



Full wwPDB NMR Structure Validation Report ⓘ

Jun 4, 2023 – 11:03 AM EDT

PDB ID : 2LHI
BMRB ID : 17850
Title : Solution structure of Ca²⁺/CNA1 peptide-bound γ CaM
Authors : Ogura, K.; Takahashi, K.; Kobashigawa, Y.; Yoshida, R.; Itoh, H.; Yazawa, M.; Inagaki, F.
Deposited on : 2011-08-10

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

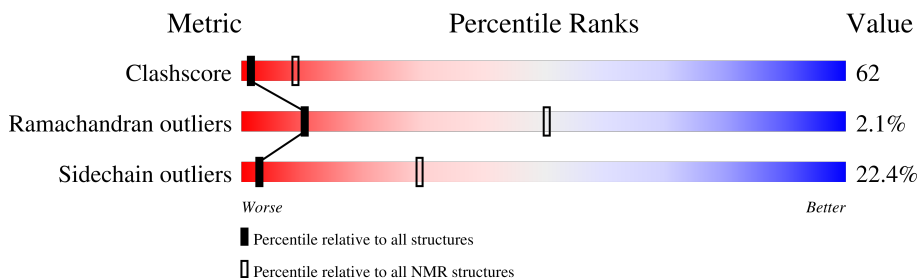
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	176	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 9 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:5-A:74, A:85-A:145, A:455-A:476 (153)	0.51	9

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2700 atoms, of which 1348 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	176	2697	833	1348	231	280	5	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P06787
A	147	GLY	-	linker	UNP P06787
A	148	SER	-	linker	UNP P06787
A	149	SER	-	linker	UNP P06787
A	150	THR	-	linker	UNP P06787
A	151	GLY	-	linker	UNP P06787

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

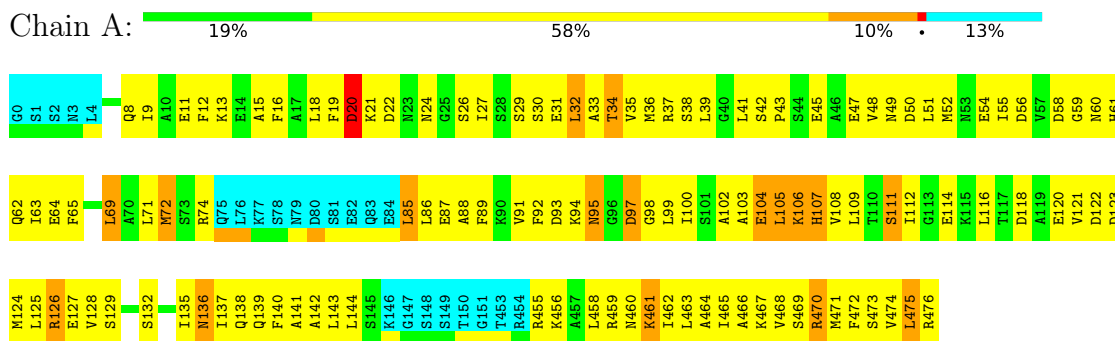
Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	3	3	3

4 Residue-property plots [i](#)

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: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



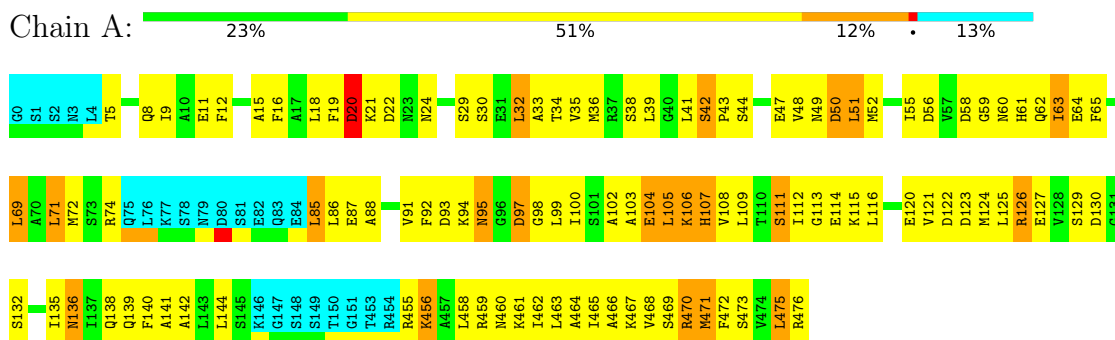
4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



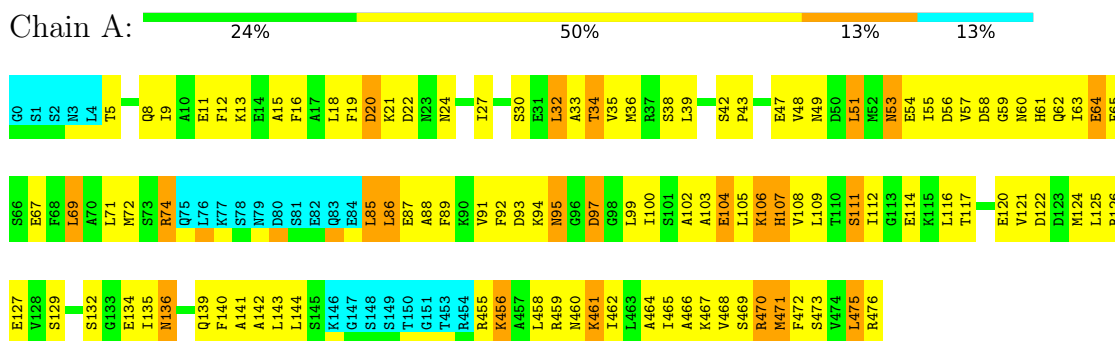
4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



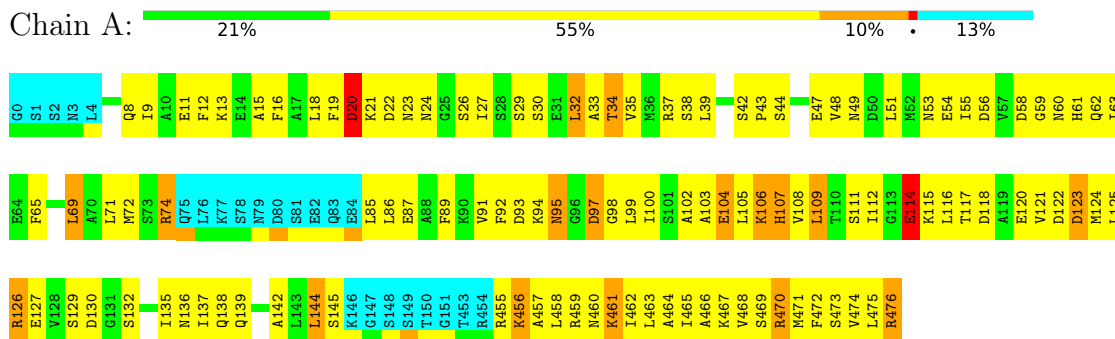
4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



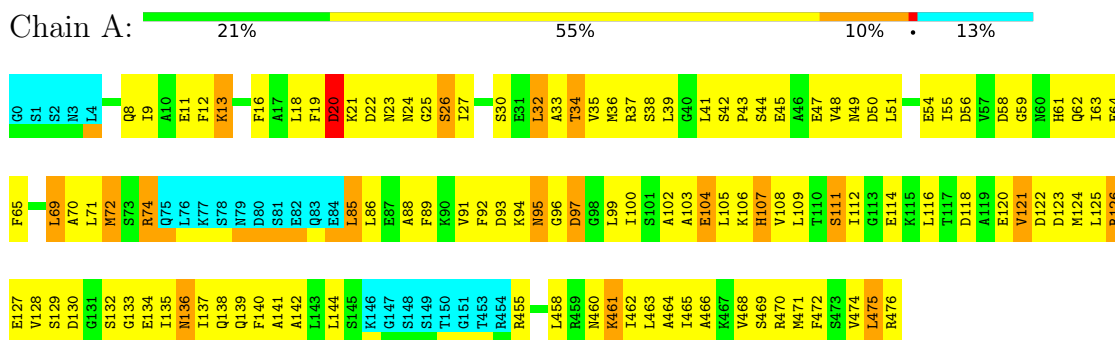
4.2.5 Score per residue for model 5

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



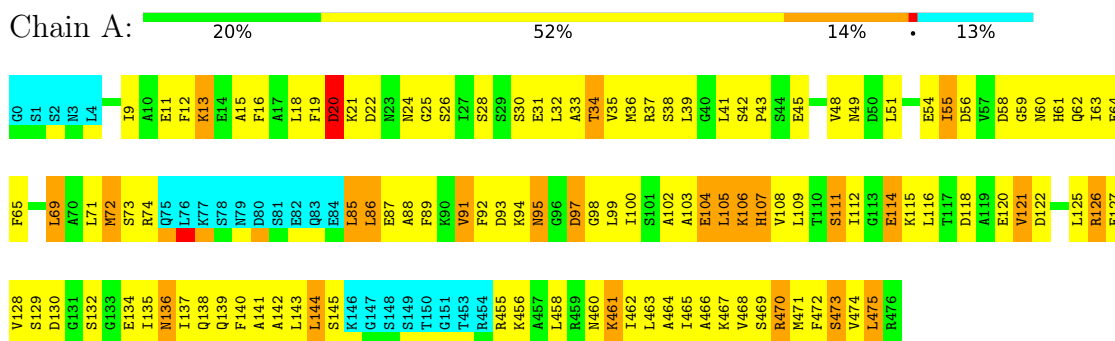
4.2.6 Score per residue for model 6

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



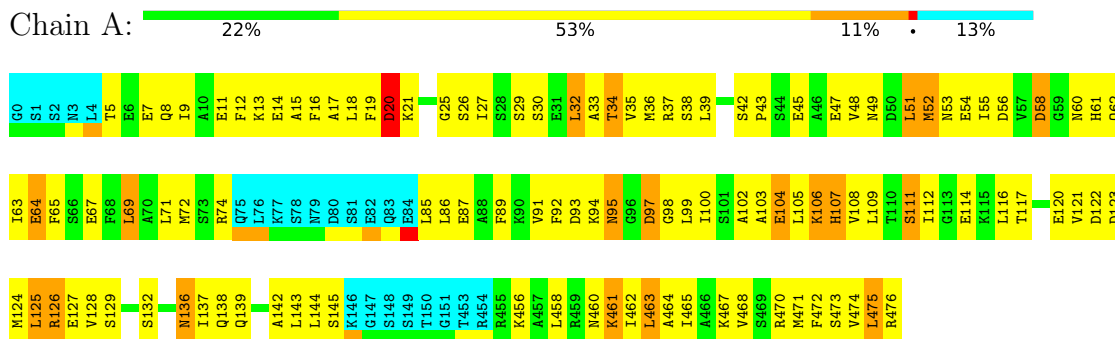
4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



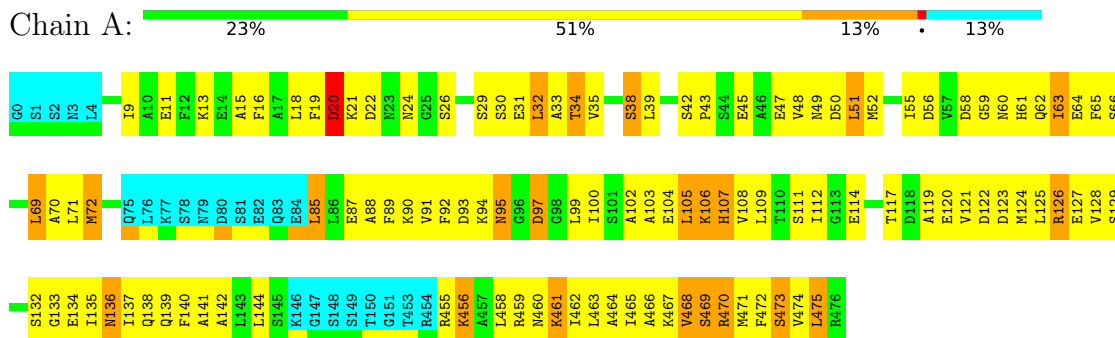
4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



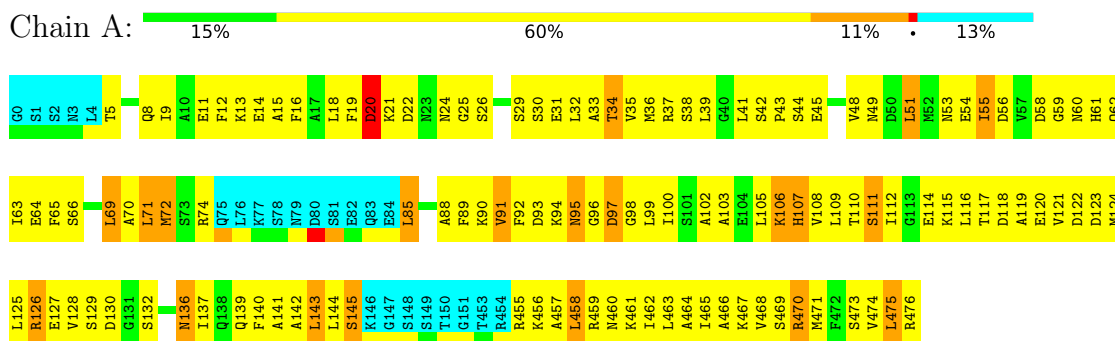
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



