Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 02:05 AM EDT

PDB ID	:	2LOX
BMRB ID	:	18229
Title	:	NMR structure of the complex between the PH domain of the Tfb1 subunit from TFIIH and Rad2
Authors	:	Lafrance-Vanasse, J.; Legault, P.; Omichinski, J.
Deposited on	:	2012-01-27

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

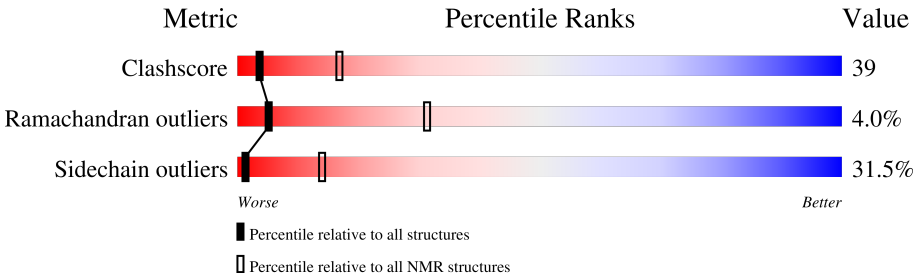
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 92%.

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	119	32% 45% 10% • 9% •
2	B	52	38% 62%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:3-A:51, A:58-A:64, A:86-A:114 (85)	0.23	13
2	A:66-A:84 (19)	1.07	12

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2132 atoms, of which 1072 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA polymerase II transcription factor B subunit 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	115	1820	559	919	161	176	5	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	expression tag	UNP P32776
A	116	GLY	-	expression tag	UNP P32776
A	117	ASN	-	expression tag	UNP P32776
A	118	SER	-	expression tag	UNP P32776
A	119	SER	-	expression tag	UNP P32776

- Molecule 2 is a protein called DNA repair protein RAD2.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	20	312	100	153	22	37	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	640	GLY	-	expression tag	UNP P07276
B	641	SER	-	expression tag	UNP P07276
B	691	TYR	-	expression tag	UNP P07276

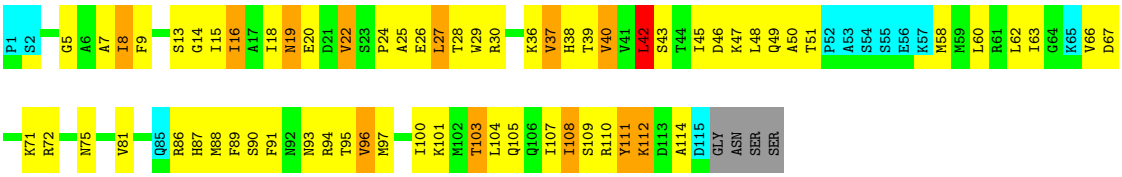
4 Residue-property plots (i)

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: RNA polymerase II transcription factor B subunit 1

Chain A: 32% 45% 10% • 9% •



• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

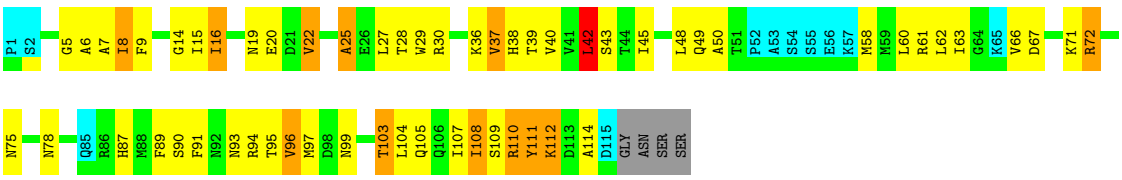
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 39% 38% 10% • 9% •



• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.2 Score per residue for model 2

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 33% 38% 17% 9% •

P1 S2 G5 A6 A7 I8 F9 E10 K11 V12 S13 G14 I15 I16 A17 I18 N19 V22 A25 E26 L27 T28 W29 R30 S31 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65 V66

D67 E68 K71 R72 E76 K83 P84 Q85 R86 H87 M88 F89 S90 F91 R94 T95 V96 M97 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

- Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.3 Score per residue for model 3

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 31% 43% 12% • 9% •

P1 S2 H3 S4 G5 I8 F9 V12 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 A25 E26 L27 T28 W29 D33 G34 D35 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 L60 R61 L62 I63 G64 K65

V66 D67 E68 S69 K70 K71 R72 K73 D74 N75 E79 V80 V81 Q85 R86 H87 M88 F89 S90 F91 R94 T95 V96 M97 D98 N99 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

- Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.4 Score per residue for model 4

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 35% 39% 13% 9% •

P1 S2 G5 A6 A7 I8 S13 G14 I15 I16 A17 I18 N19 V22 A25 E26 L27 T28 W29 R30 K36 V37 H38 T39 V40 V41 L42 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65 V66 D67 K71 R72 K73

D74 N75 N78 E79 V80 V81 P82 Q85 R86 H87 M88 F89 S90 F91 R94 T95 V96 M97 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.5 Score per residue for model 5

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 31% 41% 15% 9% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 E10 K11 V12 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 A25 E26 L27 T28 W29 R30 D35 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63

G64 K65 K70 K71 R72 N75 P82 Q85 R86 H87 M88 F89 S90 F91 R94 T95 V96 M97 D98 N99 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.6 Score per residue for model 6

• Molecule 1: RNA polymerase II transcription factor B subunit 1

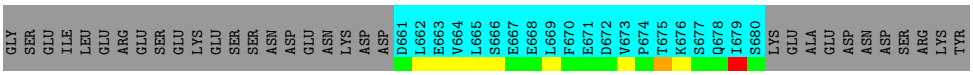
Chain A: 35% 38% 14% 9% •

P1 S2 H3 A7 I8 F9 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 A25 E26 L27 T28 W29 R30 D35 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65 V66 D67 E68

S69 K70 K71 R72 Q85 R86 H87 M88 F89 S90 F91 N92 N93 R94 T95 V96 M97 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

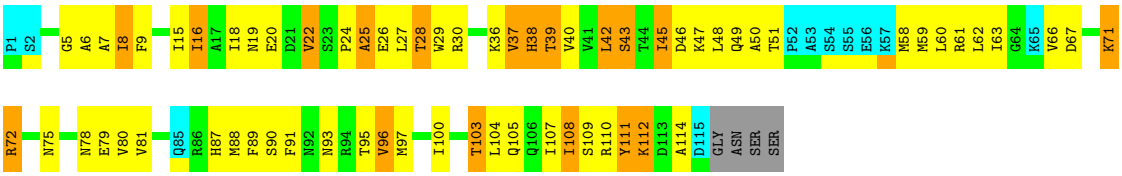
Chain B: 38% 62%



4.2.7 Score per residue for model 7

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 31% 41% 15% 9%



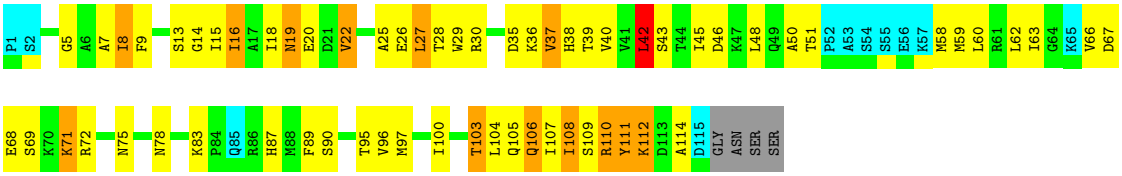
- Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

4.2.8 Score per residue for model 8

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 34% 41% 11% 9%



- Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

4.2.9 Score per residue for model 9

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 26% 45% 15% • 9% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 A25 E26 L27 T28 W29 R30 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65 V66

D67 E68 K71 R72 K73 D74 N75 N78 V81 P82 K83 P84 Q85 R86 H87 M88 F89 S90 F91 R94 T95 V96 M97 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.10 Score per residue for model 10

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 35% 36% 15% • 9% •

P1 S2 G5 A6 A7 I8 F9 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 A25 E26 L27 T28 W29 R30 D33 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65

K70 K71 R72 N75 Q85 R86 H87 M88 F89 S90 F91 N92 N93 R94 T95 V96 M97 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.11 Score per residue for model 11

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 34% 39% 15% 9% •

P1 S2 G5 A6 A7 I8 V12 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 A25 E26 L27 T28 W29 R30 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65 V66 D67

K71 R72 K73 D74 N75 V80 V81 Q85 R86 H87 M88 F89 S90 F91 N92 N93 R94 T95 V96 M97 I100 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.12 Score per residue for model 12

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 34% 39% 13% • 9% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 A25 E26 L27 T28 W29 R30 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65 V66 D67

K71 R72 K73 D74 N78 V81 Q85 R86 H87 M88 F89 S90 N93 R94 T95 V96 M97 D98 N99 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

- Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 34% 39% 12% • 9% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 A25 E26 L27 T28 W29 R30 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 L60 R61 L62 I63 G64 K65 V66 D67

K71 D74 N78 E79 V80 V81 Q85 R86 H87 M88 F89 S90 F91 R94 T95 V96 M97 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

- Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.14 Score per residue for model 14

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 36% 37% 13% • 9% •

P1 S2 G5 A6 A7 I8 F9 V12 S13 I16 A17 I18 N19 E20 D21 V22 A25 E26 L27 T28 W29 D35 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65 V66 D67

R72 V81 Q85 R86 H87 M88 F89 S90 F91 N92 N93 R94 T95 V96 M97 D98 N99 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.15 Score per residue for model 15

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 36% 38% 13% • 9% •

P1 S2 G5 A6 A7 I8 F9 S13 G14 I15 I16 A17 I18 N19 V22 S23 P24 A25 E26 L27 T28 W29 R30 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65 E68

R72 E76 K83 P84 Q85 R86 H87 M88 F89 S90 F91 N92 N93 R94 T95 V96 M97 D98 N99 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.16 Score per residue for model 16

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 29% 44% 14% 9% •

P1 S2 G5 A6 A7 I8 F9 E10 K11 V12 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 A25 E26 L27 T28 W29 R30 D35 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64

K65 V66 D67 E68 K71 R72 N75 V81 P82 K83 P84 Q85 R86 H87 M88 F89 S90 F91 N92 N93 R94 T95 V96 M97 I100 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.17 Score per residue for model 17

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 29% 43% 14% • 9% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 A25 E26 L27 T28 W29 R30 D35 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65

V66 D67 K71 R72 K73 D74 N75 E79 Q85 R86 H87 M88 F89 S90 F91 R94 T95 V96 M97 D98 N99 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

- Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.18 Score per residue for model 18

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 30% 42% 13% • 9% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 E10 K11 V12 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 A25 E26 L27 T28 W29 R30 D35 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63

G64 K65 V66 D67 E68 K71 R72 N78 V81 Q85 R86 H87 M88 F89 S90 N93 R94 T95 V96 M97 D98 N99 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

- Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.19 Score per residue for model 19

- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 34% 39% 13% • 9% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 V12 S13 G14 I15 I16 A17 I18 N19 E20 D21 V22 S23 P24 L27 T28 W29 R30 D33 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64

K65 K70 K71 R72 E79 V80 V81 Q85 R86 H87 M88 F89 S90 F91 N92 N93 R94 T95 V96 M97 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

4.2.20 Score per residue for model 20

• Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 31% 39% 16% • 9% •

P1 S2 H3 S4 G5 A6 A7 I8 F9 S13 G14 I15 I16 A17 I18 N19 V22 S23 P24 A25 E26 L27 T28 W29 R30 K36 V37 H38 T39 V40 V41 L42 S43 T44 I45 D46 K47 L48 Q49 A50 T51 P52 A53 S54 S55 E56 K57 M58 M59 L60 R61 L62 I63 G64 K65 V66 D67

K71 R72 K73 D74 N75 E76 V81 P82 Q85 R86 H87 M88 F89 S90 F91 R94 T95 V96 M97 D98 N99 I100 K101 M102 T103 L104 Q105 Q106 I107 I108 S109 R110 Y111 K112 D113 A114 D115 GLY ASN SER SER

• Molecule 2: DNA repair protein RAD2

Chain B: 38% 62%

GLY SER GLU ILE LEU GLU ARG GLU SER GLU LYS GLU SER SER ASN ASP GLU ASN LYS ASP ASP D661 L662 E663 V664 L665 S666 E667 E668 L669 F670 E671 D672 V673 P674 T675 K676 S677 Q678 I679 S680 LYS GLU ALA GLU ASP ASN ASP SER ARG LYS TYR

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1958
Number of shifts mapped to atoms	1706
Number of unparsed shifts	0
Number of shifts with mapping errors	252
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	820	839	836	65±6
2	B	0	0	0	0±0
All	All	16400	16780	16720	1293

