.08	0.12
3	0	0	1	0	21	22	0.19	0.38	0.07	0.16
4	0	1	0	1	18	20	0.18	0.31	0.07	0.16
5	0	1	0	0	16	17	0.2	0.32	0.07	0.18
6	0	1	0	1	23	25	0.19	0.33	0.07	0.18
7	0	1	0	0	19	20	0.18	0.32	0.07	0.16
8	0	0	2	0	24	26	0.17	0.31	0.07	0.14
9	0	0	2	1	20	23	0.17	0.31	0.07	0.13
10	0	0	0	1	17	18	0.19	0.32	0.07	0.16
11	1	0	2	0	18	21	0.19	0.32	0.07	0.17

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Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	1	1	0	21	23	0.17	0.31	0.07	0.13
13	1	0	2	1	23	27	0.17	0.41	0.08	0.13
14	2	0	0	2	20	24	0.18	0.33	0.07	0.15
15	3	1	0	0	19	23	0.18	0.33	0.07	0.16
16	1	3	1	0	22	27	0.17	0.38	0.07	0.15
17	1	2	0	0	25	28	0.18	0.31	0.07	0.16
18	0	2	3	1	25	31	0.17	0.32	0.07	0.15
19	2	3	2	0	19	26	0.18	0.4	0.07	0.15
20	2	0	2	0	17	21	0.18	0.3	0.07	0.16
21	3	1	0	1	17	22	0.18	0.31	0.07	0.16
22	0	1	1	1	25	28	0.17	0.33	0.08	0.14
23	1	1	1	0	22	25	0.18	0.34	0.07	0.14
24	2	0	2	0	19	23	0.19	0.37	0.07	0.16
25	3	0	2	0	20	25	0.18	0.37	0.07	0.15
26	0	0	0	0	20	20	0.18	0.3	0.07	0.18
27	0	3	0	1	16	20	0.19	0.31	0.06	0.17
28	1	0	0	1	19	21	0.19	0.31	0.07	0.18
29	1	1	2	0	22	26	0.18	0.41	0.08	0.14
30	1	0	2	1	23	27	0.17	0.4	0.07	0.15

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints,
[5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ
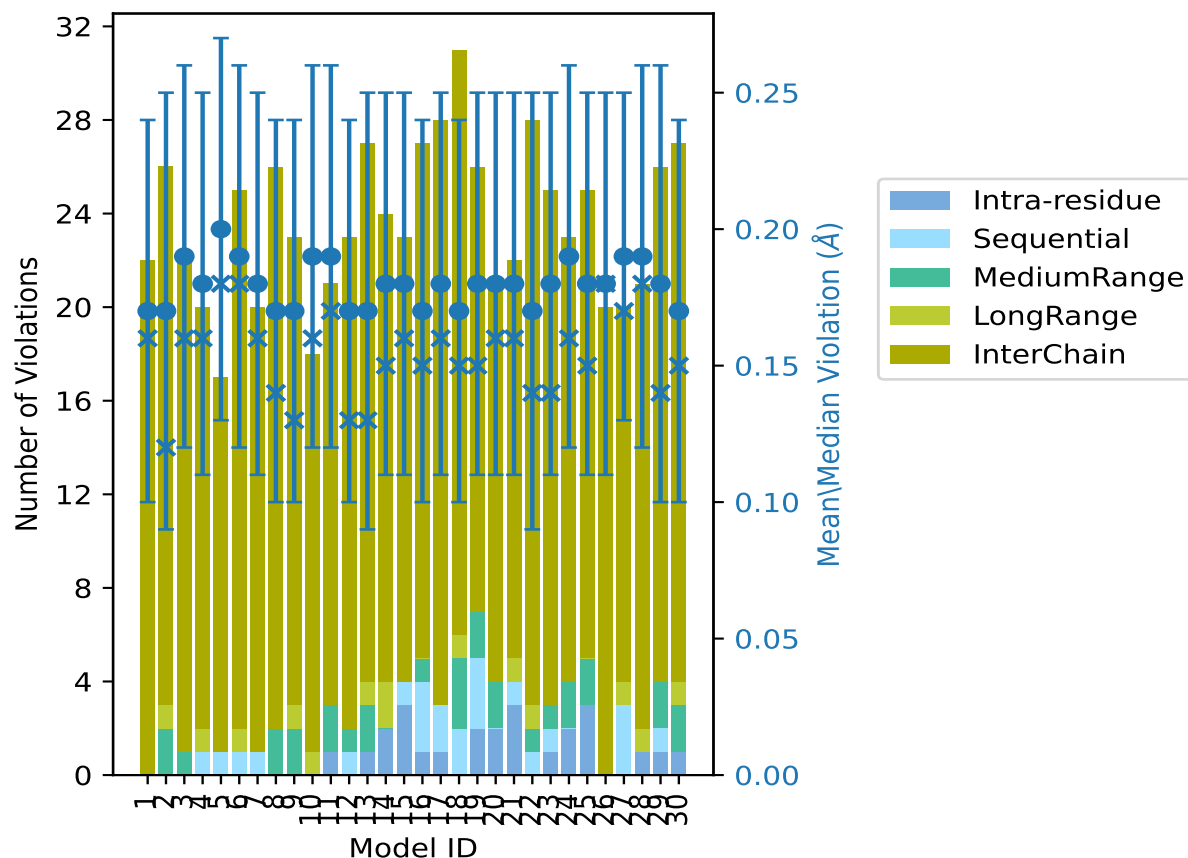
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 4019(IR:1131, SQ:911, MR:980, LR:341, IC:656) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
3	9	3	2	4	21	1	3.3
2	3	0	1	2	8	2	6.7
1	0	0	0	3	4	3	10.0
1	2	0	1	2	6	4	13.3
1	0	0	0	3	4	5	16.7
1	0	0	1	1	3	6	20.0

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Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	23.3
0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	0	0	0	10	33.3
0	0	1	0	1	2	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	1	1	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	2	2	15	50.0
0	0	1	0	1	2	16	53.3
0	0	0	0	1	1	17	56.7
0	0	0	0	2	2	18	60.0
0	0	0	0	1	1	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	2	2	24	80.0
0	0	0	0	1	1	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	2	2	28	93.3
0	0	0	0	2	2	29	96.7
0	0	0	0	8	8	30	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

9.3.1   Bar graph : Distance violation statistics for the ensemble ⓘ
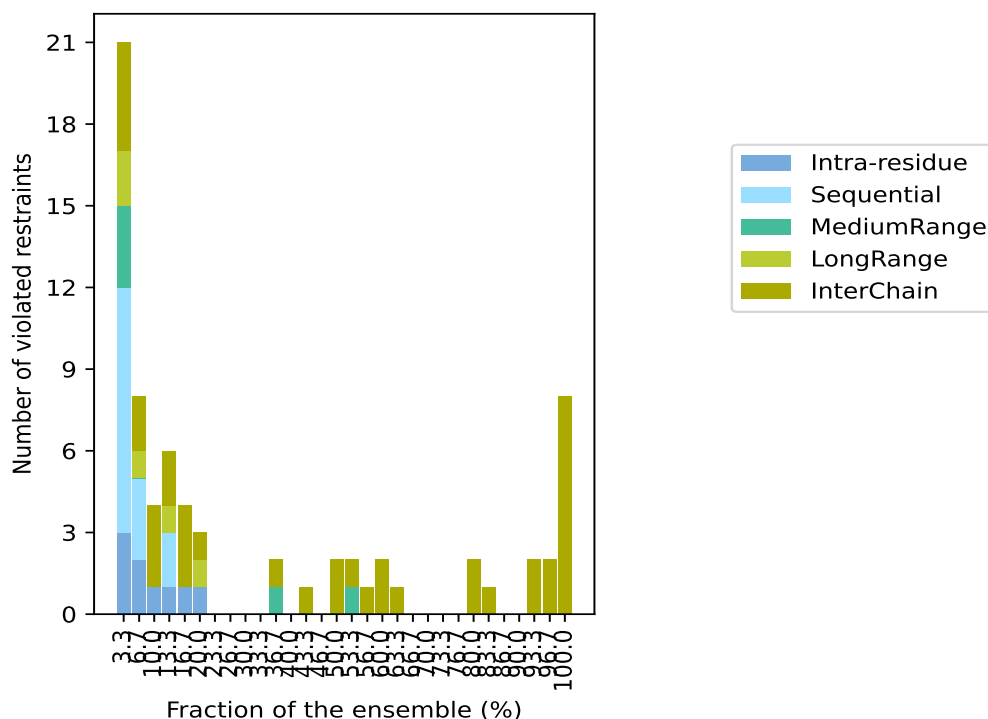
9.4   Most violated distance restraints in the ensemble ⓘ

9.4.1   Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble
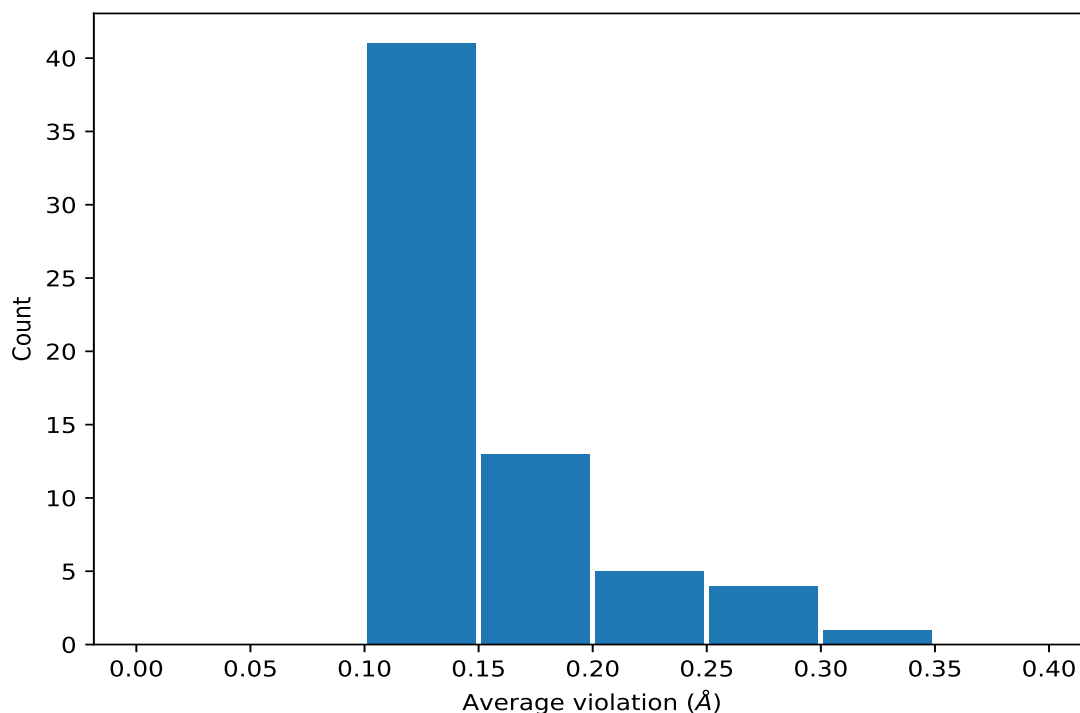
9.4.2 Table: Most violated distance restraints ⓘ

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	30	0.33	0.05	0.31
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	30	0.3	0.02	0.3
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	30	0.3	0.01	0.3
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	30	0.28	0.02	0.28
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	30	0.28	0.02	0.28
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	30	0.18	0.02	0.18
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	30	0.18	0.02	0.18
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	30	0.17	0.02	0.17
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	29	0.18	0.02	0.17
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	29	0.14	0.02	0.13
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	28	0.18	0.04	0.19
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	28	0.14	0.01	0.14
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	25	0.18	0.03	0.18
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	24	0.13	0.02	0.12
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	24	0.13	0.02	0.12
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	19	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	18	0.17	0.05	0.16
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	18	0.13	0.02	0.12
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	17	0.12	0.02	0.12
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	16	0.13	0.02	0.13
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	16	0.11	0.0	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	16	0.11	0.0	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	16	0.11	0.0	0.11
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	15	0.13	0.02	0.12
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	15	0.12	0.01	0.12
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	13	0.17	0.05	0.19
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	11	0.12	0.01	0.12
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	11	0.11	0.01	0.11
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	11	0.11	0.01	0.11
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	11	0.11	0.01	0.11
(1,1529)	1:A:353:GLN:HA	1:A:353:GLN:HG2	6	0.12	0.0	0.12
(3,57)	1:A:420:TYR:CA	1:B:401:LYS:CA	6	0.12	0.01	0.11
(3,106)	1:A:352:LEU:CA	1:A:393:HIS:CA	6	0.12	0.01	0.11
(3,56)	1:A:401:LYS:CA	1:B:420:TYR:CA	5	0.13	0.03	0.11
(3,21)	1:A:406:PHE:CA	1:B:368:LEU:CA	5	0.12	0.02	0.12
(5,90)	1:A:370:VAL:CA	1:B:409:SER:CA	5	0.12	0.01	0.12
(1,1530)	1:B:353:GLN:HA	1:B:353:GLN:HG2	5	0.12	0.0	0.12
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG2	4	0.21	0.04	0.23
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG3	4	0.21	0.04	0.23
(1,1228)	1:B:421:ASN:HB3	1:B:422:LYS:H	4	0.14	0.01	0.14
(1,1227)	1:A:421:ASN:HB3	1:A:422:LYS:H	4	0.13	0.01	0.12
(5,81)	1:A:407:LYS:CA	1:B:408:VAL:CA	4	0.13	0.01	0.13
(5,89)	1:A:409:SER:CA	1:B:370:VAL:CA	4	0.13	0.01	0.12
(5,4)	1:A:352:LEU:CA	1:A:380:LEU:CA	4	0.11	0.0	0.11
(1,3153)	1:A:414:GLU:H	1:A:414:GLU:HG2	3	0.22	0.04	0.24
(1,3153)	1:A:414:GLU:H	1:A:414:GLU:HG3	3	0.22	0.04	0.24
(3,80)	1:A:403:ILE:CA	1:B:408:VAL:CA	3	0.15	0.04	0.13
(5,101)	1:A:414:GLU:CA	1:B:404:ARG:CA	3	0.12	0.01	0.12
(5,82)	1:A:408:VAL:CA	1:B:407:LYS:CA	3	0.11	0.0	0.11
(1,363)	1:B:437:THR:HA	1:B:438:GLN:H	2	0.23	0.02	0.23
(1,362)	1:A:437:THR:HA	1:A:438:GLN:H	2	0.18	0.03	0.18
(1,2760)	1:A:361:ASN:HB2	1:A:362:SER:HB2	2	0.17	0.01	0.17
(1,2760)	1:A:361:ASN:HB2	1:A:362:SER:HB3	2	0.17	0.01	0.17
(1,2760)	1:A:361:ASN:HB3	1:A:362:SER:HB2	2	0.17	0.01	0.17
(1,2760)	1:A:361:ASN:HB3	1:A:362:SER:HB3	2	0.17	0.01	0.17
(1,2446)	1:A:436:ILE:HA	1:A:436:ILE:HD11	2	0.13	0.0	0.13
(1,2446)	1:A:436:ILE:HA	1:A:436:ILE:HD12	2	0.13	0.0	0.13
(1,2446)	1:A:436:ILE:HA	1:A:436:ILE:HD13	2	0.13	0.0	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2447)	1:B:436:ILE:HA	1:B:436:ILE:HD11	2	0.12	0.01	0.12
(1,2447)	1:B:436:ILE:HA	1:B:436:ILE:HD12	2	0.12	0.01	0.12
(1,2447)	1:B:436:ILE:HA	1:B:436:ILE:HD13	2	0.12	0.01	0.12
(3,109)	1:A:355:ILE:CA	1:A:380:LEU:CA	2	0.12	0.02	0.12
(5,95)	1:A:412:ILE:CA	1:B:403:ILE:CA	2	0.12	0.01	0.12
(5,58)	1:A:400:LEU:CA	1:B:420:TYR:CA	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5　All violated distance restraints ⓘ

