



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 06:04 PM UTC

PDB ID : 2LQW / pdb_00002lqw
BMRB ID : 18333
Title : Solution structure of phosphorylated CRKL
Authors : Jankowski, W.; Saleh, T.; Kalodimos, C.
Deposited on : 2012-03-16

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

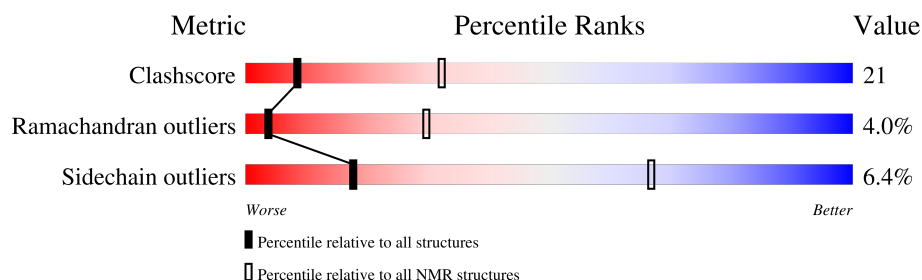
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 52%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	303	

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:104, A:125-A:180 (157)	0.80	10
2	A:238-A:247, A:254-A:295 (52)	0.86	1

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 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4705 atoms, of which 2317 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Crk-like protein.

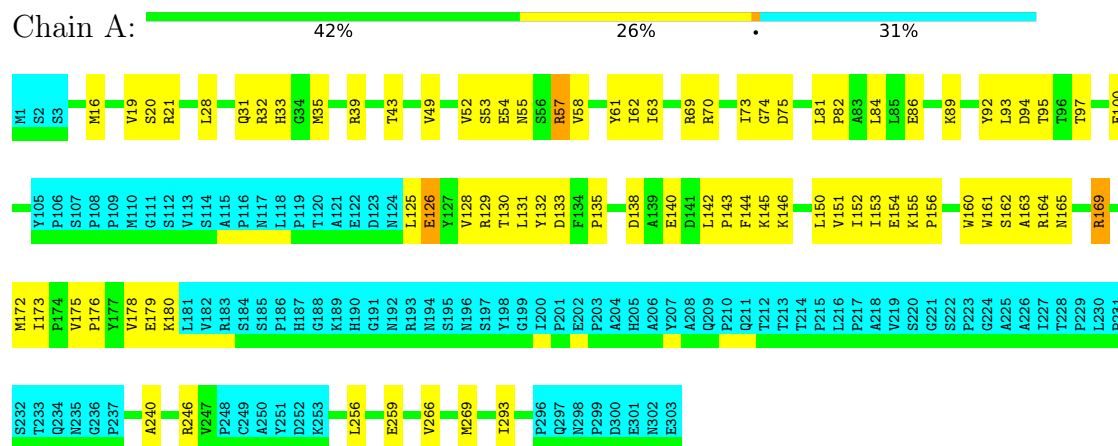
Mol	Chain	Residues	Atoms								Trace
1	A	303	Total	C	H	N	O	P	S		0
			4705	1504	2317	419	456	1	8		

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: Crk-like protein

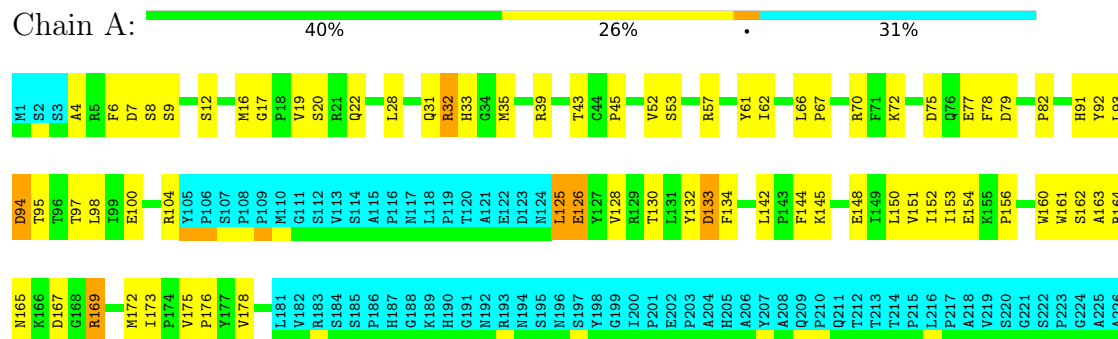


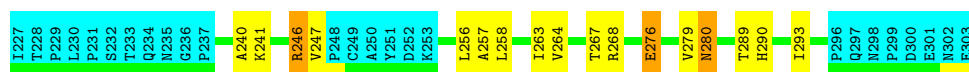
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

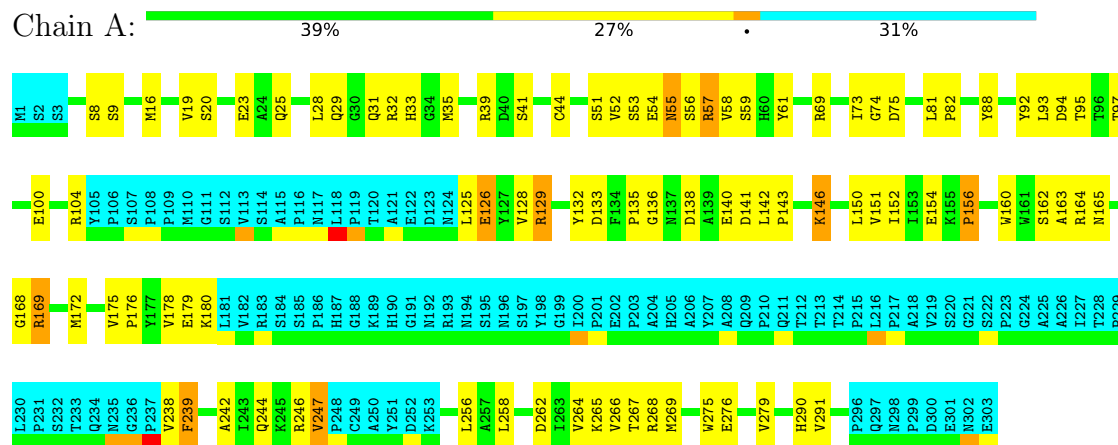
- Molecule 1: Crk-like protein





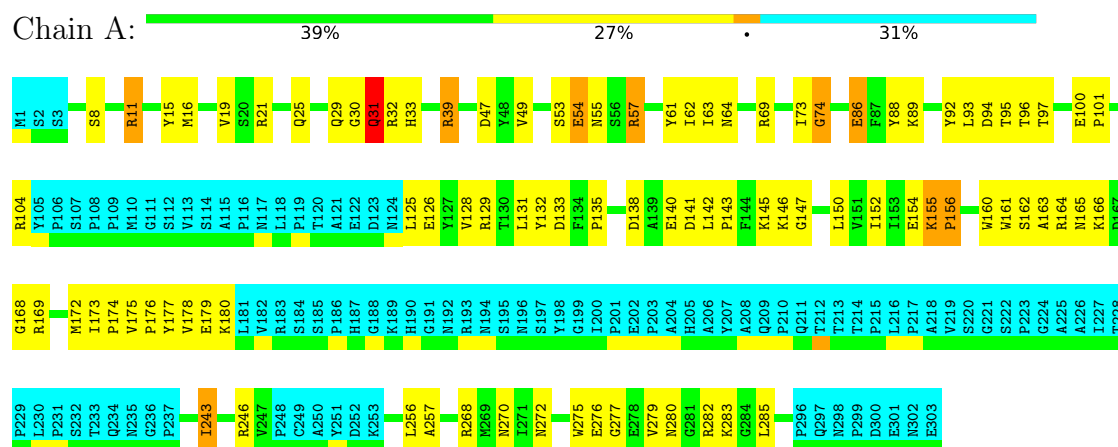
4.2.2 Score per residue for model 2

- Molecule 1: Crk-like protein



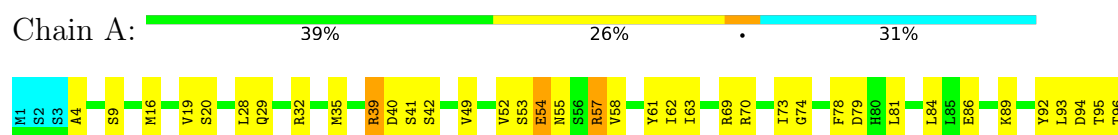
4.2.3 Score per residue for model 3

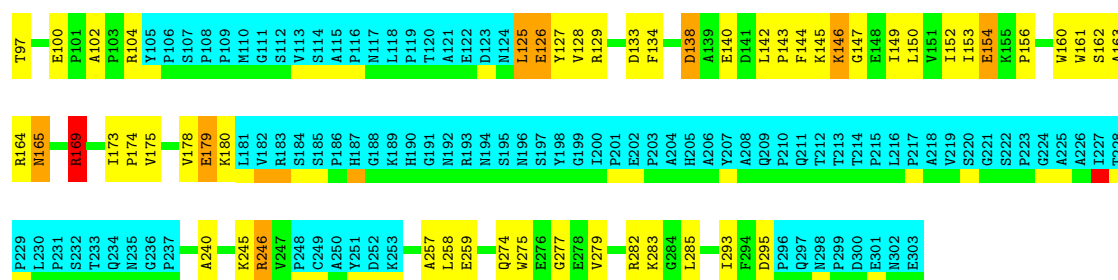
- Molecule 1: Crk-like protein



4.2.4 Score per residue for model 4

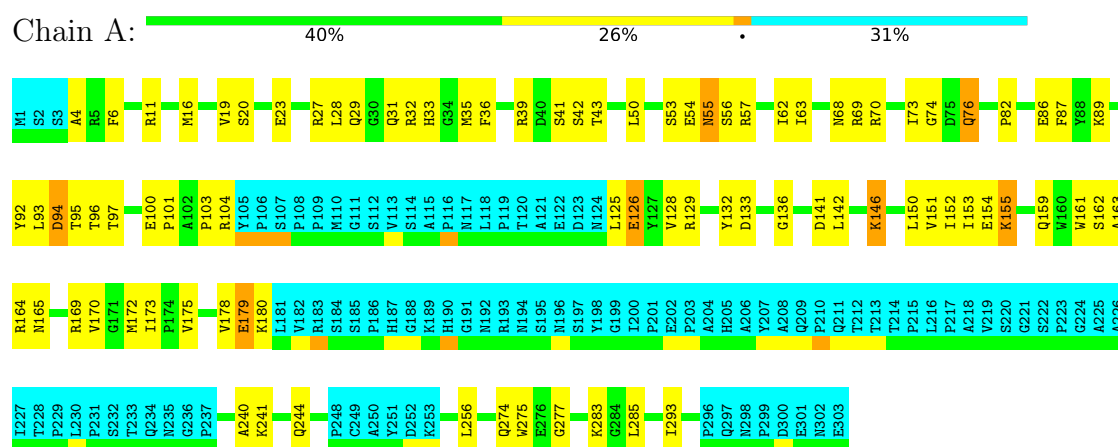
- Molecule 1: Crk-like protein





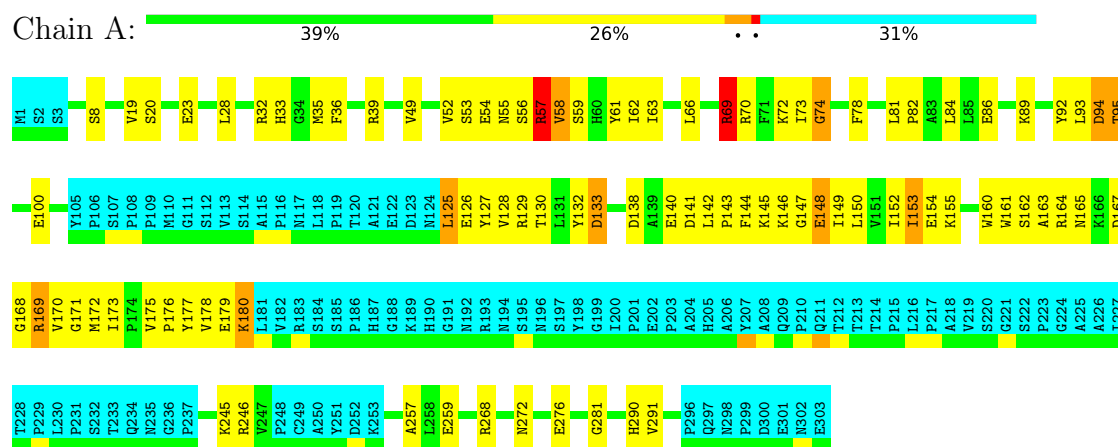
4.2.5 Score per residue for model 5

- Molecule 1: Crk-like protein



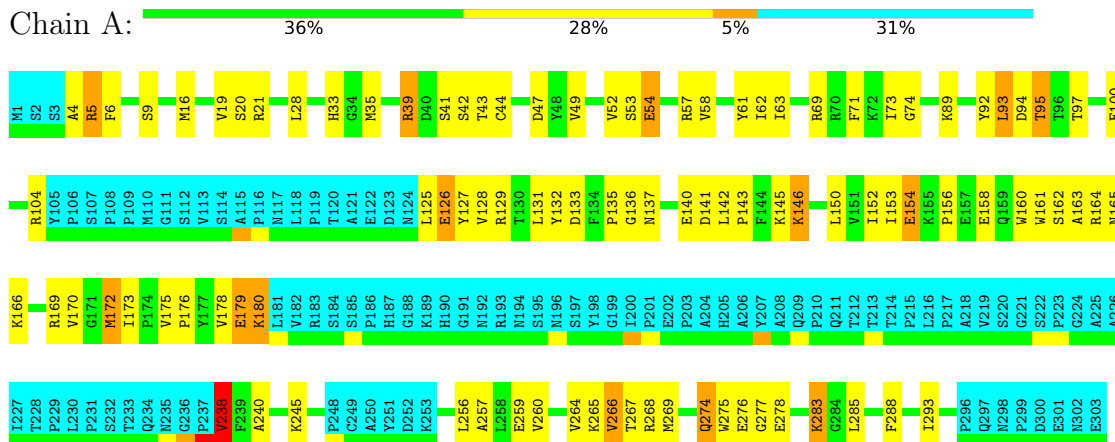
4.2.6 Score per residue for model 6

- Molecule 1: Crk-like protein



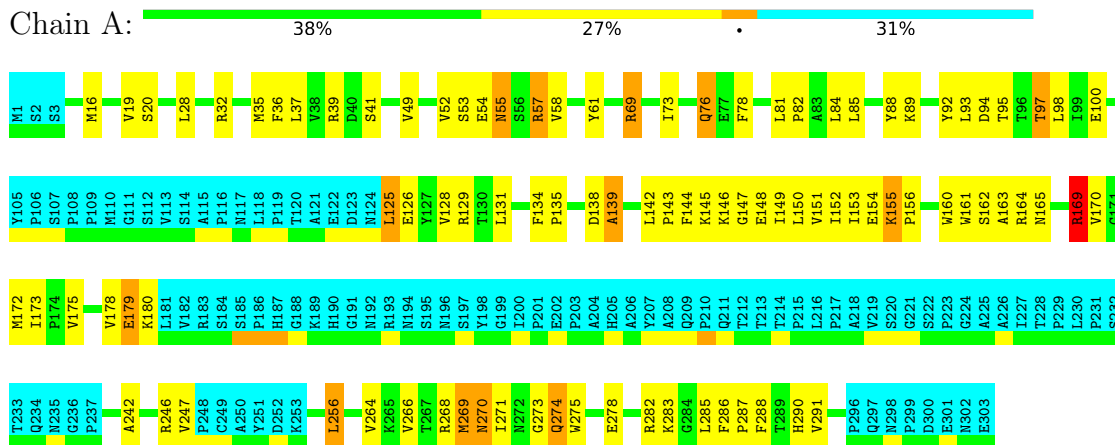
4.2.7 Score per residue for model 7

- Molecule 1: Crk-like protein



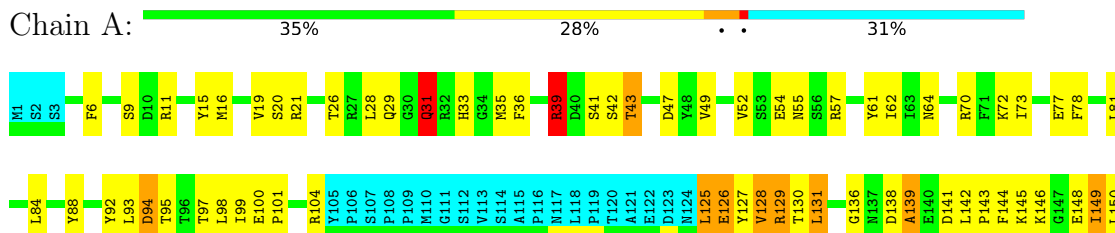
4.2.8 Score per residue for model 8

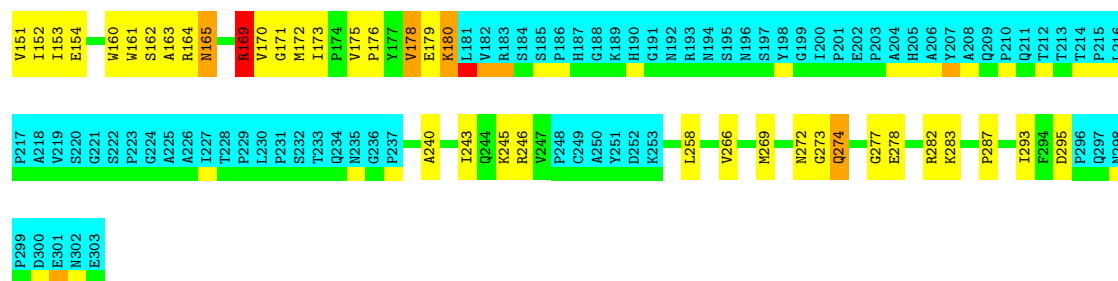
- Molecule 1: Crk-like protein



4.2.9 Score per residue for model 9

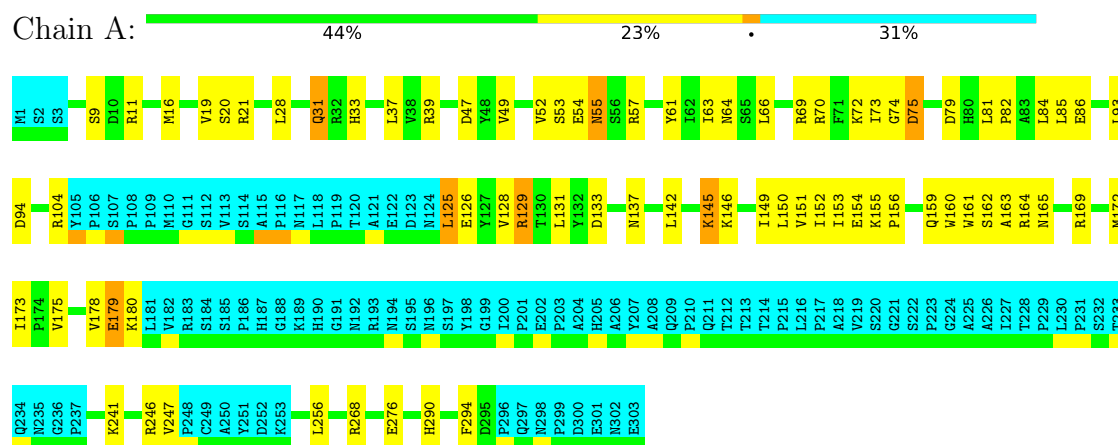
- Molecule 1: Crk-like protein





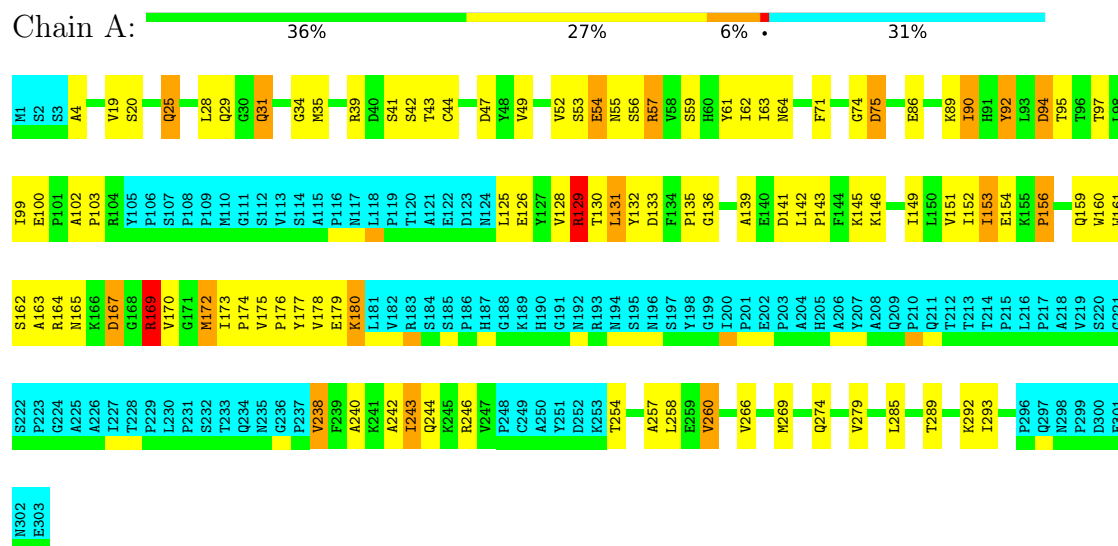
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Crk-like protein



