Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2MJE
BMRB ID	:	19718
Title	:	Reduced Yeast Adrenodoxin Homolog 1
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Deposited on	:	2014-01-07

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 (i) 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 (i)) were used in the production of this report:

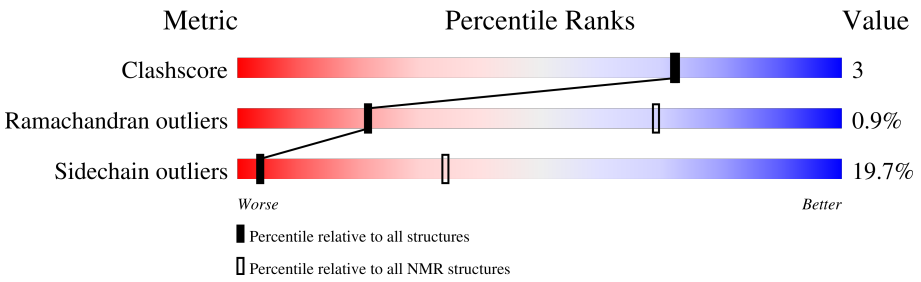
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 65%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	115	55% 17% • 25%

2 Ensemble composition and analysis (i)

This entry contains 19 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:4-A:37, A:51-A:102 (86)	0.61	10

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

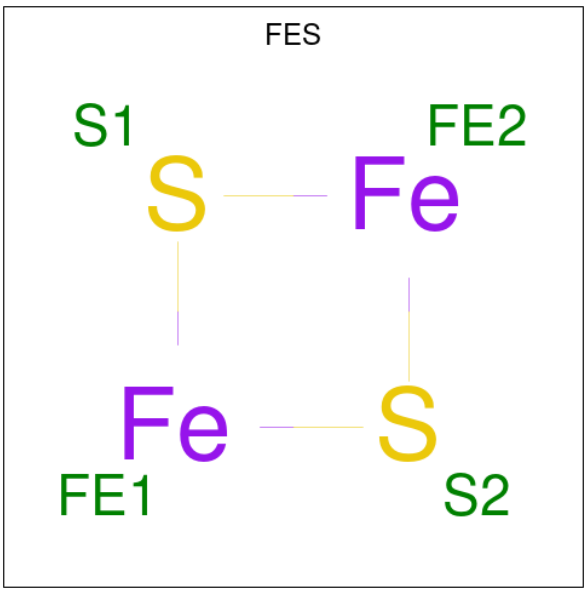
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1707 atoms, of which 826 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adrenodoxin homolog, mitochondrial.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	115	1703	535	826	143	189	10	0

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms		
			Total	Fe	S
2	A	1	4	2	2

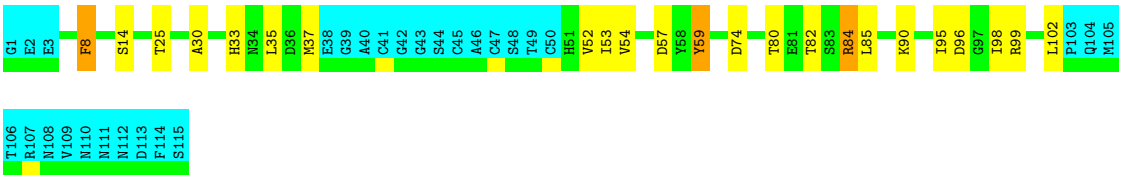
4 Residue-property plots (i)

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: Adrenodoxin homolog, mitochondrial

Chain A: 55% 17% • 25%



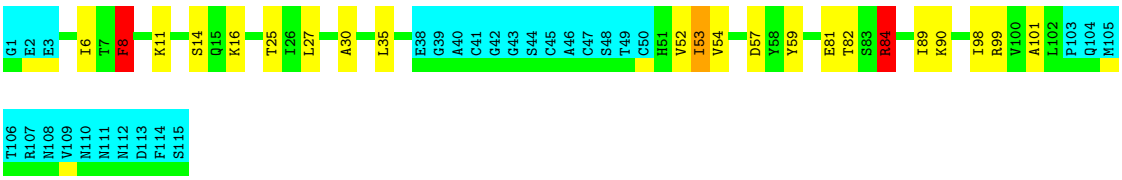
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Adrenodoxin homolog, mitochondrial

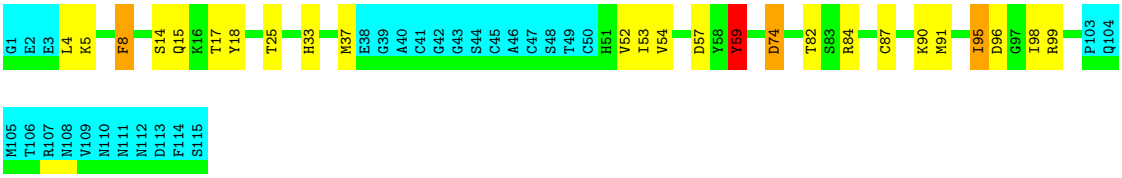
Chain A: 56% 17% •• 25%



4.2.2 Score per residue for model 2

• Molecule 1: Adrenodoxin homolog, mitochondrial

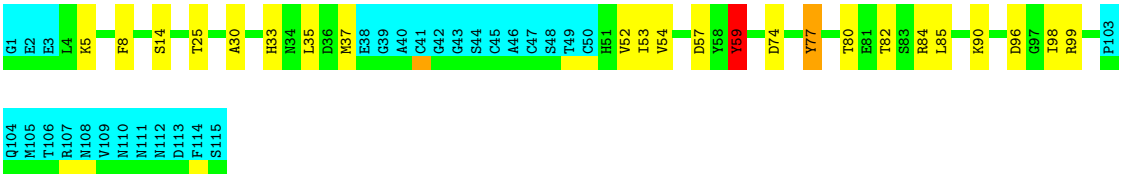
Chain A: 53% 18% •• 25%



4.2.3 Score per residue for model 3

- Molecule 1: Adrenodoxin homolog, mitochondrial

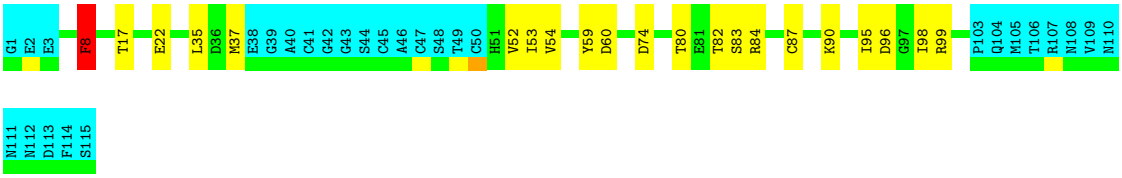
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Adrenodoxin homolog, mitochondrial

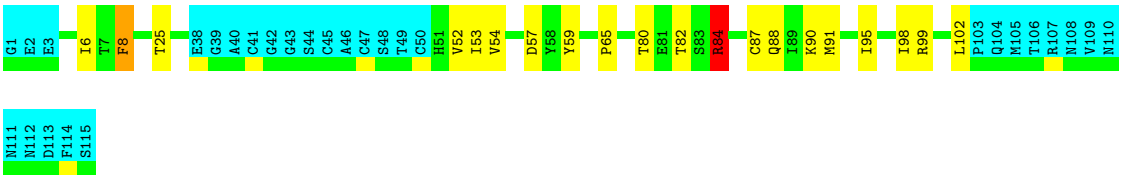
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 54% 18% • 25%

G1 E2 E3 F8 K11 S14 A30 L35 D36 M37 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 D57 Y58 Y59 L62 D74 T80 E81 T82 S83 R84 L85 G86 C87 K90 D96 G97 I98 R99 L102 P103 Q104

M105 T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.7 Score per residue for model 7

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 54% 18% • • 25%

G1 E2 E3 L4 K5 F8 S14 T25 T26 L27 H33 N34 L35 D36 M37 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 D57 Y58 Y59 D74 T80 E81 T82 S83 R84 L85 K90 I95 D96 G97 I98 R99 L102 P103

Q104 M105 T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.8 Score per residue for model 8

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 56% 17% • 25%

G1 E2 E3 F8 S14 Q15 K16 T25 H33 N34 L35 D36 M37 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 Y59 P65 D74 Y77 G78 L79 T82 S83 R84 L85 K90 D94 I98 R99 P103 Q104 M105

T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.9 Score per residue for model 9

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 55% 20% 25%

G1 E2 E3 F8 K11 S14 E19 T25 T26 L27 H33 M37 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 D57 Y58 Y59 D74 L79 T80 E81 T82 S83 R84 L85 K90 I98 R99 P103 Q104 M105 T106

R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 53% 20% • 25%

G1 E2 E3 I6 T7 F8 I9 L10 K11 S14 T25 T26 L27 A30 H33 N34 L35 D36 M37 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 D57 Y58 Y59 T80 E81 T82 S83 R84 L85 G86 K90 I95 I98 R99

V100 A101 L102 P103 Q104 M105 T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.11 Score per residue for model 11

