



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 01:10 PM EST

PDB ID : 2KE4
BMRB ID : 16129
Title : The NMR structure of the TC10 and Cdc42 interacting domain of CIP4
Authors : Kumeta, H.; Kanoh, D.; Kobashigawa, Y.; Inagaki, F.
Deposited on : 2009-01-22

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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

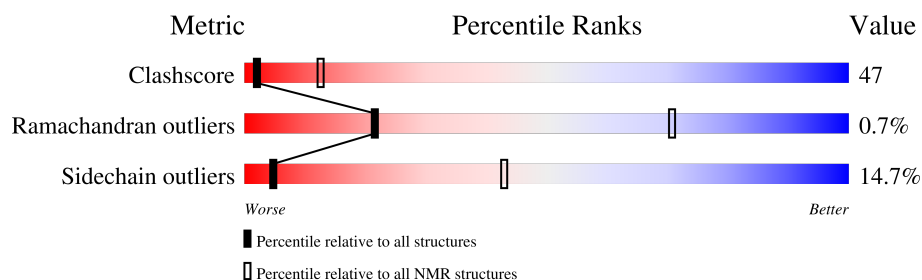
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	98	<div> <div></div> <div>27%</div> <div>50%</div> <div>5%</div> <div>18%</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:341-A:420 (80)	0.73	7

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20
2	4, 9

3 Entry composition

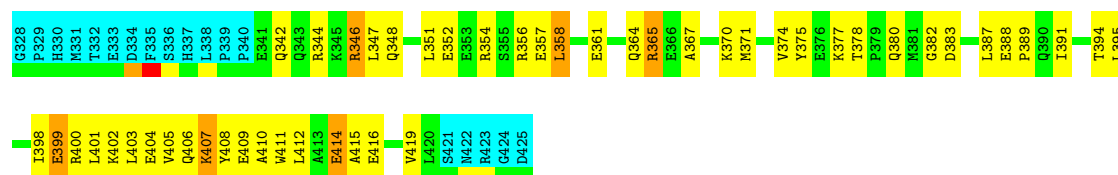
There is only 1 type of molecule in this entry. The entry contains 1610 atoms, of which 803 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cdc42-interacting protein 4.

Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1610	496	803	147	161	3	

There are 4 discrepancies between the modelled and reference sequences:

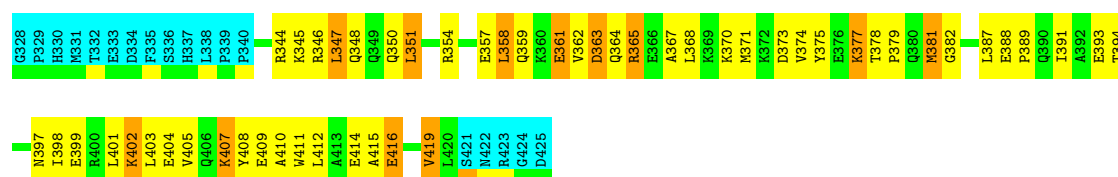
Chain	Residue	Modelled	Actual	Comment	Reference
A	328	GLY	-	expression tag	UNP Q15642
A	329	PRO	-	expression tag	UNP Q15642
A	330	HIS	-	expression tag	UNP Q15642
A	331	MET	-	expression tag	UNP Q15642



4.2.3 Score per residue for model 3

- Molecule 1: Cdc42-interacting protein 4

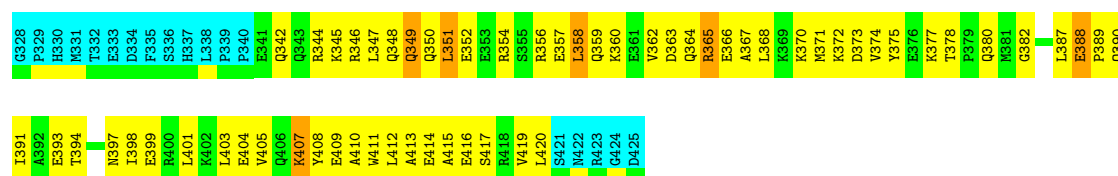
Chain A: 29% 41% 12% 18%



4.2.4 Score per residue for model 4

- Molecule 1: Cdc42-interacting protein 4

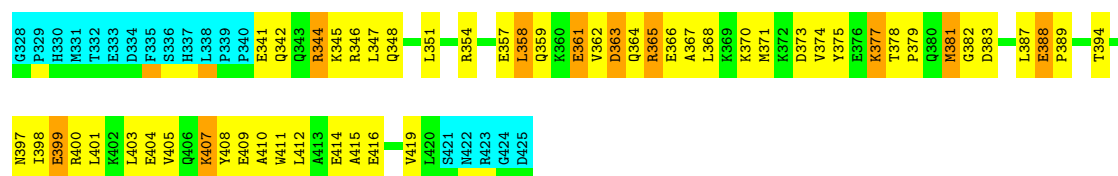
Chain A: 20% 55% 6% 18%



4.2.5 Score per residue for model 5

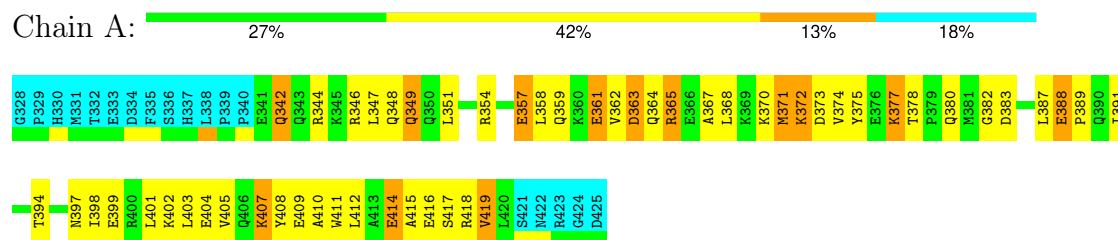
- Molecule 1: Cdc42-interacting protein 4

Chain A: 28% 44% 10% 18%



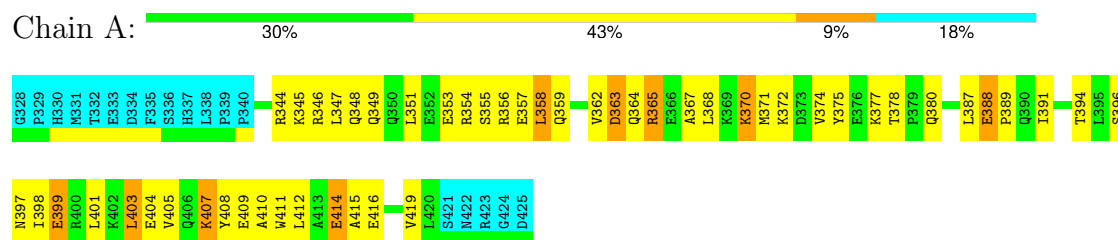
4.2.6 Score per residue for model 6

- Molecule 1: Cdc42-interacting protein 4



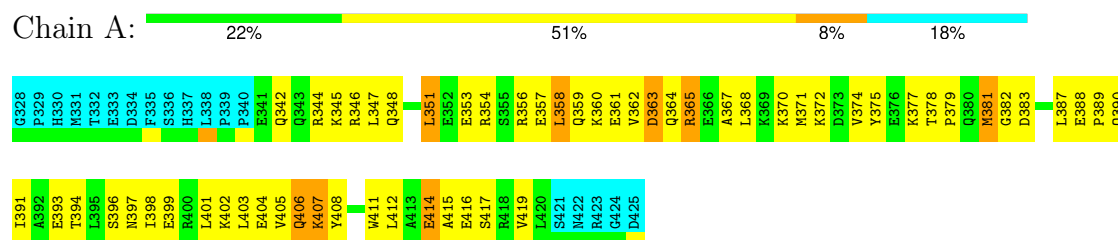
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Cdc42-interacting protein 4