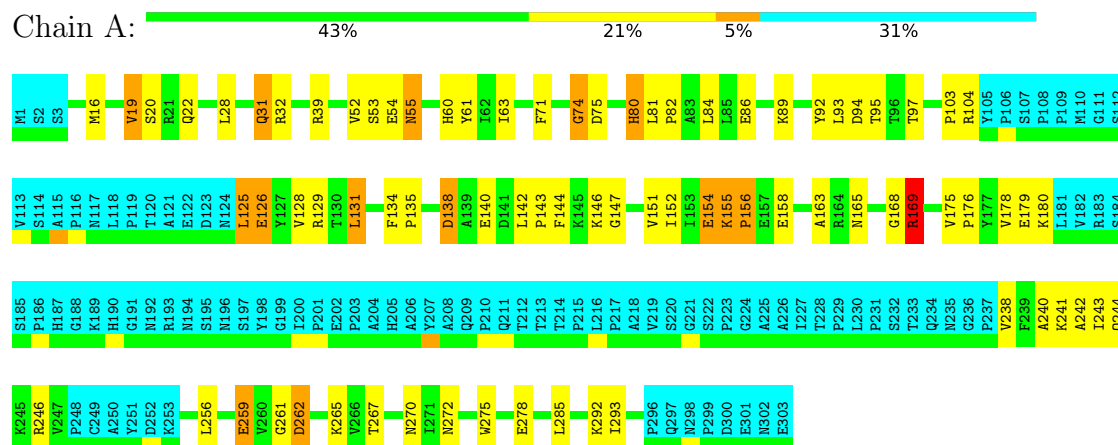
4.2.11 Score per residue for model 11

- Molecule 1: Crk-like protein



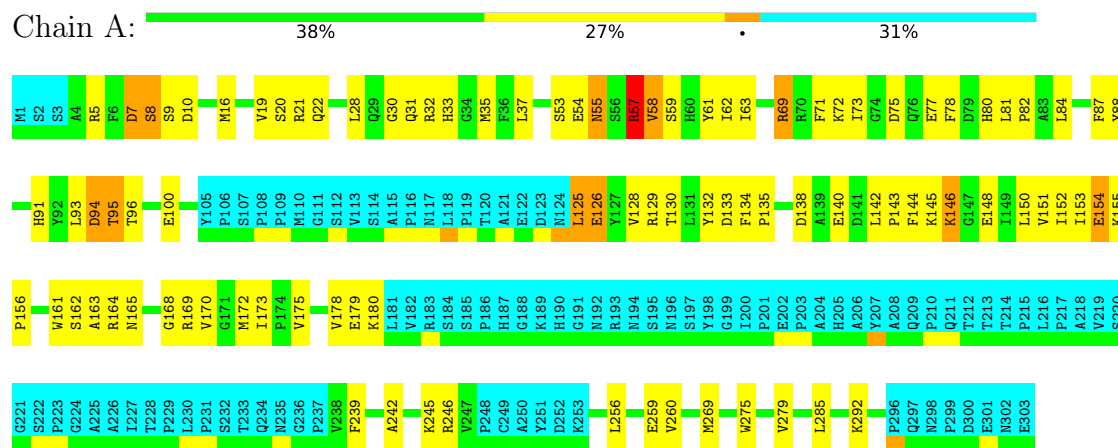
4.2.12 Score per residue for model 12

- Molecule 1: Crk-like protein



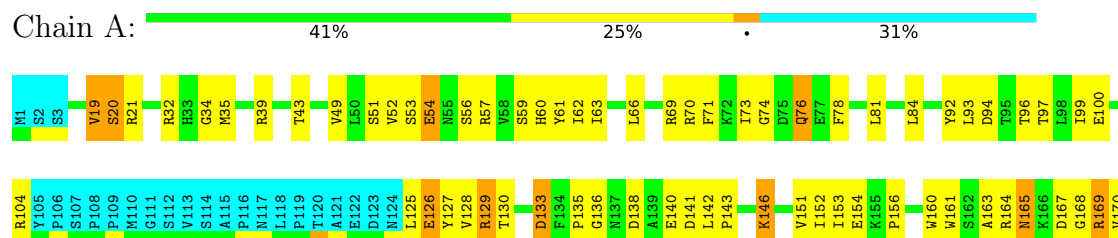
4.2.13 Score per residue for model 13

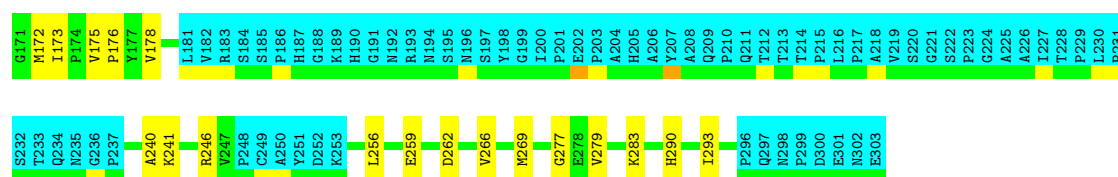
- Molecule 1: Crk-like protein



4.2.14 Score per residue for model 14

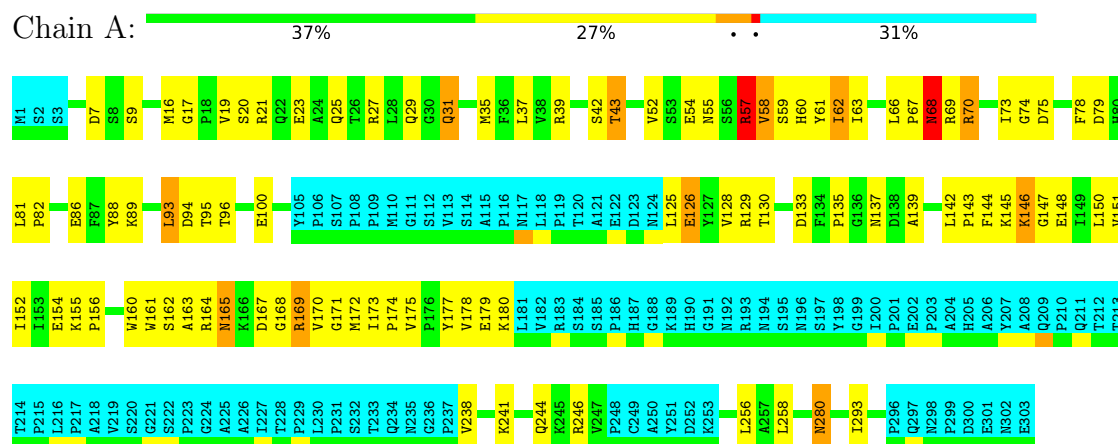
- Molecule 1: Crk-like protein





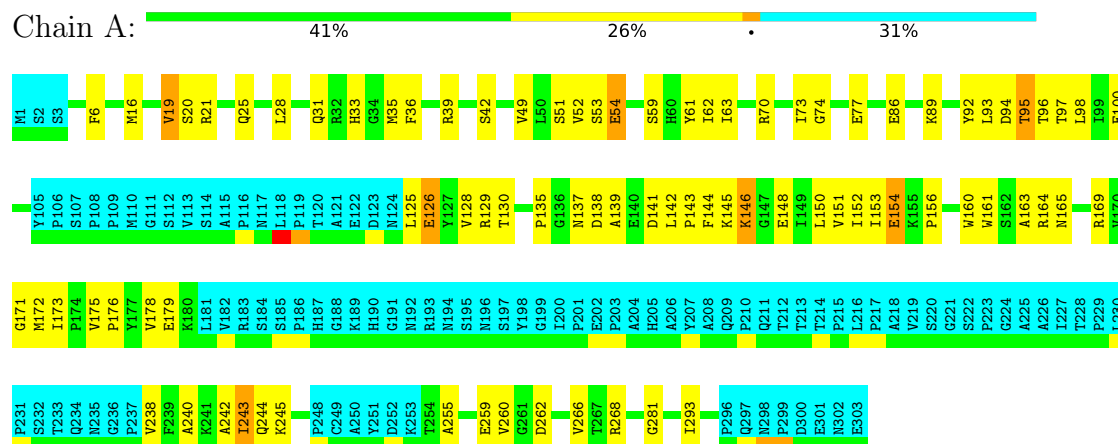
4.2.15 Score per residue for model 15

- Molecule 1: Crk-like protein



4.2.16 Score per residue for model 16

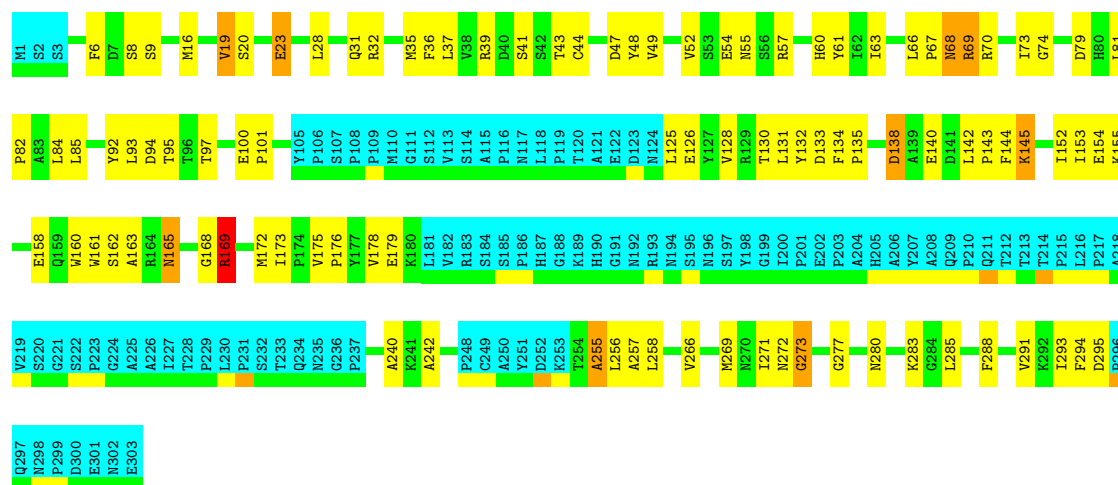
- Molecule 1: Crk-like protein



4.2.17 Score per residue for model 17

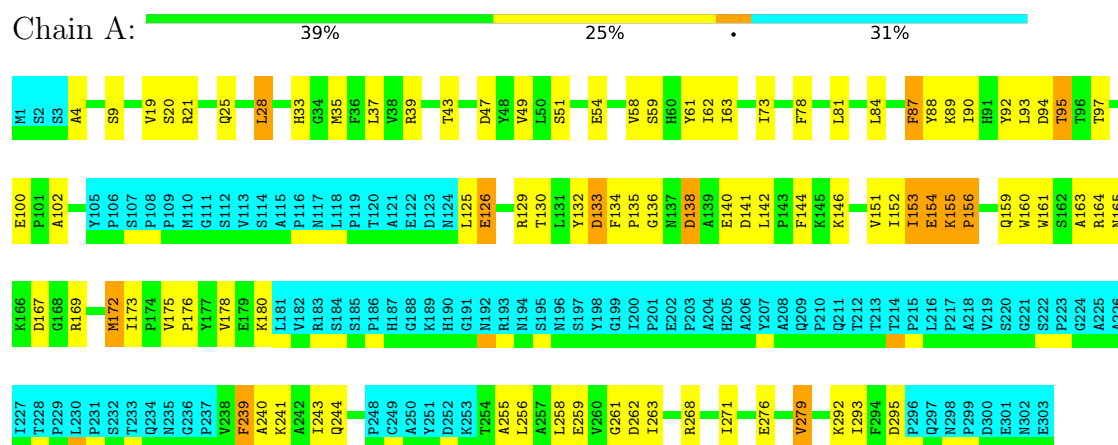
- Molecule 1: Crk-like protein





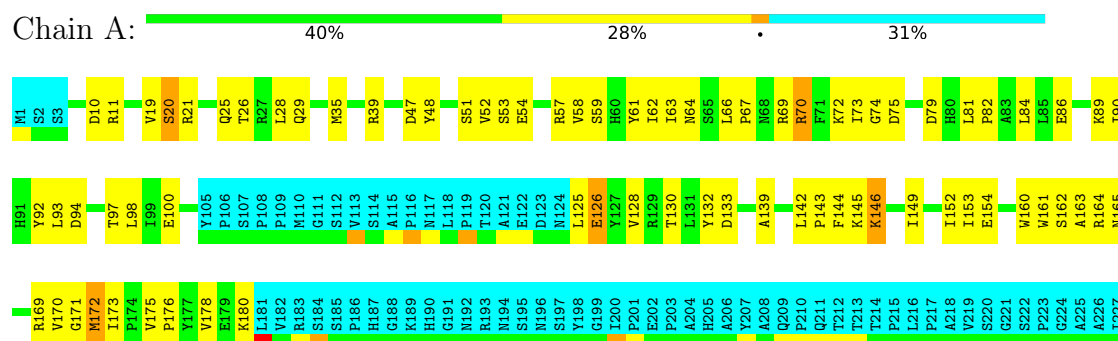
4.2.18 Score per residue for model 18

- Molecule 1: Crk-like protein



4.2.19 Score per residue for model 19

- Molecule 1: Crk-like protein

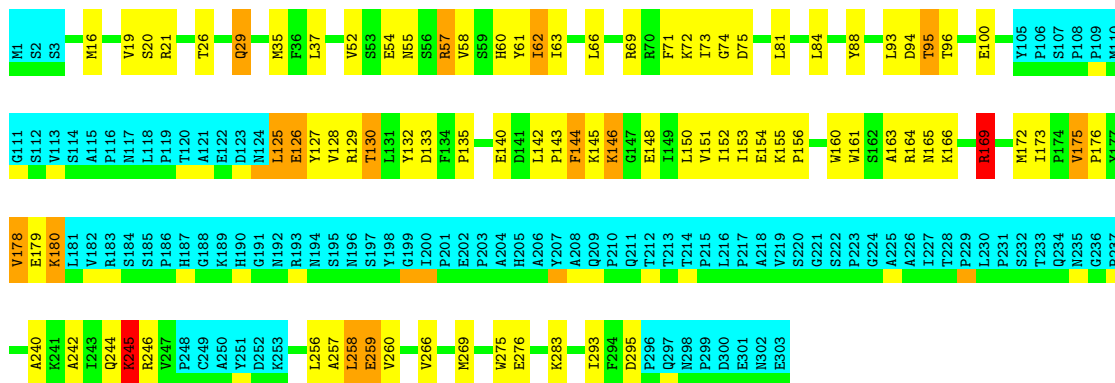




4.2.20 Score per residue for model 20

- Molecule 1: Crk-like protein

Chain A: 41% 23% 5% 31%



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	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	1952
Number of shifts mapped to atoms	1952
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	52%

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: PTR

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	0.48±0.03	0±0/1745 (0.0± 0.0%)	0.78±0.04	0±1/2366 (0.0± 0.0%)
All	All	0.48	2/34900 (0.0%)	0.78	10/47320 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±1.1
All	All	0	16

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
1	A	266	VAL	CA-CB	5.25	1.61	1.54	7	1
1	A	238	VAL	N-CA	5.16	1.52	1.46	7	1

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
1	A	57	ARG	N-CA-CB	-7.17	98.38	110.49	15	2
1	A	68	ASN	CA-CB-CG	6.89	119.49	112.60	15	1
1	A	57	ARG	N-CA-C	6.42	124.47	110.80	15	2
1	A	68	ASN	N-CA-CB	5.49	119.76	110.49	15	1
1	A	238	VAL	CB-CA-C	-5.43	102.38	111.29	7	1
1	A	30	GLY	N-CA-C	-5.32	108.15	114.48	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	175	VAL	CB-CA-C	-5.20	108.83	114.35	20	1
1	A	266	VAL	CB-CA-C	5.02	117.66	110.33	7	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	169	ARG	Sidechain	10
1	A	39	ARG	Sidechain	1
1	A	178	VAL	Peptide	1
1	A	56	SER	Peptide	1
1	A	57	ARG	Sidechain	1
1	A	129	ARG	Sidechain	1
1	A	68	ASN	Peptide	1

6.2 Too-close contacts

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	1701	1681	1681	72±14
All	All	34020	33620	33620	1448

