



## Full wwPDB NMR Structure Validation Report ⓘ

May 7, 2025 – 04:21 pm BST

PDB ID : 9QLM / pdb\_00009qlm  
BMRB ID : 34986  
Title : Solution structure of the TAF3-PHD bound to a H3K4me3Q5ser histone tail peptide with a serotonylated glutamine  
Authors : van Ingen, H.; Gielingh, H.; Pulido-Cortes, L.; Thijssen, V.; Timmers, H.Th.M.; Jongkees, S.; Honorato, R.V.; Bonvin, A.M.J.J.; Liu, M.; Yoshisada, R.; Soares, L.R.  
Deposited on : 2025-03-21

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

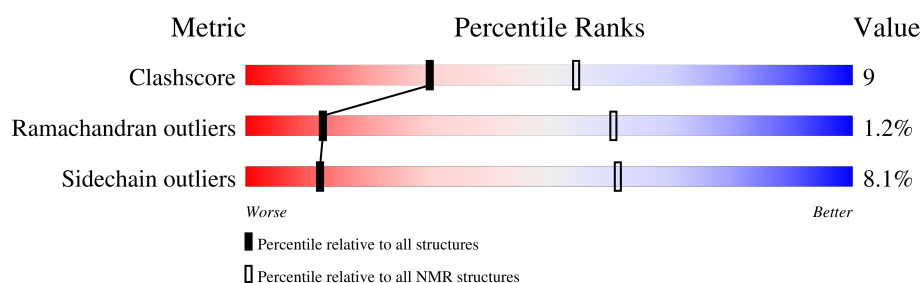
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	75	
2	B	12	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:857-A:919, B:1-B:3, B:5-B:7 (69)	0.84	8

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 5 clusters. No single-model clusters were found.

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

### 3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1366 atoms, of which 663 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms						Trace
1	A	75	Total	C	H	N	O	S	0
			1143	377	547	101	106	12	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	850	GLY	-	expression tag	UNP Q5HZG4
A	851	SER	-	expression tag	UNP Q5HZG4
A	852	HIS	-	expression tag	UNP Q5HZG4
A	853	MET	-	expression tag	UNP Q5HZG4
A	854	ALA	-	expression tag	UNP Q5HZG4
A	855	MET	-	expression tag	UNP Q5HZG4
A	856	ALA	-	expression tag	UNP Q5HZG4

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					Trace
2	B	12	Total	C	H	N	O	0
			197	55	105	20	17	

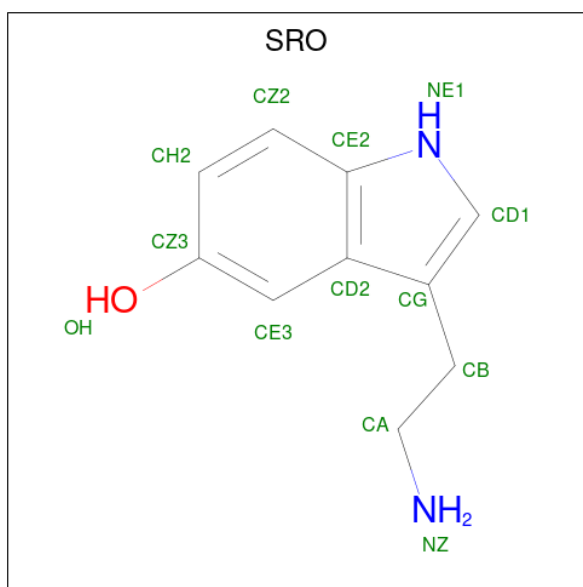
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLU	GLN	conflict	UNP P68431

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

- Molecule 4 is SEROTONIN (CCD ID: SRO) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).



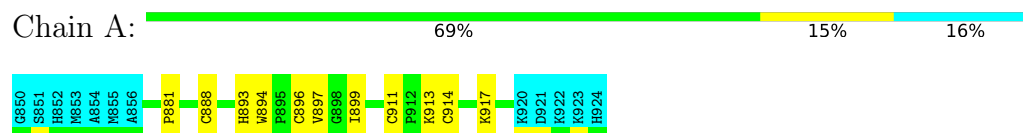
Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
4	B	1	24	10	11	2	1

## 4 Residue-property plots [i](#)

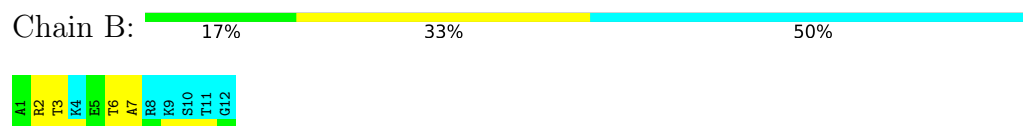
### 4.1 Average score per residue in the NMR ensemble

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: Transcription initiation factor TFIID subunit 3



- Molecule 2: Histone H3.1

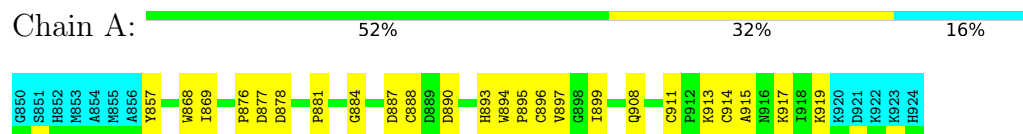


### 4.2 Scores per residue for each member of the ensemble

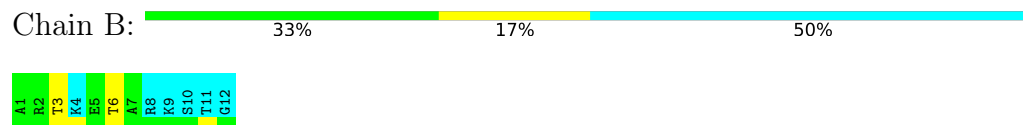
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Transcription initiation factor TFIID subunit 3