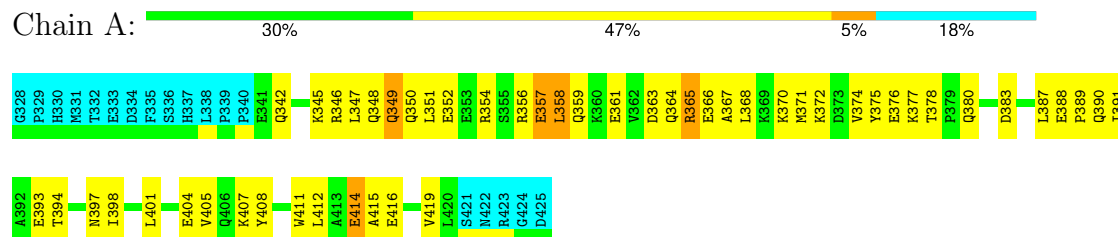
4.2.8 Score per residue for model 8

- Molecule 1: Cdc42-interacting protein 4



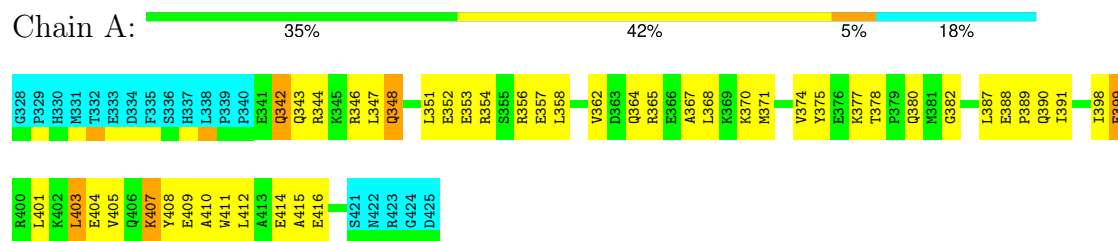
4.2.9 Score per residue for model 9

- Molecule 1: Cdc42-interacting protein 4



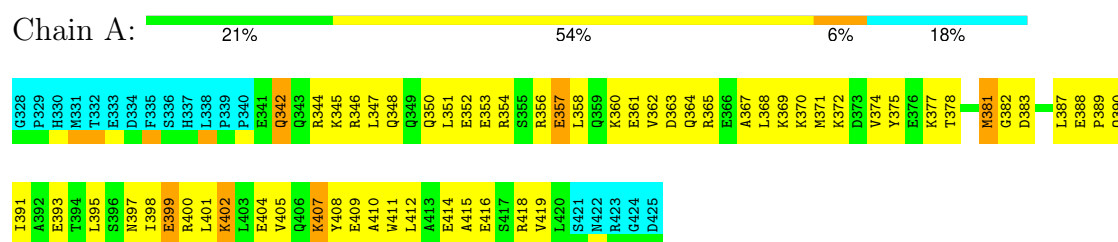
4.2.10 Score per residue for model 10

- Molecule 1: Cdc42-interacting protein 4



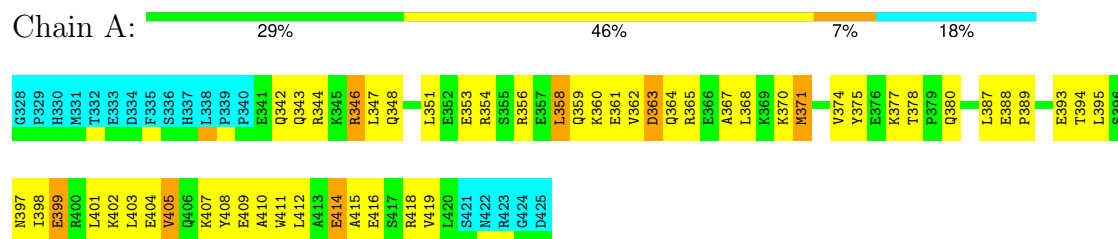
4.2.11 Score per residue for model 11

- Molecule 1: Cdc42-interacting protein 4



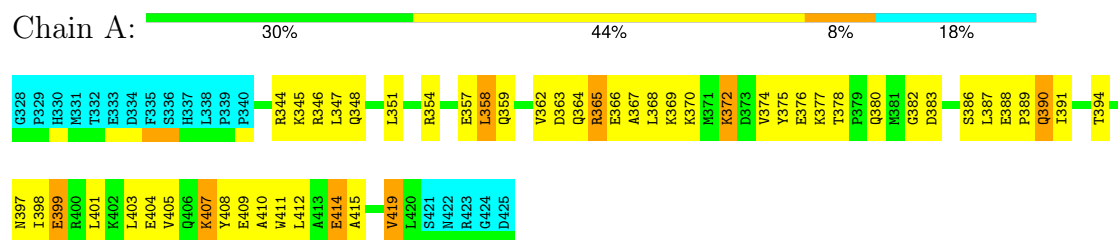
4.2.12 Score per residue for model 12

- Molecule 1: Cdc42-interacting protein 4



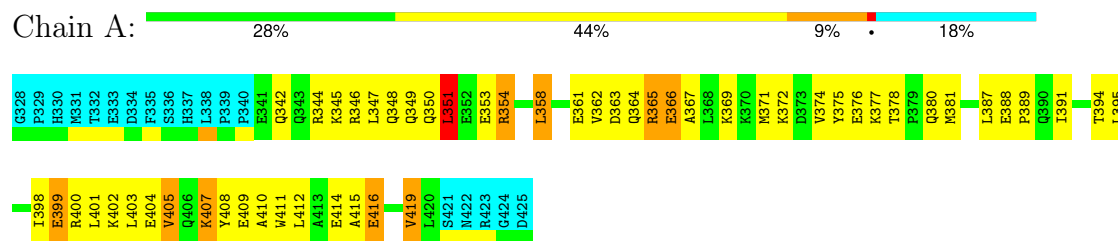
4.2.13 Score per residue for model 13

- Molecule 1: Cdc42-interacting protein 4



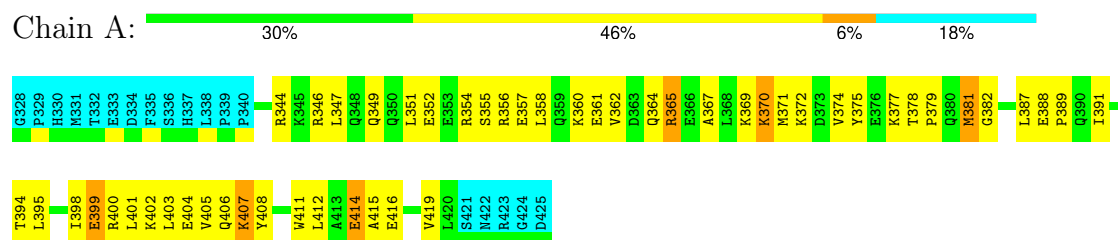
4.2.14 Score per residue for model 14

- Molecule 1: Cdc42-interacting protein 4



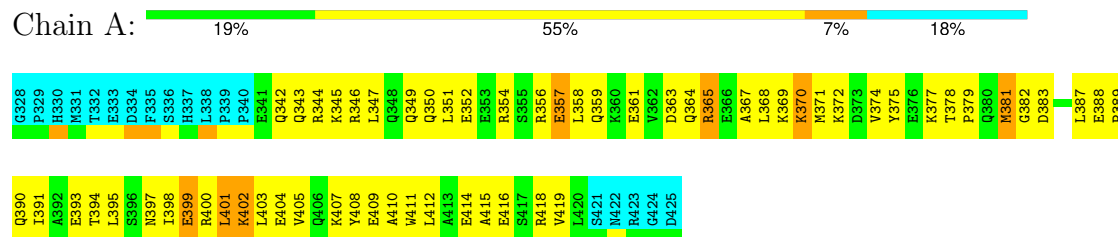
4.2.15 Score per residue for model 15

- Molecule 1: Cdc42-interacting protein 4



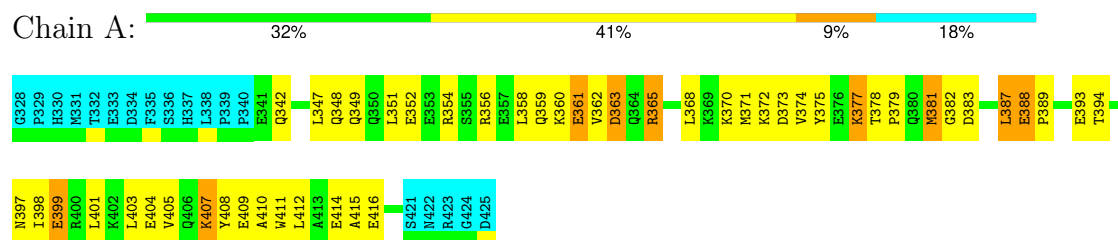
4.2.16 Score per residue for model 16

- Molecule 1: Cdc42-interacting protein 4



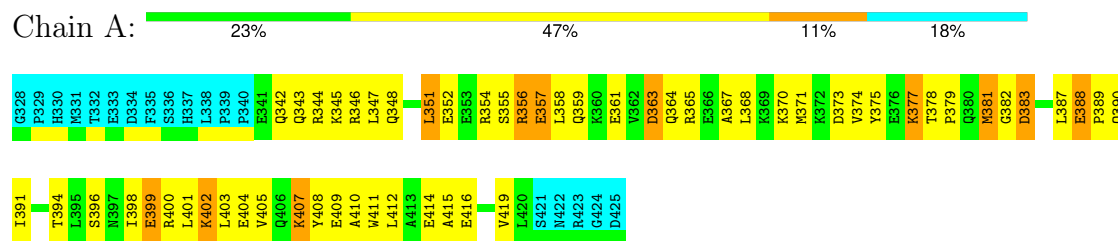
4.2.17 Score per residue for model 17

- Molecule 1: Cdc42-interacting protein 4



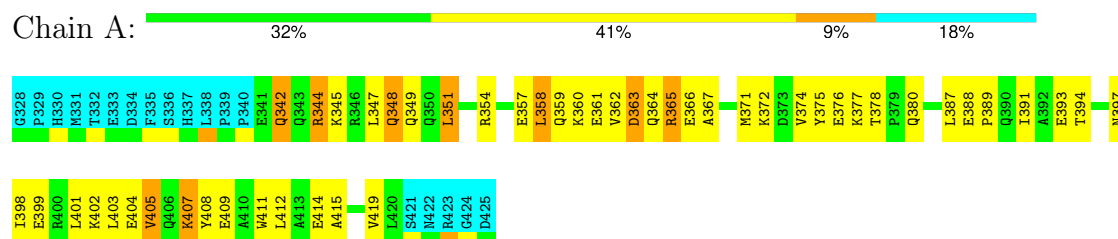
4.2.18 Score per residue for model 18

- Molecule 1: Cdc42-interacting protein 4



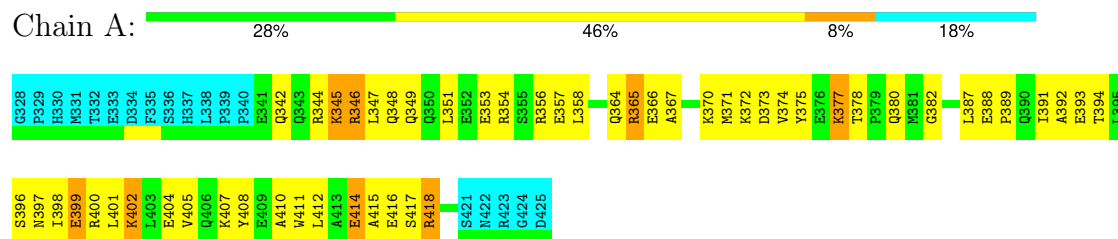
4.2.19 Score per residue for model 19

- Molecule 1: Cdc42-interacting protein 4



4.2.20 Score per residue for model 20

- Molecule 1: Cdc42-interacting protein 4



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Sparky	refinement	3.110
CYANA	structure solution	2.1

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	1287
Number of shifts mapped to atoms	1287
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality

6.1 Standard geometry

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

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	668	681	679	63±8
All	All	13360	13620	13580	1265