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:LEU:HD11	1:A:165:ASN:HB2	1.09	1.24	13	14
1:A:242:ALA:HB1	1:A:259:GLU:HA	1.00	1.33	12	3
1:A:152:ILE:HD13	1:A:163:ALA:HB2	0.98	1.36	20	20
1:A:238:VAL:H	1:A:266:VAL:HG22	0.96	1.21	7	1
1:A:238:VAL:N	1:A:266:VAL:HG22	0.95	1.75	7	1
1:A:54:GLU:HG2	1:A:57:ARG:HB3	0.93	1.41	2	1
1:A:129:ARG:HB2	1:A:179:GLU:HB3	0.93	1.39	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:LEU:HD23	1:A:152:ILE:HG21	0.92	1.40	1	2
1:A:154:GLU:HB2	1:A:162:SER:HB3	0.92	1.41	6	3
1:A:68:ASN:HD22	1:A:69:ARG:N	0.89	1.66	15	1
1:A:31:GLN:HE21	1:A:56:SER:HA	0.88	1.26	5	1
1:A:128:VAL:HG22	1:A:180:LYS:HG3	0.87	1.46	13	3
1:A:278:GLU:HG2	1:A:283:LYS:HB3	0.86	1.43	9	1
1:A:28:LEU:HB3	1:A:53:SER:HB3	0.86	1.47	11	6
1:A:57:ARG:HH21	1:A:154:GLU:HA	0.86	1.30	20	1
1:A:154:GLU:HB2	1:A:162:SER:HB2	0.86	1.46	19	10
1:A:128:VAL:HG22	1:A:180:LYS:HB3	0.86	1.45	11	5
1:A:131:LEU:HD21	1:A:179:GLU:HB2	0.86	1.43	12	2
1:A:246:ARG:HD2	1:A:290:HIS:HE1	0.85	1.31	14	2
1:A:270:ASN:H	1:A:275:TRP:CD1	0.85	1.89	8	1
1:A:28:LEU:HB3	1:A:53:SER:HB2	0.85	1.49	19	5
1:A:70:ARG:HG2	1:A:79:ASP:HA	0.85	1.48	17	2
1:A:174:PRO:HB2	1:A:177:TYR:HB2	0.84	1.49	11	2
1:A:125:LEU:HD12	1:A:152:ILE:HG21	0.84	1.49	3	15
1:A:66:LEU:HD13	1:A:69:ARG:HB2	0.83	1.47	15	1
1:A:94:ASP:HB3	1:A:154:GLU:HB2	0.83	1.48	11	1
1:A:130:THR:HG22	1:A:178:VAL:HG12	0.82	1.51	9	9
1:A:164:ARG:HA	1:A:169:ARG:O	0.82	1.74	13	18
1:A:268:ARG:HB3	1:A:276:GLU:HB3	0.82	1.50	6	3
1:A:238:VAL:HG13	1:A:266:VAL:HG13	0.82	1.51	11	1
1:A:142:LEU:HD12	1:A:143:PRO:HD2	0.81	1.52	16	9
1:A:269:MET:C	1:A:273:GLY:HA3	0.81	2.00	8	1
1:A:270:ASN:ND2	1:A:274:GLN:HA	0.81	1.89	8	1
1:A:125:LEU:HG	1:A:155:LYS:HD3	0.81	1.51	8	4
1:A:137:ASN:HA	1:A:143:PRO:HG3	0.81	1.53	7	2
1:A:129:ARG:HG2	1:A:179:GLU:HG3	0.81	1.52	11	1
1:A:19:VAL:HB	1:A:39:ARG:HD2	0.80	1.51	10	14
1:A:125:LEU:HD12	1:A:152:ILE:HG13	0.79	1.52	4	2
1:A:270:ASN:HB2	1:A:288:PHE:CD2	0.79	2.13	8	1
1:A:61:TYR:HB3	1:A:73:ILE:HD11	0.79	1.55	15	11
1:A:19:VAL:HG12	1:A:20:SER:H	0.79	1.35	15	8
1:A:138:ASP:HB2	1:A:143:PRO:HD3	0.79	1.53	16	2
1:A:239:PHE:HB2	1:A:265:LYS:HA	0.78	1.55	2	1
1:A:238:VAL:N	1:A:266:VAL:HG13	0.78	1.94	2	1
1:A:274:GLN:HE21	1:A:274:GLN:HA	0.77	1.40	7	1
1:A:129:ARG:HG2	1:A:179:GLU:HB3	0.77	1.57	10	2
1:A:94:ASP:HA	1:A:154:GLU:HG2	0.77	1.55	20	1
1:A:57:ARG:HH21	1:A:94:ASP:HB2	0.76	1.39	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:VAL:HA	1:A:180:LYS:HA	0.76	1.56	5	11
1:A:146:LYS:HD2	1:A:146:LYS:H	0.76	1.41	20	2
1:A:32:ARG:HA	1:A:35:MET:HE2	0.75	1.56	1	1
1:A:31:GLN:HB3	1:A:53:SER:HB2	0.75	1.59	3	1
1:A:246:ARG:HG2	1:A:259:GLU:HG3	0.74	1.57	12	1
1:A:57:ARG:HH12	1:A:154:GLU:HA	0.74	1.41	8	1
1:A:66:LEU:HD12	1:A:70:ARG:H	0.73	1.42	15	1
1:A:242:ALA:HB1	1:A:259:GLU:HG2	0.73	1.59	16	2
1:A:66:LEU:HD12	1:A:70:ARG:N	0.73	1.98	15	1
1:A:275:TRP:CE2	1:A:288:PHE:HB3	0.73	2.19	8	1
1:A:57:ARG:NH2	1:A:154:GLU:HA	0.73	1.99	17	4
1:A:155:LYS:HZ2	1:A:155:LYS:HB3	0.72	1.45	18	1
1:A:146:LYS:HD3	1:A:146:LYS:H	0.72	1.44	19	5
1:A:270:ASN:HB2	1:A:288:PHE:HD2	0.72	1.42	8	1
1:A:160:TRP:HB3	1:A:172:MET:HE2	0.72	1.60	15	8
1:A:57:ARG:NH2	1:A:94:ASP:HB2	0.71	1.99	20	2
1:A:154:GLU:HB3	1:A:162:SER:HB2	0.71	1.60	11	1
1:A:242:ALA:HB1	1:A:259:GLU:CA	0.71	2.15	12	2
1:A:29:GLN:HE21	1:A:29:GLN:HA	0.71	1.45	20	1
1:A:88:TYR:CD1	1:A:93:LEU:HD23	0.71	2.20	3	2
1:A:57:ARG:NH1	1:A:154:GLU:HA	0.71	2.00	8	1
1:A:129:ARG:HG3	1:A:179:GLU:HB3	0.71	1.61	4	3
1:A:142:LEU:HD11	1:A:165:ASN:HB3	0.71	1.63	14	5
1:A:165:ASN:HD21	1:A:167:ASP:HB3	0.70	1.45	6	1
1:A:94:ASP:CA	1:A:154:GLU:HB3	0.70	2.15	13	1
1:A:238:VAL:H	1:A:266:VAL:CG2	0.70	1.98	7	1
1:A:57:ARG:HD2	1:A:155:LYS:HB3	0.70	1.61	3	1
1:A:180:LYS:HD3	1:A:180:LYS:H	0.70	1.47	11	1
1:A:153:ILE:HG21	1:A:170:VAL:HG22	0.70	1.64	9	6
1:A:16:MET:SD	1:A:104:ARG:HA	0.69	2.27	7	4
1:A:275:TRP:CZ2	1:A:288:PHE:HB3	0.69	2.22	8	1
1:A:94:ASP:HA	1:A:154:GLU:HB3	0.69	1.62	13	1
1:A:150:LEU:CD2	1:A:165:ASN:HA	0.69	2.17	13	10
1:A:138:ASP:HA	1:A:141:ASP:O	0.69	1.87	9	3
1:A:153:ILE:HG21	1:A:170:VAL:HG13	0.69	1.62	11	1
1:A:243:ILE:HD12	1:A:244:GLN:HG3	0.68	1.65	18	1
1:A:69:ARG:HA	1:A:69:ARG:HE	0.68	1.46	10	4
1:A:245:LYS:HA	1:A:259:GLU:HA	0.68	1.64	4	2
1:A:95:THR:OG1	1:A:156:PRO:HB3	0.68	1.87	3	1
1:A:94:ASP:CB	1:A:154:GLU:HB2	0.68	2.19	11	1
1:A:92:TYR:HA	1:A:97:THR:HG22	0.67	1.65	3	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:ASN:HB2	1:A:94:ASP:CG	0.67	2.14	6	2
1:A:57:ARG:NE	1:A:58:VAL:H	0.67	1.85	13	3
1:A:242:ALA:CB	1:A:259:GLU:HA	0.67	2.18	16	2
1:A:20:SER:H	1:A:39:ARG:HD2	0.67	1.49	1	8
1:A:279:VAL:HG12	1:A:280:ASN:H	0.67	1.49	3	1
1:A:69:ARG:NE	1:A:69:ARG:HA	0.67	2.05	5	3
1:A:61:TYR:CE1	1:A:153:ILE:HD11	0.67	2.25	20	4
1:A:145:LYS:HB2	1:A:148:GLU:HG2	0.67	1.67	8	2
1:A:66:LEU:HD13	1:A:69:ARG:CB	0.67	2.18	15	1
1:A:63:ILE:HG13	1:A:73:ILE:HB	0.66	1.66	14	8
1:A:59:SER:HB3	1:A:61:TYR:CE2	0.66	2.25	11	2
1:A:68:ASN:HD22	1:A:69:ARG:CA	0.66	2.02	15	1
1:A:161:TRP:O	1:A:173:ILE:HG13	0.66	1.90	15	18
1:A:160:TRP:HB3	1:A:172:MET:SD	0.66	2.30	11	8
1:A:129:ARG:HB3	1:A:149:ILE:HD13	0.66	1.68	11	3
1:A:61:TYR:CE2	1:A:93:LEU:HD22	0.65	2.27	17	15
1:A:52:VAL:HG21	1:A:93:LEU:HD13	0.65	1.67	12	12
1:A:61:TYR:HE1	1:A:153:ILE:HD11	0.65	1.49	20	4
1:A:35:MET:HA	1:A:100:GLU:O	0.64	1.93	2	16
1:A:142:LEU:CD2	1:A:150:LEU:HD22	0.64	2.23	15	3
1:A:70:ARG:HB3	1:A:78:PHE:O	0.64	1.93	15	2
1:A:125:LEU:HD11	1:A:161:TRP:CZ3	0.64	2.27	10	2
1:A:16:MET:SD	1:A:104:ARG:HG2	0.64	2.32	4	3
1:A:138:ASP:HB2	1:A:143:PRO:CD	0.64	2.22	16	2
1:A:86:GLU:HA	1:A:89:LYS:HD3	0.64	1.69	4	2
1:A:152:ILE:HD12	1:A:161:TRP:HB3	0.64	1.67	15	4
1:A:243:ILE:HG12	1:A:292:LYS:HG2	0.64	1.69	18	1
1:A:66:LEU:HD12	1:A:70:ARG:HG2	0.64	1.70	19	1
1:A:142:LEU:HD21	1:A:150:LEU:HD22	0.64	1.70	15	5
1:A:241:LYS:HA	1:A:262:ASP:O	0.64	1.93	12	1
1:A:135:PRO:HA	1:A:143:PRO:HA	0.63	1.68	16	12
1:A:32:ARG:N	1:A:32:ARG:HE	0.63	1.91	1	1
1:A:126:GLU:O	1:A:151:VAL:HA	0.63	1.93	11	14
1:A:246:ARG:HB3	1:A:246:ARG:HH11	0.63	1.53	4	1
1:A:153:ILE:HG23	1:A:154:GLU:HG3	0.63	1.67	17	5
1:A:128:VAL:HG22	1:A:180:LYS:CG	0.63	2.23	15	2
1:A:72:LYS:HD3	1:A:77:GLU:HB3	0.63	1.70	13	1
1:A:93:LEU:HA	1:A:154:GLU:OE2	0.63	1.93	1	6
1:A:138:ASP:HB3	1:A:169:ARG:HD3	0.63	1.71	4	4
1:A:240:ALA:HB2	1:A:293:ILE:HD12	0.63	1.71	12	2
1:A:245:LYS:HA	1:A:259:GLU:CB	0.63	2.24	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:243:ILE:HD12	1:A:292:LYS:HG2	0.63	1.70	11	1
1:A:246:ARG:HD2	1:A:290:HIS:CE1	0.62	2.22	14	2
1:A:129:ARG:O	1:A:179:GLU:HB3	0.62	1.94	15	3
1:A:70:ARG:HD2	1:A:79:ASP:HA	0.62	1.69	15	1
1:A:142:LEU:HD11	1:A:165:ASN:CB	0.62	2.17	15	8
1:A:130:THR:HG22	1:A:178:VAL:CG1	0.62	2.24	9	2
1:A:35:MET:HG3	1:A:53:SER:HB3	0.62	1.70	14	1
1:A:128:VAL:HG21	1:A:152:ILE:HD11	0.62	1.70	9	5
1:A:129:ARG:HG2	1:A:180:LYS:O	0.62	1.94	6	1
1:A:54:GLU:CD	1:A:94:ASP:HB3	0.62	2.19	10	3
1:A:148:GLU:CD	1:A:150:LEU:HG	0.62	2.19	13	1
1:A:54:GLU:O	1:A:57:ARG:HG2	0.62	1.95	17	2
1:A:246:ARG:O	1:A:257:ALA:HA	0.61	1.93	19	6
1:A:138:ASP:OD2	1:A:169:ARG:HG2	0.61	1.95	16	2
1:A:128:VAL:HG22	1:A:180:LYS:HB2	0.61	1.72	12	6
1:A:269:MET:O	1:A:273:GLY:HA3	0.61	1.95	8	1
1:A:238:VAL:O	1:A:266:VAL:HG13	0.61	1.96	7	1
1:A:54:GLU:O	1:A:57:ARG:HG3	0.61	1.96	20	2
1:A:238:VAL:HG23	1:A:269:MET:HE3	0.61	1.73	2	1
1:A:72:LYS:HE3	1:A:75:ASP:HA	0.61	1.72	1	1
1:A:70:ARG:HB2	1:A:78:PHE:O	0.60	1.96	9	3
1:A:93:LEU:O	1:A:154:GLU:HB3	0.60	1.95	7	3
1:A:275:TRP:O	1:A:285:LEU:HD23	0.60	1.96	8	1
1:A:28:LEU:HD13	1:A:102:ALA:HB2	0.60	1.73	18	1
1:A:92:TYR:CD2	1:A:97:THR:HG23	0.60	2.32	2	4
1:A:95:THR:HG21	1:A:156:PRO:HB3	0.60	1.74	11	1
1:A:95:THR:OG1	1:A:156:PRO:HA	0.60	1.95	13	2
1:A:179:GLU:O	1:A:179:GLU:HG3	0.60	1.97	15	3
1:A:57:ARG:CD	1:A:58:VAL:H	0.60	2.10	15	2
1:A:48:TYR:HB2	1:A:63:ILE:HB	0.59	1.72	17	2
1:A:54:GLU:HG3	1:A:94:ASP:HB3	0.59	1.72	2	1
1:A:129:ARG:HH21	1:A:149:ILE:HD11	0.59	1.58	9	1
1:A:68:ASN:ND2	1:A:69:ARG:N	0.59	2.46	15	1
1:A:146:LYS:H	1:A:146:LYS:CD	0.59	2.11	20	4
1:A:19:VAL:HB	1:A:39:ARG:CD	0.59	2.27	11	4
1:A:57:ARG:HD2	1:A:58:VAL:CG2	0.59	2.28	6	1
1:A:50:LEU:HB2	1:A:63:ILE:HD11	0.59	1.75	5	1
1:A:128:VAL:HG22	1:A:180:LYS:CB	0.59	2.28	3	10
1:A:36:PHE:HB2	1:A:52:VAL:HG22	0.59	1.74	6	2
1:A:156:PRO:HG2	1:A:172:MET:SD	0.58	2.37	15	1
1:A:153:ILE:HG23	1:A:154:GLU:HG2	0.58	1.75	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:GLY:HA3	1:A:99:ILE:HB	0.58	1.75	14	1
1:A:53:SER:HA	1:A:57:ARG:O	0.58	1.98	6	3
1:A:138:ASP:CB	1:A:169:ARG:HD3	0.58	2.28	18	2
1:A:270:ASN:H	1:A:275:TRP:NE1	0.58	1.95	8	1
1:A:241:LYS:HB3	1:A:263:ILE:HD13	0.58	1.75	1	1
1:A:128:VAL:HA	1:A:179:GLU:O	0.58	1.99	9	1
1:A:154:GLU:HG3	1:A:162:SER:HB2	0.58	1.75	4	2
1:A:270:ASN:ND2	1:A:275:TRP:HD1	0.58	1.97	8	1
1:A:140:GLU:O	1:A:172:MET:HB2	0.58	1.99	3	6
1:A:180:LYS:H	1:A:180:LYS:HD2	0.58	1.59	20	2
1:A:76:GLN:HE21	1:A:76:GLN:HA	0.57	1.58	14	1
1:A:161:TRP:CZ3	1:A:180:LYS:HE2	0.57	2.34	15	1
1:A:264:VAL:O	1:A:266:VAL:HG12	0.57	1.99	7	1
1:A:239:PHE:CE1	1:A:263:ILE:HG23	0.57	2.34	18	1
1:A:133:ASP:OD1	1:A:145:LYS:HA	0.57	1.99	19	5
1:A:54:GLU:HB3	1:A:94:ASP:HB3	0.57	1.74	17	2
1:A:238:VAL:HB	1:A:269:MET:HE3	0.57	1.75	7	1
1:A:141:ASP:O	1:A:171:GLY:HA3	0.57	1.99	9	1
1:A:239:PHE:HE1	1:A:263:ILE:HG23	0.57	1.59	18	1
1:A:165:ASN:ND2	1:A:167:ASP:HB3	0.57	2.14	6	2
1:A:26:THR:O	1:A:29:GLN:HG2	0.57	1.98	9	1
1:A:238:VAL:C	1:A:266:VAL:HG13	0.57	2.24	2	1
1:A:277:GLY:O	1:A:283:LYS:HA	0.57	2.00	3	7
1:A:270:ASN:HD22	1:A:275:TRP:HD1	0.57	1.42	8	1
1:A:5:ARG:HA	1:A:5:ARG:NE	0.57	2.13	13	1
1:A:139:ALA:O	1:A:171:GLY:HA2	0.57	1.98	19	2
1:A:130:THR:HG21	1:A:144:PHE:CG	0.57	2.35	17	7
1:A:62:ILE:O	1:A:73:ILE:HA	0.57	2.00	5	5
1:A:25:GLN:O	1:A:29:GLN:HG2	0.57	1.99	2	1
1:A:162:SER:OG	1:A:172:MET:HG2	0.57	1.99	15	1
1:A:269:MET:HA	1:A:275:TRP:HB3	0.57	1.75	19	1
1:A:44:CYS:HB2	1:A:47:ASP:HB2	0.56	1.76	17	2
1:A:175:VAL:O	1:A:178:VAL:HG22	0.56	2.00	16	13
1:A:142:LEU:HB3	1:A:173:ILE:CG2	0.56	2.30	15	10
1:A:128:VAL:HA	1:A:180:LYS:HB3	0.56	1.77	7	1
1:A:129:ARG:HG2	1:A:149:ILE:HD12	0.56	1.77	8	1
1:A:255:ALA:HA	1:A:285:LEU:O	0.56	1.99	17	1
1:A:133:ASP:OD2	1:A:145:LYS:HA	0.56	2.01	1	6
1:A:16:MET:HG3	1:A:37:LEU:HB2	0.56	1.77	13	4
1:A:32:ARG:HB3	1:A:35:MET:SD	0.56	2.41	6	1
1:A:66:LEU:HB3	1:A:67:PRO:HD2	0.56	1.76	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:270:ASN:N	1:A:273:GLY:HA3	0.56	2.14	8	1
1:A:266:VAL:HG11	1:A:269:MET:HE3	0.56	1.78	17	3
1:A:49:VAL:HG22	1:A:62:ILE:HG12	0.56	1.77	18	4
1:A:136:GLY:HA3	1:A:141:ASP:HB3	0.56	1.76	11	2
1:A:87:PHE:HE1	1:A:88:TYR:CZ	0.56	2.19	18	1
1:A:148:GLU:OE1	1:A:166:LYS:HB2	0.56	2.00	20	1
1:A:165:ASN:HD22	1:A:165:ASN:C	0.56	2.09	14	3
1:A:33:HIS:NE2	1:A:55:ASN:HA	0.56	2.16	5	1
1:A:19:VAL:HG12	1:A:20:SER:N	0.55	2.15	20	9
1:A:128:VAL:CG1	1:A:178:VAL:HB	0.55	2.31	15	7
1:A:136:GLY:HA3	1:A:141:ASP:HB2	0.55	1.78	2	3
1:A:174:PRO:HB2	1:A:177:TYR:CB	0.55	2.30	11	2
1:A:33:HIS:CD2	1:A:54:GLU:HA	0.55	2.35	6	3
1:A:245:LYS:HG3	1:A:260:VAL:HG23	0.55	1.78	7	1
1:A:238:VAL:HG11	1:A:269:MET:HE3	0.55	1.78	11	1
1:A:244:GLN:HB3	1:A:259:GLU:OE2	0.55	2.02	12	1
1:A:59:SER:HB3	1:A:61:TYR:CZ	0.55	2.36	16	2
1:A:8:SER:O	1:A:82:PRO:HB3	0.55	2.00	1	2
1:A:148:GLU:OE2	1:A:150:LEU:HG	0.55	2.02	13	1
1:A:274:GLN:HB3	1:A:285:LEU:HB3	0.55	1.79	11	1
1:A:173:ILE:HD13	1:A:178:VAL:HG11	0.55	1.78	9	6
1:A:86:GLU:O	1:A:89:LYS:HG2	0.55	2.01	5	3
1:A:54:GLU:HB3	1:A:94:ASP:HB2	0.55	1.79	14	1
1:A:31:GLN:O	1:A:32:ARG:HG3	0.55	2.01	1	1
1:A:175:VAL:N	1:A:176:PRO:HD2	0.55	2.16	20	14
1:A:131:LEU:HD21	1:A:179:GLU:HG3	0.55	1.78	10	1
1:A:149:ILE:O	1:A:150:LEU:HD23	0.55	2.02	9	1
1:A:6:PHE:HB3	1:A:100:GLU:HA	0.55	1.78	17	2
1:A:127:TYR:O	1:A:180:LYS:HA	0.55	2.02	9	1
1:A:47:ASP:OD2	1:A:64:ASN:HA	0.54	2.02	3	4
1:A:128:VAL:HG13	1:A:178:VAL:HB	0.54	1.79	13	3
1:A:125:LEU:CD1	1:A:152:ILE:HG21	0.54	2.31	7	3
1:A:128:VAL:HG13	1:A:180:LYS:HB3	0.54	1.78	2	4
1:A:81:LEU:O	1:A:84:LEU:HG	0.54	2.03	8	12
1:A:238:VAL:N	1:A:266:VAL:CG2	0.54	2.61	7	1
1:A:92:TYR:CA	1:A:97:THR:HG22	0.54	2.32	14	4
1:A:142:LEU:CD1	1:A:169:ARG:HD2	0.54	2.33	17	4
1:A:16:MET:CG	1:A:37:LEU:HB2	0.54	2.32	13	6
1:A:238:VAL:HG12	1:A:293:ILE:HD11	0.54	1.79	12	1
1:A:148:GLU:OE1	1:A:150:LEU:HG	0.54	2.02	13	1
1:A:54:GLU:HB2	1:A:94:ASP:HB3	0.54	1.78	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:VAL:H	1:A:266:VAL:C	0.54	2.11	7	1
1:A:155:LYS:O	1:A:155:LYS:HG3	0.54	2.02	3	1
1:A:246:ARG:HB3	1:A:290:HIS:CE1	0.54	2.37	10	2
1:A:242:ALA:O	1:A:260:VAL:HA	0.54	2.03	11	2
1:A:138:ASP:OD1	1:A:171:GLY:HA3	0.54	2.03	16	2
1:A:92:TYR:CD1	1:A:97:THR:HG23	0.54	2.37	11	6
1:A:55:ASN:O	1:A:57:ARG:HB2	0.54	2.03	10	2
1:A:151:VAL:HB	1:A:164:ARG:CG	0.54	2.33	9	1
1:A:278:GLU:HG2	1:A:283:LYS:CB	0.54	2.29	9	1
1:A:144:PHE:CE2	1:A:173:ILE:HB	0.54	2.38	13	2
1:A:69:ARG:HG2	1:A:70:ARG:N	0.54	2.16	6	1
1:A:259:GLU:HB2	1:A:262:ASP:HB2	0.54	1.80	14	1
1:A:240:ALA:HB2	1:A:293:ILE:HD13	0.53	1.79	17	10
1:A:19:VAL:HB	1:A:39:ARG:CB	0.53	2.33	3	3
1:A:165:ASN:HB3	1:A:167:ASP:OD1	0.53	2.03	1	1
1:A:8:SER:HB3	1:A:82:PRO:HB3	0.53	1.80	6	1
1:A:142:LEU:HD21	1:A:165:ASN:HB3	0.53	1.81	6	1
1:A:20:SER:HA	1:A:42:SER:HB3	0.53	1.80	9	1
1:A:69:ARG:HA	1:A:69:ARG:NE	0.53	2.19	8	2
1:A:54:GLU:CG	1:A:57:ARG:HB3	0.53	2.26	2	1
1:A:6:PHE:HB3	1:A:101:PRO:HD3	0.53	1.80	5	3
1:A:72:LYS:HG2	1:A:77:GLU:HB3	0.53	1.80	9	1
1:A:88:TYR:CG	1:A:93:LEU:HD23	0.53	2.38	13	1
1:A:132:TYR:O	1:A:133:ASP:HB3	0.53	2.03	6	12
1:A:129:ARG:HG2	1:A:179:GLU:O	0.53	2.04	4	5
1:A:270:ASN:OD1	1:A:272:ASN:HB3	0.53	2.03	12	2
1:A:95:THR:HB	1:A:156:PRO:HA	0.53	1.80	8	3
1:A:129:ARG:N	1:A:129:ARG:HD2	0.53	2.18	11	2
1:A:129:ARG:CG	1:A:179:GLU:HB3	0.53	2.34	12	3
1:A:264:VAL:HG11	1:A:286:PHE:CZ	0.53	2.40	8	1
1:A:128:VAL:CG2	1:A:152:ILE:HD11	0.53	2.34	9	1
1:A:87:PHE:HE1	1:A:88:TYR:CE2	0.53	2.22	18	1
1:A:241:LYS:HE3	1:A:261:GLY:HA2	0.52	1.79	18	1
1:A:66:LEU:HD22	1:A:69:ARG:HH21	0.52	1.63	19	1
1:A:57:ARG:CZ	1:A:94:ASP:HB2	0.52	2.35	20	1
1:A:57:ARG:HD2	1:A:58:VAL:HG22	0.52	1.80	6	1
1:A:95:THR:CB	1:A:154:GLU:HG2	0.52	2.34	11	1
1:A:28:LEU:O	1:A:28:LEU:HG	0.52	2.03	18	1
1:A:128:VAL:CG2	1:A:180:LYS:HB3	0.52	2.30	7	2
1:A:270:ASN:N	1:A:275:TRP:NE1	0.52	2.56	8	1
1:A:128:VAL:CG2	1:A:180:LYS:HG3	0.52	2.30	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ARG:O	1:A:25:GLN:HG3	0.52	2.04	15	1
1:A:273:GLY:HA3	1:A:288:PHE:CD1	0.52	2.39	17	1
1:A:36:PHE:CD1	1:A:98:LEU:HD22	0.52	2.39	8	2
1:A:152:ILE:CD1	1:A:163:ALA:HB2	0.52	2.24	13	3
1:A:66:LEU:CD1	1:A:70:ARG:H	0.52	2.13	15	1
1:A:268:ARG:NE	1:A:268:ARG:HA	0.52	2.20	16	1
1:A:270:ASN:ND2	1:A:274:GLN:CA	0.52	2.68	8	1
1:A:151:VAL:HG11	1:A:164:ARG:NH2	0.52	2.20	9	1
1:A:66:LEU:HB2	1:A:70:ARG:O	0.52	2.04	1	3
1:A:266:VAL:HG11	1:A:275:TRP:CZ3	0.52	2.40	8	1
1:A:164:ARG:HB2	1:A:168:GLY:C	0.52	2.30	13	1
1:A:73:ILE:HD13	1:A:88:TYR:CE2	0.52	2.39	9	1
1:A:52:VAL:HB	1:A:59:SER:HB2	0.52	1.82	11	1
1:A:156:PRO:HG2	1:A:172:MET:CE	0.52	2.35	15	1
1:A:70:ARG:HB3	1:A:79:ASP:HA	0.51	1.81	1	1
1:A:55:ASN:HB3	1:A:57:ARG:HH21	0.51	1.64	6	1
1:A:93:LEU:O	1:A:154:GLU:HG2	0.51	2.05	6	1
1:A:238:VAL:CG1	1:A:266:VAL:HG13	0.51	2.33	11	1
1:A:54:GLU:HB2	1:A:57:ARG:HB3	0.51	1.82	4	1
1:A:245:LYS:HA	1:A:259:GLU:HB3	0.51	1.81	20	1
1:A:54:GLU:HB2	1:A:57:ARG:HE	0.51	1.65	9	1
1:A:32:ARG:HB3	1:A:35:MET:HE3	0.51	1.82	17	3
1:A:145:LYS:HG2	1:A:148:GLU:HG2	0.51	1.82	1	1
1:A:246:ARG:HH11	1:A:246:ARG:HB2	0.51	1.66	1	1
1:A:51:SER:HA	1:A:59:SER:O	0.51	2.05	14	5
1:A:23:GLU:O	1:A:27:ARG:HG3	0.51	2.04	15	1
1:A:264:VAL:HA	1:A:279:VAL:HG22	0.51	1.82	2	1
1:A:125:LEU:HG	1:A:155:LYS:HD2	0.51	1.82	10	2
1:A:95:THR:HB	1:A:154:GLU:HG2	0.51	1.81	11	1
1:A:25:GLN:HG3	1:A:58:VAL:HG21	0.51	1.83	18	1
1:A:66:LEU:HD12	1:A:70:ARG:HG3	0.51	1.83	1	1
1:A:270:ASN:ND2	1:A:275:TRP:CD1	0.51	2.78	8	1
1:A:151:VAL:HB	1:A:164:ARG:HG2	0.51	1.81	9	6
1:A:130:THR:HG21	1:A:144:PHE:CB	0.51	2.36	6	1
1:A:32:ARG:CB	1:A:35:MET:HE3	0.51	2.36	14	1
1:A:72:LYS:CE	1:A:75:ASP:HA	0.51	2.35	1	1
1:A:258:LEU:HD21	1:A:279:VAL:HG21	0.51	1.83	4	4
1:A:138:ASP:N	1:A:143:PRO:HD3	0.51	2.19	4	1
1:A:142:LEU:HD12	1:A:169:ARG:HD2	0.51	1.83	13	2
1:A:54:GLU:CB	1:A:94:ASP:HB3	0.51	2.35	5	3
1:A:279:VAL:HG12	1:A:280:ASN:N	0.51	2.21	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:GLU:HG2	1:A:94:ASP:HB3	0.51	1.83	9	2
1:A:142:LEU:HD13	1:A:169:ARG:O	0.51	2.06	13	2
1:A:131:LEU:HD22	1:A:131:LEU:N	0.51	2.20	12	2
1:A:94:ASP:OD1	1:A:153:ILE:HG13	0.51	2.05	11	1
1:A:135:PRO:HA	1:A:143:PRO:CA	0.50	2.37	16	2
1:A:133:ASP:HB2	1:A:146:LYS:HD3	0.50	1.83	5	1
1:A:131:LEU:CD2	1:A:179:GLU:HB2	0.50	2.26	12	1
1:A:95:THR:OG1	1:A:156:PRO:HG3	0.50	2.07	11	1
1:A:55:ASN:HD21	1:A:155:LYS:HB3	0.50	1.66	15	1
1:A:66:LEU:HD22	1:A:69:ARG:NE	0.50	2.21	15	1
1:A:129:ARG:HD2	1:A:179:GLU:OE1	0.50	2.06	4	1
1:A:54:GLU:HG2	1:A:57:ARG:HG3	0.50	1.81	11	1
1:A:57:ARG:HD2	1:A:58:VAL:N	0.50	2.21	15	1
1:A:28:LEU:CB	1:A:37:LEU:HD23	0.50	2.37	18	1
1:A:19:VAL:HB	1:A:39:ARG:HB2	0.50	1.81	5	3
1:A:238:VAL:N	1:A:266:VAL:C	0.50	2.70	7	1
1:A:153:ILE:HG21	1:A:170:VAL:CG2	0.50	2.35	9	1
