wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	7QGV
BMRB ID	:	50938
Title	:	Solid-state NMR structure of Teixobactin-Lipid II.
Authors	:	Weingarth, M.H.; Shukla, R.
Deposited on	:	2021-12-10

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

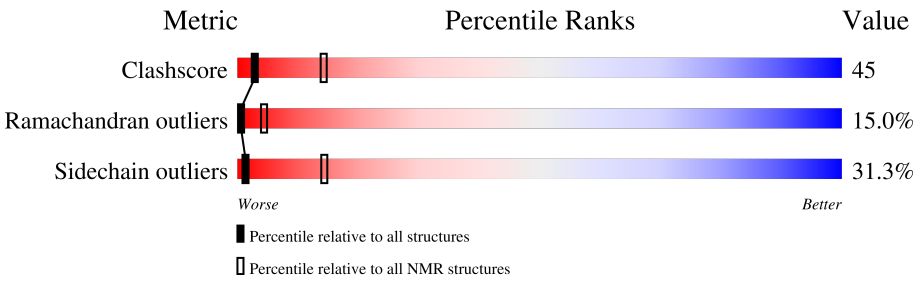
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 9%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	11	9% 45% 45%
1	B	11	9% 45% 45%
1	C	11	9% 45% 45%
1	D	11	18% 36% 45%
3	I	2	50% 50%
3	J	2	50% 50%
3	K	2	50% 50%
3	L	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
3	I	MUB	1	15	-
3	J	MUB	1	13	-
3	K	MUB	1	16	-
3	L	MUB	1	18	-

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *medoid*.

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:2-A:3, A:6-A:7, A:9-A:9, A:11-A:11, B:2-B:3, B:6-B:7, B:9-B:9, B:11-B:11, C:2-C:3, C:6-C:7, C:9-C:9, C:11-C:11, D:2-D:3, D:6-D:7, D:9-D:9, D:11-D:11 (24)	2.40	3

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 9, 11, 13, 15, 16, 17, 19, 25
2	10, 14, 23, 24
3	7, 8, 12, 18
4	21, 22
Single-model clusters	20

3 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1445 atoms, of which 737 are hydrogens and 0 are deuteriums.

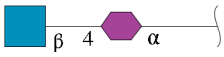
- Molecule 1 is a protein called Teixobactin.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	11	184	58	96	15	15	0
1	B	11	184	58	96	15	15	0
1	C	11	184	58	96	15	15	0
1	D	11	184	58	96	15	15	0

- Molecule 2 is a protein (with D amino acids) called Lipid II.

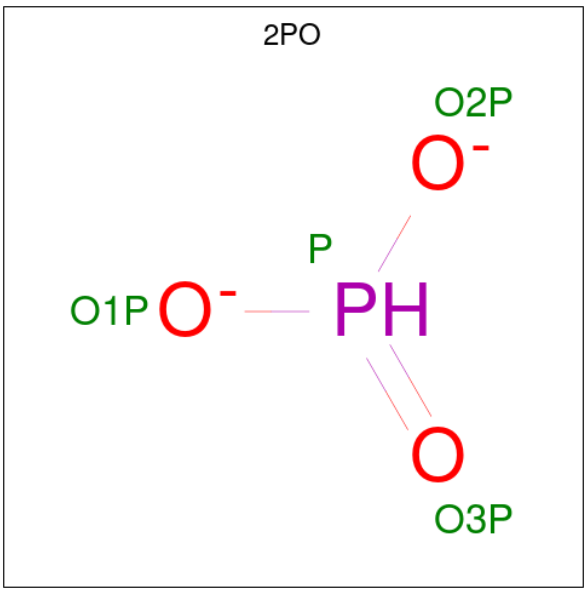
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	E	5	66	20	33	6	7	0
2	F	5	66	20	33	6	7	0
2	G	5	66	20	33	6	7	0
2	H	5	67	20	34	6	7	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid.



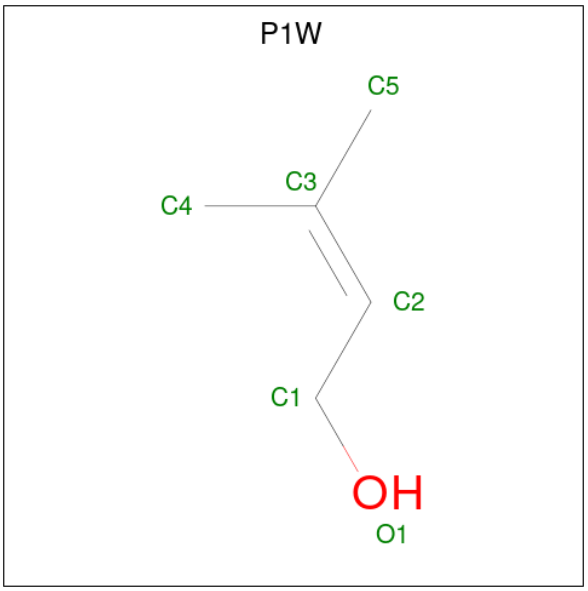
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
3	I	2	63	19	30	2	12	0
3	J	2	63	19	30	2	12	0
3	K	2	63	19	30	2	12	0
3	L	2	63	19	30	2	12	0

- Molecule 4 is PHOSPHONATE (three-letter code: 2PO) (formula: HO_3P).



Mol	Chain	Residues	Atoms		
			Total	O	P
4	A	1	4	3	1
			Total	O	P
4	A	1	4	3	1
			Total	O	P
4	B	1	4	3	1
			Total	O	P
4	B	1	4	3	1
			Total	O	P
4	C	1	4	3	1
			Total	O	P
4	C	1	4	3	1
			Total	O	P
4	D	1	4	3	1
			Total	O	P
4	D	1	4	3	1

- Molecule 5 is 3-methylbut-2-en-1-ol (three-letter code: P1W) (formula: $C_5H_{10}O$).



Mol	Chain	Residues	Atoms		
			Total	C	H
5	A	1	13	5	8
			Total	C	H
5	A	1	13	5	8
			Total	C	H
5	A	1	14	5	9
			Total	C	H
5	B	1	14	5	9
			Total	C	H
5	B	1	13	5	8
			Total	C	H
5	B	1	13	5	8
			Total	C	H
5	C	1	14	5	9
			Total	C	H
5	C	1	14	5	9
			Total	C	H
5	C	1	13	5	8
			Total	C	H
5	C	1	13	5	8
			Total	C	H
5	D	1	13	5	8
			Total	C	H
5	D	1	13	5	8

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: Teixobactin

Chain A: 9% 45% 45%

• Molecule 1: Teixobactin

Chain B: 9% 45% 45%

• Molecule 1: Teixobactin

Chain C: 9% 45% 45%

• Molecule 1: Teixobactin

Chain D: 18% 36% 45%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain I: 50% 50%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain J: 50% 50%

MUB1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain K: 50% 50%

MUB1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain L: 50% 50%

MUB1 NAG2

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

• Molecule 1: Teixobactin

Chain A: 18% 18% 18% 45%

ZAE1 I2 S3 Q4 28J5 I6 S7 T8 A9 R10 I11

• Molecule 1: Teixobactin

Chain B: 9% 27% 18% 45%

ZAE1 I2 S3 Q4 28J5 I6 S7 T8 A9 R10 I11

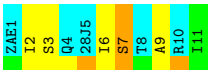
• Molecule 1: Teixobactin

Chain C: 36% 9% 9% 45%

ZAE1 Q4 28J5 I6 S7 T8 A9 R10 I11

• Molecule 1: Teixobactin

Chain D: 9% 36% 9% 45%



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain J:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain K:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain L:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry*.

Of the 25 calculated structures, 25 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
HADDOCK	structure calculation	2.4
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	79
Number of shifts mapped to atoms	78
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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: ZAE, NAG, DAL, MUB, DTH, P1W, DGN, EI4, 28J, DGL, 2PO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.94±0.19	0±0/37 (0.0± 0.0%)	1.23±0.21	0±0/44 (0.2± 0.6%)
1	B	1.08±0.22	0±0/37 (0.0± 0.0%)	1.42±0.22	0±0/44 (0.2± 0.6%)
1	C	1.12±0.19	0±0/37 (0.0± 0.0%)	1.39±0.21	0±0/44 (0.0± 0.0%)
1	D	0.86±0.17	0±0/37 (0.1± 0.5%)	1.18±0.13	0±0/44 (0.0± 0.0%)
2	E	1.78±0.18	0±0/12 (0.0± 0.0%)	2.69±0.21	1±0/12 (9.3± 2.7%)
2	F	1.82±0.20	0±0/12 (0.0± 0.0%)	2.71±0.23	1±0/12 (8.7± 1.6%)
2	G	1.85±0.22	0±0/12 (0.7± 2.3%)	2.62±0.28	1±0/12 (8.7± 1.6%)
2	H	1.83±0.20	0±0/12 (0.0± 0.0%)	2.65±0.27	1±0/12 (8.3± 0.0%)
All	All	1.27	3/4900 (0.1%)	1.71	109/5600 (1.9%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	G	3	LYS	CD-CE	5.29	1.64	1.51	9	2
1	D	3	SER	CA-CB	-5.09	1.45	1.52	12	1

5 of 10 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	E	3	LYS	CD-CE-NZ	9.09	132.61	111.70	12	25
2	G	3	LYS	CD-CE-NZ	8.93	132.24	111.70	12	25
2	F	3	LYS	CD-CE-NZ	8.77	131.88	111.70	12	25
2	H	3	LYS	CD-CE-NZ	8.70	131.70	111.70	12	25
1	A	3	SER	N-CA-CB	6.33	120.00	110.50	11	2

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	41	48	48	4±3
1	B	41	48	48	4±3
1	C	41	48	48	4±3
1	D	41	48	48	4±2
2	E	33	33	30	2±2
2	F	33	33	31	2±2
2	G	33	33	30	2±2
2	H	33	34	29	2±3
3	I	33	30	29	5±2
3	J	33	30	29	6±2
3	K	33	30	29	7±2
3	L	33	30	29	6±2
4	A	8	0	0	2±1
4	B	8	0	0	2±2
4	C	8	0	0	2±1
4	D	8	0	0	2±2
5	B	15	25	0	1±2
5	C	20	34	0	1±1
5	D	10	16	0	0±1
5	A	15	25	0	0±1
All	All	13000	13625	10653	1058

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 45.