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 53% 19% • 25%

G1 E2 E3 F8 S14 T17 T25 A30 H33 N34 L35 D36 M37 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 D55 Y59 D60 D71 T80 E81 T82 S83 R84 C87 Q88 I89 K90 D96 G97 I98 R99 L102

P103 Q104 M105 T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.12 Score per residue for model 12

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 55% 18% • 25%

G1 E2 E3 F8 K16 T25 Q31 G32 H33 N34 L35 D36 M37 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 D57 Y58 Y59 D74 T80 E81 T82 S83 R84 K90 I95 D96 G97 I98 R99 L102 P103 Q104 M105 T106

R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.13 Score per residue for model 13

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 55% 17% • • 25%

G1 E2 E3 L4 K5 F8 S14 T25 A30 H33 N34 L35 D36 M37 E38 G39 A40 C41 C42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 D57 Y58 Y59 T80 E81 T82 S83 R84 L85 K90 M91 I95 I98 R99 L102 P103 Q104 M105

T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.14 Score per residue for model 14

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 54% 18% • 25%

G1 E2 E3 F8 K11 S14 Y18 T25 A30 H33 N34 L35 D36 M37 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 D57 Y58 Y59 T80 E81 T82 S83 R84 L85 G86 C87 K90 D96 G97 I98 R99 L102

P103 Q104 M105 T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.15 Score per residue for model 15

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 54% 18% • 25%

G1 E2 E3 I6 T7 F8 S14 T25 A30 H33 N34 L35 D36 M37 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 Y59 L62 D74 T80 E81 T82 S83 R84 L85 K90 I95 D96 G97 I98 R99 L102 P103

Q104 M105 T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.16 Score per residue for model 16

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 52% 19% • • 25%

G1 E2 E3 I6 T7 F8 S14 T17 T25 I26 L27 A30 Q31 G32 H33 N34 L35 E38 G39 A40 C41 G42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 Y59 D74 T80 E81 T82 S83 R84 L85 Q88 I89 K90 M91 I95 D96 G97

I98 R99 P103 Q104 M105 T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.17 Score per residue for model 17

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A: 53% 19% • 25%

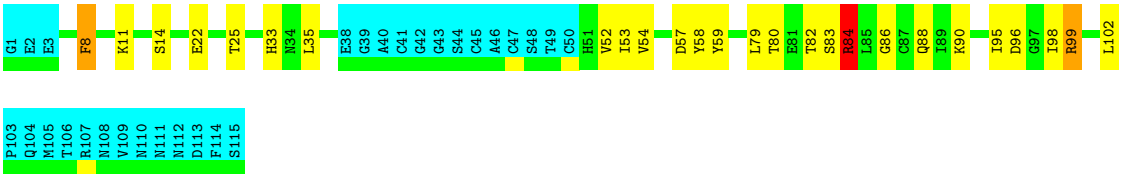
G1 E2 E3 I6 T7 F8 K11 S14 T25 A30 L35 D36 M37 E38 G39 A40 C41 C42 G43 S44 C45 A46 C47 S48 T49 C50 H51 V52 I53 V54 D57 Y58 Y59 L62 D74 T80 E81 T82 S83 K90 M91 I95 D96 G97 I98 R99 V100 A101

L102 P103 Q104 M105 T106 R107 N108 V109 N110 N111 N112 D113 F114 S115

4.2.18 Score per residue for model 18

- Molecule 1: Adrenodoxin homolog, mitochondrial

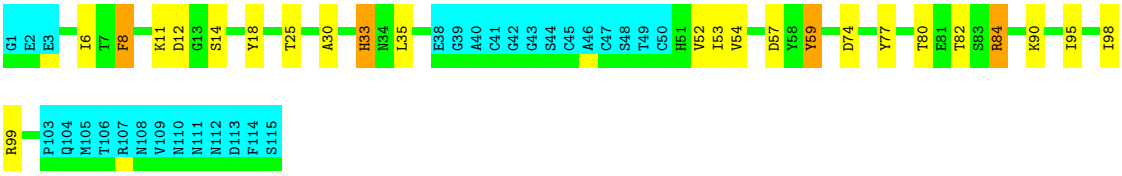
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Adrenodoxin homolog, mitochondrial

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 19 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**
CYANA	structure solution	CYANA-2.1
Amber	refinement	AMBER 11

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	792
Number of shifts mapped to atoms	792
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	65%

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: FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.67±0.01	0±0/684 (0.0± 0.0%)	1.18±0.02	3±1/928 (0.3± 0.1%)
All	All	0.67	0/12996 (0.0%)	1.18	55/17632 (0.3%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.6±1.0
All	All	0	30

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	84	ARG	NE-CZ-NH1	8.65	124.62	120.30	2	13
1	A	99	ARG	NE-CZ-NH1	8.58	124.59	120.30	15	19
1	A	84	ARG	NE-CZ-NH2	6.27	123.44	120.30	9	2
1	A	59	TYR	CB-CA-C	-6.15	98.10	110.40	11	14
1	A	8	PHE	CB-CG-CD1	-5.59	116.89	120.80	5	2
1	A	58	TYR	CB-CG-CD1	-5.49	117.71	121.00	18	1
1	A	77	TYR	CB-CG-CD1	-5.14	117.92	121.00	3	1
1	A	99	ARG	NE-CZ-NH2	-5.01	117.80	120.30	18	1
1	A	55	ASP	N-CA-CB	-5.01	101.59	110.60	11	1
1	A	54	VAL	CG1-CB-CG2	-5.00	102.89	110.90	11	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	84	ARG	Sidechain,Peptide	7
1	A	16	LYS	Peptide	3
1	A	77	TYR	Sidechain	3
1	A	59	TYR	Peptide,Sidechain	3
1	A	8	PHE	Sidechain	2
1	A	102	LEU	Peptide	2
1	A	101	ALA	Peptide	2
1	A	83	SER	Peptide	1
1	A	85	LEU	Peptide	1
1	A	79	LEU	Peptide	1
1	A	36	ASP	Peptide	1
1	A	88	GLN	Peptide	1
1	A	99	ARG	Sidechain	1

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	674	655	655	5±2
All	All	12882	12445	12445	87

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ALA:HA	1:A:35:LEU:HD12	0.54	1.77	17	11
1:A:54:VAL:HG11	1:A:59:TYR:CD1	0.53	2.39	16	8
1:A:8:PHE:CG	1:A:35:LEU:HD11	0.52	2.40	17	10
1:A:54:VAL:HG12	1:A:82:THR:HB	0.51	1.82	3	19
1:A:54:VAL:HG11	1:A:59:TYR:CG	0.50	2.42	16	1
1:A:85:LEU:H	1:A:85:LEU:HD23	0.50	1.66	14	3
1:A:59:TYR:CE1	1:A:84:ARG:HD3	0.50	2.41	7	1
1:A:84:ARG:HA	1:A:84:ARG:HE	0.49	1.68	18	1
1:A:8:PHE:CD1	1:A:35:LEU:HD11	0.47	2.45	14	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:TYR:CD2	1:A:33:HIS:CD2	0.47	3.03	19	2
1:A:79:LEU:HD21	1:A:83:SER:HB3	0.46	1.87	9	2
1:A:59:TYR:CE1	1:A:84:ARG:CD	0.46	2.99	7	1
1:A:18:TYR:CE2	1:A:33:HIS:CD2	0.45	3.04	2	1
1:A:91:MET:SD	1:A:95:ILE:HD13	0.45	2.52	2	3
1:A:62:LEU:HD11	1:A:84:ARG:HH11	0.45	1.72	15	2
1:A:62:LEU:CD1	1:A:84:ARG:HH11	0.43	2.26	6	1
1:A:6:ILE:CD1	1:A:8:PHE:CE2	0.42	3.02	17	4
1:A:91:MET:HA	1:A:95:ILE:HD11	0.42	1.89	5	1
1:A:6:ILE:HG12	1:A:8:PHE:CZ	0.41	2.51	5	3
1:A:53:ILE:HG23	1:A:101:ALA:HB3	0.41	1.93	1	1
1:A:4:LEU:HB3	1:A:95:ILE:HD11	0.41	1.91	2	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	86/115 (75%)	82±1 (95±2%)	4±1 (4±1%)	1±1 (1±1%)	21	69
All	All	1634/2185 (75%)	1549 (95%)	70 (4%)	15 (1%)	21	69

All 3 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	96	ASP	12
1	A	74	ASP	2
1	A	87	CYS	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	76/99 (77%)	61±2 (80±2%)	15±2 (20±2%)	4 34
All	All	1444/1881 (77%)	1160 (80%)	284 (20%)	4 34