1:A:179:GLU:O	1:A:180:LYS:HD3	0.50	2.06	9	1
1:A:174:PRO:HG2	1:A:177:TYR:CG	0.50	2.42	15	1
1:A:151:VAL:HG21	1:A:164:ARG:HE	0.50	1.66	9	1
1:A:31:GLN:NE2	1:A:56:SER:HA	0.50	2.09	5	1
1:A:68:ASN:HB2	1:A:70:ARG:HG2	0.50	1.82	5	1
1:A:94:ASP:O	1:A:95:THR:HG22	0.50	2.07	20	4
1:A:275:TRP:CZ2	1:A:288:PHE:CB	0.50	2.94	8	1
1:A:136:GLY:HA3	1:A:141:ASP:OD1	0.50	2.07	9	1
1:A:66:LEU:HB3	1:A:69:ARG:HE	0.50	1.65	19	1
1:A:11:ARG:O	1:A:15:TYR:HB3	0.49	2.07	3	2
1:A:69:ARG:O	1:A:70:ARG:HG2	0.49	2.07	15	1
1:A:95:THR:CB	1:A:156:PRO:HA	0.49	2.37	18	1
1:A:26:THR:HA	1:A:29:GLN:OE1	0.49	2.07	19	1
1:A:270:ASN:OD1	1:A:287:PRO:HA	0.49	2.06	8	1
1:A:238:VAL:C	1:A:266:VAL:CG1	0.49	2.85	2	1
1:A:126:GLU:CD	1:A:127:TYR:H	0.49	2.16	7	2
1:A:152:ILE:HD13	1:A:163:ALA:CB	0.49	2.26	13	1
1:A:148:GLU:CD	1:A:148:GLU:C	0.49	2.81	13	1
1:A:150:LEU:HD22	1:A:165:ASN:HA	0.49	1.84	6	6
1:A:138:ASP:HB3	1:A:141:ASP:HB2	0.49	1.85	3	1
1:A:23:GLU:O	1:A:27:ARG:HG2	0.49	2.08	5	1
1:A:130:THR:HG22	1:A:178:VAL:HG11	0.49	1.84	6	1
1:A:133:ASP:HB2	1:A:145:LYS:C	0.49	2.33	20	1
1:A:273:GLY:O	1:A:274:GLN:HG2	0.49	2.08	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:PHE:CD2	1:A:84:LEU:HB3	0.49	2.42	13	2
1:A:141:ASP:HA	1:A:172:MET:O	0.49	2.08	5	2
1:A:93:LEU:HD12	1:A:93:LEU:O	0.49	2.08	13	1
1:A:68:ASN:HD22	1:A:69:ARG:HA	0.49	1.68	15	1
1:A:57:ARG:O	1:A:57:ARG:HD2	0.49	2.08	20	1
1:A:94:ASP:HA	1:A:154:GLU:CG	0.49	2.34	20	1
1:A:282:ARG:HH11	1:A:282:ARG:HG2	0.48	1.68	4	1
1:A:17:GLY:O	1:A:39:ARG:HB2	0.48	2.07	1	1
1:A:164:ARG:HB3	1:A:170:VAL:HG22	0.48	1.85	6	1
1:A:33:HIS:HB3	1:A:54:GLU:OE1	0.48	2.09	13	2
1:A:31:GLN:C	1:A:32:ARG:HG3	0.48	2.33	1	1
1:A:154:GLU:HB3	1:A:162:SER:CB	0.48	2.36	11	1
1:A:55:ASN:HB2	1:A:94:ASP:OD2	0.48	2.08	15	1
1:A:156:PRO:HG2	1:A:172:MET:HE2	0.48	1.85	20	5
1:A:54:GLU:CG	1:A:94:ASP:HB3	0.48	2.39	5	1
1:A:94:ASP:CG	1:A:155:LYS:H	0.48	2.16	6	1
1:A:241:LYS:HG3	1:A:294:PHE:CE1	0.48	2.43	10	1
1:A:138:ASP:H	1:A:143:PRO:HD3	0.48	1.69	4	1
1:A:61:TYR:HE1	1:A:153:ILE:CD1	0.48	2.22	6	1
1:A:41:SER:HB2	1:A:49:VAL:HG23	0.48	1.86	17	1
1:A:61:TYR:CB	1:A:73:ILE:HD11	0.48	2.39	13	6
1:A:269:MET:HA	1:A:275:TRP:NE1	0.48	2.23	8	1
1:A:73:ILE:HD13	1:A:88:TYR:HE2	0.48	1.69	9	1
1:A:66:LEU:CD1	1:A:70:ARG:N	0.48	2.75	15	1
1:A:130:THR:CG2	1:A:178:VAL:HG12	0.48	2.37	16	1
1:A:57:ARG:HD2	1:A:58:VAL:H	0.48	1.68	15	1
1:A:66:LEU:HD11	1:A:72:LYS:HB2	0.48	1.84	6	3
1:A:268:ARG:HB2	1:A:276:GLU:HB2	0.48	1.84	10	1
1:A:266:VAL:HG23	1:A:276:GLU:O	0.47	2.09	2	1
1:A:41:SER:HA	1:A:49:VAL:HG23	0.47	1.86	8	2
1:A:70:ARG:CB	1:A:79:ASP:HA	0.47	2.39	1	1
1:A:62:ILE:O	1:A:73:ILE:HG13	0.47	2.09	19	2
1:A:134:PHE:HB3	1:A:144:PHE:CZ	0.47	2.44	12	7
1:A:245:LYS:HG2	1:A:259:GLU:HA	0.47	1.86	6	1
1:A:130:THR:HB	1:A:144:PHE:CD2	0.47	2.44	20	1
1:A:4:ALA:HB2	1:A:98:LEU:O	0.47	2.08	1	1
1:A:88:TYR:CG	1:A:93:LEU:HD21	0.47	2.44	2	3
1:A:126:GLU:HA	1:A:152:ILE:H	0.47	1.70	9	1
1:A:25:GLN:O	1:A:29:GLN:HB2	0.47	2.08	3	1
1:A:145:LYS:N	1:A:145:LYS:HD2	0.47	2.24	10	1
1:A:54:GLU:HB2	1:A:59:SER:OG	0.47	2.10	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:VAL:HA	1:A:180:LYS:CA	0.47	2.37	2	1
1:A:93:LEU:O	1:A:94:ASP:HB2	0.47	2.10	3	1
1:A:275:TRP:O	1:A:285:LEU:HA	0.47	2.10	12	6
1:A:33:HIS:HA	1:A:53:SER:O	0.47	2.09	16	2
1:A:63:ILE:CG2	1:A:71:PHE:HB3	0.47	2.39	7	6
1:A:128:VAL:HG13	1:A:180:LYS:HG3	0.47	1.86	11	1
1:A:28:LEU:HD22	1:A:53:SER:HB2	0.47	1.87	13	1
1:A:19:VAL:CG1	1:A:20:SER:H	0.47	2.16	15	2
1:A:86:GLU:O	1:A:89:LYS:HB3	0.47	2.10	6	1
1:A:268:ARG:O	1:A:275:TRP:HA	0.47	2.09	8	1
1:A:66:LEU:CD1	1:A:69:ARG:HB2	0.47	2.30	15	1
1:A:25:GLN:O	1:A:29:GLN:HG3	0.47	2.10	19	1
1:A:86:GLU:HA	1:A:89:LYS:HE2	0.47	1.84	19	1
1:A:166:LYS:HD3	1:A:166:LYS:C	0.47	2.35	3	1
1:A:129:ARG:HD2	1:A:179:GLU:OE2	0.47	2.10	7	1
1:A:245:LYS:CA	1:A:259:GLU:CB	0.47	2.92	20	1
1:A:70:ARG:CG	1:A:79:ASP:HA	0.47	2.40	4	1
1:A:138:ASP:CG	1:A:169:ARG:HD3	0.47	2.35	14	2
1:A:93:LEU:HA	1:A:154:GLU:OE1	0.46	2.11	18	2
1:A:94:ASP:C	1:A:96:THR:H	0.46	2.19	4	2
1:A:142:LEU:HB3	1:A:173:ILE:HG23	0.46	1.87	6	1
1:A:86:GLU:HA	1:A:89:LYS:HE3	0.46	1.85	11	1
1:A:55:ASN:HD22	1:A:94:ASP:CG	0.46	2.18	13	2
1:A:28:LEU:O	1:A:28:LEU:CG	0.46	2.63	18	1
1:A:52:VAL:HG12	1:A:54:GLU:OE2	0.46	2.09	9	1
1:A:151:VAL:O	1:A:163:ALA:HA	0.46	2.09	15	1
1:A:245:LYS:CA	1:A:259:GLU:HB3	0.46	2.41	20	1
1:A:155:LYS:HG3	1:A:161:TRP:CD1	0.46	2.45	8	3
1:A:61:TYR:CE1	1:A:153:ILE:HG13	0.46	2.45	7	2
1:A:99:ILE:HG22	1:A:100:GLU:HG3	0.46	1.86	9	1
1:A:54:GLU:CD	1:A:96:THR:HG22	0.46	2.36	14	2
1:A:256:LEU:O	1:A:258:LEU:HG	0.46	2.10	17	1
1:A:81:LEU:HB2	1:A:82:PRO:HD3	0.46	1.88	2	3
1:A:125:LEU:HD21	1:A:161:TRP:CE2	0.46	2.45	5	1
1:A:238:VAL:HB	1:A:269:MET:CE	0.46	2.40	7	1
1:A:153:ILE:HD13	1:A:170:VAL:HG21	0.46	1.85	9	1
1:A:54:GLU:HG2	1:A:57:ARG:O	0.46	2.10	11	1
1:A:16:MET:HB3	1:A:19:VAL:HG21	0.46	1.87	16	6
1:A:44:CYS:HB2	1:A:47:ASP:CB	0.46	2.41	7	1
1:A:270:ASN:N	1:A:275:TRP:HE1	0.46	2.08	8	1
1:A:246:ARG:HG3	1:A:290:HIS:CE1	0.46	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:LYS:HE3	1:A:75:ASP:O	0.46	2.11	10	1
1:A:142:LEU:HD21	1:A:150:LEU:CD2	0.46	2.41	13	1
1:A:39:ARG:HD2	1:A:49:VAL:HB	0.46	1.88	3	1
1:A:4:ALA:HB3	1:A:89:LYS:HG2	0.46	1.86	7	1
1:A:68:ASN:O	1:A:70:ARG:NH1	0.46	2.48	15	1
1:A:146:LYS:HG2	1:A:146:LYS:O	0.46	2.11	7	1
1:A:28:LEU:HD23	1:A:35:MET:HE3	0.46	1.88	9	1
1:A:49:VAL:HG22	1:A:62:ILE:HD13	0.46	1.88	11	1
1:A:21:ARG:O	1:A:25:GLN:HG2	0.46	2.11	19	2
1:A:66:LEU:HD21	1:A:72:LYS:HD3	0.45	1.88	19	1
1:A:144:PHE:CE1	1:A:173:ILE:HB	0.45	2.46	20	1
1:A:242:ALA:HA	1:A:291:VAL:HG12	0.45	1.88	19	4
1:A:28:LEU:HD21	1:A:102:ALA:HB2	0.45	1.86	4	1
1:A:174:PRO:HG2	1:A:177:TYR:CD2	0.45	2.47	15	1
1:A:244:GLN:HG2	1:A:245:LYS:HG2	0.45	1.87	16	1
1:A:269:MET:HE2	1:A:275:TRP:CH2	0.45	2.46	8	2
1:A:175:VAL:C	1:A:177:TYR:H	0.45	2.19	3	2
1:A:131:LEU:HG	1:A:179:GLU:OE1	0.45	2.12	11	1
1:A:49:VAL:HG22	1:A:62:ILE:HG13	0.45	1.88	4	1
1:A:179:GLU:C	1:A:180:LYS:HD3	0.45	2.36	6	1
1:A:131:LEU:HD11	1:A:179:GLU:HB2	0.45	1.89	12	1
1:A:29:GLN:HE22	1:A:57:ARG:HB3	0.45	1.72	15	1
1:A:6:PHE:CB	1:A:101:PRO:HD3	0.45	2.41	17	1
1:A:52:VAL:HB	1:A:59:SER:OG	0.45	2.12	2	1
1:A:138:ASP:HA	1:A:141:ASP:C	0.45	2.36	6	1
1:A:155:LYS:HE3	1:A:161:TRP:HE1	0.45	1.71	20	1
1:A:269:MET:HE2	1:A:275:TRP:CZ2	0.45	2.47	20	1
1:A:19:VAL:O	1:A:20:SER:HB2	0.45	2.12	12	2
1:A:180:LYS:N	1:A:180:LYS:HD3	0.45	2.26	19	2
1:A:91:HIS:O	1:A:92:TYR:HB2	0.45	2.12	1	1
1:A:92:TYR:N	1:A:97:THR:HG22	0.45	2.27	12	1
1:A:266:VAL:HA	1:A:277:GLY:HA2	0.45	1.88	14	1
1:A:61:TYR:HE1	1:A:153:ILE:HG13	0.45	1.72	7	2
1:A:150:LEU:HB3	1:A:163:ALA:HB1	0.45	1.88	16	3
1:A:57:ARG:HB2	1:A:58:VAL:HG23	0.45	1.87	13	1
1:A:55:ASN:O	1:A:57:ARG:HG3	0.45	2.12	15	1
1:A:125:LEU:HD21	1:A:161:TRP:CH2	0.45	2.47	15	1
1:A:165:ASN:C	1:A:167:ASP:H	0.45	2.20	15	1
1:A:245:LYS:HA	1:A:259:GLU:HB2	0.45	1.89	20	1
1:A:19:VAL:HB	1:A:39:ARG:HG2	0.45	1.89	7	1
1:A:270:ASN:CB	1:A:288:PHE:CD2	0.45	2.94	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:278:GLU:HG3	1:A:283:LYS:HB3	0.45	1.88	8	1
1:A:31:GLN:HG2	1:A:33:HIS:HD2	0.45	1.71	9	1
1:A:265:LYS:HB2	1:A:278:GLU:O	0.44	2.12	7	1
1:A:274:GLN:HA	1:A:274:GLN:NE2	0.44	2.20	7	1
1:A:86:GLU:HA	1:A:89:LYS:HD2	0.44	1.88	3	1
1:A:169:ARG:HB3	1:A:169:ARG:CZ	0.44	2.41	17	2
1:A:54:GLU:HG2	1:A:96:THR:HB	0.44	1.89	16	2
1:A:4:ALA:HB1	1:A:6:PHE:CE1	0.44	2.47	1	1
1:A:125:LEU:HD11	1:A:161:TRP:CE3	0.44	2.46	4	1
1:A:28:LEU:O	1:A:31:GLN:HB3	0.44	2.12	9	1
1:A:7:ASP:CG	1:A:8:SER:H	0.44	2.21	13	1
1:A:88:TYR:CD1	1:A:93:LEU:CD2	0.44	3.01	15	1
1:A:238:VAL:CG1	1:A:293:ILE:HD12	0.44	2.42	15	1
1:A:52:VAL:O	1:A:58:VAL:HA	0.44	2.13	8	6
1:A:39:ARG:HD3	1:A:40:ASP:O	0.44	2.12	4	1
1:A:258:LEU:O	1:A:259:GLU:HB2	0.44	2.11	20	1
1:A:128:VAL:HA	1:A:180:LYS:CB	0.44	2.43	2	1
1:A:165:ASN:ND2	1:A:168:GLY:H	0.44	2.11	14	1
1:A:69:ARG:HB3	1:A:70:ARG:HD2	0.44	1.89	19	1
1:A:54:GLU:OE1	1:A:94:ASP:HB3	0.44	2.13	10	2
1:A:180:LYS:H	1:A:180:LYS:CD	0.44	2.14	11	2
1:A:246:ARG:HD3	1:A:258:LEU:HD12	0.44	1.90	15	1
1:A:19:VAL:HG13	1:A:23:GLU:HB2	0.44	1.89	2	1
1:A:150:LEU:HA	1:A:164:ARG:O	0.44	2.13	5	1
1:A:4:ALA:HB3	1:A:89:LYS:HE3	0.44	1.88	18	1
1:A:82:PRO:O	1:A:86:GLU:HG3	0.44	2.13	5	1
1:A:32:ARG:HB2	1:A:35:MET:SD	0.44	2.53	8	1
1:A:31:GLN:HG2	1:A:33:HIS:CD2	0.44	2.47	9	1
1:A:155:LYS:HB3	1:A:155:LYS:NZ	0.44	2.28	5	1
1:A:131:LEU:HD21	1:A:179:GLU:CG	0.44	2.43	8	1
1:A:246:ARG:HB2	1:A:290:HIS:CE1	0.43	2.47	1	1
1:A:270:ASN:HA	1:A:274:GLN:N	0.43	2.27	8	1
1:A:54:GLU:O	1:A:55:ASN:HB2	0.43	2.11	13	1
1:A:94:ASP:CG	1:A:95:THR:H	0.43	2.21	9	2
1:A:102:ALA:HB1	1:A:103:PRO:HD2	0.43	1.89	11	1
1:A:57:ARG:CD	1:A:58:VAL:N	0.43	2.81	15	2
1:A:131:LEU:HG	1:A:179:GLU:HB2	0.43	1.89	7	2
1:A:54:GLU:OE1	1:A:96:THR:HB	0.43	2.13	13	1
1:A:28:LEU:C	1:A:32:ARG:HD3	0.43	2.37	1	1
1:A:81:LEU:HD23	1:A:84:LEU:HD21	0.43	1.90	12	1
1:A:36:PHE:CG	1:A:98:LEU:HD22	0.43	2.48	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:PHE:CE1	1:A:88:TYR:CZ	0.43	3.03	18	1
1:A:256:LEU:HD21	1:A:279:VAL:HB	0.43	1.91	1	2
1:A:154:GLU:CB	1:A:162:SER:HB2	0.43	2.39	11	1
1:A:78:PHE:CZ	1:A:87:PHE:CD1	0.43	3.06	18	1
1:A:125:LEU:HD11	1:A:161:TRP:CD2	0.43	2.48	3	1
1:A:256:LEU:HA	1:A:282:ARG:NH1	0.43	2.29	8	1
1:A:67:PRO:HD2	1:A:69:ARG:NH2	0.43	2.29	15	1
1:A:130:THR:HA	1:A:178:VAL:HG12	0.43	1.91	6	1
1:A:133:ASP:HB2	1:A:146:LYS:N	0.43	2.29	20	3
1:A:52:VAL:HG12	1:A:54:GLU:HG3	0.43	1.91	15	1
1:A:161:TRP:CZ3	1:A:180:LYS:CE	0.43	3.02	15	1
1:A:290:HIS:HD2	1:A:291:VAL:HG13	0.43	1.72	6	1
1:A:34:GLY:HA3	1:A:99:ILE:HD13	0.43	1.89	11	1
1:A:80:HIS:HB2	1:A:82:PRO:HD2	0.43	1.90	13	2
1:A:238:VAL:CG2	1:A:269:MET:HE3	0.43	2.43	2	1
1:A:54:GLU:O	1:A:56:SER:N	0.43	2.52	5	1
1:A:57:ARG:HE	1:A:57:ARG:H	0.43	1.57	6	1
1:A:76:GLN:HB3	1:A:78:PHE:CE2	0.43	2.49	8	1
1:A:130:THR:N	1:A:148:GLU:OE2	0.43	2.51	13	1
1:A:67:PRO:O	1:A:68:ASN:HB2	0.43	2.12	17	1
1:A:95:THR:HA	1:A:156:PRO:HA	0.43	1.91	1	1
1:A:146:LYS:HD3	1:A:146:LYS:N	0.43	2.29	2	2
1:A:57:ARG:CD	1:A:155:LYS:HB3	0.43	2.37	3	1
1:A:246:ARG:NH1	1:A:287:PRO:HD2	0.43	2.29	9	1
1:A:131:LEU:HD21	1:A:179:GLU:CB	0.43	2.31	12	1
1:A:243:ILE:H	1:A:243:ILE:HD13	0.42	1.74	16	2
1:A:126:GLU:HA	1:A:152:ILE:HB	0.42	1.91	9	1
1:A:142:LEU:HD22	1:A:163:ALA:O	0.42	2.14	13	1
1:A:161:TRP:CH2	1:A:180:LYS:HE2	0.42	2.49	15	1
1:A:268:ARG:HB2	1:A:276:GLU:HG2	0.42	1.92	1	1
1:A:148:GLU:OE1	1:A:165:ASN:HB2	0.42	2.14	6	1
1:A:82:PRO:HA	1:A:85:LEU:HD12	0.42	1.91	10	3
1:A:145:LYS:H	1:A:148:GLU:HB2	0.42	1.74	9	1
1:A:245:LYS:HA	1:A:258:LEU:O	0.42	2.13	9	1
1:A:93:LEU:C	1:A:154:GLU:HB3	0.42	2.40	12	1
1:A:154:GLU:CD	1:A:170:VAL:HG11	0.42	2.40	15	1
1:A:19:VAL:HG13	1:A:23:GLU:HB3	0.42	1.91	17	1
1:A:47:ASP:OD1	1:A:64:ASN:HA	0.42	2.14	10	1
1:A:238:VAL:HG22	1:A:266:VAL:HG12	0.42	1.91	11	1
1:A:142:LEU:HD21	1:A:165:ASN:HA	0.42	1.91	13	1
1:A:70:ARG:HD3	1:A:70:ARG:HA	0.42	1.59	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:259:GLU:O	1:A:262:ASP:HB2	0.42	2.14	18	1
1:A:92:TYR:CG	1:A:97:THR:HG23	0.42	2.49	2	1
1:A:142:LEU:CD1	1:A:165:ASN:HB2	0.42	2.40	3	1
1:A:32:ARG:HB2	1:A:35:MET:HE2	0.42	1.91	4	1
1:A:125:LEU:O	1:A:126:GLU:HG3	0.42	2.15	9	1
1:A:126:GLU:HG3	1:A:151:VAL:HG13	0.42	1.91	10	1
1:A:153:ILE:HG21	1:A:170:VAL:CG1	0.42	2.37	11	1
1:A:50:LEU:CB	1:A:63:ILE:HD11	0.42	2.44	5	1
1:A:136:GLY:HA3	1:A:141:ASP:OD2	0.42	2.14	5	1
1:A:270:ASN:ND2	1:A:275:TRP:N	0.42	2.67	8	1
1:A:31:GLN:HB3	1:A:53:SER:CB	0.42	2.40	3	1
1:A:78:PHE:CD1	1:A:84:LEU:HB3	0.42	2.49	6	1
1:A:128:VAL:HG22	1:A:179:GLU:O	0.42	2.14	6	1
1:A:54:GLU:HB3	1:A:94:ASP:OD2	0.42	2.15	7	1
1:A:82:PRO:O	1:A:86:GLU:HG2	0.42	2.15	10	1
1:A:238:VAL:CA	1:A:266:VAL:HG13	0.42	2.44	2	1
1:A:146:LYS:HD2	1:A:147:GLY:N	0.42	2.30	4	1
1:A:270:ASN:CA	1:A:273:GLY:HA3	0.42	2.45	8	1
1:A:179:GLU:HG3	1:A:180:LYS:N	0.42	2.30	9	1
1:A:159:GLN:HA	1:A:159:GLN:OE1	0.42	2.14	11	2
1:A:142:LEU:HD11	1:A:165:ASN:CG	0.42	2.39	14	1
1:A:160:TRP:CB	1:A:172:MET:HE2	0.42	2.40	15	1
1:A:32:ARG:HB3	1:A:35:MET:HB2	0.42	1.90	1	1
1:A:32:ARG:CA	1:A:35:MET:HE2	0.42	2.37	1	1
1:A:81:LEU:CB	1:A:82:PRO:HD3	0.42	2.45	2	2
1:A:54:GLU:O	1:A:57:ARG:HB3	0.42	2.15	7	1
1:A:142:LEU:HD12	1:A:143:PRO:CD	0.42	2.45	9	1
1:A:69:ARG:HD3	1:A:69:ARG:H	0.42	1.74	17	1
1:A:28:LEU:CD2	1:A:37:LEU:CD2	0.42	2.97	18	1
1:A:28:LEU:CD2	1:A:37:LEU:HD23	0.42	2.45	18	1
1:A:155:LYS:HZ2	1:A:155:LYS:CB	0.42	2.22	18	1
1:A:239:PHE:CE1	1:A:263:ILE:HD12	0.42	2.49	18	1
1:A:33:HIS:CE1	1:A:55:ASN:HA	0.42	2.49	5	1
1:A:36:PHE:HB2	1:A:50:LEU:HD11	0.42	1.92	5	1
1:A:268:ARG:HH12	1:A:276:GLU:HB3	0.42	1.75	7	1
1:A:152:ILE:HG13	1:A:161:TRP:CE3	0.42	2.50	9	1
1:A:246:ARG:CG	1:A:259:GLU:HG3	0.42	2.40	12	1
1:A:129:ARG:HG3	1:A:179:GLU:CG	0.42	2.44	15	1
1:A:70:ARG:HD2	1:A:77:GLU:HG3	0.42	1.91	16	1
1:A:125:LEU:HD11	1:A:161:TRP:CE2	0.41	2.50	3	1
1:A:54:GLU:O	1:A:55:ASN:HB3	0.41	2.14	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:269:MET:HE2	1:A:275:TRP:CE3	0.41	2.50	13	1
1:A:238:VAL:HB	1:A:266:VAL:CG1	0.41	2.45	16	1
1:A:61:TYR:CZ	1:A:93:LEU:HB2	0.41	2.49	13	1
1:A:61:TYR:HE1	1:A:153:ILE:CG1	0.41	2.28	17	1
1:A:73:ILE:HG23	1:A:73:ILE:O	0.41	2.15	17	1
1:A:138:ASP:HB3	1:A:169:ARG:CD	0.41	2.45	18	1
1:A:129:ARG:HD3	1:A:179:GLU:O	0.41	2.16	10	1
1:A:245:LYS:HG2	1:A:259:GLU:HG3	0.41	1.91	13	1
1:A:66:LEU:HB3	1:A:69:ARG:HG3	0.41	1.92	14	1
1:A:174:PRO:HB2	1:A:177:TYR:CG	0.41	2.50	3	1
1:A:138:ASP:HB2	1:A:169:ARG:HD3	0.41	1.91	14	2
1:A:238:VAL:HG13	1:A:266:VAL:CG1	0.41	2.36	11	1
1:A:31:GLN:HG3	1:A:32:ARG:H	0.41	1.76	12	1
1:A:246:ARG:HD2	1:A:256:LEU:O	0.41	2.16	13	1
1:A:275:TRP:CH2	1:A:288:PHE:HB3	0.41	2.50	7	1
1:A:94:ASP:C	1:A:154:GLU:HB3	0.41	2.41	13	1
1:A:160:TRP:CZ3	1:A:174:PRO:HD3	0.41	2.51	15	1
1:A:246:ARG:N	1:A:259:GLU:HB2	0.41	2.31	20	1
1:A:143:PRO:HD2	1:A:169:ARG:HD2	0.41	1.91	8	1
1:A:125:LEU:HG	1:A:155:LYS:CD	0.41	2.46	13	1
1:A:67:PRO:O	1:A:68:ASN:CG	0.41	2.64	15	1
1:A:165:ASN:ND2	1:A:169:ARG:H	0.41	2.12	17	1
1:A:28:LEU:C	1:A:32:ARG:CD	0.41	2.94	1	1
1:A:130:THR:HG21	1:A:144:PHE:HB2	0.41	1.93	6	1
1:A:133:ASP:HB2	1:A:146:LYS:HD2	0.41	1.91	10	1
1:A:63:ILE:HG13	1:A:73:ILE:CB	0.41	2.42	14	1
1:A:127:TYR:HB3	1:A:129:ARG:HH12	0.41	1.75	14	1
1:A:93:LEU:HD11	1:A:98:LEU:CD2	0.41	2.45	19	1
1:A:166:LYS:HD3	1:A:166:LYS:O	0.41	2.15	3	1
1:A:160:TRP:CH2	1:A:174:PRO:HG3	0.41	2.51	4	1
1:A:33:HIS:HB3	1:A:54:GLU:HG2	0.41	1.92	7	1
1:A:31:GLN:HE21	1:A:31:GLN:HA	0.41	1.76	15	1
1:A:258:LEU:CD2	1:A:279:VAL:HG21	0.41	2.46	2	1
1:A:282:ARG:HG2	1:A:282:ARG:NH1	0.41	2.30	4	1
1:A:41:SER:OG	1:A:43:THR:HG22	0.41	2.16	7	1
1:A:145:LYS:HA	1:A:145:LYS:HE2	0.41	1.93	8	1
1:A:266:VAL:HG21	1:A:275:TRP:CE3	0.41	2.51	8	1
1:A:180:LYS:HD3	1:A:180:LYS:N	0.41	2.25	11	1
1:A:243:ILE:HD13	1:A:243:ILE:H	0.41	1.76	11	1
1:A:150:LEU:HD23	1:A:165:ASN:HA	0.41	1.91	13	1
1:A:238:VAL:HB	1:A:266:VAL:HG13	0.41	1.91	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:258:LEU:HD22	1:A:264:VAL:HG22	0.41	1.92	1	1
1:A:125:LEU:HD22	1:A:155:LYS:HD3	0.41	1.92	5	1
1:A:28:LEU:HB3	1:A:53:SER:CB	0.41	2.32	8	1
1:A:54:GLU:HB2	1:A:57:ARG:NE	0.41	2.29	9	1
1:A:86:GLU:CD	1:A:89:LYS:HZ2	0.41	2.24	16	1
1:A:242:ALA:HB1	1:A:259:GLU:CG	0.41	2.40	16	1
1:A:244:GLN:O	1:A:245:LYS:HB3	0.41	2.16	20	1
1:A:16:MET:SD	1:A:104:ARG:HB3	0.40	2.57	2	1
1:A:41:SER:HB3	1:A:44:CYS:O	0.40	2.16	2	1
1:A:238:VAL:N	1:A:267:THR:N	0.40	2.70	7	1
1:A:268:ARG:O	1:A:268:ARG:HD2	0.40	2.16	7	1
1:A:31:GLN:HB3	1:A:35:MET:CE	0.40	2.46	11	1
1:A:160:TRP:O	1:A:172:MET:HE1	0.40	2.15	11	1
1:A:57:ARG:HG3	1:A:57:ARG:NH1	0.40	2.32	20	1
1:A:57:ARG:HH21	1:A:94:ASP:CG	0.40	2.23	3	1
1:A:28:LEU:O	1:A:58:VAL:HG22	0.40	2.16	4	1
1:A:19:VAL:CB	1:A:39:ARG:HD2	0.40	2.40	18	2
1:A:87:PHE:CE2	1:A:91:HIS:ND1	0.40	2.90	13	1
1:A:20:SER:H	1:A:39:ARG:CD	0.40	2.27	16	1
1:A:54:GLU:HG3	1:A:55:ASN:ND2	0.40	2.32	20	1
1:A:155:LYS:HE3	1:A:161:TRP:NE1	0.40	2.32	20	1
1:A:100:GLU:HB2	1:A:101:PRO:HD2	0.40	1.92	3	1
1:A:151:VAL:CG2	1:A:164:ARG:HE	0.40	2.30	9	1
1:A:28:LEU:HA	1:A:31:GLN:CG	0.40	2.47	17	1
1:A:275:TRP:HE3	1:A:286:PHE:CZ	0.40	2.34	8	1
1:A:266:VAL:HA	1:A:277:GLY:HA3	0.40	1.94	9	1
1:A:41:SER:HB2	1:A:44:CYS:O	0.40	2.16	11	1
1:A:131:LEU:HD12	1:A:131:LEU:H	0.40	1.76	11	1
1:A:10:ASP:OD1	1:A:10:ASP:N	0.40	2.54	13	1
1:A:54:GLU:HG3	1:A:94:ASP:OD1	0.40	2.16	13	1
1:A:63:ILE:N	1:A:63:ILE:HD12	0.40	2.31	13	1
1:A:7:ASP:C	1:A:9:SER:H	0.40	2.25	15	1
1:A:19:VAL:CG1	1:A:20:SER:N	0.40	2.83	15	1
1:A:70:ARG:HD2	1:A:77:GLU:OE2	0.40	2.17	16	1
1:A:8:SER:O	1:A:9:SER:HB3	0.40	2.17	17	1
1:A:142:LEU:CD1	1:A:169:ARG:HG2	0.40	2.47	2	1
1:A:93:LEU:HA	1:A:154:GLU:CD	0.40	2.42	3	1
1:A:175:VAL:N	1:A:176:PRO:CD	0.40	2.85	6	1
1:A:4:ALA:HA	1:A:99:ILE:HA	0.40	1.94	11	1
1:A:142:LEU:CD2	1:A:150:LEU:CD2	0.40	3.00	13	1
1:A:129:ARG:HH11	1:A:129:ARG:HG2	0.40	1.75	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:LYS:H	1:A:146:LYS:HD3	0.40	1.76	16	1
1:A:67:PRO:O	1:A:69:ARG:HD3	0.40	2.15	17	1
1:A:138:ASP:C	1:A:140:GLU:H	0.40	2.25	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/303 (69%)	172±5 (82±2%)	29±5 (14±2%)	8±2 (4±1%)	4	30
All	All	4180/6060 (69%)	3431 (82%)	582 (14%)	167 (4%)	4	30