5 of 422 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:H:4:DAL:CA	2:H:4:DAL:CB	1.65	1.75	24	3
2:F:4:DAL:CA	2:F:4:DAL:CB	1.63	1.74	24	3
2:H:5:DAL:CA	2:H:5:DAL:C	1.62	1.74	25	1
2:G:4:DAL:CA	2:G:4:DAL:CB	1.61	1.79	23	4
2:E:4:DAL:CA	2:E:4:DAL:CB	1.60	1.74	24	3

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	5/11 (45%)	3±1 (67±12%)	1±1 (18±12%)	1±1 (15±13%)	0 4
1	B	5/11 (45%)	3±1 (61±11%)	1±1 (24±13%)	1±1 (15±12%)	0 4
1	C	5/11 (45%)	3±1 (63±11%)	1±1 (25±13%)	1±1 (12±11%)	1 7
1	D	5/11 (45%)	3±1 (67±14%)	1±1 (15±13%)	1±1 (18±10%)	0 3
2	E	0	-	-	-	-
2	F	0	-	-	-	-
2	G	0	-	-	-	-
2	H	0	-	-	-	-
All	All	500/1600 (31%)	323 (65%)	102 (20%)	75 (15%)	0 4

5 of 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	7	SER	14
1	D	7	SER	14
1	A	7	SER	12
1	C	7	SER	11
1	D	9	ALA	8

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	5/5 (100%)	4±1 (82±19%)	1±1 (18±19%)	4 39
1	B	5/5 (100%)	4±1 (71±23%)	1±1 (29±23%)	2 18
1	C	5/5 (100%)	4±1 (78±14%)	1±1 (22±14%)	3 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	5/5 (100%)	4±1 (82±19%)	1±1 (18±19%)	4 37
2	E	1/1 (100%)	0±0 (32±47%)	1±0 (68±47%)	0 0
2	F	1/1 (100%)	0±0 (20±40%)	1±0 (80±40%)	0 0
2	G	1/1 (100%)	0±0 (20±40%)	1±0 (80±40%)	0 0
2	H	1/1 (100%)	0±0 (12±32%)	1±0 (88±32%)	0 0
All	All	600/600 (100%)	412 (69%)	188 (31%)	1 14

5 of 24 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	H	3	LYS	22
2	G	3	LYS	20
2	F	3	LYS	20
2	E	3	LYS	17
1	C	2	ILE	14

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

32 non-standard protein/DNA/RNA residues are 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
1	ZAE	A	1	1	11,12,13	0.54±0.12	0±0 (0±0%)
1	ZAE	C	1	1	11,12,13	0.67±0.20	0±0 (1±4%)
1	EI4	C	10	1	8,11,12	1.98±0.16	3±1 (37±9%)
1	28J	C	5	1	6,7,8	0.94±0.17	0±0 (3±6%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	ZAE	D	1	1	11,12,13	0.59±0.10	0±0 (0±1%)
1	28J	B	5	1	6,7,8	1.04±0.18	0±1 (8±11%)
1	28J	D	5	1	6,7,8	0.92±0.15	0±0 (2±5%)
1	EI4	B	10	1	8,11,12	2.05±0.16	3±1 (43±8%)
1	EI4	A	10	1	8,11,12	2.04±0.21	3±1 (41±8%)
1	28J	A	5	1	6,7,8	0.86±0.14	0±0 (2±5%)
1	ZAE	B	1	1	11,12,13	0.65±0.17	0±0 (1±3%)
1	EI4	D	10	1	8,11,12	1.87±0.16	3±1 (39±12%)

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
1	ZAE	A	1	1	13,14,16	0.69±0.14	0±0 (1±2%)
1	ZAE	C	1	1	13,14,16	0.95±0.27	1±1 (6±7%)
1	EI4	C	10	1	4,14,16	0.94±0.22	0±0 (2±9%)
1	28J	C	5	1	5,8,10	1.95±0.50	1±0 (21±7%)
1	ZAE	D	1	1	13,14,16	0.72±0.16	0±0 (1±2%)
1	28J	B	5	1	5,8,10	1.68±0.37	1±0 (22±8%)
1	28J	D	5	1	5,8,10	1.34±0.18	1±1 (15±11%)
1	EI4	B	10	1	4,14,16	0.88±0.14	0±0 (0±0%)
1	EI4	A	10	1	4,14,16	1.00±0.27	0±0 (3±8%)
1	28J	A	5	1	5,8,10	1.39±0.22	1±1 (18±11%)
1	ZAE	B	1	1	13,14,16	1.01±0.45	1±1 (6±7%)
1	EI4	D	10	1	4,14,16	0.91±0.16	0±0 (2±6%)

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
1	28J	B	5	1	-	0±0,7,8,10	-
1	28J	A	5	1	-	0±0,7,8,10	-
1	ZAE	C	1	1	-	0±0,5,8,10	0±0,1,1,1
1	EI4	C	10	1	-	0±0,5,15,17	0±0,1,1,1
1	ZAE	D	1	1	-	0±0,5,8,10	0±0,1,1,1
1	ZAE	B	1	1	-	0±0,5,8,10	0±0,1,1,1
1	EI4	B	10	1	-	0±0,5,15,17	0±0,1,1,1
1	EI4	D	10	1	-	0±0,5,15,17	0±0,1,1,1
1	28J	C	5	1	-	0±0,7,8,10	-
1	ZAE	A	1	1	-	0±0,5,8,10	0±0,1,1,1
1	28J	D	5	1	-	0±0,7,8,10	-
1	EI4	A	10	1	-	0±0,5,15,17	0±0,1,1,1

5 of 35 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	10	EI4	CG-ND1	5.19	1.52	1.46	22	25
1	A	10	EI4	CG-ND1	4.96	1.52	1.46	13	24
1	C	10	EI4	CG-ND1	4.79	1.52	1.46	1	22
1	D	10	EI4	CG-ND1	4.59	1.52	1.46	5	23
1	C	10	EI4	CE1-NE2	4.13	1.41	1.35	11	21

5 of 33 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	1	ZAE	CG-CB-CA	7.74	124.71	113.63	18	7
1	C	5	28J	CB-CA-C	6.50	102.89	112.83	18	23
1	B	5	28J	CB-CA-C	5.24	104.81	112.83	17	22
1	C	1	ZAE	CG-CB-CA	4.59	120.19	113.63	2	10
1	B	1	ZAE	CB-CA-N	4.38	103.86	110.65	7	4

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

8 monosaccharides are 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
3	MUB	I	1	4,3,2	18,19,20	1.00±0.13	1±0 (6±2%)
3	NAG	I	2	3	14,14,15	0.62±0.05	0±0 (0±1%)
3	MUB	J	1	4,3,2	18,19,20	0.97±0.07	1±0 (6±2%)
3	NAG	J	2	3	14,14,15	0.63±0.06	0±0 (0±1%)
3	MUB	K	1	4,3,2	18,19,20	0.97±0.10	1±0 (5±1%)
3	NAG	K	2	3	14,14,15	0.63±0.05	0±0 (0±1%)
3	MUB	L	1	4,3,2	18,19,20	0.96±0.09	1±0 (6±1%)
3	NAG	L	2	3	14,14,15	0.63±0.05	0±0 (0±1%)

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
3	MUB	I	1	4,3,2	21,26,28	1.36±0.08	1±1 (6±2%)
3	NAG	I	2	3	17,19,21	0.61±0.05	0±0 (0±0%)
3	MUB	J	1	4,3,2	21,26,28	1.39±0.13	2±1 (7±3%)
3	NAG	J	2	3	17,19,21	0.58±0.08	0±0 (0±0%)
3	MUB	K	1	4,3,2	21,26,28	1.38±0.10	1±1 (6±2%)
3	NAG	K	2	3	17,19,21	0.58±0.07	0±0 (0±0%)
3	MUB	L	1	4,3,2	21,26,28	1.33±0.07	1±1 (6±2%)
3	NAG	L	2	3	17,19,21	0.60±0.08	0±0 (0±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
3	MUB	I	1	4,3,2	1±0,1,8,9	0±0,10,32,34	0±0,1,1,1
3	NAG	I	2	3	-	0±0,6,23,26	0±0,1,1,1
3	MUB	J	1	4,3,2	1±0,1,8,9	0±0,10,32,34	0±0,1,1,1
3	NAG	J	2	3	-	0±0,6,23,26	0±0,1,1,1
3	MUB	K	1	4,3,2	1±0,1,8,9	0±0,10,32,34	0±0,1,1,1
3	NAG	K	2	3	-	0±0,6,23,26	0±0,1,1,1
3	MUB	L	1	4,3,2	1±0,1,8,9	0±0,10,32,34	0±0,1,1,1
3	NAG	L	2	3	-	0±0,6,23,26	0±0,1,1,1

5 of 14 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
3	I	1	MUB	C1-C2	4.12	1.48	1.52	4	1
3	K	1	MUB	C11-C9	3.81	1.59	1.51	13	24
3	I	1	MUB	C11-C9	3.53	1.58	1.51	4	24
3	J	1	MUB	C11-C9	3.52	1.58	1.51	13	24
3	L	1	MUB	C11-C9	3.42	1.58	1.51	13	25

5 of 24 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	J	1	MUB	O3-C9-C11	5.98	123.67	107.48	5	25
3	I	1	MUB	O3-C9-C11	5.20	121.54	107.48	11	25
3	K	1	MUB	O3-C9-C11	5.04	121.11	107.48	25	25
3	L	1	MUB	O3-C9-C11	4.94	120.86	107.48	10	25
3	J	1	MUB	C1-C2-N2	3.48	114.76	110.73	7	7

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

Mol	Chain	Res	Type	Atoms	Models (Total)
3	L	1	MUB	C9	18
3	K	1	MUB	C9	16
3	I	1	MUB	C9	15
3	J	1	MUB	C9	13

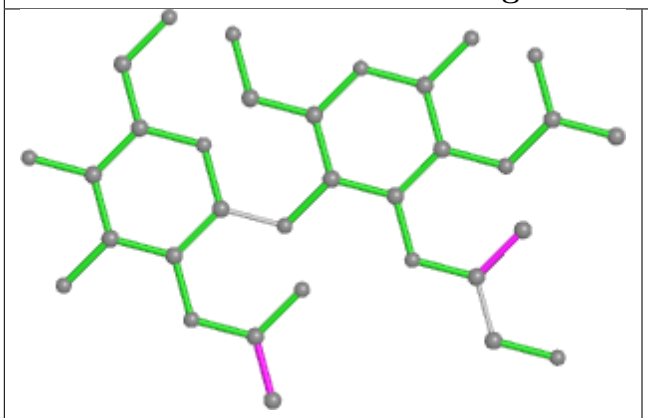
There are no torsion outliers.