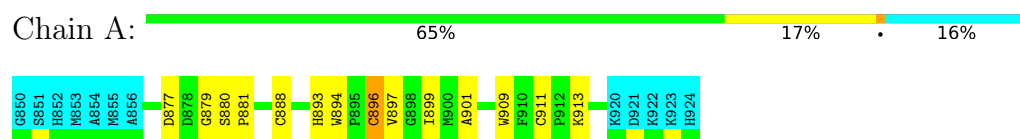


- Molecule 2: Histone H3.1

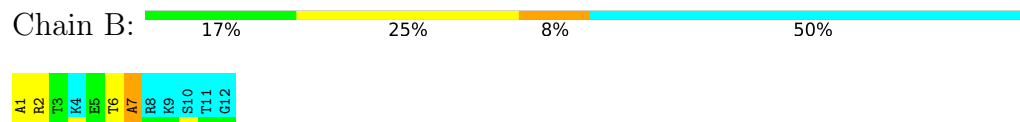


### 4.2.2 Score per residue for model 2

- Molecule 1: Transcription initiation factor TFIID subunit 3

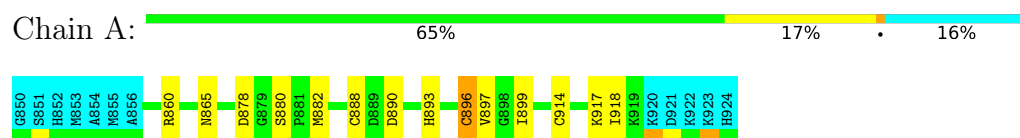


- Molecule 2: Histone H3.1

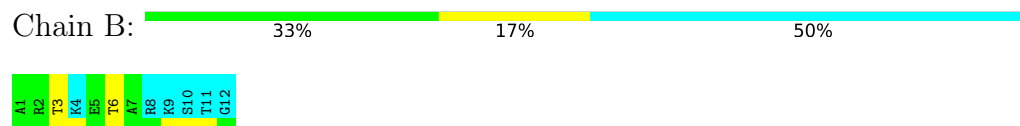


### 4.2.3 Score per residue for model 3

- Molecule 1: Transcription initiation factor TFIID subunit 3

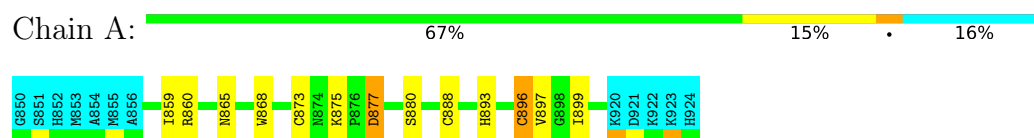


- Molecule 2: Histone H3.1

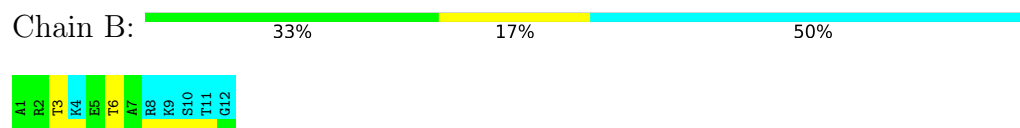


### 4.2.4 Score per residue for model 4

- Molecule 1: Transcription initiation factor TFIID subunit 3



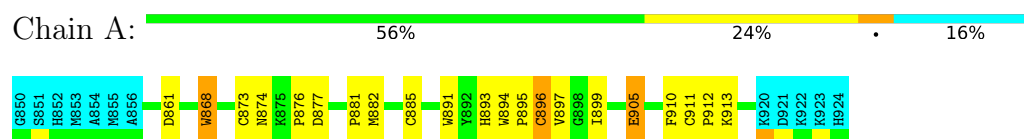
- Molecule 2: Histone H3.1



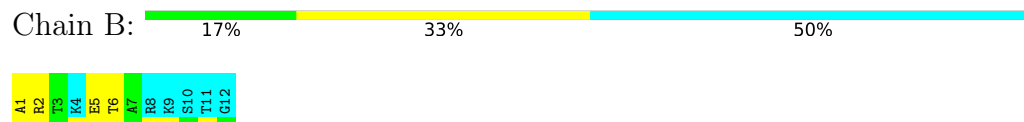


### 4.2.5 Score per residue for model 5

- Molecule 1: Transcription initiation factor TFIID subunit 3

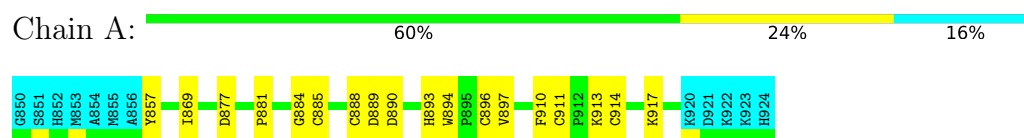


- Molecule 2: Histone H3.1

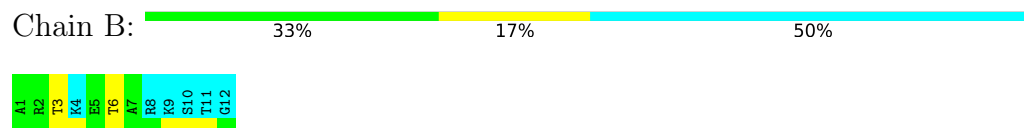


### 4.2.6 Score per residue for model 6

- Molecule 1: Transcription initiation factor TFIID subunit 3

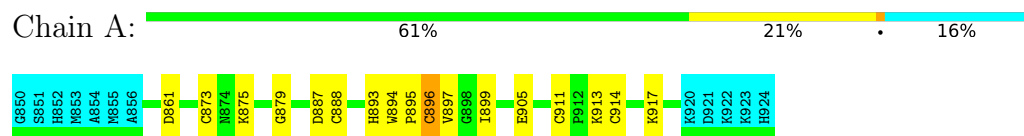


- Molecule 2: Histone H3.1

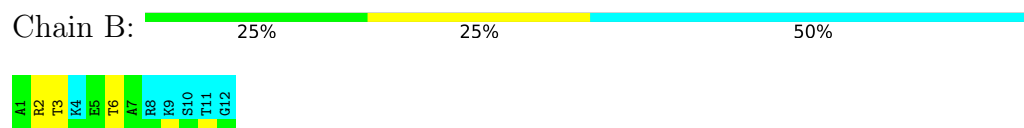


### 4.2.7 Score per residue for model 7

- Molecule 1: Transcription initiation factor TFIID subunit 3

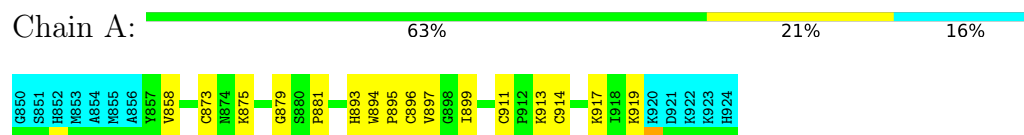


- Molecule 2: Histone H3.1

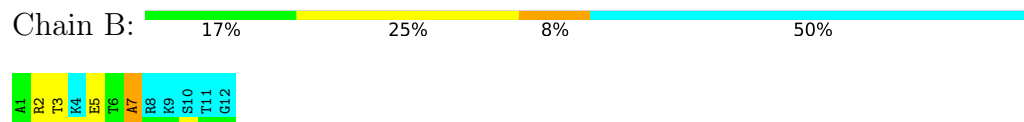


### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Transcription initiation factor TFIID subunit 3