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD11	1:A:104:LEU:HD13	0.99	1.34	1	18
1:A:107:ILE:HG22	1:A:111:TYR:CE1	0.85	2.07	7	20
1:A:16:ILE:HD11	1:A:89:PHE:CD2	0.84	2.06	19	9
1:A:16:ILE:HD11	1:A:89:PHE:CD1	0.84	2.06	13	11
1:A:107:ILE:HG22	1:A:111:TYR:HE1	0.83	1.33	7	20
1:A:48:LEU:HD22	1:A:105:GLN:NE2	0.81	1.90	14	1
1:A:42:LEU:HD11	1:A:104:LEU:CD2	0.80	2.07	4	19
1:A:45:ILE:HD12	1:A:62:LEU:HB3	0.79	1.52	1	20
1:A:14:GLY:O	1:A:15:ILE:HD13	0.79	1.78	6	15
1:A:18:ILE:HD13	1:A:103:THR:HG22	0.77	1.56	8	10
1:A:27:LEU:HD12	1:A:27:LEU:C	0.77	1.99	10	15
1:A:42:LEU:HD11	1:A:104:LEU:HD23	0.75	1.57	4	2
1:A:49:GLN:HG3	1:A:63:ILE:HD11	0.74	1.60	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:HD12	1:A:62:LEU:CB	0.73	2.14	1	20
1:A:16:ILE:HD11	1:A:89:PHE:CG	0.73	2.19	10	20
1:A:48:LEU:CD1	1:A:104:LEU:HD13	0.72	2.14	9	10
1:A:28:THR:HG22	1:A:37:VAL:CG2	0.70	2.16	20	15
1:A:112:LYS:N	1:A:112:LYS:HD2	0.70	2.02	1	20
1:A:18:ILE:HD11	1:A:100:ILE:HG23	0.67	1.67	11	4
1:A:18:ILE:HD13	1:A:103:THR:CG2	0.67	2.20	11	10
1:A:100:ILE:HG22	1:A:104:LEU:HD11	0.67	1.65	8	8
1:A:48:LEU:HD11	1:A:104:LEU:CD1	0.67	2.17	1	9
1:A:42:LEU:HD11	1:A:104:LEU:HD22	0.67	1.66	17	17
1:A:63:ILE:HG23	1:A:86:ARG:HG2	0.66	1.67	2	7
1:A:41:VAL:HG12	1:A:43:SER:OG	0.66	1.89	2	1
1:A:62:LEU:HD21	1:A:104:LEU:HD22	0.65	1.67	12	2
1:A:63:ILE:HD12	1:A:86:ARG:HD3	0.65	1.69	12	3
1:A:50:ALA:HB1	1:A:60:LEU:CD2	0.65	2.22	1	20
1:A:18:ILE:HD13	1:A:103:THR:HB	0.65	1.66	9	2
1:A:81:VAL:O	1:A:81:VAL:HG13	0.64	1.93	20	2
1:A:48:LEU:HD23	1:A:105:GLN:HE21	0.64	1.53	6	1
1:A:7:ALA:HB2	1:A:91:PHE:CZ	0.62	2.28	13	11
1:A:48:LEU:HD21	1:A:104:LEU:HB2	0.62	1.70	13	2
1:A:81:VAL:HG12	1:A:81:VAL:O	0.62	1.94	9	4
1:A:27:LEU:HD12	1:A:27:LEU:O	0.62	1.94	6	11
1:A:8:ILE:N	1:A:8:ILE:HD13	0.61	2.10	4	17
1:A:7:ALA:HB2	1:A:91:PHE:CE1	0.61	2.30	2	10
1:A:48:LEU:HD12	1:A:62:LEU:HD23	0.60	1.71	14	1
1:A:27:LEU:HB3	1:A:40:VAL:CG1	0.60	2.25	12	5
1:A:108:ILE:HA	1:A:111:TYR:CE2	0.60	2.31	6	20
1:A:80:VAL:HG12	1:A:82:PRO:HD3	0.60	1.72	4	1
1:A:19:ASN:O	1:A:22:VAL:HG23	0.59	1.97	3	19
1:A:68:GLU:HA	1:A:81:VAL:HG13	0.59	1.73	3	1
1:A:111:TYR:N	1:A:111:TYR:CD1	0.58	2.71	5	20
1:A:50:ALA:CB	1:A:60:LEU:HD22	0.58	2.28	1	20
1:A:27:LEU:C	1:A:27:LEU:CD1	0.57	2.73	10	15
1:A:18:ILE:HD12	1:A:103:THR:HB	0.57	1.75	13	7
1:A:60:LEU:HD12	1:A:91:PHE:CZ	0.57	2.35	19	1
1:A:25:ALA:HB2	1:A:107:ILE:HG21	0.57	1.75	14	9
1:A:93:ASN:HB3	1:A:96:VAL:HG23	0.57	1.76	14	6
1:A:48:LEU:HD22	1:A:108:ILE:CD1	0.56	2.31	7	1
1:A:8:ILE:HD12	1:A:13:SER:HA	0.56	1.76	11	3
1:A:62:LEU:HD12	1:A:89:PHE:CE1	0.56	2.36	14	2
1:A:16:ILE:HD11	1:A:89:PHE:CE1	0.55	2.36	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD23	1:A:105:GLN:HG2	0.55	1.78	5	3
1:A:19:ASN:OD1	1:A:22:VAL:HG22	0.54	2.02	20	1
1:A:28:THR:HG23	1:A:39:THR:HG23	0.54	1.80	7	3
1:A:27:LEU:HB3	1:A:40:VAL:HG12	0.54	1.79	4	5
1:A:62:LEU:HD12	1:A:89:PHE:HE1	0.54	1.63	14	2
1:A:89:PHE:CD1	1:A:89:PHE:N	0.53	2.77	10	5
1:A:48:LEU:HD22	1:A:105:GLN:CD	0.53	2.23	14	1
1:A:49:GLN:O	1:A:61:ARG:N	0.53	2.39	14	8
1:A:40:VAL:CG2	1:A:87:HIS:CD2	0.53	2.92	5	20
1:A:16:ILE:CD1	1:A:89:PHE:CD1	0.53	2.92	3	8
1:A:16:ILE:CG2	1:A:100:ILE:HD12	0.53	2.34	16	13
1:A:49:GLN:NE2	1:A:63:ILE:HD11	0.53	2.19	7	1
1:A:5:GLY:O	1:A:16:ILE:N	0.52	2.40	2	14
1:A:49:GLN:CG	1:A:63:ILE:HD11	0.52	2.31	1	1
1:A:50:ALA:HB1	1:A:60:LEU:HD22	0.52	1.79	1	5
1:A:100:ILE:HG22	1:A:104:LEU:HD12	0.52	1.81	12	2
1:A:14:GLY:C	1:A:15:ILE:HD13	0.52	2.24	6	10
1:A:71:LYS:HG2	1:A:81:VAL:HG23	0.52	1.80	11	1
1:A:51:THR:HG23	1:A:59:MET:HB2	0.51	1.82	17	7
1:A:63:ILE:HD12	1:A:86:ARG:HG2	0.51	1.82	17	4
1:A:15:ILE:N	1:A:30:ARG:O	0.51	2.43	16	17
1:A:16:ILE:O	1:A:16:ILE:HG22	0.50	2.05	14	5
1:A:112:LYS:N	1:A:112:LYS:CD	0.50	2.72	13	19
1:A:81:VAL:O	1:A:81:VAL:CG1	0.50	2.59	9	5
1:A:49:GLN:OE1	1:A:63:ILE:HD11	0.50	2.06	6	1
1:A:63:ILE:HD12	1:A:86:ARG:CD	0.50	2.37	6	1
1:A:27:LEU:HD22	1:A:40:VAL:HB	0.50	1.83	7	5
1:A:9:PHE:CZ	1:A:38:HIS:CD2	0.50	3.00	7	6
1:A:51:THR:HG1	1:A:58:MET:HA	0.49	1.67	9	1
1:A:50:ALA:CB	1:A:60:LEU:CD2	0.49	2.91	12	20
1:A:8:ILE:N	1:A:8:ILE:CD1	0.49	2.75	20	17
1:A:27:LEU:HD21	1:A:62:LEU:CD1	0.49	2.37	20	9
1:A:7:ALA:C	1:A:8:ILE:HD13	0.49	2.28	4	17
1:A:8:ILE:HG23	1:A:12:VAL:O	0.49	2.07	18	5
1:A:27:LEU:HG	1:A:40:VAL:CG1	0.49	2.38	5	15
1:A:29:TRP:O	1:A:37:VAL:HA	0.48	2.07	2	19
1:A:48:LEU:HD13	1:A:108:ILE:HD11	0.48	1.84	7	2
1:A:50:ALA:HB3	1:A:101:LYS:HD2	0.48	1.85	3	3
1:A:9:PHE:CE1	1:A:38:HIS:CD2	0.48	3.00	20	2
1:A:3:HIS:HA	1:A:103:THR:HG21	0.48	1.85	9	1
1:A:66:VAL:HG22	1:A:67:ASP:N	0.48	2.24	14	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:PHE:CE1	1:A:38:HIS:CE1	0.48	3.02	14	7
1:A:93:ASN:CB	1:A:96:VAL:HG23	0.48	2.38	12	10
1:A:9:PHE:HB3	1:A:29:TRP:CE2	0.48	2.43	7	14
1:A:45:ILE:CG2	1:A:62:LEU:HB3	0.47	2.38	12	20
1:A:46:ASP:N	1:A:63:ILE:O	0.47	2.48	2	17
1:A:9:PHE:CB	1:A:29:TRP:CE2	0.47	2.97	18	3
1:A:42:LEU:CB	1:A:111:TYR:OH	0.47	2.63	7	12
1:A:48:LEU:HD22	1:A:108:ILE:HG13	0.47	1.84	7	1
1:A:110:ARG:O	1:A:114:ALA:CB	0.47	2.63	18	20
1:A:112:LYS:HD2	1:A:112:LYS:H	0.47	1.69	12	19
1:A:51:THR:HG23	1:A:59:MET:HB3	0.47	1.86	7	1
1:A:98:ASP:O	1:A:102:MET:HE2	0.47	2.09	14	2
1:A:16:ILE:HG22	1:A:100:ILE:HD12	0.47	1.87	9	11
1:A:25:ALA:CB	1:A:107:ILE:HG21	0.46	2.40	7	7
1:A:107:ILE:O	1:A:110:ARG:HB2	0.46	2.10	3	5
1:A:100:ILE:HG22	1:A:104:LEU:CD1	0.46	2.40	16	4
1:A:26:GLU:OE1	1:A:41:VAL:HG22	0.46	2.10	13	1
1:A:9:PHE:CE2	1:A:38:HIS:CB	0.46	2.99	2	2
1:A:15:ILE:O	1:A:29:TRP:HA	0.46	2.10	8	13
1:A:27:LEU:HD13	1:A:62:LEU:HD11	0.46	1.87	4	4
1:A:26:GLU:HA	1:A:40:VAL:O	0.46	2.10	6	10
1:A:7:ALA:HB1	1:A:89:PHE:HB3	0.46	1.88	20	2
1:A:5:GLY:N	1:A:16:ILE:O	0.46	2.49	4	5
1:A:16:ILE:CD1	1:A:89:PHE:CD2	0.46	2.93	19	5
1:A:112:LYS:H	1:A:112:LYS:CD	0.45	2.23	4	9
1:A:3:HIS:O	1:A:18:ILE:N	0.45	2.47	20	7
1:A:40:VAL:HG22	1:A:45:ILE:HD11	0.45	1.87	7	4
1:A:102:MET:HG3	1:A:103:THR:N	0.45	2.26	5	1
1:A:48:LEU:HD23	1:A:105:GLN:NE2	0.45	2.26	6	2
1:A:24:PRO:CB	1:A:43:SER:CB	0.45	2.94	9	12
1:A:40:VAL:CG2	1:A:87:HIS:CG	0.45	2.99	20	8
1:A:112:LYS:CD	1:A:112:LYS:H	0.45	2.23	11	9
1:A:9:PHE:CZ	1:A:38:HIS:ND1	0.45	2.85	6	2
1:A:104:LEU:O	1:A:108:ILE:HG13	0.45	2.12	16	4
1:A:5:GLY:O	1:A:16:ILE:O	0.45	2.34	2	1
1:A:5:GLY:HA3	1:A:96:VAL:HG12	0.45	1.86	14	1
1:A:108:ILE:O	1:A:112:LYS:HD3	0.44	2.12	16	15
1:A:5:GLY:O	1:A:16:ILE:HB	0.44	2.12	8	10
1:A:71:LYS:HG2	1:A:81:VAL:HG22	0.44	1.88	7	1
1:A:68:GLU:CG	1:A:81:VAL:HG11	0.44	2.42	16	1
1:A:47:LYS:CG	1:A:63:ILE:CG1	0.44	2.96	13	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ALA:O	1:A:91:PHE:CD2	0.44	2.70	7	8
1:A:107:ILE:O	1:A:111:TYR:CE1	0.44	2.71	13	20
1:A:16:ILE:CD1	1:A:89:PHE:CG	0.44	3.00	14	3
1:A:28:THR:HG22	1:A:37:VAL:HG21	0.44	1.89	19	2
1:A:99:ASN:O	1:A:103:THR:OG1	0.44	2.35	5	6
1:A:9:PHE:CB	1:A:29:TRP:CD2	0.44	3.01	2	3
1:A:9:PHE:HB2	1:A:29:TRP:CE2	0.43	2.48	2	1
1:A:91:PHE:CD2	1:A:97:MET:CA	0.43	3.01	9	3
1:A:63:ILE:HA	1:A:86:ARG:HB3	0.43	1.88	16	1
1:A:81:VAL:HG22	1:A:81:VAL:O	0.43	2.13	4	1
1:A:9:PHE:CE2	1:A:38:HIS:CG	0.43	3.05	6	1
1:A:104:LEU:O	1:A:108:ILE:CG1	0.43	2.67	8	5
1:A:101:LYS:O	1:A:105:GLN:NE2	0.43	2.52	18	6
1:A:27:LEU:CD2	1:A:62:LEU:HD11	0.43	2.43	20	2
1:A:108:ILE:HA	1:A:111:TYR:CZ	0.43	2.48	18	12
1:A:41:VAL:CG1	1:A:44:THR:HG23	0.43	2.44	9	2
1:A:45:ILE:CD1	1:A:87:HIS:CD2	0.43	3.01	7	2
1:A:9:PHE:HB3	1:A:29:TRP:CZ2	0.43	2.49	7	2
1:A:45:ILE:CG2	1:A:47:LYS:O	0.43	2.66	5	3
1:A:48:LEU:CD1	1:A:62:LEU:HD23	0.43	2.43	7	1
1:A:27:LEU:HD12	1:A:28:THR:N	0.43	2.29	8	3
1:A:8:ILE:O	1:A:89:PHE:HA	0.43	2.13	14	1
1:A:59:MET:HG3	1:A:90:SER:HA	0.43	1.89	4	1
1:A:9:PHE:CZ	1:A:38:HIS:CG	0.43	3.07	12	1
1:A:48:LEU:HD23	1:A:105:GLN:CG	0.43	2.44	7	1
1:A:48:LEU:HD13	1:A:62:LEU:HD23	0.42	1.90	5	1
1:A:48:LEU:HD22	1:A:108:ILE:CG1	0.42	2.44	7	1
1:A:9:PHE:CD2	1:A:89:PHE:CE1	0.42	3.07	18	2
1:A:45:ILE:HA	1:A:63:ILE:O	0.42	2.14	13	6
1:A:102:MET:HG2	1:A:103:THR:N	0.42	2.29	20	1
1:A:50:ALA:HB2	1:A:60:LEU:HD22	0.42	1.91	5	8
1:A:45:ILE:CD1	1:A:62:LEU:HB3	0.42	2.40	16	5
1:A:108:ILE:O	1:A:111:TYR:N	0.42	2.49	11	2
1:A:42:LEU:N	1:A:42:LEU:CD2	0.42	2.83	9	15
1:A:47:LYS:HG2	1:A:63:ILE:CG1	0.42	2.45	5	1
1:A:18:ILE:HG21	1:A:107:ILE:CD1	0.42	2.45	20	1
1:A:8:ILE:HD12	1:A:13:SER:CA	0.42	2.44	3	2
1:A:25:ALA:O	1:A:26:GLU:CG	0.42	2.67	13	1
1:A:27:LEU:CD2	1:A:40:VAL:HB	0.41	2.45	7	4
1:A:103:THR:O	1:A:106:GLN:HG3	0.41	2.14	8	1
1:A:5:GLY:N	1:A:100:ILE:HD11	0.41	2.30	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLU:HG3	1:A:107:ILE:HD11	0.41	1.91	11	1
1:A:94:ARG:O	1:A:98:ASP:CB	0.41	2.69	12	1
1:A:99:ASN:O	1:A:102:MET:HG2	0.41	2.15	5	1
1:A:86:ARG:CD	1:A:86:ARG:N	0.41	2.83	16	1
1:A:99:ASN:O	1:A:102:MET:CG	0.41	2.69	5	1
1:A:60:LEU:CD1	1:A:100:ILE:CG2	0.41	2.98	7	1
1:A:24:PRO:CB	1:A:43:SER:HB2	0.41	2.46	17	3
1:A:103:THR:O	1:A:106:GLN:CG	0.41	2.69	16	1
1:A:63:ILE:CD1	1:A:86:ARG:CG	0.41	2.98	19	1
1:A:48:LEU:CD1	1:A:62:LEU:CD2	0.41	2.98	5	1
1:A:18:ILE:CD1	1:A:103:THR:HB	0.41	2.46	20	3
1:A:72:ARG:N	1:A:80:VAL:O	0.41	2.54	7	1
1:A:48:LEU:HD22	1:A:105:GLN:CG	0.41	2.46	14	1
1:A:40:VAL:CG1	1:A:42:LEU:HD22	0.41	2.46	1	2
1:A:60:LEU:O	1:A:89:PHE:N	0.41	2.54	9	1
1:A:49:GLN:N	1:A:61:ARG:O	0.41	2.48	12	1
1:A:80:VAL:O	1:A:81:VAL:O	0.41	2.38	13	1
1:A:48:LEU:HD22	1:A:105:GLN:HG2	0.41	1.92	14	1
1:A:80:VAL:HG12	1:A:81:VAL:N	0.41	2.31	19	1
1:A:22:VAL:HG21	1:A:26:GLU:CG	0.41	2.46	20	1
1:A:3:HIS:CE1	1:A:18:ILE:O	0.40	2.73	9	1
1:A:72:ARG:CD	1:A:72:ARG:N	0.40	2.85	1	1
1:A:74:ASP:O	1:A:75:ASN:CB	0.40	2.70	3	1
1:A:7:ALA:CB	1:A:91:PHE:CE1	0.40	3.04	11	1
1:A:5:GLY:CA	1:A:96:VAL:CG1	0.40	2.99	14	1
1:A:41:VAL:O	1:A:43:SER:N	0.40	2.54	14	1
1:A:28:THR:CG2	1:A:37:VAL:CG2	0.40	2.99	5	1
1:A:24:PRO:CG	1:A:43:SER:HB2	0.40	2.46	7	1
1:A:80:VAL:O	1:A:81:VAL:C	0.40	2.60	11	1
1:A:27:LEU:CD2	1:A:62:LEU:CD1	0.40	2.99	10	1
1:A:81:VAL:HG13	1:A:81:VAL:O	0.40	2.17	11	1
1:A:12:VAL:CG1	1:A:13:SER:N	0.40	2.85	18	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	104/119 (87%)	85±2 (82±2%)	14±2 (14±2%)	4±1 (4±1%)	5 31
2	B	0	-	-	-	-
All	All	2080/3420 (61%)	1708 (82%)	289 (14%)	83 (4%)	5 31