All 60 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	126	GLU	15
1	A	55	ASN	9
1	A	74	GLY	9
1	A	9	SER	8
1	A	156	PRO	8
1	A	94	ASP	7
1	A	125	LEU	6
1	A	31	GLN	6
1	A	138	ASP	5
1	A	140	GLU	5
1	A	147	GLY	5
1	A	133	ASP	4
1	A	139	ALA	4
1	A	19	VAL	4
1	A	33	HIS	3
1	A	57	ARG	3
1	A	20	SER	3
1	A	272	ASN	3
1	A	271	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	274	GLN	3
1	A	280	ASN	2
1	A	8	SER	2
1	A	4	ALA	2
1	A	41	SER	2
1	A	29	GLN	2
1	A	92	TYR	2
1	A	281	GLY	2
1	A	93	LEU	2
1	A	43	THR	2
1	A	75	ASP	2
1	A	95	THR	2
1	A	279	VAL	2
1	A	68	ASN	2
1	A	260	VAL	2
1	A	45	PRO	1
1	A	32	ARG	1
1	A	96	THR	1
1	A	42	SER	1
1	A	159	GLN	1
1	A	56	SER	1
1	A	69	ARG	1
1	A	5	ARG	1
1	A	238	VAL	1
1	A	97	THR	1
1	A	270	ASN	1
1	A	137	ASN	1
1	A	90	ILE	1
1	A	261	GLY	1
1	A	262	ASP	1
1	A	7	ASP	1
1	A	165	ASN	1
1	A	6	PHE	1
1	A	255	ALA	1
1	A	273	GLY	1
1	A	295	ASP	1
1	A	10	ASP	1
1	A	67	PRO	1
1	A	79	ASP	1
1	A	245	LYS	1
1	A	259	GLU	1

6.3.2 Protein sidechains ⓘ

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	184/261 (70%)	172±3 (94±2%)	12±3 (6±2%)	18 67
All	All	3680/5220 (70%)	3444 (94%)	236 (6%)	18 67

All 86 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	146	LYS	16
1	A	256	LEU	11
1	A	169	ARG	9
1	A	57	ARG	7
1	A	69	ARG	7
1	A	95	THR	7
1	A	54	GLU	6
1	A	154	GLU	6
1	A	179	GLU	6
1	A	129	ARG	5
1	A	155	LYS	5
1	A	243	ILE	5
1	A	180	LYS	5
1	A	43	THR	4
1	A	244	GLN	4
1	A	11	ARG	4
1	A	39	ARG	4
1	A	165	ASN	4
1	A	172	MET	4
1	A	22	GLN	3
1	A	280	ASN	3
1	A	21	ARG	3
1	A	31	GLN	3
1	A	274	GLN	3
1	A	76	GLN	3
1	A	241	LYS	3
1	A	58	VAL	3
1	A	125	LEU	3
1	A	153	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	158	GLU	3
1	A	55	ASN	3
1	A	131	LEU	3
1	A	90	ILE	3
1	A	62	ILE	3
1	A	246	ARG	2
1	A	267	THR	2
1	A	276	GLU	2
1	A	289	THR	2
1	A	239	PHE	2
1	A	262	ASP	2
1	A	282	ARG	2
1	A	29	GLN	2
1	A	126	GLU	2
1	A	96	THR	2
1	A	23	GLU	2
1	A	148	GLU	2
1	A	283	LYS	2
1	A	145	LYS	2
1	A	167	ASP	2
1	A	259	GLU	2
1	A	278	GLU	2
1	A	292	LYS	2
1	A	70	ARG	2
1	A	130	THR	2
1	A	7	ASP	1
1	A	32	ARG	1
1	A	33	HIS	1
1	A	77	GLU	1
1	A	247	VAL	1
1	A	86	GLU	1
1	A	5	ARG	1
1	A	89	LYS	1
1	A	269	MET	1
1	A	128	VAL	1
1	A	149	ILE	1
1	A	25	GLN	1
1	A	75	ASP	1
1	A	94	ASP	1
1	A	238	VAL	1
1	A	260	VAL	1
1	A	80	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	265	LYS	1
1	A	59	SER	1
1	A	138	ASP	1
1	A	133	ASP	1
1	A	68	ASN	1
1	A	137	ASN	1
1	A	28	LEU	1
1	A	47	ASP	1
1	A	87	PHE	1
1	A	159	GLN	1
1	A	26	THR	1
1	A	144	PHE	1
1	A	178	VAL	1
1	A	245	LYS	1
1	A	258	LEU	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
1	PTR	A	207	1	15,16,17	0.76±0.02	0±0 (3±3%)

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	PTR	A	207	1	17,22,24	0.65±0.01	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
1	PTR	A	207	1	-	0±0,10,11,13	0±0,1,1,1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	207	PTR	P-OH	2.06	1.63	1.59	20	10

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](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 52% for the well-defined parts and 48% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1952
Number of shifts mapped to atoms	1952
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	16

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	270	0.13 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	244	0.19 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	234	0.17 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 52%, i.e. 1524 atoms were assigned a chemical shift out of a possible 2953. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	714/1035 (69%)	333/420 (79%)	199/418 (48%)	182/197 (92%)
Sidechain	800/1653 (48%)	466/1069 (44%)	334/508 (66%)	0/76 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	10/265 (4%)	10/131 (8%)	0/125 (0%)	0/9 (0%)
Overall	1524/2953 (52%)	809/1620 (50%)	533/1051 (51%)	182/282 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 48%, i.e. 1942 atoms were assigned a chemical shift out of a possible 4054. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	932/1471 (63%)	428/595 (72%)	270/604 (45%)	234/272 (86%)
Sidechain	1000/2270 (44%)	571/1471 (39%)	429/703 (61%)	0/96 (0%)
Aromatic	10/313 (3%)	10/155 (6%)	0/146 (0%)	0/12 (0%)
Overall	1942/4054 (48%)	1009/2221 (45%)	699/1453 (48%)	234/380 (62%)

7.1.4 Statistically unusual chemical shifts ⓘ

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.