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 47.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:351:LEU:HD11	1:A:409:GLU:CG	0.95	1.92	4	12
1:A:401:LEU:O	1:A:405:VAL:HG23	0.91	1.64	20	11
1:A:351:LEU:CD1	1:A:405:VAL:HG22	0.91	1.96	18	2
1:A:370:LYS:O	1:A:374:VAL:HG13	0.90	1.67	6	16
1:A:351:LEU:HD11	1:A:409:GLU:HG3	0.83	1.50	4	9
1:A:357:GLU:OE1	1:A:401:LEU:HD21	0.82	1.75	7	6
1:A:397:ASN:O	1:A:401:LEU:HD12	0.82	1.74	12	8
1:A:357:GLU:CD	1:A:401:LEU:HD21	0.81	1.95	18	6
1:A:375:TYR:CE2	1:A:387:LEU:HD11	0.81	2.10	12	15
1:A:357:GLU:OE2	1:A:401:LEU:HD21	0.81	1.73	1	5
1:A:368:LEU:HD22	1:A:390:GLN:NE2	0.81	1.91	13	2
1:A:354:ARG:HB3	1:A:405:VAL:HG22	0.80	1.54	6	10
1:A:348:GLN:HG3	1:A:412:LEU:HD11	0.79	1.54	1	4
1:A:374:VAL:HG23	1:A:375:TYR:CD1	0.78	2.13	20	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:365:ARG:NH1	1:A:395:LEU:HD11	0.77	1.95	15	2
1:A:351:LEU:HD23	1:A:405:VAL:HG22	0.77	1.55	14	2
1:A:358:LEU:HA	1:A:401:LEU:HD13	0.77	1.56	6	15
1:A:351:LEU:HD21	1:A:409:GLU:HG3	0.77	1.52	18	2
1:A:399:GLU:O	1:A:403:LEU:HD22	0.77	1.79	18	1
1:A:344:ARG:HA	1:A:347:LEU:HD12	0.77	1.56	15	3
1:A:344:ARG:NH2	1:A:419:VAL:HG21	0.76	1.95	4	3
1:A:358:LEU:HD22	1:A:358:LEU:O	0.76	1.79	4	1
1:A:399:GLU:O	1:A:403:LEU:HD23	0.76	1.80	5	10
1:A:365:ARG:HB3	1:A:398:ILE:HD11	0.74	1.59	4	6
1:A:344:ARG:HH21	1:A:415:ALA:C	0.74	1.85	8	1
1:A:368:LEU:HD13	1:A:390:GLN:HG2	0.74	1.58	16	4
1:A:344:ARG:NH2	1:A:412:LEU:HD12	0.74	1.97	3	1
1:A:361:GLU:OE2	1:A:394:THR:HG23	0.74	1.82	14	1
1:A:357:GLU:OE1	1:A:401:LEU:HD11	0.73	1.84	18	1
1:A:358:LEU:C	1:A:358:LEU:HD13	0.72	2.05	9	1
1:A:351:LEU:CD2	1:A:405:VAL:HG13	0.71	2.15	17	1
1:A:348:GLN:CG	1:A:412:LEU:HD11	0.70	2.16	11	16
1:A:351:LEU:HD11	1:A:409:GLU:HG2	0.70	1.62	4	11
1:A:357:GLU:HG3	1:A:401:LEU:HD21	0.70	1.64	15	2
1:A:351:LEU:HD21	1:A:409:GLU:CG	0.69	2.18	18	5
1:A:354:ARG:HB3	1:A:405:VAL:HG23	0.69	1.64	10	5
1:A:351:LEU:HD23	1:A:408:TYR:CB	0.68	2.19	1	3
1:A:378:THR:HG22	1:A:380:GLN:HG2	0.68	1.65	20	10
1:A:354:ARG:HH21	1:A:404:GLU:CD	0.68	1.91	16	1
1:A:357:GLU:CG	1:A:401:LEU:HD21	0.68	2.18	15	2
1:A:387:LEU:O	1:A:391:ILE:HD12	0.67	1.89	3	10
1:A:347:LEU:HD13	1:A:411:TRP:CB	0.67	2.20	4	14
1:A:371:MET:O	1:A:374:VAL:HG22	0.67	1.89	12	14
1:A:351:LEU:CD1	1:A:405:VAL:HG13	0.66	2.20	11	3
1:A:394:THR:O	1:A:398:ILE:HD12	0.66	1.91	2	9
1:A:351:LEU:HD12	1:A:405:VAL:HG13	0.66	1.68	20	3
1:A:362:VAL:HG23	1:A:398:ILE:HG12	0.66	1.68	19	11
1:A:348:GLN:HG2	1:A:412:LEU:HD11	0.66	1.68	8	10
1:A:375:TYR:CE1	1:A:382:GLY:N	0.65	2.65	6	5
1:A:361:GLU:OE1	1:A:394:THR:HG23	0.63	1.93	19	1
1:A:388:GLU:N	1:A:389:PRO:CD	0.63	2.61	8	20
1:A:351:LEU:HD21	1:A:405:VAL:HG13	0.63	1.70	17	2
1:A:365:ARG:CB	1:A:398:ILE:HD11	0.63	2.22	4	6
1:A:358:LEU:O	1:A:358:LEU:HD23	0.62	1.93	17	8
1:A:407:LYS:O	1:A:411:TRP:CD1	0.62	2.52	11	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:344:ARG:NH2	1:A:419:VAL:HG23	0.62	2.08	11	1
1:A:362:VAL:HG22	1:A:365:ARG:CZ	0.62	2.24	11	1
1:A:365:ARG:HB2	1:A:398:ILE:HD11	0.61	1.71	9	5
1:A:346:ARG:NH2	1:A:349:GLN:HE22	0.61	1.92	20	1
1:A:404:GLU:O	1:A:408:TYR:CD2	0.61	2.53	2	18
1:A:371:MET:O	1:A:375:TYR:CD2	0.61	2.54	15	5
1:A:358:LEU:C	1:A:358:LEU:HD23	0.61	2.16	1	3
1:A:351:LEU:HD21	1:A:409:GLU:HG2	0.61	1.72	13	2
1:A:351:LEU:HD12	1:A:405:VAL:HG22	0.61	1.71	18	1
1:A:358:LEU:HD23	1:A:358:LEU:O	0.60	1.96	1	2
1:A:344:ARG:HH12	1:A:416:GLU:N	0.60	1.94	11	1
1:A:371:MET:O	1:A:375:TYR:CE2	0.60	2.54	6	4
1:A:354:ARG:O	1:A:401:LEU:HD22	0.60	1.96	15	4
1:A:358:LEU:HB2	1:A:401:LEU:HD22	0.60	1.74	9	1
1:A:351:LEU:HD23	1:A:408:TYR:HB3	0.59	1.74	19	1
1:A:347:LEU:HD22	1:A:411:TRP:HE3	0.59	1.57	3	2
1:A:364:GLN:HA	1:A:367:ALA:HB3	0.59	1.73	1	5
1:A:364:GLN:NE2	1:A:368:LEU:HD21	0.58	2.12	6	6
1:A:346:ARG:N	1:A:346:ARG:HE	0.58	1.96	20	1
1:A:404:GLU:HA	1:A:407:LYS:HZ3	0.58	1.58	11	1
1:A:351:LEU:HD22	1:A:408:TYR:HB3	0.58	1.76	18	1
1:A:378:THR:HG22	1:A:381:MET:HG3	0.58	1.75	14	1
1:A:362:VAL:HG23	1:A:398:ILE:HD13	0.57	1.76	11	2
1:A:364:GLN:HE21	1:A:368:LEU:HD21	0.57	1.58	6	7
1:A:378:THR:HG22	1:A:380:GLN:CG	0.56	2.30	7	2
1:A:371:MET:C	1:A:374:VAL:HG22	0.56	2.21	17	4
1:A:407:LYS:O	1:A:411:TRP:CG	0.56	2.59	19	20
1:A:351:LEU:HD23	1:A:408:TYR:HB2	0.56	1.78	1	2
1:A:375:TYR:CD2	1:A:383:ASP:C	0.56	2.79	17	6
1:A:354:ARG:CB	1:A:405:VAL:HG22	0.56	2.30	8	8
1:A:372:LYS:HD2	1:A:391:ILE:HD11	0.56	1.76	4	4
1:A:368:LEU:HD11	1:A:394:THR:OG1	0.56	2.00	17	6
1:A:375:TYR:CE2	1:A:387:LEU:CD1	0.55	2.89	20	1
1:A:344:ARG:NH2	1:A:419:VAL:CG2	0.55	2.70	4	4
1:A:341:GLU:HG3	1:A:419:VAL:HG11	0.55	1.77	5	1
1:A:387:LEU:HD22	1:A:390:GLN:NE2	0.55	2.17	8	1
1:A:361:GLU:CD	1:A:401:LEU:HD12	0.55	2.22	15	1
1:A:372:LYS:NZ	1:A:391:ILE:CD1	0.55	2.71	7	1
1:A:368:LEU:HD22	1:A:390:GLN:CD	0.55	2.21	13	1
1:A:368:LEU:HD22	1:A:390:GLN:OE1	0.54	2.02	16	1
1:A:351:LEU:HD23	1:A:405:VAL:HG13	0.54	1.80	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:408:TYR:O	1:A:412:LEU:HD23	0.54	2.03	7	16
1:A:354:ARG:HH21	1:A:404:GLU:HG3	0.54	1.63	20	10
1:A:347:LEU:HD13	1:A:411:TRP:HB3	0.54	1.80	3	3
1:A:362:VAL:CG2	1:A:398:ILE:HD13	0.53	2.32	11	3
1:A:378:THR:HG23	1:A:380:GLN:HG2	0.53	1.78	14	1
1:A:357:GLU:HG3	1:A:401:LEU:HD22	0.53	1.80	10	2
1:A:375:TYR:CD2	1:A:387:LEU:HD11	0.53	2.38	19	4
1:A:358:LEU:HD13	1:A:359:GLN:N	0.53	2.18	4	1
1:A:398:ILE:HA	1:A:401:LEU:HD12	0.53	1.80	10	1
1:A:365:ARG:CD	1:A:365:ARG:C	0.53	2.77	4	8
1:A:371:MET:CB	1:A:387:LEU:HD13	0.53	2.33	12	5
1:A:344:ARG:HH21	1:A:419:VAL:HG21	0.53	1.60	4	2
1:A:351:LEU:CD1	1:A:405:VAL:CG1	0.53	2.86	11	2
1:A:365:ARG:HD3	1:A:398:ILE:HD12	0.53	1.80	11	1
1:A:358:LEU:HD22	1:A:358:LEU:C	0.52	2.24	4	1
1:A:347:LEU:HD22	1:A:408:TYR:CD1	0.52	2.40	8	2
1:A:351:LEU:HD12	1:A:351:LEU:O	0.52	2.04	18	1
1:A:361:GLU:OE2	1:A:401:LEU:HD11	0.52	2.03	17	1
1:A:344:ARG:NH1	1:A:416:GLU:CG	0.52	2.72	3	1
1:A:407:LYS:CB	1:A:407:LYS:NZ	0.52	2.72	10	3
1:A:346:ARG:HH21	1:A:349:GLN:HE22	0.52	1.48	20	1
1:A:372:LYS:CG	1:A:387:LEU:HD12	0.52	2.34	11	1
1:A:372:LYS:NZ	1:A:391:ILE:HD13	0.51	2.20	7	1
1:A:395:LEU:O	1:A:399:GLU:CG	0.51	2.59	11	5
1:A:365:ARG:HE	1:A:395:LEU:HD11	0.51	1.66	16	1
1:A:350:GLN:CB	1:A:408:TYR:CZ	0.51	2.94	4	1
1:A:358:LEU:C	1:A:358:LEU:CD2	0.51	2.79	13	11
1:A:375:TYR:CE1	1:A:382:GLY:HA3	0.51	2.41	17	8
1:A:344:ARG:CZ	1:A:416:GLU:CD	0.51	2.79	10	5
1:A:365:ARG:NH1	1:A:398:ILE:HD13	0.51	2.20	14	1
1:A:345:LYS:HB2	1:A:346:ARG:HH21	0.51	1.66	20	1
1:A:375:TYR:CE1	1:A:382:GLY:CA	0.51	2.93	6	3
1:A:388:GLU:N	1:A:389:PRO:HD2	0.50	2.21	8	20
1:A:398:ILE:O	1:A:402:LYS:CD	0.50	2.59	2	5
1:A:357:GLU:CD	1:A:401:LEU:CD2	0.50	2.80	10	3
1:A:359:GLN:O	1:A:363:ASP:CB	0.50	2.59	5	13
1:A:351:LEU:HD12	1:A:351:LEU:C	0.50	2.27	18	1
1:A:387:LEU:O	1:A:391:ILE:CD1	0.50	2.60	15	6
1:A:371:MET:O	1:A:387:LEU:CD1	0.50	2.60	5	6
1:A:400:ARG:O	1:A:404:GLU:CG	0.50	2.59	16	6
1:A:387:LEU:O	1:A:391:ILE:CG1	0.50	2.60	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:345:LYS:O	1:A:345:LYS:CD	0.50	2.60	1	2
1:A:375:TYR:O	1:A:379:PRO:CD	0.50	2.60	5	5
1:A:344:ARG:NH2	1:A:348:GLN:NE2	0.49	2.60	7	1
1:A:394:THR:O	1:A:398:ILE:CD1	0.49	2.60	8	7
1:A:387:LEU:HD22	1:A:390:GLN:HE22	0.49	1.67	8	1
1:A:345:LYS:NZ	1:A:349:GLN:NE2	0.49	2.60	7	1
1:A:342:GLN:NE2	1:A:345:LYS:NZ	0.49	2.60	11	1
1:A:351:LEU:HD22	1:A:408:TYR:CB	0.49	2.37	18	1
1:A:344:ARG:NH2	1:A:419:VAL:HG11	0.49	2.22	4	2
1:A:344:ARG:NH1	1:A:419:VAL:CG2	0.49	2.76	8	1
1:A:407:LYS:HD3	1:A:411:TRP:CZ2	0.49	2.43	18	10
1:A:394:THR:O	1:A:398:ILE:CG1	0.49	2.61	8	4
1:A:354:ARG:O	1:A:401:LEU:CD2	0.49	2.61	15	1
1:A:346:ARG:CD	1:A:346:ARG:N	0.49	2.76	2	1
1:A:364:GLN:O	1:A:367:ALA:N	0.48	2.46	13	19
1:A:407:LYS:O	1:A:411:TRP:N	0.48	2.46	11	20
1:A:378:THR:CG2	1:A:380:GLN:OE1	0.48	2.61	2	1
1:A:402:LYS:CB	1:A:402:LYS:NZ	0.48	2.75	16	2
1:A:371:MET:O	1:A:387:LEU:HD11	0.48	2.08	17	5
1:A:368:LEU:HD12	1:A:391:ILE:HA	0.48	1.85	11	2
1:A:371:MET:O	1:A:374:VAL:CG2	0.48	2.60	17	1
1:A:375:TYR:O	1:A:379:PRO:CG	0.48	2.62	5	6
1:A:354:ARG:CB	1:A:405:VAL:HG23	0.48	2.36	10	1
1:A:365:ARG:HG3	1:A:398:ILE:HD11	0.48	1.85	11	1
1:A:344:ARG:NH2	1:A:412:LEU:CD1	0.48	2.73	3	1
1:A:344:ARG:CG	1:A:345:LYS:N	0.48	2.76	14	4
1:A:354:ARG:HB2	1:A:405:VAL:HG22	0.48	1.84	17	2
1:A:361:GLU:OE2	1:A:401:LEU:HD12	0.48	2.08	15	1
1:A:397:ASN:O	1:A:401:LEU:CD1	0.48	2.60	13	3
1:A:407:LYS:HD3	1:A:411:TRP:CH2	0.48	2.43	17	7
1:A:350:GLN:HB3	1:A:408:TYR:CE2	0.48	2.44	14	1
1:A:352:GLU:O	1:A:356:ARG:CG	0.48	2.62	17	7
1:A:371:MET:CE	1:A:375:TYR:OH	0.47	2.62	19	2
1:A:392:ALA:O	1:A:396:SER:CB	0.47	2.62	20	1
1:A:378:THR:O	1:A:381:MET:CG	0.47	2.63	1	9