9.5.1　Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
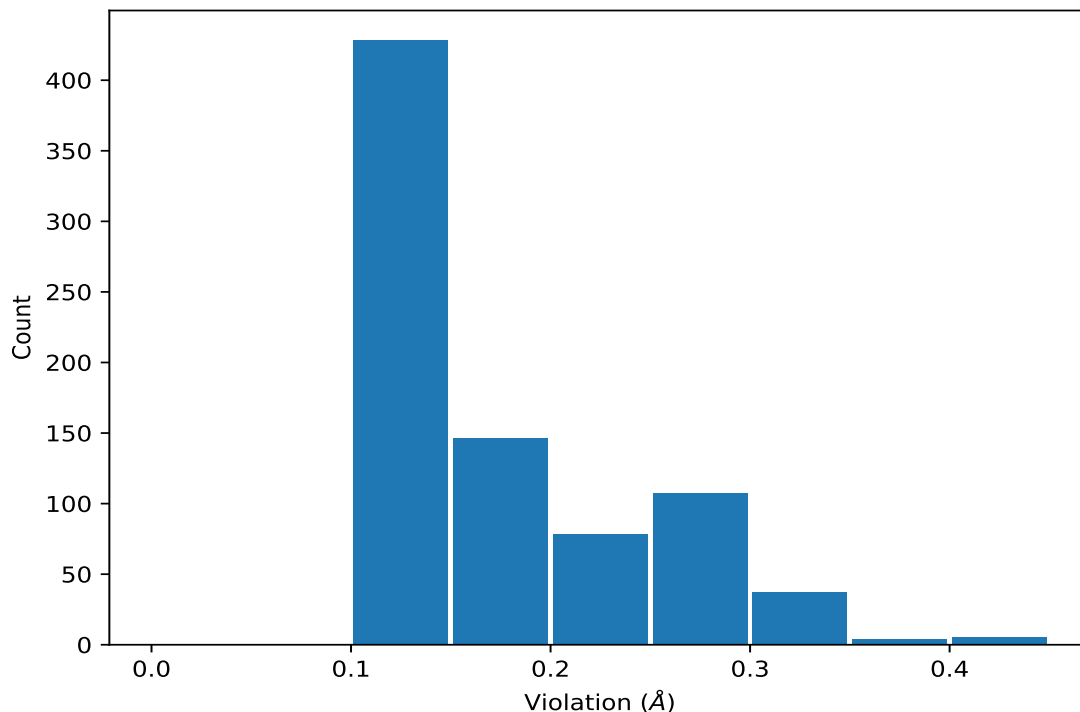
9.5.2　Table : All distance violations ⓘ

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	2	0.41
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	13	0.41
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	29	0.41
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	30	0.4
(1,1040)	1:B:409:SER:H	1:B:412:ILE:HB	19	0.4
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	3	0.38
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	16	0.38
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	24	0.37
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	25	0.37
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	23	0.34
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	14	0.33
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	15	0.33
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	13	0.33
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	13	0.33
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	6	0.33
(1,1409)	1:A:439:VAL:HB	1:A:440:LEU:H	22	0.33
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	1	0.32
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	5	0.32
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	6	0.32
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	7	0.32
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	5	0.32
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	10	0.32
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	18	0.32
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	19	0.32
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	22	0.32
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	10	0.32
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	11	0.32
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	18	0.32
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	23	0.32
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	29	0.32
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	30	0.32
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	4	0.31
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	8	0.31
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	9	0.31
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	12	0.31
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	21	0.31
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	28	0.31
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	4	0.31
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	17	0.31
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	29	0.31
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	4	0.31
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	8	0.31
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	21	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	27	0.31
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	6	0.31
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	22	0.31
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	10	0.3
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	20	0.3
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	22	0.3
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	23	0.3
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	26	0.3
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	27	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	2	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	3	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	8	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	11	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	14	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	16	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	21	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	27	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	28	0.3
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	30	0.3
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	2	0.3
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	5	0.3
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	15	0.3
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	19	0.3
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	22	0.3
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	24	0.3
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	25	0.3
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	28	0.3
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	20	0.3
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	28	0.3
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	7	0.3
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	14	0.3
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	28	0.3
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	17	0.29
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	18	0.29
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	6	0.29
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	12	0.29
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	15	0.29
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	20	0.29
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	25	0.29
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	3	0.29
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	6	0.29
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	17	0.29
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	20	0.29
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	26	0.29
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	1	0.29
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	7	0.29
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	8	0.29
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	9	0.29
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	14	0.29
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	22	0.29
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	1	0.29
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	9	0.29
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	11	0.29
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	12	0.29
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	19	0.29
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	20	0.29
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	1	0.28
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	7	0.28
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	9	0.28
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	24	0.28
(5,108)	1:A:404:ARG:CA	1:B:416:SER:CA	26	0.28
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	1	0.28
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	7	0.28
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	9	0.28