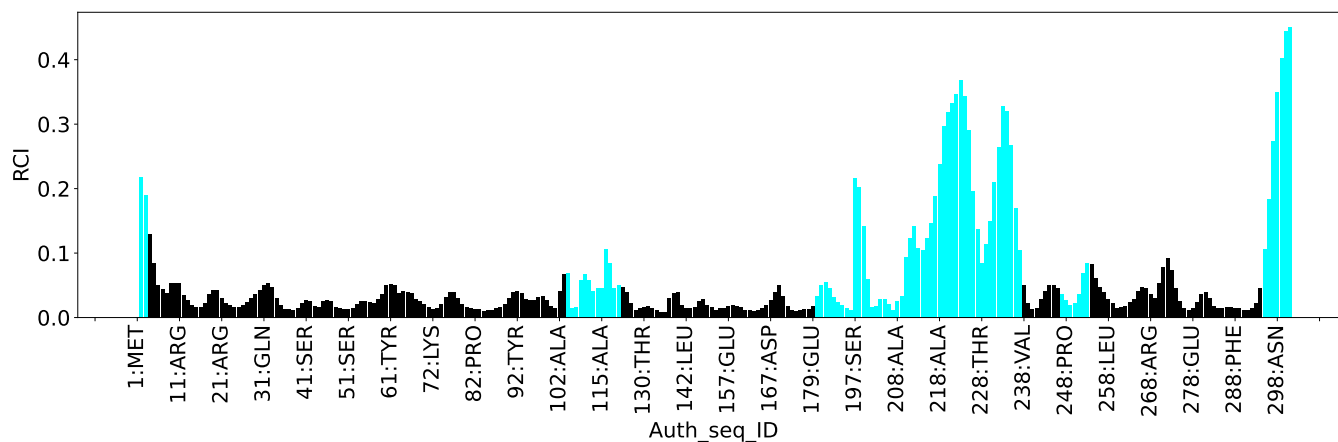
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	1	MET	HE1	10.20	-0.03 – 3.80	21.7
1	A	1	MET	HE2	10.20	-0.03 – 3.80	21.7
1	A	1	MET	HE3	10.20	-0.03 – 3.80	21.7
1	A	231	PRO	CD	42.81	45.11 – 55.58	-7.2
1	A	206	ALA	CA	40.20	43.52 – 62.81	-6.7
1	A	101	PRO	CA	53.31	55.85 – 70.84	-6.7
1	A	201	PRO	CA	53.89	55.85 – 70.84	-6.3
1	A	269	MET	HG3	0.14	0.54 – 4.26	-6.1
1	A	85	LEU	HD21	-0.74	-0.65 – 2.13	-5.3
1	A	85	LEU	HD22	-0.74	-0.65 – 2.13	-5.3
1	A	85	LEU	HD23	-0.74	-0.65 – 2.13	-5.3
1	A	84	LEU	HA	1.92	2.04 – 6.55	-5.3
1	A	21	ARG	HG2	0.24	0.26 – 2.87	-5.1
1	A	93	LEU	HD21	-0.67	-0.65 – 2.13	-5.1
1	A	93	LEU	HD22	-0.67	-0.65 – 2.13	-5.1
1	A	93	LEU	HD23	-0.67	-0.65 – 2.13	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication

of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3525
Intra-residue ($ i-j =0$)	711
Sequential ($ i-j =1$)	968
Medium range ($ i-j >1$ and $ i-j <5$)	427
Long range ($ i-j \geq 5$)	1418
Inter-chain	0
Hydrogen bond restraints	1
Disulfide bond restraints	0
Total dihedral-angle restraints	176
Number of unmapped restraints	0
Number of restraints per residue	12.2
Number of long range restraints per residue ¹	4.7

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	13.7	0.2
0.2-0.5 (Medium)	13.4	0.5
>0.5 (Large)	0.6	0.74

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)	14.7	9.34
10.0-20.0 (Medium)	0.1	13.03
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

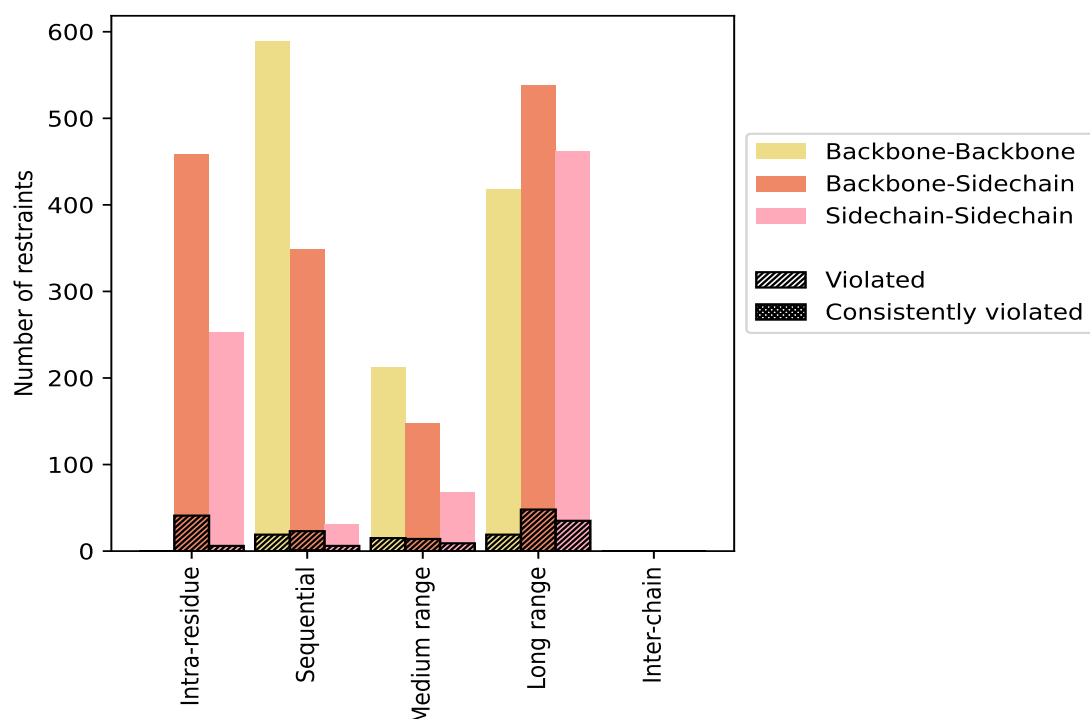
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	711	20.2	47	6.6	1.3	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	458	13.0	41	9.0	1.2	0	0.0	0.0
Sidechain-Sidechain	253	7.2	6	2.4	0.2	0	0.0	0.0
Sequential ($i-j =1$)	968	27.5	47	4.9	1.3	0	0.0	0.0
Backbone-Backbone	589	16.7	19	3.2	0.5	0	0.0	0.0
Backbone-Sidechain	348	9.9	22	6.3	0.6	0	0.0	0.0
Sidechain-Sidechain	31	0.9	6	19.4	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	427	12.1	38	8.9	1.1	0	0.0	0.0
Backbone-Backbone	212	6.0	15	7.1	0.4	0	0.0	0.0
Backbone-Sidechain	147	4.2	14	9.5	0.4	0	0.0	0.0
Sidechain-Sidechain	68	1.9	9	13.2	0.3	0	0.0	0.0
Long range ($i-j \geq 5$)	1418	40.2	102	7.2	2.9	0	0.0	0.0
Backbone-Backbone	418	11.9	19	4.5	0.5	0	0.0	0.0
Backbone-Sidechain	538	15.3	48	8.9	1.4	0	0.0	0.0
Sidechain-Sidechain	462	13.1	35	7.6	1.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	1	0.0	1	100.0	0.0	1	100.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3525	100.0	235	6.7	6.7	1	0.0	0.0
Backbone-Backbone	1219	34.6	53	4.3	1.5	0	0.0	0.0
Backbone-Sidechain	1492	42.3	126	8.4	3.6	1	0.1	0.0
Sidechain-Sidechain	814	23.1	56	6.9	1.6	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	9	3	3	7	0	22	0.22	0.42	0.1	0.18
2	10	6	5	13	0	34	0.23	0.54	0.11	0.21
3	7	10	3	10	0	30	0.25	0.73	0.15	0.2
4	7	8	6	10	0	31	0.2	0.48	0.1	0.16
5	13	4	3	11	0	31	0.23	0.46	0.12	0.17
6	8	8	8	12	0	36	0.25	0.51	0.12	0.22
7	9	8	7	10	0	34	0.2	0.4	0.09	0.16
8	9	8	7	14	0	38	0.25	0.57	0.13	0.24
9	13	9	3	19	0	44	0.26	0.5	0.11	0.24
10	3	8	2	7	0	20	0.26	0.49	0.13	0.23

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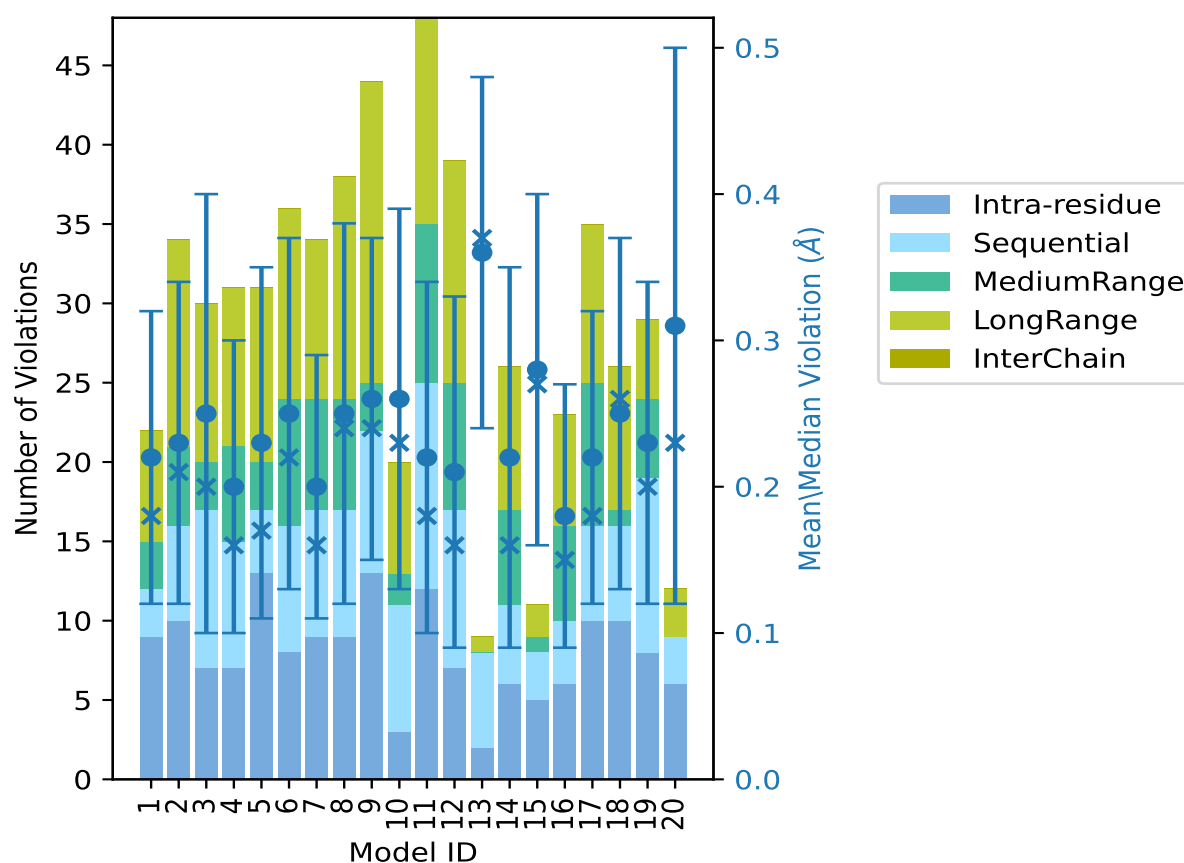
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	12	13	10	13	0	48	0.22	0.53	0.12	0.18
12	7	10	8	14	0	39	0.21	0.5	0.12	0.16
13	2	6	0	1	0	9	0.36	0.55	0.12	0.37
14	6	5	6	9	0	26	0.22	0.5	0.13	0.16
15	5	3	1	2	0	11	0.28	0.51	0.12	0.27
16	6	4	6	7	0	23	0.18	0.4	0.09	0.15
17	10	6	9	10	0	35	0.22	0.5	0.1	0.18
18	10	6	1	9	0	26	0.25	0.49	0.12	0.26
19	8	11	5	5	0	29	0.23	0.47	0.11	0.2
20	6	3	0	3	0	12	0.31	0.74	0.19	0.23

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

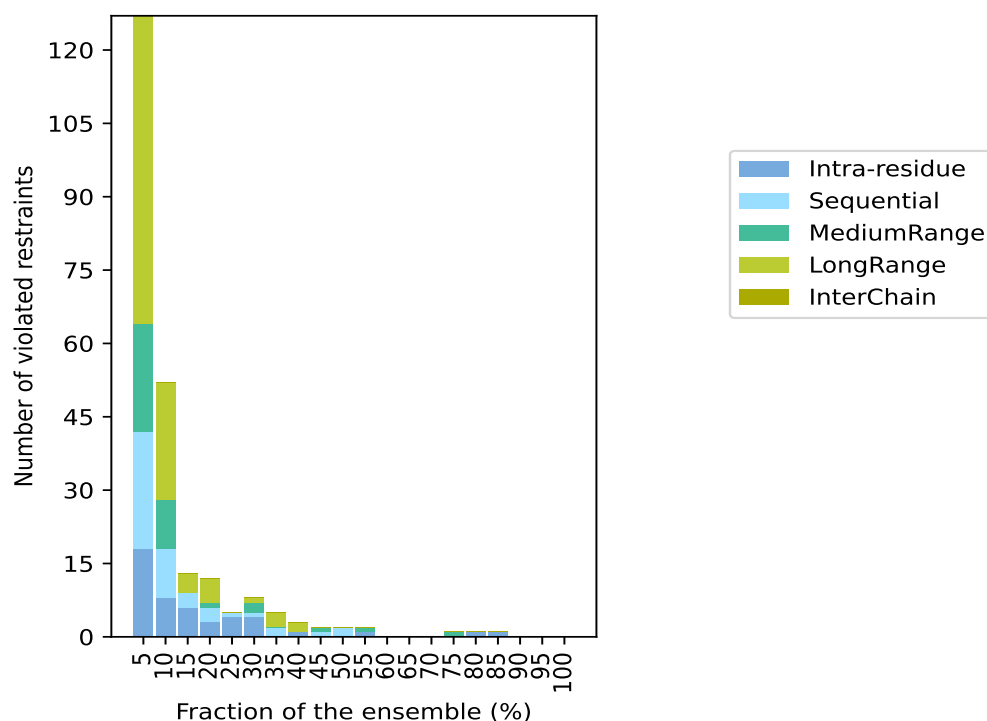
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3290(IR:664, SQ:921, MR:389, LR:1316, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
18	24	22	63	0	127	1	5.0
8	10	10	24	0	52	2	10.0
6	3	0	4	0	13	3	15.0
3	3	1	5	0	12	4	20.0
4	1	0	0	0	5	5	25.0
4	1	2	1	0	8	6	30.0
0	2	0	3	0	5	7	35.0
1	0	0	2	0	3	8	40.0
0	1	1	0	0	2	9	45.0
0	2	0	0	0	2	10	50.0
1	0	1	0	0	2	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	1	0	0	1	15	75.0
1	0	0	0	0	1	16	80.0
1	0	0	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

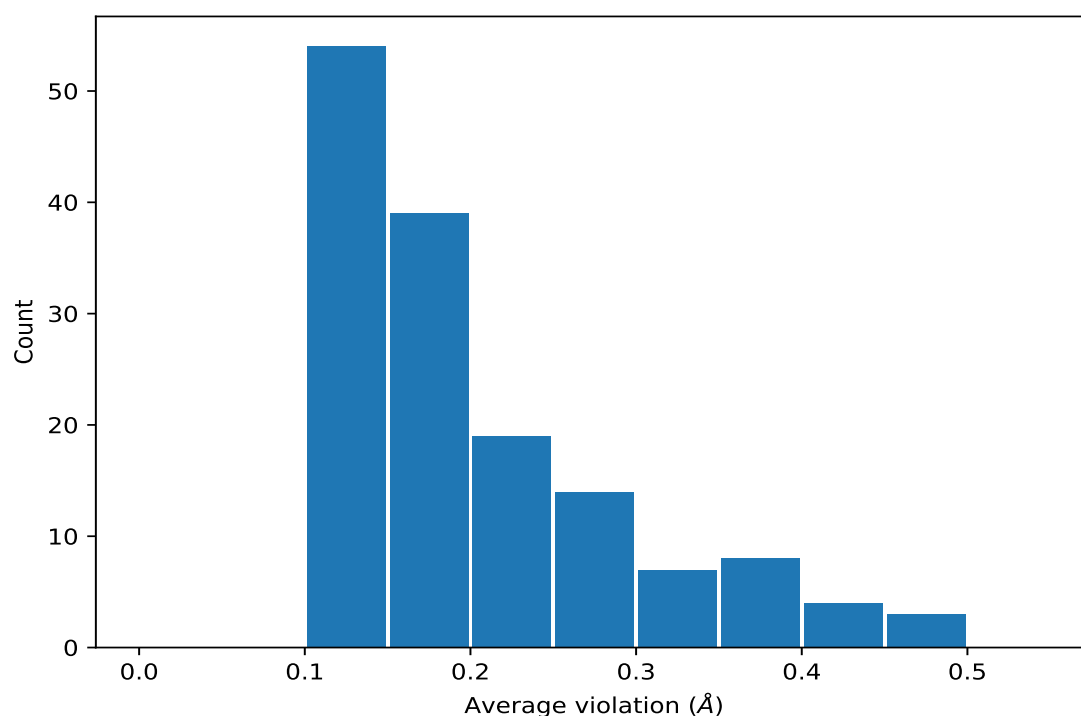
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	20	0.25	0.01	0.25
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	17	0.43	0.08	0.44
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	16	0.42	0.02	0.43
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	15	0.16	0.04	0.15
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	11	0.21	0.04	0.21
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	11	0.2	0.06	0.23
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	10	0.33	0.16	0.37
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	10	0.26	0.07	0.28
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	9	0.36	0.14	0.4
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	9	0.14	0.02	0.13
(1,2630)	1:207:A:PTR:HA	1:207:A:PTR:HD1	8	0.33	0.11	0.34
(1,458)	1:33:A:HIS:HE2	1:56:A:SER:HA	8	0.18	0.06	0.17
(1,2017)	1:152:A:ILE:H	1:163:A:ALA:HB1	8	0.13	0.02	0.12
(1,2640)	1:223:A:PRO:HA	1:224:A:GLY:H	7	0.45	0.06	0.48
(1,2642)	1:226:A:ALA:HA	1:227:A:ILE:H	7	0.38	0.12	0.41
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD2	7	0.22	0.12	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD3	7	0.22	0.12	0.18
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD2	7	0.22	0.12	0.18
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD3	7	0.22	0.12	0.18
(1,1437)	1:127:A:TYR:H	1:180:A:LYS:HA	7	0.18	0.07	0.15
(1,858)	1:61:A:TYR:HH	1:94:A:ASP:HA	7	0.15	0.04	0.13
(1,2307)	1:164:A:ARG:HA	1:165:A:ASN:HB2	6	0.43	0.05	0.42
(1,2365)	1:169:A:ARG:H	1:169:A:ARG:HB2	6	0.36	0.21	0.3
(1,1742)	1:138:A:ASP:H	1:138:A:ASP:HB2	6	0.36	0.02	0.36
(1,3284)	1:272:A:ASN:HD21	1:274:A:GLN:H	6	0.28	0.13	0.24
(1,2330)	1:165:A:ASN:H	1:165:A:ASN:HB2	6	0.23	0.01	0.24
(1,1762)	1:139:A:ALA:HA	1:171:A:GLY:HA3	6	0.17	0.02	0.18
(1,1395)	1:120:A:THR:H	1:120:A:THR:HB	6	0.17	0.06	0.15
(1,1758)	1:139:A:ALA:H	1:141:A:ASP:H	6	0.15	0.02	0.16
(1,1063)	1:78:A:PHE:HA	1:78:A:PHE:HD1	5	0.29	0.08	0.29
(1,2361)	1:167:A:ASP:H	1:167:A:ASP:HB2	5	0.28	0.09	0.32
(1,1410)	1:123:A:ASP:H	1:123:A:ASP:HB2	5	0.25	0.11	0.24
(1,1393)	1:115:A:ALA:H	1:116:A:PRO:HD2	5	0.24	0.08	0.25
(1,2564)	1:182:A:VAL:H	1:182:A:VAL:HG11	5	0.22	0.08	0.19
(1,2637)	1:220:A:SER:HA	1:221:A:GLY:H	4	0.34	0.12	0.34
(1,2086)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	4	0.27	0.04	0.28
(1,2265)	1:162:A:SER:HB2	1:163:A:ALA:HA	4	0.26	0.02	0.26
(1,1462)	1:127:A:TYR:HD1	1:150:A:LEU:H	4	0.2	0.1	0.18
(1,2636)	1:217:A:PRO:HA	1:218:A:ALA:H	4	0.19	0.03	0.2
(1,699)	1:49:A:VAL:HG21	1:62:A:ILE:HG12	4	0.17	0.06	0.16
(1,699)	1:49:A:VAL:HG22	1:62:A:ILE:HG12	4	0.17	0.06	0.16
(1,699)	1:49:A:VAL:HG23	1:62:A:ILE:HG12	4	0.17	0.06	0.16
(1,410)	1:30:A:GLY:H	1:53:A:SER:HG	4	0.17	0.05	0.15
(1,280)	1:21:A:ARG:HE	1:60:A:HIS:HD2	4	0.15	0.02	0.14
(1,776)	1:52:A:VAL:HB	1:61:A:TYR:H	4	0.14	0.03	0.14
(1,805)	1:54:A:GLU:HA	1:57:A:ARG:H	4	0.14	0.02	0.14
(1,2409)	1:172:A:MET:HA	1:172:A:MET:HE2	4	0.11	0.01	0.12
(1,2413)	1:172:A:MET:HB2	1:172:A:MET:HE1	4	0.11	0.0	0.11
(1,1405)	1:122:A:GLU:HA	1:123:A:ASP:H	3	0.36	0.02	0.37
(1,1920)	1:146:A:LYS:HA	1:146:A:LYS:HD2	3	0.36	0.01	0.37
(1,1910)	1:145:A:LYS:HA	1:146:A:LYS:HD2	3	0.25	0.08	0.22
(1,2698)	1:239:A:PHE:HA	1:239:A:PHE:HD1	3	0.25	0.1	0.3
(1,1779)	1:141:A:ASP:H	1:141:A:ASP:HB2	3	0.19	0.05	0.2
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD11	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD12	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD13	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD11	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD12	3	0.19	0.06	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD13	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD11	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD12	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD13	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD11	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD12	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD13	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD11	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD12	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD13	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD11	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD12	3	0.19	0.06	0.18
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD13	3	0.19	0.06	0.18
(1,2890)	1:246:A:ARG:HE	1:286:A:PHE:HA	3	0.17	0.03	0.15
(1,827)	1:59:A:SER:H	1:59:A:SER:HG	3	0.15	0.01	0.14
(1,2219)	1:161:A:TRP:HA	1:172:A:MET:HG2	3	0.14	0.02	0.15
(1,413)	1:30:A:GLY:HA2	1:56:A:SER:HA	3	0.13	0.02	0.13
(1,2093)	1:155:A:LYS:HG2	1:155:A:LYS:HE2	3	0.13	0.02	0.12
(1,1918)	1:146:A:LYS:H	1:147:A:GLY:H	3	0.12	0.01	0.13
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD11	3	0.12	0.01	0.12
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD12	3	0.12	0.01	0.12
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD13	3	0.12	0.01	0.12
(1,2458)	1:174:A:PRO:HB2	1:177:A:TYR:HB2	2	0.48	0.05	0.48
(1,2458)	1:174:A:PRO:HB3	1:177:A:TYR:HB2	2	0.48	0.05	0.48
(1,2568)	1:182:A:VAL:HA	1:182:A:VAL:HG13	2	0.4	0.0	0.4
(1,2094)	1:155:A:LYS:HG2	1:156:A:PRO:HD2	2	0.36	0.18	0.36
(1,3233)	1:268:A:ARG:H	1:276:A:GLU:H	2	0.36	0.01	0.36
(1,3201)	1:266:A:VAL:HB	1:269:A:MET:HE3	2	0.34	0.1	0.34
(1,1916)	1:145:A:LYS:HG2	1:146:A:LYS:H	2	0.32	0.04	0.32
(1,23)	1:62:A:ILE:HG12	1:207:A:PTR:HD2	2	0.31	0.08	0.31
(1,23)	1:62:A:ILE:HG13	1:207:A:PTR:HD2	2	0.31	0.08	0.31
(1,3285)	1:273:A:GLY:H	1:274:A:GLN:H	2	0.3	0.12	0.3
(1,1431)	1:126:A:GLU:HA	1:126:A:GLU:HG2	2	0.25	0.01	0.25
(1,2902)	1:247:A:VAL:H	1:247:A:VAL:HG23	2	0.25	0.02	0.25
(1,3260)	1:270:A:ASN:H	1:275:A:TRP:HD1	2	0.25	0.02	0.25
(1,8)	1:60:A:HIS:HB2	1:207:A:PTR:HD2	2	0.24	0.09	0.24
(1,8)	1:60:A:HIS:HB3	1:207:A:PTR:HD2	2	0.24	0.09	0.24
(1,1915)	1:145:A:LYS:HB2	1:148:A:GLU:HG2	2	0.24	0.08	0.24
(1,2687)	1:238:A:VAL:HB	1:266:A:VAL:HG12	2	0.23	0.05	0.23
(1,2864)	1:244:A:GLN:HE21	1:245:A:LYS:H	2	0.23	0.08	0.23
(1,2686)	1:238:A:VAL:HB	1:266:A:VAL:HG11	2	0.22	0.01	0.22
(1,972)	1:67:A:PRO:HA	1:69:A:ARG:HE	2	0.22	0.01	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,974)	1:68:A:ASN:H	1:70:A:ARG:H	2	0.21	0.05	0.21
(1,2641)	1:225:A:ALA:H	1:225:A:ALA:HB1	2	0.2	0.01	0.2
(1,1623)	1:131:A:LEU:HG	1:179:A:GLU:H	2	0.19	0.05	0.19
(1,2625)	1:199:A:GLY:H	1:200:A:ILE:H	2	0.18	0.06	0.18
(1,415)	1:31:A:GLN:H	1:53:A:SER:HG	2	0.17	0.02	0.17
(1,20)	1:62:A:ILE:HG12	1:207:A:PTR:HB2	2	0.16	0.06	0.16
(1,20)	1:62:A:ILE:HG12	1:207:A:PTR:HB3	2	0.16	0.06	0.16
(1,20)	1:62:A:ILE:HG13	1:207:A:PTR:HB2	2	0.16	0.06	0.16
(1,20)	1:62:A:ILE:HG13	1:207:A:PTR:HB3	2	0.16	0.06	0.16
(1,1421)	1:125:A:LEU:HA	1:152:A:ILE:HB	2	0.16	0.06	0.16
(1,2150)	1:158:A:GLU:H	1:158:A:GLU:HB2	2	0.16	0.01	0.16
(1,1423)	1:125:A:LEU:HA	1:161:A:TRP:HE3	2	0.15	0.01	0.15
(1,1756)	1:139:A:ALA:H	1:140:A:GLU:H	2	0.15	0.02	0.15
(1,817)	1:58:A:VAL:H	1:60:A:HIS:HD2	2	0.15	0.04	0.15
(1,2537)	1:178:A:VAL:HG13	1:178:A:VAL:HG21	2	0.15	0.0	0.15
(1,417)	1:32:A:ARG:H	1:32:A:ARG:HE	2	0.15	0.0	0.15
(1,1884)	1:144:A:PHE:HE1	1:177:A:TYR:HB2	2	0.15	0.03	0.15
(1,2931)	1:250:A:ALA:H	1:251:A:TYR:H	2	0.14	0.01	0.14
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG11	2	0.13	0.01	0.13
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG12	2	0.13	0.01	0.13
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG13	2	0.13	0.01	0.13
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG21	2	0.13	0.01	0.13
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG22	2	0.13	0.01	0.13
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG23	2	0.13	0.01	0.13
(1,1769)	1:140:A:GLU:H	1:142:A:LEU:HA	2	0.13	0.0	0.13
(1,2600)	1:187:A:HIS:H	1:187:A:HIS:HB2	2	0.13	0.03	0.13
(1,2877)	1:246:A:ARG:H	1:259:A:GLU:HA	2	0.13	0.03	0.13
(1,291)	1:21:A:ARG:HH12	1:51:A:SER:HG	2	0.12	0.02	0.12
(1,3252)	1:269:A:MET:HE3	1:286:A:PHE:HZ	2	0.12	0.02	0.12
(1,877)	1:62:A:ILE:HB	1:63:A:ILE:HA	2	0.12	0.0	0.12
(1,1324)	1:96:A:THR:HG1	1:99:A:ILE:HD13	2	0.12	0.01	0.12
(1,1556)	1:129:A:ARG:HD2	1:181:A:LEU:HA	2	0.12	0.0	0.12
(1,2084)	1:155:A:LYS:HA	1:162:A:SER:HG	2	0.12	0.01	0.12
(1,2947)	1:252:A:ASP:H	1:253:A:LYS:HA	2	0.12	0.01	0.12
(1,1542)	1:129:A:ARG:HA	1:178:A:VAL:HB	2	0.12	0.02	0.12
(1,456)	1:33:A:HIS:HE2	1:55:A:ASN:H	2	0.12	0.0	0.12
(1,2026)	1:152:A:ILE:HA	1:163:A:ALA:HB1	2	0.12	0.0	0.12
(1,2894)	1:246:A:ARG:HH12	1:290:A:HIS:HE2	2	0.12	0.0	0.12
(1,935)	1:65:A:SER:HG	1:67:A:PRO:HA	2	0.11	0.0	0.11
(1,1502)	1:128:A:VAL:HB	1:163:A:ALA:HB1	2	0.11	0.01	0.11
(1,1812)	1:142:A:LEU:HA	1:143:A:PRO:HD2	2	0.11	0.0	0.11
(1,2956)	1:253:A:LYS:HA	1:255:A:ALA:HB2	2	0.11	0.0	0.11