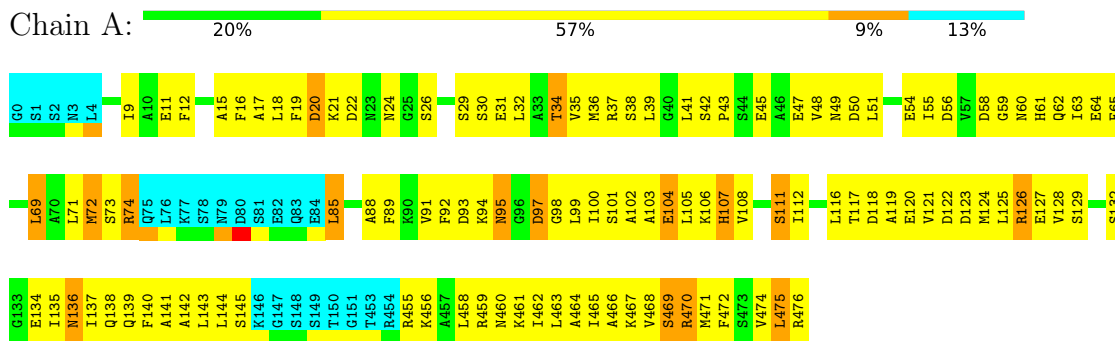
4.2.10 Score per residue for model 10

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



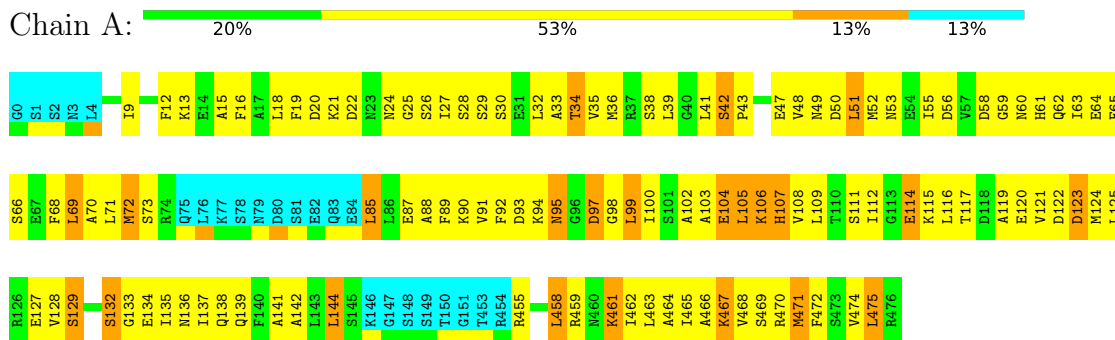
4.2.11 Score per residue for model 11

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



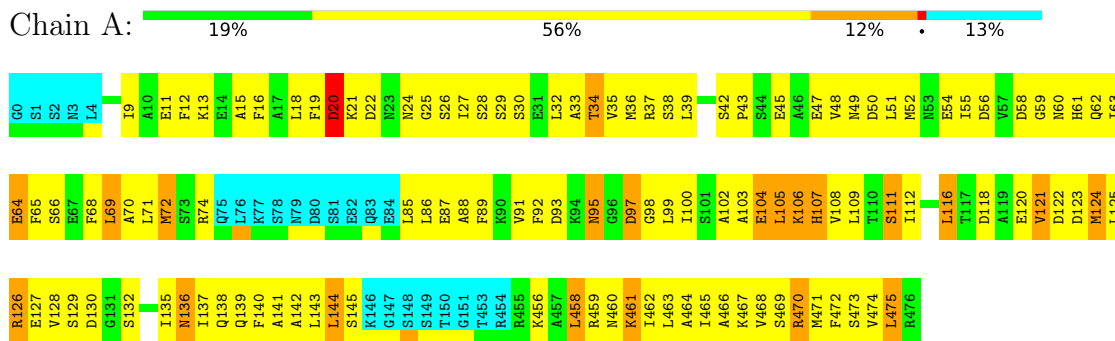
4.2.12 Score per residue for model 12

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



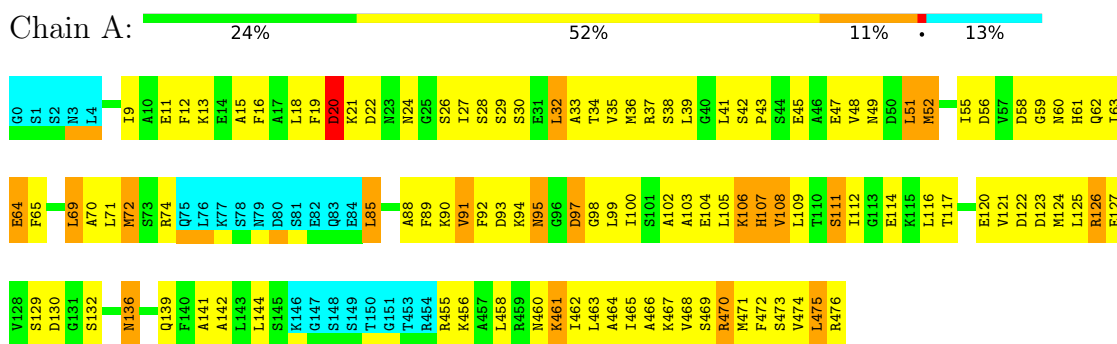
4.2.13 Score per residue for model 13

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



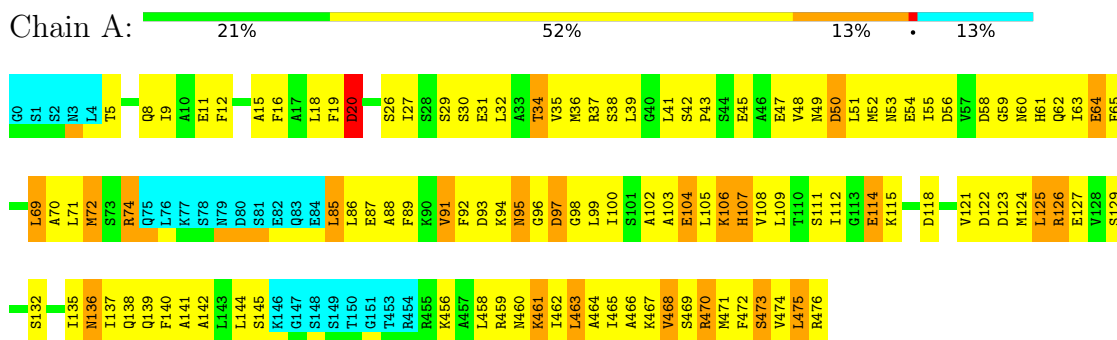
4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



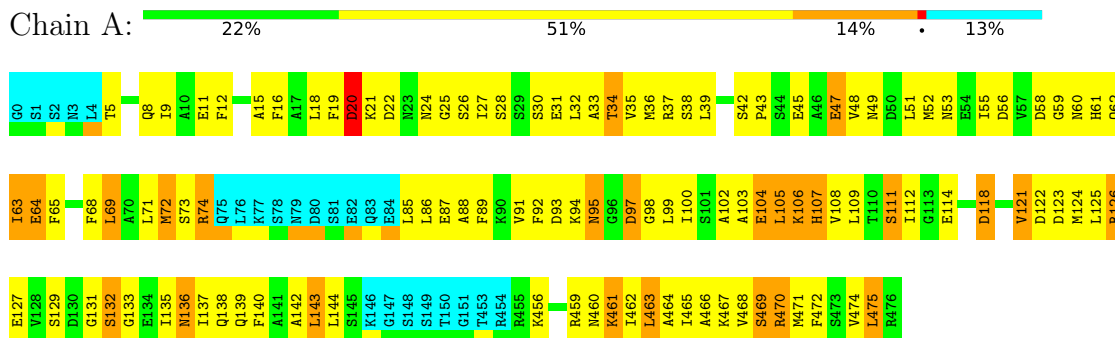
4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



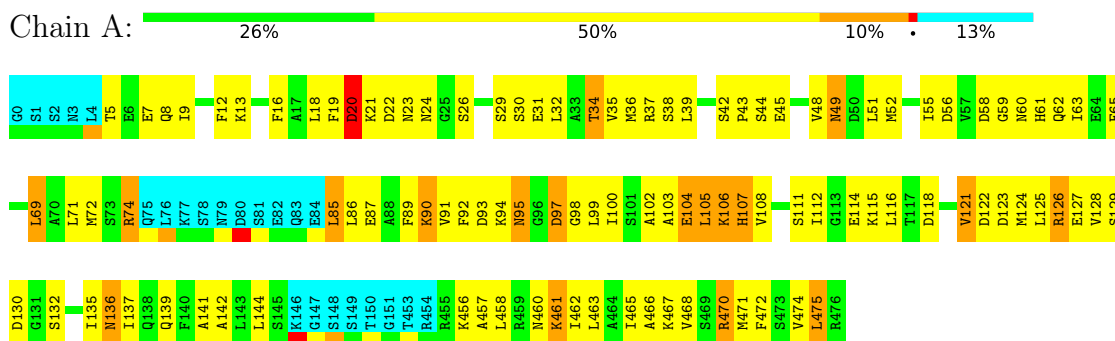
4.2.18 Score per residue for model 18

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



4.2.19 Score per residue for model 19

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



4.2.20 Score per residue for model 20

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



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	3.113
CYANA	geometry optimization	2.1
CYANA	structure solution	2.1
TALOS	structure solution	2003.027.13.05

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	2204
Number of shifts mapped to atoms	2204
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	1182	1190	1182	146±8
All	All	23700	23800	23640	2917