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	12	0.28
(5,107)	1:A:416:SER:CA	1:B:404:ARG:CA	16	0.28
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	10	0.28
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	11	0.28
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	12	0.28
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	15	0.28
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	17	0.28
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	24	0.28
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	26	0.28
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	8	0.28
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	10	0.28
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	17	0.28
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	18	0.28
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	2	0.27
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	4	0.27
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	18	0.27
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	21	0.27
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	25	0.27
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	5	0.27
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	21	0.27
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	24	0.27
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	26	0.27
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	27	0.27
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	3	0.26
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	5	0.26
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	23	0.26
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	27	0.26
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	29	0.26
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	3	0.26
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	4	0.26
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	16	0.26
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	23	0.26
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	25	0.26
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	29	0.26
(1,3153)	1:A:414:GLU:H	1:A:414:GLU:HG2	17	0.26
(1,3153)	1:A:414:GLU:H	1:A:414:GLU:HG3	17	0.26
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	11	0.25
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	19	0.25
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	30	0.25
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	15	0.25
(1,675)	1:A:380:LEU:HD11	1:A:382:SER:H	18	0.25
(1,675)	1:A:380:LEU:HD12	1:A:382:SER:H	18	0.25
(1,675)	1:A:380:LEU:HD13	1:A:382:SER:H	18	0.25
(1,363)	1:B:437:THR:HA	1:B:438:GLN:H	23	0.25
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	13	0.24
(3,98)	1:A:403:ILE:CA	1:B:416:SER:CA	16	0.24
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	13	0.24
(3,97)	1:A:416:SER:CA	1:B:403:ILE:CA	30	0.24
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	25	0.24
(1,3153)	1:A:414:GLU:H	1:A:414:GLU:HG2	16	0.24
(1,3153)	1:A:414:GLU:H	1:A:414:GLU:HG3	16	0.24
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	3	0.23
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	17	0.23
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	11	0.23
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	24	0.23
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	3	0.23
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	16	0.23
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	25	0.23
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	4	0.23
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	21	0.23
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	19	0.23
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG2	15	0.23
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG3	15	0.23
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG2	25	0.23
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG3	25	0.23
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG2	30	0.23
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG3	30	0.23
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	16	0.22
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	8	0.22
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	17	0.22
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	2	0.22
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	13	0.22
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	29	0.22
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	30	0.22
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	2	0.22
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	13	0.22
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	24	0.22
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	29	0.22
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	18	0.22
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	20	0.22
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	9	0.22
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	20	0.22
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	6	0.21
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	8	0.21
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	11	0.21
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	17	0.21
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	18	0.21
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	28	0.21
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	24	0.21
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	11	0.21
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	18	0.21
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	28	0.21
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	8	0.21
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	10	0.21
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	22	0.21
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	27	0.21
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	28	0.21
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	6	0.21
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	8	0.21
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	28	0.21
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:B:437:THR:HA	1:B:438:GLN:H	17	0.21
(1,362)	1:A:437:THR:HA	1:A:438:GLN:H	27	0.21
(5,80)	1:A:407:LYS:CA	1:B:407:LYS:CA	19	0.2
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	6	0.2
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	25	0.2
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	26	0.2
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	29	0.2
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	6	0.2
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	30	0.2
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	6	0.2
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	7	0.2