1:A:342:GLN:O	1:A:345:LYS:N	0.47	2.48	4	5
1:A:358:LEU:C	1:A:358:LEU:CD1	0.47	2.80	9	1
1:A:358:LEU:HD23	1:A:358:LEU:C	0.47	2.30	17	4
1:A:399:GLU:O	1:A:403:LEU:CD2	0.47	2.60	13	5
1:A:346:ARG:O	1:A:347:LEU:C	0.47	2.52	2	7
1:A:356:ARG:CD	1:A:357:GLU:N	0.47	2.78	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:347:LEU:O	1:A:351:LEU:CB	0.47	2.62	11	4
1:A:365:ARG:CD	1:A:398:ILE:CD1	0.47	2.92	10	1
1:A:348:GLN:O	1:A:351:LEU:CB	0.47	2.62	4	1
1:A:361:GLU:HB2	1:A:394:THR:HG23	0.47	1.86	15	1
1:A:349:GLN:NE2	1:A:349:GLN:H	0.47	2.08	1	1
1:A:411:TRP:O	1:A:415:ALA:N	0.47	2.48	9	20
1:A:371:MET:HE3	1:A:375:TYR:CZ	0.47	2.45	19	2
1:A:354:ARG:HD2	1:A:401:LEU:HD23	0.46	1.87	4	2
1:A:354:ARG:CB	1:A:405:VAL:CG2	0.46	2.93	17	1
1:A:374:VAL:HG23	1:A:375:TYR:CE1	0.46	2.45	12	4
1:A:365:ARG:CB	1:A:398:ILE:CD1	0.46	2.94	4	5
1:A:367:ALA:O	1:A:370:LYS:N	0.46	2.48	13	5
1:A:394:THR:HG22	1:A:398:ILE:HD11	0.46	1.87	12	2
1:A:362:VAL:HG22	1:A:398:ILE:HD13	0.46	1.86	15	1
1:A:353:GLU:O	1:A:356:ARG:N	0.46	2.49	8	6
1:A:364:GLN:O	1:A:367:ALA:HB3	0.46	2.10	10	5
1:A:360:LYS:CB	1:A:360:LYS:NZ	0.46	2.79	8	1
1:A:347:LEU:O	1:A:351:LEU:N	0.46	2.48	13	7
1:A:358:LEU:O	1:A:361:GLU:N	0.46	2.49	8	3
1:A:342:GLN:O	1:A:342:GLN:NE2	0.46	2.49	19	1
1:A:411:TRP:O	1:A:414:GLU:N	0.46	2.49	3	19
1:A:347:LEU:HD22	1:A:408:TYR:CE1	0.46	2.46	8	1
1:A:343:GLN:O	1:A:346:ARG:CG	0.46	2.64	12	1
1:A:399:GLU:O	1:A:403:LEU:HD13	0.46	2.11	18	1
1:A:350:GLN:HB2	1:A:408:TYR:CZ	0.46	2.46	3	2
1:A:372:LYS:CE	1:A:391:ILE:CD1	0.46	2.93	4	2
1:A:402:LYS:O	1:A:405:VAL:N	0.45	2.49	19	9
1:A:344:ARG:NH2	1:A:416:GLU:CD	0.45	2.70	20	2
1:A:351:LEU:CD2	1:A:408:TYR:CB	0.45	2.94	19	1
1:A:351:LEU:HD13	1:A:405:VAL:HG22	0.45	1.88	19	1
1:A:344:ARG:CZ	1:A:416:GLU:CG	0.45	2.94	16	2
1:A:401:LEU:O	1:A:404:GLU:N	0.45	2.49	18	4
1:A:416:GLU:O	1:A:419:VAL:N	0.45	2.50	4	8
1:A:368:LEU:O	1:A:371:MET:N	0.45	2.49	6	6
1:A:345:LYS:O	1:A:349:GLN:NE2	0.45	2.50	7	3
1:A:357:GLU:OE1	1:A:401:LEU:CD2	0.45	2.63	10	1
1:A:346:ARG:CG	1:A:347:LEU:N	0.45	2.79	15	1
1:A:399:GLU:O	1:A:403:LEU:CG	0.45	2.65	10	4
1:A:365:ARG:HE	1:A:395:LEU:HD21	0.45	1.71	12	1
1:A:347:LEU:HD23	1:A:411:TRP:HE3	0.45	1.70	1	1
1:A:361:GLU:O	1:A:365:ARG:N	0.45	2.49	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:347:LEU:HD13	1:A:411:TRP:HB2	0.45	1.87	8	11
1:A:359:GLN:O	1:A:363:ASP:N	0.45	2.50	6	5
1:A:361:GLU:O	1:A:394:THR:CG2	0.45	2.64	18	1
1:A:410:ALA:O	1:A:414:GLU:CG	0.45	2.65	3	15
1:A:372:LYS:O	1:A:376:GLU:N	0.45	2.49	19	4
1:A:361:GLU:N	1:A:361:GLU:OE1	0.45	2.50	3	2
1:A:373:ASP:O	1:A:377:LYS:CG	0.45	2.65	20	8
1:A:357:GLU:OE2	1:A:401:LEU:CD2	0.45	2.64	2	1
1:A:361:GLU:N	1:A:361:GLU:OE2	0.45	2.50	5	2
1:A:362:VAL:HG23	1:A:398:ILE:CD1	0.45	2.41	10	2
1:A:365:ARG:HG3	1:A:398:ILE:CD1	0.45	2.41	11	3
1:A:364:GLN:O	1:A:365:ARG:C	0.45	2.55	18	8
1:A:414:GLU:O	1:A:418:ARG:NE	0.45	2.50	6	2
1:A:354:ARG:O	1:A:358:LEU:N	0.45	2.49	19	1
1:A:344:ARG:NH1	1:A:416:GLU:OE1	0.45	2.50	6	1
1:A:397:ASN:O	1:A:400:ARG:N	0.45	2.50	16	2
1:A:375:TYR:CZ	1:A:382:GLY:HA3	0.44	2.47	2	9
1:A:405:VAL:O	1:A:405:VAL:CG1	0.44	2.65	18	4
1:A:357:GLU:N	1:A:357:GLU:CD	0.44	2.70	8	1
1:A:415:ALA:O	1:A:418:ARG:N	0.44	2.50	11	2
1:A:393:GLU:O	1:A:397:ASN:ND2	0.44	2.50	4	4
1:A:368:LEU:HD13	1:A:390:GLN:HG3	0.44	1.89	18	2
1:A:396:SER:O	1:A:400:ARG:NE	0.44	2.50	18	1
1:A:413:ALA:O	1:A:417:SER:CB	0.44	2.65	4	1
1:A:414:GLU:O	1:A:418:ARG:CD	0.44	2.65	6	1
1:A:350:GLN:O	1:A:351:LEU:C	0.44	2.56	14	1
1:A:394:THR:O	1:A:398:ILE:N	0.44	2.50	13	3
1:A:402:LYS:O	1:A:405:VAL:HG12	0.44	2.12	19	3
1:A:344:ARG:NH1	1:A:416:GLU:CD	0.44	2.71	6	2
1:A:344:ARG:NE	1:A:416:GLU:CG	0.44	2.81	7	2
1:A:372:LYS:HG3	1:A:387:LEU:HD12	0.44	1.89	11	1
1:A:371:MET:HA	1:A:371:MET:CE	0.44	2.43	12	1
1:A:347:LEU:O	1:A:349:GLN:N	0.44	2.51	16	2
1:A:368:LEU:N	1:A:368:LEU:HD23	0.44	2.27	9	1
1:A:352:GLU:O	1:A:356:ARG:N	0.44	2.51	15	1
1:A:361:GLU:OE1	1:A:401:LEU:HD11	0.43	2.12	6	1
1:A:350:GLN:O	1:A:353:GLU:N	0.43	2.50	11	1
1:A:355:SER:O	1:A:358:LEU:N	0.43	2.50	18	1
1:A:347:LEU:HD22	1:A:411:TRP:HB2	0.43	1.90	19	1
1:A:342:GLN:NE2	1:A:346:ARG:NH1	0.43	2.67	10	1
1:A:398:ILE:CG2	1:A:402:LYS:NZ	0.43	2.81	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:407:LYS:CE	1:A:411:TRP:CZ2	0.43	3.02	17	1
1:A:411:TRP:O	1:A:412:LEU:C	0.43	2.57	2	13
1:A:358:LEU:HD13	1:A:358:LEU:C	0.43	2.34	4	1
1:A:372:LYS:HE3	1:A:391:ILE:CD1	0.43	2.44	4	4
1:A:389:PRO:O	1:A:393:GLU:CB	0.43	2.66	16	1
1:A:347:LEU:CB	1:A:412:LEU:CD2	0.43	2.97	19	1
1:A:371:MET:CE	1:A:375:TYR:CZ	0.43	3.02	19	1
1:A:354:ARG:HB2	1:A:405:VAL:CG2	0.43	2.44	17	1
1:A:372:LYS:CD	1:A:391:ILE:HD11	0.43	2.44	4	1
1:A:372:LYS:O	1:A:375:TYR:N	0.43	2.52	6	1
1:A:347:LEU:HB3	1:A:412:LEU:CD2	0.43	2.44	19	1
1:A:347:LEU:HD22	1:A:411:TRP:CE3	0.43	2.44	3	1
1:A:361:GLU:N	1:A:361:GLU:CD	0.43	2.72	17	2
1:A:344:ARG:HH21	1:A:416:GLU:N	0.43	2.12	8	1
1:A:358:LEU:C	1:A:360:LYS:N	0.43	2.71	12	1
1:A:351:LEU:HD13	1:A:405:VAL:HA	0.43	1.89	18	1
1:A:344:ARG:CZ	1:A:416:GLU:HG2	0.43	2.44	16	1
1:A:365:ARG:HG3	1:A:366:GLU:N	0.43	2.29	20	1
1:A:391:ILE:O	1:A:394:THR:N	0.42	2.52	4	2
1:A:358:LEU:O	1:A:360:LYS:N	0.42	2.52	12	1
1:A:371:MET:HB2	1:A:387:LEU:HD13	0.42	1.90	9	1
1:A:347:LEU:C	1:A:349:GLN:N	0.42	2.71	16	2
1:A:347:LEU:O	1:A:348:GLN:C	0.42	2.58	14	4
1:A:347:LEU:O	1:A:350:GLN:N	0.42	2.53	16	1
1:A:361:GLU:CD	1:A:401:LEU:CD1	0.42	2.88	15	1
1:A:349:GLN:C	1:A:351:LEU:N	0.42	2.73	17	3
1:A:402:LYS:CB	1:A:402:LYS:HZ3	0.42	2.28	16	1
1:A:350:GLN:NE2	1:A:353:GLU:OE1	0.42	2.53	14	1
1:A:407:LYS:HB2	1:A:411:TRP:CE2	0.42	2.49	4	15
1:A:346:ARG:O	1:A:350:GLN:N	0.42	2.52	11	2
1:A:351:LEU:CD2	1:A:409:GLU:CG	0.42	2.97	11	1
1:A:344:ARG:CD	1:A:416:GLU:HG2	0.42	2.45	5	2
1:A:365:ARG:HD3	1:A:398:ILE:CD1	0.42	2.45	11	1
1:A:371:MET:HA	1:A:374:VAL:CG2	0.42	2.45	14	2
1:A:344:ARG:CZ	1:A:416:GLU:HG3	0.42	2.45	3	1
1:A:400:ARG:CZ	1:A:400:ARG:HB3	0.42	2.45	18	1
1:A:347:LEU:HD22	1:A:411:TRP:HB3	0.41	1.91	1	1
1:A:374:VAL:O	1:A:378:THR:O	0.41	2.38	12	6
1:A:344:ARG:NH2	1:A:416:GLU:OE1	0.41	2.53	16	1
1:A:408:TYR:O	1:A:411:TRP:N	0.41	2.53	20	4
1:A:401:LEU:C	1:A:405:VAL:HG23	0.41	2.33	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:404:GLU:OE1	1:A:407:LYS:NZ	0.41	2.53	8	1
1:A:342:GLN:NE2	1:A:345:LYS:CE	0.41	2.83	11	1
1:A:344:ARG:NH2	1:A:348:GLN:HE22	0.41	2.14	12	1
1:A:346:ARG:O	1:A:350:GLN:OE1	0.41	2.39	14	1
1:A:365:ARG:CG	1:A:398:ILE:HD11	0.41	2.45	18	1
1:A:350:GLN:HB3	1:A:408:TYR:CZ	0.41	2.51	4	1
1:A:365:ARG:CG	1:A:366:GLU:N	0.41	2.83	4	5
1:A:402:LYS:O	1:A:406:GLN:CD	0.41	2.59	8	1
1:A:354:ARG:HH21	1:A:404:GLU:CG	0.41	2.27	12	1
1:A:400:ARG:CG	1:A:401:LEU:N	0.41	2.84	5	1
1:A:353:GLU:C	1:A:355:SER:N	0.41	2.74	7	1
1:A:371:MET:HA	1:A:371:MET:HE3	0.41	1.93	12	1
1:A:401:LEU:O	1:A:402:LYS:C	0.41	2.59	18	1
1:A:347:LEU:HA	1:A:408:TYR:CD1	0.41	2.51	3	1
1:A:344:ARG:CD	1:A:416:GLU:CG	0.41	2.98	5	1
1:A:351:LEU:HD23	1:A:405:VAL:CG1	0.41	2.46	5	1
1:A:349:GLN:O	1:A:352:GLU:N	0.41	2.54	4	1
1:A:364:GLN:O	1:A:368:LEU:N	0.41	2.53	8	2
1:A:351:LEU:CD2	1:A:405:VAL:HA	0.41	2.46	8	1
1:A:367:ALA:O	1:A:371:MET:N	0.41	2.53	9	1
1:A:365:ARG:HD2	1:A:398:ILE:CD1	0.41	2.46	10	1
1:A:344:ARG:NH1	1:A:416:GLU:HG2	0.41	2.31	3	1
1:A:393:GLU:O	1:A:397:ASN:CG	0.41	2.60	4	8
1:A:347:LEU:CB	1:A:412:LEU:HD22	0.41	2.45	4	2
1:A:367:ALA:O	1:A:368:LEU:C	0.41	2.59	4	1
1:A:357:GLU:OE1	1:A:357:GLU:CA	0.41	2.69	8	1
1:A:407:LYS:CB	1:A:407:LYS:HZ2	0.41	2.27	10	1
1:A:344:ARG:HB3	1:A:344:ARG:CZ	0.41	2.46	11	1
1:A:412:LEU:O	1:A:416:GLU:CG	0.41	2.69	11	1
1:A:372:LYS:HE3	1:A:391:ILE:HD12	0.41	1.93	20	1
1:A:399:GLU:OE2	1:A:400:ARG:CZ	0.41	2.69	20	1
1:A:375:TYR:O	1:A:379:PRO:CB	0.41	2.69	16	1
1:A:415:ALA:O	1:A:416:GLU:C	0.40	2.60	3	3
1:A:345:LYS:CB	1:A:346:ARG:HH21	0.40	2.29	20	1
1:A:351:LEU:HD21	1:A:409:GLU:CD	0.40	2.37	3	1
1:A:397:ASN:C	1:A:399:GLU:N	0.40	2.73	1	1
1:A:365:ARG:CD	1:A:366:GLU:N	0.40	2.84	19	2
1:A:406:GLN:O	1:A:407:LYS:C	0.40	2.60	2	1
1:A:348:GLN:O	1:A:351:LEU:N	0.40	2.54	4	1
1:A:379:PRO:O	1:A:382:GLY:O	0.40	2.39	15	1
1:A:361:GLU:OE2	1:A:401:LEU:CD1	0.40	2.68	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:419:VAL:O	1:A:420:LEU:C	0.40	2.60	4	1
1:A:357:GLU:O	1:A:361:GLU:OE1	0.40	2.40	5	1
1:A:416:GLU:O	1:A:417:SER:C	0.40	2.60	6	2
1:A:402:LYS:O	1:A:406:GLN:OE1	0.40	2.40	8	1
1:A:415:ALA:C	1:A:417:SER:N	0.40	2.74	8	1
1:A:393:GLU:CG	1:A:397:ASN:ND2	0.40	2.84	11	1
1:A:408:TYR:O	1:A:412:LEU:CD2	0.40	2.69	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	80/98 (82%)	69±2 (86±3%)	10±3 (13±3%)	1±1 (1±1%)	21	71
All	All	1600/1960 (82%)	1381 (86%)	208 (13%)	11 (1%)	21	71