There are no ring outliers.

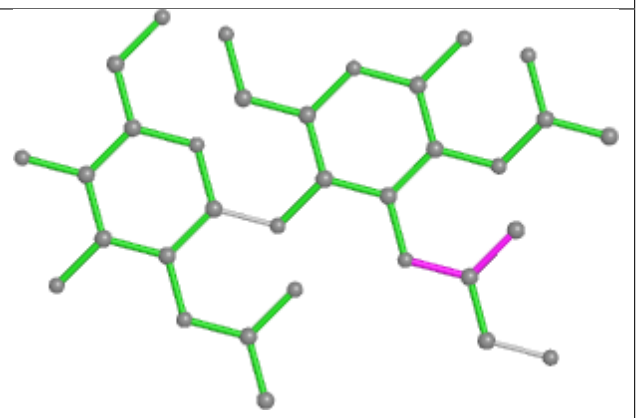
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

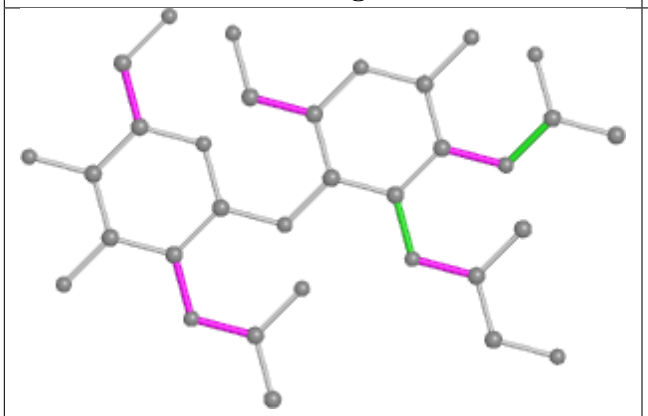
Oligosaccharide Chain I



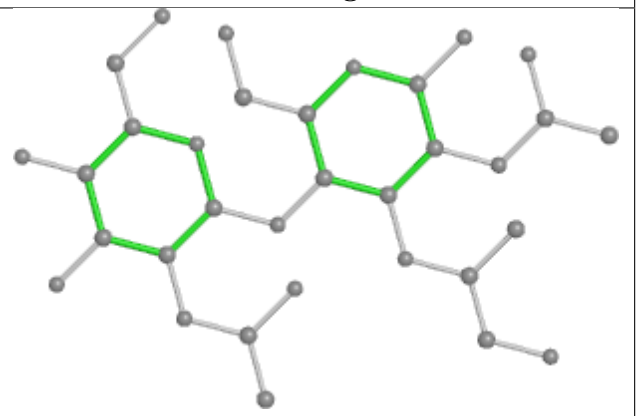
Bond lengths



Bond angles

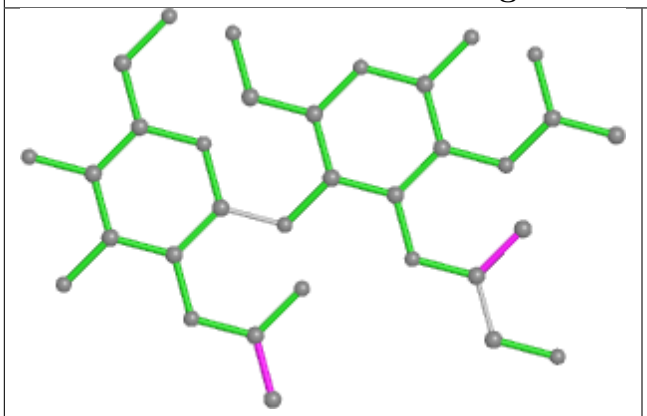


Torsions

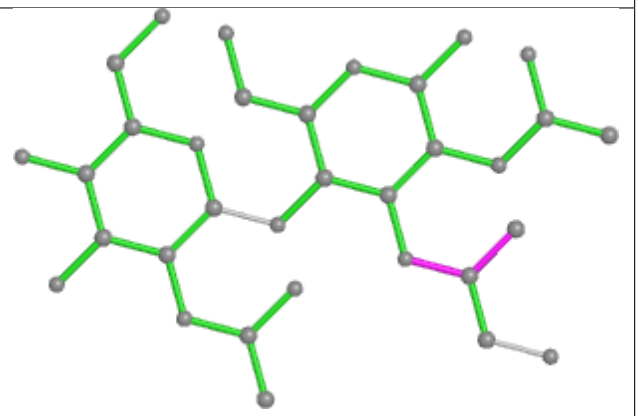


Rings

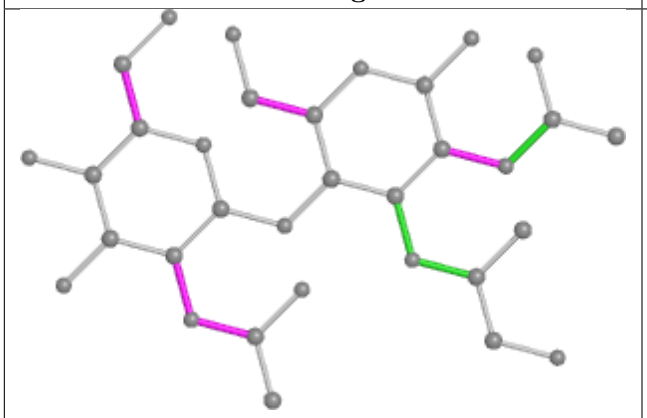
Oligosaccharide Chain J



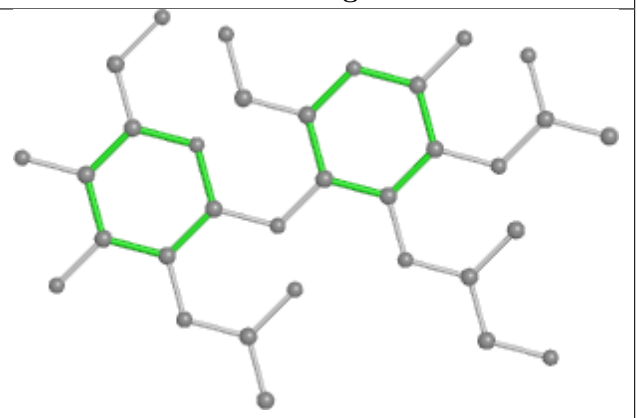
Bond lengths



Bond angles

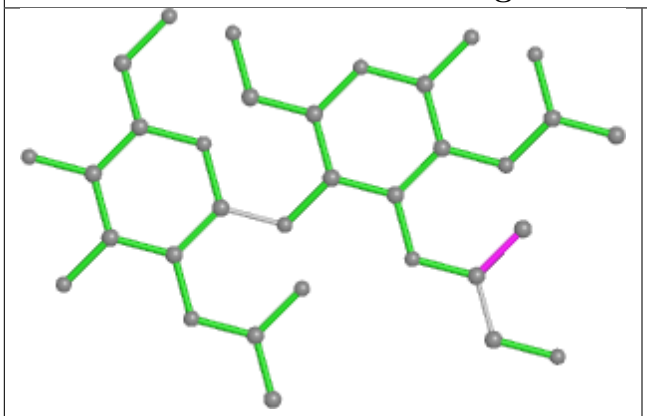


Torsions

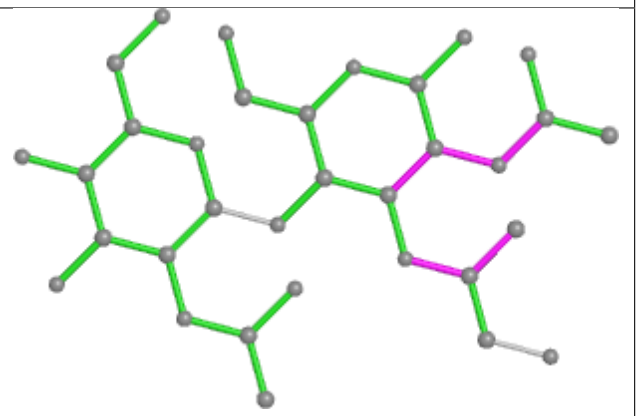


Rings

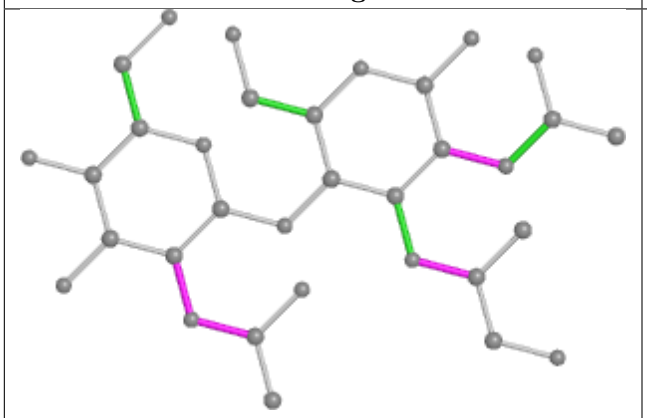
Oligosaccharide Chain K



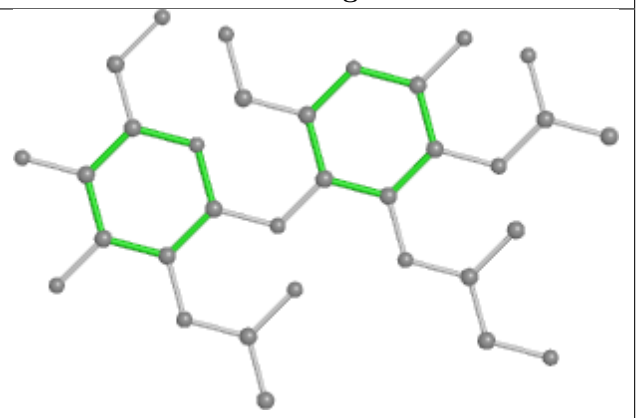
Bond lengths



Bond angles

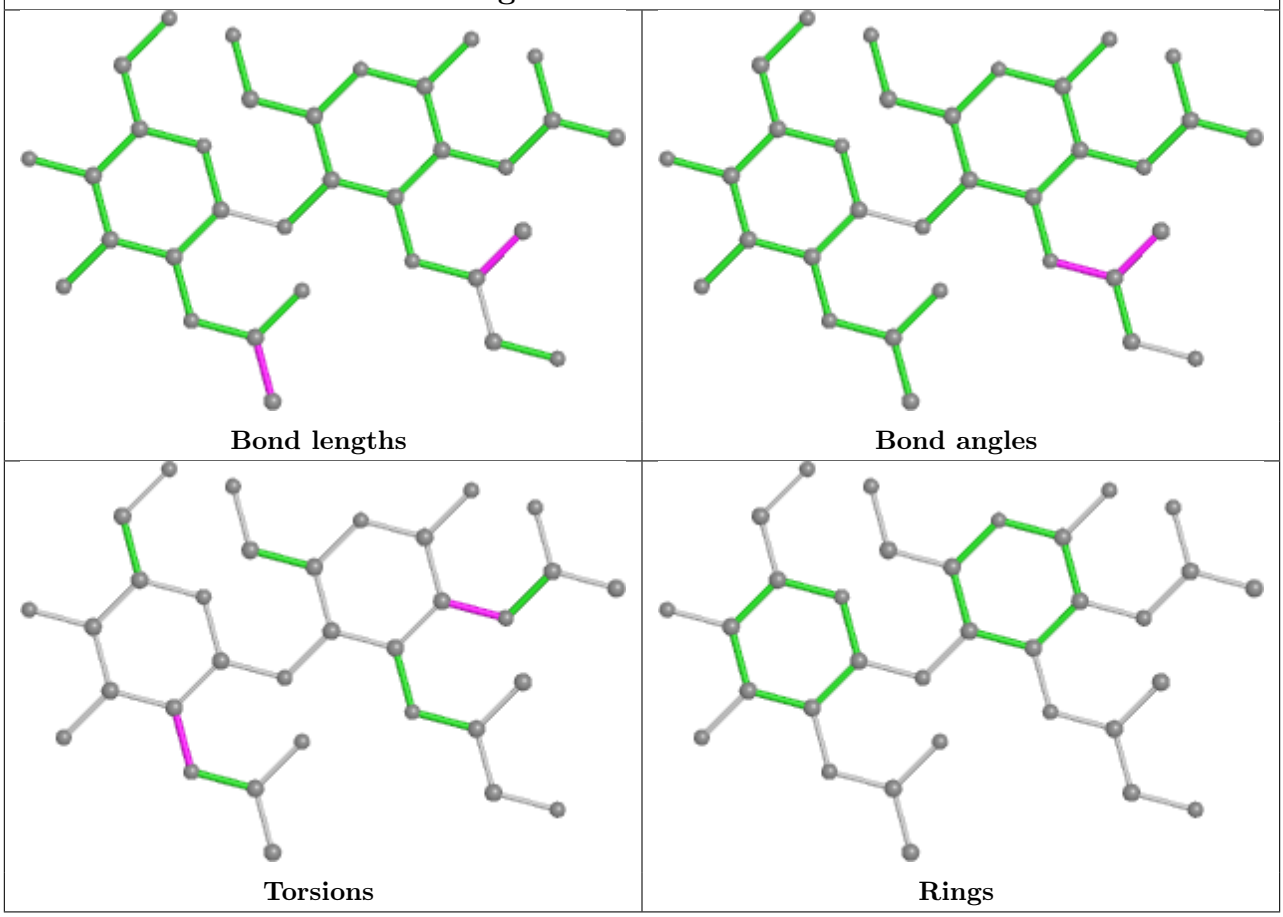


Torsions



Rings

Oligosaccharide Chain L



6.6 Ligand geometry (i)

20 ligands are 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
5	P1W	A	105	5	4,4,5	0.87±0.12	0±0 (0±0%)
4	2PO	C	105	4,5	0,3,3	0.00±0.00	-
5	P1W	D	103	4,5	4,4,5	0.90±0.26	0±0 (2±6%)
5	P1W	A	104	5	4,4,5	0.76±0.16	0±0 (1±4%)
5	P1W	B	104	4,5	4,4,5	0.85±0.28	0±0 (4±9%)
5	P1W	B	105	5	4,4,5	0.77±0.15	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	2PO	D	101	4,3	0,3,3	0.00±0.00	-
4	2PO	A	101	4,3	0,3,3	0.00±0.00	-
4	2PO	A	102	4,5	0,3,3	0.00±0.00	-
5	P1W	C	101	5	4,4,5	0.94±0.18	0±0 (4±9%)
5	P1W	C	102	5	4,4,5	0.88±0.12	0±0 (0±0%)
5	P1W	C	103	5	4,4,5	0.73±0.09	0±0 (0±0%)
4	2PO	B	103	4,5	0,3,3	0.00±0.00	-
5	P1W	C	106	4,5	4,4,5	0.76±0.24	0±0 (1±4%)
5	P1W	D	104	5	4,4,5	0.75±0.11	0±0 (0±0%)
5	P1W	B	101	5	4,4,5	0.85±0.16	0±0 (2±6%)
4	2PO	B	102	4,3	0,3,3	0.00±0.00	-
4	2PO	C	104	4,3	0,3,3	0.00±0.00	-
5	P1W	A	103	4,5	4,4,5	0.80±0.30	0±0 (2±6%)
4	2PO	D	102	4,5	0,3,3	0.00±0.00	-

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	P1W	A	105	5	4,4,5	0.59±0.17	0±0 (1±4%)
4	2PO	C	105	4,5	0,3,3	0.00±0.00	-
5	P1W	D	103	4,5	4,4,5	0.52±0.34	0±0 (2±9%)
5	P1W	A	104	5	4,4,5	0.57±0.11	0±0 (0±0%)