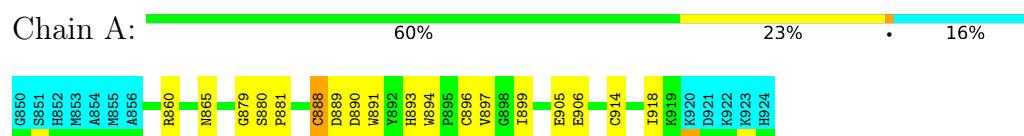


- Molecule 2: Histone H3.1

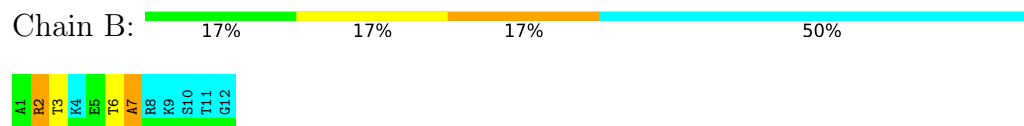


### 4.2.9 Score per residue for model 9

- Molecule 1: Transcription initiation factor TFIID subunit 3

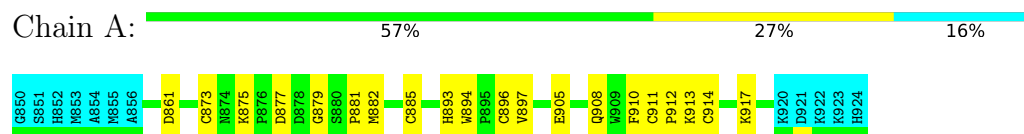


- Molecule 2: Histone H3.1



### 4.2.10 Score per residue for model 10

- Molecule 1: Transcription initiation factor TFIID subunit 3

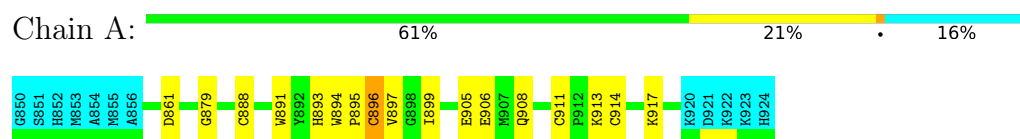


- Molecule 2: Histone H3.1

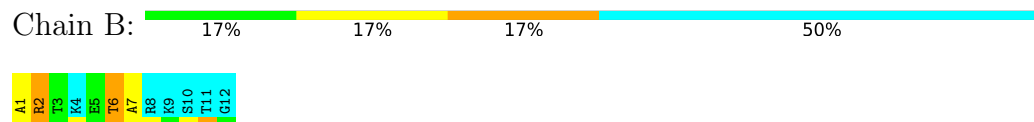


### 4.2.11 Score per residue for model 11

- Molecule 1: Transcription initiation factor TFIID subunit 3

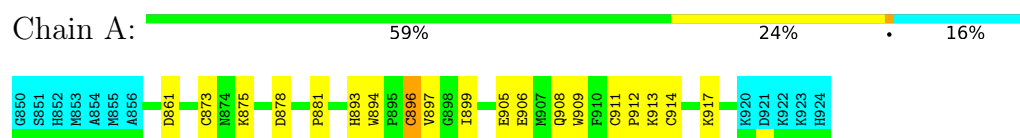


- Molecule 2: Histone H3.1

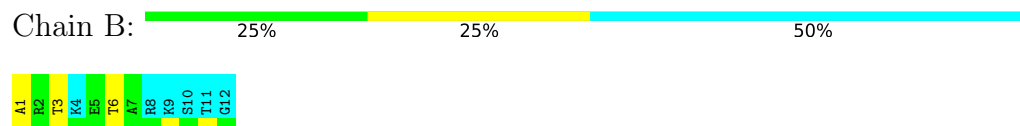


### 4.2.12 Score per residue for model 12

- Molecule 1: Transcription initiation factor TFIID subunit 3

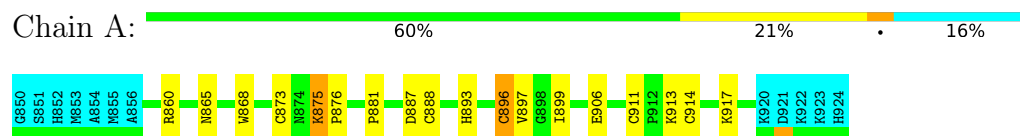


- Molecule 2: Histone H3.1

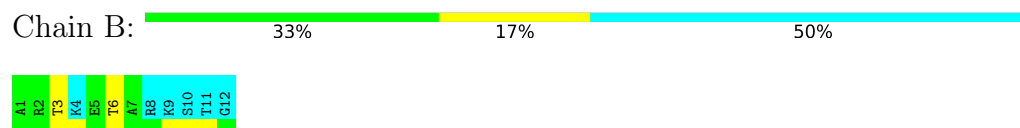


### 4.2.13 Score per residue for model 13

- Molecule 1: Transcription initiation factor TFIID subunit 3

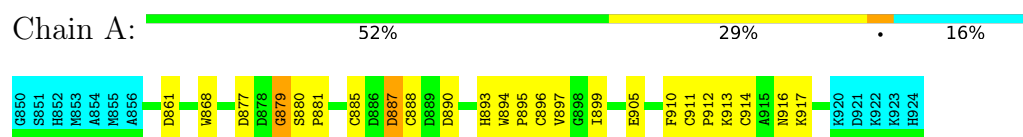


- Molecule 2: Histone H3.1

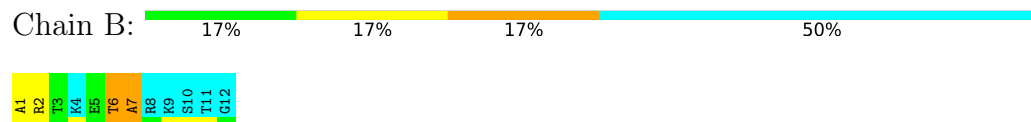


#### 4.2.14 Score per residue for model 14

- Molecule 1: Transcription initiation factor TFIID subunit 3

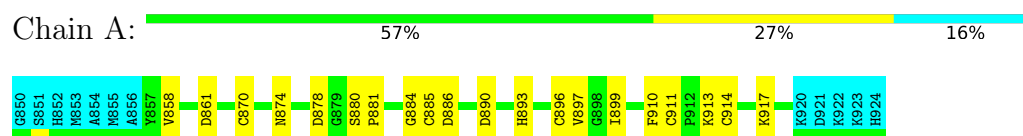


- Molecule 2: Histone H3.1

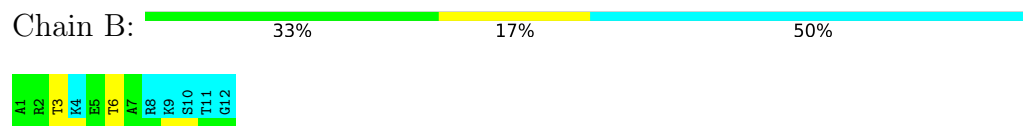


#### 4.2.15 Score per residue for model 15

- Molecule 1: Transcription initiation factor TFIID subunit 3

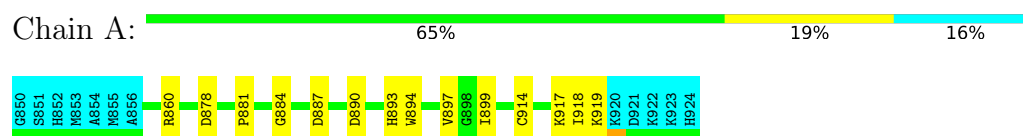


- Molecule 2: Histone H3.1

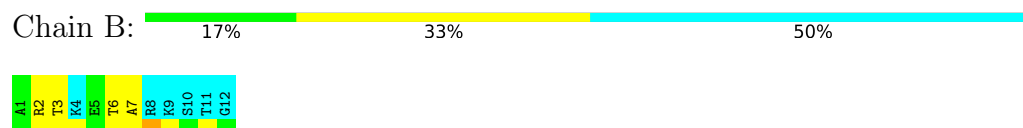


#### 4.2.16 Score per residue for model 16

- Molecule 1: Transcription initiation factor TFIID subunit 3

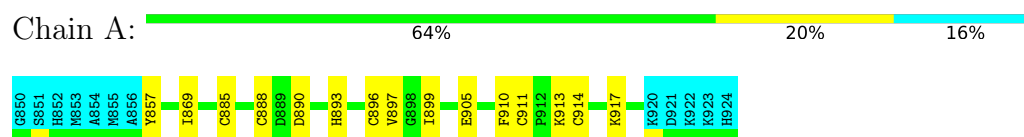


- Molecule 2: Histone H3.1

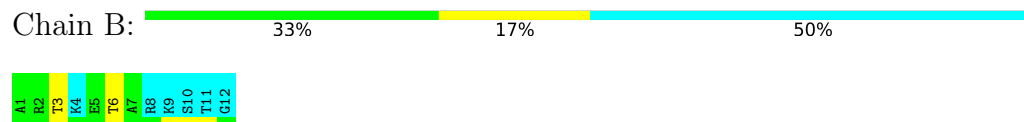


### 4.2.17 Score per residue for model 17

- Molecule 1: Transcription initiation factor TFIID subunit 3

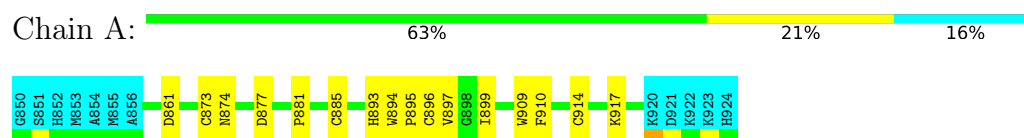


- Molecule 2: Histone H3.1



### 4.2.18 Score per residue for model 18

- Molecule 1: Transcription initiation factor TFIID subunit 3

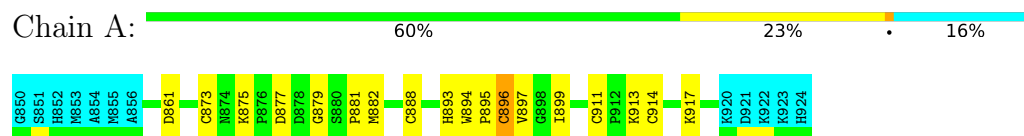


- Molecule 2: Histone H3.1

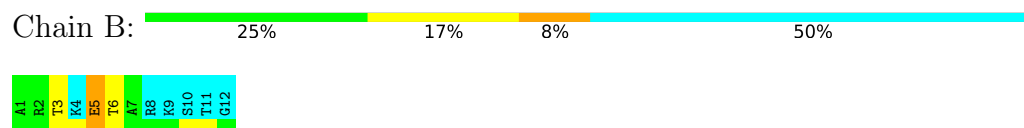


### 4.2.19 Score per residue for model 19

- Molecule 1: Transcription initiation factor TFIID subunit 3

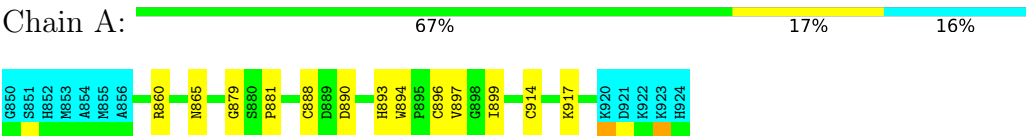


- Molecule 2: Histone H3.1

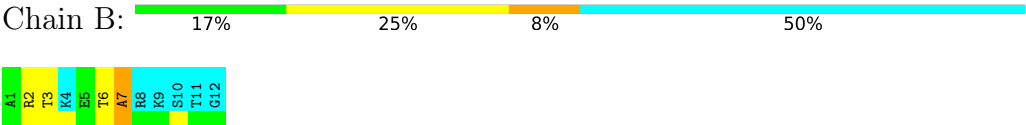


4.2.20 Score per residue for model 20

- Molecule 1: Transcription initiation factor TFIID subunit 3



- Molecule 2: Histone H3.1



## 5 Refinement protocol and experimental data overview

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

Of the 200 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
HADDOCK	refinement	
HADDOCK	structure calculation	

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	850
Number of shifts mapped to atoms	847
Number of unparsed shifts	0
Number of shifts with mapping errors	3
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SRO, M3L

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	505	452	452	9±3
2	B	43	45	45	1±1
All	All	11260	10160	10158	188

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:911:CYS:SG	1:A:913:LYS:HG3	0.68	2.28	19	7
1:A:879:GLY:O	2:B:7:ALA:HA	0.62	1.93	8	5
1:A:888:CYS:SG	1:A:913:LYS:NZ	0.62	2.72	11	8
1:A:893:HIS:HB2	1:A:896:CYS:SG	0.62	2.34	12	19
1:A:909:TRP:HB3	2:B:1:ALA:HB2	0.60	1.72	2	3
1:A:868:TRP:O	1:A:876:PRO:HA	0.56	2.00	13	3
1:A:873:CYS:SG	1:A:875:LYS:HD3	0.56	2.40	10	1
1:A:873:CYS:SG	1:A:875:LYS:NZ	0.56	2.78	13	2
1:A:881:PRO:HB2	1:A:894:TRP:CD2	0.55	2.37	18	12
1:A:893:HIS:O	1:A:897:VAL:HG22	0.54	2.03	12	12
1:A:888:CYS:SG	1:A:890:ASP:HB2	0.54	2.42	6	3

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:885:CYS:SG	1:A:910:PHE:HA	0.54	2.42	17	7
1:A:887:ASP:CG	1:A:917:LYS:HZ1	0.54	2.10	14	1
1:A:911:CYS:SG	1:A:913:LYS:HB2	0.54	2.43	15	5
1:A:897:VAL:HG23	1:A:899:ILE:HG12	0.53	1.80	18	18
1:A:914:CYS:SG	1:A:917:LYS:NZ	0.52	2.81	16	12
1:A:870:CYS:O	1:A:874:ASN:HA	0.51	2.06	15	1
1:A:879:GLY:CA	2:B:7:ALA:HA	0.49	2.37	9	1
1:A:860:ARG:HA	1:A:865:ASN:O	0.49	2.07	13	5
1:A:905:GLU:CD	2:B:2:ARG:HH21	0.49	2.16	9	1
1:A:873:CYS:SG	1:A:875:LYS:HB2	0.48	2.48	10	2
1:A:873:CYS:SG	1:A:875:LYS:HB3	0.47	2.49	7	2
1:A:914:CYS:O	1:A:917:LYS:HG2	0.46	2.09	10	7
1:A:873:CYS:HB2	1:A:875:LYS:NZ	0.46	2.24	8	1
1:A:905:GLU:HA	2:B:1:ALA:O	0.46	2.10	10	5
1:A:877:ASP:HB2	1:A:882:MET:SD	0.46	2.51	10	2
1:A:884:GLY:HA2	1:A:890:ASP:O	0.45	2.12	6	4
1:A:894:TRP:N	1:A:895:PRO:HD2	0.45	2.27	14	8
1:A:881:PRO:HB2	1:A:894:TRP:CE2	0.45	2.47	12	1
1:A:911:CYS:HB2	1:A:912:PRO:HD2	0.44	1.89	10	4
1:A:905:GLU:OE2	2:B:2:ARG:HD3	0.44	2.11	11	1
1:A:905:GLU:OE2	2:B:2:ARG:HA	0.44	2.12	7	1
1:A:881:PRO:HB2	1:A:894:TRP:CE3	0.44	2.46	8	2
1:A:894:TRP:CZ3	1:A:901:ALA:HA	0.44	2.48	2	1
1:A:857:TYR:HB3	1:A:869:ILE:O	0.44	2.13	1	3
1:A:914:CYS:O	1:A:918:ILE:HG12	0.44	2.13	9	2
1:A:885:CYS:SG	1:A:886:ASP:N	0.43	2.90	15	1
1:A:877:ASP:HB3	1:A:882:MET:SD	0.43	2.53	19	1
1:A:911:CYS:SG	1:A:913:LYS:NZ	0.42	2.87	2	2
1:A:891:TRP:CD1	1:A:891:TRP:N	0.42	2.87	9	1
1:A:915:ALA:O	1:A:919:LYS:HG2	0.42	2.14	1	1
1:A:914:CYS:O	1:A:918:ILE:HG13	0.42	2.14	16	1
1:A:911:CYS:SG	1:A:913:LYS:HD3	0.42	2.54	17	1
1:A:881:PRO:CB	2:B:5:GLU:HB2	0.42	2.44	19	1
1:A:912:PRO:O	1:A:916:ASN:HB2	0.42	2.15	14	1
1:A:879:GLY:HA2	2:B:6:THR:O	0.42	2.15	11	2
1:A:873:CYS:O	1:A:874:ASN:HB2	0.41	2.15	5	2
1:A:881:PRO:HB3	2:B:5:GLU:HB2	0.41	1.93	19	1
1:A:888:CYS:SG	1:A:889:ASP:N	0.40	2.93	9	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	63/75 (84%)	55±3 (87±5%)	8±3 (13±4%)	0±1 (1±1%)	21	71
2	B	5/12 (42%)	4±1 (75±22%)	1±1 (17±18%)	0±1 (8±12%)	1	14
All	All	1360/1740 (78%)	1168 (86%)	175 (13%)	17 (1%)	13	60

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	7	ALA	6
1	A	888	CYS	4
1	A	879	GLY	3
2	B	5	GLU	2
1	A	878	ASP	1
1	A	858	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	55/64 (86%)	52±1 (95±2%)	3±1 (5±2%)	25	78
2	B	4/8 (50%)	2±0 (44±11%)	2±0 (56±11%)	0	0
All	All	1180/1440 (82%)	1084 (92%)	96 (8%)	12	61

All 18 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)
2	B	6	THR	18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
2	B	3	THR	16
2	B	2	ARG	10
1	A	896	CYS	9
1	A	861	ASP	9
1	A	880	SER	6
1	A	887	ASP	5
1	A	908	GLN	4
1	A	906	GLU	4
1	A	878	ASP	3
1	A	890	ASP	3
1	A	868	TRP	2
1	A	905	GLU	2
1	A	877	ASP	1
1	A	889	ASP	1
1	A	875	LYS	1
1	A	860	ARG	1
2	B	5	GLU	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	M3L	B	4	2	10,11,12	0.49±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard

deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	M3L	B	4	2	9,14,16	0.45±0.02	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	B	4	2	-	0±0,9,10,12	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	SRO	B	101	2	12,14,14	0.81±0.03	0±0 (1±2%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	SRO	B	101	2	12,19,19	0.97±0.02	1±0 (8±1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SRO	B	101	2	-	0±0,3,3,3	0±0,2,2,2

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	B	101	SRO	CE3-CD2	2.09	1.38	1.42	18	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	101	SRO	CH2-CZ2-CE2	2.54	117.65	120.84	13	20
4	B	101	SRO	CZ3-CE3-CD2	2.03	119.22	120.64	7	1