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	15	0.2
(3,80)	1:A:403:ILE:CA	1:B:408:VAL:CA	14	0.2
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	6	0.2
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	1	0.2
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	10	0.2
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	18	0.2
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	27	0.2
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	14	0.2
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	6	0.2
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	7	0.19
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	9	0.19
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	12	0.19
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	14	0.19
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	15	0.19
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	2	0.19
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	15	0.19
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	18	0.19
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	22	0.19
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	2	0.19
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	25	0.19
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	26	0.19
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	29	0.19
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	1	0.19
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	9	0.19
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	12	0.19
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	3	0.19
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	30	0.19
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	3	0.19
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	7	0.19
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	9	0.19
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	23	0.19
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	1	0.19
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	12	0.19
(1,3427)	1:B:361:ASN:HB2	1:B:362:SER:HB2	18	0.19
(1,3427)	1:B:361:ASN:HB2	1:B:362:SER:HB3	18	0.19
(1,3427)	1:B:361:ASN:HB3	1:B:362:SER:HB2	18	0.19
(1,3427)	1:B:361:ASN:HB3	1:B:362:SER:HB3	18	0.19
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	1	0.18
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	5	0.18
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	26	0.18
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	29	0.18
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	13	0.18
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	23	0.18
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	28	0.18
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	13	0.18
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	18	0.18
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	28	0.18
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	2	0.18
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	3	0.18
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	5	0.18
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	14	0.18
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	21	0.18
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	26	0.18
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	27	0.18
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	29	0.18
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	23	0.18
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	11	0.18
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	26	0.18
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	5	0.18
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	26	0.18
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	11	0.18
(3,56)	1:A:401:LYS:CA	1:B:420:TYR:CA	7	0.18
(1,2760)	1:A:361:ASN:HB2	1:A:362:SER:HB2	6	0.18
(1,2760)	1:A:361:ASN:HB2	1:A:362:SER:HB3	6	0.18
(1,2760)	1:A:361:ASN:HB3	1:A:362:SER:HB2	6	0.18
(1,2760)	1:A:361:ASN:HB3	1:A:362:SER:HB3	6	0.18
(1,1029)	1:A:408:VAL:HG11	1:A:409:SER:H	19	0.18
(1,1029)	1:A:408:VAL:HG12	1:A:409:SER:H	19	0.18
(1,1029)	1:A:408:VAL:HG13	1:A:409:SER:H	19	0.18
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	2	0.17
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	4	0.17
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	21	0.17
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	24	0.17
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	27	0.17
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	1	0.17
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	4	0.17
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	9	0.17
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	10	0.17
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	12	0.17
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	27	0.17
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	30	0.17
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	1	0.17
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	10	0.17
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	12	0.17
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	22	0.17
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	23	0.17
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	16	0.17
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	4	0.17
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	13	0.17
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	22	0.17
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	23	0.17
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	30	0.17
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	16	0.17
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	6	0.17
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	15	0.17
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	4	0.17
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	17	0.17
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	21	0.17
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	24	0.17
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	19	0.17
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	15	0.17
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	11	0.17
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	18	0.17
(1,3153)	1:A:414:GLU:H	1:A:414:GLU:HG2	24	0.17
(1,3153)	1:A:414:GLU:H	1:A:414:GLU:HG3	24	0.17
(1,2621)	1:B:418:MET:HE1	1:B:419:LEU:H	21	0.17
(1,2621)	1:B:418:MET:HE2	1:B:419:LEU:H	21	0.17
(1,2621)	1:B:418:MET:HE3	1:B:419:LEU:H	21	0.17
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	3	0.16
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	10	0.16
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	16	0.16
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	25	0.16