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	419	VAL	4
1	A	349	GLN	3
1	A	348	GLN	2
1	A	351	LEU	1
1	A	401	LEU	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	73/89 (82%)	62±2 (85±3%)	11±2 (15±3%)	5	43
All	All	1460/1780 (82%)	1245 (85%)	215 (15%)	5	43

All 39 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	377	LYS	19
1	A	399	GLU	18
1	A	365	ARG	16
1	A	407	LYS	15
1	A	342	GLN	11
1	A	358	LEU	11
1	A	363	ASP	11
1	A	414	GLU	10
1	A	381	MET	9
1	A	388	GLU	7
1	A	403	LEU	7
1	A	360	LYS	6
1	A	345	LYS	6
1	A	351	LEU	6
1	A	402	LYS	5
1	A	383	ASP	5
1	A	357	GLU	5
1	A	369	LYS	5
1	A	346	ARG	4
1	A	361	GLU	4
1	A	370	LYS	4
1	A	416	GLU	3
1	A	372	LYS	3
1	A	405	VAL	3
1	A	347	LEU	2
1	A	356	ARG	2
1	A	344	ARG	2
1	A	371	MET	2
1	A	396	SER	2
1	A	406	GLN	2
1	A	366	GLU	2
1	A	349	GLN	1
1	A	348	GLN	1
1	A	386	SER	1
1	A	390	GLN	1
1	A	354	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	355	SER	1
1	A	387	LEU	1
1	A	418	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1287
Number of shifts mapped to atoms	1287
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	98	-0.46 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	95	0.22 ± 0.04	None needed (< 0.5 ppm)
$^{13}\text{C}'$	87	-0.53 ± 0.13	Should be applied
^{15}N	90	0.18 ± 0.19	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1091 atoms were assigned a chemical shift out of a possible 1172. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	390/395 (99%)	158/158 (100%)	155/160 (97%)	77/77 (100%)
Sidechain	677/747 (91%)	446/475 (94%)	214/232 (92%)	17/40 (42%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	24/30 (80%)	14/14 (100%)	9/15 (60%)	1/1 (100%)
Overall	1091/1172 (93%)	618/647 (96%)	378/407 (93%)	95/118 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1286 atoms were assigned a chemical shift out of a possible 1393. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	467/481 (97%)	192/193 (99%)	185/196 (94%)	90/92 (98%)
Sidechain	779/858 (91%)	513/546 (94%)	247/268 (92%)	19/44 (43%)
Aromatic	40/54 (74%)	23/27 (85%)	16/24 (67%)	1/3 (33%)
Overall	1286/1393 (92%)	728/766 (95%)	448/488 (92%)	110/139 (79%)