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 62.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:ILE:HG21	1:A:465:ILE:HD11	1.11	1.20	16	20
1:A:85:LEU:HD11	1:A:141:ALA:HB2	1.08	1.22	12	8
1:A:9:ILE:HG22	1:A:65:PHE:CZ	1.05	1.85	12	18
1:A:39:LEU:HD13	1:A:465:ILE:HG23	1.05	1.28	14	20
1:A:69:LEU:HD13	1:A:70:ALA:N	0.99	1.73	9	5
1:A:85:LEU:HD21	1:A:141:ALA:HB2	0.98	1.05	20	1
1:A:51:LEU:HD21	1:A:471:MET:HE3	0.97	1.33	1	1
1:A:85:LEU:HD22	1:A:144:LEU:HD12	0.97	1.33	3	8
1:A:85:LEU:HD21	1:A:141:ALA:CB	0.96	1.91	20	2
1:A:32:LEU:HD22	1:A:48:VAL:HG13	0.95	1.36	16	20
1:A:92:PHE:CZ	1:A:108:VAL:HG11	0.92	1.99	18	20
1:A:54:GLU:C	1:A:55:ILE:HD13	0.91	1.85	10	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:LEU:CD1	1:A:141:ALA:HB2	0.90	1.96	12	8
1:A:85:LEU:CD2	1:A:141:ALA:HB2	0.89	1.97	20	4
1:A:15:ALA:HB1	1:A:464:ALA:HB2	0.88	1.46	2	15
1:A:88:ALA:HB2	1:A:466:ALA:HB2	0.87	1.46	6	17
1:A:114:GLU:OE1	1:A:116:LEU:HD13	0.87	1.69	5	2
1:A:125:LEU:HD13	1:A:133:GLY:O	0.87	1.70	18	3
1:A:460:ASN:OD1	1:A:463:LEU:HD12	0.87	1.69	20	1
1:A:71:LEU:HD21	1:A:471:MET:SD	0.86	2.10	9	13
1:A:39:LEU:CD1	1:A:465:ILE:HG23	0.85	2.00	5	20
1:A:105:LEU:CD1	1:A:135:ILE:HD11	0.85	2.00	20	8
1:A:85:LEU:HD11	1:A:141:ALA:CB	0.85	2.01	12	7
1:A:121:VAL:O	1:A:125:LEU:HD22	0.84	1.71	8	3
1:A:109:LEU:HD12	1:A:116:LEU:HD12	0.84	1.47	10	2
1:A:464:ALA:O	1:A:468:VAL:HG22	0.83	1.73	20	5
1:A:112:ILE:HG21	1:A:465:ILE:CD1	0.82	2.04	19	18
1:A:112:ILE:CG2	1:A:465:ILE:HD11	0.82	2.04	10	8
1:A:98:GLY:O	1:A:99:LEU:HD23	0.81	1.72	12	17
1:A:137:ILE:HG23	1:A:138:GLN:OE1	0.81	1.75	2	2
1:A:18:LEU:HD21	1:A:461:LYS:HG3	0.81	1.52	15	11
1:A:85:LEU:CD2	1:A:144:LEU:HD12	0.81	2.06	3	5
1:A:51:LEU:HD11	1:A:471:MET:HE3	0.78	1.54	17	3
1:A:19:PHE:CZ	1:A:468:VAL:HG11	0.78	2.13	15	20
1:A:18:LEU:HD21	1:A:461:LYS:HG2	0.77	1.56	11	8
1:A:102:ALA:HA	1:A:125:LEU:HD11	0.76	1.56	12	3
1:A:14:GLU:OE2	1:A:457:ALA:HB1	0.76	1.79	16	1
1:A:51:LEU:HB2	1:A:475:LEU:HD22	0.76	1.54	1	7
1:A:92:PHE:CE1	1:A:462:ILE:HG23	0.75	2.16	12	19
1:A:92:PHE:CE2	1:A:108:VAL:HG11	0.74	2.18	14	20
1:A:85:LEU:HG	1:A:144:LEU:HD12	0.74	1.59	4	2
1:A:105:LEU:HD23	1:A:121:VAL:CG2	0.73	2.13	6	3
1:A:36:MET:HE2	1:A:41:LEU:HD13	0.73	1.60	1	6
1:A:69:LEU:HD13	1:A:69:LEU:C	0.73	2.04	10	5
1:A:461:LYS:O	1:A:465:ILE:HD12	0.72	1.82	6	13
1:A:105:LEU:HD11	1:A:135:ILE:HD11	0.72	1.60	20	4
1:A:88:ALA:HB2	1:A:466:ALA:CB	0.72	2.15	7	7
1:A:110:THR:HG23	1:A:115:LYS:HG2	0.72	1.61	10	1
1:A:106:LYS:HG2	1:A:121:VAL:HG21	0.72	1.61	8	10
1:A:86:LEU:HD12	1:A:86:LEU:C	0.72	2.05	4	5
1:A:47:GLU:HB3	1:A:475:LEU:HD21	0.72	1.60	18	8
1:A:61:HIS:CG	1:A:61:HIS:O	0.72	2.42	5	11
1:A:460:ASN:HA	1:A:463:LEU:HD22	0.72	1.62	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:LEU:HD13	1:A:114:GLU:OE1	0.71	1.85	10	1
1:A:69:LEU:C	1:A:69:LEU:HD12	0.71	2.05	2	12
1:A:9:ILE:N	1:A:9:ILE:HD13	0.71	2.01	5	20
1:A:32:LEU:C	1:A:32:LEU:HD23	0.71	2.06	6	16
1:A:105:LEU:HD23	1:A:121:VAL:HG23	0.70	1.63	5	6
1:A:18:LEU:HD21	1:A:461:LYS:CG	0.70	2.17	17	9
1:A:39:LEU:HD23	1:A:111:SER:OG	0.70	1.87	2	10
1:A:85:LEU:HG	1:A:141:ALA:HB2	0.70	1.64	10	3
1:A:15:ALA:HB1	1:A:464:ALA:CB	0.70	2.15	2	4
1:A:55:ILE:HG13	1:A:71:LEU:HD22	0.70	1.64	20	4
1:A:9:ILE:HG22	1:A:65:PHE:HZ	0.70	1.47	14	14
1:A:144:LEU:HD23	1:A:144:LEU:N	0.69	2.02	14	12
1:A:55:ILE:HD13	1:A:55:ILE:N	0.69	2.01	10	4
1:A:51:LEU:C	1:A:51:LEU:HD13	0.69	2.07	13	12
1:A:69:LEU:HD12	1:A:69:LEU:O	0.69	1.87	7	15
1:A:85:LEU:HB3	1:A:137:ILE:HD11	0.69	1.64	5	5
1:A:116:LEU:HD23	1:A:120:GLU:HB3	0.69	1.64	1	5
1:A:124:MET:HE1	1:A:458:LEU:HD11	0.69	1.64	12	2
1:A:475:LEU:HD12	1:A:475:LEU:O	0.68	1.88	20	6
1:A:102:ALA:HB1	1:A:121:VAL:CG1	0.68	2.19	6	7
1:A:71:LEU:HD21	1:A:471:MET:CE	0.68	2.18	18	8
1:A:31:GLU:O	1:A:34:THR:HG22	0.68	1.88	18	11
1:A:47:GLU:CB	1:A:475:LEU:HD21	0.68	2.18	6	2
1:A:50:ASP:OD1	1:A:475:LEU:HD13	0.68	1.88	3	1
1:A:85:LEU:HD22	1:A:144:LEU:CD1	0.68	2.17	3	2
1:A:85:LEU:CD1	1:A:140:PHE:CD2	0.67	2.77	11	4
1:A:92:PHE:CZ	1:A:108:VAL:CG1	0.67	2.77	12	20
1:A:55:ILE:HG21	1:A:71:LEU:HB2	0.67	1.67	9	7
1:A:51:LEU:HD11	1:A:471:MET:HB3	0.67	1.66	3	2
1:A:36:MET:CE	1:A:41:LEU:HD13	0.66	2.20	11	6
1:A:39:LEU:HD13	1:A:465:ILE:CG2	0.66	2.18	5	6
1:A:85:LEU:CG	1:A:141:ALA:HB2	0.66	2.21	10	1
1:A:99:LEU:HD23	1:A:136:ASN:HB3	0.66	1.67	6	10
1:A:139:GLN:O	1:A:142:ALA:HB3	0.66	1.91	3	19
1:A:51:LEU:HD21	1:A:471:MET:CE	0.66	2.16	1	3
1:A:51:LEU:HD21	1:A:471:MET:HB3	0.66	1.65	17	9
1:A:61:HIS:CD2	1:A:61:HIS:O	0.66	2.49	17	8
1:A:61:HIS:O	1:A:61:HIS:CG	0.65	2.50	13	8
1:A:21:LYS:HE3	1:A:34:THR:HG21	0.65	1.68	8	11
1:A:112:ILE:HD13	1:A:465:ILE:HD11	0.65	1.66	18	4
1:A:32:LEU:HD23	1:A:33:ALA:N	0.65	2.06	1	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:HIS:O	1:A:61:HIS:CD2	0.65	2.50	3	11
1:A:55:ILE:HD12	1:A:71:LEU:HD13	0.65	1.68	8	8
1:A:51:LEU:HD11	1:A:471:MET:HE2	0.65	1.68	7	2
1:A:32:LEU:HD22	1:A:48:VAL:CG1	0.65	2.19	6	10
1:A:105:LEU:HD21	1:A:124:MET:SD	0.64	2.32	8	3
1:A:92:PHE:CZ	1:A:462:ILE:HG23	0.64	2.28	12	1
1:A:65:PHE:CD1	1:A:65:PHE:O	0.64	2.51	16	20
1:A:51:LEU:C	1:A:51:LEU:HD23	0.64	2.12	11	3
1:A:97:ASP:OD2	1:A:99:LEU:HD12	0.63	1.94	6	19
1:A:85:LEU:HD13	1:A:140:PHE:CE2	0.63	2.28	11	2
1:A:107:HIS:CD2	1:A:108:VAL:HG23	0.63	2.29	12	19
1:A:50:ASP:CG	1:A:475:LEU:HD13	0.63	2.14	3	1
1:A:21:LYS:CE	1:A:34:THR:HG21	0.63	2.24	18	5
1:A:72:MET:HG3	1:A:467:LYS:HZ3	0.62	1.54	17	2
1:A:55:ILE:HG21	1:A:71:LEU:HD22	0.62	1.71	11	2
1:A:85:LEU:HD21	1:A:141:ALA:HA	0.62	1.69	7	7
1:A:116:LEU:HD22	1:A:120:GLU:HB3	0.62	1.72	12	3
1:A:459:ARG:O	1:A:463:LEU:HD13	0.62	1.93	10	5
1:A:137:ILE:HG23	1:A:138:GLN:HE21	0.61	1.53	12	5
1:A:19:PHE:CE2	1:A:35:VAL:HG11	0.61	2.30	16	3
1:A:19:PHE:CZ	1:A:468:VAL:HG21	0.61	2.30	2	7
1:A:19:PHE:CE1	1:A:468:VAL:HG11	0.61	2.30	15	2
1:A:69:LEU:HD22	1:A:69:LEU:O	0.61	1.95	12	5
1:A:105:LEU:HD12	1:A:135:ILE:HD11	0.61	1.72	9	5
1:A:470:ARG:NH1	1:A:474:VAL:HG21	0.61	2.11	18	1
1:A:16:PHE:CE2	1:A:20:ASP:OD2	0.61	2.54	1	19
1:A:50:ASP:OD2	1:A:475:LEU:HD13	0.61	1.94	3	1
1:A:71:LEU:HD11	1:A:471:MET:SD	0.61	2.35	13	3
1:A:72:MET:CB	1:A:467:LYS:HZ3	0.61	2.09	17	1
1:A:9:ILE:HG23	1:A:69:LEU:HD22	0.60	1.72	7	6
1:A:18:LEU:CD2	1:A:112:ILE:HD12	0.60	2.25	19	10
1:A:11:GLU:HB3	1:A:456:LYS:HZ3	0.60	1.54	5	1
1:A:92:PHE:HE2	1:A:105:LEU:HD12	0.60	1.55	14	2
1:A:9:ILE:HG22	1:A:65:PHE:CE1	0.60	2.30	20	5
1:A:116:LEU:CD2	1:A:124:MET:CE	0.60	2.79	19	3
1:A:87:GLU:O	1:A:91:VAL:HG23	0.60	1.96	12	10
1:A:14:GLU:HG3	1:A:457:ALA:HB1	0.60	1.73	17	1
1:A:92:PHE:CE1	1:A:108:VAL:HG11	0.60	2.32	20	17
1:A:109:LEU:HD12	1:A:116:LEU:CD1	0.60	2.26	7	2
1:A:32:LEU:CD2	1:A:48:VAL:HG13	0.59	2.24	9	5
1:A:105:LEU:HD22	1:A:125:LEU:HD11	0.59	1.74	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:VAL:HG11	1:A:142:ALA:CB	0.59	2.28	10	9
1:A:92:PHE:CE2	1:A:105:LEU:HD12	0.59	2.32	14	3
1:A:92:PHE:CE2	1:A:108:VAL:CG1	0.59	2.86	10	15
1:A:137:ILE:HG23	1:A:138:GLN:NE2	0.59	2.11	12	5
1:A:72:MET:CG	1:A:467:LYS:HZ3	0.59	2.11	17	1
1:A:13:LYS:CG	1:A:65:PHE:CE1	0.59	2.85	1	9
1:A:135:ILE:CD1	1:A:143:LEU:HD11	0.59	2.28	7	2
1:A:55:ILE:HD11	1:A:471:MET:SD	0.59	2.38	19	3
1:A:106:LYS:HB3	1:A:121:VAL:HG21	0.58	1.73	17	8
1:A:69:LEU:HD12	1:A:69:LEU:C	0.58	2.19	3	3
1:A:107:HIS:CD2	1:A:108:VAL:N	0.58	2.72	14	20
1:A:122:ASP:HA	1:A:125:LEU:HD12	0.58	1.75	13	2
1:A:16:PHE:CZ	1:A:20:ASP:OD2	0.58	2.57	17	2
1:A:463:LEU:HG	1:A:467:LYS:HZ2	0.58	1.59	10	1
1:A:99:LEU:HD22	1:A:136:ASN:OD1	0.57	2.00	20	4
1:A:85:LEU:CD2	1:A:141:ALA:CB	0.57	2.83	4	2
1:A:50:ASP:HB3	1:A:475:LEU:HD13	0.57	1.74	11	2
1:A:456:LYS:HE3	1:A:457:ALA:HB2	0.57	1.77	5	1
1:A:15:ALA:O	1:A:68:PHE:CZ	0.57	2.58	17	5
1:A:86:LEU:HD12	1:A:87:GLU:N	0.57	2.14	19	7
1:A:105:LEU:HD13	1:A:135:ILE:HD11	0.57	1.75	6	4
1:A:92:PHE:CB	1:A:100:ILE:HD13	0.56	2.29	8	19
1:A:14:GLU:CD	1:A:457:ALA:HB1	0.56	2.20	10	1
1:A:16:PHE:CZ	1:A:64:GLU:C	0.56	2.78	17	12
1:A:92:PHE:HE1	1:A:462:ILE:HG23	0.56	1.58	10	17
1:A:51:LEU:HD21	1:A:471:MET:HE1	0.56	1.76	6	1
1:A:85:LEU:HD11	1:A:141:ALA:CA	0.56	2.31	10	11
1:A:85:LEU:HD13	1:A:140:PHE:CD2	0.56	2.36	11	4
1:A:19:PHE:CE2	1:A:35:VAL:CG1	0.56	2.89	16	3
1:A:124:MET:CE	1:A:458:LEU:HD11	0.55	2.31	12	1
1:A:475:LEU:HD12	1:A:475:LEU:C	0.55	2.21	20	2
1:A:109:LEU:HD11	1:A:458:LEU:HD11	0.55	1.79	13	1
1:A:58:ASP:OD1	1:A:58:ASP:N	0.55	2.40	8	1
1:A:55:ILE:HD12	1:A:71:LEU:CD1	0.55	2.32	2	4
1:A:51:LEU:HD13	1:A:51:LEU:O	0.55	2.02	18	8
1:A:107:HIS:NE2	1:A:108:VAL:HG23	0.55	2.16	10	13
1:A:18:LEU:CD1	1:A:464:ALA:HB3	0.55	2.32	1	7
1:A:41:LEU:HD11	1:A:469:SER:OG	0.54	2.03	6	1
1:A:9:ILE:HG23	1:A:69:LEU:CD2	0.54	2.32	7	3
1:A:139:GLN:O	1:A:142:ALA:CB	0.54	2.56	3	17
1:A:49:ASN:OD1	1:A:61:HIS:CE1	0.54	2.61	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:GLU:HB3	1:A:475:LEU:HD11	0.54	1.79	6	1
1:A:54:GLU:O	1:A:55:ILE:HD13	0.54	2.03	17	6
1:A:85:LEU:O	1:A:89:PHE:N	0.54	2.41	10	16
1:A:51:LEU:HD12	1:A:472:PHE:HA	0.54	1.78	11	1
1:A:55:ILE:HD12	1:A:71:LEU:HD12	0.54	1.80	7	3
1:A:33:ALA:HB1	1:A:37:ARG:NH2	0.54	2.17	18	1
1:A:36:MET:HE1	1:A:472:PHE:CG	0.54	2.38	12	8
1:A:112:ILE:HD11	1:A:461:LYS:HG2	0.53	1.79	4	1
1:A:19:PHE:CD1	1:A:27:ILE:HD13	0.53	2.38	12	2
1:A:66:SER:O	1:A:69:LEU:CD1	0.53	2.56	9	5
1:A:87:GLU:O	1:A:91:VAL:CG2	0.53	2.56	19	11
1:A:109:LEU:HD12	1:A:114:GLU:CB	0.53	2.33	4	4
1:A:32:LEU:HD11	1:A:51:LEU:HD12	0.53	1.80	5	4
1:A:102:ALA:HB1	1:A:121:VAL:HG11	0.53	1.80	6	4