All 13 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	71	LYS	18
1	A	42	LEU	13
1	A	75	ASN	11
1	A	25	ALA	10
1	A	78	ASN	8
1	A	93	ASN	6
1	A	81	VAL	4
1	A	79	GLU	3
1	A	45	ILE	3
1	A	70	LYS	3
1	A	82	PRO	2
1	A	31	SER	1
1	A	22	VAL	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	93/106 (88%)	64±4 (68±4%)	29±4 (32±4%)	1 14
2	B	0	-	-	-
All	All	1860/3120 (60%)	1274 (68%)	586 (32%)	1 14

All 62 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	16	ILE	20
1	A	22	VAL	20
1	A	36	LYS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	37	VAL	20
1	A	39	THR	20
1	A	95	THR	20
1	A	97	MET	20
1	A	103	THR	20
1	A	108	ILE	20
1	A	111	TYR	20
1	A	112	LYS	20
1	A	42	LEU	19
1	A	72	ARG	19
1	A	96	VAL	19
1	A	90	SER	18
1	A	8	ILE	17
1	A	105	GLN	15
1	A	13	SER	15
1	A	27	LEU	15
1	A	20	GLU	14
1	A	94	ARG	14
1	A	19	ASN	13
1	A	40	VAL	13
1	A	86	ARG	13
1	A	43	SER	12
1	A	109	SER	12
1	A	58	MET	11
1	A	88	MET	10
1	A	110	ARG	8
1	A	26	GLU	8
1	A	35	ASP	8
1	A	68	GLU	6
1	A	74	ASP	6
1	A	28	THR	5
1	A	47	LYS	5
1	A	83	LYS	5
1	A	75	ASN	5
1	A	49	GLN	5
1	A	106	GLN	5
1	A	11	LYS	4
1	A	73	LYS	4
1	A	101	LYS	4
1	A	76	GLU	3
1	A	33	ASP	3
1	A	81	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	89	PHE	3
1	A	102	MET	3
1	A	9	PHE	2
1	A	70	LYS	2
1	A	61	ARG	2
1	A	69	SER	2
1	A	79	GLU	2
1	A	71	LYS	2
1	A	4	SER	2
1	A	67	ASP	2
1	A	30	ARG	2
1	A	10	GLU	1
1	A	31	SER	1
1	A	59	MET	1
1	A	38	HIS	1
1	A	78	ASN	1
1	A	21	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)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 93% 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	1958
Number of shifts mapped to atoms	1706
Number of unparsed shifts	0
Number of shifts with mapping errors	252
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 3 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	LEU	HD11	0.855	0.005	2
1	A	48	LEU	HD12	0.855	0.005	2
1	A	48	LEU	HD13	0.855	0.005	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 252 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	117	ASN	H	8.317	.	1
1	A	117	ASN	N	118.871	.	1
1	A	118	SER	H	8.329	.	1
1	A	118	SER	N	116.555	.	1
1	A	116	GLY	H	8.217	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	GLY	N	108.816	.	1
1	A	119	SER	H	8.016	.	1
1	A	119	SER	N	123.353	.	1
1	A	118	SER	C	173.789	.	1
1	A	116	GLY	C	174.366	.	1
1	A	117	ASN	C	175.359	.	1
1	A	118	SER	CB	63.939	0.001	1
1	A	118	SER	CA	58.41	0.013	1
1	A	116	GLY	CA	45.802	.	1
1	A	117	ASN	CA	53.229	0.022	1
1	A	117	ASN	CB	39.193	0.012	1
1	A	119	SER	CB	64.719	0.043	1
1	A	119	SER	CA	60.007	0.019	1
1	A	116	GLY	HA3	4.003	0.001	1
1	A	116	GLY	HA2	4.003	0.001	1
1	A	117	ASN	HA	4.852	0.001	1
1	A	117	ASN	HB3	2.9	0.003	2
1	A	117	ASN	HB2	2.822	0.002	2
1	A	118	SER	HA	4.557	0.003	1
1	A	118	SER	HB3	3.931	0.005	2
1	A	118	SER	HB2	3.931	0.005	2
1	A	119	SER	HA	4.306	0.002	1
1	A	119	SER	HB3	3.875	0.002	2
1	A	119	SER	HB2	3.875	0.002	2
1	A	117	ASN	ND2	113.528	.	1
1	A	117	ASN	HD21	7.663	.	1
1	A	117	ASN	HD22	6.941	.	1
1	B	646	ARG	HE	7.272	.	1
1	B	646	ARG	NE	124.512	.	1
1	B	684	GLU	H	8.313	.	1
1	B	684	GLU	N	120.022	.	1
1	B	681	LYS	H	8.42	.	1
1	B	681	LYS	N	124.077	.	1
1	B	644	LEU	H	8.243	.	1
1	B	644	LEU	N	126.349	.	1
1	B	657	ASN	H	8.454	.	1
1	B	657	ASN	N	119.502	.	1
1	B	686	ASN	H	8.37	.	1
1	B	686	ASN	N	119.403	.	1
1	B	645	GLU	H	8.64	.	1
1	B	645	GLU	N	123.191	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	654	ASN	H	8.496	.	1
1	B	654	ASN	N	120.907	.	1
1	B	690	LYS	H	8.124	.	1
1	B	690	LYS	N	122.478	.	1
1	B	653	SER	H	8.409	.	1
1	B	653	SER	N	117.859	.	1
1	B	652	SER	H	8.371	.	1
1	B	652	SER	N	117.099	.	1
1	B	649	GLU	H	8.43	.	1
1	B	649	GLU	N	122.77	.	1
1	B	648	SER	H	8.326	.	1
1	B	648	SER	N	116.353	.	1
1	B	688	SER	H	8.196	.	1
1	B	688	SER	N	116.057	.	1
1	B	647	GLU	H	8.553	.	1
1	B	647	GLU	N	122.357	.	1
1	B	651	GLU	H	8.459	.	1
1	B	651	GLU	N	122.132	.	1
1	B	683	ALA	H	8.244	.	1
1	B	683	ALA	N	124.346	.	1
1	B	683	ALA	C	177.889	.	1
1	B	645	GLU	C	176.413	.	1
1	B	690	LYS	C	176.363	.	1
1	B	643	ILE	C	176.117	.	1
1	B	656	GLU	C	176.309	.	1
1	B	685	ASP	C	176.312	.	1
1	B	644	LEU	C	176.764	.	1
1	B	652	SER	C	174.62	.	1
1	B	650	LYS	C	176.683	.	1
1	B	646	ARG	C	176.494	.	1
1	B	648	SER	C	174.72	.	1
1	B	660	ASP	C	176.172	.	1
1	B	651	GLU	C	176.624	.	1
1	B	687	ASP	C	176.631	.	1
1	B	647	GLU	C	176.799	.	1
1	B	682	GLU	C	176.442	.	1
1	B	689	ARG	H	8.116	.	1
1	B	689	ARG	N	122.433	.	1
1	B	689	ARG	C	174.692	.	1
1	B	688	SER	C	175.935	.	1
1	B	646	ARG	H	8.307	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	646	ARG	N	121.703	.	1
1	B	682	GLU	H	8.449	.	1
1	B	682	GLU	N	121.869	.	1
1	B	685	ASP	H	8.506	.	1
1	B	685	ASP	N	121.35	.	1
1	B	684	GLU	C	176.09	.	1
1	B	681	LYS	C	176.743	.	1
1	B	684	GLU	CA	56.509	.	1
1	B	684	GLU	CB	30.207	.	1
1	B	681	LYS	CB	33.037	0.0	1
1	B	681	LYS	CA	56.571	0.0	1
1	B	644	LEU	CB	42.369	.	1
1	B	644	LEU	CA	55.212	.	1
1	B	657	ASN	CB	38.994	.	1
1	B	657	ASN	CA	53.394	.	1
1	B	686	ASN	CB	39.218	.	1
1	B	686	ASN	CA	53.954	.	1
1	B	645	GLU	CA	56.974	.	1
1	B	654	ASN	CA	53.414	.	1
1	B	654	ASN	CB	39.171	.	1
1	B	690	LYS	CB	33.021	.	1
1	B	690	LYS	CA	56.203	.	1
1	B	652	SER	CA	58.265	.	1
1	B	652	SER	CB	63.885	.	1
1	B	649	GLU	CA	56.974	.	1
1	B	649	GLU	CB	30.196	.	1
1	B	648	SER	CA	58.679	.	1
1	B	648	SER	CB	63.77	.	1
1	B	688	SER	CA	58.689	.	1
1	B	688	SER	CB	63.591	.	1
1	B	651	GLU	CA	56.722	.	1
1	B	651	GLU	CB	30.229	.	1
1	B	683	ALA	CB	19.346	.	1
1	B	683	ALA	CA	52.68	.	1
1	B	685	ASP	CB	41.143	.	1
1	B	685	ASP	CA	54.347	.	1
1	B	643	ILE	CB	38.518	.	1
1	B	643	ILE	CA	61.194	.	1
1	B	656	GLU	CB	30.3	.	1
1	B	656	GLU	CA	56.864	.	1
1	B	689	ARG	CA	56.228	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	689	ARG	CB	30.57	.	1
1	B	660	ASP	CB	41.226	.	1
1	B	660	ASP	CA	54.605	.	1
1	B	687	ASP	CB	41.166	.	1
1	B	687	ASP	CA	54.842	.	1
1	B	647	GLU	CB	30.123	.	1
1	B	647	GLU	CA	56.974	.	1
1	B	650	LYS	CB	33.225	.	1
1	B	650	LYS	CA	56.443	.	1
1	B	682	GLU	CA	56.858	0.014	1
1	B	682	GLU	CB	30.059	0.013	1
1	B	646	ARG	CB	30.988	.	1
1	B	646	ARG	CA	56.161	.	1
1	B	653	SER	CA	58.293	.	1
1	B	653	SER	CB	63.846	.	1
1	B	653	SER	C	174.407	.	1
1	B	690	LYS	CG	24.521	.	1
1	B	690	LYS	CD	29.046	.	1
1	B	690	LYS	CE	42.471	.	1
1	B	644	LEU	CG	27.089	.	1
1	B	644	LEU	CD2	23.922	.	2
1	B	647	GLU	CG	36.33	.	1
1	B	646	ARG	CG	27.089	.	1
1	B	646	ARG	CD	43.331	.	1
1	B	650	LYS	CE	42.17	.	1
1	B	650	LYS	CD	29.147	.	1
1	B	650	LYS	CG	24.739	.	1
1	B	645	GLU	CG	36.33	.	1
1	B	681	LYS	CE	42.143	0.013	1
1	B	681	LYS	CD	28.975	0.013	1
1	B	681	LYS	CG	24.701	0.0	1
1	B	684	GLU	CG	36.282	.	1
1	B	651	GLU	CG	36.243	.	1
1	B	682	GLU	CG	36.307	0.0	1
1	B	645	GLU	CB	30.123	.	1
1	B	644	LEU	CD1	24.882	.	2
1	B	689	ARG	CD	43.289	.	1
1	B	689	ARG	CG	27.055	.	1
1	B	681	LYS	HA	4.359	0.0	1
1	B	681	LYS	HB3	1.896	0.0	2
1	B	681	LYS	HB2	1.812	0.0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	681	LYS	HG3	1.479	0.003	2
1	B	681	LYS	HG2	1.48	0.003	2
1	B	681	LYS	HD3	1.728	0.002	1
1	B	681	LYS	HD2	1.728	0.002	1
1	B	681	LYS	HE3	3.038	0.002	2
1	B	681	LYS	HE2	3.038	0.001	2
1	B	682	GLU	HA	4.282	0.002	1
1	B	682	GLU	HB2	2.119	0.004	2
1	B	682	GLU	HB3	1.998	0.002	2
1	B	682	GLU	HG3	2.338	0.001	1
1	B	682	GLU	HG2	2.338	0.001	1
1	B	683	ALA	HA	4.336	.	1
1	B	683	ALA	HB1	1.45	.	1
1	B	683	ALA	HB2	1.45	.	1
1	B	683	ALA	HB3	1.45	.	1
1	B	684	GLU	HB2	2.124	.	2
1	B	684	GLU	HA	4.387	.	1
1	B	684	GLU	HB3	2.004	.	2
1	B	684	GLU	HG2	2.337	.	1
1	B	684	GLU	HG3	2.337	.	1
1	B	685	ASP	HA	4.651	.	1
1	B	685	ASP	HB3	2.762	.	2
1	B	685	ASP	HB2	2.684	.	2
1	B	686	ASN	HA	4.662	.	1
1	B	644	LEU	HA	4.372	.	1
1	B	644	LEU	HB2	1.685	.	1
1	B	644	LEU	HB3	1.685	.	1
1	B	644	LEU	HD11	0.967	.	1
1	B	644	LEU	HD12	0.967	.	1
1	B	644	LEU	HD13	0.967	.	1
1	B	644	LEU	HG	1.685	.	1
1	B	644	LEU	HD21	0.967	.	1
1	B	644	LEU	HD22	0.967	.	1
1	B	644	LEU	HD23	0.967	.	1
1	B	645	GLU	HA	4.314	.	1
1	B	645	GLU	HB3	2.112	.	2
1	B	645	GLU	HB2	2.007	.	2
1	B	645	GLU	HG2	2.338	.	1
1	B	645	GLU	HG3	2.338	.	1
1	B	646	ARG	HA	4.372	.	1
1	B	647	GLU	HA	4.314	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	646	ARG	HB3	1.915	.	2
1	B	646	ARG	HB2	1.825	.	2
1	B	646	ARG	HG2	1.685	.	1
1	B	646	ARG	HG3	1.685	.	1
1	B	646	ARG	HD3	3.254	.	1
1	B	646	ARG	HD2	3.254	.	1
1	B	648	SER	HA	4.444	.	1
1	B	647	GLU	HB3	2.112	.	2
1	B	647	GLU	HB2	2.007	.	2
1	B	647	GLU	HG2	2.338	.	1
1	B	647	GLU	HG3	2.338	.	1
1	B	649	GLU	HA	4.314	.	1
1	B	648	SER	HB2	3.924	.	1
1	B	648	SER	HB3	3.924	.	1
1	B	690	LYS	HA	4.317	.	1
1	B	688	SER	HA	4.406	.	1
1	B	690	LYS	HE3	3.027	.	1
1	B	690	LYS	HE2	3.027	.	1
1	B	690	LYS	HD3	1.702	.	1
1	B	690	LYS	HD2	1.702	.	1
1	B	690	LYS	HG3	1.426	.	1
1	B	690	LYS	HG2	1.426	.	1
1	B	690	LYS	HB3	1.695	.	2
1	B	690	LYS	HB2	1.811	.	2
1	B	689	ARG	HD2	3.192	.	1
1	B	689	ARG	HD3	3.192	.	1
1	B	689	ARG	HG3	1.588	.	1
1	B	689	ARG	HG2	1.588	.	1
1	B	689	ARG	HB2	1.798	.	1
1	B	689	ARG	HB3	1.798	.	1
1	B	689	ARG	HA	4.317	.	1
1	B	688	SER	HB2	3.938	.	1
1	B	688	SER	HB3	3.938	.	1
1	B	654	ASN	ND2	113.243	.	1
1	B	657	ASN	HD22	7.639	.	1
1	B	654	ASN	HD21	6.921	.	1
1	B	657	ASN	ND2	112.704	.	1
1	B	657	ASN	HD21	6.936	.	1
1	B	654	ASN	HD22	7.64	.	1
1	B	686	ASN	ND2	112.412	.	1
1	B	686	ASN	HD22	6.96	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	686	ASN	HD21	7.64	.	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
$^{13}C_{\alpha}$	164	-0.21 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	158	-0.07 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	154	0.05 ± 0.11	None needed (< 0.5 ppm)
^{15}N	153	-0.14 ± 0.24	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 1328 atoms were assigned a chemical shift out of a possible 1441. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	515/519 (99%)	210/210 (100%)	204/208 (98%)	101/101 (100%)
Sidechain	762/847 (90%)	522/549 (95%)	228/262 (87%)	12/36 (33%)
Aromatic	51/75 (68%)	27/37 (73%)	23/31 (74%)	1/7 (14%)
Overall	1328/1441 (92%)	759/796 (95%)	455/501 (91%)	114/144 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1703 atoms were assigned a chemical shift out of a possible 1836. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	663/668 (99%)	269/269 (100%)	265/270 (98%)	129/129 (100%)
Sidechain	981/1083 (91%)	671/700 (96%)	296/342 (87%)	14/41 (34%)
Aromatic	59/85 (69%)	31/42 (74%)	27/36 (75%)	1/7 (14%)
Overall	1703/1836 (93%)	971/1011 (96%)	588/648 (91%)	144/177 (81%)