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	30	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	5	0.16
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	7	0.16
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	8	0.16
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	11	0.16
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	20	0.16
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	21	0.16
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	4	0.16
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	7	0.16
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	8	0.16
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	9	0.16
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	20	0.16
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	27	0.16
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	10	0.16
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	24	0.16
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	25	0.16
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	30	0.16
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	16	0.16
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	20	0.16
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	19	0.16
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	20	0.16
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	15	0.16
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	17	0.16
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	14	0.16
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	16	0.16
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	17	0.16
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	7	0.16
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	11	0.16
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	15	0.16
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	6	0.16
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	4	0.16
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	4	0.16
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	17	0.16
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	18	0.16
(3,21)	1:A:406:PHE:CA	1:B:368:LEU:CA	14	0.16
(1,890)	1:B:401:LYS:H	1:B:401:LYS:HB2	19	0.16
(1,889)	1:A:401:LYS:H	1:A:401:LYS:HB2	19	0.16
(1,2760)	1:A:361:ASN:HB2	1:A:362:SER:HB2	4	0.16
(1,2760)	1:A:361:ASN:HB2	1:A:362:SER:HB3	4	0.16
(1,2760)	1:A:361:ASN:HB3	1:A:362:SER:HB2	4	0.16
(1,2760)	1:A:361:ASN:HB3	1:A:362:SER:HB3	4	0.16
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	22	0.15
(5,89)	1:A:409:SER:CA	1:B:370:VAL:CA	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	24	0.15
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	3	0.15
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	5	0.15
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	16	0.15
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	17	0.15
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	21	0.15
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	3	0.15
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	24	0.15
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	29	0.15
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	16	0.15
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	19	0.15
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	22	0.15
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	22	0.15
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	25	0.15
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	18	0.15
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	28	0.15
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	14	0.15
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	28	0.15
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	6	0.15
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	8	0.15
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	19	0.15
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	21	0.15
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	23	0.15
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	27	0.15
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	28	0.15
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	8	0.15
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	27	0.15
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	28	0.15
(3,57)	1:A:420:TYR:CA	1:B:401:LYS:CA	30	0.15
(1,1227)	1:A:421:ASN:HB3	1:A:422:LYS:H	5	0.15
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	19	0.14
(5,90)	1:A:370:VAL:CA	1:B:409:SER:CA	18	0.14
(5,81)	1:A:407:LYS:CA	1:B:408:VAL:CA	6	0.14
(5,81)	1:A:407:LYS:CA	1:B:408:VAL:CA	19	0.14
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	14	0.14
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	29	0.14
(5,101)	1:A:414:GLU:CA	1:B:404:ARG:CA	19	0.14
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	20	0.14
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	10	0.14
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	23	0.14
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	10	0.14
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	18	0.14
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	19	0.14
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	6	0.14
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	22	0.14
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	23	0.14
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	5	0.14
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	21	0.14
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	22	0.14
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	1	0.14
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	3	0.14
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	5	0.14
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	13	0.14
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	14	0.14
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	22	0.14
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	5	0.14
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	11	0.14
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	13	0.14
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	19	0.14
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	21	0.14
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	24	0.14
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	25	0.14
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	25	0.14
(3,109)	1:A:355:ILE:CA	1:A:380:LEU:CA	14	0.14
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG2	24	0.14
(1,3713)	1:B:414:GLU:H	1:B:414:GLU:HG3	24	0.14
(1,362)	1:A:437:THR:HA	1:A:438:GLN:H	17	0.14
(1,1228)	1:B:421:ASN:HB3	1:B:422:LYS:H	18	0.14
(1,1228)	1:B:421:ASN:HB3	1:B:422:LYS:H	27	0.14
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	20	0.13