7.1.4 Statistically unusual chemical shifts ⓘ

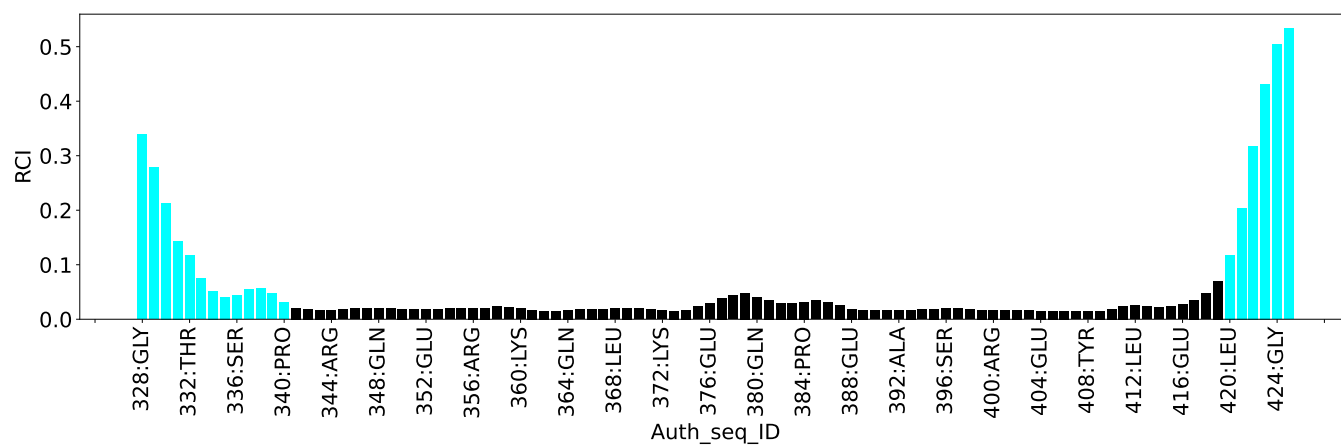
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	418	ARG	NE	109.79	76.53 – 92.65	15.6
1	A	423	ARG	NE	109.62	76.53 – 92.65	15.5
1	A	354	ARG	NE	109.59	76.53 – 92.65	15.5
1	A	356	ARG	NE	109.33	76.53 – 92.65	15.3
1	A	346	ARG	NE	108.85	76.53 – 92.65	15.1
1	A	344	ARG	NE	108.36	76.53 – 92.65	14.7
1	A	400	ARG	NE	107.36	76.53 – 92.65	14.1
1	A	407	LYS	HG2	0.01	0.13 – 2.61	-5.5
1	A	411	TRP	CE2	171.11	105.29 – 170.61	5.1

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

8.1 Conformationally restricting restraints

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	1979
Intra-residue ($ i-j =0$)	629
Sequential ($ i-j =1$)	516
Medium range ($ i-j >1$ and $ i-j <5$)	571
Long range ($ i-j \geq 5$)	263
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	20.2
Number of long range restraints per residue ¹	2.7

¹Long 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

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

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)	0.8	0.2
0.2-0.5 (Medium)	0.6	0.3
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model [i](#)

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

9 Distance violation analysis ⓘ

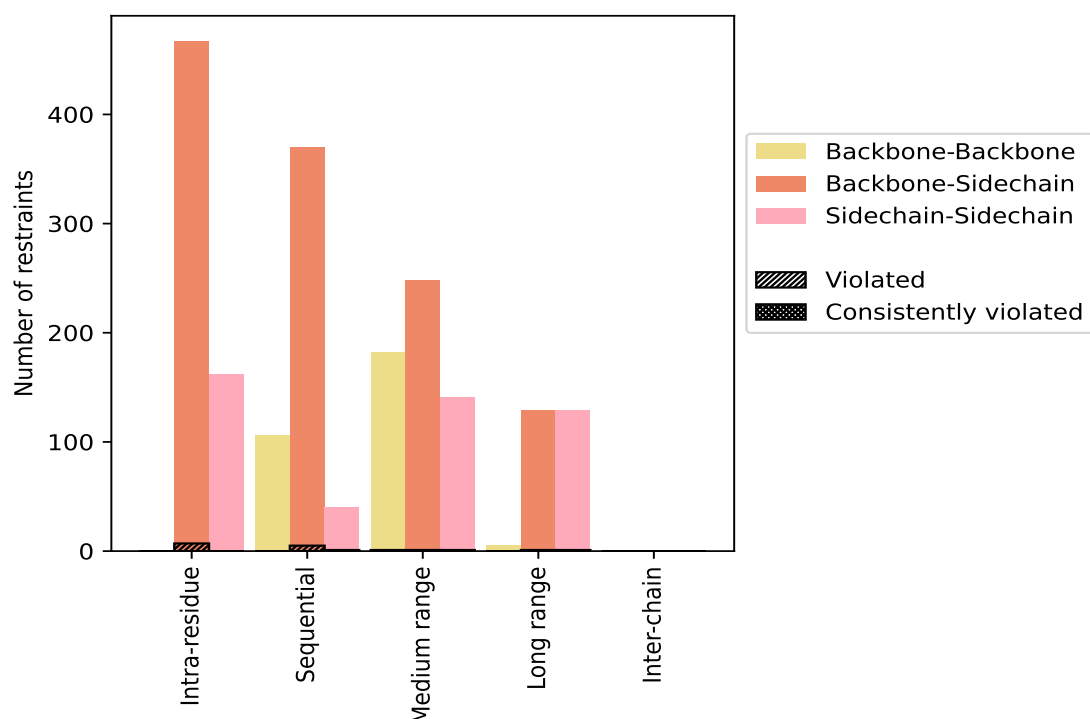
9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	629	31.8	7	1.1	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	467	23.6	7	1.5	0.4	0	0.0	0.0
Sidechain-Sidechain	162	8.2	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	516	26.1	6	1.2	0.3	0	0.0	0.0
Backbone-Backbone	106	5.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	370	18.7	5	1.4	0.3	0	0.0	0.0
Sidechain-Sidechain	40	2.0	1	2.5	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	571	28.9	3	0.5	0.2	0	0.0	0.0
Backbone-Backbone	182	9.2	1	0.5	0.1	0	0.0	0.0
Backbone-Sidechain	248	12.5	1	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	141	7.1	1	0.7	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	263	13.3	2	0.8	0.1	0	0.0	0.0
Backbone-Backbone	5	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	129	6.5	1	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	129	6.5	1	0.8	0.1	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	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	1979	100.0	18	0.9	0.9	0	0.0	0.0
Backbone-Backbone	293	14.8	1	0.3	0.1	0	0.0	0.0
Backbone-Sidechain	1214	61.3	14	1.2	0.7	0	0.0	0.0
Sidechain-Sidechain	472	23.9	3	0.6	0.2	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 [i](#)