7.1.4 Statistically unusual chemical shifts (i)

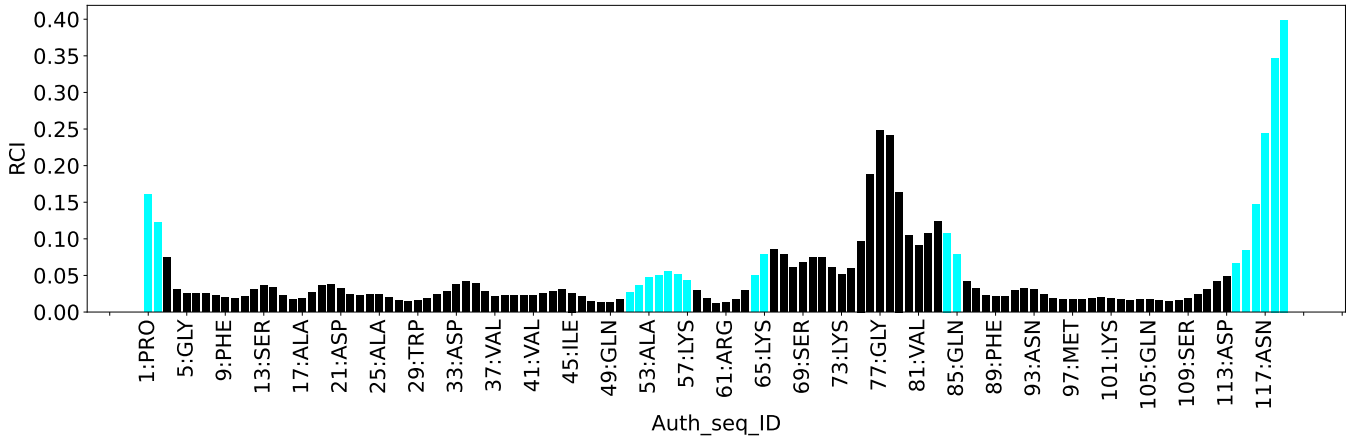
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	646	ARG	NE	124.51	76.53 – 92.65	24.8
1	A	10	GLU	HG3	0.61	1.20 – 3.30	-7.8
1	A	89	PHE	CZ	117.69	121.82 – 136.66	-7.8
1	A	10	GLU	HG2	1.11	1.24 – 3.30	-5.6
1	A	101	LYS	CG	19.14	19.35 – 30.45	-5.2

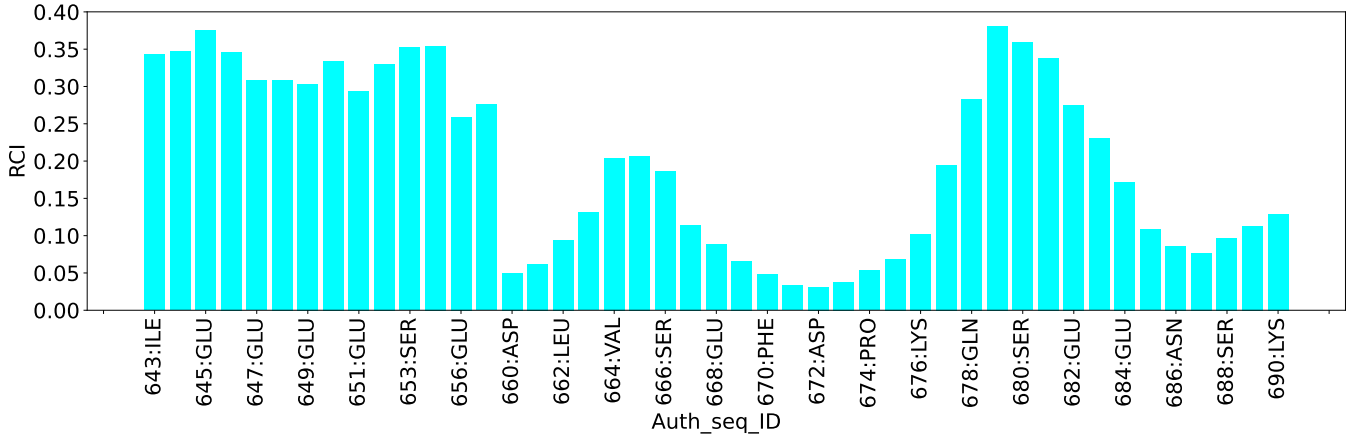
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:



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	1617
Intra-residue (|i-j|=0)	377
Sequential (|i-j|=1)	409
Medium range (|i-j|>1 and |i-j|<5)	240
Long range (|i-j|≥5)	480
Inter-chain	75
Hydrogen bond restraints	36
Disulfide bond restraints	0
Total dihedral-angle restraints	158
Number of unmapped restraints	2
Number of restraints per residue	10.4
Number of long range restraints per residue[1]	3.0

[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)	10.2	0.2
0.2-0.5 (Medium)	1.1	0.49
>0.5 (Large)	0.8	0.86

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.8	1.8
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

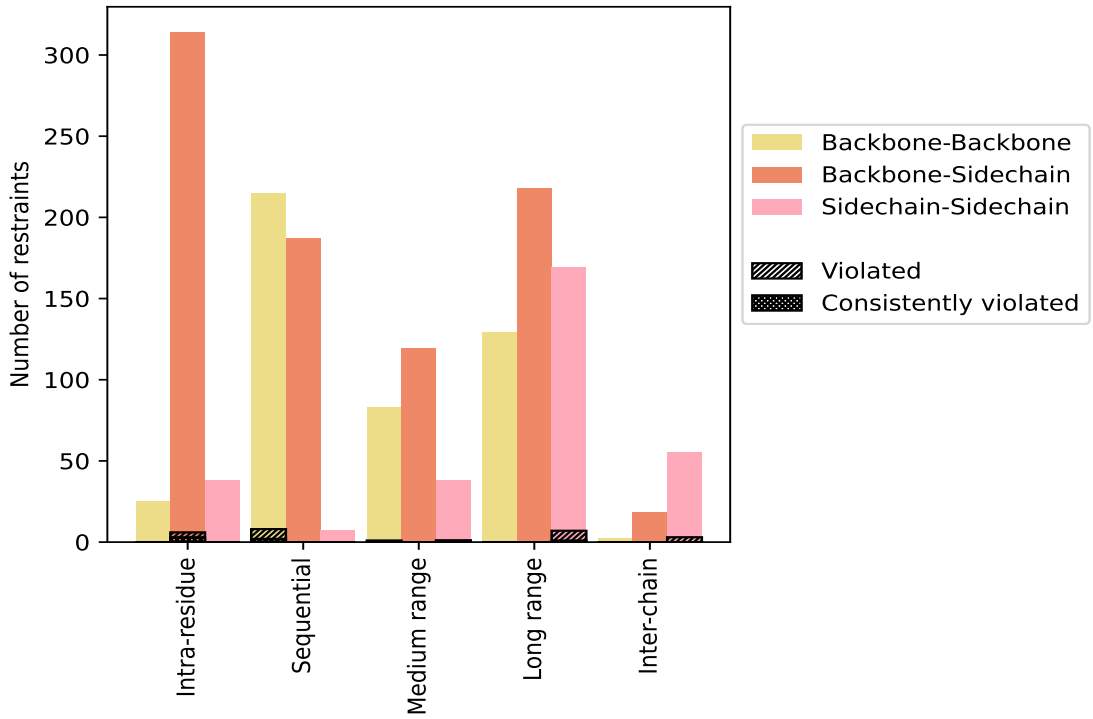
9.1 Summary of distance violations (i)