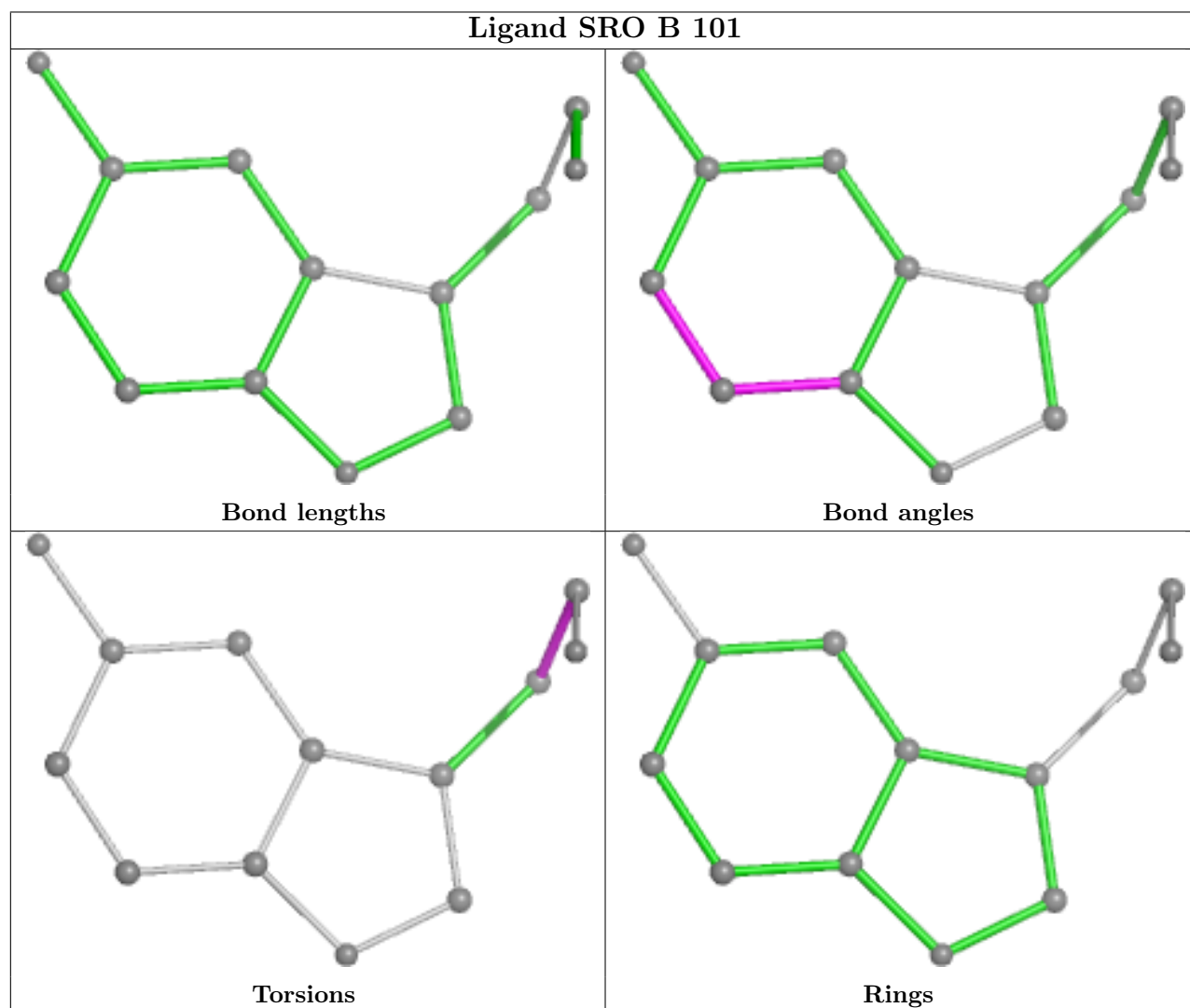
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 74% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	850
Number of shifts mapped to atoms	847
Number of unparsed shifts	0
Number of shifts with mapping errors	3
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

- No matching atom found in the structure. All 3 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	1	ALA	H	10.507	0.00	1
1	B	101	SRO	HE1	10.016	0.00	1
1	B	101	SRO	HZ	7.71	0.00	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	74	$-0.29 \pm 0.23$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	63	$0.19 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	64	$-0.46 \pm 0.42$	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 81%, i.e. 720 atoms were assigned a chemical shift out of a possible 890. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	252/336 (75%)	135/136 (99%)	62/138 (45%)	55/62 (89%)
Sidechain	389/459 (85%)	271/296 (92%)	113/148 (76%)	5/15 (33%)
Aromatic	79/95 (83%)	42/47 (89%)	31/42 (74%)	6/6 (100%)
Overall	720/890 (81%)	448/479 (94%)	206/328 (63%)	66/83 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 821 atoms were assigned a chemical shift out of a possible 1113. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	305/423 (72%)	167/172 (97%)	74/172 (43%)	64/79 (81%)
Sidechain	429/579 (74%)	305/373 (82%)	119/184 (65%)	5/22 (23%)
Aromatic	87/111 (78%)	46/55 (84%)	35/46 (76%)	6/10 (60%)
Overall	821/1113 (74%)	518/600 (86%)	228/402 (57%)	75/111 (68%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

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

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	884	GLY	HA3	1.04	2.08 – 5.71	-7.9
1	A	881	PRO	HB3	-0.38	0.25 – 3.76	-6.8
1	A	871	PRO	HD2	1.53	1.93 – 5.38	-6.2
1	A	870	CYS	N	145.01	98.14 – 142.06	5.7
1	A	881	PRO	HB2	0.18	0.37 – 3.78	-5.5
1	A	862	GLU	HG2	1.21	1.24 – 3.30	-5.1

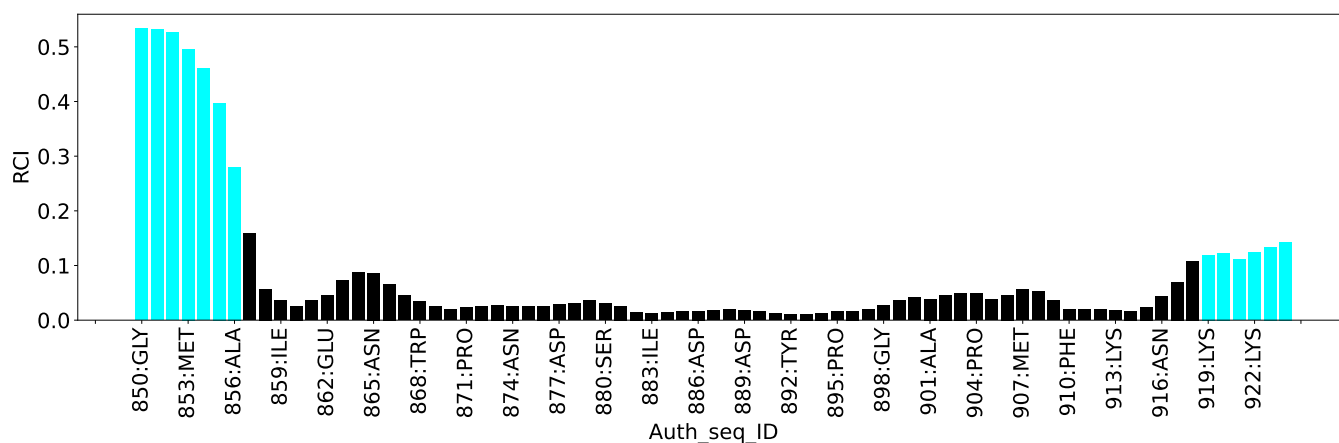
### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

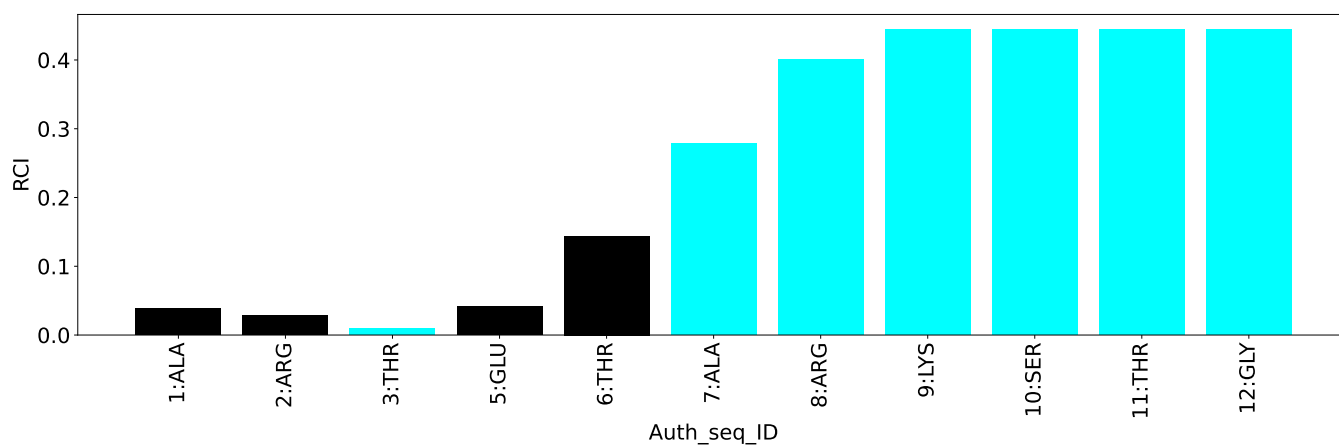


composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	404
Intra-residue ( $ i-j =0$ )	139
Sequential ( $ i-j =1$ )	84
Medium range ( $ i-j >1$ and $ i-j <5$ )	26
Long range ( $ i-j \geq 5$ )	32
Inter-chain	123
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	24
Number of restraints per residue	4.5
Number of long range restraints per residue <sup>1</sup>	0.4

<sup>1</sup>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

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

#### 8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	2.3	0.2
0.2-0.5 (Medium)	4.6	0.5
>0.5 (Large)	9.6	2.32

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

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis ⓘ

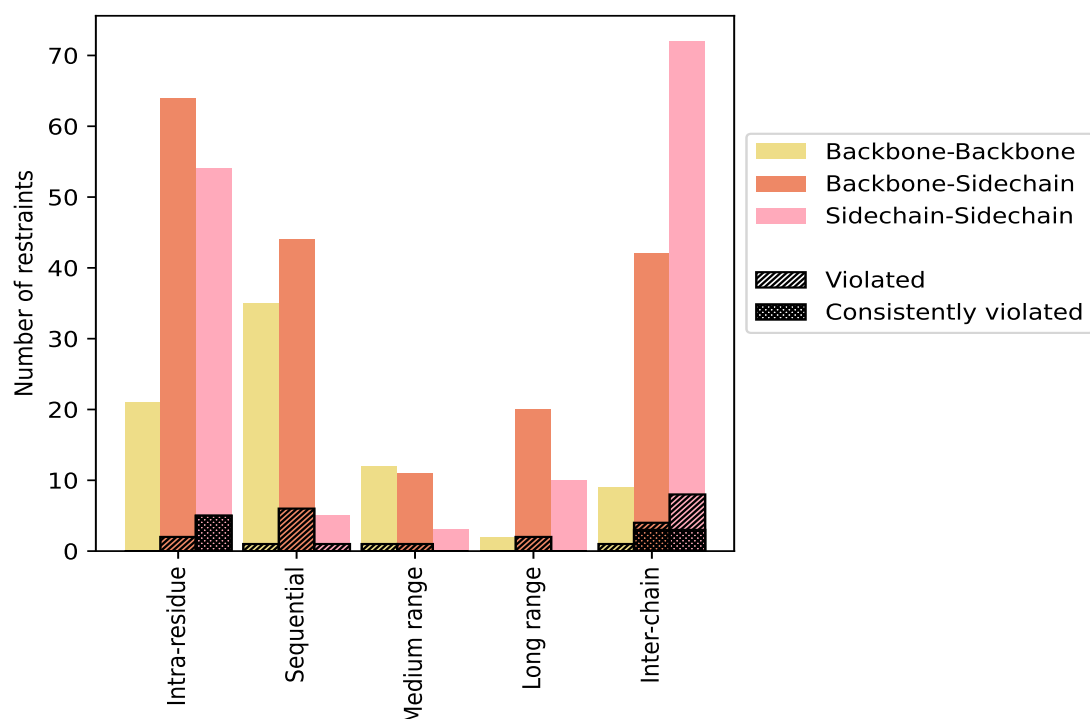
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>139</b>	<b>34.4</b>	<b>7</b>	<b>5.0</b>	<b>1.7</b>	<b>5</b>	<b>3.6</b>	<b>1.2</b>
Backbone-Backbone	21	5.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	64	15.8	2	3.1	0.5	0	0.0	0.0
Sidechain-Sidechain	54	13.4	5	9.3	1.2	5	9.3	1.2
<b>Sequential (<math> i-j =1</math>)</b>	<b>84</b>	<b>20.8</b>	<b>8</b>	<b>9.5</b>	<b>2.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	35	8.7	1	2.9	0.2	0	0.0	0.0
Backbone-Sidechain	44	10.9	6	13.6	1.5	0	0.0	0.0
Sidechain-Sidechain	5	1.2	1	20.0	0.2	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>26</b>	<b>6.4</b>	<b>2</b>	<b>7.7</b>	<b>0.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	12	3.0	1	8.3	0.2	0	0.0	0.0
Backbone-Sidechain	11	2.7	1	9.1	0.2	0	0.0	0.0
Sidechain-Sidechain	3	0.7	0	0.0	0.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>32</b>	<b>7.9</b>	<b>2</b>	<b>6.2</b>	<b>0.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	2	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	20	5.0	2	10.0	0.5	0	0.0	0.0
Sidechain-Sidechain	10	2.5	0	0.0	0.0	0	0.0	0.0
<b>Inter-chain</b>	<b>123</b>	<b>30.4</b>	<b>13</b>	<b>10.6</b>	<b>3.2</b>	<b>6</b>	<b>4.9</b>	<b>1.5</b>
Backbone-Backbone	9	2.2	1	11.1	0.2	0	0.0	0.0
Backbone-Sidechain	42	10.4	4	9.5	1.0	3	7.1	0.7
Sidechain-Sidechain	72	17.8	8	11.1	2.0	3	4.2	0.7
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Total</b>	<b>404</b>	<b>100.0</b>	<b>32</b>	<b>7.9</b>	<b>7.9</b>	<b>11</b>	<b>2.7</b>	<b>2.7</b>
Backbone-Backbone	79	19.6	3	3.8	0.7	0	0.0	0.0
Backbone-Sidechain	181	44.8	15	8.3	3.7	3	1.7	0.7
Sidechain-Sidechain	144	35.6	14	9.7	3.5	8	5.6	2.0