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	52	VAL	19
1	A	53	ILE	19
1	A	90	LYS	19
1	A	98	ILE	19
1	A	8	PHE	18
1	A	25	THR	17
1	A	14	SER	16
1	A	80	THR	16
1	A	57	ASP	14
1	A	37	MET	14
1	A	33	HIS	13
1	A	74	ASP	11
1	A	95	ILE	11
1	A	102	LEU	9
1	A	11	LYS	8
1	A	59	TYR	7
1	A	84	ARG	6
1	A	85	LEU	6
1	A	27	LEU	5
1	A	87	CYS	5
1	A	5	LYS	4
1	A	17	THR	4
1	A	88	GLN	3
1	A	22	GLU	2
1	A	60	ASP	2
1	A	65	PRO	2
1	A	83	SER	2
1	A	31	GLN	2
1	A	81	GLU	1
1	A	89	ILE	1
1	A	15	GLN	1
1	A	79	LEU	1
1	A	94	ASP	1
1	A	19	GLU	1
1	A	9	ILE	1
1	A	71	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	91	MET	1
1	A	62	LEU	1
1	A	12	ASP	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	FES	A	201	1	0,4,4	0.00±0.00	-

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	FES	A	201	1	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	A	201	1	-	-	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 65% for the well-defined parts and 54% 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	792
Number of shifts mapped to atoms	792
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	88	0.16 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	83	0.17 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	79	0.15 ± 0.14	None needed (< 0.5 ppm)
^{15}N	79	0.58 ± 0.39	None needed (imprecise)

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 65%, i.e. 746 atoms were assigned a chemical shift out of a possible 1145. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	385/430 (90%)	156/175 (89%)	155/172 (90%)	74/83 (89%)
Sidechain	361/655 (55%)	186/425 (44%)	171/214 (80%)	4/16 (25%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/60 (0%)	0/29 (0%)	0/29 (0%)	0/2 (0%)
Overall	746/1145 (65%)	342/629 (54%)	326/415 (79%)	78/101 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 54%, i.e. 792 atoms were assigned a chemical shift out of a possible 1456. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	414/577 (72%)	168/236 (71%)	167/230 (73%)	79/111 (71%)
Sidechain	378/809 (47%)	194/522 (37%)	180/263 (68%)	4/24 (17%)
Aromatic	0/70 (0%)	0/34 (0%)	0/34 (0%)	0/2 (0%)
Overall	792/1456 (54%)	362/792 (46%)	347/527 (66%)	83/137 (61%)

7.1.4 Statistically unusual chemical shifts (i)

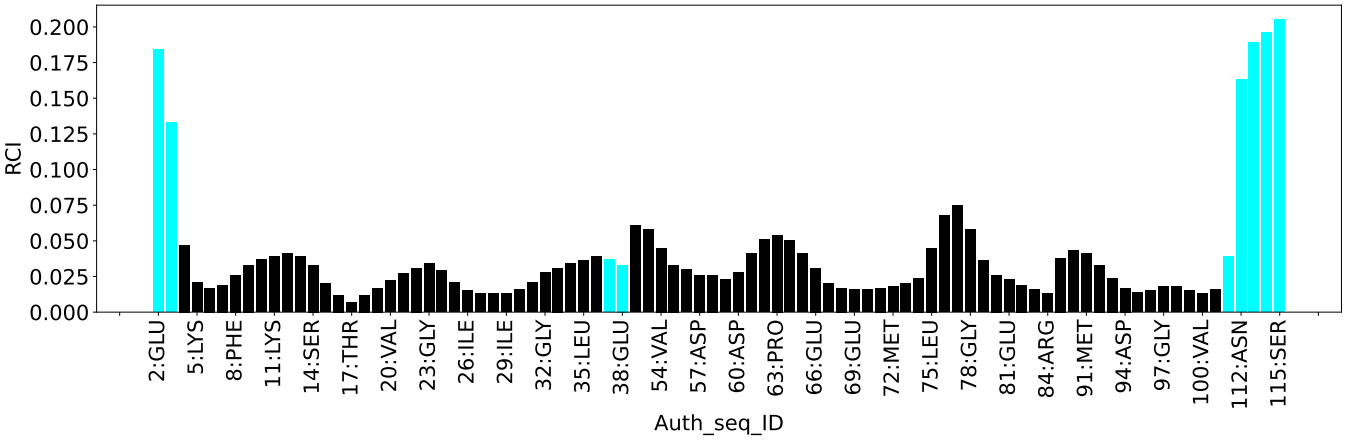
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	17	THR	N	0.00	91.89 – 138.78	-24.6

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:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
2:GLU
5:LYS
8:PHE
11:LYS
14:SER
17:THR
20:VAL
23:GLY
26:ILE
29:ILE
32:GLY
35:LEU
38:GLU
54:VAL
57:ASP
60:ASP
63:PRO
66:GLU
69:GLU
72:MET
75:LEU
78:GLY
81:GLU
84:ARG
91:MET
94:ASP
97:GLY
100:VAL
112:ASN
115:SER
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1360
Intra-residue (|i-j|=0)	253
Sequential (|i-j|=1)	403
Medium range (|i-j|>1 and |i-j|<5)	256
Long range (|i-j|≥5)	448
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	11.8
Number of long range restraints per residue[1]	3.9

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	16.2	0.2
0.2-0.5 (Medium)	2.8	0.48
>0.5 (Large)	1.8	1.57

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 (i)

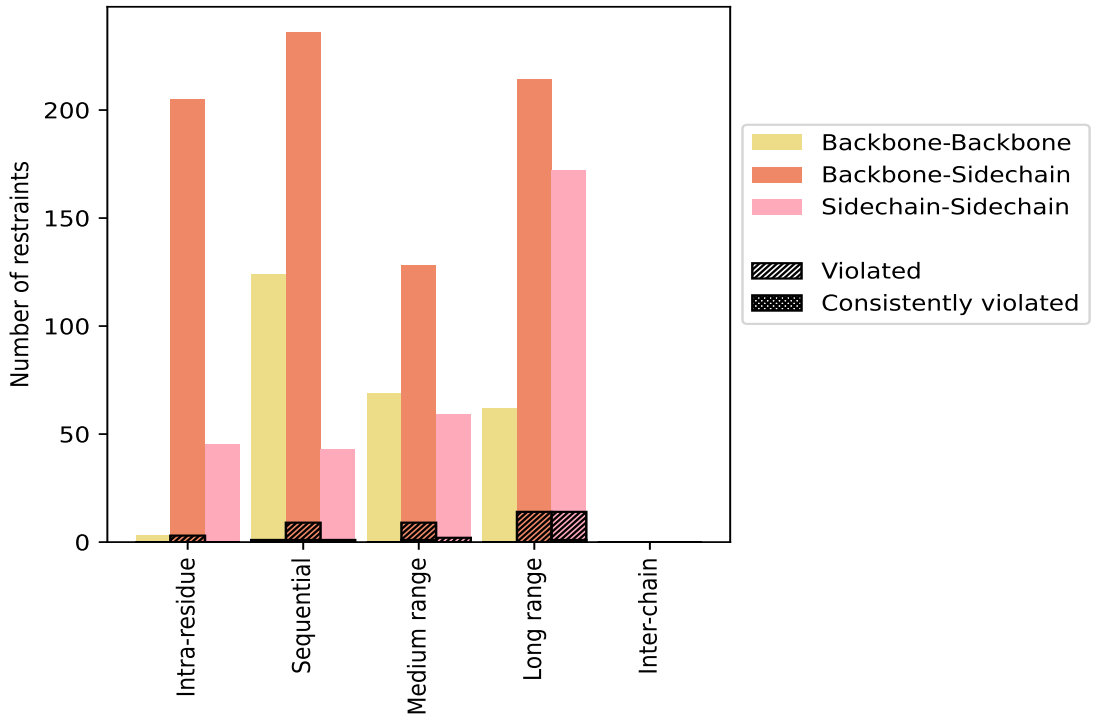
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	253	18.6	3	1.2	0.2	0	0.0	0.0
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	205	15.1	3	1.5	0.2	0	0.0	0.0
Sidechain-Sidechain	45	3.3	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	403	29.6	11	2.7	0.8	1	0.2	0.1
Backbone-Backbone	124	9.1	1	0.8	0.1	0	0.0	0.0
Backbone-Sidechain	236	17.4	9	3.8	0.7	1	0.4	0.1
Sidechain-Sidechain	43	3.2	1	2.3	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	256	18.8	11	4.3	0.8	1	0.4	0.1
Backbone-Backbone	69	5.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	128	9.4	9	7.0	0.7	1	0.8	0.1
Sidechain-Sidechain	59	4.3	2	3.4	0.1	0	0.0	0.0
Long range (|i-j|≥5)	448	32.9	28	6.2	2.1	1	0.2	0.1
Backbone-Backbone	62	4.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	214	15.7	14	6.5	1.0	0	0.0	0.0
Sidechain-Sidechain	172	12.6	14	8.1	1.0	1	0.6	0.1
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	1360	100.0	53	3.9	3.9	3	0.2	0.2
Backbone-Backbone	258	19.0	1	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	783	57.6	35	4.5	2.6	2	0.3	0.1
Sidechain-Sidechain	319	23.5	17	5.3	1.2	1	0.3	0.1