5	P1W	B	104	4,5	4,4,5	0.61±0.25	0±0 (0±0%)
5	P1W	B	105	5	4,4,5	0.56±0.14	0±0 (0±0%)
4	2PO	D	101	4,3	0,3,3	0.00±0.00	-
4	2PO	A	101	4,3	0,3,3	0.00±0.00	-
4	2PO	A	102	4,5	0,3,3	0.00±0.00	-
5	P1W	C	101	5	4,4,5	0.58±0.18	0±0 (0±0%)
5	P1W	C	102	5	4,4,5	0.57±0.15	0±0 (0±0%)
5	P1W	C	103	5	4,4,5	0.59±0.13	0±0 (0±0%)
4	2PO	B	103	4,5	0,3,3	0.00±0.00	-
5	P1W	C	106	4,5	4,4,5	0.60±0.25	0±0 (0±0%)
5	P1W	D	104	5	4,4,5	0.54±0.13	0±0 (0±0%)
5	P1W	B	101	5	4,4,5	0.65±0.15	0±0 (0±0%)
4	2PO	B	102	4,3	0,3,3	0.00±0.00	-

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	2PO	C	104	4,3	0,3,3	0.00±0.00	-
5	P1W	A	103	4,5	4,4,5	0.59±0.28	0±0 (0±0%)
4	2PO	D	102	4,5	0,3,3	0.00±0.00	-

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
5	P1W	A	105	5	-	0±0,2,2,3	-
5	P1W	C	101	5	-	0±0,2,2,3	-
5	P1W	C	102	5	-	0±0,2,2,3	-
5	P1W	A	104	5	-	0±0,2,2,3	-
5	P1W	B	105	5	-	0±0,2,2,3	-
5	P1W	A	103	4,5	-	0±0,2,2,3	-
5	P1W	C	106	4,5	-	0±0,2,2,3	-
5	P1W	D	103	4,5	-	0±0,2,2,3	-
5	P1W	C	103	5	-	0±0,2,2,3	-
5	P1W	B	104	4,5	-	0±0,2,2,3	-
5	P1W	D	104	5	-	0±0,2,2,3	-
5	P1W	B	101	5	-	0±0,2,2,3	-

5 of 8 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
5	D	103	P1W	C2-C3	2.65	1.22	1.33	5	1
5	A	103	P1W	C5-C3	2.56	1.57	1.50	4	2
5	B	104	P1W	C5-C3	2.45	1.57	1.50	13	4
5	D	103	P1W	C4-C3	2.35	1.56	1.50	2	1
5	C	101	P1W	C4-C3	2.23	1.56	1.50	1	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
5	D	103	P1W	C1-C2-C3	2.87	118.20	126.31	5	1
5	D	103	P1W	C5-C3-C4	2.15	119.36	114.60	5	1
5	A	105	P1W	C1-C2-C3	2.01	120.62	126.31	15	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	23-F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
23	F	2:DGL	C	3:LYS	N	2.99

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 9% for the well-defined parts and 9% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping (i)

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

Total number of shifts	79
Number of shifts mapped to atoms	78
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	28J	H2	8.5	.	.