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	6	3	0	1	7	17	0.74	1.73	0.56	0.53
2	6	1	0	1	8	16	0.77	1.54	0.51	0.62
3	5	4	0	0	7	16	0.79	1.54	0.48	0.89
4	6	2	0	1	7	16	0.8	1.66	0.53	0.84
5	5	2	1	1	8	17	0.85	1.61	0.5	0.81
6	6	3	0	1	7	17	0.79	1.66	0.56	0.93
7	6	5	0	0	6	17	0.8	1.63	0.53	0.93
8	6	0	0	1	8	15	0.87	1.58	0.52	0.8
9	6	1	0	0	7	14	0.79	1.5	0.51	0.84
10	6	0	2	1	8	17	0.72	1.55	0.56	0.41

*Continued on next page...*

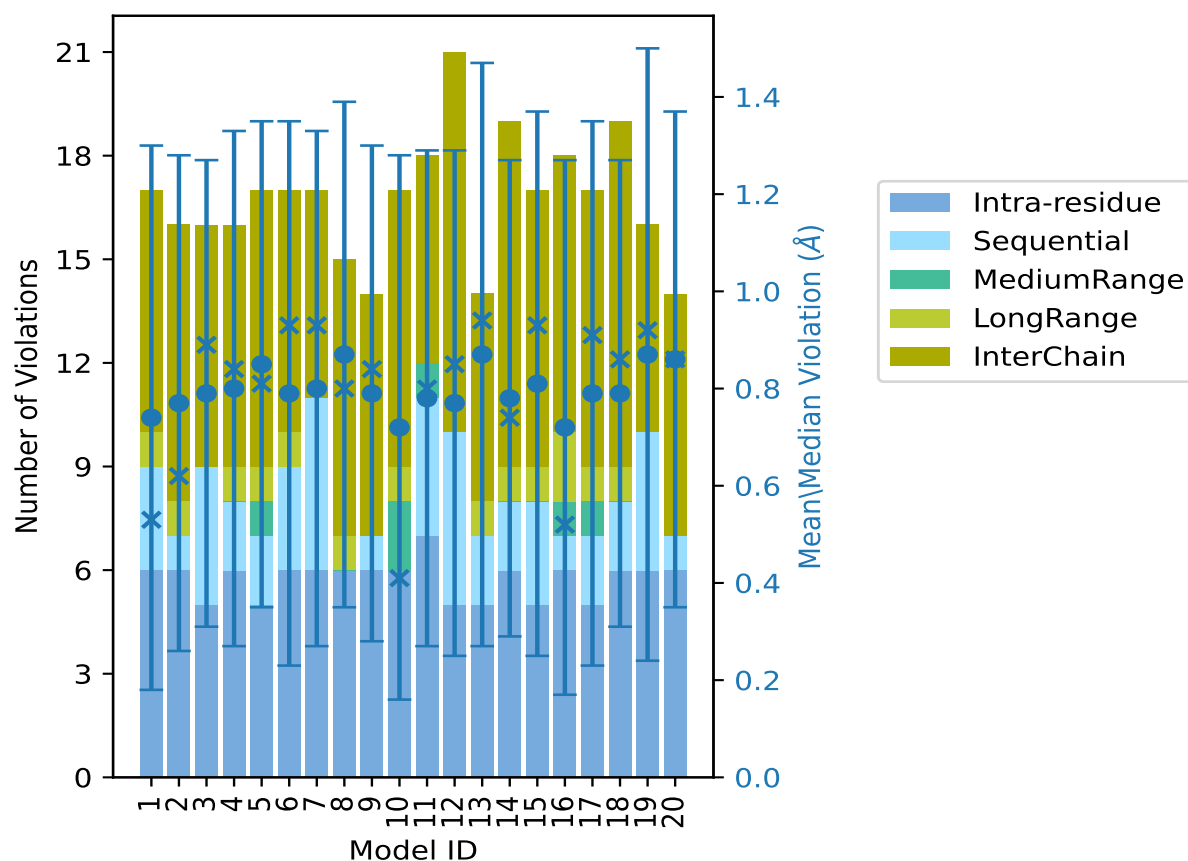
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	7	4	1	0	6	18	0.78	1.76	0.51	0.8
12	5	5	0	0	11	21	0.77	1.69	0.52	0.85
13	5	2	0	1	6	14	0.87	1.71	0.6	0.94
14	6	2	0	1	10	19	0.78	1.52	0.49	0.74
15	5	3	0	1	8	17	0.81	1.72	0.56	0.93
16	6	1	1	2	8	18	0.72	1.65	0.55	0.52
17	5	2	1	1	8	17	0.79	1.69	0.56	0.91
18	6	2	0	1	10	19	0.79	1.65	0.48	0.86
19	6	4	0	0	6	16	0.87	2.32	0.63	0.92
20	6	1	0	0	7	14	0.86	1.54	0.51	0.86

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble

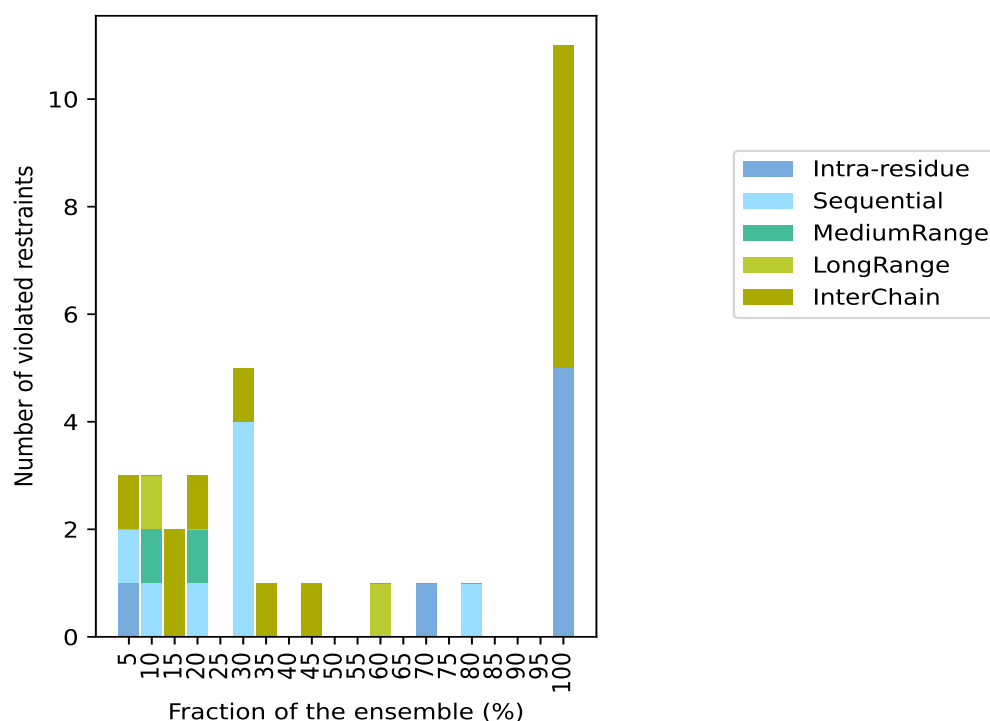
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 372(IR:132, SQ:76, MR:24, LR:30, IC:110) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
1	1	0	0	1	3	1	5.0
0	1	1	1	0	3	2	10.0
0	0	0	0	2	2	3	15.0
0	1	1	0	1	3	4	20.0
0	0	0	0	0	0	5	25.0
0	4	0	0	1	5	6	30.0
0	0	0	0	1	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	1	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	0	0	0	13	65.0
1	0	0	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	1	0	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
5	0	0	0	6	11	20	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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

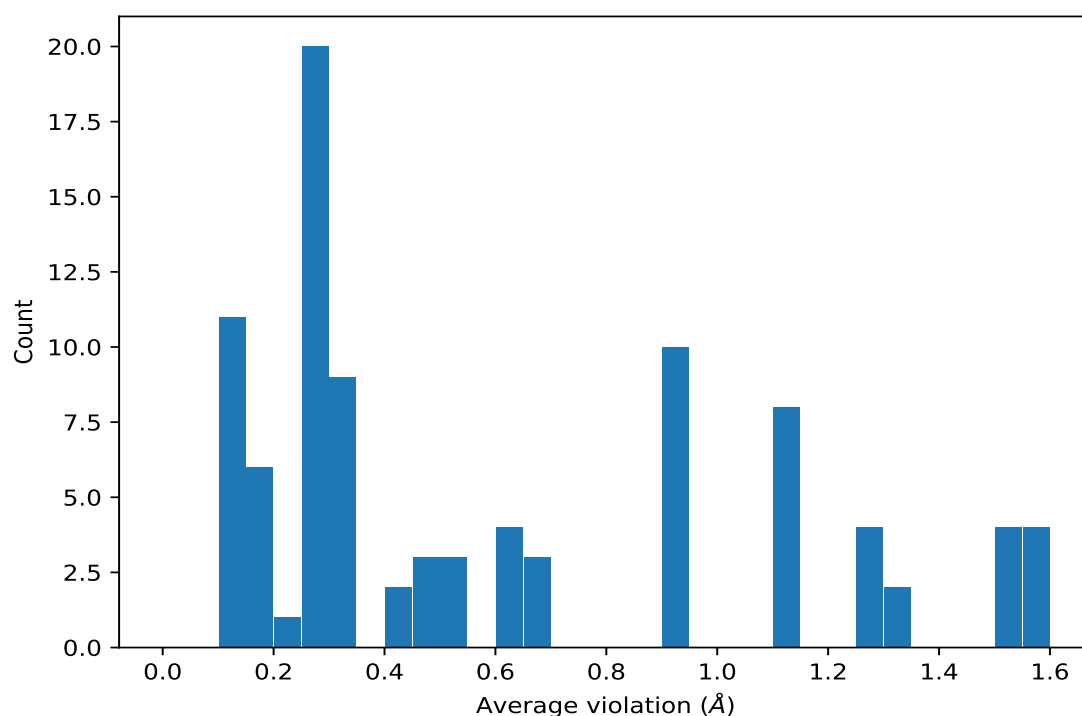


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	20	1.55	0.14	1.54
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	20	1.55	0.14	1.54
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	20	1.55	0.14	1.54
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	20	1.55	0.14	1.54
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	20	1.54	0.23	1.49
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	20	1.54	0.23	1.49
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	20	1.54	0.06	1.52
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	20	1.54	0.06	1.52
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	20	1.3	0.24	1.43
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	20	1.3	0.24	1.43
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	20	1.26	0.2	1.25
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	20	1.26	0.2	1.25
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	20	1.26	0.2	1.25
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	20	1.26	0.2	1.25
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	20	1.11	0.07	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	20	1.11	0.07	1.1