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)	377	23.3	6	1.6	0.4	3	0.8	0.2
Backbone-Backbone	25	1.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	314	19.4	6	1.9	0.4	3	1.0	0.2
Sidechain-Sidechain	38	2.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	409	25.3	8	2.0	0.5	2	0.5	0.1
Backbone-Backbone	215	13.3	8	3.7	0.5	2	0.9	0.1
Backbone-Sidechain	187	11.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	7	0.4	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	240	14.8	2	0.8	0.1	1	0.4	0.1
Backbone-Backbone	83	5.1	1	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	119	7.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	38	2.4	1	2.6	0.1	1	2.6	0.1
Long range (|i-j|≥5)	480	29.7	7	1.5	0.4	1	0.2	0.1
Backbone-Backbone	93	5.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	218	13.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	169	10.5	7	4.1	0.4	1	0.6	0.1
Inter-chain	75	4.6	3	4.0	0.2	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	18	1.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	55	3.4	3	5.5	0.2	0	0.0	0.0
Hydrogen bond	36	2.2	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	1617	100.0	26	1.6	1.6	7	0.4	0.4
Backbone-Backbone	454	28.1	9	2.0	0.6	2	0.4	0.1
Backbone-Sidechain	856	52.9	6	0.7	0.4	3	0.4	0.2
Sidechain-Sidechain	307	19.0	11	3.6	0.7	2	0.7	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	4	3	1	2	1	11	0.2	0.67	0.15	0.17
2	5	2	2	2	2	13	0.22	0.54	0.13	0.19
3	3	3	2	2	1	11	0.22	0.86	0.21	0.18
4	5	2	2	2	2	13	0.19	0.66	0.14	0.16
5	4	3	2	1	1	11	0.22	0.86	0.21	0.17
6	5	2	2	1	1	11	0.21	0.72	0.16	0.18
7	4	3	1	1	1	10	0.23	0.86	0.21	0.16
8	4	5	2	2	2	15	0.2	0.86	0.18	0.14
9	5	3	2	1	3	14	0.23	0.86	0.19	0.17
10	4	3	2	2	0	11	0.15	0.21	0.04	0.14
11	4	5	2	1	1	13	0.2	0.83	0.19	0.15

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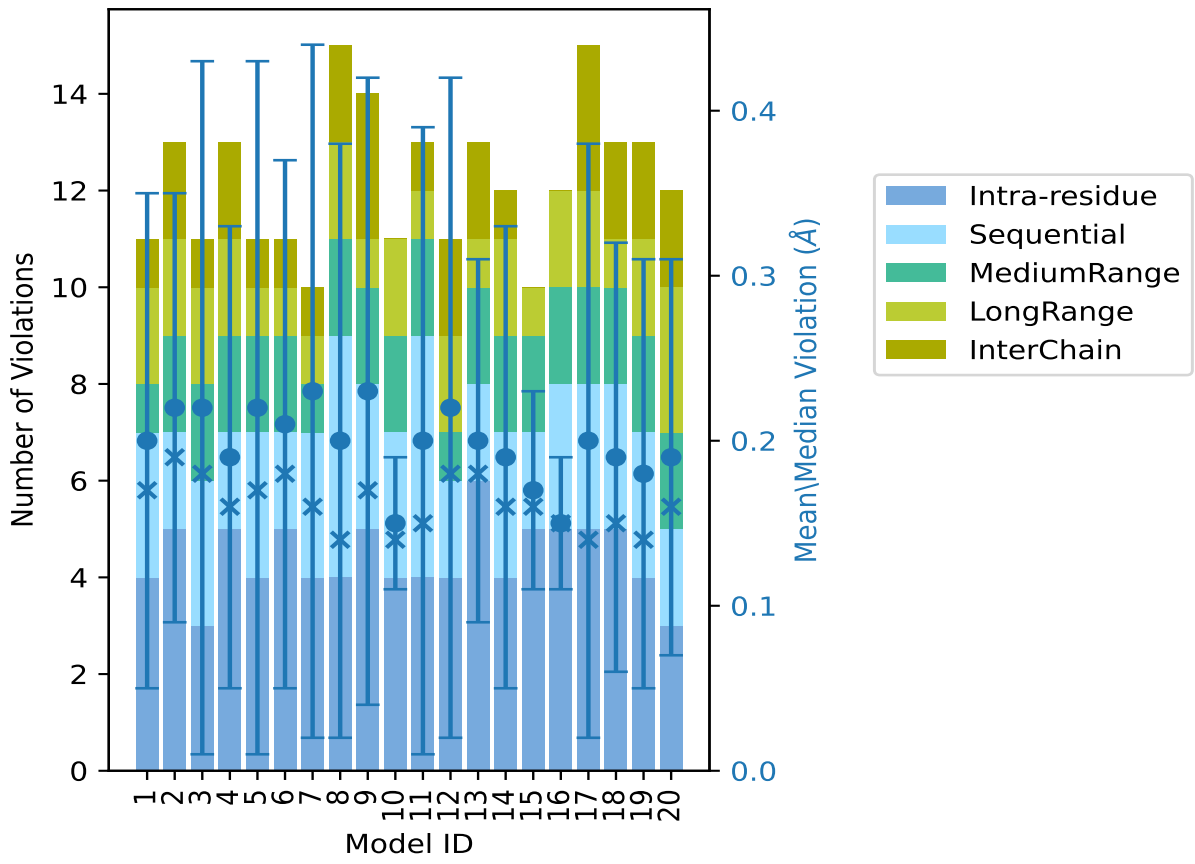
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	4	2	1	2	2	11	0.22	0.84	0.2	0.18
13	6	2	2	1	2	13	0.2	0.49	0.11	0.18
14	4	3	2	2	1	12	0.19	0.66	0.14	0.16
15	5	2	2	1	0	10	0.17	0.33	0.06	0.16
16	5	3	2	2	0	12	0.15	0.21	0.04	0.15
17	5	3	2	2	3	15	0.2	0.86	0.18	0.14
18	5	3	2	1	2	13	0.19	0.62	0.13	0.15
19	4	3	2	2	2	13	0.18	0.6	0.13	0.14
20	3	2	2	3	2	12	0.19	0.56	0.12	0.16

[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

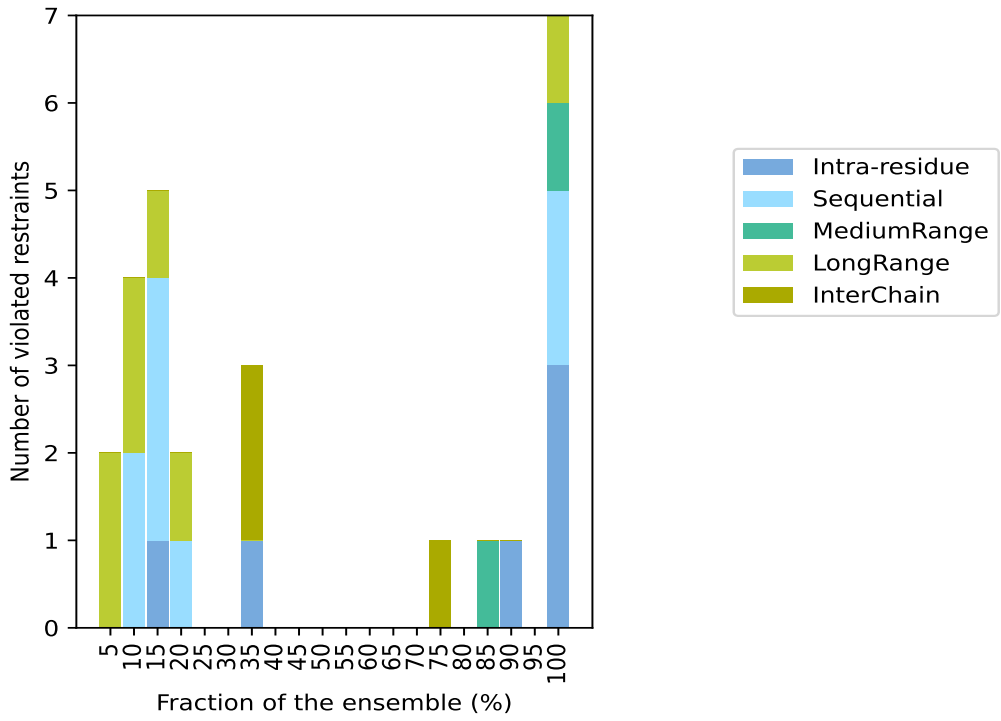
9.3 Distance violation statistics for the ensemble (i)

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, 1555(IR:371, SQ:401, MR:238, LR:473, IC:72) 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]	%
0	0	0	2	0	2	1	5.0
0	2	0	2	0	4	2	10.0
1	3	0	1	0	5	3	15.0
0	1	0	1	0	2	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
1	0	0	0	2	3	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	1	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	1	0	0	1	17	85.0
1	0	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
3	2	1	1	0	7	20	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

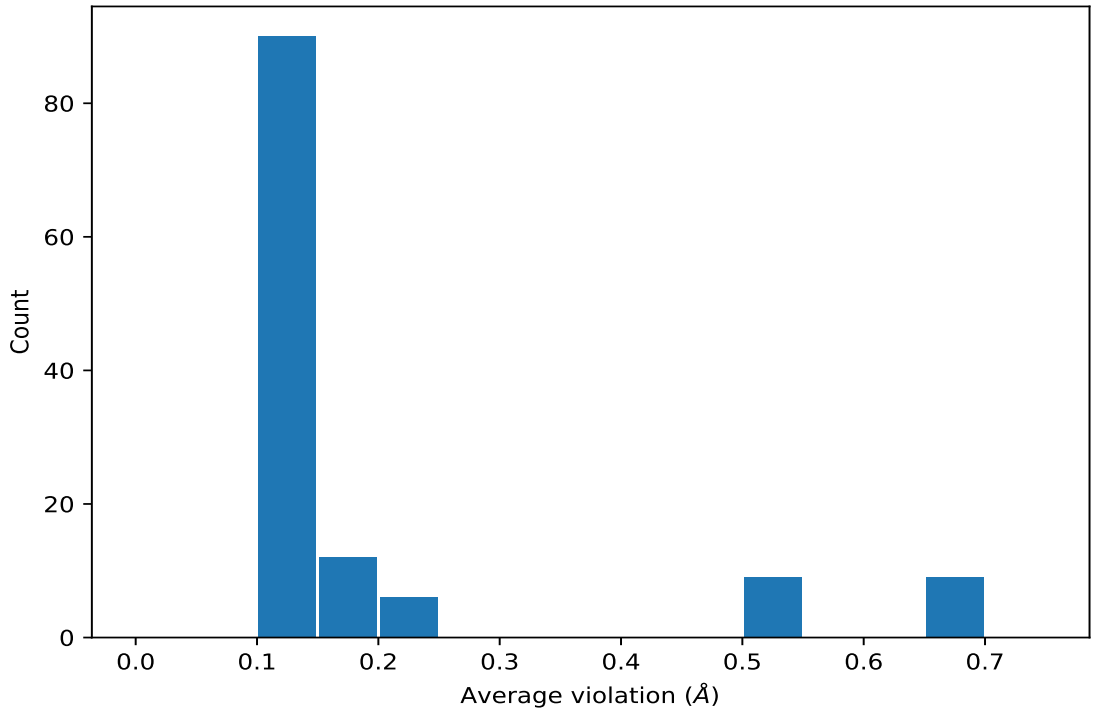
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	20	0.22	0.03	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	20	0.22	0.03	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	20	0.22	0.03	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	20	0.22	0.03	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	20	0.22	0.03	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	20	0.22	0.03	0.22
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	20	0.19	0.01	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	20	0.19	0.0	0.19
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	20	0.18	0.0	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	20	0.18	0.01	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	20	0.18	0.01	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	20	0.18	0.01	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	20	0.18	0.01	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	20	0.18	0.01	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	20	0.18	0.01	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	20	0.18	0.01	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	20	0.18	0.01	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	20	0.18	0.01	0.18
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	20	0.14	0.0	0.14
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	20	0.12	0.0	0.12
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	18	0.11	0.0	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	17	0.11	0.0	0.11
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	15	0.69	0.16	0.66
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	15	0.69	0.16	0.66
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	15	0.69	0.16	0.66
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	15	0.69	0.16	0.66
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	15	0.69	0.16	0.66
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	15	0.69	0.16	0.66
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	15	0.69	0.16	0.66
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	15	0.69	0.16	0.66
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	15	0.69	0.16	0.66
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD21	7	0.53	0.26	0.51
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD22	7	0.53	0.26	0.51
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD23	7	0.53	0.26	0.51
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD21	7	0.53	0.26	0.51
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD22	7	0.53	0.26	0.51
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD23	7	0.53	0.26	0.51
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD21	7	0.53	0.26	0.51
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD22	7	0.53	0.26	0.51
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD23	7	0.53	0.26	0.51
(1,701)	1:A:95:THR:H	1:A:95:THR:HB	7	0.14	0.0	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG22	7	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG23	7	0.13	0.01	0.13
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD21	4	0.13	0.02	0.12
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD22	4	0.13	0.02	0.12
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD23	4	0.13	0.02	0.12
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD21	4	0.13	0.02	0.12
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD22	4	0.13	0.02	0.12
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD23	4	0.13	0.02	0.12
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD21	4	0.13	0.02	0.12
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD22	4	0.13	0.02	0.12
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD23	4	0.13	0.02	0.12
(1,564)	1:A:75:ASN:H	1:A:74:ASP:HA	4	0.12	0.0	0.12
(1,603)	1:A:81:VAL:H	1:A:81:VAL:HB	3	0.15	0.0	0.15
(1,1)	1:A:2:SER:H	1:A:1:PRO:HA	3	0.12	0.0	0.12
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD11	3	0.12	0.0	0.12
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD12	3	0.12	0.0	0.12
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD13	3	0.12	0.0	0.12
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD11	3	0.12	0.0	0.12
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD12	3	0.12	0.0	0.12
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD13	3	0.12	0.0	0.12
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD11	3	0.12	0.0	0.12
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD12	3	0.12	0.0	0.12
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD13	3	0.12	0.0	0.12
(1,1465)	2:B:667:GLU:H	2:B:666:SER:HA	3	0.11	0.0	0.11
(1,1278)	1:A:79:GLU:HA	1:A:78:ASN:HA	3	0.11	0.0	0.11