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 9%, i.e. 39 atoms were assigned a chemical shift out of a possible 424. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	24/160 (15%)	6/64 (9%)	12/64 (19%)	6/32 (19%)
Sidechain	15/264 (6%)	0/180 (0%)	15/80 (19%)	0/4 (0%)
Overall	39/424 (9%)	6/244 (2%)	27/144 (19%)	6/36 (17%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts (i)

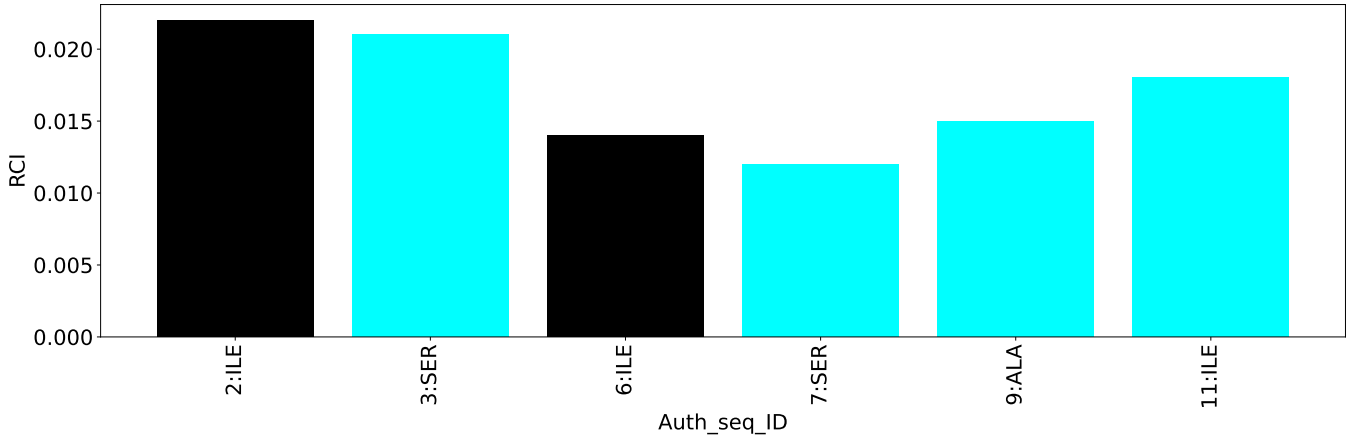
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	7	SER	H	11.20	5.45 – 11.10	5.2

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	183
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	0
Medium range (|i-j|>1 and |i-j|<5)	0
Long range (|i-j|≥5)	0
Inter-chain	127
Hydrogen bond restraints	56
Disulfide bond restraints	0
Total dihedral-angle restraints	40
Number of unmapped restraints	0
Number of restraints per residue	2.7
Number of long range restraints per residue[1]	0.0

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	1.8	0.2
0.2-0.5 (Medium)	3.9	0.5
>0.5 (Large)	2.7	2.02

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	12.9	9.89
10.0-20.0 (Medium)	7.1	19.94
>20.0 (Large)	1.3	34.84

9 Distance violation analysis (i)

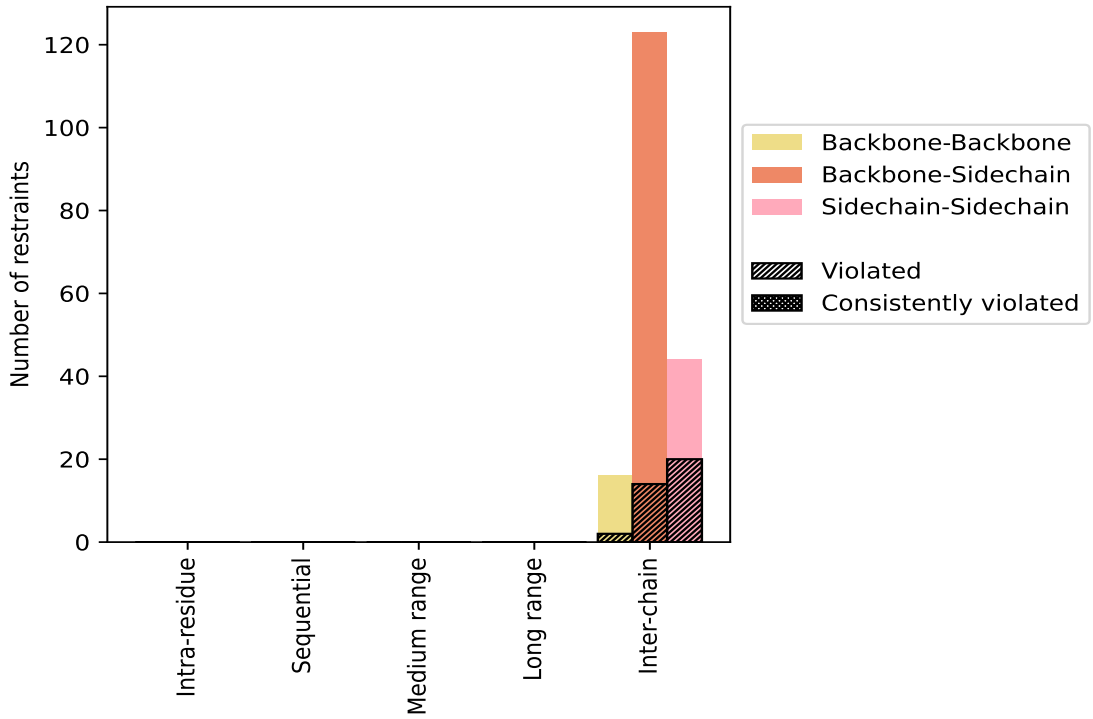
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	127	69.4	24	18.9	13.1	0	0.0	0.0
Backbone-Backbone	16	8.7	2	12.5	1.1	0	0.0	0.0
Backbone-Sidechain	67	36.6	2	3.0	1.1	0	0.0	0.0
Sidechain-Sidechain	44	24.0	20	45.5	10.9	0	0.0	0.0
Hydrogen bond	56	30.6	12	21.4	6.6	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	183	100.0	36	19.7	19.7	0	0.0	0.0
Backbone-Backbone	16	8.7	2	12.5	1.1	0	0.0	0.0
Backbone-Sidechain	123	67.2	14	11.4	7.7	0	0.0	0.0
Sidechain-Sidechain	44	24.0	20	45.5	10.9	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	16	16	0.54	0.79	0.21	0.61
2	0	0	0	0	8	8	0.11	0.12	0.01	0.11
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	10	10	0.45	0.83	0.21	0.34
7	0	0	0	0	22	22	0.49	0.98	0.28	0.43
8	0	0	0	0	16	16	0.85	2.02	0.7	0.56
9	0	0	0	0	14	14	0.31	0.61	0.14	0.22
10	0	0	0	0	6	6	0.18	0.18	0.0	0.18
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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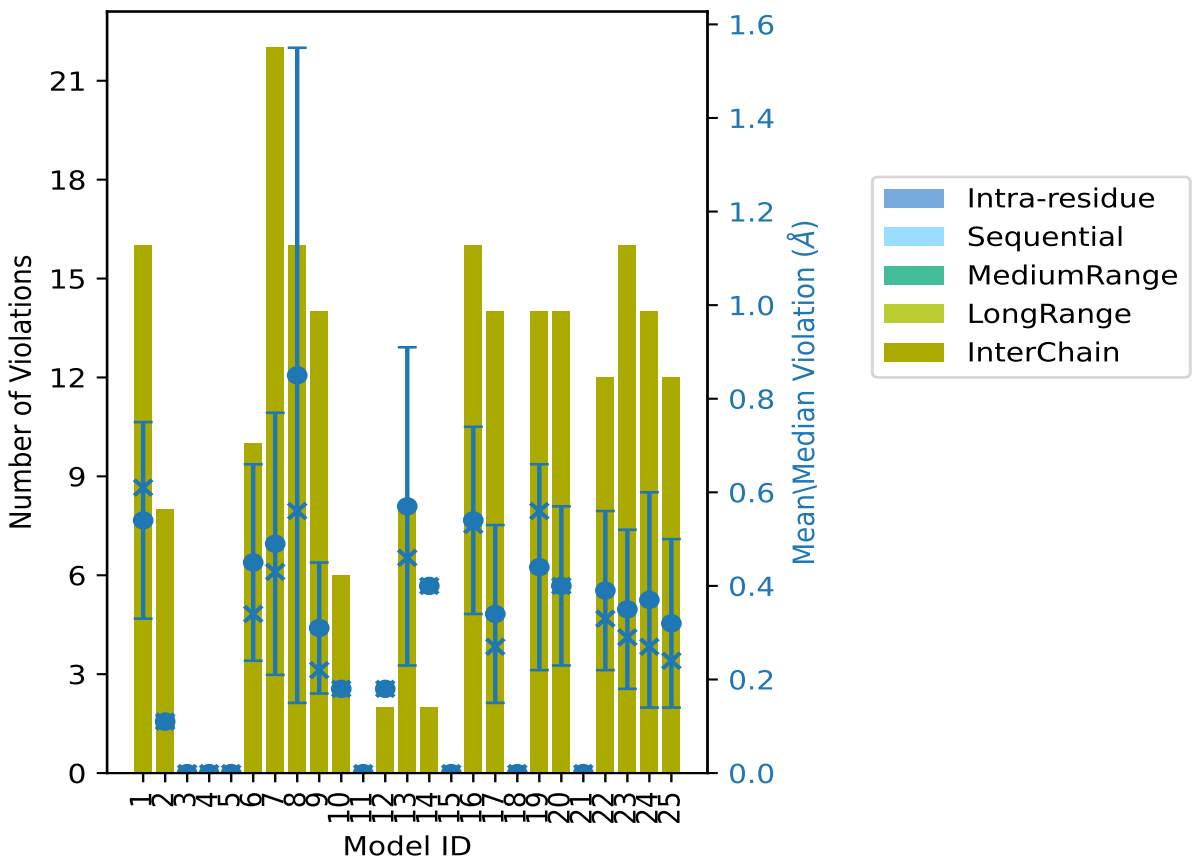
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	0	2	2	0.18	0.18	0.0	0.18
13	0	0	0	0	8	8	0.57	1.11	0.34	0.46
14	0	0	0	0	2	2	0.4	0.4	0.0	0.4
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	16	16	0.54	0.99	0.2	0.53
17	0	0	0	0	14	14	0.34	0.77	0.19	0.27
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	14	14	0.44	0.71	0.22	0.56
20	0	0	0	0	14	14	0.4	0.63	0.17	0.4
21	0	0	0	0	0	0	0.0	0.0	0.0	0.0
22	0	0	0	0	12	12	0.39	0.64	0.17	0.33
23	0	0	0	0	16	16	0.35	0.74	0.17	0.29
24	0	0	0	0	14	14	0.37	0.87	0.23	0.27
25	0	0	0	0	12	12	0.32	0.67	0.18	0.24