[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	4	5	7	0	17	0.16	0.39	0.07	0.14
2	0	5	4	11	0	20	0.33	1.57	0.43	0.14
3	1	3	7	13	0	24	0.25	1.18	0.28	0.14
4	1	4	3	13	0	21	0.37	1.26	0.42	0.14
5	1	4	5	12	0	22	0.27	1.03	0.28	0.16
6	1	5	5	9	0	20	0.16	0.42	0.07	0.15
7	0	4	6	10	0	20	0.17	0.66	0.12	0.14
8	2	4	4	8	0	18	0.22	1.05	0.22	0.14
9	1	5	5	8	0	19	0.15	0.33	0.05	0.15
10	2	7	6	9	0	24	0.24	1.16	0.28	0.16
11	1	4	3	11	0	19	0.17	0.54	0.09	0.16

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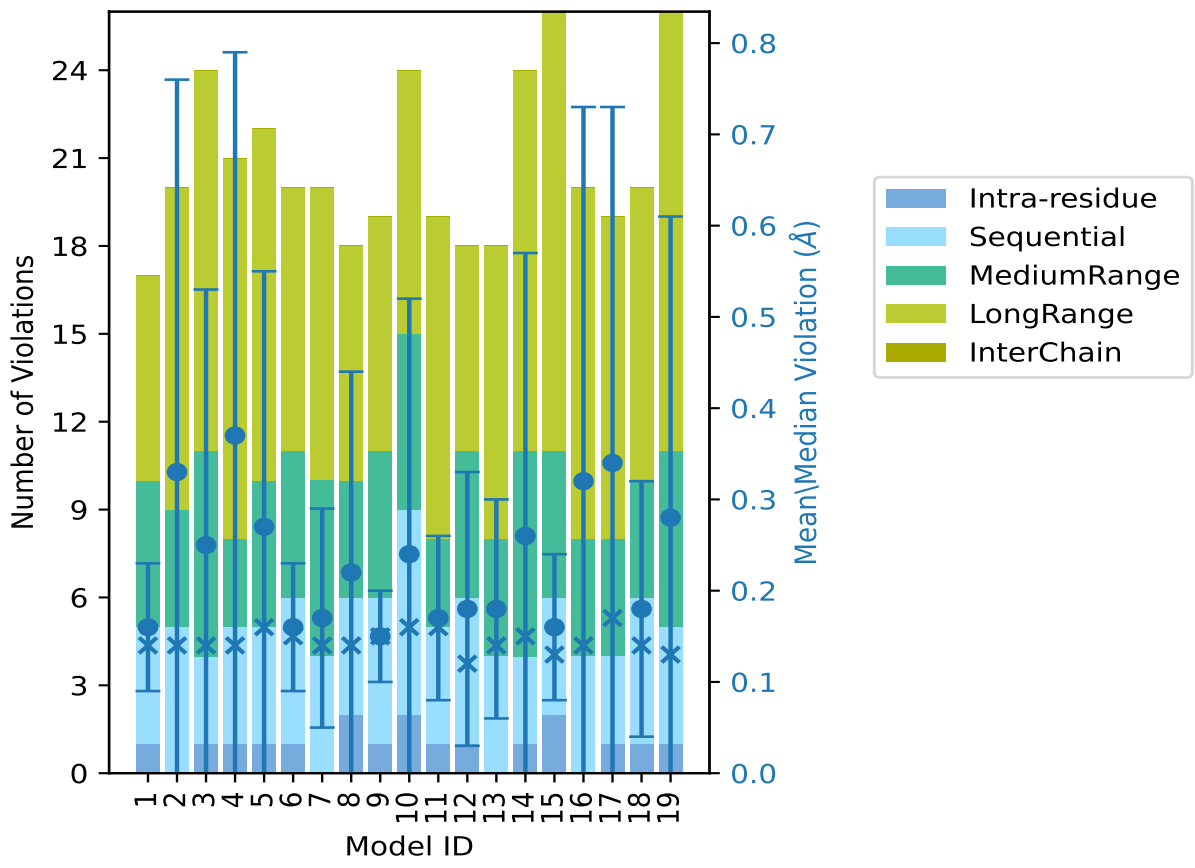
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	5	5	7	0	18	0.18	0.76	0.15	0.12
13	0	4	4	10	0	18	0.18	0.62	0.12	0.14
14	1	3	7	13	0	24	0.26	1.24	0.31	0.15
15	2	4	5	15	0	26	0.16	0.43	0.08	0.13
16	0	4	4	12	0	20	0.32	1.46	0.41	0.14
17	1	3	4	11	0	19	0.34	1.45	0.39	0.17
18	1	5	4	10	0	20	0.18	0.76	0.14	0.14
19	1	4	6	15	0	26	0.28	1.36	0.33	0.13

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

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

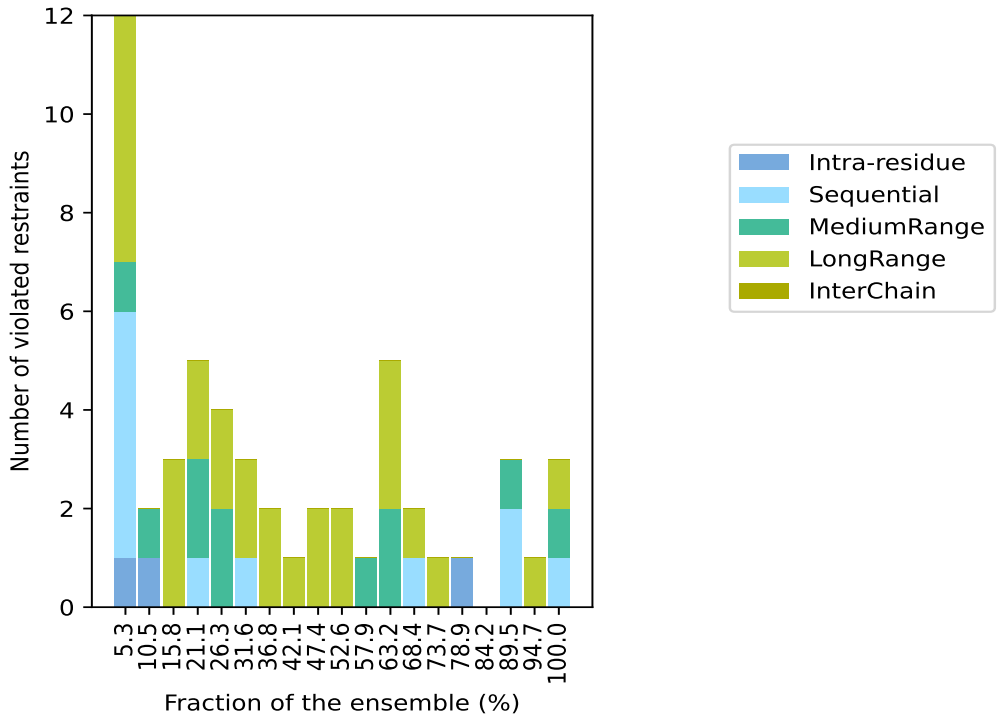
9.3 Distance violation statistics for the ensemble (i)

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, 1307(IR:250, SQ:392, MR:245, LR:420, 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]	%
1	5	1	5	0	12	1	5.3
1	0	1	0	0	2	2	10.5
0	0	0	3	0	3	3	15.8
0	1	2	2	0	5	4	21.1
0	0	2	2	0	4	5	26.3
0	1	0	2	0	3	6	31.6
0	0	0	2	0	2	7	36.8
0	0	0	1	0	1	8	42.1
0	0	0	2	0	2	9	47.4
0	0	0	2	0	2	10	52.6
0	0	1	0	0	1	11	57.9
0	0	2	3	0	5	12	63.2
0	1	0	1	0	2	13	68.4
0	0	0	1	0	1	14	73.7
1	0	0	0	0	1	15	78.9
0	0	0	0	0	0	16	84.2
0	2	1	0	0	3	17	89.5
0	0	0	1	0	1	18	94.7
0	1	1	1	0	3	19	100.0