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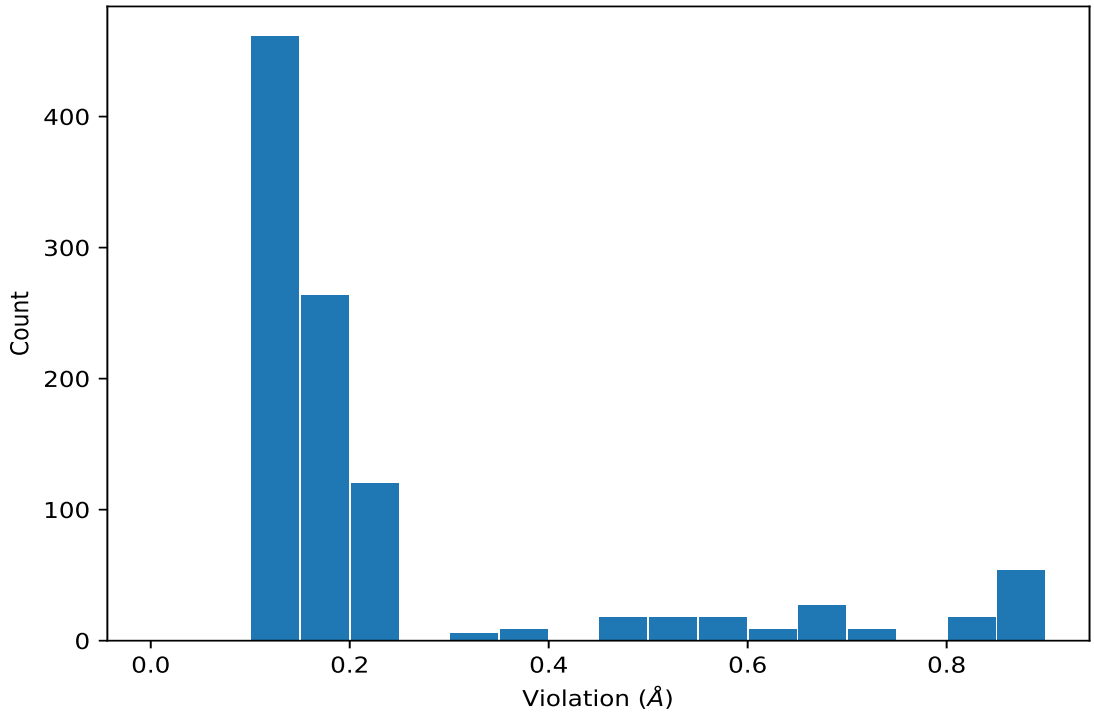
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1172)	1:A:50:ALA:HB1	1:A:101:LYS:HD2	2	0.14	0.01	0.14
(1,1172)	1:A:50:ALA:HB1	1:A:101:LYS:HD3	2	0.14	0.01	0.14
(1,1172)	1:A:50:ALA:HB2	1:A:101:LYS:HD2	2	0.14	0.01	0.14
(1,1172)	1:A:50:ALA:HB2	1:A:101:LYS:HD3	2	0.14	0.01	0.14
(1,1172)	1:A:50:ALA:HB3	1:A:101:LYS:HD2	2	0.14	0.01	0.14
(1,1172)	1:A:50:ALA:HB3	1:A:101:LYS:HD3	2	0.14	0.01	0.14
(1,1466)	2:B:669:LEU:H	2:B:668:GLU:HA	2	0.12	0.0	0.12
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG11	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG12	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG13	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG21	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG22	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG23	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG11	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG12	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG13	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG21	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG22	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG23	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG11	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG12	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG13	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG21	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG22	2	0.11	0.0	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG23	2	0.11	0.0	0.11
(1,1463)	2:B:678:GLN:H	2:B:677:SER:HA	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)
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD21	9	0.86
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD22	9	0.86
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD23	9	0.86
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD21	9	0.86
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD22	9	0.86
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD23	9	0.86
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD21	9	0.86
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD22	9	0.86
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD23	9	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	3	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	3	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	3	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	3	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	3	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	3	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	3	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	3	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	3	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	5	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	5	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	5	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	5	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	5	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	5	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	5	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	5	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	5	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	7	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	7	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	7	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	7	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	7	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	7	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	7	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	7	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	7	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	8	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	8	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	8	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	8	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	8	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	8	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	8	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	8	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	8	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	17	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	17	0.86
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	17	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	17	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	17	0.86
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	17	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	17	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	17	0.86
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	17	0.86
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD21	12	0.84
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD22	12	0.84
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD23	12	0.84
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD21	12	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD22	12	0.84
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD23	12	0.84
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD21	12	0.84
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD22	12	0.84
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD23	12	0.84
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	11	0.83
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	11	0.83
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	11	0.83
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	11	0.83
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	11	0.83
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	11	0.83
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	11	0.83
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	11	0.83
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	11	0.83
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	6	0.72
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	6	0.72
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	6	0.72
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	6	0.72
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	6	0.72
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	6	0.72
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	6	0.72
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	6	0.72
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	6	0.72
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD21	1	0.67
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD22	1	0.67
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD23	1	0.67
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD21	1	0.67
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD22	1	0.67
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD23	1	0.67
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD21	1	0.67
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD22	1	0.67
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD23	1	0.67
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	4	0.66
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	4	0.66
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	4	0.66
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	4	0.66
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	4	0.66
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	4	0.66
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	4	0.66
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	4	0.66
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	4	0.66
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	14	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	14	0.66
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	14	0.66
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	14	0.66
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	14	0.66
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	14	0.66
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	14	0.66
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	14	0.66
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	14	0.66
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	18	0.62
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	18	0.62
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	18	0.62
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	18	0.62
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	18	0.62
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	18	0.62
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	18	0.62
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	18	0.62
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	18	0.62
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	19	0.6
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	19	0.6
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	19	0.6
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	19	0.6
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	19	0.6
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	19	0.6
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	19	0.6
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	19	0.6
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	19	0.6
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	20	0.56
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	20	0.56
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	20	0.56
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	20	0.56
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	20	0.56
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	20	0.56
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	20	0.56
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	20	0.56
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	20	0.56
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	2	0.54
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	2	0.54
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	2	0.54
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	2	0.54
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	2	0.54
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	2	0.54
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	2	0.54
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	2	0.54
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD21	2	0.51
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD22	2	0.51
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD23	2	0.51
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD21	2	0.51
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD22	2	0.51
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD23	2	0.51
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD21	2	0.51
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD22	2	0.51
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD23	2	0.51
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD21	13	0.49
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD22	13	0.49
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD23	13	0.49
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD21	13	0.49
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD22	13	0.49
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD23	13	0.49
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD21	13	0.49
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD22	13	0.49
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD23	13	0.49
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	9	0.46
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	9	0.46
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	9	0.46
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	9	0.46
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	9	0.46
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	9	0.46
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	9	0.46
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	9	0.46
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	9	0.46
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD11	13	0.39
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD12	13	0.39
(1,1500)	1:A:59:MET:HE1	2:B:665:LEU:HD13	13	0.39
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD11	13	0.39
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD12	13	0.39
(1,1500)	1:A:59:MET:HE2	2:B:665:LEU:HD13	13	0.39
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD11	13	0.39
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD12	13	0.39
(1,1500)	1:A:59:MET:HE3	2:B:665:LEU:HD13	13	0.39
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	15	0.33
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	15	0.33
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	15	0.33
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	15	0.33
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	15	0.33
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	6	0.23
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	6	0.23
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	6	0.23
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	6	0.23
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	6	0.23
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	6	0.23
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	7	0.23
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	7	0.23
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	7	0.23
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	7	0.23
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	7	0.23
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	7	0.23
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	9	0.23
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	9	0.23
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	9	0.23
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	9	0.23
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	9	0.23
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	9	0.23
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	18	0.23
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	18	0.23
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	18	0.23
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	18	0.23
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	18	0.23
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	18	0.23
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	2	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	2	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	2	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	2	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	2	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	2	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	3	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	3	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	3	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	3	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	3	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	3	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	8	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	8	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	8	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	8	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	8	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	13	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	13	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	13	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	13	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	13	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	13	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	20	0.22
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	20	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	20	0.22
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	20	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	20	0.22
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	20	0.22
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	6	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	1	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	1	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	1	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	1	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	1	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	1	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	5	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	5	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	5	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	5	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	5	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	5	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	10	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	10	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	10	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	10	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	10	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	10	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	11	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	11	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	11	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	11	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	11	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	11	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	12	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	12	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	12	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	12	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	12	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	16	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	16	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	16	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	16	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	16	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	16	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	17	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	17	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	17	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	17	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	17	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	17	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	19	0.21
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	19	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	19	0.21
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	19	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	19	0.21
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	19	0.21
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	2	0.2
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	3	0.2
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	5	0.2
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	11	0.2
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	20	0.2
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	4	0.2
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	4	0.2
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	4	0.2
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	4	0.2
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	4	0.2
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	4	0.2
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE1	14	0.2
(1,1409)	1:A:107:ILE:HG21	1:A:111:TYR:HE2	14	0.2
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE1	14	0.2
(1,1409)	1:A:107:ILE:HG22	1:A:111:TYR:HE2	14	0.2
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE1	14	0.2
(1,1409)	1:A:107:ILE:HG23	1:A:111:TYR:HE2	14	0.2
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	7	0.19
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	8	0.19
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	9	0.19
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	13	0.19
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	15	0.19
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	16	0.19
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	17	0.19
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	18	0.19
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	19	0.19
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD21	17	0.19
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD22	17	0.19
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD23	17	0.19
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD21	17	0.19
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD22	17	0.19
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD23	17	0.19
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD21	17	0.19
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD22	17	0.19
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD23	17	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	1	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	2	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	4	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	5	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	7	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	9	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	10	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	11	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	12	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	13	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	14	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	15	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	16	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	17	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	18	0.19
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	20	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	2	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	2	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	2	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	2	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	2	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	2	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	2	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	2	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	2	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	3	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	3	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	3	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	3	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	3	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	3	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	3	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	3	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	8	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	8	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	8	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	8	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	8	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	8	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	8	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	8	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	8	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	13	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	13	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	13	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	13	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	13	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	13	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	13	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	13	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	13	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	16	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	16	0.19
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	16	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	16	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	16	0.19
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	16	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	16	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	16	0.19
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	16	0.19
(1,1072)	1:A:29:TRP:HD1	1:A:16:ILE:HG12	2	0.19
(1,1072)	1:A:29:TRP:HD1	1:A:16:ILE:HG13	2	0.19
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	1	0.18
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	12	0.18
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD21	8	0.18
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD22	8	0.18
(1,1501)	1:A:59:MET:HE1	2:B:665:LEU:HD23	8	0.18
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD21	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD22	8	0.18
(1,1501)	1:A:59:MET:HE2	2:B:665:LEU:HD23	8	0.18
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD21	8	0.18
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD22	8	0.18
(1,1501)	1:A:59:MET:HE3	2:B:665:LEU:HD23	8	0.18
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	3	0.18
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	6	0.18
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	8	0.18
(1,1467)	2:B:668:GLU:H	2:B:667:GLU:HA	19	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	1	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	2	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	3	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	4	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	5	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	6	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	8	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	9	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	10	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	11	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	12	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	13	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	14	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	15	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	16	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	17	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	18	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	19	0.18
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	20	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	6	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	6	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	6	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	6	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	6	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	6	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	6	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	6	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	6	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	9	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	9	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	9	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	9	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	9	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	9	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	9	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	9	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	11	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	11	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	11	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	11	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	11	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	11	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	11	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	11	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	11	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	12	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	12	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	12	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	12	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	12	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	12	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	12	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	12	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	12	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	14	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	14	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	14	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	14	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	14	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	14	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	14	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	14	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	14	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	17	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	17	0.18
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	17	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	17	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	17	0.18
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	17	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	17	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	17	0.18
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	17	0.18
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	4	0.17
(1,231)	1:A:29:TRP:H	1:A:29:TRP:HD1	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	1	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	1	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	1	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	1	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	1	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	1	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	1	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	1	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	1	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	4	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	4	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	4	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	4	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	4	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	4	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	4	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	4	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	4	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	5	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	5	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	5	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	5	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	5	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	5	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	5	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	5	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	5	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	10	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	10	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	10	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	10	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	10	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	10	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	10	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	10	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	10	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	15	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	15	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	15	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	15	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	15	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	15	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	15	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	15	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	18	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	18	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	18	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	18	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	18	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	18	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	18	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	18	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	18	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	19	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	19	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	19	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	19	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	19	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	19	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	19	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	19	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	19	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	20	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	20	0.17
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	20	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	20	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	20	0.17
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	20	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	20	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	20	0.17
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	20	0.17
(1,603)	1:A:81:VAL:H	1:A:81:VAL:HB	9	0.16
(1,1282)	1:A:80:VAL:HA	1:A:80:VAL:HB	7	0.16
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB1	7	0.16
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB2	7	0.16
(1,1206)	1:A:60:LEU:HD21	1:A:50:ALA:HB3	7	0.16
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB1	7	0.16
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB2	7	0.16
(1,1206)	1:A:60:LEU:HD22	1:A:50:ALA:HB3	7	0.16
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB1	7	0.16
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB2	7	0.16
(1,1206)	1:A:60:LEU:HD23	1:A:50:ALA:HB3	7	0.16
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD21	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD22	4	0.16
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD23	4	0.16
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD21	4	0.16
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD22	4	0.16
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD23	4	0.16
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD21	4	0.16
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD22	4	0.16
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD23	4	0.16
(1,701)	1:A:95:THR:H	1:A:95:THR:HB	4	0.15
(1,701)	1:A:95:THR:H	1:A:95:THR:HB	16	0.15
(1,603)	1:A:81:VAL:H	1:A:81:VAL:HB	13	0.15
(1,603)	1:A:81:VAL:H	1:A:81:VAL:HB	18	0.15
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	9	0.15
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	11	0.15
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	18	0.15
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG11	9	0.15
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG12	9	0.15
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG13	9	0.15
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG21	9	0.15
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG22	9	0.15
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG23	9	0.15
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG11	9	0.15
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG12	9	0.15
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG13	9	0.15
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG21	9	0.15
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG22	9	0.15
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG23	9	0.15
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG11	9	0.15
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG12	9	0.15
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG13	9	0.15
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG21	9	0.15
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG22	9	0.15
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG23	9	0.15
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG11	9	0.15
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG12	9	0.15
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG13	9	0.15
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG21	9	0.15
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG22	9	0.15
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG23	9	0.15
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG11	9	0.15
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG12	9	0.15
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG13	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG21	9	0.15
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG22	9	0.15
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG23	9	0.15
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG11	9	0.15
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG12	9	0.15
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG13	9	0.15
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG21	9	0.15
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG22	9	0.15
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG23	9	0.15
(1,701)	1:A:95:THR:H	1:A:95:THR:HB	2	0.14
(1,701)	1:A:95:THR:H	1:A:95:THR:HB	6	0.14
(1,701)	1:A:95:THR:H	1:A:95:THR:HB	13	0.14
(1,701)	1:A:95:THR:H	1:A:95:THR:HB	15	0.14
(1,701)	1:A:95:THR:H	1:A:95:THR:HB	17	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	1	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	2	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	3	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	4	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	5	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	6	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	7	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	8	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	10	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	12	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	13	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	14	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	15	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	16	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	17	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	19	0.14
(1,365)	1:A:44:THR:H	1:A:44:THR:HB	20	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG11	4	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG12	4	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG13	4	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG21	4	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG22	4	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG23	4	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG11	4	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG12	4	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG13	4	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG21	4	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG22	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG23	4	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG11	4	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG12	4	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG13	4	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG21	4	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG22	4	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG23	4	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG11	4	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG12	4	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG13	4	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG21	4	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG22	4	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG23	4	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG11	4	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG12	4	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG13	4	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG21	4	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG22	4	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG23	4	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG11	4	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG12	4	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG13	4	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG21	4	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG22	4	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG23	4	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG11	12	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG12	12	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG13	12	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG21	12	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG22	12	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG23	12	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG11	12	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG12	12	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG13	12	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG21	12	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG22	12	0.14
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG23	12	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG11	12	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG12	12	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG13	12	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG21	12	0.14
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG22	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG23	12	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG11	12	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG12	12	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG13	12	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG21	12	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG22	12	0.14
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG23	12	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG11	12	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG12	12	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG13	12	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG21	12	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG22	12	0.14
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG23	12	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG11	12	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG12	12	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG13	12	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG21	12	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG22	12	0.14
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG23	12	0.14
(1,1172)	1:A:50:ALA:HB1	1:A:101:LYS:HD2	14	0.14
(1,1172)	1:A:50:ALA:HB1	1:A:101:LYS:HD3	14	0.14
(1,1172)	1:A:50:ALA:HB2	1:A:101:LYS:HD2	14	0.14
(1,1172)	1:A:50:ALA:HB2	1:A:101:LYS:HD3	14	0.14
(1,1172)	1:A:50:ALA:HB3	1:A:101:LYS:HD2	14	0.14
(1,1172)	1:A:50:ALA:HB3	1:A:101:LYS:HD3	14	0.14
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG11	18	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG12	18	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG13	18	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG21	18	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG22	18	0.13
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG23	18	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG11	18	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG12	18	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG13	18	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG21	18	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG22	18	0.13
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG23	18	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG11	18	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG12	18	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG13	18	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG21	18	0.13
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG22	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG23	18	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG11	18	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG12	18	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG13	18	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG21	18	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG22	18	0.13
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG23	18	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG11	18	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG12	18	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG13	18	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG21	18	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG22	18	0.13
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG23	18	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG11	18	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG12	18	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG13	18	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG21	18	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG22	18	0.13
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG23	18	0.13
(1,1172)	1:A:50:ALA:HB1	1:A:101:LYS:HD2	3	0.13
(1,1172)	1:A:50:ALA:HB1	1:A:101:LYS:HD3	3	0.13
(1,1172)	1:A:50:ALA:HB2	1:A:101:LYS:HD2	3	0.13
(1,1172)	1:A:50:ALA:HB2	1:A:101:LYS:HD3	3	0.13
(1,1172)	1:A:50:ALA:HB3	1:A:101:LYS:HD2	3	0.13
(1,1172)	1:A:50:ALA:HB3	1:A:101:LYS:HD3	3	0.13
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD21	12	0.13
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD22	12	0.13
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD23	12	0.13
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD21	12	0.13
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD22	12	0.13
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD23	12	0.13
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD21	12	0.13
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD22	12	0.13
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD23	12	0.13
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	1	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	2	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	5	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	6	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	7	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	9	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	10	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	15	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	16	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	18	0.12
(1,564)	1:A:75:ASN:H	1:A:74:ASP:HA	7	0.12
(1,564)	1:A:75:ASN:H	1:A:74:ASP:HA	10	0.12
(1,564)	1:A:75:ASN:H	1:A:74:ASP:HA	16	0.12
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	2	0.12
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	6	0.12
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	16	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG11	19	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG12	19	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG13	19	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG21	19	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG22	19	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG23	19	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG11	19	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG12	19	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG13	19	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG21	19	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG22	19	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG23	19	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG11	19	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG12	19	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG13	19	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG21	19	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG22	19	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG23	19	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG11	19	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG12	19	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG13	19	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG21	19	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG22	19	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG23	19	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG11	19	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG12	19	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG13	19	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG21	19	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG22	19	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG23	19	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG11	19	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG12	19	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG13	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG21	19	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG22	19	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG23	19	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG11	20	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG12	20	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG13	20	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG21	20	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG22	20	0.12
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG23	20	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG11	20	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG12	20	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG13	20	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG21	20	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG22	20	0.12
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG23	20	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG11	20	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG12	20	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG13	20	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG21	20	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG22	20	0.12
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG23	20	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG11	20	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG12	20	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG13	20	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG21	20	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG22	20	0.12
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG23	20	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG11	20	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG12	20	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG13	20	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG21	20	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG22	20	0.12
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG23	20	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG11	20	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG12	20	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG13	20	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG21	20	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG22	20	0.12
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG23	20	0.12
(1,1466)	2:B:669:LEU:H	2:B:668:GLU:HA	8	0.12
(1,1466)	2:B:669:LEU:H	2:B:668:GLU:HA	11	0.12
(1,1465)	2:B:667:GLU:H	2:B:666:SER:HA	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	11	0.12
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD11	10	0.12
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD12	10	0.12
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD13	10	0.12
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD11	10	0.12
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD12	10	0.12
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD13	10	0.12
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD11	10	0.12
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD12	10	0.12
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD13	10	0.12
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD11	20	0.12
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD12	20	0.12
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD13	20	0.12
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD11	20	0.12
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD12	20	0.12
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD13	20	0.12
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD11	20	0.12
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD12	20	0.12
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD13	20	0.12
(1,1)	1:A:2:SER:H	1:A:1:PRO:HA	1	0.12
(1,1)	1:A:2:SER:H	1:A:1:PRO:HA	14	0.12
(1,1)	1:A:2:SER:H	1:A:1:PRO:HA	17	0.12
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	3	0.11
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	4	0.11
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	8	0.11
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	11	0.11
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	12	0.11
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	13	0.11
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	17	0.11
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	19	0.11
(1,828)	1:A:109:SER:H	1:A:108:ILE:HA	20	0.11
(1,564)	1:A:75:ASN:H	1:A:74:ASP:HA	8	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	3	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	4	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	5	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	8	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	9	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	10	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	11	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	13	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	14	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	17	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	18	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	19	0.11
(1,371)	1:A:45:ILE:H	1:A:43:SER:H	20	0.11
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG11	17	0.11
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG12	17	0.11
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG13	17	0.11
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG21	17	0.11
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG22	17	0.11
(1,1573)	1:A:48:LEU:HD11	2:B:673:VAL:HG23	17	0.11
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG11	17	0.11
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG12	17	0.11
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG13	17	0.11
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG21	17	0.11
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG22	17	0.11
(1,1573)	1:A:48:LEU:HD12	2:B:673:VAL:HG23	17	0.11
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG11	17	0.11
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG12	17	0.11
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG13	17	0.11
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG21	17	0.11
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG22	17	0.11
(1,1573)	1:A:48:LEU:HD13	2:B:673:VAL:HG23	17	0.11
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG11	17	0.11
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG12	17	0.11
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG13	17	0.11
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG21	17	0.11
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG22	17	0.11
(1,1573)	1:A:48:LEU:HD21	2:B:673:VAL:HG23	17	0.11
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG11	17	0.11
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG12	17	0.11
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG13	17	0.11
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG21	17	0.11
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG22	17	0.11
(1,1573)	1:A:48:LEU:HD22	2:B:673:VAL:HG23	17	0.11
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG11	17	0.11
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG12	17	0.11
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG13	17	0.11
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG21	17	0.11
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG22	17	0.11
(1,1573)	1:A:48:LEU:HD23	2:B:673:VAL:HG23	17	0.11
(1,1465)	2:B:667:GLU:H	2:B:666:SER:HA	9	0.11
(1,1465)	2:B:667:GLU:H	2:B:666:SER:HA	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1463)	2:B:678:GLN:H	2:B:677:SER:HA	11	0.11
(1,1463)	2:B:678:GLN:H	2:B:677:SER:HA	18	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	1	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	2	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	4	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	5	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	6	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	7	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	8	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	9	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	10	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	12	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	13	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	14	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	15	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	16	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	17	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	18	0.11
(1,1345)	1:A:95:THR:HB	1:A:95:THR:HA	19	0.11
(1,1278)	1:A:79:GLU:HA	1:A:78:ASN:HA	3	0.11
(1,1278)	1:A:79:GLU:HA	1:A:78:ASN:HA	5	0.11
(1,1278)	1:A:79:GLU:HA	1:A:78:ASN:HA	19	0.11
(1,1211)	1:A:62:LEU:HB2	1:A:45:ILE:HD11	1	0.11
(1,1211)	1:A:62:LEU:HB2	1:A:45:ILE:HD12	1	0.11
(1,1211)	1:A:62:LEU:HB2	1:A:45:ILE:HD13	1	0.11
(1,1211)	1:A:62:LEU:HB3	1:A:45:ILE:HD11	1	0.11
(1,1211)	1:A:62:LEU:HB3	1:A:45:ILE:HD12	1	0.11
(1,1211)	1:A:62:LEU:HB3	1:A:45:ILE:HD13	1	0.11
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD21	16	0.11
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD22	16	0.11
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD23	16	0.11
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD21	16	0.11
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD22	16	0.11
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD23	16	0.11
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD21	16	0.11
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD22	16	0.11
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD23	16	0.11
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD21	17	0.11
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD22	17	0.11
(1,1122)	1:A:42:LEU:HD11	1:A:104:LEU:HD23	17	0.11
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD21	17	0.11
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD22	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:A:42:LEU:HD12	1:A:104:LEU:HD23	17	0.11
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD21	17	0.11
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD22	17	0.11
(1,1122)	1:A:42:LEU:HD13	1:A:104:LEU:HD23	17	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG11	19	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG12	19	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG13	19	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG21	19	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG22	19	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG23	19	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG11	19	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG12	19	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG13	19	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG21	19	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG22	19	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG23	19	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG11	19	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG12	19	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG13	19	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG21	19	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG22	19	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG23	19	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG11	20	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG12	20	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG13	20	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG21	20	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG22	20	0.11
(1,1066)	1:A:28:THR:HG21	1:A:37:VAL:HG23	20	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG11	20	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG12	20	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG13	20	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG21	20	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG22	20	0.11
(1,1066)	1:A:28:THR:HG22	1:A:37:VAL:HG23	20	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG11	20	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG12	20	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG13	20	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG21	20	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG22	20	0.11
(1,1066)	1:A:28:THR:HG23	1:A:37:VAL:HG23	20	0.11
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD11	8	0.11
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD12	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:A:27:LEU:HD21	1:A:62:LEU:HD13	8	0.11
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD11	8	0.11
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD12	8	0.11
(1,1060)	1:A:27:LEU:HD22	1:A:62:LEU:HD13	8	0.11
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD11	8	0.11
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD12	8	0.11
(1,1060)	1:A:27:LEU:HD23	1:A:62:LEU:HD13	8	0.11