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

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



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

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 103(IR:0, SQ:0, MR:0, LR:0, IC:103) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	2	2	1	4.0
0	0	0	0	2	2	2	8.0
0	0	0	0	0	0	3	12.0
0	0	0	0	0	0	4	16.0
0	0	0	0	2	2	5	20.0
0	0	0	0	2	2	6	24.0

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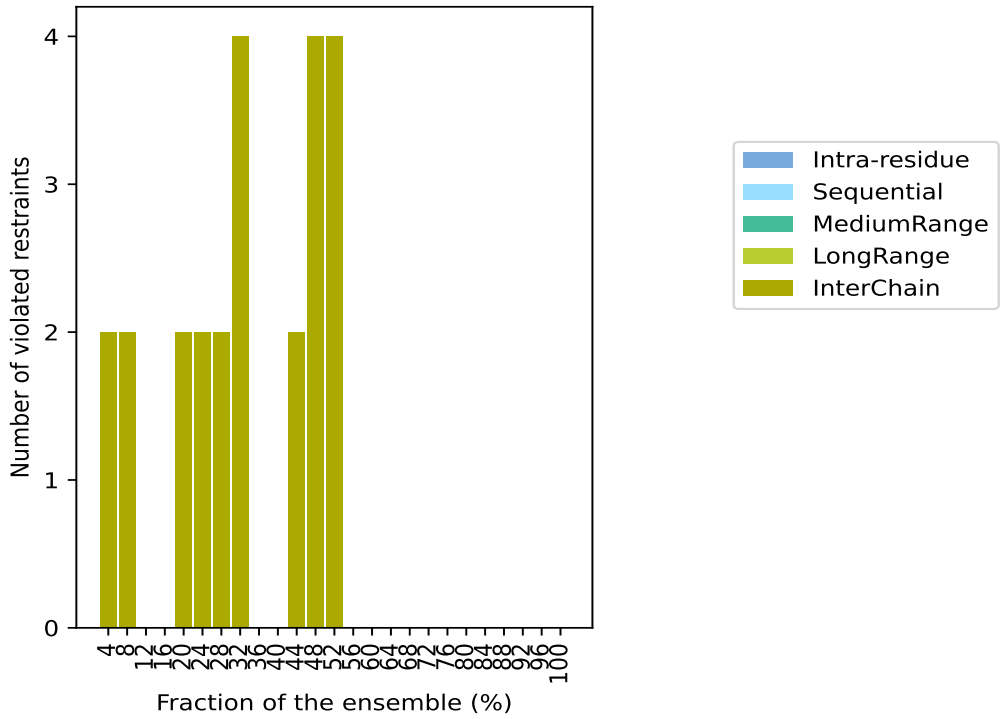
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	2	2	7	28.0
0	0	0	0	4	4	8	32.0
0	0	0	0	0	0	9	36.0
0	0	0	0	0	0	10	40.0
0	0	0	0	2	2	11	44.0
0	0	0	0	4	4	12	48.0
0	0	0	0	4	4	13	52.0
0	0	0	0	0	0	14	56.0
0	0	0	0	0	0	15	60.0
0	0	0	0	0	0	16	64.0
0	0	0	0	0	0	17	68.0
0	0	0	0	0	0	18	72.0
0	0	0	0	0	0	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	0	0	0	21	84.0
0	0	0	0	0	0	22	88.0
0	0	0	0	0	0	23	92.0
0	0	0	0	0	0	24	96.0
0	0	0	0	0	0	25	100.0

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

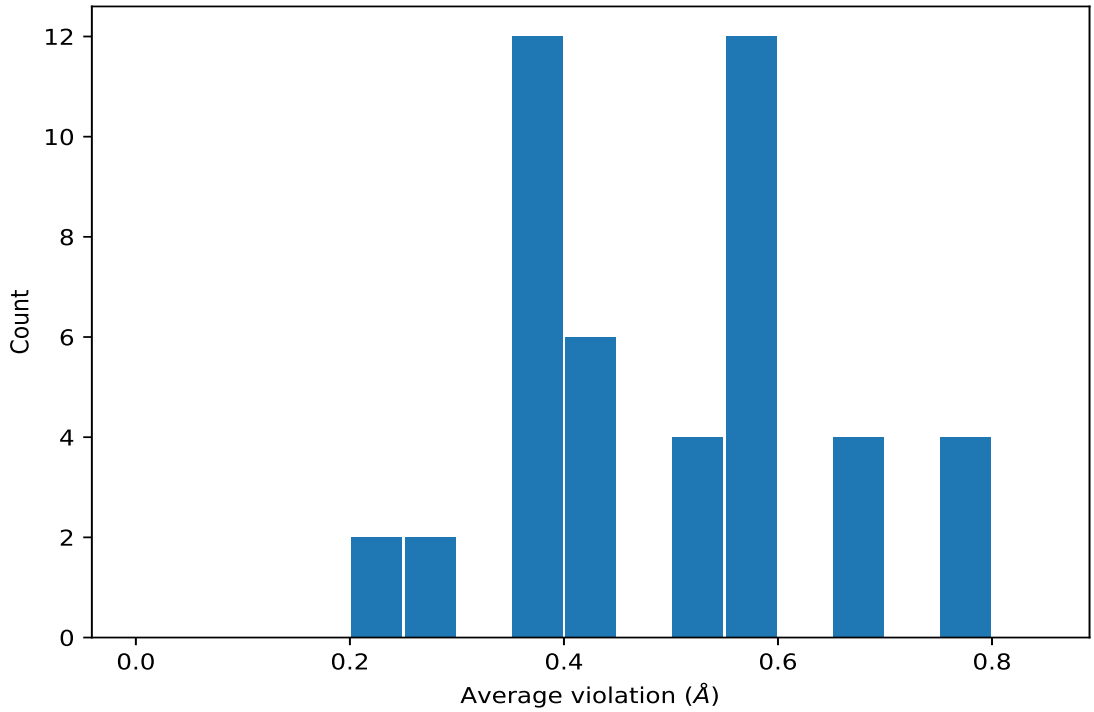
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,25)	1:6:B:ILE:CD1	1:1:C:ZAE:CG	13	0.38	0.18	0.32
(1,25)	1:6:B:ILE:CD1	1:1:A:ZAE:CG	13	0.38	0.18	0.32
(1,57)	1:6:B:ILE:CD1	1:1:C:ZAE:CG	13	0.38	0.18	0.32
(1,57)	1:6:B:ILE:CD1	1:1:A:ZAE:CG	13	0.38	0.18	0.32
(1,14)	1:5:B:28J:CG1	1:1:C:ZAE:CG	13	0.26	0.07	0.24
(1,46)	1:5:B:28J:CG1	1:1:C:ZAE:CG	13	0.26	0.07	0.24
(1,88)	1:6:C:ILE:CD1	1:1:B:ZAE:CD2	12	0.57	0.3	0.53
(1,88)	1:6:C:ILE:CD1	1:1:D:ZAE:CD2	12	0.57	0.3	0.53
(1,88)	1:6:C:ILE:CD1	1:1:D:ZAE:CD1	12	0.57	0.3	0.53
(1,88)	1:6:C:ILE:CD1	1:1:B:ZAE:CD1	12	0.57	0.3	0.53
(1,120)	1:6:C:ILE:CD1	1:1:B:ZAE:CD2	12	0.57	0.3	0.53
(1,120)	1:6:C:ILE:CD1	1:1:D:ZAE:CD2	12	0.57	0.3	0.53
(1,120)	1:6:C:ILE:CD1	1:1:D:ZAE:CD1	12	0.57	0.3	0.53
(1,120)	1:6:C:ILE:CD1	1:1:B:ZAE:CD1	12	0.57	0.3	0.53
(1,89)	1:6:C:ILE:CD1	1:1:B:ZAE:CG	12	0.57	0.19	0.62
(1,89)	1:6:C:ILE:CD1	1:1:D:ZAE:CG	12	0.57	0.19	0.62

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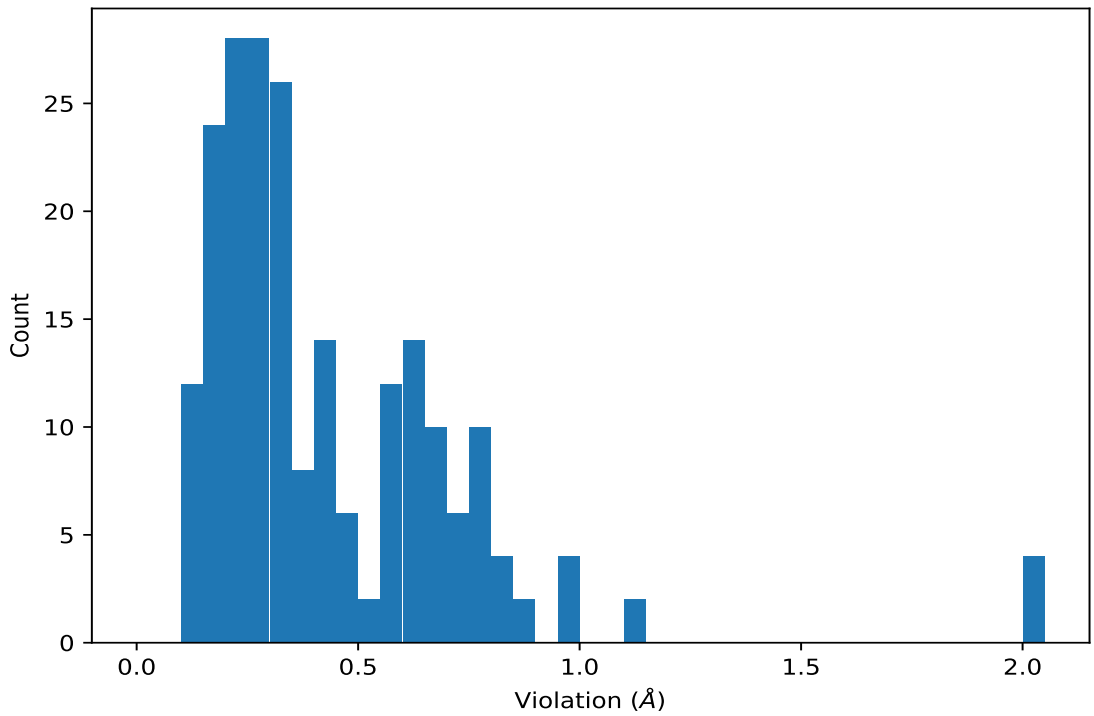
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,121)	1:6:C:ILE:CD1	1:1:B:ZAE:CG	12	0.57	0.19	0.62
(1,121)	1:6:C:ILE:CD1	1:1:D:ZAE:CG	12	0.57	0.19	0.62
(1,78)	1:5:C:28J:CG1	1:1:B:ZAE:CG	11	0.23	0.07	0.25
(1,110)	1:5:C:28J:CG1	1:1:B:ZAE:CG	11	0.23	0.07	0.25