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	20	1.11	0.07	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	20	1.11	0.07	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	20	1.11	0.07	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	20	1.11	0.07	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	20	1.11	0.07	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	20	1.11	0.07	1.1
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	20	0.93	0.2	0.92
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	20	0.93	0.2	0.92
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	20	0.93	0.2	0.92
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	20	0.93	0.2	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	20	0.93	0.01	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	20	0.93	0.01	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	20	0.93	0.01	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	20	0.93	0.01	0.93
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	20	0.34	0.01	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	20	0.34	0.01	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	20	0.34	0.01	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	20	0.34	0.01	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	20	0.34	0.01	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	20	0.34	0.01	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	20	0.34	0.01	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	20	0.34	0.01	0.34
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	20	0.3	0.0	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	20	0.3	0.0	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	20	0.3	0.0	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	20	0.3	0.0	0.3
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	20	0.27	0.01	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	20	0.27	0.01	0.27

*Continued on next page...*

*Continued from previous page...*

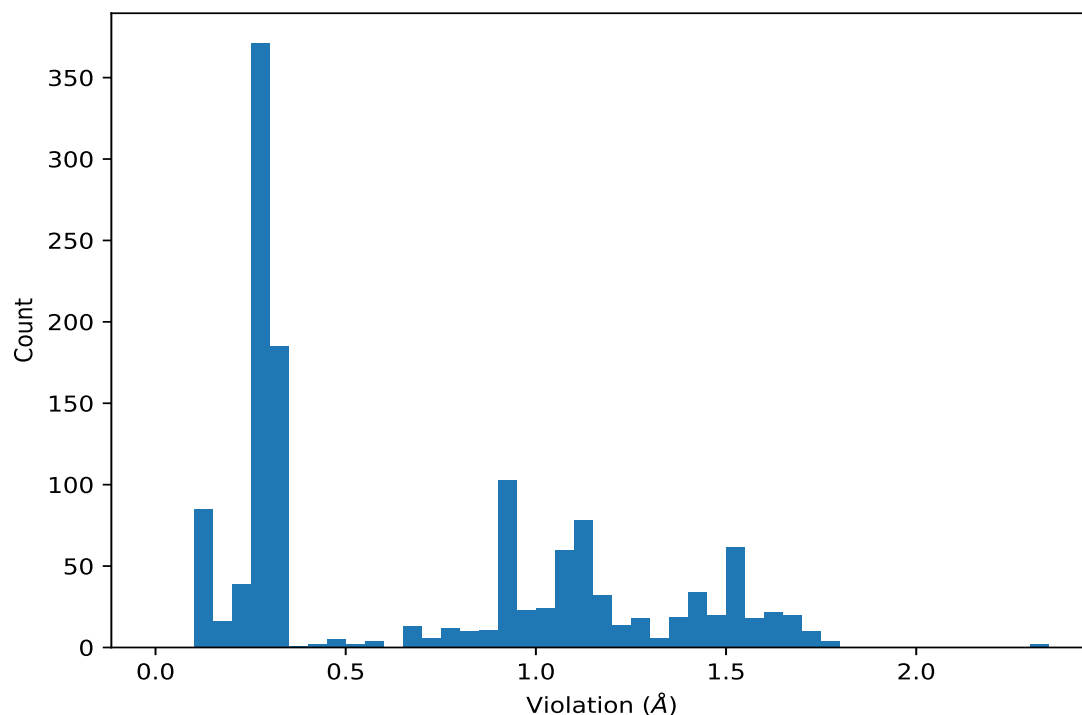
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG3	16	0.9	0.37	1.0
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG2	16	0.9	0.37	1.0
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	14	0.45	0.14	0.44
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	12	0.16	0.04	0.15
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	12	0.16	0.04	0.15
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	9	0.12	0.02	0.12
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	9	0.12	0.02	0.12
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	9	0.12	0.02	0.12
(1,115)	2:4:B:M3L:HM32	1:868:A:TRP:HE1	7	0.62	0.29	0.75
(1,115)	2:4:B:M3L:HM12	1:868:A:TRP:HE1	7	0.62	0.29	0.75
(1,115)	2:4:B:M3L:HM31	1:868:A:TRP:HE1	7	0.62	0.29	0.75
(1,115)	2:4:B:M3L:HM23	1:868:A:TRP:HE1	7	0.62	0.29	0.75
(1,123)	2:4:B:M3L:HM12	1:891:A:TRP:HD1	6	0.69	0.42	0.69
(1,123)	2:4:B:M3L:HM22	1:891:A:TRP:HD1	6	0.69	0.42	0.69
(1,123)	2:4:B:M3L:HM21	1:891:A:TRP:HD1	6	0.69	0.42	0.69
(1,103)	2:4:B:M3L:HE2	2:5:B:GLU:HA	6	0.31	0.3	0.2
(1,296)	1:880:A:SER:H	1:881:A:PRO:HA	6	0.18	0.05	0.18
(1,107)	2:4:B:M3L:HG2	2:5:B:GLU:H	6	0.17	0.05	0.16
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG21	6	0.14	0.04	0.13
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG22	6	0.14	0.04	0.13
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG23	6	0.14	0.04	0.13
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG21	6	0.14	0.04	0.13
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG22	6	0.14	0.04	0.13
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG23	6	0.14	0.04	0.13
(1,100)	2:4:B:M3L:HD2	2:5:B:GLU:H	4	0.52	0.19	0.59
(1,105)	2:4:B:M3L:HE2	1:891:A:TRP:HE3	4	0.23	0.05	0.24
(1,228)	2:6:B:THR:HA	2:8:B:ARG:H	4	0.14	0.02	0.14
(1,124)	2:4:B:M3L:HM33	1:891:A:TRP:HE1	3	0.4	0.25	0.33
(1,124)	2:4:B:M3L:HM22	1:891:A:TRP:HE1	3	0.4	0.25	0.33
(1,241)	2:6:B:THR:H	1:879:A:GLY:HA2	3	0.16	0.03	0.15
(1,241)	2:6:B:THR:H	1:879:A:GLY:HA3	3	0.16	0.03	0.15
(1,57)	2:3:B:THR:HA	2:4:B:M3L:HM22	2	0.52	0.17	0.52
(1,57)	2:3:B:THR:HA	2:4:B:M3L:HM33	2	0.52	0.17	0.52
(1,112)	2:4:B:M3L:HM22	2:6:B:THR:H	2	0.48	0.33	0.48
(1,112)	2:4:B:M3L:HM23	2:6:B:THR:H	2	0.48	0.33	0.48
(1,289)	1:878:A:ASP:H	1:893:A:HIS:HD2	2	0.15	0.05	0.15

<sup>1</sup>Number of violated models, <sup>2</sup>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)
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	19	2.32
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	19	2.32
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	11	1.76
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	11	1.76
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	11	1.76
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	11	1.76
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	1	1.73
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	1	1.73
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	1	1.73
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	1	1.73

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	15	1.72
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	15	1.72
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	13	1.71
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	13	1.71
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	13	1.71
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	13	1.71
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	13	1.7
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	13	1.7
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	12	1.69
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	12	1.69
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	17	1.69
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	17	1.69
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	19	1.68
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	19	1.68
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	4	1.66
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	4	1.66
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	4	1.66
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	4	1.66
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	6	1.66
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	6	1.66
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	6	1.66
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	6	1.66
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	17	1.66
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	17	1.66
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	17	1.66
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	17	1.66
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	18	1.65
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	18	1.65
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	18	1.65
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	18	1.65
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	16	1.65
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	16	1.65
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	16	1.65
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	16	1.65
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	6	1.65
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	6	1.65
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	1	1.63
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	1	1.63
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	7	1.63
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	7	1.63
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	13	1.63
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	13	1.63

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	7	1.62
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	7	1.62
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	7	1.62
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	7	1.62
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	5	1.61
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	5	1.61
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	15	1.59
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	15	1.59
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	8	1.58
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	8	1.58
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	19	1.57
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	19	1.57
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	19	1.57
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	19	1.57
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	1	1.55
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	1	1.55
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	10	1.55
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	10	1.55
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	15	1.55
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	15	1.55
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	15	1.55
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	15	1.55
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	8	1.55
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	8	1.55
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	20	1.54
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	20	1.54
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	20	1.54
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	20	1.54
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	13	1.54
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	13	1.54
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	6	1.54
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	6	1.54
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	2	1.54
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	2	1.54
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	2	1.54
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	2	1.54
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	3	1.54
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	3	1.54
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	3	1.54
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	3	1.54
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	2	1.53
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	2	1.53

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	3	1.53
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	3	1.53
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	16	1.53
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	16	1.53
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	8	1.52
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	8	1.52
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	10	1.52
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	10	1.52
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	12	1.52
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	12	1.52
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	5	1.52
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	5	1.52
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	5	1.52
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	5	1.52
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	8	1.52
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	8	1.52
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	8	1.52
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	8	1.52
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	14	1.52
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	14	1.52
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	14	1.52
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	14	1.52
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	16	1.51
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	16	1.51
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	4	1.51
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	4	1.51
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	14	1.51
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	14	1.51
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	18	1.51
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	18	1.51
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	20	1.51
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	20	1.51
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	9	1.5
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	9	1.5
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	9	1.5
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	9	1.5
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	12	1.5
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	12	1.5
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	7	1.5
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	7	1.5
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	11	1.5
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	11	1.5

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	17	1.5
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	17	1.5
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	2	1.49
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	2	1.49
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	4	1.49
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	4	1.49
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	6	1.48
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	6	1.48
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	9	1.48
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	9	1.48
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	17	1.47
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	17	1.47
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	18	1.47
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	18	1.47
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	18	1.47
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	18	1.47
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	3	1.47
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	3	1.47
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	15	1.46
(1,174)	4:101:B:SRO:HZ2	1:901:A:ALA:HA	15	1.46
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	5	1.46
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	5	1.46
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	12	1.45
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	12	1.45
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	12	1.45
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	12	1.45
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	11	1.43
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	11	1.43
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	11	1.43
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	11	1.43
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	1	1.43
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	1	1.43
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	5	1.43
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	5	1.43
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	20	1.43
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	20	1.43
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	9	1.43
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	9	1.43
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	9	1.43
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	9	1.43
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	20	1.43
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	20	1.43