10 Dihedral-angle violation analysis (i)

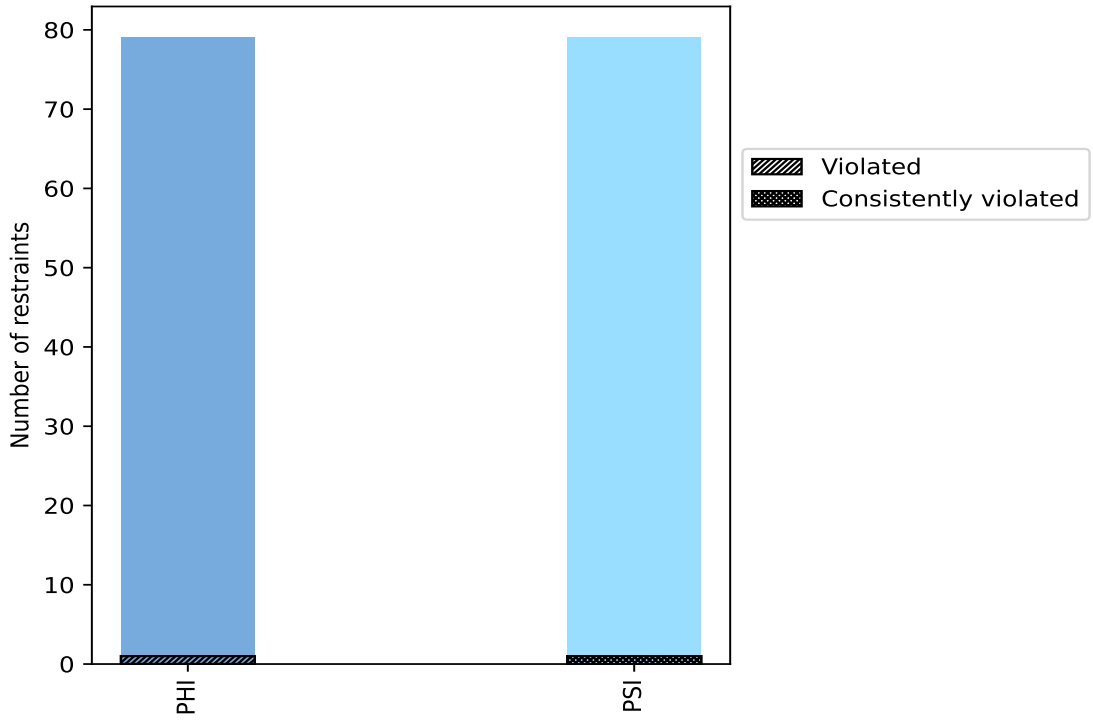
10.1 Summary of dihedral-angle violations (i)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	79	50.0	1	1.3	0.6	0	0.0	0.0
PSI	79	50.0	1	1.3	0.6	1	1.3	0.6
Total	158	100.0	2	1.3	1.3	1	0.6	0.6