(5,99)	1:A:413:MET:CA	1:B:404:ARG:CA	23	0.13
(5,95)	1:A:412:ILE:CA	1:B:403:ILE:CA	15	0.13
(5,90)	1:A:370:VAL:CA	1:B:409:SER:CA	6	0.13
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	14	0.13
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	15	0.13
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	25	0.13
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	12	0.13
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	24	0.13
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	5	0.13
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	21	0.13
(3,80)	1:A:403:ILE:CA	1:B:408:VAL:CA	23	0.13
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	3	0.13
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	8	0.13
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	11	0.13
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	14	0.13
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	23	0.13
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	24	0.13
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	28	0.13
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	29	0.13
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	24	0.13
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	6	0.13
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	7	0.13
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	10	0.13
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	24	0.13
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	26	0.13
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	3	0.13
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	4	0.13
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	7	0.13
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	10	0.13
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	2	0.13
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	9	0.13
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	10	0.13
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	16	0.13
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	17	0.13
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	25	0.13
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	29	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	1	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	2	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	3	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	7	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	10	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	12	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	15	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	26	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	29	0.13
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	30	0.13
(3,106)	1:A:352:LEU:CA	1:A:393:HIS:CA	13	0.13
(3,106)	1:A:352:LEU:CA	1:A:393:HIS:CA	21	0.13
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	24	0.13
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	24	0.13
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	24	0.13
(1,2615)	1:B:418:MET:HA	1:B:418:MET:HE1	21	0.13
(1,2615)	1:B:418:MET:HA	1:B:418:MET:HE2	21	0.13
(1,2615)	1:B:418:MET:HA	1:B:418:MET:HE3	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2447)	1:B:436:ILE:HA	1:B:436:ILE:HD11	28	0.13
(1,2447)	1:B:436:ILE:HA	1:B:436:ILE:HD12	28	0.13
(1,2447)	1:B:436:ILE:HA	1:B:436:ILE:HD13	28	0.13
(1,2446)	1:A:436:ILE:HA	1:A:436:ILE:HD11	11	0.13
(1,2446)	1:A:436:ILE:HA	1:A:436:ILE:HD12	11	0.13
(1,2446)	1:A:436:ILE:HA	1:A:436:ILE:HD13	11	0.13
(1,2446)	1:A:436:ILE:HA	1:A:436:ILE:HD11	29	0.13
(1,2446)	1:A:436:ILE:HA	1:A:436:ILE:HD12	29	0.13
(1,2446)	1:A:436:ILE:HA	1:A:436:ILE:HD13	29	0.13
(1,1503)	1:A:352:LEU:HD21	1:A:380:LEU:HA	30	0.13
(1,1503)	1:A:352:LEU:HD22	1:A:380:LEU:HA	30	0.13
(1,1503)	1:A:352:LEU:HD23	1:A:380:LEU:HA	30	0.13
(1,1406)	1:B:440:LEU:H	1:B:441:ASN:H	27	0.13
(1,1228)	1:B:421:ASN:HB3	1:B:422:LYS:H	15	0.13
(1,1228)	1:B:421:ASN:HB3	1:B:422:LYS:H	29	0.13
(1,1227)	1:A:421:ASN:HB3	1:A:422:LYS:H	12	0.13
(5,90)	1:A:370:VAL:CA	1:B:409:SER:CA	8	0.12
(5,89)	1:A:409:SER:CA	1:B:370:VAL:CA	8	0.12
(5,89)	1:A:409:SER:CA	1:B:370:VAL:CA	19	0.12
(5,89)	1:A:409:SER:CA	1:B:370:VAL:CA	28	0.12
(5,81)	1:A:407:LYS:CA	1:B:408:VAL:CA	17	0.12
(5,77)	1:A:365:ILE:CA	1:B:406:PHE:CA	14	0.12
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	15	0.12
(5,76)	1:A:406:PHE:CA	1:B:365:ILE:CA	19	0.12
(5,4)	1:A:352:LEU:CA	1:A:380:LEU:CA	14	0.12
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	2	0.12
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	6	0.12
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	13	0.12
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	15	0.12
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	17	0.12
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	22	0.12
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	23	0.12
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	26	0.12
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	2	0.12
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	13	0.12
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	15	0.12
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	16	0.12
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	17	0.12
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	23	0.12
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	25	0.12
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	30	0.12
(5,101)	1:A:414:GLU:CA	1:B:404:ARG:CA	23	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,100)	1:A:404:ARG:CA	1:B:413:MET:CA	19	0.12
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	9	0.12
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	30	0.12
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	26	0.12
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	9	0.12
(3,80)	1:A:403:ILE:CA	1:B:408:VAL:CA	22	0.12
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	13	0.12
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	15	0.12
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	29	0.12
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	3	0.12
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	6	0.12
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	2	0.12
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	13	0.12
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	13	0.12
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	25	0.12
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	29	0.12
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	30	0.12
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	1	0.12
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	8	0.12
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	9	0.12