1:A:470:ARG:CD	1:A:474:VAL:CG2	0.53	2.86	15	1
1:A:112:ILE:CD1	1:A:461:LYS:CG	0.53	2.87	12	7
1:A:71:LEU:HD21	1:A:471:MET:HE2	0.53	1.79	18	1
1:A:58:ASP:OD1	1:A:59:GLY:N	0.53	2.41	19	19
1:A:13:LYS:HG3	1:A:65:PHE:CE1	0.53	2.39	1	8
1:A:61:HIS:O	1:A:62:GLN:CG	0.53	2.57	18	11
1:A:70:ALA:O	1:A:74:ARG:CB	0.53	2.57	15	5
1:A:121:VAL:CG1	1:A:122:ASP:N	0.53	2.72	19	19
1:A:105:LEU:CD1	1:A:135:ILE:CD1	0.53	2.85	3	4
1:A:140:PHE:CZ	1:A:144:LEU:HD11	0.53	2.39	15	1
1:A:51:LEU:C	1:A:51:LEU:CD2	0.53	2.78	11	5
1:A:456:LYS:CB	1:A:459:ARG:NH2	0.53	2.72	9	2
1:A:116:LEU:HD13	1:A:124:MET:HE3	0.52	1.81	8	2
1:A:91:VAL:CG1	1:A:92:PHE:N	0.52	2.72	14	7
1:A:13:LYS:HG2	1:A:65:PHE:CE1	0.52	2.39	19	7
1:A:8:GLN:O	1:A:12:PHE:CD2	0.52	2.63	4	5
1:A:102:ALA:HB1	1:A:121:VAL:HG13	0.52	1.81	8	1
1:A:43:PRO:HA	1:A:472:PHE:CZ	0.52	2.40	6	1
1:A:18:LEU:HD22	1:A:112:ILE:HB	0.52	1.80	8	6
1:A:99:LEU:HD23	1:A:136:ASN:CB	0.52	2.34	9	3
1:A:19:PHE:HB2	1:A:27:ILE:HD13	0.52	1.82	18	11
1:A:92:PHE:CD2	1:A:105:LEU:HD22	0.52	2.40	1	1
1:A:13:LYS:HG3	1:A:65:PHE:CZ	0.52	2.40	19	11
1:A:36:MET:SD	1:A:41:LEU:HD13	0.52	2.45	16	3
1:A:135:ILE:HD12	1:A:143:LEU:HD11	0.52	1.80	7	2
1:A:463:LEU:O	1:A:466:ALA:HB3	0.52	2.05	12	2
1:A:51:LEU:C	1:A:51:LEU:CD1	0.52	2.78	16	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HD13	1:A:120:GLU:HB3	0.52	1.83	13	2
1:A:124:MET:O	1:A:127:GLU:CG	0.51	2.59	11	9
1:A:16:PHE:CZ	1:A:65:PHE:N	0.51	2.78	3	7
1:A:470:ARG:O	1:A:473:SER:N	0.51	2.43	14	10
1:A:128:VAL:HG11	1:A:142:ALA:HB1	0.51	1.80	10	2
1:A:19:PHE:CE2	1:A:35:VAL:HB	0.51	2.40	17	9
1:A:105:LEU:HD22	1:A:125:LEU:CD1	0.51	2.35	15	2
1:A:85:LEU:HD12	1:A:137:ILE:HD12	0.51	1.81	9	5
1:A:13:LYS:HA	1:A:65:PHE:CE1	0.51	2.41	16	1
1:A:31:GLU:O	1:A:34:THR:CG2	0.51	2.59	1	11
1:A:51:LEU:O	1:A:51:LEU:HD13	0.51	2.05	8	3
1:A:103:ALA:O	1:A:107:HIS:N	0.51	2.44	6	17
1:A:106:LYS:O	1:A:109:LEU:N	0.51	2.44	14	10
1:A:121:VAL:HG13	1:A:122:ASP:N	0.51	2.21	15	13
1:A:29:SER:O	1:A:48:VAL:HG11	0.51	2.05	2	1
1:A:15:ALA:N	1:A:461:LYS:HZ1	0.51	2.04	4	1
1:A:118:ASP:O	1:A:122:ASP:CB	0.51	2.59	7	6
1:A:86:LEU:C	1:A:86:LEU:CD1	0.51	2.79	4	2
1:A:58:ASP:OD1	1:A:58:ASP:C	0.51	2.50	6	19
1:A:18:LEU:O	1:A:35:VAL:CG2	0.50	2.60	6	14
1:A:50:ASP:OD2	1:A:475:LEU:CD1	0.50	2.58	3	1
1:A:106:LYS:CB	1:A:121:VAL:HG21	0.50	2.36	5	3
1:A:99:LEU:CD2	1:A:136:ASN:OD1	0.50	2.59	19	5
1:A:105:LEU:HD23	1:A:135:ILE:HD11	0.50	1.82	12	1
1:A:51:LEU:HD23	1:A:472:PHE:HA	0.50	1.83	15	1
1:A:43:PRO:HB3	1:A:472:PHE:CE1	0.50	2.42	6	13
1:A:106:LYS:CG	1:A:121:VAL:HG21	0.50	2.35	15	5
1:A:139:GLN:O	1:A:142:ALA:N	0.50	2.44	18	20
1:A:125:LEU:O	1:A:129:SER:N	0.50	2.44	5	19
1:A:13:LYS:CB	1:A:65:PHE:CZ	0.50	2.94	16	1
1:A:56:ASP:OD2	1:A:60:ASN:N	0.50	2.44	18	15
1:A:125:LEU:O	1:A:127:GLU:N	0.50	2.45	18	20
1:A:19:PHE:CE1	1:A:35:VAL:HB	0.50	2.42	15	11
1:A:29:SER:OG	1:A:48:VAL:CG1	0.50	2.60	14	4
1:A:52:MET:HB2	1:A:63:ILE:HD11	0.50	1.84	2	4
1:A:112:ILE:CD1	1:A:461:LYS:CD	0.50	2.90	10	2
1:A:109:LEU:O	1:A:112:ILE:CG1	0.50	2.60	12	7
1:A:103:ALA:O	1:A:105:LEU:N	0.50	2.44	19	20
1:A:19:PHE:HZ	1:A:468:VAL:HG11	0.50	1.61	6	7
1:A:19:PHE:CD2	1:A:35:VAL:HB	0.50	2.42	16	9
1:A:32:LEU:C	1:A:32:LEU:CD2	0.50	2.80	1	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:CD2	1:A:471:MET:SD	0.50	2.99	13	3
1:A:9:ILE:CG2	1:A:65:PHE:CZ	0.49	2.79	12	6
1:A:470:ARG:HH11	1:A:474:VAL:HG21	0.49	1.66	18	1
1:A:19:PHE:CD1	1:A:35:VAL:HB	0.49	2.43	10	11
1:A:116:LEU:CD2	1:A:124:MET:HE3	0.49	2.36	17	2
1:A:9:ILE:HG23	1:A:69:LEU:HG	0.49	1.84	20	2
1:A:98:GLY:O	1:A:99:LEU:CD2	0.49	2.59	14	15
1:A:39:LEU:CD2	1:A:111:SER:OG	0.49	2.60	10	9
1:A:74:ARG:CG	1:A:74:ARG:O	0.49	2.60	15	7
1:A:456:LYS:NZ	1:A:460:ASN:ND2	0.49	2.60	20	1
1:A:467:LYS:O	1:A:470:ARG:N	0.49	2.46	10	10
1:A:141:ALA:O	1:A:145:SER:N	0.49	2.46	13	4
1:A:37:ARG:CG	1:A:38:SER:N	0.49	2.75	5	13
1:A:69:LEU:C	1:A:69:LEU:CD1	0.49	2.81	13	11
1:A:52:MET:CB	1:A:63:ILE:HD11	0.49	2.38	2	5
1:A:72:MET:SD	1:A:72:MET:N	0.49	2.85	6	9
1:A:102:ALA:O	1:A:105:LEU:N	0.49	2.45	11	19
1:A:116:LEU:HD13	1:A:124:MET:CE	0.49	2.38	8	2
1:A:51:LEU:HD21	1:A:471:MET:C	0.49	2.28	9	2
1:A:97:ASP:OD1	1:A:99:LEU:N	0.49	2.45	7	19
1:A:51:LEU:C	1:A:51:LEU:HD22	0.49	2.28	4	2
1:A:51:LEU:CD2	1:A:471:MET:O	0.49	2.61	9	3
1:A:11:GLU:CB	1:A:456:LYS:HZ3	0.48	2.21	5	1
1:A:56:ASP:OD2	1:A:61:HIS:N	0.48	2.46	10	5
1:A:105:LEU:HD13	1:A:109:LEU:HD23	0.48	1.84	12	1
1:A:43:PRO:HB3	1:A:472:PHE:CZ	0.48	2.44	5	6
1:A:132:SER:OG	1:A:133:GLY:N	0.48	2.46	9	2
1:A:458:LEU:HD22	1:A:461:LYS:NZ	0.48	2.23	13	1
1:A:114:GLU:CG	1:A:461:LYS:NZ	0.48	2.76	14	1
1:A:27:ILE:O	1:A:52:MET:CE	0.48	2.62	16	3
1:A:51:LEU:HD11	1:A:471:MET:CE	0.48	2.39	14	3
1:A:127:GLU:OE1	1:A:455:ARG:CZ	0.48	2.61	2	1
1:A:9:ILE:N	1:A:9:ILE:CD1	0.48	2.71	3	7
1:A:88:ALA:CB	1:A:466:ALA:HB2	0.48	2.36	7	1
1:A:144:LEU:N	1:A:144:LEU:CD2	0.48	2.73	14	7
1:A:11:GLU:CD	1:A:456:LYS:CD	0.48	2.81	18	2
1:A:11:GLU:O	1:A:460:ASN:ND2	0.48	2.47	16	14
1:A:19:PHE:CE2	1:A:35:VAL:CB	0.48	2.96	16	4
1:A:114:GLU:O	1:A:114:GLU:CG	0.48	2.61	10	1
1:A:105:LEU:HD13	1:A:125:LEU:CD1	0.48	2.39	17	1
1:A:45:GLU:O	1:A:49:ASN:ND2	0.48	2.47	19	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LYS:HE2	1:A:65:PHE:CE2	0.48	2.44	5	2
1:A:36:MET:HE3	1:A:472:PHE:HB2	0.48	1.86	7	1
1:A:102:ALA:CA	1:A:125:LEU:HD11	0.48	2.35	12	1
1:A:114:GLU:HG3	1:A:461:LYS:HZ2	0.48	1.69	14	1
1:A:456:LYS:HB2	1:A:459:ARG:HH21	0.48	1.69	16	1
1:A:129:SER:O	1:A:132:SER:N	0.47	2.47	19	17
1:A:13:LYS:CG	1:A:65:PHE:CZ	0.47	2.97	19	2
1:A:36:MET:HE1	1:A:472:PHE:CB	0.47	2.39	12	1
1:A:128:VAL:CG2	1:A:143:LEU:CD1	0.47	2.92	13	1
1:A:89:PHE:CE1	1:A:137:ILE:N	0.47	2.81	12	4
1:A:144:LEU:HD21	1:A:462:ILE:HD12	0.47	1.85	19	1
1:A:56:ASP:OD1	1:A:58:ASP:OD1	0.47	2.33	20	20
1:A:33:ALA:HB2	1:A:48:VAL:HG21	0.47	1.85	9	7
1:A:459:ARG:CG	1:A:460:ASN:N	0.47	2.76	13	3
1:A:31:GLU:O	1:A:34:THR:CB	0.47	2.61	20	4
1:A:36:MET:SD	1:A:41:LEU:CD1	0.47	3.02	16	2
1:A:143:LEU:O	1:A:459:ARG:NH1	0.47	2.48	11	3
1:A:466:ALA:O	1:A:469:SER:N	0.47	2.48	2	5
1:A:50:ASP:OD1	1:A:51:LEU:N	0.47	2.48	3	1
1:A:36:MET:HE1	1:A:472:PHE:CD2	0.47	2.45	17	1
1:A:95:ASN:OD1	1:A:96:GLY:N	0.47	2.47	6	4
1:A:16:PHE:CE2	1:A:65:PHE:HB2	0.47	2.43	16	1
1:A:95:ASN:ND2	1:A:95:ASN:C	0.47	2.68	1	16
1:A:103:ALA:C	1:A:105:LEU:N	0.47	2.68	9	20
1:A:19:PHE:HZ	1:A:468:VAL:HG21	0.47	1.70	13	5
1:A:114:GLU:CD	1:A:115:LYS:N	0.47	2.68	12	3
1:A:13:LYS:HB2	1:A:65:PHE:CZ	0.47	2.45	16	1
1:A:49:ASN:HD22	1:A:49:ASN:N	0.47	2.08	19	1
1:A:11:GLU:OE1	1:A:456:LYS:CG	0.47	2.63	18	1
1:A:135:ILE:HD12	1:A:143:LEU:CD1	0.47	2.40	7	1
1:A:52:MET:HE1	1:A:61:HIS:O	0.47	2.09	12	2
1:A:144:LEU:HD13	1:A:463:LEU:CD1	0.47	2.39	17	1
1:A:461:LYS:HZ3	1:A:461:LYS:N	0.47	2.07	19	1
1:A:49:ASN:O	1:A:53:ASN:N	0.47	2.48	2	9
1:A:114:GLU:OE2	1:A:116:LEU:N	0.47	2.48	5	1
1:A:109:LEU:O	1:A:114:GLU:N	0.46	2.48	4	6
1:A:105:LEU:O	1:A:108:VAL:N	0.46	2.48	9	1
1:A:472:PHE:CD1	1:A:475:LEU:HD23	0.46	2.45	14	1
1:A:72:MET:SD	1:A:467:LYS:CD	0.46	3.03	5	2
1:A:18:LEU:HD22	1:A:112:ILE:HD12	0.46	1.85	4	2
1:A:8:GLN:O	1:A:12:PHE:CE2	0.46	2.68	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:LYS:HD2	1:A:121:VAL:HG11	0.46	1.86	11	1
1:A:71:LEU:CD1	1:A:471:MET:SD	0.46	3.03	13	1
1:A:461:LYS:N	1:A:461:LYS:NZ	0.46	2.62	19	1
1:A:42:SER:N	1:A:43:PRO:HD3	0.46	2.24	5	19
1:A:121:VAL:O	1:A:124:MET:N	0.46	2.49	8	14
1:A:141:ALA:O	1:A:144:LEU:N	0.46	2.49	13	2
1:A:56:ASP:OD1	1:A:62:GLN:O	0.46	2.34	14	20
1:A:120:GLU:CD	1:A:120:GLU:N	0.46	2.69	2	1
1:A:460:ASN:HA	1:A:463:LEU:HD12	0.46	1.88	7	8
1:A:21:LYS:CE	1:A:34:THR:CG2	0.46	2.93	18	2
1:A:106:LYS:CG	1:A:121:VAL:HG11	0.46	2.40	5	1
1:A:19:PHE:O	1:A:21:LYS:N	0.46	2.49	8	15
1:A:136:ASN:O	1:A:140:PHE:N	0.46	2.47	13	8
1:A:467:LYS:O	1:A:469:SER:N	0.46	2.49	9	7
1:A:13:LYS:HG3	1:A:14:GLU:N	0.46	2.25	16	1
1:A:12:PHE:O	1:A:15:ALA:N	0.46	2.49	16	1
1:A:125:LEU:C	1:A:127:GLU:N	0.46	2.69	7	20
1:A:85:LEU:HD12	1:A:137:ILE:CD1	0.46	2.41	2	3
1:A:136:ASN:C	1:A:138:GLN:N	0.46	2.69	13	7
1:A:36:MET:HE1	1:A:472:PHE:HB2	0.46	1.87	15	2
1:A:92:PHE:CB	1:A:100:ILE:CD1	0.46	2.94	14	15
1:A:469:SER:O	1:A:472:PHE:N	0.46	2.49	2	3
1:A:22:ASP:OD1	1:A:24:ASN:CB	0.46	2.64	4	4
1:A:51:LEU:HD21	1:A:471:MET:SD	0.46	2.51	4	2
1:A:114:GLU:O	1:A:115:LYS:CG	0.46	2.64	5	2
1:A:464:ALA:O	1:A:468:VAL:CG2	0.46	2.59	5	3
1:A:90:LYS:CB	1:A:90:LYS:NZ	0.46	2.79	19	1
1:A:89:PHE:CE2	1:A:137:ILE:HB	0.45	2.46	12	3
1:A:466:ALA:O	1:A:467:LYS:C	0.45	2.55	2	3
1:A:103:ALA:O	1:A:107:HIS:HB3	0.45	2.11	19	7
1:A:467:LYS:C	1:A:469:SER:N	0.45	2.69	16	7
1:A:22:ASP:OD1	1:A:24:ASN:N	0.45	2.50	3	17
1:A:35:VAL:O	1:A:38:SER:N	0.45	2.49	1	14
1:A:134:GLU:O	1:A:139:GLN:NE2	0.45	2.50	11	8
1:A:71:LEU:O	1:A:74:ARG:N	0.45	2.49	18	3
1:A:24:ASN:OD1	1:A:25:GLY:N	0.45	2.50	6	3
1:A:105:LEU:CD1	1:A:109:LEU:HD23	0.45	2.41	12	1
1:A:456:LYS:NZ	1:A:460:ASN:HD22	0.45	2.09	20	1
1:A:128:VAL:HB	1:A:142:ALA:HB3	0.45	1.86	1	1
1:A:108:VAL:O	1:A:111:SER:N	0.45	2.50	3	2
1:A:72:MET:CE	1:A:467:LYS:CD	0.45	2.94	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:SER:OG	1:A:61:HIS:NE2	0.45	2.49	12	1
1:A:55:ILE:CD1	1:A:471:MET:SD	0.45	3.04	19	2
1:A:25:GLY:O	1:A:64:GLU:CG	0.45	2.65	13	9
1:A:117:THR:O	1:A:120:GLU:N	0.45	2.50	5	9
1:A:51:LEU:HD11	1:A:471:MET:HE1	0.45	1.87	2	1
1:A:5:THR:O	1:A:8:GLN:N	0.45	2.50	10	10
1:A:119:ALA:O	1:A:123:ASP:N	0.45	2.50	10	1