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



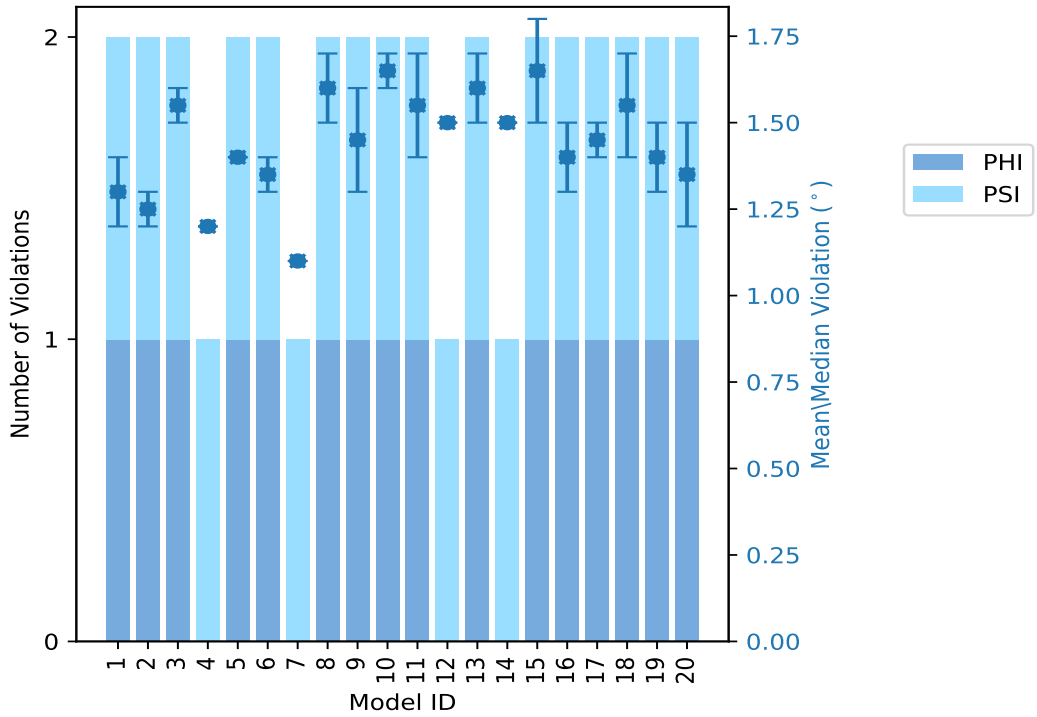
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	1	1	2	1.3	1.4	0.1	1.3
2	1	1	2	1.25	1.3	0.05	1.25
3	1	1	2	1.55	1.6	0.05	1.55
4	0	1	1	1.2	1.2	0.0	1.2
5	1	1	2	1.4	1.4	0.0	1.4
6	1	1	2	1.35	1.4	0.05	1.35
7	0	1	1	1.1	1.1	0.0	1.1
8	1	1	2	1.6	1.7	0.1	1.6
9	1	1	2	1.45	1.6	0.15	1.45
10	1	1	2	1.65	1.7	0.05	1.65
11	1	1	2	1.55	1.7	0.15	1.55
12	0	1	1	1.5	1.5	0.0	1.5
13	1	1	2	1.6	1.7	0.1	1.6
14	0	1	1	1.5	1.5	0.0	1.5
15	1	1	2	1.65	1.8	0.15	1.65
16	1	1	2	1.4	1.5	0.1	1.4
17	1	1	2	1.45	1.5	0.05	1.45
18	1	1	2	1.55	1.7	0.15	1.55
19	1	1	2	1.4	1.5	0.1	1.4
20	1	1	2	1.35	1.5	0.15	1.35

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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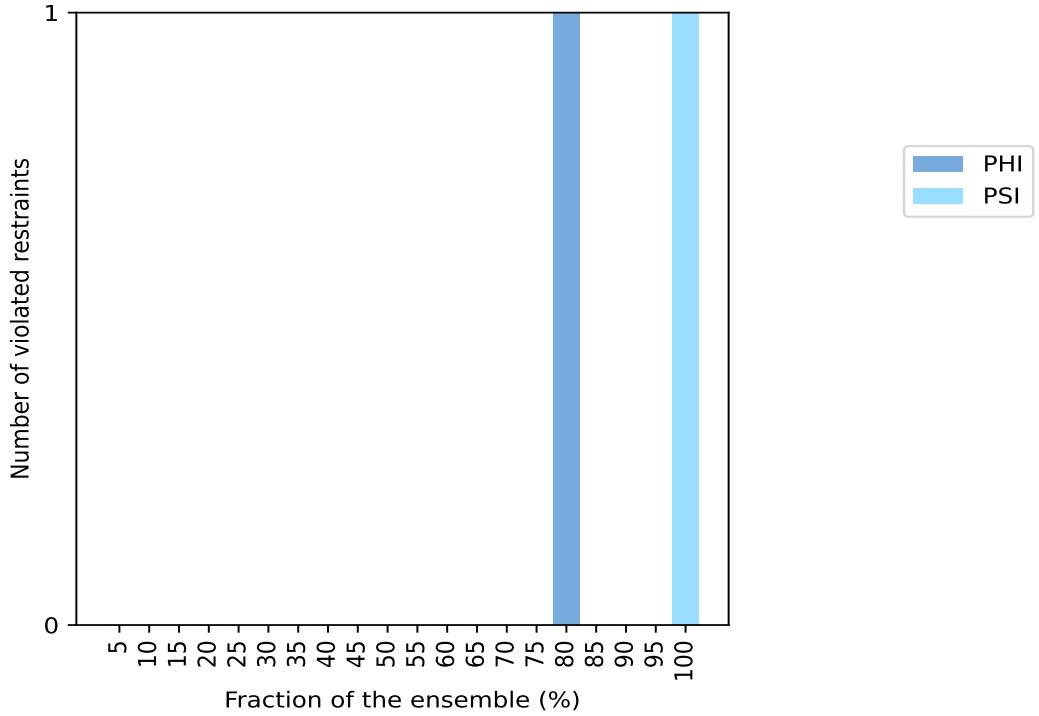
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	1	1	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)

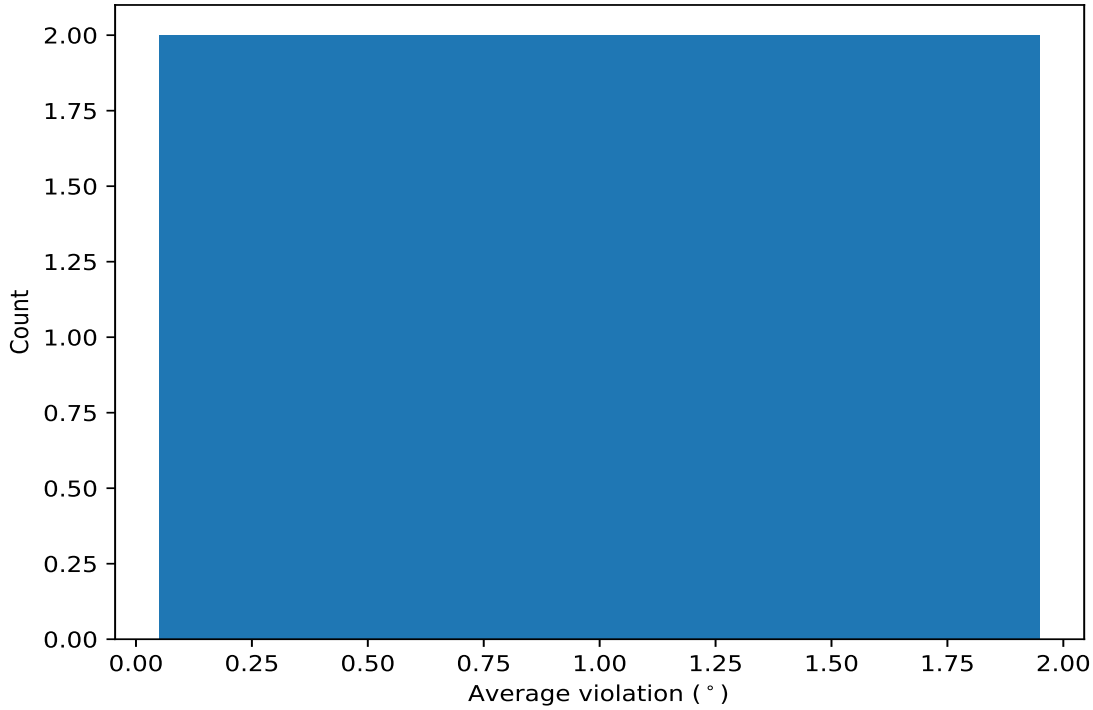


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

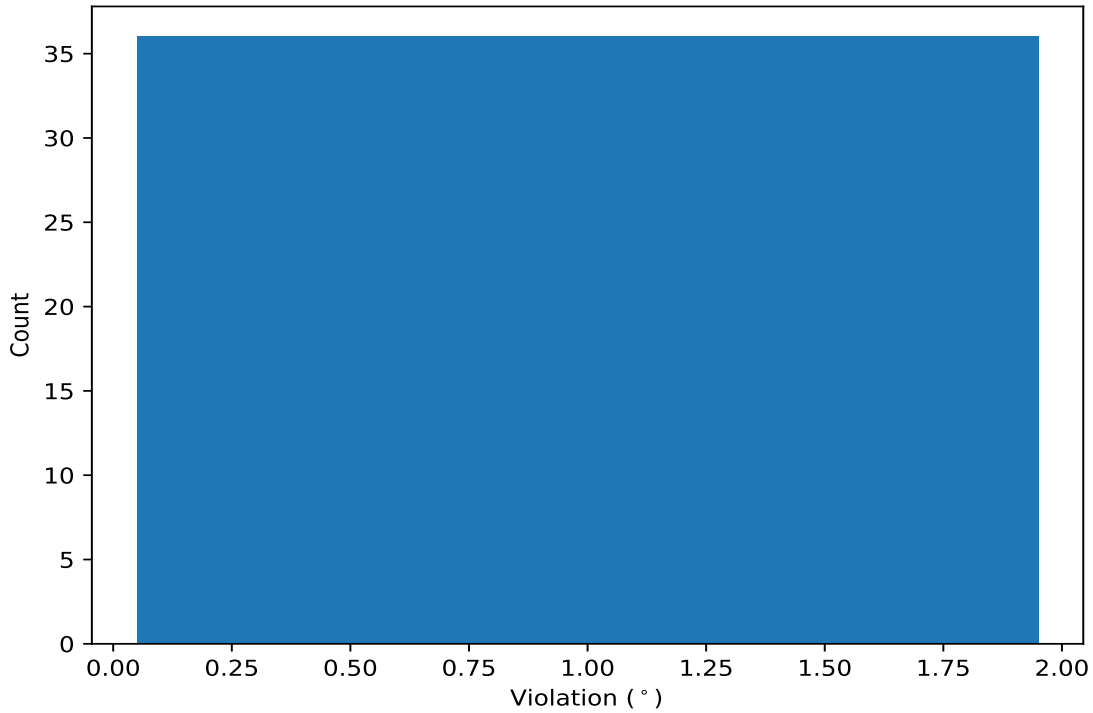
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	20	1.46	0.15	1.5
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	16	1.44	0.19	1.4

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints (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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	15	1.8
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	10	1.7
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	13	1.7
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	18	1.7
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	8	1.7
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	11	1.7
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	3	1.6
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	9	1.6
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	10	1.6
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	8	1.5
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	3	1.5
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	12	1.5
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	13	1.5
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	14	1.5
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	15	1.5
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	16	1.5
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	17	1.5
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	19	1.5
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	20	1.5
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	5	1.4
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	11	1.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	17	1.4
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	1	1.4
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	5	1.4
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	6	1.4
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	18	1.4
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	2	1.3
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	6	1.3
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	9	1.3
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	16	1.3
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	19	1.3
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	1	1.2
(1,19)	1:A:15:ILE:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	20	1.2
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	2	1.2
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	4	1.2
(1,140)	2:B:667:GLU:N	2:B:667:GLU:CA	2:B:667:GLU:C	2:B:668:GLU:N	7	1.1