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	20	1.43
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	20	1.43
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	11	1.43
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	11	1.43
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	5	1.42
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	5	1.42
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	5	1.42
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	5	1.42
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	10	1.42
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	10	1.42
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	10	1.42
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	10	1.42
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	10	1.42
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	10	1.42
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG3	12	1.4
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	10	1.39
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	10	1.39
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	10	1.39
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	10	1.39
(1,123)	2:4:B:M3L:HM12	1:891:A:TRP:HD1	14	1.38
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG3	4	1.38
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	14	1.35
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	14	1.35
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	14	1.35
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	14	1.35
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	16	1.35
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	16	1.35
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	16	1.35
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	16	1.35
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	16	1.35
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	16	1.35
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	20	1.35
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	20	1.35
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	9	1.34
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	9	1.34
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	8	1.32
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	8	1.32
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	8	1.32
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	8	1.32
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	18	1.29
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	18	1.29
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	14	1.27

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	14	1.27
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG3	7	1.27
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	19	1.26
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	19	1.26
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	19	1.26
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	19	1.26
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG3	15	1.26
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	2	1.25
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	2	1.25
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	2	1.25
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	2	1.25
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	2	1.25
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	2	1.25
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	2	1.25
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	2	1.25
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	7	1.24
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	7	1.24
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	7	1.24
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	7	1.24
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	2	1.23
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	2	1.23
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	2	1.23
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	2	1.23
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	13	1.22
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	13	1.22
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	13	1.22
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	13	1.22
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	14	1.22
(1,144)	2:5:B:GLU:HA	4:101:B:SRO:HZ2	14	1.22
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	18	1.2
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	18	1.2
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	9	1.2
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	9	1.2
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	9	1.2
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	9	1.2
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	9	1.2
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	9	1.2
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	9	1.2
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	9	1.2
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	4	1.18
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	4	1.18
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	4	1.18

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	4	1.18
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	7	1.16
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	7	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	8	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	8	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	8	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	8	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	8	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	8	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	8	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	8	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	10	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	10	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	10	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	10	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	10	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	10	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	10	1.16
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	10	1.16
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	6	1.15
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	6	1.15
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	6	1.15
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	6	1.15
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	2	1.15
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	2	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	5	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	5	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	5	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	5	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	5	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	5	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	5	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	5	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	18	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	18	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	18	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	18	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	18	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	18	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	18	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	18	1.15
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	20	1.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	20	1.14
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	20	1.14
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	20	1.14
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	20	1.14
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	20	1.14
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	20	1.14
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	20	1.14
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	17	1.13
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	17	1.13
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	17	1.13
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	17	1.13
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	14	1.13
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	14	1.13
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	14	1.13
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	14	1.13
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	14	1.13
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	14	1.13
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	14	1.13
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	14	1.13
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	19	1.13
(1,152)	2:5:B:GLU:HB2	4:101:B:SRO:HZ2	19	1.13
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	19	1.13
(1,152)	2:5:B:GLU:HB3	4:101:B:SRO:HZ2	19	1.13
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	16	1.12
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	16	1.12
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	16	1.12
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	16	1.12
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	16	1.12
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	16	1.12
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	16	1.12
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	16	1.12
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	12	1.11
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	12	1.11
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	12	1.11
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	12	1.11
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	12	1.11
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	12	1.11
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	12	1.11
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	12	1.11
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	3	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	3	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	3	1.1

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	3	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	3	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	3	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	3	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	3	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	7	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	7	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	7	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	7	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	7	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	7	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	7	1.1
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	7	1.1
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	11	1.08
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	11	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	4	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	4	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	4	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	4	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	4	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	4	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	4	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	4	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	11	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	11	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	11	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	11	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	11	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	11	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	11	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	11	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	15	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	15	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	15	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	15	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	15	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	15	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	15	1.08
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	15	1.08
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	15	1.07
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	15	1.07
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	15	1.07

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	15	1.07
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	19	1.06
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	19	1.06
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	6	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	6	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	6	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	6	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	6	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	6	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	6	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	6	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	13	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	13	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	13	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	13	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	13	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	13	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	13	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	13	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	17	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	17	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	17	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	17	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	17	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	17	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	17	1.05
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	17	1.05
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	17	1.05
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	17	1.05
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	17	1.05
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	17	1.05
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	12	1.04
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	12	1.04
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	12	1.04
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	12	1.04
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	1	1.04
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	1	1.04
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	1	1.04
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	1	1.04
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	1	1.04
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	1	1.04
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	1	1.04

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	1	1.04
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	1	1.04
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	1	1.04
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	1	1.04
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	1	1.04
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	6	1.01
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	6	1.01
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	6	1.01
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	6	1.01
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	11	1.01
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	11	1.01
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	11	1.01
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	11	1.01
(1,115)	2:4:B:M3L:HM23	1:868:A:TRP:HE1	12	0.99
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	3	0.98
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	3	0.98
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	3	0.98
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	3	0.98
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	13	0.98
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	13	0.98
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	13	0.98
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	13	0.98
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	12	0.98
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	12	0.98
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	12	0.98
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	12	0.98
(1,123)	2:4:B:M3L:HM12	1:891:A:TRP:HD1	18	0.98
(1,103)	2:4:B:M3L:HE2	2:5:B:GLU:HA	5	0.97
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	7	0.96
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	7	0.96
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	7	0.96
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	7	0.96
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	15	0.96
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	15	0.96
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	15	0.96
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	15	0.96
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG2	11	0.95
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	5	0.94
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	5	0.94
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	5	0.94
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	5	0.94
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	10	0.94

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	10	0.94
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	10	0.94
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	10	0.94
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	19	0.94
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	19	0.94
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	19	0.94
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	19	0.94
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	19	0.94
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA1	19	0.94
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	19	0.94
(1,166)	4:101:B:SRO:HZ2	4:101:B:SRO:HA2	19	0.94
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	1	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	1	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	1	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	1	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	2	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	2	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	2	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	2	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	4	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	4	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	4	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	4	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	6	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	6	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	6	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	6	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	7	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	7	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	7	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	7	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	8	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	8	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	8	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	8	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	9	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	9	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	9	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	9	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	15	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	15	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	15	0.93

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	15	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	20	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	20	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	20	0.93
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	20	0.93
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	9	0.92
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	9	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	3	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	3	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	3	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	3	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	11	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	11	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	11	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	11	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	12	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	12	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	12	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	12	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	14	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	14	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	14	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	14	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	16	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	16	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	16	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	16	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	18	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	18	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	18	0.92
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	18	0.92
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	16	0.92
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	16	0.92
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	16	0.92
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	16	0.92
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	1	0.91
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	1	0.91
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB2	1	0.91
(1,210)	4:101:B:SRO:HE3	1:880:A:SER:HB3	1	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	13	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	13	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	13	0.91

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	13	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	17	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	17	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	17	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	17	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	19	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	19	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	19	0.91
(1,200)	4:101:B:SRO:HD1	4:101:B:SRO:HE3	19	0.91
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	4	0.91
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	4	0.91
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	4	0.91
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	4	0.91
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	3	0.89
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	3	0.89
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	3	0.89
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	3	0.89
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	3	0.89
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	3	0.89
(1,115)	2:4:B:M3L:HM12	1:868:A:TRP:HE1	18	0.88
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	18	0.86
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	18	0.86
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	18	0.86
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	18	0.86
(1,123)	2:4:B:M3L:HM22	1:891:A:TRP:HD1	12	0.85
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	14	0.81
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	14	0.81
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	14	0.81
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	14	0.81
(1,112)	2:4:B:M3L:HM23	2:6:B:THR:H	5	0.81
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	8	0.8
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	8	0.8
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	8	0.8
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	8	0.8
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	20	0.79
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	20	0.79
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	20	0.79
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	20	0.79
(1,115)	2:4:B:M3L:HM12	1:868:A:TRP:HE1	8	0.79
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	4	0.78
(1,209)	4:101:B:SRO:HE3	1:880:A:SER:HA	4	0.78
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	9	0.77

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	9	0.77
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	9	0.77
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	9	0.77
(1,115)	2:4:B:M3L:HM32	1:868:A:TRP:HE1	5	0.75
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	10	0.74
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	10	0.74
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	10	0.74
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	10	0.74
(1,124)	2:4:B:M3L:HM33	1:891:A:TRP:HE1	14	0.74
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG2	18	0.72
(1,100)	2:4:B:M3L:HD2	2:5:B:GLU:H	3	0.7
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	8	0.7
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	2	0.69
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	2	0.69
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	2	0.69
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	2	0.69
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	18	0.69
(1,57)	2:3:B:THR:HA	2:4:B:M3L:HM33	11	0.68
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	5	0.67
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	5	0.67
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG2	5	0.67
(1,165)	4:101:B:SRO:HZ2	2:5:B:GLU:HG3	5	0.67
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG2	14	0.65
(1,100)	2:4:B:M3L:HD2	2:5:B:GLU:H	12	0.59
(1,100)	2:4:B:M3L:HD2	2:5:B:GLU:H	15	0.59
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	16	0.58
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG2	5	0.58
(1,123)	2:4:B:M3L:HM12	1:891:A:TRP:HD1	20	0.53
(1,115)	2:4:B:M3L:HM12	1:868:A:TRP:HE1	14	0.5
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	4	0.49
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	2	0.48
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	11	0.48
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	14	0.47
(1,25)	2:1:B:ALA:HA	2:2:B:ARG:HG2	16	0.47
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	7	0.42
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	10	0.41
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	1	0.39
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	19	0.35
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	19	0.35
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	19	0.35
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	19	0.35
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	19	0.35

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	19	0.35
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	19	0.35
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	19	0.35
(1,57)	2:3:B:THR:HA	2:4:B:M3L:HM22	19	0.35
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	1	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	1	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	1	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	1	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	1	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	1	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	1	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	1	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	4	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	4	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	4	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	4	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	4	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	4	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	4	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	4	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	5	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	5	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	5	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	5	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	5	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	5	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	5	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	5	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	6	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	6	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	6	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	6	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	6	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	6	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	6	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	6	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	7	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	7	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	7	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	7	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	7	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	7	0.34

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	7	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	7	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	10	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	10	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	10	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	10	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	10	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	10	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	10	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	10	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	11	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	11	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	11	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	11	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	11	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	11	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	11	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	11	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	13	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	13	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	13	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	13	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	13	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	13	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	13	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	13	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	14	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	14	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	14	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	14	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	14	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	14	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	14	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	14	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	15	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	15	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	15	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	15	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	15	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	15	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	15	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	15	0.34

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	20	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	20	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	20	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	20	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	20	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	20	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	20	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	20	0.34
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	3	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	3	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	3	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	3	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	3	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	3	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	3	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	3	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	8	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	8	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	8	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	8	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	8	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	8	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	8	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	8	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	9	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	9	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	9	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	9	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	9	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	9	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	9	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	9	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	12	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	12	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	12	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	12	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	12	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	12	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	12	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	12	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	16	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	16	0.33