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

The following table provides the 10 worst performing restraints, sorted by the violation 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)
(2,16)	1:7:A:SER:O	1:3:B:SER:H	8	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:7:A:SER:O	1:3:B:SER:H	8	2.02
(2,8)	1:7:A:SER:O	1:3:B:SER:H	8	2.02
(2,4)	1:7:A:SER:O	1:3:B:SER:H	8	2.02
(1,120)	1:6:C:ILE:CD1	1:1:B:ZAE:CD2	13	1.11
(1,88)	1:6:C:ILE:CD1	1:1:B:ZAE:CD2	13	1.11
(1,120)	1:6:C:ILE:CD1	1:1:B:ZAE:CD2	16	0.99
(1,88)	1:6:C:ILE:CD1	1:1:B:ZAE:CD2	16	0.99
(1,120)	1:6:C:ILE:CD1	1:1:D:ZAE:CD1	7	0.98
(1,88)	1:6:C:ILE:CD1	1:1:D:ZAE:CD1	7	0.98

10 Dihedral-angle violation analysis (i)

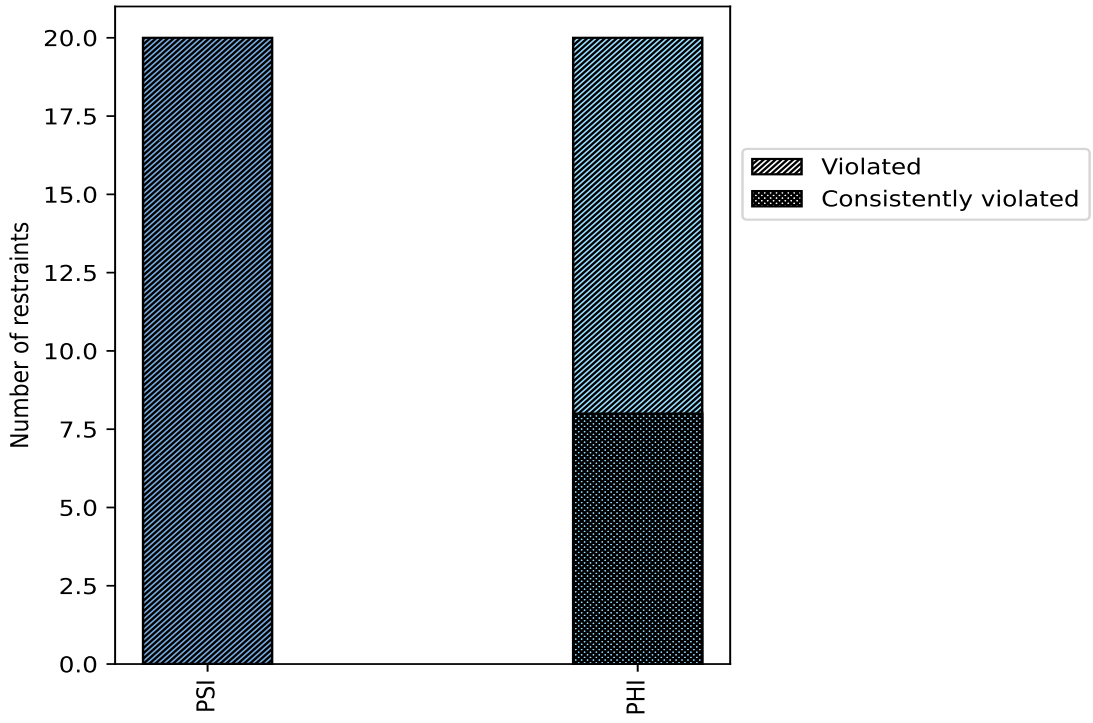
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	20	50.0	20	100.0	50.0	0	0.0	0.0
PHI	20	50.0	20	100.0	50.0	8	40.0	20.0
Total	40	100.0	40	100.0	100.0	8	20.0	20.0

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

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



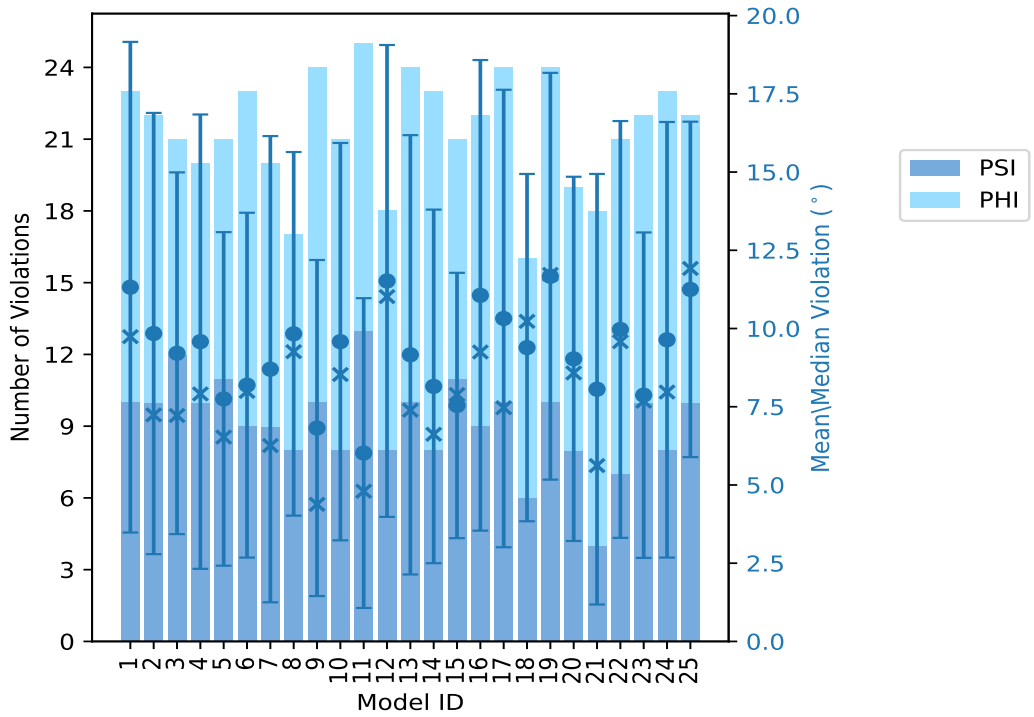
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	10	13	23	11.32	31.68	7.84	9.74
2	10	12	22	9.84	28.72	7.05	7.24
3	12	9	21	9.21	18.18	5.78	7.22
4	10	10	20	9.58	34.75	7.26	7.91
5	11	10	21	7.75	19.92	5.33	6.53
6	9	14	23	8.19	17.8	5.51	7.99
7	9	11	20	8.7	26.9	7.45	6.26
8	8	9	17	9.83	22.79	5.81	9.26
9	10	14	24	6.82	20.1	5.37	4.38
10	8	13	21	9.58	24.36	6.35	8.53
11	13	12	25	6.02	19.32	4.95	4.8
12	8	10	18	11.52	34.84	7.54	11.02
13	10	14	24	9.16	26.67	7.02	7.39
14	8	15	23	8.15	22.62	5.65	6.62
15	11	10	21	7.54	15.22	4.24	7.89
16	9	13	22	11.06	28.68	7.52	9.25
17	10	14	24	10.32	27.7	7.31	7.47
18	6	10	16	9.39	20.24	5.55	10.23
19	10	14	24	11.67	24.72	6.5	11.73
20	8	11	19	9.03	23.77	5.82	8.58
21	4	14	18	8.06	25.1	6.88	5.62
22	7	14	21	9.97	22.62	6.66	9.58
23	10	12	22	7.87	19.89	5.2	7.68
24	8	15	23	9.64	27.21	6.96	7.97
25	10	12	22	11.25	25.1	5.36	11.92

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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

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

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	1	4.0
1	0	1	2	8.0
1	3	4	3	12.0
2	0	2	4	16.0
1	0	1	5	20.0
2	0	2	6	24.0
2	2	4	7	28.0
1	2	3	8	32.0
0	0	0	9	36.0
1	2	3	10	40.0
0	0	0	11	44.0