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

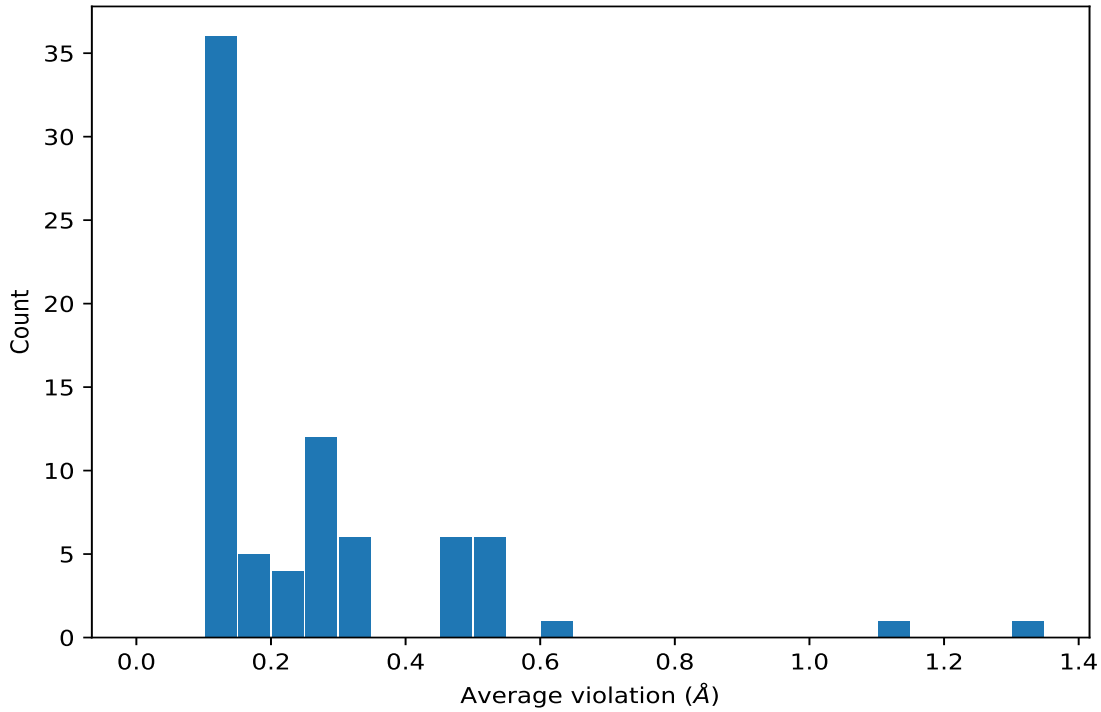
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	19	0.22	0.01	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	19	0.22	0.01	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	19	0.22	0.01	0.22
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	19	0.21	0.03	0.21
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	19	0.15	0.02	0.15
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	18	0.14	0.02	0.14
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	17	0.16	0.02	0.16
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	17	0.15	0.02	0.15
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	17	0.14	0.01	0.14
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	15	0.16	0.02	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	15	0.16	0.02	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	15	0.16	0.02	0.16
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	14	0.18	0.03	0.18
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	13	0.33	0.26	0.23
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	13	0.33	0.26	0.23
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	13	0.33	0.26	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	13	0.33	0.26	0.23
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	13	0.33	0.26	0.23
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	13	0.33	0.26	0.23
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	13	0.13	0.01	0.13
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	12	0.49	0.27	0.4
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	12	0.49	0.27	0.4
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	12	0.49	0.27	0.4
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	12	0.49	0.27	0.4
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	12	0.49	0.27	0.4
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	12	0.49	0.27	0.4
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	12	0.14	0.02	0.14
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	12	0.13	0.02	0.12
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	12	0.12	0.01	0.12
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	12	0.12	0.01	0.12
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	12	0.11	0.01	0.11
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	11	0.12	0.01	0.12
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	10	1.14	0.36	1.25
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	10	0.12	0.01	0.11
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	9	1.3	0.16	1.26
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	9	0.63	0.2	0.7
(1,1080)	1:A:73:LEU:HD11	1:A:83:SER:HB2	8	0.52	0.26	0.51
(1,1080)	1:A:73:LEU:HD12	1:A:83:SER:HB2	8	0.52	0.26	0.51
(1,1080)	1:A:73:LEU:HD13	1:A:83:SER:HB2	8	0.52	0.26	0.51
(1,1080)	1:A:73:LEU:HD21	1:A:83:SER:HB2	8	0.52	0.26	0.51
(1,1080)	1:A:73:LEU:HD22	1:A:83:SER:HB2	8	0.52	0.26	0.51
(1,1080)	1:A:73:LEU:HD23	1:A:83:SER:HB2	8	0.52	0.26	0.51
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD11	7	0.28	0.09	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD12	7	0.28	0.09	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD13	7	0.28	0.09	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD21	7	0.28	0.09	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD22	7	0.28	0.09	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD23	7	0.28	0.09	0.26
(1,905)	1:A:59:TYR:HD1	1:A:82:THR:HB	7	0.12	0.01	0.12
(1,905)	1:A:59:TYR:HD2	1:A:82:THR:HB	7	0.12	0.01	0.12
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD2	6	0.28	0.12	0.24
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD3	6	0.28	0.12	0.24
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD2	6	0.28	0.12	0.24
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD3	6	0.28	0.12	0.24
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD2	6	0.28	0.12	0.24
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD3	6	0.28	0.12	0.24
(1,1344)	1:A:101:ALA:HA	1:A:102:LEU:HB3	6	0.14	0.02	0.14
(1,318)	1:A:10:LEU:HG	1:A:15:GLN:H	6	0.12	0.01	0.12