1:A:44:SER:O	1:A:47:GLU:N	0.45	2.50	20	1
1:A:43:PRO:HB3	1:A:472:PHE:CD1	0.45	2.46	6	1
1:A:106:LYS:CD	1:A:121:VAL:HG11	0.45	2.41	6	1
1:A:13:LYS:CE	1:A:65:PHE:CE2	0.45	3.00	10	1
1:A:51:LEU:CD1	1:A:471:MET:SD	0.45	3.05	10	1
1:A:49:ASN:OD1	1:A:61:HIS:ND1	0.45	2.50	12	1
1:A:29:SER:HB3	1:A:61:HIS:CE1	0.45	2.46	8	1
1:A:129:SER:OG	1:A:133:GLY:N	0.45	2.50	12	1
1:A:112:ILE:CD1	1:A:461:LYS:HG2	0.45	2.42	8	12
1:A:125:LEU:O	1:A:126:ARG:C	0.45	2.55	8	18
1:A:464:ALA:O	1:A:468:VAL:N	0.45	2.49	14	7
1:A:85:LEU:HD11	1:A:141:ALA:HA	0.45	1.89	11	1
1:A:28:SER:OG	1:A:61:HIS:CD2	0.45	2.70	12	1
1:A:129:SER:OG	1:A:132:SER:N	0.45	2.50	12	1
1:A:460:ASN:O	1:A:463:LEU:N	0.45	2.50	15	1
1:A:33:ALA:O	1:A:37:ARG:NE	0.45	2.50	18	1
1:A:47:GLU:C	1:A:49:ASN:N	0.45	2.69	12	7
1:A:102:ALA:O	1:A:106:LYS:N	0.45	2.50	11	6
1:A:28:SER:OG	1:A:29:SER:N	0.45	2.49	12	1
1:A:72:MET:CA	1:A:467:LYS:NZ	0.45	2.80	17	1
1:A:51:LEU:HD21	1:A:471:MET:CB	0.45	2.41	5	2
1:A:119:ALA:O	1:A:123:ASP:CB	0.45	2.64	11	2
1:A:112:ILE:CD1	1:A:461:LYS:HG3	0.45	2.42	12	1
1:A:19:PHE:CD2	1:A:27:ILE:HD13	0.45	2.46	14	1
1:A:116:LEU:CD2	1:A:124:MET:HE2	0.45	2.42	19	1
1:A:19:PHE:CE1	1:A:35:VAL:CG1	0.45	3.00	20	1
1:A:74:ARG:O	1:A:74:ARG:CD	0.44	2.66	15	2
1:A:35:VAL:HG12	1:A:36:MET:N	0.44	2.26	19	2
1:A:102:ALA:O	1:A:106:LYS:CG	0.44	2.66	9	4
1:A:455:ARG:O	1:A:458:LEU:N	0.44	2.50	1	2
1:A:47:GLU:O	1:A:49:ASN:N	0.44	2.51	12	6
1:A:470:ARG:HD2	1:A:474:VAL:CG2	0.44	2.43	15	1
1:A:464:ALA:C	1:A:466:ALA:N	0.44	2.70	3	13
1:A:456:LYS:HZ2	1:A:457:ALA:HA	0.44	1.72	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:465:ILE:O	1:A:469:SER:CB	0.44	2.65	4	4
1:A:113:GLY:O	1:A:115:LYS:CG	0.44	2.65	3	1
1:A:47:GLU:O	1:A:51:LEU:N	0.44	2.50	16	5
1:A:114:GLU:OE2	1:A:116:LEU:CG	0.44	2.66	12	1
1:A:136:ASN:O	1:A:138:GLN:N	0.44	2.51	13	1
1:A:457:ALA:O	1:A:461:LYS:NZ	0.44	2.49	19	1
1:A:55:ILE:O	1:A:56:ASP:C	0.44	2.56	12	19
1:A:69:LEU:C	1:A:69:LEU:HD22	0.44	2.33	9	3
1:A:19:PHE:CD2	1:A:35:VAL:CG2	0.44	3.00	12	1
1:A:462:ILE:HA	1:A:465:ILE:HD12	0.44	1.90	15	1
1:A:7:GLU:OE2	1:A:456:LYS:NZ	0.44	2.51	16	1
1:A:466:ALA:O	1:A:470:ARG:N	0.43	2.50	1	2
1:A:66:SER:O	1:A:70:ALA:HB2	0.43	2.13	10	1
1:A:15:ALA:HB2	1:A:460:ASN:OD1	0.43	2.13	14	1
1:A:56:ASP:OD2	1:A:59:GLY:CA	0.43	2.66	20	2
1:A:28:SER:C	1:A:52:MET:CE	0.43	2.87	13	1
1:A:9:ILE:C	1:A:11:GLU:N	0.43	2.72	16	1
1:A:20:ASP:O	1:A:23:ASN:ND2	0.43	2.51	1	4
1:A:92:PHE:HB3	1:A:100:ILE:HD13	0.43	1.89	14	7
1:A:16:PHE:CE1	1:A:64:GLU:O	0.43	2.72	7	2
1:A:105:LEU:HD13	1:A:125:LEU:HD11	0.43	1.90	17	1
1:A:49:ASN:C	1:A:51:LEU:N	0.43	2.72	3	7
1:A:469:SER:O	1:A:470:ARG:C	0.43	2.56	2	2
1:A:36:MET:HE3	1:A:41:LEU:HD13	0.43	1.89	11	1
1:A:112:ILE:HD13	1:A:461:LYS:HG2	0.43	1.89	1	1
1:A:129:SER:O	1:A:130:ASP:C	0.43	2.57	1	10
1:A:15:ALA:HA	1:A:18:LEU:CD1	0.43	2.43	2	11
1:A:128:VAL:HG21	1:A:139:GLN:O	0.43	2.14	10	2
1:A:87:GLU:HB2	1:A:466:ALA:HB1	0.43	1.89	15	1
1:A:474:VAL:O	1:A:475:LEU:C	0.43	2.57	1	11
1:A:474:VAL:C	1:A:476:ARG:N	0.43	2.70	2	3
1:A:11:GLU:OE2	1:A:456:LYS:NZ	0.43	2.51	7	1
1:A:464:ALA:O	1:A:468:VAL:HG13	0.43	2.14	11	2
1:A:142:ALA:O	1:A:145:SER:C	0.43	2.57	10	2
1:A:55:ILE:N	1:A:55:ILE:CD1	0.43	2.69	10	1
1:A:474:VAL:HG13	1:A:475:LEU:N	0.43	2.29	9	5
1:A:66:SER:C	1:A:69:LEU:HD12	0.43	2.34	9	3
1:A:72:MET:N	1:A:72:MET:SD	0.43	2.91	11	3
1:A:129:SER:C	1:A:131:GLY:N	0.43	2.71	16	1
1:A:11:GLU:OE1	1:A:456:LYS:CD	0.43	2.67	18	1
1:A:466:ALA:O	1:A:469:SER:CB	0.43	2.67	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:471:MET:HA	1:A:474:VAL:HG12	0.43	1.90	13	5
1:A:469:SER:O	1:A:471:MET:N	0.43	2.51	20	1
1:A:105:LEU:HD23	1:A:121:VAL:HG22	0.43	1.86	6	1
1:A:109:LEU:CD1	1:A:458:LEU:HD11	0.43	2.44	13	1
1:A:33:ALA:CB	1:A:37:ARG:HH21	0.43	2.26	18	1
1:A:464:ALA:O	1:A:466:ALA:N	0.43	2.52	4	3
1:A:105:LEU:CD1	1:A:105:LEU:C	0.43	2.87	12	1
1:A:32:LEU:HD11	1:A:51:LEU:CD1	0.43	2.43	13	1
1:A:57:VAL:HG23	1:A:67:GLU:HG2	0.42	1.91	4	2
1:A:97:ASP:OD1	1:A:99:LEU:O	0.42	2.36	4	2
1:A:102:ALA:HB2	1:A:125:LEU:HD11	0.42	1.90	14	1
1:A:474:VAL:O	1:A:476:ARG:N	0.42	2.52	2	2
1:A:21:LYS:NZ	1:A:34:THR:HG21	0.42	2.29	8	1
1:A:116:LEU:HD22	1:A:124:MET:CE	0.42	2.44	14	1
1:A:462:ILE:O	1:A:466:ALA:N	0.42	2.51	19	1
1:A:92:PHE:HE2	1:A:105:LEU:HD13	0.42	1.74	1	1
1:A:87:GLU:HA	1:A:90:LYS:HZ2	0.42	1.75	2	1
1:A:467:LYS:O	1:A:468:VAL:C	0.42	2.58	16	15
1:A:125:LEU:HD13	1:A:125:LEU:N	0.42	2.29	17	1
1:A:116:LEU:CD1	1:A:124:MET:CE	0.42	2.98	8	1
1:A:85:LEU:HD11	1:A:141:ALA:N	0.42	2.29	10	1
1:A:470:ARG:HD3	1:A:474:VAL:CG2	0.42	2.44	15	3
1:A:470:ARG:HD3	1:A:474:VAL:HG23	0.42	1.91	20	1
1:A:129:SER:O	1:A:132:SER:CB	0.42	2.67	4	3
1:A:13:LYS:HE3	1:A:65:PHE:CE2	0.42	2.50	10	1
1:A:51:LEU:HD21	1:A:471:MET:HE2	0.42	1.91	11	1
1:A:127:GLU:CD	1:A:455:ARG:NH1	0.42	2.73	2	1
1:A:85:LEU:O	1:A:88:ALA:N	0.42	2.53	4	1
1:A:61:HIS:C	1:A:62:GLN:CG	0.42	2.88	6	1
1:A:52:MET:SD	1:A:61:HIS:C	0.42	2.98	14	4
1:A:49:ASN:OD1	1:A:61:HIS:NE2	0.42	2.50	10	1
1:A:460:ASN:O	1:A:460:ASN:OD1	0.42	2.38	10	1
1:A:92:PHE:HB3	1:A:100:ILE:CD1	0.42	2.44	14	1
1:A:85:LEU:O	1:A:89:PHE:CB	0.42	2.68	16	1
1:A:109:LEU:C	1:A:114:GLU:O	0.42	2.58	10	4
1:A:143:LEU:C	1:A:459:ARG:NH1	0.42	2.73	1	1
1:A:102:ALA:O	1:A:106:LYS:HG3	0.42	2.15	9	6
1:A:120:GLU:OE2	1:A:120:GLU:CA	0.42	2.67	2	1
1:A:136:ASN:OD1	1:A:139:GLN:OE1	0.42	2.38	10	3
1:A:85:LEU:HG	1:A:141:ALA:CB	0.42	2.45	1	2
1:A:56:ASP:OD1	1:A:60:ASN:OD1	0.42	2.38	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:ALA:O	1:A:104:GLU:C	0.42	2.58	19	13
1:A:11:GLU:OE1	1:A:456:LYS:CE	0.42	2.68	4	1
1:A:72:MET:O	1:A:467:LYS:NZ	0.42	2.52	4	1
1:A:11:GLU:C	1:A:13:LYS:N	0.42	2.73	13	1
1:A:109:LEU:HD12	1:A:114:GLU:CG	0.42	2.45	16	1
1:A:105:LEU:CD2	1:A:124:MET:SD	0.42	3.08	17	1
1:A:39:LEU:HD11	1:A:465:ILE:HG23	0.42	1.87	18	1
1:A:112:ILE:HG21	1:A:465:ILE:CG1	0.42	2.45	4	1
1:A:464:ALA:O	1:A:465:ILE:C	0.42	2.58	9	4
1:A:460:ASN:C	1:A:462:ILE:N	0.42	2.73	15	1
1:A:121:VAL:C	1:A:123:ASP:N	0.41	2.73	15	9
1:A:129:SER:O	1:A:132:SER:OG	0.41	2.39	8	1
1:A:128:VAL:CG1	1:A:142:ALA:CB	0.41	2.98	10	1
1:A:36:MET:CE	1:A:472:PHE:HB2	0.41	2.45	12	3
1:A:114:GLU:HG3	1:A:461:LYS:HZ3	0.41	1.74	8	1
1:A:66:SER:O	1:A:69:LEU:HD12	0.41	2.15	13	2
1:A:19:PHE:CE1	1:A:35:VAL:HG11	0.41	2.49	20	1
1:A:95:ASN:ND2	1:A:95:ASN:O	0.41	2.53	13	4
1:A:461:LYS:HE2	1:A:461:LYS:CA	0.41	2.45	4	1
1:A:106:LYS:HG2	1:A:121:VAL:HG11	0.41	1.92	5	1
1:A:112:ILE:HD12	1:A:461:LYS:HD3	0.41	1.92	6	1
1:A:125:LEU:N	1:A:125:LEU:HD13	0.41	2.30	8	1
1:A:112:ILE:CD1	1:A:461:LYS:HD3	0.41	2.44	10	1
1:A:144:LEU:N	1:A:144:LEU:HD23	0.41	2.30	13	1
1:A:58:ASP:OD2	1:A:67:GLU:OE2	0.41	2.38	8	1
1:A:105:LEU:HD13	1:A:125:LEU:CD2	0.41	2.46	9	1
1:A:104:GLU:O	1:A:108:VAL:CG2	0.41	2.68	11	1
1:A:22:ASP:OD1	1:A:22:ASP:C	0.41	2.59	20	2
1:A:27:ILE:O	1:A:52:MET:HE1	0.41	2.16	8	1
1:A:116:LEU:CD1	1:A:124:MET:HE1	0.41	2.46	8	1
1:A:143:LEU:C	1:A:145:SER:N	0.41	2.73	11	1
1:A:469:SER:C	1:A:471:MET:N	0.41	2.72	20	1
1:A:125:LEU:C	1:A:129:SER:OG	0.41	2.58	7	2
1:A:19:PHE:O	1:A:21:LYS:CD	0.41	2.68	20	2
1:A:14:GLU:O	1:A:17:ALA:N	0.41	2.54	8	1
1:A:103:ALA:HA	1:A:106:LYS:CG	0.41	2.46	18	1
1:A:39:LEU:HD23	1:A:111:SER:HG	0.41	1.76	1	1
1:A:55:ILE:CG2	1:A:71:LEU:HD13	0.41	2.44	2	1
1:A:13:LYS:HE2	1:A:65:PHE:CD2	0.41	2.50	5	1
1:A:55:ILE:CG2	1:A:71:LEU:HD12	0.41	2.45	7	1
1:A:88:ALA:O	1:A:91:VAL:HG12	0.41	2.16	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:VAL:HG21	1:A:142:ALA:HB3	0.41	1.93	10	1
1:A:141:ALA:C	1:A:143:LEU:N	0.41	2.73	13	1
1:A:95:ASN:OD1	1:A:95:ASN:C	0.41	2.59	15	1
1:A:71:LEU:CD2	1:A:471:MET:CE	0.41	2.98	16	1
1:A:12:PHE:CG	1:A:69:LEU:HB2	0.41	2.50	18	3
1:A:456:LYS:CB	1:A:456:LYS:NZ	0.41	2.84	4	1
1:A:117:THR:C	1:A:119:ALA:N	0.41	2.74	9	2
1:A:124:MET:O	1:A:143:LEU:HD21	0.41	2.16	10	1
1:A:50:ASP:OD1	1:A:50:ASP:C	0.41	2.59	3	1
1:A:38:SER:O	1:A:111:SER:OG	0.41	2.39	18	2
1:A:135:ILE:HG22	1:A:139:GLN:HE21	0.41	1.75	5	1
1:A:14:GLU:CD	1:A:457:ALA:CB	0.41	2.88	10	1
1:A:128:VAL:CG1	1:A:142:ALA:HB1	0.41	2.46	10	1
1:A:136:ASN:OD1	1:A:139:GLN:CD	0.41	2.59	10	1
1:A:29:SER:CB	1:A:61:HIS:CE1	0.41	3.03	12	1
1:A:50:ASP:O	1:A:54:GLU:CG	0.41	2.69	1	1
1:A:72:MET:HA	1:A:467:LYS:CE	0.41	2.46	1	1
1:A:47:GLU:O	1:A:48:VAL:C	0.41	2.59	12	4
1:A:114:GLU:C	1:A:115:LYS:CG	0.41	2.89	12	1
1:A:131:GLY:O	1:A:132:SER:C	0.41	2.60	18	1
1:A:17:ALA:O	1:A:18:LEU:C	0.40	2.59	11	1
1:A:128:VAL:HG22	1:A:143:LEU:HD21	0.40	1.93	11	1
1:A:136:ASN:O	1:A:137:ILE:C	0.40	2.58	13	1
1:A:91:VAL:O	1:A:94:LYS:NZ	0.40	2.51	14	1
1:A:475:LEU:O	1:A:476:ARG:C	0.40	2.60	14	1
1:A:33:ALA:O	1:A:37:ARG:CG	0.40	2.69	20	1
1:A:50:ASP:O	1:A:54:GLU:CD	0.40	2.60	1	1
1:A:35:VAL:O	1:A:36:MET:C	0.40	2.59	11	2
1:A:8:GLN:CD	1:A:11:GLU:OE2	0.40	2.60	15	1
1:A:72:MET:HE3	1:A:467:LYS:CB	0.40	2.46	18	1
1:A:106:LYS:O	1:A:110:THR:N	0.40	2.55	2	1
1:A:456:LYS:NZ	1:A:456:LYS:CB	0.40	2.84	3	1
1:A:463:LEU:CG	1:A:467:LYS:HZ2	0.40	2.28	10	1
1:A:65:PHE:O	1:A:69:LEU:HD23	0.40	2.16	18	1
1:A:26:SER:CB	1:A:62:GLN:OE1	0.40	2.69	6	1
1:A:106:LYS:O	1:A:107:HIS:C	0.40	2.59	15	2
1:A:114:GLU:OE2	1:A:116:LEU:HD13	0.40	2.16	17	1
1:A:58:ASP:OD2	1:A:60:ASN:CG	0.40	2.60	9	1
1:A:107:HIS:O	1:A:111:SER:OG	0.40	2.39	14	1
1:A:72:MET:CB	1:A:467:LYS:NZ	0.40	2.83	17	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	152/176 (86%)	118±2 (77±1%)	31±2 (21±1%)	3±1 (2±1%)	10	50
All	All	3040/3520 (86%)	2350 (77%)	626 (21%)	64 (2%)	10	50