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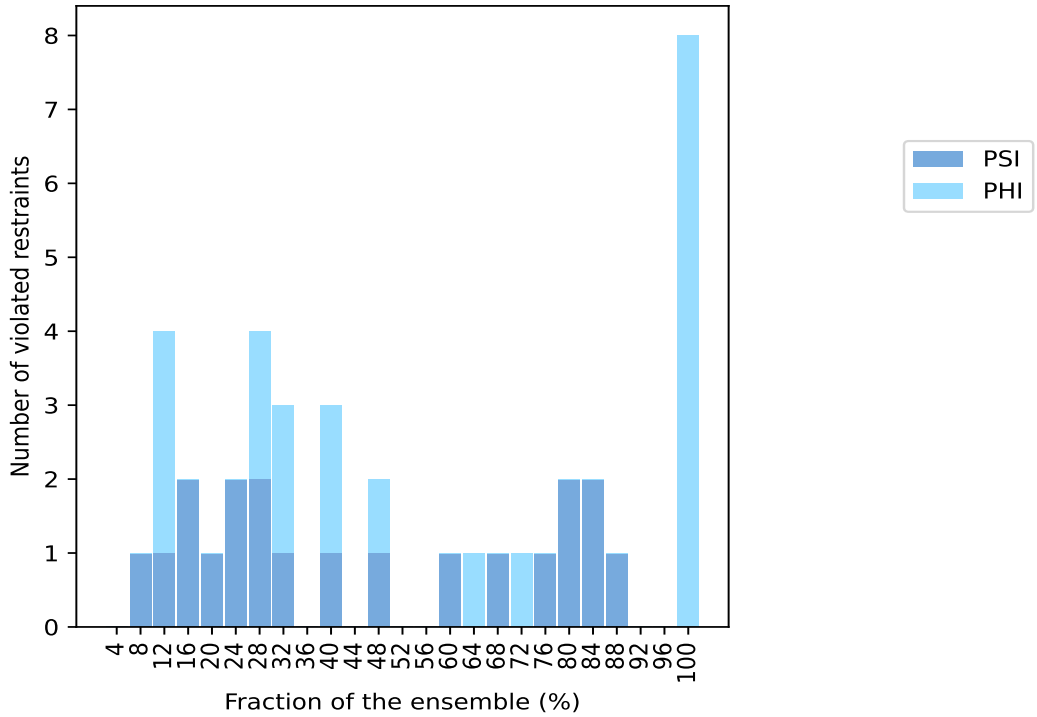
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	1	2	12	48.0
0	0	0	13	52.0
0	0	0	14	56.0
1	0	1	15	60.0
0	1	1	16	64.0
1	0	1	17	68.0
0	1	1	18	72.0
1	0	1	19	76.0
2	0	2	20	80.0
2	0	2	21	84.0
1	0	1	22	88.0
0	0	0	23	92.0
0	0	0	24	96.0
0	8	8	25	100.0

[1] Number of models with violations

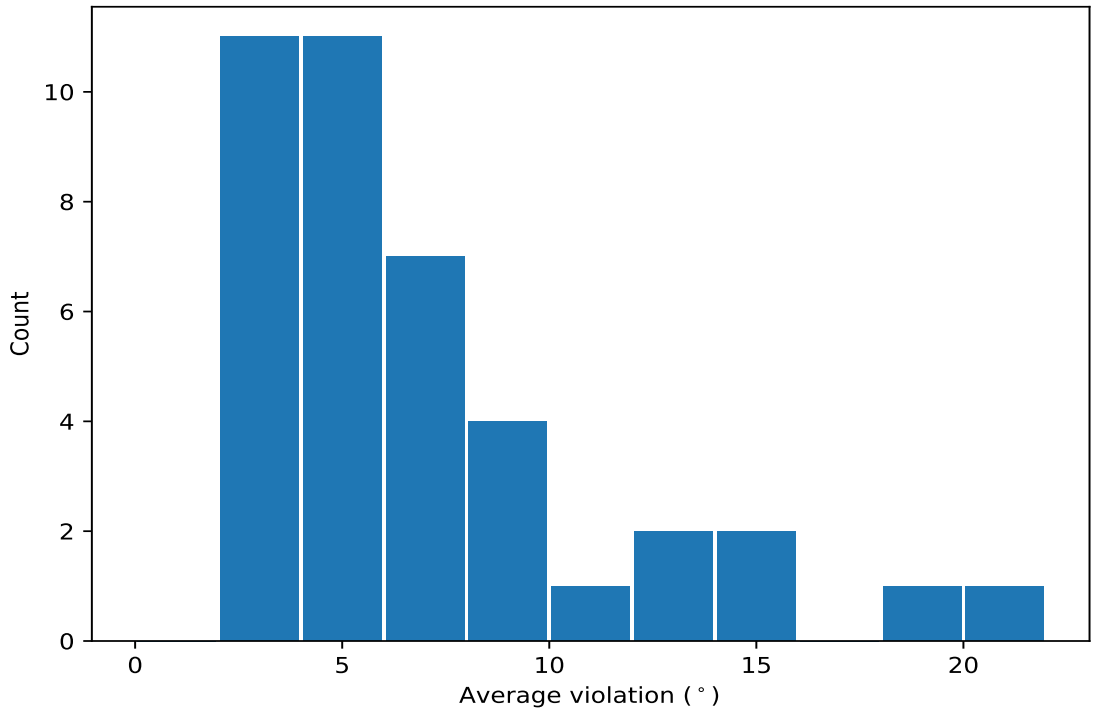
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

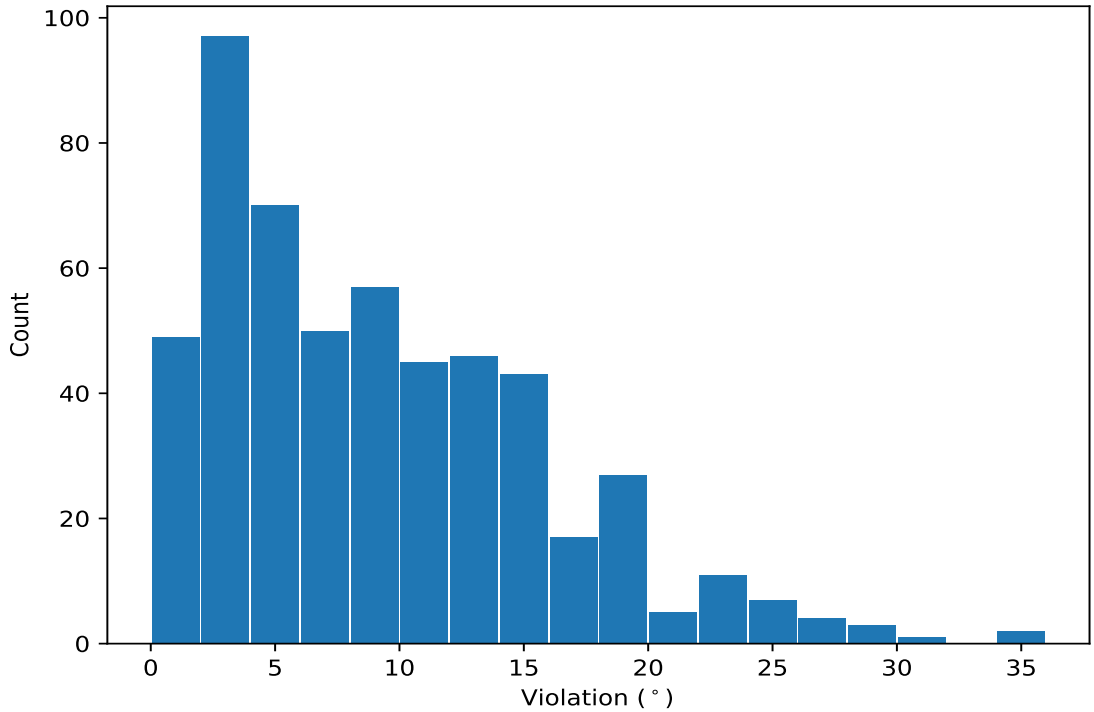
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,14)	1:4:B:DGN:C	1:5:B:28J:N	1:5:B:28J:CA	1:5:B:28J:C	25	20.15	5.37	19.32
(1,24)	1:4:C:DGN:C	1:5:C:28J:N	1:5:C:28J:CA	1:5:C:28J:C	25	19.36	6.69	19.55
(1,25)	1:5:C:28J:C	1:6:C:ILE:N	1:6:C:ILE:CA	1:6:C:ILE:C	25	15.85	5.56	15.66
(1,15)	1:5:B:28J:C	1:6:B:ILE:N	1:6:B:ILE:CA	1:6:B:ILE:C	25	15.28	6.19	14.05
(1,34)	1:4:D:DGN:C	1:5:D:28J:N	1:5:D:28J:CA	1:5:D:28J:C	25	13.83	2.36	14.01
(1,4)	1:4:A:DGN:C	1:5:A:28J:N	1:5:A:28J:CA	1:5:A:28J:C	25	13.69	3.8	13.35
(1,35)	1:5:D:28J:C	1:6:D:ILE:N	1:6:D:ILE:CA	1:6:D:ILE:C	25	11.58	3.52	12.39
(1,5)	1:5:A:28J:C	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	25	9.47	3.63	9.08
(1,38)	1:4:D:DGN:N	1:4:D:DGN:CA	1:4:D:DGN:C	1:5:D:28J:N	22	9.05	3.15	9.16
(1,8)	1:4:A:DGN:N	1:4:A:DGN:CA	1:4:A:DGN:C	1:5:A:28J:N	21	8.45	3.69	8.07

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table provides the list of violationsfor the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	1:4:B:DGN:C	1:5:B:28J:N	1:5:B:28J:CA	1:5:B:28J:C	12	34.84
(1,24)	1:4:C:DGN:C	1:5:C:28J:N	1:5:C:28J:CA	1:5:C:28J:C	4	34.75
(1,15)	1:5:B:28J:C	1:6:B:ILE:N	1:6:B:ILE:CA	1:6:B:ILE:C	1	31.68
(1,24)	1:4:C:DGN:C	1:5:C:28J:N	1:5:C:28J:CA	1:5:C:28J:C	2	28.72
(1,14)	1:4:B:DGN:C	1:5:B:28J:N	1:5:B:28J:CA	1:5:B:28J:C	16	28.68
(1,24)	1:4:C:DGN:C	1:5:C:28J:N	1:5:C:28J:CA	1:5:C:28J:C	16	28.34
(1,14)	1:4:B:DGN:C	1:5:B:28J:N	1:5:B:28J:CA	1:5:B:28J:C	17	27.7
(1,4)	1:4:A:DGN:C	1:5:A:28J:N	1:5:A:28J:CA	1:5:A:28J:C	24	27.21
(1,25)	1:5:C:28J:C	1:6:C:ILE:N	1:6:C:ILE:CA	1:6:C:ILE:C	7	26.9
(1,15)	1:5:B:28J:C	1:6:B:ILE:N	1:6:B:ILE:CA	1:6:B:ILE:C	13	26.67