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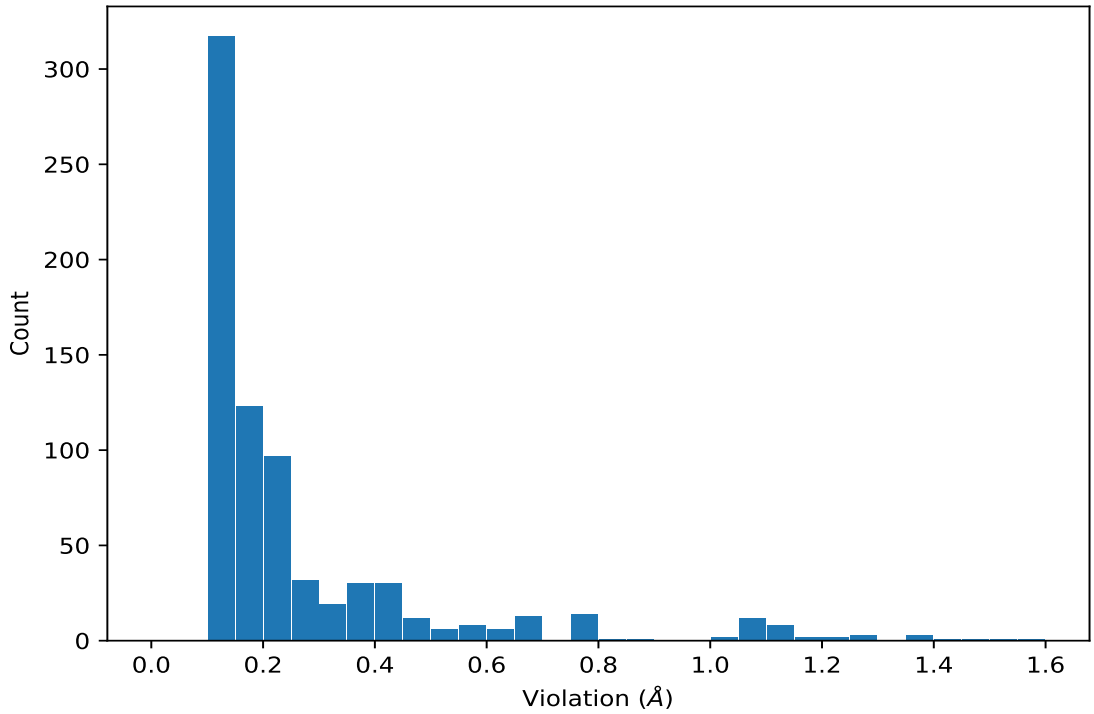
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,634)	1:A:31:GLN:HA	1:A:34:ASN:HD22	5	0.12	0.0	0.12
(1,377)	1:A:15:GLN:HB2	1:A:17:THR:H	5	0.12	0.0	0.12
(1,377)	1:A:15:GLN:HB3	1:A:17:THR:H	5	0.12	0.0	0.12
(1,93)	1:A:6:ILE:HG13	1:A:29:ILE:HB	5	0.11	0.0	0.11
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE1	5	0.11	0.01	0.11
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE2	5	0.11	0.01	0.11
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG21	4	0.13	0.01	0.13
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG22	4	0.13	0.01	0.13
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG23	4	0.13	0.01	0.13
(2,2)	2:A:201:FES:FE1	1:A:72:MET:CA	4	0.13	0.03	0.12
(1,796)	1:A:54:VAL:HB	1:A:83:SER:HA	4	0.12	0.01	0.12
(1,1303)	1:A:95:ILE:HG13	1:A:97:GLY:H	4	0.12	0.01	0.12
(1,691)	1:A:35:LEU:HB3	1:A:37:MET:HB2	4	0.11	0.0	0.11
(1,269)	1:A:9:ILE:HG12	1:A:101:ALA:HA	3	0.12	0.0	0.12
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG21	3	0.12	0.01	0.11
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG22	3	0.12	0.01	0.11
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG23	3	0.12	0.01	0.11
(2,5)	2:A:201:FES:FE1	1:A:25:THR:CA	3	0.11	0.0	0.11
(1,461)	1:A:22:GLU:H	1:A:22:GLU:HG3	2	0.12	0.0	0.12
(1,642)	1:A:31:GLN:HB3	1:A:33:HIS:H	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard 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)
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	2	1.57
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	2	1.5
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	16	1.46
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	17	1.45
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	16	1.39
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	17	1.36
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	19	1.36
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	4	1.26
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	4	1.26
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	19	1.25
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	14	1.24
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	14	1.24
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	3	1.18
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	10	1.16
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	10	1.15
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	4	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	4	1.12
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	4	1.12
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	4	1.12
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	4	1.12
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	4	1.12
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	3	1.1
(1,1080)	1:A:73:LEU:HD11	1:A:83:SER:HB2	4	1.09
(1,1080)	1:A:73:LEU:HD12	1:A:83:SER:HB2	4	1.09
(1,1080)	1:A:73:LEU:HD13	1:A:83:SER:HB2	4	1.09
(1,1080)	1:A:73:LEU:HD21	1:A:83:SER:HB2	4	1.09
(1,1080)	1:A:73:LEU:HD22	1:A:83:SER:HB2	4	1.09
(1,1080)	1:A:73:LEU:HD23	1:A:83:SER:HB2	4	1.09
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	8	1.05
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	8	1.05
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	8	1.05
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	8	1.05
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	8	1.05
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	8	1.05
(1,311)	1:A:10:LEU:HB2	1:A:15:GLN:HE22	5	1.03
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	5	1.01
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	16	0.87
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	2	0.84
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	12	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	12	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	12	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	12	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	12	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	12	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	18	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	18	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	18	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	18	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	18	0.76
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	18	0.76
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	17	0.75
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	19	0.75
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	4	0.7
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	5	0.67
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	5	0.67
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	5	0.67
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	5	0.67
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	5	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	5	0.67
(1,1080)	1:A:73:LEU:HD11	1:A:83:SER:HB2	7	0.66
(1,1080)	1:A:73:LEU:HD12	1:A:83:SER:HB2	7	0.66
(1,1080)	1:A:73:LEU:HD13	1:A:83:SER:HB2	7	0.66
(1,1080)	1:A:73:LEU:HD21	1:A:83:SER:HB2	7	0.66
(1,1080)	1:A:73:LEU:HD22	1:A:83:SER:HB2	7	0.66
(1,1080)	1:A:73:LEU:HD23	1:A:83:SER:HB2	7	0.66
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	13	0.62
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	13	0.62
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	13	0.62
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	13	0.62
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	13	0.62
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	13	0.62
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	5	0.59
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	14	0.58
(1,1080)	1:A:73:LEU:HD11	1:A:83:SER:HB2	16	0.58
(1,1080)	1:A:73:LEU:HD12	1:A:83:SER:HB2	16	0.58
(1,1080)	1:A:73:LEU:HD13	1:A:83:SER:HB2	16	0.58
(1,1080)	1:A:73:LEU:HD21	1:A:83:SER:HB2	16	0.58
(1,1080)	1:A:73:LEU:HD22	1:A:83:SER:HB2	16	0.58
(1,1080)	1:A:73:LEU:HD23	1:A:83:SER:HB2	16	0.58
(1,1080)	1:A:73:LEU:HD11	1:A:83:SER:HB2	11	0.54
(1,1080)	1:A:73:LEU:HD12	1:A:83:SER:HB2	11	0.54
(1,1080)	1:A:73:LEU:HD13	1:A:83:SER:HB2	11	0.54
(1,1080)	1:A:73:LEU:HD21	1:A:83:SER:HB2	11	0.54
(1,1080)	1:A:73:LEU:HD22	1:A:83:SER:HB2	11	0.54
(1,1080)	1:A:73:LEU:HD23	1:A:83:SER:HB2	11	0.54
(1,1080)	1:A:73:LEU:HD11	1:A:83:SER:HB2	17	0.48
(1,1080)	1:A:73:LEU:HD12	1:A:83:SER:HB2	17	0.48
(1,1080)	1:A:73:LEU:HD13	1:A:83:SER:HB2	17	0.48
(1,1080)	1:A:73:LEU:HD21	1:A:83:SER:HB2	17	0.48
(1,1080)	1:A:73:LEU:HD22	1:A:83:SER:HB2	17	0.48
(1,1080)	1:A:73:LEU:HD23	1:A:83:SER:HB2	17	0.48
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	19	0.47
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	19	0.47
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	19	0.47
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	19	0.47
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	19	0.47
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	19	0.47
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD2	8	0.43
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD3	8	0.43
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD2	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD3	8	0.43
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD2	8	0.43
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD3	8	0.43
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD2	15	0.43
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD3	15	0.43
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD2	15	0.43
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD3	15	0.43
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD2	15	0.43
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD3	15	0.43
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	3	0.43
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	3	0.43
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	3	0.43
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	3	0.43
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	3	0.43
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	3	0.43
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	6	0.42
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	6	0.42
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	6	0.42
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	6	0.42
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	6	0.42
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	6	0.42
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	2	0.41
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	2	0.41
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	2	0.41
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	2	0.41
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	2	0.41
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	2	0.41
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	14	0.39
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	14	0.39
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	14	0.39
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	14	0.39
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	14	0.39
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	14	0.39
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD11	1	0.39
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD12	1	0.39
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD13	1	0.39
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD21	1	0.39
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD22	1	0.39
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD23	1	0.39
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD11	19	0.37
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD12	19	0.37
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD13	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD21	19	0.37
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD22	19	0.37
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD23	19	0.37
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	8	0.36
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	8	0.36
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	8	0.36
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	8	0.36
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	8	0.36
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	8	0.36
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD11	15	0.36
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD12	15	0.36
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD13	15	0.36
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD21	15	0.36
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD22	15	0.36
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD23	15	0.36
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	3	0.35
(1,1080)	1:A:73:LEU:HD11	1:A:83:SER:HB2	19	0.34
(1,1080)	1:A:73:LEU:HD12	1:A:83:SER:HB2	19	0.34
(1,1080)	1:A:73:LEU:HD13	1:A:83:SER:HB2	19	0.34
(1,1080)	1:A:73:LEU:HD21	1:A:83:SER:HB2	19	0.34
(1,1080)	1:A:73:LEU:HD22	1:A:83:SER:HB2	19	0.34
(1,1080)	1:A:73:LEU:HD23	1:A:83:SER:HB2	19	0.34
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	9	0.33
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	9	0.33
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	9	0.33
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	9	0.33
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	9	0.33
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	9	0.33
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	17	0.32
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	17	0.32
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	17	0.32
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	17	0.32
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	17	0.32
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	17	0.32
(1,1080)	1:A:73:LEU:HD11	1:A:83:SER:HB2	15	0.3
(1,1080)	1:A:73:LEU:HD12	1:A:83:SER:HB2	15	0.3
(1,1080)	1:A:73:LEU:HD13	1:A:83:SER:HB2	15	0.3
(1,1080)	1:A:73:LEU:HD21	1:A:83:SER:HB2	15	0.3
(1,1080)	1:A:73:LEU:HD22	1:A:83:SER:HB2	15	0.3
(1,1080)	1:A:73:LEU:HD23	1:A:83:SER:HB2	15	0.3
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	18	0.28
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	19	0.27
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	19	0.27
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	19	0.27
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	19	0.27
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	19	0.27
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	5	0.27
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	5	0.27
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	5	0.27
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	5	0.27
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	5	0.27
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	5	0.27
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD2	10	0.26
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD3	10	0.26
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD2	10	0.26
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD3	10	0.26
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD2	10	0.26
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD3	10	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD11	13	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD12	13	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD13	13	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD21	13	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD22	13	0.26
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD23	13	0.26
(1,257)	1:A:9:ILE:HA	1:A:15:GLN:HE22	10	0.25
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	1	0.24
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	1	0.24
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	1	0.24
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	5	0.24
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	5	0.24
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	5	0.24
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	6	0.24
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	6	0.24
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	6	0.24
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	12	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	12	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	12	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	13	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	13	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	13	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	14	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	14	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	18	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	18	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	18	0.23