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 [i](#)

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	1	0	0	0	0	1	0.13	0.13	0.0	0.13
2	0	1	0	0	0	1	0.18	0.18	0.0	0.18
3	0	0	1	0	0	1	0.11	0.11	0.0	0.11
4	0	1	0	0	0	1	0.25	0.25	0.0	0.25
5	0	1	0	0	0	1	0.26	0.26	0.0	0.26
6	1	0	1	0	0	2	0.12	0.12	0.0	0.12
7	3	0	0	0	0	3	0.17	0.2	0.02	0.17
8	0	0	0	1	0	1	0.1	0.1	0.0	0.1
9	1	0	1	0	0	2	0.2	0.3	0.1	0.2
10	1	1	0	0	0	2	0.12	0.13	0.01	0.12

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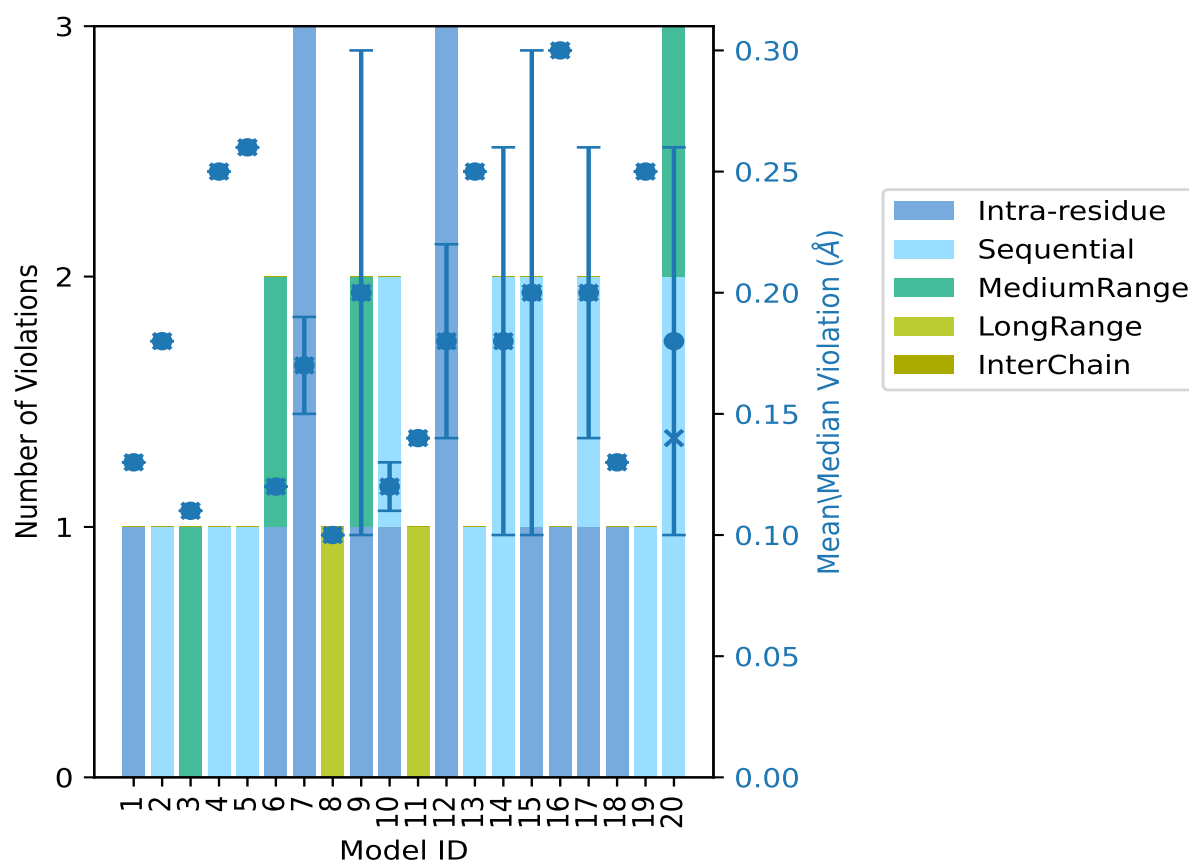
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	1	0	1	0.14	0.14	0.0	0.14
12	3	0	0	0	0	3	0.18	0.22	0.04	0.18
13	0	1	0	0	0	1	0.25	0.25	0.0	0.25
14	0	2	0	0	0	2	0.18	0.25	0.08	0.18
15	1	1	0	0	0	2	0.2	0.3	0.1	0.2
16	1	0	0	0	0	1	0.3	0.3	0.0	0.3
17	1	1	0	0	0	2	0.2	0.27	0.06	0.2
18	1	0	0	0	0	1	0.13	0.13	0.0	0.13
19	0	1	0	0	0	1	0.25	0.25	0.0	0.25
20	0	2	1	0	0	3	0.18	0.29	0.08	0.14

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard 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

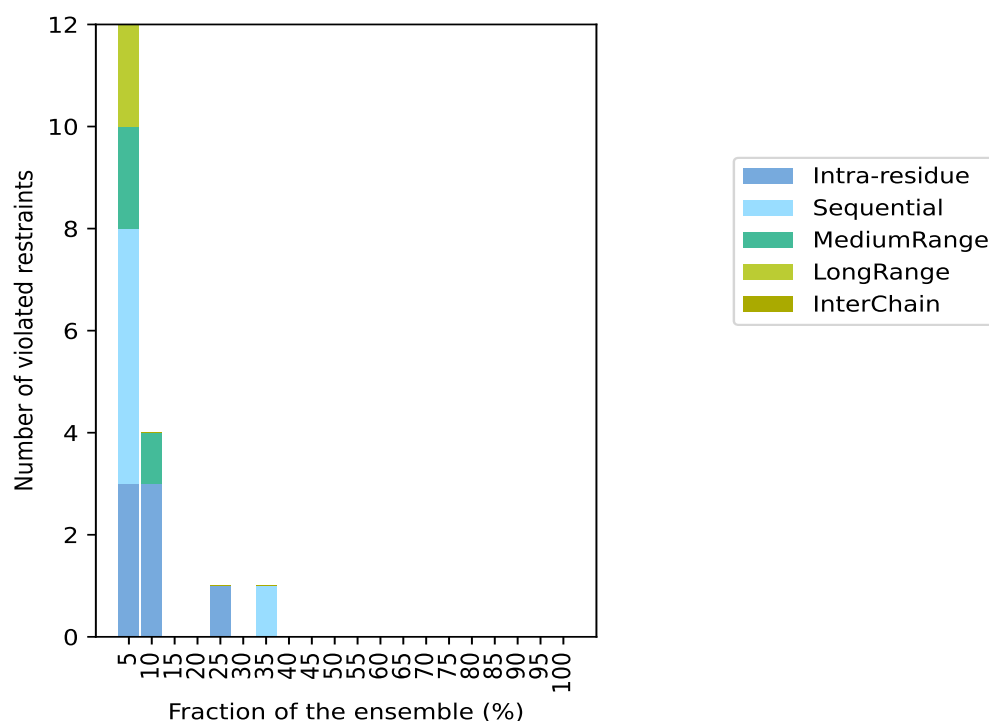
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1961(IR:622, SQ:510, MR:568, LR:261, IC:0) restraints are 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	5	2	2	0	12	1	5.0
3	0	1	0	0	4	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
1	0	0	0	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	1	0	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

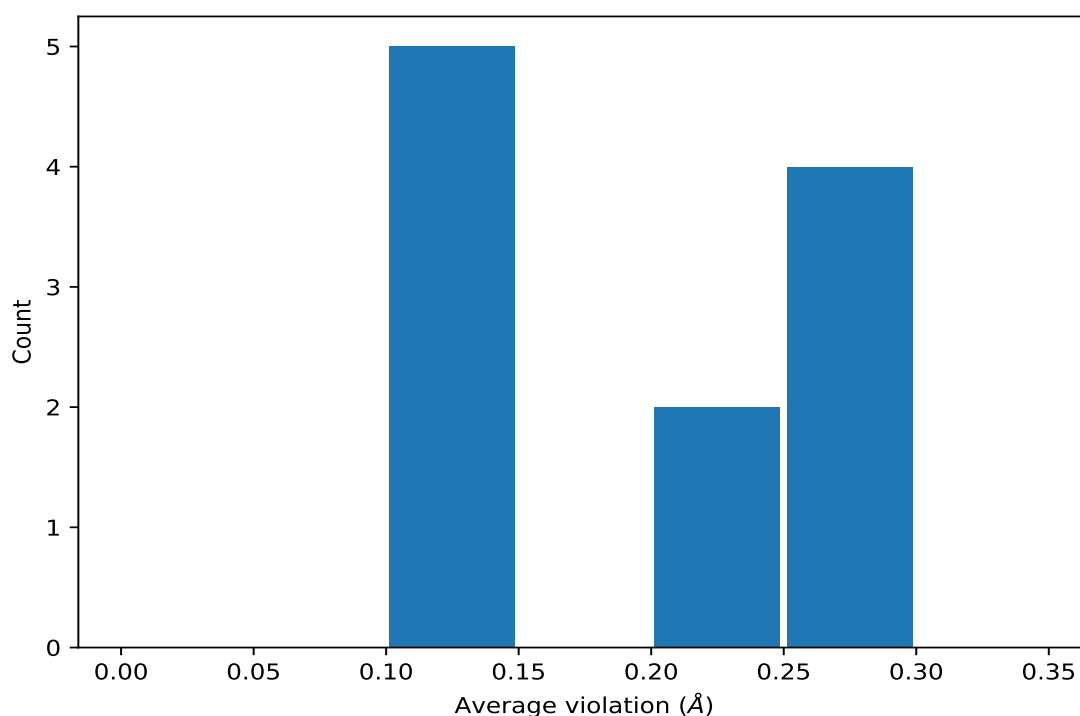
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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 [i](#)

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.