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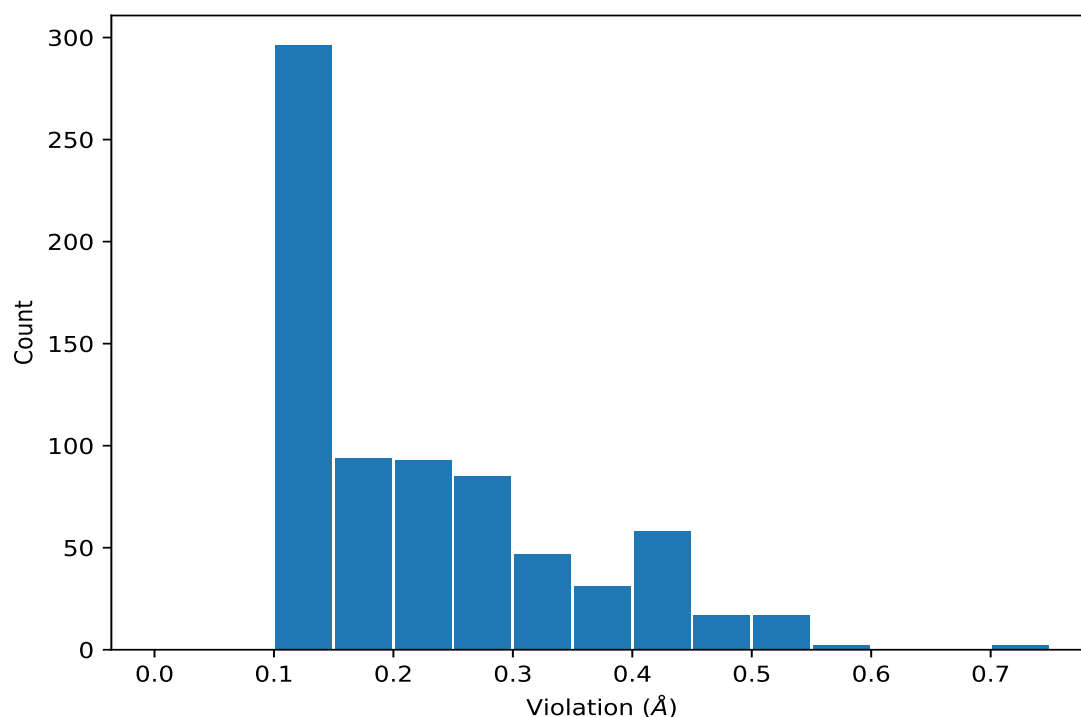
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3013)	1:256:A:LEU:HD11	1:279:A:VAL:HB	2	0.11	0.0	0.11
(1,3013)	1:256:A:LEU:HD12	1:279:A:VAL:HB	2	0.11	0.0	0.11
(1,3013)	1:256:A:LEU:HD13	1:279:A:VAL:HB	2	0.11	0.0	0.11
(1,3013)	1:256:A:LEU:HD21	1:279:A:VAL:HB	2	0.11	0.0	0.11
(1,3013)	1:256:A:LEU:HD22	1:279:A:VAL:HB	2	0.11	0.0	0.11
(1,3013)	1:256:A:LEU:HD23	1:279:A:VAL:HB	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1880)	1:144:A:PHE:HD1	1:145:A:LYS:H	20	0.74
(1,2365)	1:169:A:ARG:H	1:169:A:ARG:HB2	3	0.73
(1,3270)	1:270:A:ASN:HD21	1:275:A:TRP:HD1	8	0.57
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	13	0.55
(1,2365)	1:169:A:ARG:H	1:169:A:ARG:HB2	2	0.54
(1,2094)	1:155:A:LYS:HG2	1:156:A:PRO:HD2	3	0.54
(1,1560)	1:130:A:THR:H	1:144:A:PHE:HD1	20	0.54
(1,2458)	1:174:A:PRO:HB2	1:177:A:TYR:HB2	11	0.53
(1,2458)	1:174:A:PRO:HB3	1:177:A:TYR:HB2	11	0.53
(1,2640)	1:223:A:PRO:HA	1:224:A:GLY:H	6	0.51
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	3	0.51
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	15	0.51
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	20	0.51
(1,3284)	1:272:A:ASN:HD21	1:274:A:GLN:H	12	0.5
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	6	0.5
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	9	0.5
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	14	0.5
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	11	0.5
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	14	0.5
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	17	0.5
(1,2307)	1:164:A:ARG:HA	1:165:A:ASN:HB2	9	0.5
(1,2640)	1:223:A:PRO:HA	1:224:A:GLY:H	10	0.49
(1,2640)	1:223:A:PRO:HA	1:224:A:GLY:H	12	0.49
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	18	0.49
(1,2640)	1:223:A:PRO:HA	1:224:A:GLY:H	13	0.48
(1,2630)	1:207:A:PTR:HA	1:207:A:PTR:HD1	4	0.48
(1,2307)	1:164:A:ARG:HA	1:165:A:ASN:HB2	4	0.48
(1,2637)	1:220:A:SER:HA	1:221:A:GLY:H	19	0.47
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	6	0.47
(1,3499)	1:294:A:PHE:H	1:294:A:PHE:HE1	6	0.46
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	10	0.46
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	10	0.46
(1,1386)	1:112:A:SER:HA	1:112:A:SER:HG	5	0.46
(1,2642)	1:226:A:ALA:HA	1:227:A:ILE:H	8	0.45
(1,2642)	1:226:A:ALA:HA	1:227:A:ILE:H	9	0.45
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	2	0.45
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	5	0.45
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	13	0.45
(1,3201)	1:266:A:VAL:HB	1:269:A:MET:HE3	2	0.44
(1,2642)	1:226:A:ALA:HA	1:227:A:ILE:H	18	0.44
(1,2640)	1:223:A:PRO:HA	1:224:A:GLY:H	8	0.44
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	6	0.44
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	12	0.44
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	14	0.44
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	15	0.44
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD2	10	0.44
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD3	10	0.44
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD2	10	0.44
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD3	10	0.44
(1,2637)	1:220:A:SER:HA	1:221:A:GLY:H	8	0.43
(1,2630)	1:207:A:PTR:HA	1:207:A:PTR:HD1	5	0.43
(1,2630)	1:207:A:PTR:HA	1:207:A:PTR:HD1	12	0.43
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	2	0.43
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	8	0.43
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	19	0.43
(1,2515)	1:177:A:TYR:HB2	1:178:A:VAL:HG12	11	0.43
(1,2458)	1:174:A:PRO:HB2	1:177:A:TYR:HB2	3	0.43
(1,2458)	1:174:A:PRO:HB3	1:177:A:TYR:HB2	3	0.43
(1,2307)	1:164:A:ARG:HA	1:165:A:ASN:HB2	5	0.43
(1,2115)	1:156:A:PRO:HD2	1:162:A:SER:HA	11	0.43
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	3	0.43
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	8	0.43
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	11	0.43
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	20	0.43
(1,3285)	1:273:A:GLY:H	1:274:A:GLN:H	9	0.42
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	5	0.42
(1,2307)	1:164:A:ARG:HA	1:165:A:ASN:HB2	14	0.42
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	1	0.42
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	17	0.42
(1,2950)	1:252:A:ASP:HA	1:255:A:ALA:HB1	17	0.41
(1,2642)	1:226:A:ALA:HA	1:227:A:ILE:H	13	0.41
(1,2642)	1:226:A:ALA:HA	1:227:A:ILE:H	19	0.41
(1,2640)	1:223:A:PRO:HA	1:224:A:GLY:H	19	0.41
(1,2568)	1:182:A:VAL:HA	1:182:A:VAL:HG13	14	0.41
(1,2065)	1:154:A:GLU:HA	1:155:A:LYS:HB2	19	0.41
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	6	0.41
(1,2692)	1:238:A:VAL:HG11	1:266:A:VAL:HG12	11	0.4
(1,2692)	1:238:A:VAL:HG12	1:266:A:VAL:HG12	11	0.4
(1,2692)	1:238:A:VAL:HG13	1:266:A:VAL:HG12	11	0.4
(1,2692)	1:238:A:VAL:HG21	1:266:A:VAL:HG12	11	0.4
(1,2692)	1:238:A:VAL:HG22	1:266:A:VAL:HG12	11	0.4
(1,2692)	1:238:A:VAL:HG23	1:266:A:VAL:HG12	11	0.4
(1,2673)	1:237:A:PRO:HA	1:238:A:VAL:H	7	0.4
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2568)	1:182:A:VAL:HA	1:182:A:VAL:HG13	11	0.4
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	5	0.4
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	16	0.4
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	18	0.4
(1,1636)	1:132:A:TYR:HB2	1:132:A:TYR:HD1	19	0.4
(1,1467)	1:127:A:TYR:HE1	1:164:A:ARG:HE	9	0.4
(1,1410)	1:123:A:ASP:H	1:123:A:ASP:HB2	5	0.4
(1,1063)	1:78:A:PHE:HA	1:78:A:PHE:HD1	1	0.4
(1,11)	1:61:A:TYR:HA	1:208:A:ALA:HB1	8	0.4
(1,11)	1:61:A:TYR:HA	1:208:A:ALA:HB2	8	0.4
(1,11)	1:61:A:TYR:HA	1:208:A:ALA:HB3	8	0.4
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	9	0.39
(1,1742)	1:138:A:ASP:H	1:138:A:ASP:HB2	9	0.39
(1,1742)	1:138:A:ASP:H	1:138:A:ASP:HB2	18	0.39
(1,1409)	1:122:A:GLU:HB2	1:123:A:ASP:HA	7	0.39
(1,1403)	1:122:A:GLU:H	1:122:A:GLU:HB2	1	0.39
(1,23)	1:62:A:ILE:HG12	1:207:A:PTR:HD2	9	0.39
(1,23)	1:62:A:ILE:HG13	1:207:A:PTR:HD2	9	0.39
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	7	0.38
(1,2630)	1:207:A:PTR:HA	1:207:A:PTR:HD1	15	0.38
(1,1405)	1:122:A:GLU:HA	1:123:A:ASP:H	12	0.38
(1,394)	1:28:A:LEU:HG	1:37:A:LEU:HD23	18	0.38
(1,3520)	1:94:A:ASP:HA	1:154:A:GLU:HB2	13	0.37
(1,3520)	1:94:A:ASP:HA	1:154:A:GLU:HB3	13	0.37
(1,3284)	1:272:A:ASN:HD21	1:274:A:GLN:H	9	0.37
(1,3233)	1:268:A:ARG:H	1:276:A:GLU:H	7	0.37
(1,2642)	1:226:A:ALA:HA	1:227:A:ILE:H	11	0.37
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	13	0.37
(1,2597)	1:186:A:PRO:HB2	1:187:A:HIS:H	8	0.37
(1,2365)	1:169:A:ARG:H	1:169:A:ARG:HB2	17	0.37
(1,2307)	1:164:A:ARG:HA	1:165:A:ASN:HB2	6	0.37
(1,2307)	1:164:A:ARG:HA	1:165:A:ASN:HB2	17	0.37
(1,1920)	1:146:A:LYS:HA	1:146:A:LYS:HD2	6	0.37
(1,1920)	1:146:A:LYS:HA	1:146:A:LYS:HD2	18	0.37
(1,1733)	1:136:A:GLY:HA2	1:137:A:ASN:HB2	7	0.37
(1,1405)	1:122:A:GLU:HA	1:123:A:ASP:H	19	0.37
(1,1393)	1:115:A:ALA:H	1:116:A:PRO:HD2	12	0.37
(1,3124)	1:262:A:ASP:HA	1:263:A:ILE:H	12	0.36
(1,2564)	1:182:A:VAL:H	1:182:A:VAL:HG11	9	0.36
(1,1916)	1:145:A:LYS:HG2	1:146:A:LYS:H	3	0.36
(1,1910)	1:145:A:LYS:HA	1:146:A:LYS:HD2	18	0.36
(1,1742)	1:138:A:ASP:H	1:138:A:ASP:HB2	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	10	0.35
(1,1899)	1:145:A:LYS:H	1:145:A:LYS:HB2	1	0.35
(1,1742)	1:138:A:ASP:H	1:138:A:ASP:HB2	2	0.35
(1,1742)	1:138:A:ASP:H	1:138:A:ASP:HB2	12	0.35
(1,1739)	1:137:A:ASN:HA	1:143:A:PRO:HB2	17	0.35
(1,3233)	1:268:A:ARG:H	1:276:A:GLU:H	2	0.34
(1,2698)	1:239:A:PHE:HA	1:239:A:PHE:HD1	11	0.34
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	10	0.34
(1,2361)	1:167:A:ASP:H	1:167:A:ASP:HB2	9	0.34
(1,1920)	1:146:A:LYS:HA	1:146:A:LYS:HD2	9	0.34
(1,1742)	1:138:A:ASP:H	1:138:A:ASP:HB2	17	0.34
(1,1462)	1:127:A:TYR:HD1	1:150:A:LEU:H	9	0.34
(1,1405)	1:122:A:GLU:HA	1:123:A:ASP:H	8	0.34
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD2	3	0.34
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD3	3	0.34
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD2	3	0.34
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD3	3	0.34
(1,3287)	1:273:A:GLY:H	1:275:A:TRP:HE1	8	0.33
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	2	0.33
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	16	0.33
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	17	0.33
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	1	0.33
(1,2361)	1:167:A:ASP:H	1:167:A:ASP:HB2	1	0.33
(1,1410)	1:123:A:ASP:H	1:123:A:ASP:HB2	17	0.33
(1,1063)	1:78:A:PHE:HA	1:78:A:PHE:HD1	6	0.33
(1,8)	1:60:A:HIS:HB2	1:207:A:PTR:HD2	14	0.33
(1,8)	1:60:A:HIS:HB3	1:207:A:PTR:HD2	14	0.33
(1,2693)	1:238:A:VAL:HG11	1:269:A:MET:HE1	11	0.32
(1,2693)	1:238:A:VAL:HG12	1:269:A:MET:HE1	11	0.32
(1,2693)	1:238:A:VAL:HG13	1:269:A:MET:HE1	11	0.32
(1,2693)	1:238:A:VAL:HG21	1:269:A:MET:HE1	11	0.32
(1,2693)	1:238:A:VAL:HG22	1:269:A:MET:HE1	11	0.32
(1,2693)	1:238:A:VAL:HG23	1:269:A:MET:HE1	11	0.32
(1,2660)	1:233:A:THR:HB	1:234:A:GLN:HA	8	0.32
(1,2640)	1:223:A:PRO:HA	1:224:A:GLY:H	3	0.32
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	15	0.32
(1,2361)	1:167:A:ASP:H	1:167:A:ASP:HB2	10	0.32
(1,2361)	1:167:A:ASP:H	1:167:A:ASP:HB2	18	0.32
(1,2086)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	5	0.32
(1,1089)	1:80:A:HIS:H	1:80:A:HIS:HD2	5	0.32
(1,3522)	1:94:A:ASP:HA	1:156:A:PRO:HD2	11	0.31
(1,3522)	1:94:A:ASP:HA	1:156:A:PRO:HD3	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3284)	1:272:A:ASN:HD21	1:274:A:GLN:H	8	0.31
(1,2864)	1:244:A:GLN:HE21	1:245:A:LYS:H	11	0.31
(1,2609)	1:187:A:HIS:HB2	1:190:A:HIS:HD2	7	0.31
(1,1915)	1:145:A:LYS:HB2	1:148:A:GLU:HG2	8	0.31
(1,1437)	1:127:A:TYR:H	1:180:A:LYS:HA	11	0.31
(1,2698)	1:239:A:PHE:HA	1:239:A:PHE:HD1	4	0.3
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	15	0.3
(1,2630)	1:207:A:PTR:HA	1:207:A:PTR:HD1	2	0.3
(1,458)	1:33:A:HIS:HE2	1:56:A:SER:HA	9	0.3
(1,3301)	1:275:A:TRP:H	1:275:A:TRP:HE3	8	0.29
(1,3267)	1:270:A:ASN:HA	1:273:A:GLY:H	6	0.29
(1,2086)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	8	0.29
(1,1916)	1:145:A:LYS:HG2	1:146:A:LYS:H	8	0.29
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	19	0.29
(1,1083)	1:78:A:PHE:HE2	1:87:A:PHE:HD2	18	0.29
(1,1063)	1:78:A:PHE:HA	1:78:A:PHE:HD1	3	0.29
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	12	0.29
(1,2687)	1:238:A:VAL:HB	1:266:A:VAL:HG12	7	0.28
(1,2630)	1:207:A:PTR:HA	1:207:A:PTR:HD1	18	0.28
(1,2265)	1:162:A:SER:HB2	1:163:A:ALA:HA	6	0.28
(1,1393)	1:115:A:ALA:H	1:116:A:PRO:HD2	7	0.28
(1,380)	1:28:A:LEU:H	1:28:A:LEU:HD21	18	0.28
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	15	0.27
(1,3260)	1:270:A:ASN:H	1:275:A:TRP:HD1	8	0.27
(1,3240)	1:269:A:MET:HA	1:275:A:TRP:HA	2	0.27
(1,2902)	1:247:A:VAL:H	1:247:A:VAL:HG23	12	0.27
(1,2265)	1:162:A:SER:HB2	1:163:A:ALA:HA	10	0.27
(1,1448)	1:127:A:TYR:HA	1:151:A:VAL:HA	9	0.27
(1,1395)	1:120:A:THR:H	1:120:A:THR:HB	9	0.27
(1,1392)	1:114:A:SER:HG	1:115:A:ALA:H	3	0.27
(1,1063)	1:78:A:PHE:HA	1:78:A:PHE:HD1	9	0.27
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	1	0.26
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	10	0.26
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	13	0.26
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	16	0.26
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	20	0.26
(1,2637)	1:220:A:SER:HA	1:221:A:GLY:H	2	0.26
(1,2086)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	17	0.26
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	6	0.26
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	18	0.26
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD11	5	0.26
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD12	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD13	5	0.26
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD11	5	0.26
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD12	5	0.26
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD13	5	0.26
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD11	5	0.26
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD12	5	0.26
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD13	5	0.26
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD11	5	0.26
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD12	5	0.26
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD13	5	0.26
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD11	5	0.26
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD12	5	0.26
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD13	5	0.26
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD11	5	0.26
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD12	5	0.26
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD13	5	0.26
(1,1437)	1:127:A:TYR:H	1:180:A:LYS:HA	10	0.26
(1,1431)	1:126:A:GLU:HA	1:126:A:GLU:HG2	7	0.26
(1,1387)	1:114:A:SER:H	1:114:A:SER:HB2	14	0.26
(1,1071)	1:78:A:PHE:HD1	1:84:A:LEU:HA	6	0.26
(1,974)	1:68:A:ASN:H	1:70:A:ARG:H	19	0.26
(1,824)	1:58:A:VAL:HB	1:60:A:HIS:HD2	11	0.26
(1,699)	1:49:A:VAL:HG21	1:62:A:ILE:HG12	18	0.26
(1,699)	1:49:A:VAL:HG22	1:62:A:ILE:HG12	18	0.26
(1,699)	1:49:A:VAL:HG23	1:62:A:ILE:HG12	18	0.26
(1,410)	1:30:A:GLY:H	1:53:A:SER:HG	9	0.26
(1,406)	1:29:A:GLN:HA	1:30:A:GLY:H	11	0.26
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	2	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	3	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	4	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	6	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	7	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	8	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	9	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	11	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	12	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	17	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	18	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	19	0.25
(1,2951)	1:252:A:ASP:HA	1:255:A:ALA:HB2	17	0.25
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	7	0.25
(1,2265)	1:162:A:SER:HB2	1:163:A:ALA:HA	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1779)	1:141:A:ASP:H	1:141:A:ASP:HB2	16	0.25
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	5	0.25
(1,1553)	1:129:A:ARG:HG2	1:181:A:LEU:H	8	0.25
(1,1462)	1:127:A:TYR:HD1	1:150:A:LEU:H	6	0.25
(1,1393)	1:115:A:ALA:H	1:116:A:PRO:HD2	13	0.25
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	19	0.25
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	5	0.24
(2,41)	1:166:A:LYS:N	1:165:A:ASN:O	14	0.24
(1,3201)	1:266:A:VAL:HB	1:269:A:MET:HE3	7	0.24
(1,2625)	1:199:A:GLY:H	1:200:A:ILE:H	11	0.24
(1,2365)	1:169:A:ARG:H	1:169:A:ARG:HB2	9	0.24
(1,2330)	1:165:A:ASN:H	1:165:A:ASN:HB2	4	0.24
(1,2330)	1:165:A:ASN:H	1:165:A:ASN:HB2	5	0.24
(1,2330)	1:165:A:ASN:H	1:165:A:ASN:HB2	14	0.24
(1,2265)	1:162:A:SER:HB2	1:163:A:ALA:HA	17	0.24
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	16	0.24
(1,1623)	1:131:A:LEU:HG	1:179:A:GLU:H	12	0.24
(1,1469)	1:127:A:TYR:HH	1:164:A:ARG:HH21	9	0.24
(1,1431)	1:126:A:GLU:HA	1:126:A:GLU:HG2	4	0.24
(1,1410)	1:123:A:ASP:H	1:123:A:ASP:HB2	20	0.24
(1,858)	1:61:A:TYR:HH	1:94:A:ASP:HA	2	0.24
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	6	0.24
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD2	6	0.24
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD3	6	0.24
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD2	6	0.24
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD3	6	0.24
(1,3517)	1:298:A:ASN:HA	1:300:A:ASP:H	19	0.23
(1,3260)	1:270:A:ASN:H	1:275:A:TRP:HD1	2	0.23
(1,3119)	1:260:A:VAL:HG23	1:261:A:GLY:H	1	0.23
(1,2902)	1:247:A:VAL:H	1:247:A:VAL:HG23	2	0.23
(1,2686)	1:238:A:VAL:HB	1:266:A:VAL:HG11	2	0.23
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	2	0.23
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	19	0.23
(1,2630)	1:207:A:PTR:HA	1:207:A:PTR:HD1	3	0.23
(1,2564)	1:182:A:VAL:H	1:182:A:VAL:HG11	2	0.23
(1,2330)	1:165:A:ASN:H	1:165:A:ASN:HB2	9	0.23
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	17	0.23
(1,1395)	1:120:A:THR:H	1:120:A:THR:HB	15	0.23
(1,411)	1:30:A:GLY:H	1:56:A:SER:HA	5	0.23
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	19	0.23
(1,23)	1:62:A:ILE:HG12	1:207:A:PTR:HD2	4	0.23
(1,23)	1:62:A:ILE:HG13	1:207:A:PTR:HD2	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3242)	1:269:A:MET:HA	1:276:A:GLU:H	8	0.22
(1,3203)	1:266:A:VAL:HB	1:276:A:GLU:H	7	0.22
(1,2890)	1:246:A:ARG:HE	1:286:A:PHE:HA	9	0.22
(1,2686)	1:238:A:VAL:HB	1:266:A:VAL:HG11	7	0.22
(1,2636)	1:217:A:PRO:HA	1:218:A:ALA:H	20	0.22
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	3	0.22
(1,2606)	1:187:A:HIS:HB2	1:187:A:HIS:HD2	16	0.22
(1,2330)	1:165:A:ASN:H	1:165:A:ASN:HB2	6	0.22
(1,2330)	1:165:A:ASN:H	1:165:A:ASN:HB2	17	0.22
(1,2159)	1:159:A:GLN:H	1:159:A:GLN:HG2	11	0.22
(1,1910)	1:145:A:LYS:HA	1:146:A:LYS:HD2	9	0.22
(1,1906)	1:145:A:LYS:H	1:148:A:GLU:HB2	9	0.22
(1,1896)	1:144:A:PHE:HE2	1:174:A:PRO:HG2	20	0.22
(1,1421)	1:125:A:LEU:HA	1:152:A:ILE:HB	9	0.22
(1,972)	1:67:A:PRO:HA	1:69:A:ARG:HE	14	0.22
(1,620)	1:41:A:SER:HA	1:43:A:THR:H	4	0.22
(1,458)	1:33:A:HIS:HE2	1:56:A:SER:HA	3	0.22
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	3	0.22
(1,20)	1:62:A:ILE:HG12	1:207:A:PTR:HB2	4	0.22
(1,20)	1:62:A:ILE:HG12	1:207:A:PTR:HB3	4	0.22
(1,20)	1:62:A:ILE:HG13	1:207:A:PTR:HB2	4	0.22
(1,20)	1:62:A:ILE:HG13	1:207:A:PTR:HB3	4	0.22
(1,3299)	1:274:A:GLN:HA	1:288:A:PHE:H	8	0.21
(1,2826)	1:242:A:ALA:HB2	1:260:A:VAL:HA	16	0.21
(1,2641)	1:225:A:ALA:H	1:225:A:ALA:HB1	7	0.21
(1,2636)	1:217:A:PRO:HA	1:218:A:ALA:H	11	0.21
(1,1673)	1:133:A:ASP:HB2	1:145:A:LYS:HB2	4	0.21
(1,1447)	1:127:A:TYR:HA	1:151:A:VAL:H	9	0.21
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	9	0.21
(1,972)	1:67:A:PRO:HA	1:69:A:ARG:HE	6	0.21
(1,965)	1:66:A:LEU:HD11	1:70:A:ARG:H	15	0.21
(1,965)	1:66:A:LEU:HD12	1:70:A:ARG:H	15	0.21
(1,965)	1:66:A:LEU:HD13	1:70:A:ARG:H	15	0.21
(1,965)	1:66:A:LEU:HD21	1:70:A:ARG:H	15	0.21
(1,965)	1:66:A:LEU:HD22	1:70:A:ARG:H	15	0.21
(1,965)	1:66:A:LEU:HD23	1:70:A:ARG:H	15	0.21
(1,914)	1:64:A:ASN:H	1:64:A:ASN:HD21	14	0.21
(1,458)	1:33:A:HIS:HE2	1:56:A:SER:HA	12	0.21
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	7	0.21
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	14	0.21
(1,4)	1:49:A:VAL:HG11	1:207:A:PTR:HE2	6	0.21
(1,4)	1:49:A:VAL:HG12	1:207:A:PTR:HE2	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:49:A:VAL:HG13	1:207:A:PTR:HE2	6	0.21
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	11	0.2
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	18	0.2
(1,2086)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	9	0.2
(1,1779)	1:141:A:ASP:H	1:141:A:ASP:HB2	5	0.2
(1,1762)	1:139:A:ALA:HA	1:171:A:GLY:HA3	9	0.2
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	10	0.2
(1,1072)	1:78:A:PHE:HD1	1:87:A:PHE:HD2	19	0.2
(1,1055)	1:76:A:GLN:H	1:88:A:TYR:HH	9	0.2
(1,699)	1:49:A:VAL:HG21	1:62:A:ILE:HG12	6	0.2
(1,699)	1:49:A:VAL:HG22	1:62:A:ILE:HG12	6	0.2
(1,699)	1:49:A:VAL:HG23	1:62:A:ILE:HG12	6	0.2
(1,626)	1:41:A:SER:HG	1:43:A:THR:H	11	0.2
(1,458)	1:33:A:HIS:HE2	1:56:A:SER:HA	11	0.2
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	1	0.2
(1,3285)	1:273:A:GLY:H	1:274:A:GLN:H	19	0.19
(1,3110)	1:260:A:VAL:HA	1:262:A:ASP:H	12	0.19
(1,2641)	1:225:A:ALA:H	1:225:A:ALA:HB1	10	0.19
(1,2637)	1:220:A:SER:HA	1:221:A:GLY:H	10	0.19
(1,2564)	1:182:A:VAL:H	1:182:A:VAL:HG11	3	0.19
(1,2094)	1:155:A:LYS:HG2	1:156:A:PRO:HD2	19	0.19
(1,1762)	1:139:A:ALA:HA	1:171:A:GLY:HA3	4	0.19
(1,1762)	1:139:A:ALA:HA	1:171:A:GLY:HA3	8	0.19
(1,1603)	1:131:A:LEU:H	1:131:A:LEU:HD11	11	0.19
(1,1603)	1:131:A:LEU:H	1:131:A:LEU:HD12	11	0.19
(1,1603)	1:131:A:LEU:H	1:131:A:LEU:HD13	11	0.19
(1,1603)	1:131:A:LEU:H	1:131:A:LEU:HD21	11	0.19
(1,1603)	1:131:A:LEU:H	1:131:A:LEU:HD22	11	0.19
(1,1603)	1:131:A:LEU:H	1:131:A:LEU:HD23	11	0.19
(1,1395)	1:120:A:THR:H	1:120:A:THR:HB	20	0.19
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	1	0.19
(1,971)	1:67:A:PRO:HA	1:69:A:ARG:H	17	0.19
(1,817)	1:58:A:VAL:H	1:60:A:HIS:HD2	12	0.19
(1,415)	1:31:A:GLN:H	1:53:A:SER:HG	1	0.19
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	2	0.19
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	17	0.19
(1,3284)	1:272:A:ASN:HD21	1:274:A:GLN:H	17	0.18
(1,2934)	1:250:A:ALA:HA	1:252:A:ASP:H	4	0.18
(1,2687)	1:238:A:VAL:HB	1:266:A:VAL:HG12	11	0.18
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	4	0.18
(1,2636)	1:217:A:PRO:HA	1:218:A:ALA:H	4	0.18
(1,1910)	1:145:A:LYS:HA	1:146:A:LYS:HD2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD11	9	0.18
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD12	9	0.18
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD13	9	0.18
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD11	9	0.18
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD12	9	0.18
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD13	9	0.18
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD11	9	0.18
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD12	9	0.18
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD13	9	0.18
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD11	9	0.18
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD12	9	0.18
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD13	9	0.18
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD11	9	0.18
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD12	9	0.18
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD13	9	0.18
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD11	9	0.18
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD12	9	0.18
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD13	9	0.18
(1,1438)	1:127:A:TYR:H	1:181:A:LEU:H	6	0.18
(1,1412)	1:123:A:ASP:H	1:124:A:ASN:H	3	0.18
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	17	0.18
(1,823)	1:58:A:VAL:HB	1:60:A:HIS:H	11	0.18
(1,815)	1:58:A:VAL:H	1:58:A:VAL:HB	6	0.18
(1,554)	1:37:A:LEU:HG	1:28:A:LEU:HD21	18	0.18
(1,554)	1:37:A:LEU:HG	1:28:A:LEU:HD22	18	0.18
(1,554)	1:37:A:LEU:HG	1:28:A:LEU:HD23	18	0.18
(1,280)	1:21:A:ARG:HE	1:60:A:HIS:HD2	12	0.18
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	12	0.18
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD2	17	0.18
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD3	17	0.18
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD2	17	0.18
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD3	17	0.18
(1,3284)	1:272:A:ASN:HD21	1:274:A:GLN:H	6	0.17
(1,3262)	1:270:A:ASN:H	1:276:A:GLU:H	8	0.17
(1,2923)	1:249:A:CYS:H	1:255:A:ALA:HB2	17	0.17
(1,2564)	1:182:A:VAL:H	1:182:A:VAL:HG11	11	0.17
(1,2365)	1:169:A:ARG:H	1:169:A:ARG:HB2	11	0.17
(1,2150)	1:158:A:GLU:H	1:158:A:GLU:HB2	7	0.17
(1,2017)	1:152:A:ILE:H	1:163:A:ALA:HB1	2	0.17
(1,1884)	1:144:A:PHE:HE1	1:177:A:TYR:HB2	3	0.17
(1,1762)	1:139:A:ALA:HA	1:171:A:GLY:HA3	11	0.17
(1,1758)	1:139:A:ALA:H	1:141:A:ASP:H	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:139:A:ALA:H	1:141:A:ASP:H	14	0.17
(1,1756)	1:139:A:ALA:H	1:140:A:GLU:H	11	0.17
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	8	0.17
(1,1437)	1:127:A:TYR:H	1:180:A:LYS:HA	16	0.17
(1,827)	1:59:A:SER:H	1:59:A:SER:HG	1	0.17
(1,776)	1:52:A:VAL:HB	1:61:A:TYR:H	6	0.17
(1,776)	1:52:A:VAL:HB	1:61:A:TYR:H	17	0.17
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	5	0.17
(1,3273)	1:271:A:ILE:H	1:272:A:ASN:H	6	0.16
(1,2877)	1:246:A:ARG:H	1:259:A:GLU:HA	12	0.16
(1,2600)	1:187:A:HIS:H	1:187:A:HIS:HB2	12	0.16
(1,2093)	1:155:A:LYS:HG2	1:155:A:LYS:HE2	19	0.16
(1,1915)	1:145:A:LYS:HB2	1:148:A:GLU:HG2	16	0.16
(1,1762)	1:139:A:ALA:HA	1:171:A:GLY:HA3	16	0.16
(1,1758)	1:139:A:ALA:H	1:141:A:ASP:H	2	0.16
(1,1758)	1:139:A:ALA:H	1:141:A:ASP:H	4	0.16
(1,1729)	1:136:A:GLY:HA3	1:141:A:ASP:HB2	2	0.16
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	11	0.16
(1,1423)	1:125:A:LEU:HA	1:161:A:TRP:HE3	10	0.16
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	3	0.16
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	7	0.16
(1,1063)	1:78:A:PHE:HA	1:78:A:PHE:HD1	19	0.16
(1,974)	1:68:A:ASN:H	1:70:A:ARG:H	14	0.16
(1,413)	1:30:A:GLY:HA2	1:56:A:SER:HA	1	0.16
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	4	0.16
(1,3284)	1:272:A:ASN:HD21	1:274:A:GLN:H	19	0.15
(1,2916)	1:248:A:PRO:HA	1:255:A:ALA:HB2	17	0.15
(1,2890)	1:246:A:ARG:HE	1:286:A:PHE:HA	2	0.15
(1,2890)	1:246:A:ARG:HE	1:286:A:PHE:HA	17	0.15
(1,2864)	1:244:A:GLN:HE21	1:245:A:LYS:H	7	0.15
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	3	0.15
(1,2566)	1:182:A:VAL:H	1:183:A:ARG:H	4	0.15
(1,2537)	1:178:A:VAL:HG13	1:178:A:VAL:HG21	5	0.15
(1,2537)	1:178:A:VAL:HG13	1:178:A:VAL:HG21	7	0.15
(1,2219)	1:161:A:TRP:HA	1:172:A:MET:HG2	5	0.15
(1,2219)	1:161:A:TRP:HA	1:172:A:MET:HG2	17	0.15
(1,2150)	1:158:A:GLU:H	1:158:A:GLU:HB2	17	0.15
(1,2017)	1:152:A:ILE:H	1:163:A:ALA:HB1	18	0.15
(1,1905)	1:145:A:LYS:H	1:148:A:GLU:HA	6	0.15
(1,1710)	1:134:A:PHE:HD2	1:144:A:PHE:HZ	15	0.15
(1,1459)	1:127:A:TYR:HB2	1:181:A:LEU:H	11	0.15
(1,1437)	1:127:A:TYR:H	1:180:A:LYS:HA	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:123:A:ASP:H	1:123:A:ASP:HB2	2	0.15
(1,1393)	1:115:A:ALA:H	1:116:A:PRO:HD2	1	0.15
(1,1393)	1:115:A:ALA:H	1:116:A:PRO:HD2	19	0.15
(1,1279)	1:92:A:TYR:HD2	1:97:A:THR:HG22	12	0.15
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	6	0.15
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	14	0.15
(1,1064)	1:78:A:PHE:HA	1:78:A:PHE:HE1	1	0.15
(1,858)	1:61:A:TYR:HH	1:94:A:ASP:HA	5	0.15
(1,805)	1:54:A:GLU:HA	1:57:A:ARG:H	11	0.15
(1,417)	1:32:A:ARG:H	1:32:A:ARG:HE	2	0.15
(1,415)	1:31:A:GLN:H	1:53:A:SER:HG	12	0.15
(1,410)	1:30:A:GLY:H	1:53:A:SER:HG	5	0.15
(1,396)	1:28:A:LEU:HG	1:102:A:ALA:HB2	18	0.15
(1,280)	1:21:A:ARG:HE	1:60:A:HIS:HD2	6	0.15
(1,249)	1:20:A:SER:H	1:23:A:GLU:H	16	0.15
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	1	0.15
(1,8)	1:60:A:HIS:HB2	1:207:A:PTR:HD2	20	0.15
(1,8)	1:60:A:HIS:HB3	1:207:A:PTR:HD2	20	0.15
(1,3252)	1:269:A:MET:HE3	1:286:A:PHE:HZ	8	0.14
(1,2931)	1:250:A:ALA:H	1:251:A:TYR:H	4	0.14
(1,2705)	1:239:A:PHE:HA	1:265:A:LYS:HA	7	0.14
(1,2636)	1:217:A:PRO:HA	1:218:A:ALA:H	14	0.14
(1,2365)	1:169:A:ARG:H	1:169:A:ARG:HB2	8	0.14
(1,2017)	1:152:A:ILE:H	1:163:A:ALA:HB1	3	0.14
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD11	15	0.14
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD12	15	0.14
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD13	15	0.14
(1,1831)	1:142:A:LEU:HD11	1:143:A:PRO:HD2	12	0.14
(1,1831)	1:142:A:LEU:HD11	1:143:A:PRO:HD3	12	0.14
(1,1831)	1:142:A:LEU:HD12	1:143:A:PRO:HD2	12	0.14
(1,1831)	1:142:A:LEU:HD12	1:143:A:PRO:HD3	12	0.14
(1,1831)	1:142:A:LEU:HD13	1:143:A:PRO:HD2	12	0.14
(1,1831)	1:142:A:LEU:HD13	1:143:A:PRO:HD3	12	0.14
(1,1831)	1:142:A:LEU:HD21	1:143:A:PRO:HD2	12	0.14
(1,1831)	1:142:A:LEU:HD21	1:143:A:PRO:HD3	12	0.14
(1,1831)	1:142:A:LEU:HD22	1:143:A:PRO:HD2	12	0.14
(1,1831)	1:142:A:LEU:HD22	1:143:A:PRO:HD3	12	0.14
(1,1831)	1:142:A:LEU:HD23	1:143:A:PRO:HD2	12	0.14
(1,1831)	1:142:A:LEU:HD23	1:143:A:PRO:HD3	12	0.14
(1,1758)	1:139:A:ALA:H	1:141:A:ASP:H	17	0.14
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	1	0.14
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1623)	1:131:A:LEU:HG	1:179:A:GLU:H	9	0.14
(1,1460)	1:127:A:TYR:HB2	1:182:A:VAL:H	7	0.14
(1,1437)	1:127:A:TYR:H	1:180:A:LYS:HA	12	0.14
(1,1423)	1:125:A:LEU:HA	1:161:A:TRP:HE3	5	0.14
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	2	0.14
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	8	0.14
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	12	0.14
(1,858)	1:61:A:TYR:HH	1:94:A:ASP:HA	4	0.14
(1,827)	1:59:A:SER:H	1:59:A:SER:HG	4	0.14
(1,827)	1:59:A:SER:H	1:59:A:SER:HG	5	0.14
(1,805)	1:54:A:GLU:HA	1:57:A:ARG:H	2	0.14
(1,805)	1:54:A:GLU:HA	1:57:A:ARG:H	8	0.14
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG11	8	0.14
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG12	8	0.14
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG13	8	0.14
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG21	8	0.14
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG22	8	0.14
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG23	8	0.14
(1,458)	1:33:A:HIS:HE2	1:56:A:SER:HA	10	0.14
(1,417)	1:32:A:ARG:H	1:32:A:ARG:HE	7	0.14
(1,410)	1:30:A:GLY:H	1:53:A:SER:HG	11	0.14
(1,372)	1:27:A:ARG:H	1:28:A:LEU:HG	18	0.14
(1,291)	1:21:A:ARG:HH12	1:51:A:SER:HG	3	0.14
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	17	0.14
(1,2947)	1:252:A:ASP:H	1:253:A:LYS:HA	14	0.13
(1,2931)	1:250:A:ALA:H	1:251:A:TYR:H	10	0.13
(1,2699)	1:239:A:PHE:HA	1:239:A:PHE:HE1	2	0.13
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	12	0.13
(1,2631)	1:210:A:PRO:HA	1:211:A:GLN:H	13	0.13
(1,2564)	1:182:A:VAL:H	1:182:A:VAL:HG11	17	0.13
(1,2084)	1:155:A:LYS:HA	1:162:A:SER:HG	12	0.13
(1,2017)	1:152:A:ILE:H	1:163:A:ALA:HB1	4	0.13
(1,1965)	1:150:A:LEU:HA	1:165:A:ASN:HA	3	0.13
(1,1918)	1:146:A:LYS:H	1:147:A:GLY:H	2	0.13
(1,1918)	1:146:A:LYS:H	1:147:A:GLY:H	11	0.13
(1,1828)	1:142:A:LEU:HG	1:165:A:ASN:HB2	4	0.13
(1,1779)	1:141:A:ASP:H	1:141:A:ASP:HB2	8	0.13
(1,1769)	1:140:A:GLU:H	1:142:A:LEU:HA	5	0.13
(1,1769)	1:140:A:GLU:H	1:142:A:LEU:HA	7	0.13
(1,1762)	1:139:A:ALA:HA	1:171:A:GLY:HA3	17	0.13
(1,1756)	1:139:A:ALA:H	1:140:A:GLU:H	9	0.13
(1,1616)	1:131:A:LEU:HA	1:146:A:LYS:HB2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1561)	1:130:A:THR:H	1:145:A:LYS:H	1	0.13
(1,1542)	1:129:A:ARG:HA	1:178:A:VAL:HB	12	0.13
(1,1324)	1:96:A:THR:HG1	1:99:A:ILE:HD13	16	0.13
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	5	0.13
(1,858)	1:61:A:TYR:HH	1:94:A:ASP:HA	9	0.13
(1,858)	1:61:A:TYR:HH	1:94:A:ASP:HA	14	0.13
(1,858)	1:61:A:TYR:HH	1:94:A:ASP:HA	16	0.13
(1,858)	1:61:A:TYR:HH	1:94:A:ASP:HA	18	0.13
(1,825)	1:58:A:VAL:HB	1:60:A:HIS:HE2	11	0.13
(1,459)	1:33:A:HIS:HE2	1:56:A:SER:HG	6	0.13
(1,458)	1:33:A:HIS:HE2	1:56:A:SER:HA	1	0.13
(1,458)	1:33:A:HIS:HE2	1:56:A:SER:HA	5	0.13
(1,413)	1:30:A:GLY:HA2	1:56:A:SER:HA	9	0.13
(1,410)	1:30:A:GLY:H	1:53:A:SER:HG	3	0.13
(1,280)	1:21:A:ARG:HE	1:60:A:HIS:HD2	2	0.13
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	10	0.13
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	16	0.13
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD2	16	0.13
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD3	16	0.13
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD2	16	0.13
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD3	16	0.13
(1,2894)	1:246:A:ARG:HH12	1:290:A:HIS:HE2	6	0.12
(1,2882)	1:246:A:ARG:HA	1:290:A:HIS:HE1	14	0.12
(1,2752)	1:240:A:ALA:HB3	1:264:A:VAL:HB	2	0.12
(1,2698)	1:239:A:PHE:HA	1:239:A:PHE:HD1	20	0.12
(1,2630)	1:207:A:PTR:HA	1:207:A:PTR:HD1	19	0.12
(1,2625)	1:199:A:GLY:H	1:200:A:ILE:H	3	0.12
(1,2409)	1:172:A:MET:HA	1:172:A:MET:HE2	2	0.12
(1,2409)	1:172:A:MET:HA	1:172:A:MET:HE2	11	0.12
(1,2093)	1:155:A:LYS:HG2	1:155:A:LYS:HE2	9	0.12
(1,2093)	1:155:A:LYS:HG2	1:155:A:LYS:HE2	11	0.12
(1,2026)	1:152:A:ILE:HA	1:163:A:ALA:HB1	6	0.12
(1,2017)	1:152:A:ILE:H	1:163:A:ALA:HB1	8	0.12
(1,2017)	1:152:A:ILE:H	1:163:A:ALA:HB1	16	0.12
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD11	9	0.12
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD12	9	0.12
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD13	9	0.12
(1,1884)	1:144:A:PHE:HE1	1:177:A:TYR:HB2	11	0.12
(1,1758)	1:139:A:ALA:H	1:141:A:ASP:H	18	0.12
(1,1632)	1:132:A:TYR:HA	1:132:A:TYR:HE1	19	0.12
(1,1556)	1:129:A:ARG:HD2	1:181:A:LEU:HA	4	0.12
(1,1556)	1:129:A:ARG:HD2	1:181:A:LEU:HA	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD11	7	0.12
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD12	7	0.12
(1,1507)	1:128:A:VAL:HG11	1:152:A:ILE:HD13	7	0.12
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD11	7	0.12
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD12	7	0.12
(1,1507)	1:128:A:VAL:HG12	1:152:A:ILE:HD13	7	0.12
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD11	7	0.12
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD12	7	0.12
(1,1507)	1:128:A:VAL:HG13	1:152:A:ILE:HD13	7	0.12
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD11	7	0.12
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD12	7	0.12
(1,1507)	1:128:A:VAL:HG21	1:152:A:ILE:HD13	7	0.12
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD11	7	0.12
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD12	7	0.12
(1,1507)	1:128:A:VAL:HG22	1:152:A:ILE:HD13	7	0.12
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD11	7	0.12
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD12	7	0.12
(1,1507)	1:128:A:VAL:HG23	1:152:A:ILE:HD13	7	0.12
(1,1502)	1:128:A:VAL:HB	1:163:A:ALA:HB1	14	0.12
(1,1462)	1:127:A:TYR:HD1	1:150:A:LEU:H	10	0.12
(1,1410)	1:123:A:ASP:H	1:123:A:ASP:HB2	16	0.12
(1,1309)	1:95:A:THR:HG22	1:96:A:THR:HB	11	0.12
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	4	0.12
(1,877)	1:62:A:ILE:HB	1:63:A:ILE:HA	5	0.12
(1,877)	1:62:A:ILE:HB	1:63:A:ILE:HA	19	0.12
(1,802)	1:54:A:GLU:H	1:59:A:SER:H	8	0.12
(1,699)	1:49:A:VAL:HG21	1:62:A:ILE:HG12	14	0.12
(1,699)	1:49:A:VAL:HG22	1:62:A:ILE:HG12	14	0.12
(1,699)	1:49:A:VAL:HG23	1:62:A:ILE:HG12	14	0.12
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG11	9	0.12
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG12	9	0.12
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG13	9	0.12
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG21	9	0.12
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG22	9	0.12
(1,625)	1:41:A:SER:HA	1:49:A:VAL:HG23	9	0.12
(1,456)	1:33:A:HIS:HE2	1:55:A:ASN:H	8	0.12
(1,408)	1:29:A:GLN:HA	1:31:A:GLN:H	11	0.12
(1,284)	1:21:A:ARG:HH11	1:39:A:ARG:HH12	14	0.12
(1,280)	1:21:A:ARG:HE	1:60:A:HIS:HD2	19	0.12
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	7	0.12
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD2	11	0.12
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD3	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD2	11	0.12
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD3	11	0.12
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD2	12	0.12
(1,29)	1:74:A:GLY:HA2	1:210:A:PRO:HD3	12	0.12
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD2	12	0.12
(1,29)	1:74:A:GLY:HA3	1:210:A:PRO:HD3	12	0.12
(1,15)	1:61:A:TYR:HD1	1:209:A:GLN:HA	19	0.12
(1,15)	1:61:A:TYR:HD2	1:209:A:GLN:HA	19	0.12
(1,14)	1:61:A:TYR:HA	1:209:A:GLN:HA	19	0.12
(1,3252)	1:269:A:MET:HE3	1:286:A:PHE:HZ	10	0.11
(1,3145)	1:263:A:ILE:HD11	1:294:A:PHE:HE2	7	0.11
(1,3013)	1:256:A:LEU:HD11	1:279:A:VAL:HB	5	0.11
(1,3013)	1:256:A:LEU:HD12	1:279:A:VAL:HB	5	0.11
(1,3013)	1:256:A:LEU:HD13	1:279:A:VAL:HB	5	0.11
(1,3013)	1:256:A:LEU:HD21	1:279:A:VAL:HB	5	0.11
(1,3013)	1:256:A:LEU:HD22	1:279:A:VAL:HB	5	0.11
(1,3013)	1:256:A:LEU:HD23	1:279:A:VAL:HB	5	0.11
(1,3013)	1:256:A:LEU:HD11	1:279:A:VAL:HB	14	0.11
(1,3013)	1:256:A:LEU:HD12	1:279:A:VAL:HB	14	0.11
(1,3013)	1:256:A:LEU:HD13	1:279:A:VAL:HB	14	0.11
(1,3013)	1:256:A:LEU:HD21	1:279:A:VAL:HB	14	0.11
(1,3013)	1:256:A:LEU:HD22	1:279:A:VAL:HB	14	0.11
(1,3013)	1:256:A:LEU:HD23	1:279:A:VAL:HB	14	0.11
(1,2956)	1:253:A:LYS:HA	1:255:A:ALA:HB2	7	0.11
(1,2956)	1:253:A:LYS:HA	1:255:A:ALA:HB2	11	0.11
(1,2952)	1:253:A:LYS:H	1:255:A:ALA:H	17	0.11
(1,2947)	1:252:A:ASP:H	1:253:A:LYS:HA	3	0.11
(1,2894)	1:246:A:ARG:HH12	1:290:A:HIS:HE2	1	0.11
(1,2638)	1:221:A:GLY:HA2	1:222:A:SER:H	18	0.11
(1,2610)	1:187:A:HIS:HE1	1:190:A:HIS:HD2	11	0.11
(1,2593)	1:185:A:SER:HG	1:186:A:PRO:HD2	4	0.11
(1,2579)	1:183:A:ARG:HB2	1:184:A:SER:H	4	0.11
(1,2413)	1:172:A:MET:HB2	1:172:A:MET:HE1	7	0.11
(1,2413)	1:172:A:MET:HB2	1:172:A:MET:HE1	18	0.11
(1,2413)	1:172:A:MET:HB2	1:172:A:MET:HE1	19	0.11
(1,2409)	1:172:A:MET:HA	1:172:A:MET:HE2	4	0.11
(1,2219)	1:161:A:TRP:HA	1:172:A:MET:HG2	7	0.11
(1,2084)	1:155:A:LYS:HA	1:162:A:SER:HG	17	0.11
(1,2026)	1:152:A:ILE:HA	1:163:A:ALA:HB1	9	0.11
(1,2017)	1:152:A:ILE:H	1:163:A:ALA:HB1	10	0.11
(1,2017)	1:152:A:ILE:H	1:163:A:ALA:HB1	12	0.11
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD11	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD12	7	0.11
(1,1960)	1:150:A:LEU:HA	1:150:A:LEU:HD13	7	0.11
(1,1944)	1:149:A:ILE:HA	1:149:A:ILE:HD12	18	0.11
(1,1918)	1:146:A:LYS:H	1:147:A:GLY:H	9	0.11
(1,1840)	1:142:A:LEU:HD11	1:143:A:PRO:HD2	12	0.11
(1,1840)	1:142:A:LEU:HD12	1:143:A:PRO:HD2	12	0.11
(1,1840)	1:142:A:LEU:HD13	1:143:A:PRO:HD2	12	0.11
(1,1840)	1:142:A:LEU:HD21	1:143:A:PRO:HD2	12	0.11
(1,1840)	1:142:A:LEU:HD22	1:143:A:PRO:HD2	12	0.11
(1,1840)	1:142:A:LEU:HD23	1:143:A:PRO:HD2	12	0.11
(1,1812)	1:142:A:LEU:HA	1:143:A:PRO:HD2	12	0.11
(1,1812)	1:142:A:LEU:HA	1:143:A:PRO:HD2	17	0.11
(1,1735)	1:137:A:ASN:H	1:142:A:LEU:HA	17	0.11
(1,1466)	1:127:A:TYR:HE1	1:151:A:VAL:HA	9	0.11
(1,1437)	1:127:A:TYR:H	1:180:A:LYS:HA	5	0.11
(1,1421)	1:125:A:LEU:HA	1:152:A:ILE:HB	18	0.11
(1,1395)	1:120:A:THR:H	1:120:A:THR:HB	5	0.11
(1,1395)	1:120:A:THR:H	1:120:A:THR:HB	7	0.11
(1,1395)	1:120:A:THR:H	1:120:A:THR:HB	8	0.11
(1,1324)	1:96:A:THR:HG1	1:99:A:ILE:HD13	11	0.11
(1,1200)	1:87:A:PHE:HZ	1:91:A:HIS:HE1	16	0.11
(1,1081)	1:78:A:PHE:HZ	1:88:A:TYR:HH	18	0.11
(1,1074)	1:78:A:PHE:HE1	1:84:A:LEU:HA	6	0.11
(1,979)	1:68:A:ASN:HA	1:70:A:ARG:H	6	0.11
(1,935)	1:65:A:SER:HG	1:67:A:PRO:HA	4	0.11
(1,935)	1:65:A:SER:HG	1:67:A:PRO:HA	16	0.11
(1,817)	1:58:A:VAL:H	1:60:A:HIS:HD2	6	0.11
(1,805)	1:54:A:GLU:HA	1:57:A:ARG:H	12	0.11
(1,776)	1:52:A:VAL:HB	1:61:A:TYR:H	19	0.11
(1,775)	1:52:A:VAL:HB	1:60:A:HIS:HA	14	0.11
(1,699)	1:49:A:VAL:HG21	1:62:A:ILE:HG12	7	0.11
(1,699)	1:49:A:VAL:HG22	1:62:A:ILE:HG12	7	0.11
(1,699)	1:49:A:VAL:HG23	1:62:A:ILE:HG12	7	0.11
(1,458)	1:33:A:HIS:HE2	1:56:A:SER:HA	2	0.11
(1,456)	1:33:A:HIS:HE2	1:55:A:ASN:H	4	0.11
(1,449)	1:33:A:HIS:HD2	1:56:A:SER:HA	12	0.11
(1,413)	1:30:A:GLY:HA2	1:56:A:SER:HA	5	0.11
(1,368)	1:26:A:THR:HG21	1:27:A:ARG:H	11	0.11
(1,291)	1:21:A:ARG:HH12	1:51:A:SER:HG	12	0.11
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	14	0.11
(1,20)	1:62:A:ILE:HG12	1:207:A:PTR:HB2	15	0.11
(1,20)	1:62:A:ILE:HG12	1:207:A:PTR:HB3	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:62:A:ILE:HG13	1:207:A:PTR:HB2	15	0.11
(1,20)	1:62:A:ILE:HG13	1:207:A:PTR:HB3	15	0.11
(1,3380)	1:280:A:ASN:H	1:280:A:ASN:HD21	7	0.1
(1,3286)	1:273:A:GLY:H	1:275:A:TRP:HD1	8	0.1
(1,2910)	1:247:A:VAL:HA	1:257:A:ALA:HB2	3	0.1
(1,2901)	1:247:A:VAL:H	1:247:A:VAL:HG21	12	0.1
(1,2877)	1:246:A:ARG:H	1:259:A:GLU:HA	16	0.1
(1,2642)	1:226:A:ALA:HA	1:227:A:ILE:H	16	0.1
(1,2633)	1:211:A:GLN:HB2	1:212:A:THR:HA	9	0.1
(1,2626)	1:202:A:GLU:HA	1:203:A:PRO:HD2	17	0.1
(1,2626)	1:202:A:GLU:HA	1:203:A:PRO:HD3	17	0.1
(1,2600)	1:187:A:HIS:H	1:187:A:HIS:HB2	8	0.1
(1,2416)	1:172:A:MET:HB2	1:173:A:ILE:HA	11	0.1
(1,2413)	1:172:A:MET:HB2	1:172:A:MET:HE1	3	0.1
(1,2409)	1:172:A:MET:HA	1:172:A:MET:HE2	16	0.1
(1,2361)	1:167:A:ASP:H	1:167:A:ASP:HB2	11	0.1
(1,2181)	1:160:A:TRP:HA	1:172:A:MET:HE2	5	0.1
(1,1631)	1:132:A:TYR:HA	1:132:A:TYR:HD1	12	0.1
(1,1542)	1:129:A:ARG:HA	1:178:A:VAL:HB	2	0.1
(1,1502)	1:128:A:VAL:HB	1:163:A:ALA:HB1	1	0.1
(1,1462)	1:127:A:TYR:HD1	1:150:A:LEU:H	14	0.1
(1,1446)	1:127:A:TYR:HA	1:150:A:LEU:HB2	3	0.1
(1,1437)	1:127:A:TYR:H	1:180:A:LYS:HA	8	0.1
(1,776)	1:52:A:VAL:HB	1:61:A:TYR:H	11	0.1
(1,273)	1:21:A:ARG:HA	1:39:A:ARG:HH21	2	0.1
(1,193)	1:16:A:MET:H	1:19:A:VAL:HB	8	0.1
(1,74)	1:8:A:SER:HG	1:86:A:GLU:H	3	0.1