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	4	0.23
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	7	0.23
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	11	0.23
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	14	0.23
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	14	0.23
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	14	0.23
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	14	0.23
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	14	0.23
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	14	0.23
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD11	7	0.23
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD12	7	0.23
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD13	7	0.23
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD21	7	0.23
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD22	7	0.23
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD23	7	0.23
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	3	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	3	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	3	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	7	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	7	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	7	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	8	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	8	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	8	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	9	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	9	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	9	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	19	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	19	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	19	0.22
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	1	0.22
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	8	0.22
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	10	0.22
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	14	0.22
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	3	0.22
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	8	0.22
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD2	6	0.22
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD3	6	0.22
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD2	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD3	6	0.22
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD2	6	0.22
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD3	6	0.22
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	2	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	2	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	2	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	4	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	4	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	4	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	15	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	15	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	15	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	17	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	17	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	17	0.21
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	6	0.21
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	13	0.21
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	10	0.2
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	10	0.2
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	10	0.2
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	12	0.2
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	17	0.2
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	19	0.2
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	11	0.2
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	18	0.2
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD2	3	0.2
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD3	3	0.2
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD2	3	0.2
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD3	3	0.2
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD2	3	0.2
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD3	3	0.2
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	17	0.2
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	17	0.2
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	17	0.2
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	17	0.2
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	17	0.2
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	17	0.2
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	11	0.19
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	11	0.19
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	11	0.19
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD11	16	0.19
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD12	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:A:6:ILE:HG13	1:A:35:LEU:HD13	16	0.19
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	2	0.19
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	3	0.19
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	9	0.19
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	12	0.19
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	14	0.19
(1,1080)	1:A:73:LEU:HD11	1:A:83:SER:HB2	18	0.19
(1,1080)	1:A:73:LEU:HD12	1:A:83:SER:HB2	18	0.19
(1,1080)	1:A:73:LEU:HD13	1:A:83:SER:HB2	18	0.19
(1,1080)	1:A:73:LEU:HD21	1:A:83:SER:HB2	18	0.19
(1,1080)	1:A:73:LEU:HD22	1:A:83:SER:HB2	18	0.19
(1,1080)	1:A:73:LEU:HD23	1:A:83:SER:HB2	18	0.19
(2,2)	2:A:201:FES:FE1	1:A:72:MET:CA	11	0.18
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	5	0.18
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	16	0.18
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	6	0.18
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	15	0.18
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	5	0.18
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	5	0.18
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	5	0.18
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	5	0.18
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	13	0.18
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	19	0.18
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	9	0.18
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	9	0.18
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	9	0.18
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	9	0.18
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	9	0.18
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	9	0.18
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD11	11	0.18
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD12	11	0.18
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD13	11	0.18
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD21	11	0.18
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD22	11	0.18
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD23	11	0.18
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	11	0.18
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	17	0.17
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	1	0.17
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	6	0.17
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	12	0.17
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	15	0.17
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	5	0.17
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	10	0.17
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	14	0.17
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	3	0.17
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	3	0.17
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	3	0.17
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	8	0.17
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	8	0.17
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	8	0.17
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	18	0.17
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	18	0.17
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	18	0.17
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	4	0.17
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	11	0.17
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	17	0.17
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD11	6	0.17
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD12	6	0.17
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD13	6	0.17
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD21	6	0.17
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD22	6	0.17
(1,175)	1:A:8:PHE:H	1:A:102:LEU:HD23	6	0.17
(1,1344)	1:A:101:ALA:HA	1:A:102:LEU:HB3	10	0.17
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	2	0.17
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	18	0.16
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	1	0.16
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	2	0.16
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	3	0.16
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	5	0.16
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	6	0.16
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	11	0.16
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	19	0.16
(1,892)	1:A:59:TYR:HB2	1:A:60:ASP:HA	15	0.16
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	5	0.16
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	13	0.16
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	9	0.16
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	17	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	1	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	1	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	1	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	6	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	6	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	10	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	10	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	10	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	11	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	11	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	11	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	15	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	15	0.16
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	15	0.16
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	9	0.16
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	2	0.16
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	3	0.16
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	9	0.16
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	10	0.16
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	16	0.16
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	13	0.16
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	13	0.16
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	13	0.16
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	13	0.16
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	13	0.16
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	13	0.16
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	16	0.16
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	16	0.16
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	16	0.16
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	16	0.16
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	16	0.16
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	16	0.16
(1,1350)	1:A:113:ASP:HA	1:A:114:PHE:H	10	0.16
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	4	0.16
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	12	0.16
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	14	0.16
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	15	0.16
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	17	0.16
(1,1197)	1:A:84:ARG:HA	1:A:85:LEU:HB3	10	0.16
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	3	0.15
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	5	0.15
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	4	0.15
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	9	0.15
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	10	0.15
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	13	0.15
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	14	0.15
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	1	0.15
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	9	0.15
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	9	0.15
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	9	0.15
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	12	0.15
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	12	0.15
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	12	0.15
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	14	0.15
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	14	0.15
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	14	0.15
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	7	0.15
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	8	0.15
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	10	0.15
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	11	0.15
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	17	0.15
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	7	0.15
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	15	0.15
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	18	0.15
(1,1344)	1:A:101:ALA:HA	1:A:102:LEU:HB3	9	0.15
(1,1344)	1:A:101:ALA:HA	1:A:102:LEU:HB3	16	0.15
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	6	0.15
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	7	0.15
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	10	0.15
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	18	0.15
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	2	0.14
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	2	0.14
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	2	0.14
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	2	0.14
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	2	0.14
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	2	0.14
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	7	0.14
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	4	0.14
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	7	0.14
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	8	0.14
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	14	0.14
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	15	0.14
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	17	0.14
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	7	0.14
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	2	0.14