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	12	0.12
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	20	0.12
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	21	0.12
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	27	0.12
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	1	0.12
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	8	0.12
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	9	0.12
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	12	0.12
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	16	0.12
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	18	0.12
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	20	0.12
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	26	0.12
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	27	0.12
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	7	0.12
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	12	0.12
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	20	0.12
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	24	0.12
(3,67)	1:A:412:ILE:CA	1:B:404:ARG:CA	26	0.12
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	9	0.12
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	14	0.12
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	20	0.12
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	23	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,56)	1:A:401:LYS:CA	1:B:420:TYR:CA	22	0.12
(3,21)	1:A:406:PHE:CA	1:B:368:LEU:CA	18	0.12
(3,21)	1:A:406:PHE:CA	1:B:368:LEU:CA	23	0.12
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	2	0.12
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	3	0.12
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	8	0.12
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	13	0.12
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	14	0.12
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	16	0.12
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	18	0.12
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	30	0.12
(1,644)	1:B:379:GLU:HG3	1:B:380:LEU:H	16	0.12
(1,637)	1:A:379:GLU:HG2	1:A:380:LEU:H	16	0.12
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	2	0.12
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	2	0.12
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	2	0.12
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	13	0.12
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	13	0.12
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	13	0.12
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	30	0.12
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	30	0.12
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	30	0.12
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	2	0.12
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	2	0.12
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	2	0.12
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	13	0.12
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	13	0.12
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	13	0.12
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	16	0.12
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	16	0.12
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	16	0.12
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	25	0.12
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	25	0.12
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	25	0.12
(1,2447)	1:B:436:ILE:HA	1:B:436:ILE:HD11	23	0.12
(1,2447)	1:B:436:ILE:HA	1:B:436:ILE:HD12	23	0.12
(1,2447)	1:B:436:ILE:HA	1:B:436:ILE:HD13	23	0.12
(1,1530)	1:B:353:GLN:HA	1:B:353:GLN:HG2	14	0.12
(1,1530)	1:B:353:GLN:HA	1:B:353:GLN:HG2	15	0.12
(1,1530)	1:B:353:GLN:HA	1:B:353:GLN:HG2	20	0.12
(1,1530)	1:B:353:GLN:HA	1:B:353:GLN:HG2	21	0.12
(1,1530)	1:B:353:GLN:HA	1:B:353:GLN:HG2	25	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:A:353:GLN:HA	1:A:353:GLN:HG2	14	0.12
(1,1529)	1:A:353:GLN:HA	1:A:353:GLN:HG2	15	0.12
(1,1529)	1:A:353:GLN:HA	1:A:353:GLN:HG2	20	0.12
(1,1529)	1:A:353:GLN:HA	1:A:353:GLN:HG2	21	0.12
(1,1529)	1:A:353:GLN:HA	1:A:353:GLN:HG2	25	0.12
(1,1227)	1:A:421:ASN:HB3	1:A:422:LYS:H	7	0.12
(5,95)	1:A:412:ILE:CA	1:B:403:ILE:CA	17	0.11
(5,90)	1:A:370:VAL:CA	1:B:409:SER:CA	17	0.11
(5,90)	1:A:370:VAL:CA	1:B:409:SER:CA	28	0.11
(5,82)	1:A:408:VAL:CA	1:B:407:LYS:CA	4	0.11
(5,82)	1:A:408:VAL:CA	1:B:407:LYS:CA	8	0.11
(5,82)	1:A:408:VAL:CA	1:B:407:LYS:CA	18	0.11
(5,81)	1:A:407:LYS:CA	1:B:408:VAL:CA	8	0.11
(5,58)	1:A:400:LEU:CA	1:B:420:TYR:CA	18	0.11
(5,58)	1:A:400:LEU:CA	1:B:420:TYR:CA	30	0.11
(5,4)	1:A:352:LEU:CA	1:A:380:LEU:CA	2	0.11
(5,4)	1:A:352:LEU:CA	1:A:380:LEU:CA	6	0.11
(5,4)	1:A:352:LEU:CA	1:A:380:LEU:CA	9	0.11
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	9	0.11
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	11	0.11
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	12	0.11
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	18	0.11
(5,13)	1:A:360:LYS:CA	1:B:365:ILE:CA	30	0.11
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	1	0.11
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	6	0.11
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	12	0.11
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	22	0.11
(5,12)	1:A:365:ILE:CA	1:B:360:LYS:CA	26	0.11
(5,102)	1:A:404:ARG:CA	1:B:414:GLU:CA	6	0.11
(5,101)	1:A:414:GLU:CA	1:B:404:ARG:CA	22	0.11
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	1	0.11
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	2	0.11
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	3	0.11
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	12	0.11
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	13	0.11
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	26	0.11
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	27	0.11
(3,92)	1:A:403:ILE:CA	1:B:413:MET:CA	29	0.11
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	1	0.11
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	2	0.11
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	7	0.11
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	13	0.11
(3,91)	1:A:413:MET:CA	1:B:403:ILE:CA	16	0.11
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	1	0.11
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	8	0.11
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	11	0.11
(3,82)	1:A:406:PHE:CA	1:B:408:VAL:CA	28	0.11
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	1	0.11
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	4	0.11
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	7	0.11
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	8	0.11
(3,81)	1:A:408:VAL:CA	1:B:406:PHE:CA	22	0.11
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	1	0.11