All 7 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	104	GLU	19
1	A	126	ARG	19
1	A	20	ASP	17
1	A	114	GLU	3
1	A	468	VAL	3
1	A	132	SER	2
1	A	470	ARG	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	130/150 (87%)	101±2 (78±2%)	29±2 (22±2%)	3	29
All	All	2600/3000 (87%)	2017 (78%)	583 (22%)	3	29

All 69 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	34	THR	20
1	A	63	ILE	20
1	A	69	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	93	ASP	20
1	A	95	ASN	20
1	A	97	ASP	20
1	A	107	HIS	20
1	A	136	ASN	20
1	A	475	LEU	20
1	A	20	ASP	19
1	A	30	SER	19
1	A	111	SER	19
1	A	458	LEU	19
1	A	94	LYS	18
1	A	106	LYS	17
1	A	470	ARG	17
1	A	26	SER	16
1	A	72	MET	16
1	A	461	LYS	16
1	A	85	LEU	15
1	A	456	LYS	14
1	A	476	ARG	13
1	A	74	ARG	13
1	A	64	GLU	11
1	A	105	LEU	11
1	A	32	LEU	10
1	A	123	ASP	8
1	A	51	LEU	8
1	A	91	VAL	7
1	A	50	ASP	7
1	A	44	SER	6
1	A	469	SER	6
1	A	121	VAL	6
1	A	90	LYS	6
1	A	463	LEU	5
1	A	29	SER	5
1	A	143	LEU	5
1	A	118	ASP	5
1	A	144	LEU	5
1	A	471	MET	4
1	A	114	GLU	4
1	A	473	SER	4
1	A	47	GLU	3
1	A	42	SER	3
1	A	145	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	13	LYS	3
1	A	28	SER	3
1	A	125	LEU	3
1	A	115	LYS	3
1	A	23	ASN	2
1	A	38	SER	2
1	A	71	LEU	2
1	A	86	LEU	2
1	A	55	ILE	2
1	A	52	MET	2
1	A	99	LEU	2
1	A	116	LEU	2
1	A	120	GLU	1
1	A	53	ASN	1
1	A	109	LEU	1
1	A	58	ASP	1
1	A	73	SER	1
1	A	101	SER	1
1	A	129	SER	1
1	A	467	LYS	1
1	A	124	MET	1
1	A	108	VAL	1
1	A	132	SER	1
1	A	49	ASN	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 monosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 94% 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 [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	2204
Number of shifts mapped to atoms	2204
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	176	-0.42 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	165	0.18 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	165	-0.48 ± 0.14	None needed (< 0.5 ppm)
^{15}N	175	0.34 ± 0.22	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 94%, i.e. 1944 atoms were assigned a chemical shift out of a possible 2061. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	764/771 (99%)	313/313 (100%)	299/306 (98%)	152/152 (100%)
Sidechain	1103/1186 (93%)	741/771 (96%)	343/373 (92%)	19/42 (45%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	77/104 (74%)	48/53 (91%)	29/49 (59%)	0/2 (0%)
Overall	1944/2061 (94%)	1102/1137 (97%)	671/728 (92%)	171/196 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 2197 atoms were assigned a chemical shift out of a possible 2331. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	877/889 (99%)	361/362 (100%)	341/352 (97%)	175/175 (100%)
Sidechain	1243/1338 (93%)	832/866 (96%)	387/421 (92%)	24/51 (47%)
Aromatic	77/104 (74%)	48/53 (91%)	29/49 (59%)	0/2 (0%)
Overall	2197/2331 (94%)	1241/1281 (97%)	757/822 (92%)	199/228 (87%)

7.1.4 Statistically unusual chemical shifts [i](#)

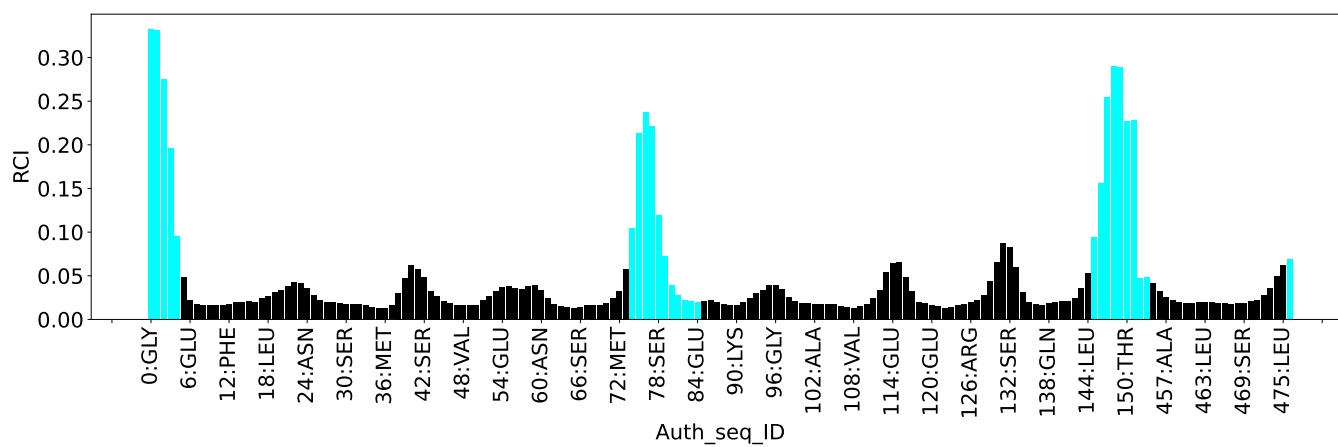
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	5	THR	HG1	5.66	0.08 – 2.19	21.4
1	A	34	THR	HG1	5.56	0.08 – 2.19	21.0
1	A	110	THR	HG1	5.18	0.08 – 2.19	19.1

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. 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	3899
Intra-residue ($ i-j =0$)	1008
Sequential ($ i-j =1$)	989
Medium range ($ i-j >1$ and $ i-j <5$)	997
Long range ($ i-j \geq 5$)	905
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	22.2
Number of long range restraints per residue ¹	5.1

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)	10.0	0.2
0.2-0.5 (Medium)	3.3	0.49
>0.5 (Large)	1.1	0.64