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	9	0.14
(1,796)	1:A:54:VAL:HB	1:A:83:SER:HA	5	0.14
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	17	0.14
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	17	0.14
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	1	0.14
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	16	0.14
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	19	0.14
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	18	0.14
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG21	6	0.14
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG22	6	0.14
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG23	6	0.14
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	13	0.14
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	15	0.14
(1,318)	1:A:10:LEU:HG	1:A:15:GLN:H	4	0.14
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	13	0.14
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	1	0.13
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	10	0.13
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	15	0.13
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	9	0.13
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	10	0.13
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	13	0.13
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	19	0.13
(1,905)	1:A:59:TYR:HD1	1:A:82:THR:HB	2	0.13
(1,905)	1:A:59:TYR:HD2	1:A:82:THR:HB	2	0.13
(1,905)	1:A:59:TYR:HD1	1:A:82:THR:HB	19	0.13
(1,905)	1:A:59:TYR:HD2	1:A:82:THR:HB	19	0.13
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	16	0.13
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	17	0.13
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	7	0.13
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	19	0.13
(1,796)	1:A:54:VAL:HB	1:A:83:SER:HA	3	0.13
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	7	0.13
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	8	0.13
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE1	4	0.13
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE2	4	0.13
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	11	0.13
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	14	0.13
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	17	0.13
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	4	0.13
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	4	0.13
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	4	0.13
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	6	0.13
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	12	0.13
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	18	0.13
(1,634)	1:A:31:GLN:HA	1:A:34:ASN:HD22	3	0.13
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG21	1	0.13
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG22	1	0.13
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG23	1	0.13
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG21	8	0.13
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG22	8	0.13
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG23	8	0.13
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	1	0.13
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	3	0.13
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	9	0.13
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	10	0.13
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	3	0.13
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	4	0.13
(1,320)	1:A:10:LEU:HG	1:A:15:GLN:HE22	18	0.13
(1,318)	1:A:10:LEU:HG	1:A:15:GLN:H	2	0.13
(1,269)	1:A:9:ILE:HG12	1:A:101:ALA:HA	18	0.13
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	6	0.13
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	6	0.13
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	15	0.13
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	15	0.13
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	19	0.13
(1,1303)	1:A:95:ILE:HG13	1:A:97:GLY:H	3	0.13
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG21	3	0.13
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG22	3	0.13
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG23	3	0.13
(2,6)	2:A:201:FES:FE2	1:A:25:THR:CA	13	0.12
(2,2)	2:A:201:FES:FE1	1:A:72:MET:CA	19	0.12
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD11	7	0.12
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD12	7	0.12
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD13	7	0.12
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD21	7	0.12
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD22	7	0.12
(1,979)	1:A:65:PRO:HB2	1:A:73:LEU:HD23	7	0.12
(1,93)	1:A:6:ILE:HG13	1:A:29:ILE:HB	3	0.12
(1,93)	1:A:6:ILE:HG13	1:A:29:ILE:HB	15	0.12
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	6	0.12
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	8	0.12
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	13	0.12
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	14	0.12
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	2	0.12
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	1:A:59:TYR:HD1	1:A:82:THR:HB	3	0.12
(1,905)	1:A:59:TYR:HD2	1:A:82:THR:HB	3	0.12
(1,905)	1:A:59:TYR:HD1	1:A:82:THR:HB	6	0.12
(1,905)	1:A:59:TYR:HD2	1:A:82:THR:HB	6	0.12
(1,905)	1:A:59:TYR:HD1	1:A:82:THR:HB	13	0.12
(1,905)	1:A:59:TYR:HD2	1:A:82:THR:HB	13	0.12
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	8	0.12
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	3	0.12
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	4	0.12
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	6	0.12
(1,796)	1:A:54:VAL:HB	1:A:83:SER:HA	14	0.12
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	16	0.12
(1,744)	1:A:53:ILE:HA	1:A:84:ARG:HB3	4	0.12
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD11	19	0.12
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD12	19	0.12
(1,739)	1:A:53:ILE:HA	1:A:53:ILE:HD13	19	0.12
(1,691)	1:A:35:LEU:HB3	1:A:37:MET:HB2	10	0.12
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	3	0.12
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	13	0.12
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	14	0.12
(1,634)	1:A:31:GLN:HA	1:A:34:ASN:HD22	2	0.12
(1,634)	1:A:31:GLN:HA	1:A:34:ASN:HD22	8	0.12
(1,634)	1:A:31:GLN:HA	1:A:34:ASN:HD22	12	0.12
(1,634)	1:A:31:GLN:HA	1:A:34:ASN:HD22	17	0.12
(1,461)	1:A:22:GLU:H	1:A:22:GLU:HG3	10	0.12
(1,461)	1:A:22:GLU:H	1:A:22:GLU:HG3	15	0.12
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	8	0.12
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG21	12	0.12
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG22	12	0.12
(1,387)	1:A:16:LYS:HA	1:A:17:THR:HG23	12	0.12
(1,377)	1:A:15:GLN:HB2	1:A:17:THR:H	1	0.12
(1,377)	1:A:15:GLN:HB3	1:A:17:THR:H	1	0.12
(1,377)	1:A:15:GLN:HB2	1:A:17:THR:H	6	0.12
(1,377)	1:A:15:GLN:HB3	1:A:17:THR:H	6	0.12
(1,377)	1:A:15:GLN:HB2	1:A:17:THR:H	12	0.12
(1,377)	1:A:15:GLN:HB3	1:A:17:THR:H	12	0.12
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	6	0.12
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	7	0.12
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	8	0.12
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	11	0.12
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	12	0.12
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	15	0.12
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	18	0.12
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	19	0.12
(1,318)	1:A:10:LEU:HG	1:A:15:GLN:H	10	0.12
(1,318)	1:A:10:LEU:HG	1:A:15:GLN:H	13	0.12
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD2	7	0.12
(1,290)	1:A:9:ILE:HG21	1:A:99:ARG:HD3	7	0.12
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD2	7	0.12
(1,290)	1:A:9:ILE:HG22	1:A:99:ARG:HD3	7	0.12
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD2	7	0.12
(1,290)	1:A:9:ILE:HG23	1:A:99:ARG:HD3	7	0.12
(1,269)	1:A:9:ILE:HG12	1:A:101:ALA:HA	3	0.12
(1,269)	1:A:9:ILE:HG12	1:A:101:ALA:HA	9	0.12
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	7	0.12
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	7	0.12
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	8	0.12
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	8	0.12
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	11	0.12
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	11	0.12
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	16	0.12
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	16	0.12
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	11	0.12
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	11	0.12
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	11	0.12
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	11	0.12
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	11	0.12
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	11	0.12
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG21	15	0.12
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG22	15	0.12
(1,227)	1:A:8:PHE:HD1	1:A:26:ILE:HG23	15	0.12
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG21	15	0.12
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG22	15	0.12
(1,227)	1:A:8:PHE:HD2	1:A:26:ILE:HG23	15	0.12
(1,1344)	1:A:101:ALA:HA	1:A:102:LEU:HB3	2	0.12
(1,1344)	1:A:101:ALA:HA	1:A:102:LEU:HB3	4	0.12
(1,1344)	1:A:101:ALA:HA	1:A:102:LEU:HB3	18	0.12
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	1	0.12
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	9	0.12
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	16	0.12
(1,1303)	1:A:95:ILE:HG13	1:A:97:GLY:H	15	0.12
(1,1303)	1:A:95:ILE:HG13	1:A:97:GLY:H	16	0.12
(1,1166)	1:A:80:THR:HG21	1:A:81:GLU:HB2	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1166)	1:A:80:THR:HG22	1:A:81:GLU:HB2	2	0.12
(1,1166)	1:A:80:THR:HG23	1:A:81:GLU:HB2	2	0.12
(1,1145)	1:A:79:LEU:HG	1:A:83:SER:H	3	0.12
(2,5)	2:A:201:FES:FE1	1:A:25:THR:CA	12	0.11
(2,5)	2:A:201:FES:FE1	1:A:25:THR:CA	15	0.11
(2,5)	2:A:201:FES:FE1	1:A:25:THR:CA	19	0.11
(2,3)	2:A:201:FES:FE2	1:A:72:MET:CA	15	0.11
(2,2)	2:A:201:FES:FE1	1:A:72:MET:CA	1	0.11
(2,2)	2:A:201:FES:FE1	1:A:72:MET:CA	5	0.11
(1,93)	1:A:6:ILE:HG13	1:A:29:ILE:HB	7	0.11
(1,93)	1:A:6:ILE:HG13	1:A:29:ILE:HB	10	0.11
(1,93)	1:A:6:ILE:HG13	1:A:29:ILE:HB	16	0.11
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	5	0.11
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	9	0.11
(1,927)	1:A:60:ASP:HB2	1:A:62:LEU:H	19	0.11
(1,92)	1:A:6:ILE:HG12	1:A:99:ARG:HA	12	0.11
(1,905)	1:A:59:TYR:HD1	1:A:82:THR:HB	11	0.11
(1,905)	1:A:59:TYR:HD2	1:A:82:THR:HB	11	0.11
(1,905)	1:A:59:TYR:HD1	1:A:82:THR:HB	14	0.11
(1,905)	1:A:59:TYR:HD2	1:A:82:THR:HB	14	0.11
(1,893)	1:A:59:TYR:HB2	1:A:61:ALA:H	18	0.11
(1,829)	1:A:55:ASP:HB2	1:A:58:TYR:H	14	0.11
(1,803)	1:A:54:VAL:HG11	1:A:84:ARG:HD3	14	0.11
(1,803)	1:A:54:VAL:HG12	1:A:84:ARG:HD3	14	0.11
(1,803)	1:A:54:VAL:HG13	1:A:84:ARG:HD3	14	0.11
(1,796)	1:A:54:VAL:HB	1:A:83:SER:HA	6	0.11
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	2	0.11
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	4	0.11
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	11	0.11
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	12	0.11
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	13	0.11
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	15	0.11
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	17	0.11
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	18	0.11
(1,794)	1:A:54:VAL:HB	1:A:82:THR:HB	19	0.11
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE1	1	0.11
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE2	1	0.11
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE1	9	0.11
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE2	9	0.11
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE1	15	0.11
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE2	15	0.11
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE1	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:A:54:VAL:HB	1:A:59:TYR:HE2	18	0.11
(1,790)	1:A:54:VAL:HB	1:A:59:TYR:HA	16	0.11
(1,749)	1:A:53:ILE:HG12	1:A:54:VAL:HA	6	0.11
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	2	0.11
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	4	0.11
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	5	0.11
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	7	0.11
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	15	0.11
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	16	0.11
(1,748)	1:A:53:ILE:HG12	1:A:101:ALA:H	19	0.11
(1,691)	1:A:35:LEU:HB3	1:A:37:MET:HB2	14	0.11
(1,691)	1:A:35:LEU:HB3	1:A:37:MET:HB2	16	0.11
(1,691)	1:A:35:LEU:HB3	1:A:37:MET:HB2	19	0.11
(1,662)	1:A:33:HIS:HB2	1:A:35:LEU:H	5	0.11
(1,642)	1:A:31:GLN:HB3	1:A:33:HIS:H	14	0.11
(1,642)	1:A:31:GLN:HB3	1:A:33:HIS:H	18	0.11
(1,489)	1:A:23:GLY:HA2	1:A:90:LYS:HD2	4	0.11
(1,489)	1:A:23:GLY:HA2	1:A:90:LYS:HD3	4	0.11
(1,489)	1:A:23:GLY:HA3	1:A:90:LYS:HD2	4	0.11
(1,489)	1:A:23:GLY:HA3	1:A:90:LYS:HD3	4	0.11
(1,389)	1:A:16:LYS:HB2	1:A:17:THR:H	12	0.11
(1,377)	1:A:15:GLN:HB2	1:A:17:THR:H	5	0.11
(1,377)	1:A:15:GLN:HB3	1:A:17:THR:H	5	0.11
(1,377)	1:A:15:GLN:HB2	1:A:17:THR:H	10	0.11
(1,377)	1:A:15:GLN:HB3	1:A:17:THR:H	10	0.11
(1,371)	1:A:15:GLN:HA	1:A:16:LYS:HB3	5	0.11
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	7	0.11
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	9	0.11
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	10	0.11
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	11	0.11
(1,363)	1:A:14:SER:HB2	1:A:16:LYS:HG3	14	0.11
(1,318)	1:A:10:LEU:HG	1:A:15:GLN:H	5	0.11
(1,318)	1:A:10:LEU:HG	1:A:15:GLN:H	15	0.11
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	1	0.11
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	1	0.11
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	9	0.11
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	9	0.11
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	12	0.11
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	12	0.11
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	13	0.11
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	13	0.11
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	14	0.11
(1,228)	1:A:8:PHE:HD1	1:A:29:ILE:HB	19	0.11
(1,228)	1:A:8:PHE:HD2	1:A:29:ILE:HB	19	0.11
(1,1322)	1:A:99:ARG:HB2	1:A:100:VAL:HA	5	0.11
(1,1303)	1:A:95:ILE:HG13	1:A:97:GLY:H	7	0.11
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG21	11	0.11
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG22	11	0.11
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG23	11	0.11
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG21	18	0.11
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG22	18	0.11
(1,1198)	1:A:84:ARG:HB2	1:A:89:ILE:HG23	18	0.11
(1,1139)	1:A:79:LEU:HA	1:A:79:LEU:HD21	8	0.11
(1,1139)	1:A:79:LEU:HA	1:A:79:LEU:HD22	8	0.11
(1,1139)	1:A:79:LEU:HA	1:A:79:LEU:HD23	8	0.11
(1,1127)	1:A:77:TYR:HB2	1:A:78:GLY:HA3	19	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found