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	2	0.11
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	9	0.11
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	12	0.11
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	14	0.11
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	16	0.11
(3,78)	1:A:363:LEU:CA	1:B:408:VAL:CA	30	0.11
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	1	0.11
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	2	0.11
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	4	0.11
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	12	0.11
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	13	0.11
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	16	0.11
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	17	0.11
(3,77)	1:A:408:VAL:CA	1:B:363:LEU:CA	22	0.11
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	29	0.11
(3,73)	1:A:407:LYS:CA	1:B:406:PHE:CA	30	0.11
(3,72)	1:A:406:PHE:CA	1:B:407:LYS:CA	2	0.11
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	4	0.11
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	5	0.11
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	18	0.11
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	25	0.11
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	29	0.11
(3,69)	1:A:413:MET:CA	1:B:405:ARG:CA	30	0.11
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	2	0.11
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	23	0.11
(3,68)	1:A:405:ARG:CA	1:B:413:MET:CA	29	0.11
(3,66)	1:A:404:ARG:CA	1:B:412:ILE:CA	22	0.11
(3,62)	1:A:403:ILE:CA	1:B:365:ILE:CA	16	0.11
(3,57)	1:A:420:TYR:CA	1:B:401:LYS:CA	7	0.11
(3,57)	1:A:420:TYR:CA	1:B:401:LYS:CA	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,57)	1:A:420:TYR:CA	1:B:401:LYS:CA	17	0.11
(3,57)	1:A:420:TYR:CA	1:B:401:LYS:CA	19	0.11
(3,57)	1:A:420:TYR:CA	1:B:401:LYS:CA	21	0.11
(3,56)	1:A:401:LYS:CA	1:B:420:TYR:CA	3	0.11
(3,56)	1:A:401:LYS:CA	1:B:420:TYR:CA	17	0.11
(3,56)	1:A:401:LYS:CA	1:B:420:TYR:CA	25	0.11
(3,21)	1:A:406:PHE:CA	1:B:368:LEU:CA	11	0.11
(3,21)	1:A:406:PHE:CA	1:B:368:LEU:CA	22	0.11
(3,20)	1:A:368:LEU:CA	1:B:406:PHE:CA	18	0.11
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	22	0.11
(3,11)	1:A:364:LYS:CA	1:B:364:LYS:CA	26	0.11
(3,109)	1:A:355:ILE:CA	1:A:380:LEU:CA	27	0.11
(3,106)	1:A:352:LEU:CA	1:A:393:HIS:CA	4	0.11
(3,106)	1:A:352:LEU:CA	1:A:393:HIS:CA	18	0.11
(3,106)	1:A:352:LEU:CA	1:A:393:HIS:CA	22	0.11
(3,106)	1:A:352:LEU:CA	1:A:393:HIS:CA	28	0.11
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	8	0.11
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	8	0.11
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	8	0.11
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	9	0.11
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	9	0.11
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	9	0.11
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	11	0.11
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	11	0.11
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	11	0.11
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	18	0.11
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	18	0.11
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	18	0.11
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	20	0.11
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	20	0.11
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	20	0.11
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	25	0.11
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	25	0.11
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	25	0.11
(1,387)	1:B:365:ILE:HD11	1:B:367:ASN:H	29	0.11
(1,387)	1:B:365:ILE:HD12	1:B:367:ASN:H	29	0.11
(1,387)	1:B:365:ILE:HD13	1:B:367:ASN:H	29	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	3	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	3	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	3	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	8	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	8	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	9	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	9	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	9	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	11	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	11	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	11	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	12	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	12	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	12	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	18	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	18	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	18	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	20	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	20	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	20	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	22	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	22	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	22	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	23	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	23	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	23	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	24	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	24	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	24	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	29	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	29	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	29	0.11
(1,386)	1:A:365:ILE:HD11	1:A:367:ASN:H	30	0.11
(1,386)	1:A:365:ILE:HD12	1:A:367:ASN:H	30	0.11
(1,386)	1:A:365:ILE:HD13	1:A:367:ASN:H	30	0.11
(1,3686)	1:B:409:SER:H	1:B:412:ILE:HG12	19	0.11
(1,3686)	1:B:409:SER:H	1:B:412:ILE:HG13	19	0.11
(1,3656)	1:B:401:LYS:HB2	1:B:402:LYS:H	19	0.11
(1,3656)	1:B:401:LYS:HB3	1:B:402:LYS:H	19	0.11
(1,3069)	1:A:401:LYS:HB2	1:A:402:LYS:H	19	0.11
(1,3069)	1:A:401:LYS:HB3	1:A:402:LYS:H	19	0.11
(1,2255)	1:A:408:VAL:HG21	1:B:406:PHE:HE1	17	0.11
(1,2255)	1:A:408:VAL:HG21	1:B:406:PHE:HE2	17	0.11
(1,2255)	1:A:408:VAL:HG22	1:B:406:PHE:HE1	17	0.11
(1,2255)	1:A:408:VAL:HG22	1:B:406:PHE:HE2	17	0.11
(1,2255)	1:A:408:VAL:HG23	1:B:406:PHE:HE1	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2255)	1:A:408:VAL:HG23	1:B:406:PHE:HE2	17	0.11
(1,1529)	1:A:353:GLN:HA	1:A:353:GLN:HG2	13	0.11
(1,1521)	1:A:352:LEU:HD11	1:A:380:LEU:HA	10	0.11
(1,1521)	1:A:352:LEU:HD12	1:A:380:LEU:HA	10	0.11
(1,1521)	1:A:352:LEU:HD13	1:A:380:LEU:HA	10	0.11
(1,1227)	1:A:421:ASN:HB3	1:A:422:LYS:H	16	0.11

10 Dihedral-angle violation analysis ⓘ

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value