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

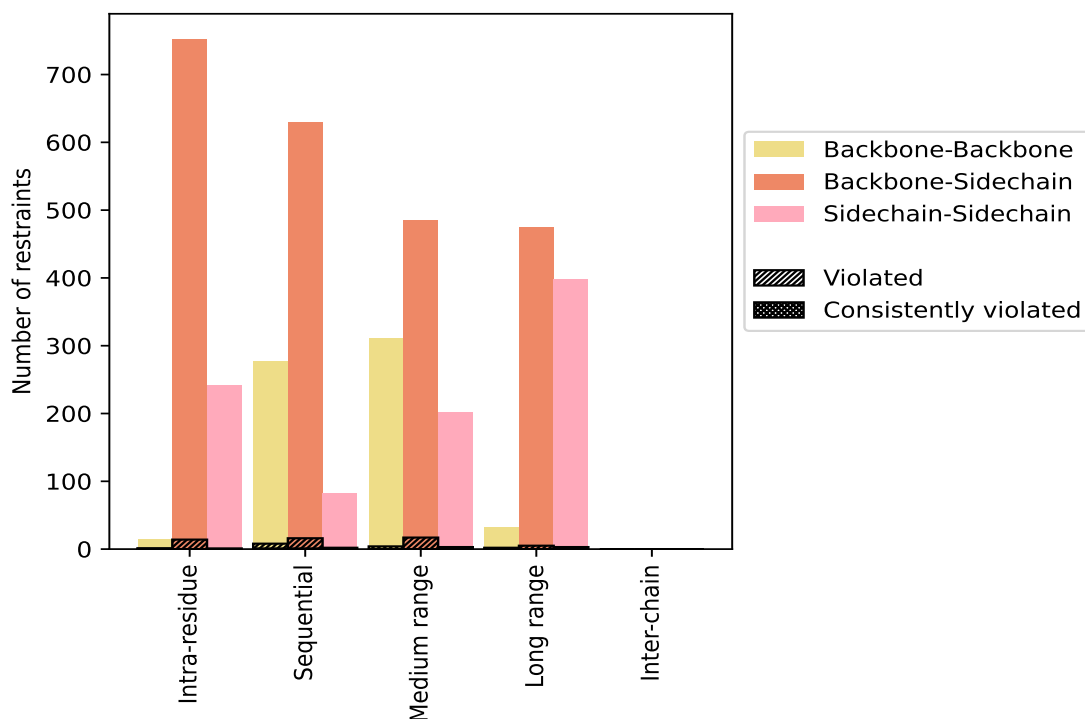
9.1 Summary of distance violations

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 ($i-j =0$)	1008	25.9	16	1.6	0.4	1	0.1	0.0
Backbone-Backbone	14	0.4	1	7.1	0.0	1	7.1	0.0
Backbone-Sidechain	752	19.3	14	1.9	0.4	0	0.0	0.0
Sidechain-Sidechain	242	6.2	1	0.4	0.0	0	0.0	0.0
Sequential ($i-j =1$)	989	25.4	26	2.6	0.7	2	0.2	0.1
Backbone-Backbone	277	7.1	8	2.9	0.2	1	0.4	0.0
Backbone-Sidechain	630	16.2	16	2.5	0.4	1	0.2	0.0
Sidechain-Sidechain	82	2.1	2	2.4	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	997	25.6	24	2.4	0.6	0	0.0	0.0
Backbone-Backbone	311	8.0	4	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	485	12.4	17	3.5	0.4	0	0.0	0.0
Sidechain-Sidechain	201	5.2	3	1.5	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	905	23.2	10	1.1	0.3	0	0.0	0.0
Backbone-Backbone	32	0.8	2	6.2	0.1	0	0.0	0.0
Backbone-Sidechain	475	12.2	5	1.1	0.1	0	0.0	0.0
Sidechain-Sidechain	398	10.2	3	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	3899	100.0	76	1.9	1.9	3	0.1	0.1
Backbone-Backbone	634	16.3	15	2.4	0.4	2	0.3	0.1
Backbone-Sidechain	2342	60.1	52	2.2	1.3	1	0.0	0.0
Sidechain-Sidechain	923	23.7	9	1.0	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 disulfid 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	4	6	4	4	0	18	0.18	0.53	0.11	0.14
2	4	8	2	0	0	14	0.21	0.62	0.14	0.14
3	4	5	3	1	0	13	0.2	0.63	0.15	0.13
4	4	3	4	2	0	13	0.21	0.57	0.13	0.16
5	3	6	2	3	0	14	0.21	0.55	0.12	0.16
6	4	5	3	0	0	12	0.23	0.49	0.13	0.18
7	5	5	4	0	0	14	0.22	0.48	0.12	0.18
8	3	3	5	1	0	12	0.23	0.58	0.17	0.13
9	3	3	7	2	0	15	0.19	0.63	0.14	0.13
10	3	8	7	1	0	19	0.17	0.57	0.11	0.13
11	3	10	3	2	0	18	0.19	0.55	0.1	0.16

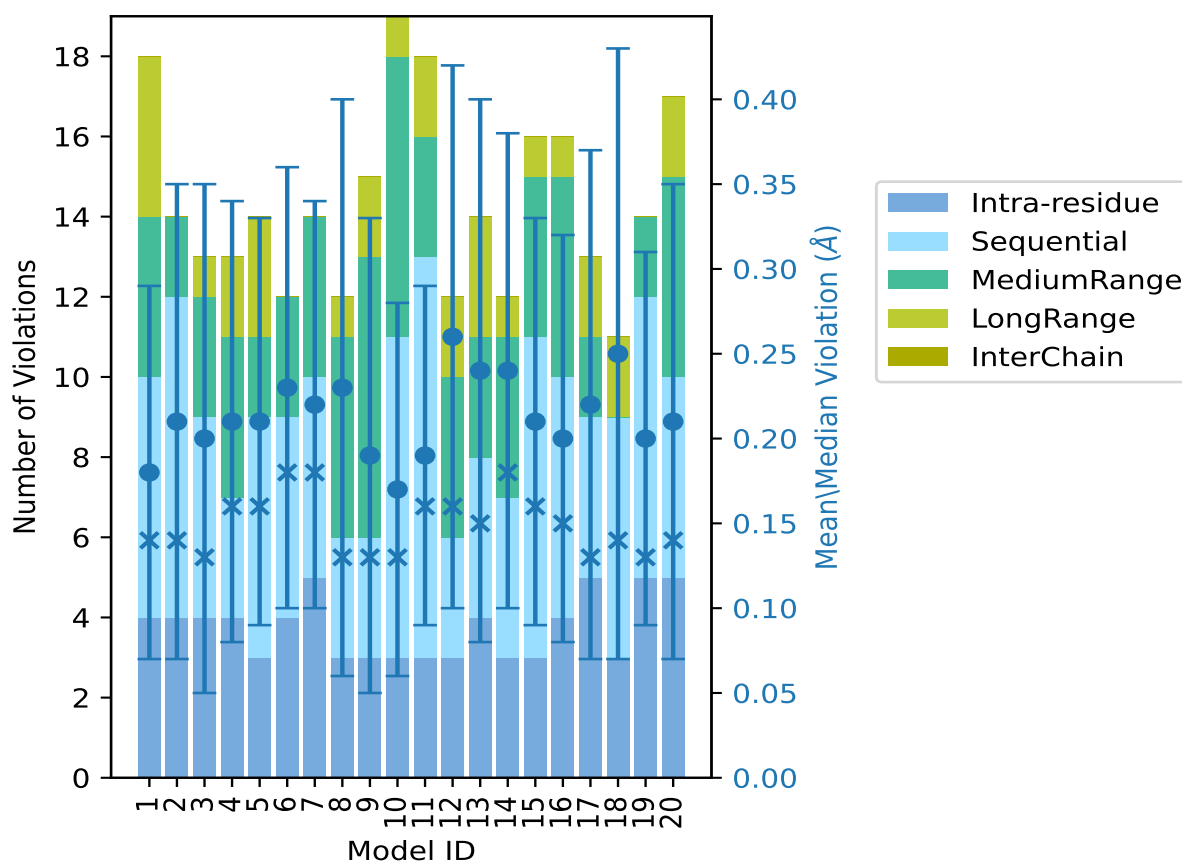
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
12	3	3	4	2	0	12	0.26	0.63	0.16	0.16
13	4	4	3	3	0	14	0.24	0.6	0.16	0.15
14	3	4	4	1	0	12	0.24	0.62	0.14	0.18
15	3	8	4	1	0	16	0.21	0.59	0.12	0.16
16	4	6	5	1	0	16	0.2	0.58	0.12	0.15
17	5	4	2	2	0	13	0.22	0.57	0.15	0.13
18	3	6	0	2	0	11	0.25	0.64	0.18	0.14
19	5	7	2	0	0	14	0.2	0.45	0.11	0.13
20	5	5	5	2	0	17	0.21	0.63	0.14	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 [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

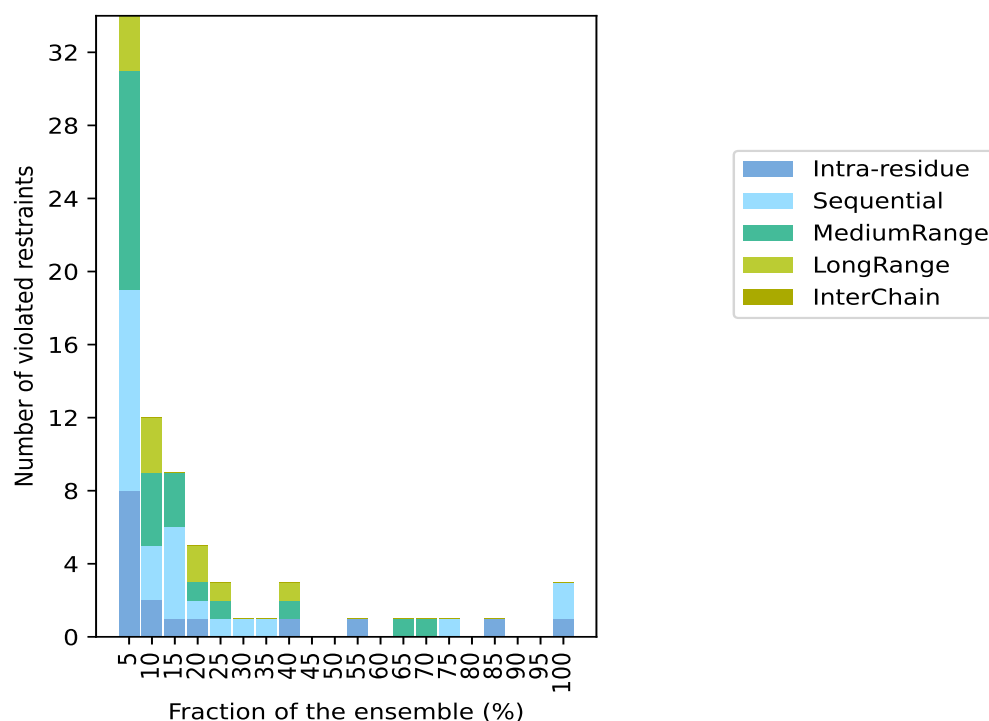
9.3 Distance violation statistics for the ensemble [i](#)

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, 3823(IR:992, SQ:963, MR:973, LR:895, 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	%
8	11	12	3	0	34	1	5.0
2	3	4	3	0	12	2	10.0
1	5	3	0	0	9	3	15.0
1	1	1	2	0	5	4	20.0
0	1	1	1	0	3	5	25.0
0	1	0	0	0	1	6	30.0
0	1	0	0	0	1	7	35.0
1	0	1	1	0	3	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
1	0	0	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	1	0	0	1	13	65.0
0	0	1	0	0	1	14	70.0
0	1	0	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
1	0	0	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
1	2	0	0	0	3	20	100.0

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

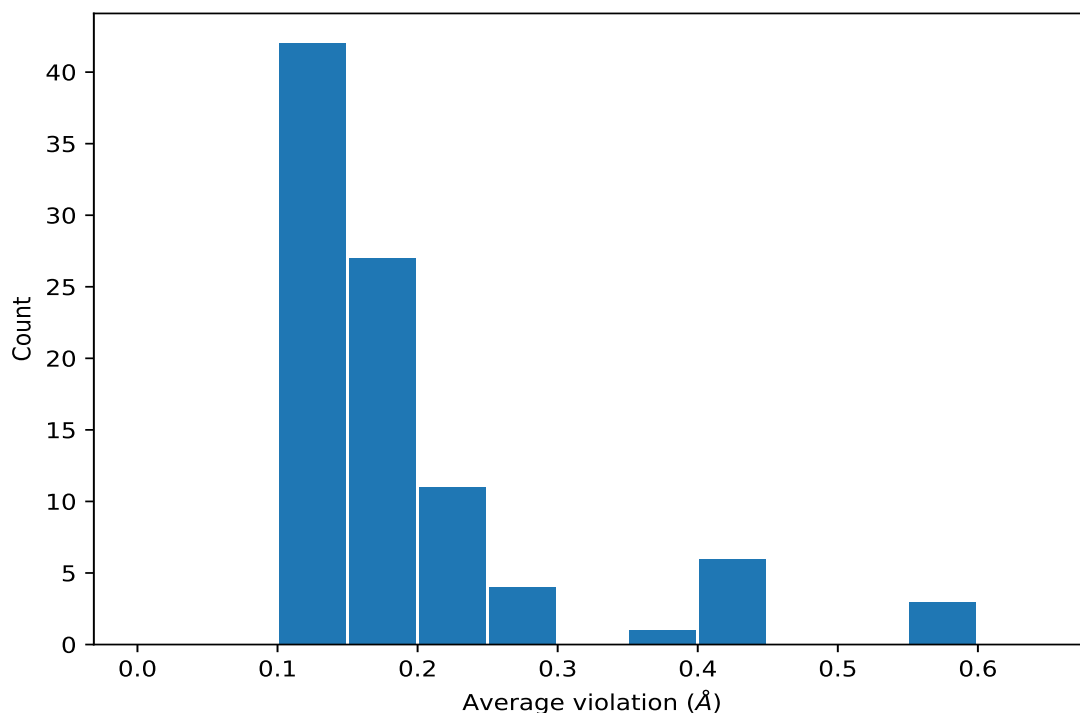
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	20	0.56	0.09	0.58
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	20	0.56	0.09	0.58
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	20	0.56	0.09	0.58
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	20	0.36	0.06	0.38
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	20	0.21	0.01	0.21
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	17	0.15	0.02	0.15
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	15	0.13	0.0	0.13
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	14	0.13	0.01	0.14
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	13	0.13	0.02	0.13
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	11	0.27	0.07	0.29
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	11	0.27	0.07	0.29
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	11	0.27	0.07	0.29
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD11	8	0.4	0.21	0.55
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD12	8	0.4	0.21	0.55
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD13	8	0.4	0.21	0.55
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB2	8	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB3	8	0.13	0.02	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB2	8	0.13	0.02	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB3	8	0.13	0.02	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB1	8	0.13	0.01	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB2	8	0.13	0.01	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB3	8	0.13	0.01	0.12
(1,1981)	1:A:474:VAL:HG21	1:A:475:LEU:H	7	0.14	0.01	0.14
(1,1981)	1:A:474:VAL:HG22	1:A:475:LEU:H	7	0.14	0.01	0.14
(1,1981)	1:A:474:VAL:HG23	1:A:475:LEU:H	7	0.14	0.01	0.14
(1,2933)	1:A:473:SER:HB2	1:A:474:VAL:HB	6	0.14	0.02	0.14
(1,2933)	1:A:473:SER:HB3	1:A:474:VAL:HB	6	0.14	0.02	0.14
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD1	5	0.17	0.03	0.17
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD2	5	0.17	0.03	0.17
(1,451)	1:A:473:SER:HA	1:A:474:VAL:H	5	0.16	0.03	0.16
(1,166)	1:A:66:SER:H	1:A:69:LEU:HG	5	0.13	0.01	0.12
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD21	4	0.43	0.04	0.44
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD22	4	0.43	0.04	0.44
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD23	4	0.43	0.04	0.44
(1,1459)	1:A:145:SER:HA	1:A:146:LYS:H	4	0.22	0.04	0.23
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB2	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB3	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB2	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB3	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB2	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB3	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB2	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB3	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB2	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB3	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB2	4	0.19	0.07	0.18
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB3	4	0.19	0.07	0.18
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD1	4	0.12	0.01	0.12
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD2	4	0.12	0.01	0.12
(1,289)	1:A:135:ILE:H	1:A:139:GLN:HB3	4	0.12	0.01	0.12
(1,162)	1:A:112:ILE:H	1:A:113:GLY:HA3	3	0.22	0.08	0.24
(1,223)	1:A:5:THR:H	1:A:8:GLN:HA	3	0.21	0.01	0.21
(1,2572)	1:A:57:VAL:HB	1:A:58:ASP:HA	3	0.21	0.0	0.21
(1,611)	1:A:51:LEU:HG	1:A:52:MET:H	3	0.17	0.01	0.16
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG11	3	0.16	0.02	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG12	3	0.16	0.02	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG13	3	0.16	0.02	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG21	3	0.16	0.02	0.17