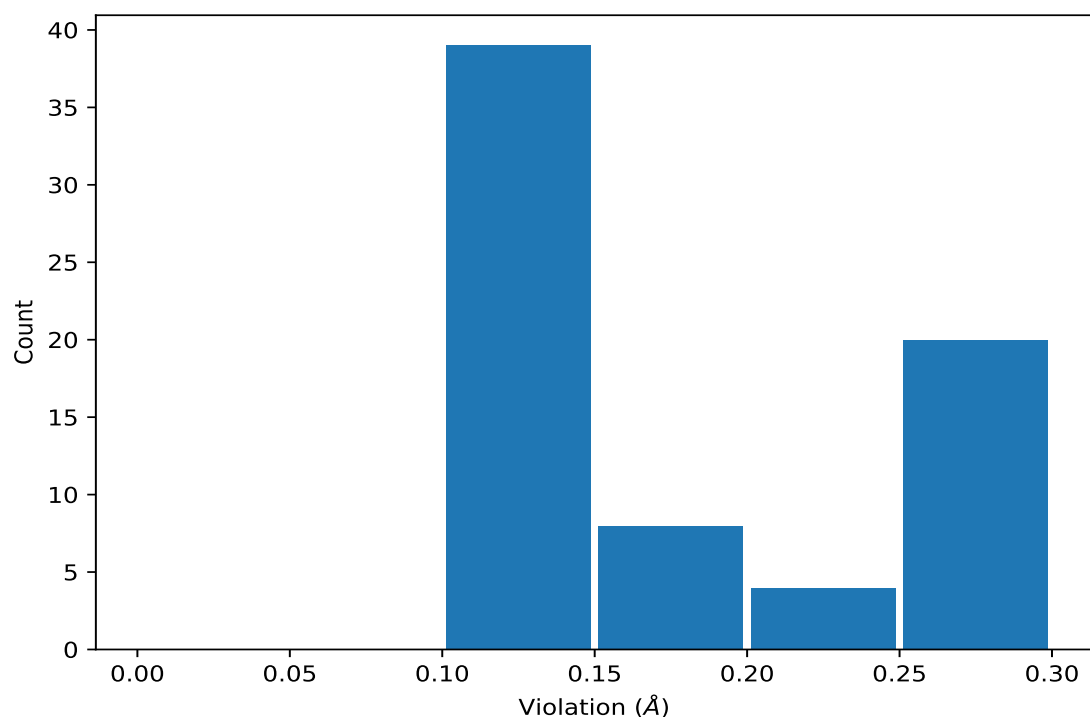
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1714)	1:365:A:ARG:HB2	1:366:A:GLU:H	7	0.26	0.01	0.25
(1,1714)	1:365:A:ARG:HB3	1:366:A:GLU:H	7	0.26	0.01	0.25
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD2	5	0.26	0.05	0.3
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD3	5	0.26	0.05	0.3
(1,371)	1:370:A:LYS:H	1:370:A:LYS:HD2	2	0.2	0.02	0.2
(1,371)	1:370:A:LYS:H	1:370:A:LYS:HD3	2	0.2	0.02	0.2
(1,1196)	1:370:A:LYS:HA	1:370:A:LYS:HE2	2	0.14	0.01	0.14
(1,1196)	1:370:A:LYS:HA	1:370:A:LYS:HE3	2	0.14	0.01	0.14
(1,1766)	1:372:A:LYS:H	1:372:A:LYS:HD2	2	0.12	0.02	0.12
(1,1766)	1:372:A:LYS:H	1:372:A:LYS:HD3	2	0.12	0.02	0.12
(1,1407)	1:371:A:MET:HA	1:374:A:VAL:HA	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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 [i](#)

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)
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD2	9	0.3
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD3	9	0.3
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD2	15	0.3
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD3	15	0.3
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD2	16	0.3
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD3	16	0.3
(1,1714)	1:365:A:ARG:HB2	1:366:A:GLU:H	20	0.29
(1,1714)	1:365:A:ARG:HB3	1:366:A:GLU:H	20	0.29
(1,1714)	1:365:A:ARG:HB2	1:366:A:GLU:H	17	0.27
(1,1714)	1:365:A:ARG:HB3	1:366:A:GLU:H	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1714)	1:365:A:ARG:HB2	1:366:A:GLU:H	5	0.26
(1,1714)	1:365:A:ARG:HB3	1:366:A:GLU:H	5	0.26
(1,1714)	1:365:A:ARG:HB2	1:366:A:GLU:H	4	0.25
(1,1714)	1:365:A:ARG:HB3	1:366:A:GLU:H	4	0.25
(1,1714)	1:365:A:ARG:HB2	1:366:A:GLU:H	13	0.25
(1,1714)	1:365:A:ARG:HB3	1:366:A:GLU:H	13	0.25
(1,1714)	1:365:A:ARG:HB2	1:366:A:GLU:H	14	0.25
(1,1714)	1:365:A:ARG:HB3	1:366:A:GLU:H	14	0.25
(1,1714)	1:365:A:ARG:HB2	1:366:A:GLU:H	19	0.25
(1,1714)	1:365:A:ARG:HB3	1:366:A:GLU:H	19	0.25
(1,371)	1:370:A:LYS:H	1:370:A:LYS:HD2	12	0.22
(1,371)	1:370:A:LYS:H	1:370:A:LYS:HD3	12	0.22
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD2	7	0.2
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD3	7	0.2
(1,1522)	1:346:A:ARG:HG2	1:347:A:LEU:H	2	0.18
(1,1522)	1:346:A:ARG:HG3	1:347:A:LEU:H	2	0.18
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD2	12	0.18
(1,1053)	1:370:A:LYS:HA	1:370:A:LYS:HD3	12	0.18
(1,371)	1:370:A:LYS:H	1:370:A:LYS:HD2	7	0.17
(1,371)	1:370:A:LYS:H	1:370:A:LYS:HD3	7	0.17
(1,1196)	1:370:A:LYS:HA	1:370:A:LYS:HE2	7	0.15
(1,1196)	1:370:A:LYS:HA	1:370:A:LYS:HE3	7	0.15
(1,1766)	1:372:A:LYS:H	1:372:A:LYS:HD2	17	0.14
(1,1766)	1:372:A:LYS:H	1:372:A:LYS:HD3	17	0.14
(1,1718)	1:365:A:ARG:HG2	1:398:A:ILE:HG21	11	0.14
(1,1718)	1:365:A:ARG:HG2	1:398:A:ILE:HG22	11	0.14
(1,1718)	1:365:A:ARG:HG2	1:398:A:ILE:HG23	11	0.14
(1,1718)	1:365:A:ARG:HG3	1:398:A:ILE:HG21	11	0.14
(1,1718)	1:365:A:ARG:HG3	1:398:A:ILE:HG22	11	0.14
(1,1718)	1:365:A:ARG:HG3	1:398:A:ILE:HG23	11	0.14
(1,1515)	1:345:A:LYS:HG2	1:346:A:ARG:H	20	0.14
(1,1515)	1:345:A:LYS:HG3	1:346:A:ARG:H	20	0.14
(1,1545)	1:348:A:GLN:HA	1:348:A:GLN:HG2	10	0.13
(1,1545)	1:348:A:GLN:HA	1:348:A:GLN:HG3	10	0.13
(1,1196)	1:370:A:LYS:HA	1:370:A:LYS:HE2	12	0.13
(1,1196)	1:370:A:LYS:HA	1:370:A:LYS:HE3	12	0.13
(1,1184)	1:345:A:LYS:H	1:345:A:LYS:HE2	1	0.13
(1,1184)	1:345:A:LYS:H	1:345:A:LYS:HE3	1	0.13
(1,1148)	1:357:A:GLU:HA	1:357:A:GLU:HG2	18	0.13
(1,1407)	1:371:A:MET:HA	1:374:A:VAL:HA	6	0.12
(1,892)	1:338:A:LEU:HD21	1:339:A:PRO:HD2	10	0.12
(1,892)	1:338:A:LEU:HD22	1:339:A:PRO:HD2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:338:A:LEU:HD23	1:339:A:PRO:HD2	10	0.12
(1,1766)	1:372:A:LYS:H	1:372:A:LYS:HD2	6	0.11
(1,1766)	1:372:A:LYS:H	1:372:A:LYS:HD3	6	0.11
(1,1507)	1:344:A:ARG:HE	1:347:A:LEU:HD11	3	0.11
(1,1507)	1:344:A:ARG:HE	1:347:A:LEU:HD12	3	0.11
(1,1507)	1:344:A:ARG:HE	1:347:A:LEU:HD13	3	0.11
(1,1507)	1:344:A:ARG:HE	1:347:A:LEU:HD21	3	0.11
(1,1507)	1:344:A:ARG:HE	1:347:A:LEU:HD22	3	0.11
(1,1507)	1:344:A:ARG:HE	1:347:A:LEU:HD23	3	0.11
(1,256)	1:342:A:GLN:HG2	1:345:A:LYS:H	20	0.11
(1,256)	1:342:A:GLN:HG3	1:345:A:LYS:H	20	0.11
(1,1407)	1:371:A:MET:HA	1:374:A:VAL:HA	9	0.1
(1,1216)	1:383:A:ASP:HA	1:384:A:PRO:HB2	15	0.1
(1,1022)	1:351:A:LEU:HD11	1:408:A:TYR:H	8	0.1
(1,1022)	1:351:A:LEU:HD12	1:408:A:TYR:H	8	0.1
(1,1022)	1:351:A:LEU:HD13	1:408:A:TYR:H	8	0.1
(1,955)	1:405:A:VAL:HG21	1:406:A:GLN:H	14	0.1
(1,955)	1:405:A:VAL:HG22	1:406:A:GLN:H	14	0.1
(1,955)	1:405:A:VAL:HG23	1:406:A:GLN:H	14	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found