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	16	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	16	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	16	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	16	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	16	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	16	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	17	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	17	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	17	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	17	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	17	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	17	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	17	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	17	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	18	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	18	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	18	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	18	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	18	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	18	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	18	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	18	0.33
(1,124)	2:4:B:M3L:HM33	1:891:A:TRP:HE1	18	0.33
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	20	0.33
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	2	0.32
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	2	0.32
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	2	0.32
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	2	0.32
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	2	0.32
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB1	2	0.32
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	2	0.32
(1,167)	4:101:B:SRO:HZ2	4:101:B:SRO:HB2	2	0.32
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	6	0.32
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	2	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	2	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	2	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	2	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	4	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	4	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	4	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	4	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	10	0.31

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	10	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	10	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	10	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	11	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	11	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	11	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	11	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	20	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	20	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	20	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	20	0.31
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	9	0.31
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	1	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	1	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	1	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	1	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	3	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	3	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	3	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	3	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	5	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	5	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	5	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	5	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	6	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	6	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	6	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	6	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	7	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	7	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	7	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	7	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	8	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	8	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	8	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	8	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	9	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	9	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	9	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	9	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	12	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	12	0.3

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	12	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	12	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	13	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	13	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	13	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	13	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	14	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	14	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	14	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	14	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	15	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	15	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	15	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	15	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	16	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	16	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	16	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	16	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	17	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	17	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	17	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	17	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	18	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	18	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	18	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	18	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	19	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	19	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	19	0.3
(1,207)	4:101:B:SRO:HE3	4:101:B:SRO:HZ2	19	0.3
(1,133)	2:4:B:M3L:H	2:4:B:M3L:HM23	11	0.3
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	2	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	2	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	2	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	2	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	2	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	2	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	2	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	2	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	2	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	2	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	2	0.29

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	2	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	2	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	2	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	2	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	2	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	9	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	9	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	9	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	9	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	9	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	9	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	9	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	9	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	9	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	9	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	9	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	9	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	9	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	9	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	9	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	9	0.29
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	9	0.29
(1,114)	2:4:B:M3L:HM21	1:868:A:TRP:HD1	12	0.29
(1,105)	2:4:B:M3L:HE2	1:891:A:TRP:HE3	12	0.29
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	8	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	10	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	10	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	10	0.28

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	10	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	10	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	10	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	10	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	10	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	10	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	10	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	10	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	10	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	10	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	10	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	10	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	10	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	18	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	18	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	18	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	18	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	18	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	18	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	18	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	18	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	18	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	18	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	18	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	18	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	18	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	18	0.28
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	18	0.28
(1,107)	2:4:B:M3L:HG2	2:5:B:GLU:H	3	0.28
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	3	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	3	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	3	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	3	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	3	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	3	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	3	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	3	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	3	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	3	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	3	0.27

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	3	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	3	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	3	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	3	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	4	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	4	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	4	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	4	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	4	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	4	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	4	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	4	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	4	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	4	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	4	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	4	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	4	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	4	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	4	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	4	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	5	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	5	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	5	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	5	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	5	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	5	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	5	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	5	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	5	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	5	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	5	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	5	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	5	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	5	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	5	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	5	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	7	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	7	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	7	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	7	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	7	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	7	0.27

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	7	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	7	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	7	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	7	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	7	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	7	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	7	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	7	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	7	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	7	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	11	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	11	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	11	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	11	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	11	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	11	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	11	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	11	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	11	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	11	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	11	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	11	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	11	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	11	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	11	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	11	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	12	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	12	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	12	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	12	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	12	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	12	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	12	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	12	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	12	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	12	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	12	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	12	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	12	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	12	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	12	0.27

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	14	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	14	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	14	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	14	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	14	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	14	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	14	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	14	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	14	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	14	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	14	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	14	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	14	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	14	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	14	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	14	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	16	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	16	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	16	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	16	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	16	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	16	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	16	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	16	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	16	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	16	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	16	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	16	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	16	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	16	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	16	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	16	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	20	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	20	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	20	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	20	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	20	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	20	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	20	0.27
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	20	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	20	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	20	0.27

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	20	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	20	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	20	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	20	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	20	0.27
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	20	0.27
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	17	0.26
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	17	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	1	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	1	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	1	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	1	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	1	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	1	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	1	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	1	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	1	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	1	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	1	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	1	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	1	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	1	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	1	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	1	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	6	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	6	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	6	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	6	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	6	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	6	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	6	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	6	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	6	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	6	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	6	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	6	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	6	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	6	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	6	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	6	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	13	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	13	0.26

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	13	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	13	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	13	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	13	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	13	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	13	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	13	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	13	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	13	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	13	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	13	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	13	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	13	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	13	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	15	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	15	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	15	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	15	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	15	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	15	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	15	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	15	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	15	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	15	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	15	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	15	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	15	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	15	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	15	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	15	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	17	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	17	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	17	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	17	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	17	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	17	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	17	0.26
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	17	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	17	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	17	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	17	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	17	0.26

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	17	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	17	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	17	0.26
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	17	0.26
(1,104)	2:4:B:M3L:HE2	2:5:B:GLU:H	7	0.25
(1,296)	1:880:A:SER:H	1:881:A:PRO:HA	7	0.24
(1,123)	2:4:B:M3L:HM21	1:891:A:TRP:HD1	17	0.24
(1,105)	2:4:B:M3L:HE2	1:891:A:TRP:HE3	17	0.24
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	19	0.23
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	19	0.23
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	19	0.23
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	19	0.23
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	19	0.23
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB1	19	0.23
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	19	0.23
(1,190)	4:101:B:SRO:HA1	4:101:B:SRO:HB2	19	0.23
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	19	0.23
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	19	0.23
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	19	0.23
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	19	0.23
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	19	0.23
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB1	19	0.23
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	19	0.23
(1,190)	4:101:B:SRO:HA2	4:101:B:SRO:HB2	19	0.23
(1,105)	2:4:B:M3L:HE2	1:891:A:TRP:HE3	15	0.23
(1,296)	1:880:A:SER:H	1:881:A:PRO:HA	19	0.22
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG21	17	0.22
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG22	17	0.22
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG23	17	0.22
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG21	17	0.22
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG22	17	0.22
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG23	17	0.22
(1,296)	1:880:A:SER:H	1:881:A:PRO:HA	12	0.21
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	13	0.21
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	13	0.21
(1,115)	2:4:B:M3L:HM12	1:868:A:TRP:HE1	9	0.21
(1,103)	2:4:B:M3L:HE2	2:5:B:GLU:HA	4	0.21
(1,103)	2:4:B:M3L:HE2	2:5:B:GLU:HA	7	0.21
(1,91)	2:4:B:M3L:HA	2:4:B:M3L:HE2	19	0.21
(1,289)	1:878:A:ASP:H	1:893:A:HIS:HD2	2	0.2
(1,241)	2:6:B:THR:H	1:879:A:GLY:HA2	8	0.2
(1,241)	2:6:B:THR:H	1:879:A:GLY:HA3	8	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	2:4:B:M3L:HM31	1:868:A:TRP:HE1	10	0.2
(1,103)	2:4:B:M3L:HE2	2:5:B:GLU:HA	18	0.2
(1,107)	2:4:B:M3L:HG2	2:5:B:GLU:H	12	0.19
(1,100)	2:4:B:M3L:HD2	2:5:B:GLU:H	6	0.19
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	1	0.18
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	1	0.18
(1,228)	2:6:B:THR:HA	2:8:B:ARG:H	11	0.18
(1,123)	2:4:B:M3L:HM12	1:891:A:TRP:HD1	2	0.18
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	2	0.18
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	2	0.18
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	2	0.18
(1,107)	2:4:B:M3L:HG2	2:5:B:GLU:H	15	0.17
(1,103)	2:4:B:M3L:HE2	2:5:B:GLU:HA	11	0.17
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	5	0.16
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	5	0.16
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	18	0.16
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	18	0.16
(1,107)	2:4:B:M3L:HG2	2:5:B:GLU:H	1	0.16
(1,296)	1:880:A:SER:H	1:881:A:PRO:HA	3	0.15
(1,296)	1:880:A:SER:H	1:881:A:PRO:HA	11	0.15
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	6	0.15
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	6	0.15
(1,241)	2:6:B:THR:H	1:879:A:GLY:HA2	16	0.15
(1,241)	2:6:B:THR:H	1:879:A:GLY:HA3	16	0.15
(1,228)	2:6:B:THR:HA	2:8:B:ARG:H	16	0.15
(1,112)	2:4:B:M3L:HM22	2:6:B:THR:H	10	0.15
(1,105)	2:4:B:M3L:HE2	1:891:A:TRP:HE3	6	0.15
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	14	0.14
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	14	0.14
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	16	0.14
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	16	0.14
(1,241)	2:6:B:THR:H	1:879:A:GLY:HA2	10	0.14
(1,241)	2:6:B:THR:H	1:879:A:GLY:HA3	10	0.14
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG21	13	0.14
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG22	13	0.14
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG23	13	0.14
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG21	13	0.14
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG22	13	0.14
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG23	13	0.14
(1,228)	2:6:B:THR:HA	2:8:B:ARG:H	10	0.13
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG21	1	0.13
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG22	1	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG23	1	0.13
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG21	1	0.13
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG22	1	0.13
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG23	1	0.13
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG21	6	0.13
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG22	6	0.13
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG23	6	0.13
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG21	6	0.13
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG22	6	0.13
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG23	6	0.13
(1,124)	2:4:B:M3L:HM22	1:891:A:TRP:HE1	12	0.13
(1,107)	2:4:B:M3L:HG2	2:5:B:GLU:H	13	0.13
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	16	0.13
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	16	0.13
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	16	0.13
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	8	0.12
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	8	0.12
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	10	0.12
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	10	0.12
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	15	0.12
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	15	0.12
(1,228)	2:6:B:THR:HA	2:8:B:ARG:H	17	0.12
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG21	19	0.12
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG22	19	0.12
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG23	19	0.12
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG21	19	0.12
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG22	19	0.12
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG23	19	0.12
(1,103)	2:4:B:M3L:HE2	2:5:B:GLU:HA	14	0.12
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	3	0.12
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	3	0.12
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	3	0.12
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	5	0.12
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	5	0.12
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	5	0.12
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	14	0.12
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	14	0.12
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	14	0.12
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	15	0.12
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	15	0.12
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	15	0.12
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	18	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	18	0.12
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	18	0.12
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG21	12	0.11
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG22	12	0.11
(1,157)	2:5:B:GLU:HB2	2:6:B:THR:HG23	12	0.11
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG21	12	0.11
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG22	12	0.11
(1,157)	2:5:B:GLU:HB3	2:6:B:THR:HG23	12	0.11
(1,107)	2:4:B:M3L:HG2	2:5:B:GLU:H	7	0.11
(1,296)	1:880:A:SER:H	1:881:A:PRO:HA	9	0.1
(1,289)	1:878:A:ASP:H	1:893:A:HIS:HD2	16	0.1
(1,266)	1:868:A:TRP:HB2	1:878:A:ASP:H	4	0.1
(1,266)	1:868:A:TRP:HB3	1:878:A:ASP:H	4	0.1
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	1	0.1
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	1	0.1
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	1	0.1
(1,8)	2:1:B:ALA:HB1	1:902:A:ALA:HA	4	0.1
(1,8)	2:1:B:ALA:HB2	1:902:A:ALA:HA	4	0.1
(1,8)	2:1:B:ALA:HB3	1:902:A:ALA:HA	4	0.1

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found