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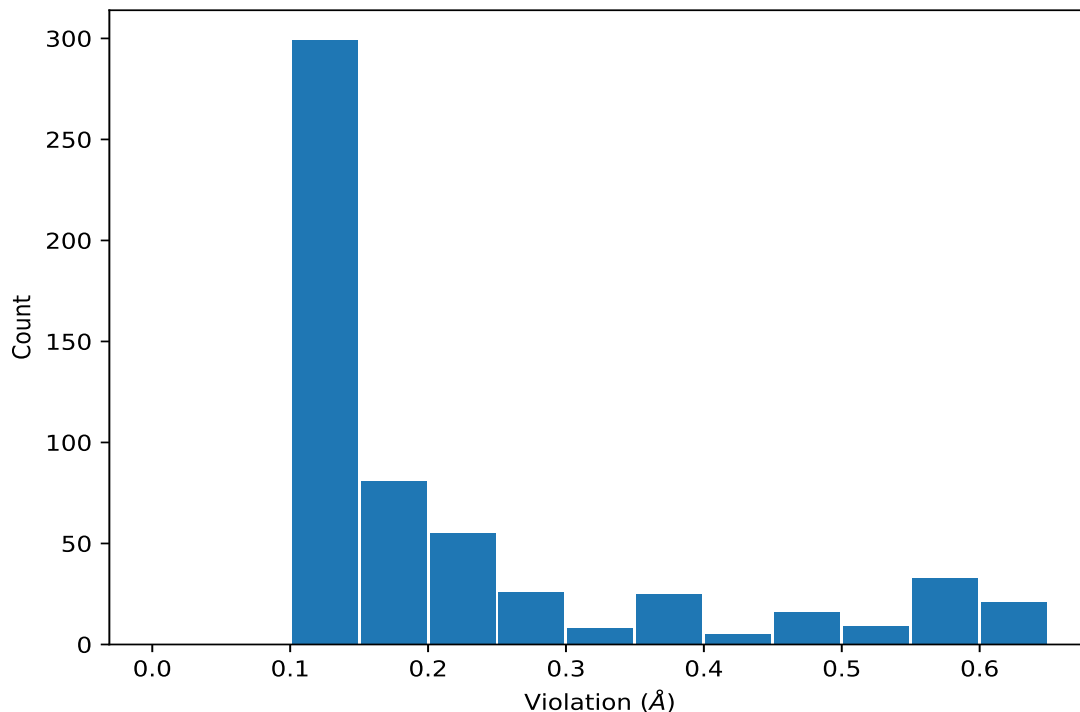
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG22	3	0.16	0.02	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG23	3	0.16	0.02	0.17
(1,1268)	1:A:4:LEU:H	1:A:8:GLN:HG3	3	0.16	0.02	0.15
(1,2059)	1:A:91:VAL:HG21	1:A:92:PHE:HD1	3	0.13	0.01	0.13
(1,2059)	1:A:91:VAL:HG21	1:A:92:PHE:HD2	3	0.13	0.01	0.13
(1,2059)	1:A:91:VAL:HG22	1:A:92:PHE:HD1	3	0.13	0.01	0.13
(1,2059)	1:A:91:VAL:HG22	1:A:92:PHE:HD2	3	0.13	0.01	0.13
(1,2059)	1:A:91:VAL:HG23	1:A:92:PHE:HD1	3	0.13	0.01	0.13
(1,2059)	1:A:91:VAL:HG23	1:A:92:PHE:HD2	3	0.13	0.01	0.13
(1,2260)	1:A:476:ARG:H	1:A:476:ARG:HG2	3	0.13	0.0	0.13
(1,817)	1:A:68:PHE:HB2	1:A:71:LEU:H	3	0.11	0.0	0.11
(1,2779)	1:A:126:ARG:HA	1:A:131:GLY:HA3	2	0.3	0.18	0.3
(1,3591)	1:A:105:LEU:HD11	1:A:106:LYS:HA	2	0.21	0.03	0.21
(1,3591)	1:A:105:LEU:HD12	1:A:106:LYS:HA	2	0.21	0.03	0.21
(1,3591)	1:A:105:LEU:HD13	1:A:106:LYS:HA	2	0.21	0.03	0.21
(1,3591)	1:A:105:LEU:HD21	1:A:106:LYS:HA	2	0.21	0.03	0.21
(1,3591)	1:A:105:LEU:HD22	1:A:106:LYS:HA	2	0.21	0.03	0.21
(1,3591)	1:A:105:LEU:HD23	1:A:106:LYS:HA	2	0.21	0.03	0.21
(1,812)	1:A:71:LEU:H	1:A:72:MET:HB2	2	0.17	0.02	0.17
(1,812)	1:A:71:LEU:H	1:A:72:MET:HB3	2	0.17	0.02	0.17
(1,649)	1:A:467:LYS:H	1:A:467:LYS:HD2	2	0.16	0.01	0.16
(1,649)	1:A:467:LYS:H	1:A:467:LYS:HD3	2	0.16	0.01	0.16
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD11	2	0.15	0.04	0.15
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD12	2	0.15	0.04	0.15
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD13	2	0.15	0.04	0.15
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD21	2	0.15	0.04	0.15
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD22	2	0.15	0.04	0.15
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD23	2	0.15	0.04	0.15
(1,1297)	1:A:67:GLU:HG3	1:A:70:ALA:H	2	0.14	0.02	0.14
(1,1409)	1:A:102:ALA:H	1:A:105:LEU:HB2	2	0.14	0.01	0.14
(1,179)	1:A:66:SER:H	1:A:70:ALA:H	2	0.12	0.01	0.12
(1,60)	1:A:94:LYS:HG2	1:A:96:GLY:H	2	0.12	0.0	0.12
(1,60)	1:A:94:LYS:HG3	1:A:96:GLY:H	2	0.12	0.0	0.12
(1,129)	1:A:98:GLY:H	1:A:99:LEU:HB2	2	0.11	0.0	0.11
(1,1081)	1:A:144:LEU:HA	1:A:459:ARG:HE	2	0.11	0.0	0.11
(1,1610)	1:A:57:VAL:H	1:A:67:GLU:H	2	0.11	0.0	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)
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	18	0.64
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	18	0.64
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	18	0.64
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	3	0.63
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	3	0.63
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	3	0.63
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	9	0.63
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	9	0.63
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	9	0.63
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	12	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	12	0.63
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	12	0.63
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	20	0.63
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	20	0.63
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	20	0.63
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	2	0.62
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	2	0.62
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	2	0.62
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	14	0.62
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	14	0.62
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	14	0.62
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	13	0.6
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	13	0.6
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	13	0.6
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	15	0.59
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	15	0.59
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	15	0.59
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	8	0.58
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	8	0.58
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	8	0.58
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	16	0.58
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	16	0.58
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	16	0.58
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD11	17	0.57
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD12	17	0.57
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD13	17	0.57
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	4	0.57
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	4	0.57
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	4	0.57
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	10	0.57
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	10	0.57
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	10	0.57
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD11	13	0.56
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD12	13	0.56
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD13	13	0.56
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD11	5	0.55
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD12	5	0.55
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD13	5	0.55
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD11	18	0.55
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD12	18	0.55
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD13	18	0.55
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	11	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	11	0.55
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	11	0.55
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD11	8	0.54
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD12	8	0.54
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD13	8	0.54
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	1	0.53
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	1	0.53
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	1	0.53
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	17	0.52
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	17	0.52
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	17	0.52
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	6	0.49
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	6	0.49
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	6	0.49
(1,2779)	1:A:126:ARG:HA	1:A:131:GLY:HA3	12	0.48
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD21	20	0.48
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD22	20	0.48
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD23	20	0.48
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	7	0.48
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	7	0.48
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	7	0.48
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD21	6	0.46
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD22	6	0.46
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD23	6	0.46
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	19	0.45
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	19	0.45
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	19	0.45
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD21	7	0.42
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD22	7	0.42
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD23	7	0.42
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	5	0.4
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	16	0.4
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	9	0.39
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	12	0.39
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	19	0.39
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	3	0.38
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	4	0.38
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	7	0.38
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	13	0.38
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	14	0.38
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	15	0.38
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD21	4	0.37
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD22	4	0.37
(1,2139)	1:A:85:LEU:H	1:A:85:LEU:HD23	4	0.37
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	6	0.37
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	18	0.37
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	20	0.37
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	2	0.36
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	8	0.36
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	11	0.36
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	12	0.36
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	12	0.36
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	12	0.36
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	14	0.36
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	14	0.36
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	14	0.36
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	1	0.35
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	19	0.32
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	19	0.32
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	19	0.32
(1,162)	1:A:112:ILE:H	1:A:113:GLY:HA3	10	0.31
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	15	0.31
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	15	0.31
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	15	0.31
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	2	0.3
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	2	0.3
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	2	0.3
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB2	1	0.29
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB3	1	0.29
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB2	1	0.29
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB3	1	0.29
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB2	1	0.29
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB3	1	0.29
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB2	1	0.29
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB3	1	0.29
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB2	1	0.29
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB3	1	0.29
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB2	1	0.29
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB3	1	0.29
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	3	0.29
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	3	0.29
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	3	0.29
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	16	0.28
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	16	0.28
(1,1710)	1:A:112:ILE:HD11	1:A:113:GLY:HA2	5	0.27
(1,1710)	1:A:112:ILE:HD12	1:A:113:GLY:HA2	5	0.27
(1,1710)	1:A:112:ILE:HD13	1:A:113:GLY:HA2	5	0.27
(1,1459)	1:A:145:SER:HA	1:A:146:LYS:H	2	0.26
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	10	0.25
(1,3591)	1:A:105:LEU:HD11	1:A:106:LYS:HA	14	0.24
(1,3591)	1:A:105:LEU:HD12	1:A:106:LYS:HA	14	0.24
(1,3591)	1:A:105:LEU:HD13	1:A:106:LYS:HA	14	0.24
(1,3591)	1:A:105:LEU:HD21	1:A:106:LYS:HA	14	0.24
(1,3591)	1:A:105:LEU:HD22	1:A:106:LYS:HA	14	0.24
(1,3591)	1:A:105:LEU:HD23	1:A:106:LYS:HA	14	0.24
(1,162)	1:A:112:ILE:H	1:A:113:GLY:HA3	7	0.24
(1,1459)	1:A:145:SER:HA	1:A:146:LYS:H	13	0.24
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	1	0.23
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	7	0.23
(1,3163)	1:A:13:LYS:HB2	1:A:14:GLU:H	16	0.23
(1,3163)	1:A:13:LYS:HB3	1:A:14:GLU:H	16	0.23
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	8	0.22
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	11	0.22
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	12	0.22
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	17	0.22
(1,2495)	1:A:461:LYS:HB3	1:A:461:LYS:HE2	19	0.22
(1,2495)	1:A:461:LYS:HB3	1:A:461:LYS:HE3	19	0.22
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD1	13	0.22
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD2	13	0.22
(1,223)	1:A:5:THR:H	1:A:8:GLN:HA	14	0.22
(1,1459)	1:A:145:SER:HA	1:A:146:LYS:H	15	0.22
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	2	0.21
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	5	0.21
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	9	0.21
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	13	0.21
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	15	0.21
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	16	0.21
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	18	0.21
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	20	0.21
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB2	20	0.21
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB3	20	0.21
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB2	20	0.21
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB3	20	0.21
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB2	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB3	20	0.21
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB2	20	0.21
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB3	20	0.21
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB2	20	0.21
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB3	20	0.21
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB2	20	0.21
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB3	20	0.21
(1,2572)	1:A:57:VAL:HB	1:A:58:ASP:HA	5	0.21
(1,2572)	1:A:57:VAL:HB	1:A:58:ASP:HA	10	0.21
(1,2572)	1:A:57:VAL:HB	1:A:58:ASP:HA	11	0.21
(1,223)	1:A:5:THR:H	1:A:8:GLN:HA	6	0.21
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	3	0.2
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	4	0.2
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	6	0.2
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	14	0.2
(1,45)	1:A:113:GLY:H	1:A:113:GLY:HA3	19	0.2
(1,223)	1:A:5:THR:H	1:A:8:GLN:HA	7	0.2
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	9	0.2
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	9	0.2
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	9	0.2
(1,812)	1:A:71:LEU:H	1:A:72:MET:HB2	11	0.19
(1,812)	1:A:71:LEU:H	1:A:72:MET:HB3	11	0.19
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	8	0.19
(1,451)	1:A:473:SER:HA	1:A:474:VAL:H	15	0.19
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD11	7	0.19
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD12	7	0.19
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD13	7	0.19
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD21	7	0.19
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD22	7	0.19
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD23	7	0.19
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	1	0.19
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	1	0.19
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	1	0.19
(1,611)	1:A:51:LEU:HG	1:A:52:MET:H	3	0.18
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	17	0.18
(1,425)	1:A:460:ASN:H	1:A:461:LYS:HB3	19	0.18
(1,3591)	1:A:105:LEU:HD11	1:A:106:LYS:HA	10	0.18
(1,3591)	1:A:105:LEU:HD12	1:A:106:LYS:HA	10	0.18
(1,3591)	1:A:105:LEU:HD13	1:A:106:LYS:HA	10	0.18
(1,3591)	1:A:105:LEU:HD21	1:A:106:LYS:HA	10	0.18
(1,3591)	1:A:105:LEU:HD22	1:A:106:LYS:HA	10	0.18
(1,3591)	1:A:105:LEU:HD23	1:A:106:LYS:HA	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3494)	1:A:85:LEU:HD11	1:A:89:PHE:H	4	0.18
(1,3494)	1:A:85:LEU:HD12	1:A:89:PHE:H	4	0.18
(1,3494)	1:A:85:LEU:HD13	1:A:89:PHE:H	4	0.18
(1,3494)	1:A:85:LEU:HD21	1:A:89:PHE:H	4	0.18
(1,3494)	1:A:85:LEU:HD22	1:A:89:PHE:H	4	0.18
(1,3494)	1:A:85:LEU:HD23	1:A:89:PHE:H	4	0.18
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG11	11	0.18
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG12	11	0.18
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG13	11	0.18
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG21	11	0.18
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG22	11	0.18
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG23	11	0.18
(1,2933)	1:A:473:SER:HB2	1:A:474:VAL:HB	15	0.18
(1,2933)	1:A:473:SER:HB3	1:A:474:VAL:HB	15	0.18
(1,1268)	1:A:4:LEU:H	1:A:8:GLN:HG3	6	0.18
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	6	0.17
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	7	0.17
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	15	0.17
(1,451)	1:A:473:SER:HA	1:A:474:VAL:H	20	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG11	5	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG12	5	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG13	5	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG21	5	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG22	5	0.17
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG23	5	0.17
(1,3140)	1:A:9:ILE:HG21	1:A:13:LYS:HE2	16	0.17
(1,3140)	1:A:9:ILE:HG21	1:A:13:LYS:HE3	16	0.17
(1,3140)	1:A:9:ILE:HG22	1:A:13:LYS:HE2	16	0.17
(1,3140)	1:A:9:ILE:HG22	1:A:13:LYS:HE3	16	0.17
(1,3140)	1:A:9:ILE:HG23	1:A:13:LYS:HE2	16	0.17
(1,3140)	1:A:9:ILE:HG23	1:A:13:LYS:HE3	16	0.17
(1,2933)	1:A:473:SER:HB2	1:A:474:VAL:HB	11	0.17
(1,2933)	1:A:473:SER:HB3	1:A:474:VAL:HB	11	0.17
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB2	11	0.17
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB3	11	0.17
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB2	11	0.17
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB3	11	0.17
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD1	5	0.17
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD2	5	0.17
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD1	17	0.17
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD2	17	0.17
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	12	0.16
(1,649)	1:A:467:LYS:H	1:A:467:LYS:HD2	2	0.16
(1,649)	1:A:467:LYS:H	1:A:467:LYS:HD3	2	0.16
(1,611)	1:A:51:LEU:HG	1:A:52:MET:H	4	0.16
(1,611)	1:A:51:LEU:HG	1:A:52:MET:H	12	0.16
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	4	0.16
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	12	0.16
(1,451)	1:A:473:SER:HA	1:A:474:VAL:H	11	0.16
(1,1981)	1:A:474:VAL:HG21	1:A:475:LEU:H	1	0.16
(1,1981)	1:A:474:VAL:HG22	1:A:475:LEU:H	1	0.16
(1,1981)	1:A:474:VAL:HG23	1:A:475:LEU:H	1	0.16
(1,1981)	1:A:474:VAL:HG21	1:A:475:LEU:H	6	0.16
(1,1981)	1:A:474:VAL:HG22	1:A:475:LEU:H	6	0.16
(1,1981)	1:A:474:VAL:HG23	1:A:475:LEU:H	6	0.16
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	10	0.16
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	10	0.16
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	10	0.16
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	1	0.15
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	9	0.15
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	13	0.15
(1,812)	1:A:71:LEU:H	1:A:72:MET:HB2	7	0.15
(1,812)	1:A:71:LEU:H	1:A:72:MET:HB3	7	0.15
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	15	0.15
(1,649)	1:A:467:LYS:H	1:A:467:LYS:HD2	13	0.15
(1,649)	1:A:467:LYS:H	1:A:467:LYS:HD3	13	0.15
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	1	0.15
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	13	0.15
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	14	0.15
(1,451)	1:A:473:SER:HA	1:A:474:VAL:H	18	0.15
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB1	13	0.15
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB2	13	0.15
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB3	13	0.15
(1,2854)	1:A:13:LYS:HA	1:A:13:LYS:HG2	16	0.15
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB2	10	0.15
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB3	10	0.15
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB2	10	0.15
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB3	10	0.15
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD11	4	0.15
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD12	4	0.15
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD13	4	0.15
(1,2059)	1:A:91:VAL:HG21	1:A:92:PHE:HD1	5	0.15
(1,2059)	1:A:91:VAL:HG21	1:A:92:PHE:HD2	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2059)	1:A:91:VAL:HG22	1:A:92:PHE:HD1	5	0.15
(1,2059)	1:A:91:VAL:HG22	1:A:92:PHE:HD2	5	0.15
(1,2059)	1:A:91:VAL:HG23	1:A:92:PHE:HD1	5	0.15
(1,2059)	1:A:91:VAL:HG23	1:A:92:PHE:HD2	5	0.15
(1,166)	1:A:66:SER:H	1:A:69:LEU:HG	9	0.15
(1,1459)	1:A:145:SER:HA	1:A:146:LYS:H	16	0.15
(1,1297)	1:A:67:GLU:HG3	1:A:70:ALA:H	20	0.15
(1,1268)	1:A:4:LEU:H	1:A:8:GLN:HG3	7	0.15
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD11	11	0.15
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD12	11	0.15
(1,1022)	1:A:85:LEU:H	1:A:85:LEU:HD13	11	0.15
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD1	13	0.14
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD2	13	0.14
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	4	0.14
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	10	0.14
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	15	0.14
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	20	0.14
(1,848)	1:A:86:LEU:H	1:A:87:GLU:HG2	15	0.14
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	16	0.14
(1,697)	1:A:467:LYS:HD2	1:A:468:VAL:H	2	0.14
(1,697)	1:A:467:LYS:HD3	1:A:468:VAL:H	2	0.14
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	3	0.14
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	20	0.14
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB1	1	0.14
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB2	1	0.14
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB3	1	0.14
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB2	15	0.14
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB3	15	0.14
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB2	15	0.14
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB3	15	0.14
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB2	15	0.14
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB3	15	0.14
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB2	15	0.14
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB3	15	0.14
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB2	15	0.14
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB3	15	0.14
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB2	15	0.14
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB3	15	0.14
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG11	10	0.14
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG12	10	0.14
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG13	10	0.14
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG21	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG22	10	0.14
(1,3371)	1:A:56:ASP:H	1:A:57:VAL:HG23	10	0.14
(1,2933)	1:A:473:SER:HB2	1:A:474:VAL:HB	18	0.14
(1,2933)	1:A:473:SER:HB3	1:A:474:VAL:HB	18	0.14
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB2	12	0.14
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB3	12	0.14
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB2	12	0.14
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB3	12	0.14
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD1	8	0.14
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD2	8	0.14
(1,1981)	1:A:474:VAL:HG21	1:A:475:LEU:H	2	0.14
(1,1981)	1:A:474:VAL:HG22	1:A:475:LEU:H	2	0.14
(1,1981)	1:A:474:VAL:HG23	1:A:475:LEU:H	2	0.14
(1,1981)	1:A:474:VAL:HG21	1:A:475:LEU:H	15	0.14
(1,1981)	1:A:474:VAL:HG22	1:A:475:LEU:H	15	0.14
(1,1981)	1:A:474:VAL:HG23	1:A:475:LEU:H	15	0.14
(1,1981)	1:A:474:VAL:HG21	1:A:475:LEU:H	18	0.14
(1,1981)	1:A:474:VAL:HG22	1:A:475:LEU:H	18	0.14
(1,1981)	1:A:474:VAL:HG23	1:A:475:LEU:H	18	0.14
(1,1981)	1:A:474:VAL:HG21	1:A:475:LEU:H	20	0.14
(1,1981)	1:A:474:VAL:HG22	1:A:475:LEU:H	20	0.14
(1,1981)	1:A:474:VAL:HG23	1:A:475:LEU:H	20	0.14
(1,1409)	1:A:102:ALA:H	1:A:105:LEU:HB2	14	0.14
(1,1268)	1:A:4:LEU:H	1:A:8:GLN:HG3	14	0.14
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD1	5	0.13
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD2	5	0.13
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	6	0.13
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	11	0.13
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	5	0.13
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	9	0.13
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	14	0.13
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	20	0.13
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	2	0.13
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	9	0.13
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	11	0.13
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	18	0.13
(1,515)	1:A:105:LEU:HD21	1:A:106:LYS:H	1	0.13
(1,515)	1:A:105:LEU:HD22	1:A:106:LYS:H	1	0.13
(1,515)	1:A:105:LEU:HD23	1:A:106:LYS:H	1	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	1	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	2	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	5	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	6	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	7	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	10	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	11	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	13	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	14	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	16	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	17	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	19	0.13
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	20	0.13
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB1	16	0.13
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB2	16	0.13
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB3	16	0.13
(1,2933)	1:A:473:SER:HB2	1:A:474:VAL:HB	1	0.13
(1,2933)	1:A:473:SER:HB3	1:A:474:VAL:HB	1	0.13
(1,2933)	1:A:473:SER:HB2	1:A:474:VAL:HB	2	0.13
(1,2933)	1:A:473:SER:HB3	1:A:474:VAL:HB	2	0.13
(1,289)	1:A:135:ILE:H	1:A:139:GLN:HB3	17	0.13
(1,2855)	1:A:13:LYS:HA	1:A:13:LYS:HD2	16	0.13
(1,2779)	1:A:126:ARG:HA	1:A:131:GLY:HA3	1	0.13
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD1	18	0.13
(1,2268)	1:A:85:LEU:HG	1:A:140:PHE:HD2	18	0.13
(1,2260)	1:A:476:ARG:H	1:A:476:ARG:HG2	3	0.13
(1,2260)	1:A:476:ARG:H	1:A:476:ARG:HG2	5	0.13
(1,2260)	1:A:476:ARG:H	1:A:476:ARG:HG2	17	0.13
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD11	6	0.13
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD12	6	0.13
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD13	6	0.13
(1,2137)	1:A:85:LEU:HA	1:A:85:LEU:HD21	7	0.13
(1,2137)	1:A:85:LEU:HA	1:A:85:LEU:HD22	7	0.13
(1,2137)	1:A:85:LEU:HA	1:A:85:LEU:HD23	7	0.13
(1,2059)	1:A:91:VAL:HG21	1:A:92:PHE:HD1	18	0.13
(1,2059)	1:A:91:VAL:HG21	1:A:92:PHE:HD2	18	0.13
(1,2059)	1:A:91:VAL:HG22	1:A:92:PHE:HD1	18	0.13
(1,2059)	1:A:91:VAL:HG22	1:A:92:PHE:HD2	18	0.13
(1,2059)	1:A:91:VAL:HG23	1:A:92:PHE:HD1	18	0.13
(1,2059)	1:A:91:VAL:HG23	1:A:92:PHE:HD2	18	0.13
(1,1981)	1:A:474:VAL:HG21	1:A:475:LEU:H	11	0.13
(1,1981)	1:A:474:VAL:HG22	1:A:475:LEU:H	11	0.13
(1,1981)	1:A:474:VAL:HG23	1:A:475:LEU:H	11	0.13
(1,179)	1:A:66:SER:H	1:A:70:ALA:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:A:66:SER:H	1:A:69:LEU:HG	12	0.13
(1,1409)	1:A:102:ALA:H	1:A:105:LEU:HB2	10	0.13
(1,1237)	1:A:77:LYS:H	1:A:78:SER:H	19	0.13
(1,1154)	1:A:47:GLU:HB2	1:A:50:ASP:H	12	0.13
(1,1053)	1:A:114:GLU:H	1:A:115:LYS:HA	19	0.13
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD1	17	0.12
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD2	17	0.12
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	2	0.12
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	3	0.12
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	17	0.12
(1,817)	1:A:68:PHE:HB2	1:A:71:LEU:H	5	0.12
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	1	0.12
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	4	0.12
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	8	0.12
(1,60)	1:A:94:LYS:HG2	1:A:96:GLY:H	20	0.12
(1,60)	1:A:94:LYS:HG3	1:A:96:GLY:H	20	0.12
(1,589)	1:A:61:HIS:H	1:A:61:HIS:HD2	19	0.12
(1,461)	1:A:131:GLY:HA3	1:A:132:SER:H	15	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB1	3	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB2	3	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB3	3	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB1	5	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB2	5	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB3	5	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB1	11	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB2	11	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB3	11	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB1	20	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB2	20	0.12
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB3	20	0.12
(1,289)	1:A:135:ILE:H	1:A:139:GLN:HB3	13	0.12
(1,2887)	1:A:81:SER:HA	1:A:84:GLU:H	8	0.12
(1,2793)	1:A:90:LYS:HA	1:A:90:LYS:HG3	19	0.12
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB2	1	0.12
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB3	1	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB2	1	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB3	1	0.12
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB2	2	0.12
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB3	2	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB2	2	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB3	2	0.12
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB2	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB3	16	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB2	16	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB3	16	0.12
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB2	19	0.12
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB3	19	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB2	19	0.12
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB3	19	0.12
(1,2328)	1:A:90:LYS:HA	1:A:90:LYS:HD2	20	0.12
(1,2328)	1:A:90:LYS:HA	1:A:90:LYS:HD3	20	0.12
(1,2187)	1:A:85:LEU:HD11	1:A:141:ALA:H	4	0.12
(1,2187)	1:A:85:LEU:HD12	1:A:141:ALA:H	4	0.12
(1,2187)	1:A:85:LEU:HD13	1:A:141:ALA:H	4	0.12
(1,2059)	1:A:91:VAL:HG21	1:A:92:PHE:HD1	10	0.12
(1,2059)	1:A:91:VAL:HG21	1:A:92:PHE:HD2	10	0.12
(1,2059)	1:A:91:VAL:HG22	1:A:92:PHE:HD1	10	0.12
(1,2059)	1:A:91:VAL:HG22	1:A:92:PHE:HD2	10	0.12
(1,2059)	1:A:91:VAL:HG23	1:A:92:PHE:HD1	10	0.12
(1,2059)	1:A:91:VAL:HG23	1:A:92:PHE:HD2	10	0.12
(1,179)	1:A:66:SER:H	1:A:70:ALA:H	1	0.12
(1,166)	1:A:66:SER:H	1:A:69:LEU:HG	10	0.12
(1,166)	1:A:66:SER:H	1:A:69:LEU:HG	20	0.12
(1,1297)	1:A:67:GLU:HG3	1:A:70:ALA:H	9	0.12
(1,1215)	1:A:130:ASP:H	1:A:139:GLN:HE22	12	0.12
(1,1080)	1:A:459:ARG:HA	1:A:459:ARG:HE	1	0.12
(1,1066)	1:A:100:ILE:HG21	1:A:104:GLU:H	4	0.12
(1,1066)	1:A:100:ILE:HG22	1:A:104:GLU:H	4	0.12
(1,1066)	1:A:100:ILE:HG23	1:A:104:GLU:H	4	0.12
(1,1052)	1:A:113:GLY:HA2	1:A:114:GLU:H	10	0.12
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD1	18	0.11
(1,911)	1:A:89:PHE:H	1:A:140:PHE:HD2	18	0.11
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	8	0.11
(1,875)	1:A:69:LEU:H	1:A:71:LEU:HB2	16	0.11
(1,817)	1:A:68:PHE:HB2	1:A:71:LEU:H	3	0.11
(1,817)	1:A:68:PHE:HB2	1:A:71:LEU:H	7	0.11
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	7	0.11
(1,802)	1:A:121:VAL:HB	1:A:123:ASP:H	10	0.11
(1,799)	1:A:58:ASP:HB2	1:A:60:ASN:H	16	0.11
(1,60)	1:A:94:LYS:HG2	1:A:96:GLY:H	15	0.11
(1,60)	1:A:94:LYS:HG3	1:A:96:GLY:H	15	0.11
(1,513)	1:A:80:ASP:H	1:A:81:SER:H	9	0.11
(1,471)	1:A:91:VAL:HG21	1:A:93:ASP:H	10	0.11
(1,471)	1:A:91:VAL:HG22	1:A:93:ASP:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:A:91:VAL:HG23	1:A:93:ASP:H	10	0.11
(1,451)	1:A:473:SER:HA	1:A:474:VAL:H	2	0.11
(1,3849)	1:A:467:LYS:H	1:A:467:LYS:HE2	17	0.11
(1,3849)	1:A:467:LYS:H	1:A:467:LYS:HE3	17	0.11
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB1	9	0.11
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB2	9	0.11
(1,370)	1:A:129:SER:H	1:A:142:ALA:HB3	9	0.11
(1,369)	1:A:126:ARG:HG3	1:A:129:SER:H	8	0.11
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB2	10	0.11
(1,3459)	1:A:76:LEU:HD11	1:A:81:SER:HB3	10	0.11
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB2	10	0.11
(1,3459)	1:A:76:LEU:HD12	1:A:81:SER:HB3	10	0.11
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB2	10	0.11
(1,3459)	1:A:76:LEU:HD13	1:A:81:SER:HB3	10	0.11
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB2	10	0.11
(1,3459)	1:A:76:LEU:HD21	1:A:81:SER:HB3	10	0.11
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB2	10	0.11
(1,3459)	1:A:76:LEU:HD22	1:A:81:SER:HB3	10	0.11
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB2	10	0.11
(1,3459)	1:A:76:LEU:HD23	1:A:81:SER:HB3	10	0.11
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD11	10	0.11
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD12	10	0.11
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD13	10	0.11
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD21	10	0.11
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD22	10	0.11
(1,3422)	1:A:71:LEU:HA	1:A:71:LEU:HD23	10	0.11
(1,2959)	1:A:90:LYS:HD2	1:A:91:VAL:HA	19	0.11
(1,2959)	1:A:90:LYS:HD3	1:A:91:VAL:HA	19	0.11
(1,2933)	1:A:473:SER:HB2	1:A:474:VAL:HB	6	0.11
(1,2933)	1:A:473:SER:HB3	1:A:474:VAL:HB	6	0.11
(1,289)	1:A:135:ILE:H	1:A:139:GLN:HB3	8	0.11
(1,289)	1:A:135:ILE:H	1:A:139:GLN:HB3	15	0.11
(1,2795)	1:A:89:PHE:HB2	1:A:90:LYS:HA	16	0.11
(1,2494)	1:A:112:ILE:HD11	1:A:461:LYS:HE2	4	0.11
(1,2494)	1:A:112:ILE:HD11	1:A:461:LYS:HE3	4	0.11
(1,2494)	1:A:112:ILE:HD12	1:A:461:LYS:HE2	4	0.11
(1,2494)	1:A:112:ILE:HD12	1:A:461:LYS:HE3	4	0.11
(1,2494)	1:A:112:ILE:HD13	1:A:461:LYS:HE2	4	0.11
(1,2494)	1:A:112:ILE:HD13	1:A:461:LYS:HE3	4	0.11
(1,2456)	1:A:47:GLU:HA	1:A:50:ASP:HB2	3	0.11
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB2	9	0.11
(1,2378)	1:A:83:GLN:HG2	1:A:86:LEU:HB3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB2	9	0.11
(1,2378)	1:A:83:GLN:HG3	1:A:86:LEU:HB3	9	0.11
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD11	20	0.11
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD12	20	0.11
(1,2184)	1:A:85:LEU:HA	1:A:85:LEU:HD13	20	0.11
(1,2100)	1:A:76:LEU:HD11	1:A:80:ASP:HB2	9	0.11
(1,2100)	1:A:76:LEU:HD11	1:A:80:ASP:HB3	9	0.11
(1,2100)	1:A:76:LEU:HD12	1:A:80:ASP:HB2	9	0.11
(1,2100)	1:A:76:LEU:HD12	1:A:80:ASP:HB3	9	0.11
(1,2100)	1:A:76:LEU:HD13	1:A:80:ASP:HB2	9	0.11
(1,2100)	1:A:76:LEU:HD13	1:A:80:ASP:HB3	9	0.11
(1,166)	1:A:66:SER:H	1:A:69:LEU:HG	13	0.11
(1,1637)	1:A:64:GLU:H	1:A:68:PHE:HA	19	0.11
(1,162)	1:A:112:ILE:H	1:A:113:GLY:HA3	11	0.11
(1,1610)	1:A:57:VAL:H	1:A:67:GLU:H	9	0.11
(1,1610)	1:A:57:VAL:H	1:A:67:GLU:H	14	0.11
(1,1370)	1:A:71:LEU:HB3	1:A:74:ARG:H	10	0.11
(1,129)	1:A:98:GLY:H	1:A:99:LEU:HB2	3	0.11
(1,129)	1:A:98:GLY:H	1:A:99:LEU:HB2	8	0.11
(1,1177)	1:A:470:ARG:HE	1:A:471:MET:HA	17	0.11
(1,1081)	1:A:144:LEU:HA	1:A:459:ARG:HE	1	0.11
(1,1081)	1:A:144:LEU:HA	1:A:459:ARG:HE	11	0.11

10 Dihedral-angle violation analysis

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