10 Dihedral-angle violation analysis [i](#)

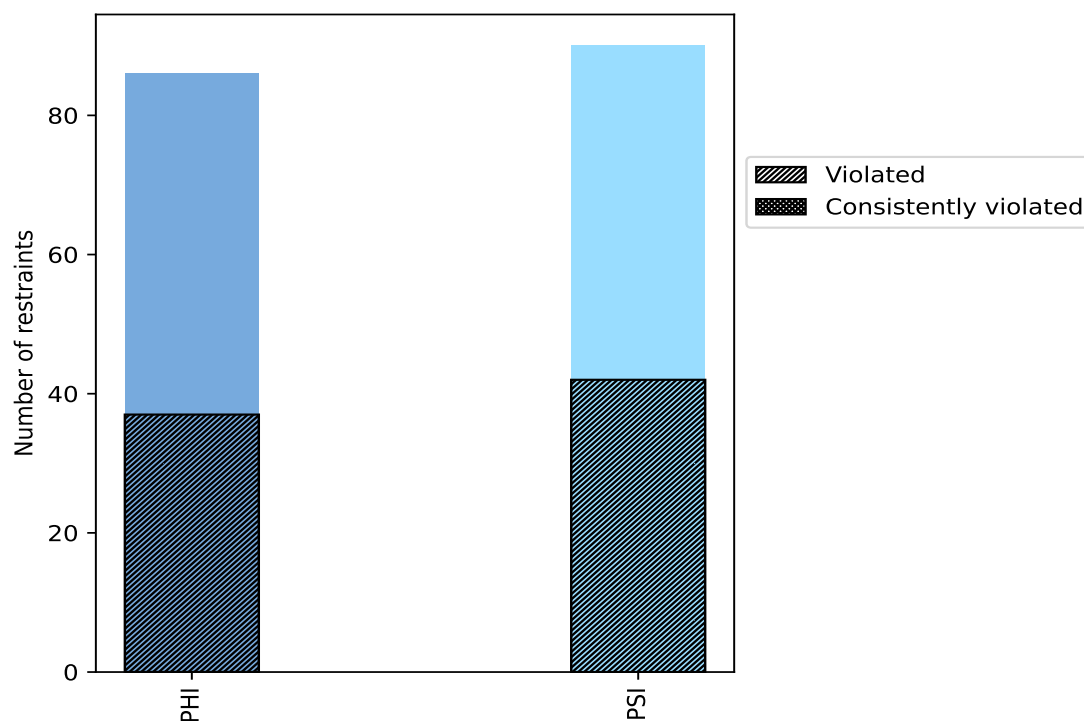
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	86	48.9	37	43.0	21.0	0	0.0	0.0
PSI	90	51.1	42	46.7	23.9	0	0.0	0.0
Total	176	100.0	79	44.9	44.9	0	0.0	0.0

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](#)



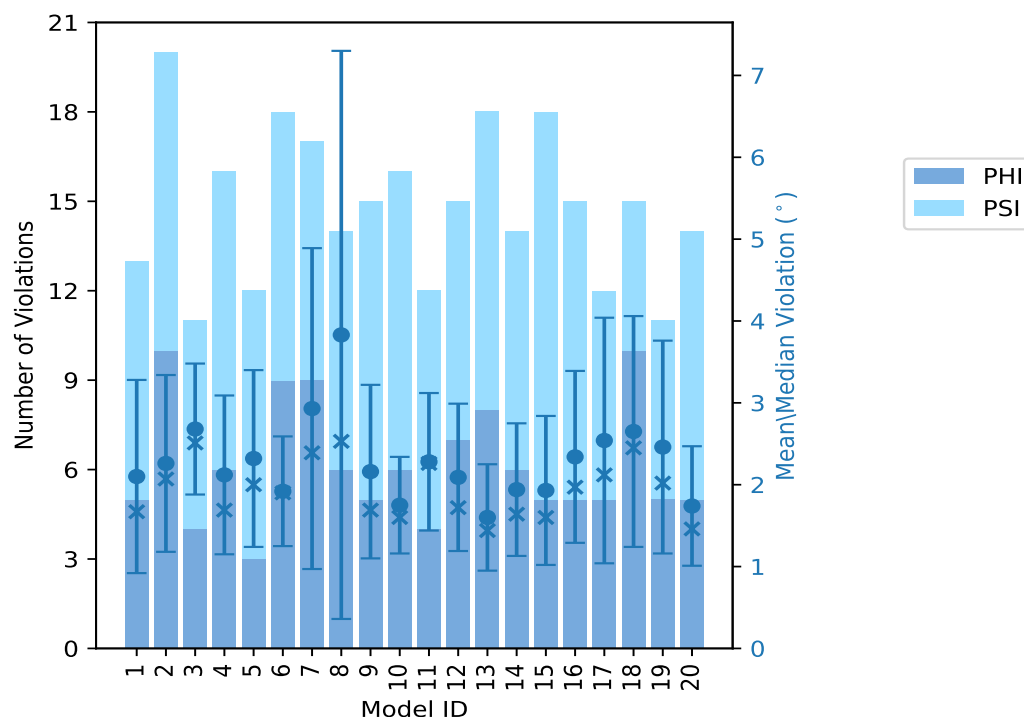
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	5	8	13	2.1	4.95	1.18	1.67
2	10	10	20	2.26	5.39	1.08	2.07
3	4	7	11	2.68	3.73	0.8	2.51
4	6	10	16	2.12	3.95	0.97	1.69
5	3	9	12	2.32	4.61	1.08	2.0
6	9	9	18	1.92	3.42	0.67	1.9
7	9	8	17	2.93	9.34	1.96	2.39
8	6	8	14	3.83	13.03	3.47	2.53
9	5	10	15	2.16	4.16	1.06	1.69
10	6	10	16	1.75	3.47	0.59	1.6
11	4	8	12	2.28	4.24	0.84	2.26
12	7	8	15	2.09	4.11	0.9	1.72
13	8	10	18	1.6	3.93	0.65	1.44
14	6	8	14	1.94	4.14	0.81	1.64
15	5	13	18	1.93	4.63	0.91	1.6
16	5	10	15	2.34	5.24	1.05	1.97
17	5	7	12	2.54	6.26	1.5	2.12
18	10	5	15	2.65	6.21	1.41	2.45
19	5	6	11	2.46	5.14	1.3	2.02
20	5	9	14	1.74	3.64	0.73	1.46

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
19	13	32	1	5.0
4	7	11	2	10.0
3	8	11	3	15.0
2	2	4	4	20.0
2	1	3	5	25.0
2	1	3	6	30.0
1	4	5	7	35.0
0	1	1	8	40.0
2	0	2	9	45.0
0	1	1	10	50.0
0	1	1	11	55.0

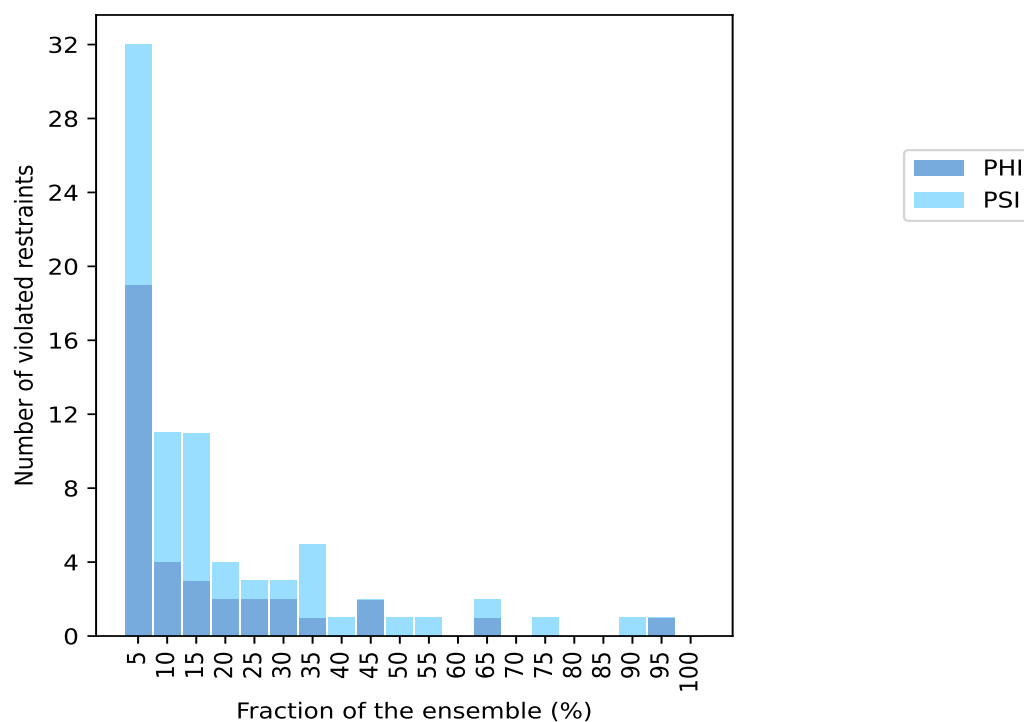
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
1	1	2	13	65.0
0	0	0	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
1	0	1	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

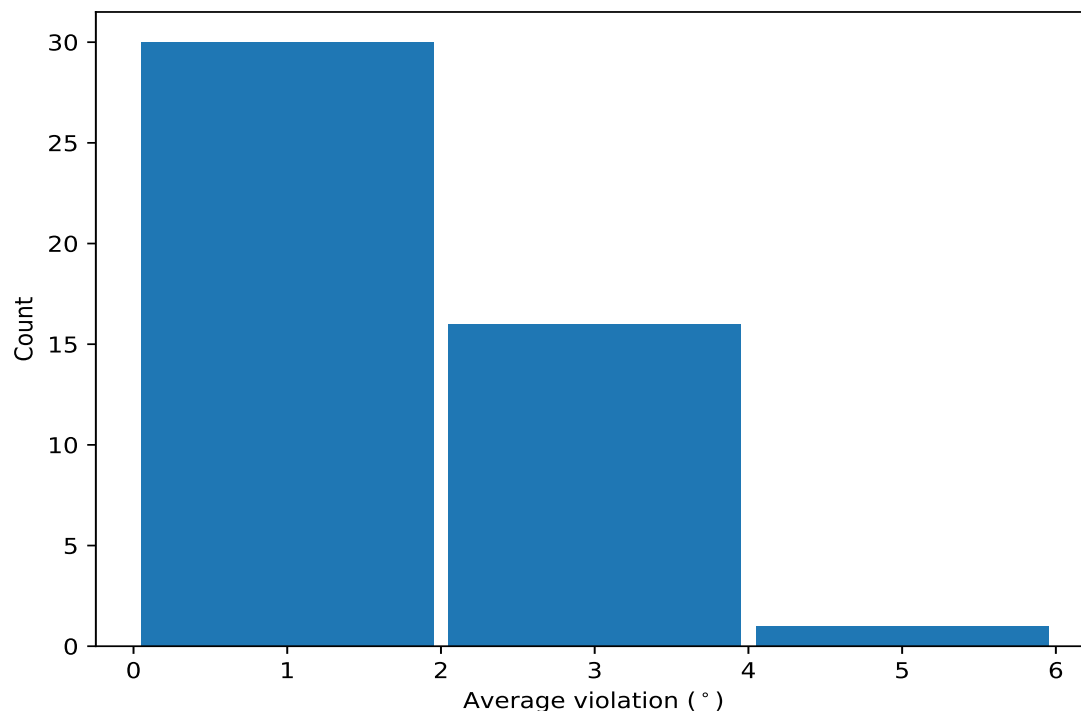


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	19	2.43	0.44	2.46
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	18	2.94	1.03	2.8
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	15	3.5	1.33	3.9
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	13	2.55	0.91	2.39
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	13	1.96	0.49	2.02
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	11	3.12	0.92	3.47
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	10	3.73	1.8	3.51
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	9	1.72	0.32	1.69
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	9	1.37	0.35	1.2
(1,87)	1:87:A:PHE:N	1:87:A:PHE:CA	1:87:A:PHE:C	1:88:A:TYR:N	8	1.52	0.28	1.52
(1,106)	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	1:154:A:GLU:N	7	2.09	0.95	1.8
(1,101)	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1:151:A:VAL:N	7	1.98	0.43	1.9
(1,20)	1:23:A:GLU:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	7	1.84	0.37	1.91
(1,69)	1:71:A:PHE:N	1:71:A:PHE:CA	1:71:A:PHE:C	1:72:A:LYS:N	7	1.45	0.32	1.3
(1,162)	1:278:A:GLU:N	1:278:A:GLU:CA	1:278:A:GLU:C	1:279:A:VAL:N	7	1.36	0.26	1.51
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ILE:N	6	1.85	0.71	1.8
(1,59)	1:61:A:TYR:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	6	1.59	0.4	1.64
(1,171)	1:290:A:HIS:C	1:291:A:VAL:N	1:291:A:VAL:CA	1:291:A:VAL:C	6	1.56	0.53	1.32
(1,93)	1:128:A:VAL:C	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	5	2.48	1.27	1.91
(1,73)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:GLY:N	5	1.89	0.91	1.37

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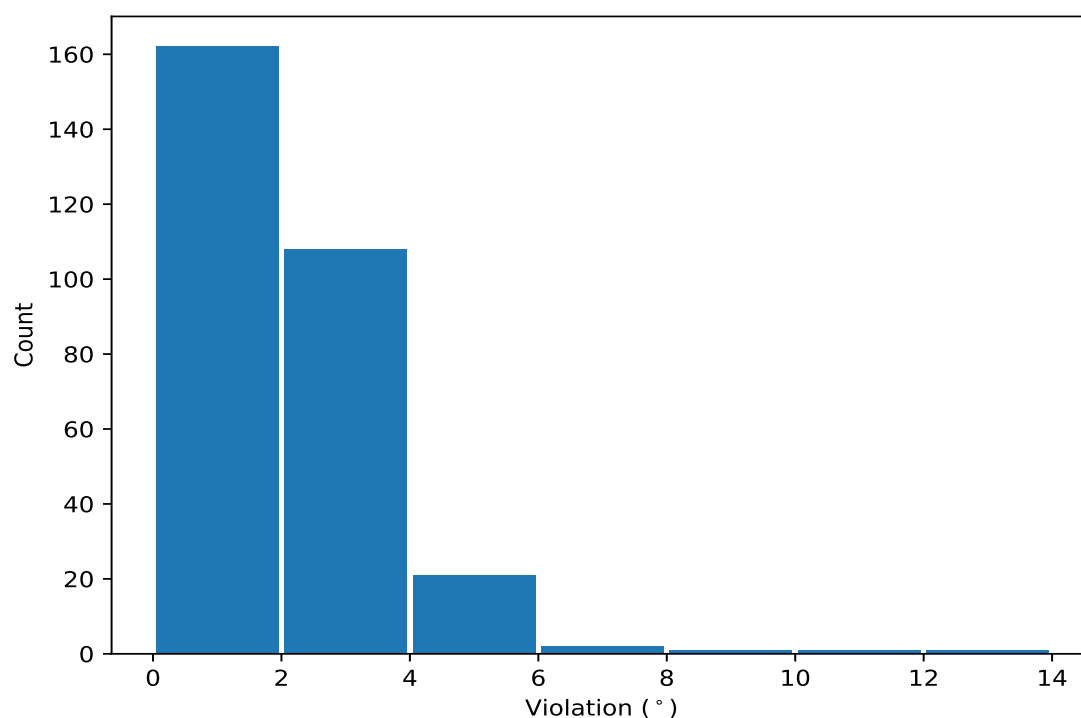
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,55)	1:59:A:SER:C	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	5	1.69	0.57	1.45
(1,133)	1:238:A:VAL:C	1:239:A:PHE:N	1:239:A:PHE:CA	1:239:A:PHE:C	4	4.98	2.87	4.54
(1,155)	1:274:A:GLN:C	1:275:A:TRP:N	1:275:A:TRP:CA	1:275:A:TRP:C	4	3.47	3.94	1.26
(1,90)	1:127:A:TYR:N	1:127:A:TYR:CA	1:127:A:TYR:C	1:128:A:VAL:N	4	1.7	0.26	1.71
(1,7)	1:14:A:TRP:N	1:14:A:TRP:CA	1:14:A:TRP:C	1:15:A:TYR:N	4	1.27	0.2	1.23
(1,151)	1:267:A:THR:C	1:268:A:ARG:N	1:268:A:ARG:CA	1:268:A:ARG:C	3	3.22	1.42	4.08
(1,53)	1:58:A:VAL:C	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	3	3.13	0.98	3.7
(1,67)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:PRO:N	3	3.04	0.2	3.15
(1,38)	1:40:A:ASP:N	1:40:A:ASP:CA	1:40:A:ASP:C	1:41:A:SER:N	3	2.39	1.57	1.37
(1,147)	1:265:A:LYS:C	1:266:A:VAL:N	1:266:A:VAL:CA	1:266:A:VAL:C	3	2.2	0.53	1.99
(1,103)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:ILE:N	3	1.96	0.24	1.82
(1,15)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:GLN:N	3	1.92	0.5	2.27
(1,164)	1:283:A:LYS:N	1:283:A:LYS:CA	1:283:A:LYS:C	1:284:A:GLY:N	3	1.78	0.57	1.86
(1,50)	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	1:54:A:GLU:N	3	1.6	0.39	1.49
(1,96)	1:130:A:THR:N	1:130:A:THR:CA	1:130:A:THR:C	1:131:A:LEU:N	3	1.48	0.13	1.48
(1,138)	1:241:A:LYS:N	1:241:A:LYS:CA	1:241:A:LYS:C	1:242:A:ALA:N	3	1.29	0.24	1.12
(1,23)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:THR:N	2	2.95	0.61	2.95
(1,136)	1:240:A:ALA:N	1:240:A:ALA:CA	1:240:A:ALA:C	1:241:A:LYS:N	2	2.35	0.36	2.35
(1,153)	1:268:A:ARG:C	1:269:A:MET:N	1:269:A:MET:CA	1:269:A:MET:C	2	1.92	0.87	1.92
(1,119)	1:169:A:ARG:C	1:170:A:VAL:N	1:170:A:VAL:CA	1:170:A:VAL:C	2	1.85	0.43	1.85
(1,16)	1:21:A:ARG:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	2	1.72	0.53	1.72
(1,109)	1:159:A:GLN:C	1:160:A:TRP:N	1:160:A:TRP:CA	1:160:A:TRP:C	2	1.71	0.71	1.71
(1,154)	1:269:A:MET:N	1:269:A:MET:CA	1:269:A:MET:C	1:270:A:ASN:N	2	1.5	0.15	1.5
(1,77)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ALA:N	2	1.43	0.29	1.43
(1,89)	1:88:A:TYR:N	1:88:A:TYR:CA	1:88:A:TYR:C	1:89:A:LYS:N	2	1.33	0.06	1.33
(1,104)	1:152:A:ILE:N	1:152:A:ILE:CA	1:152:A:ILE:C	1:153:A:ILE:N	2	1.25	0.07	1.25
(1,110)	1:160:A:TRP:N	1:160:A:TRP:CA	1:160:A:TRP:C	1:161:A:TRP:N	2	1.02	0.01	1.02

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



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

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,156)	1:275:A:TRP:N	1:275:A:TRP:CA	1:275:A:TRP:C	1:276:A:GLU:N	8	13.03
(1,155)	1:274:A:GLN:C	1:275:A:TRP:N	1:275:A:TRP:CA	1:275:A:TRP:C	8	10.29
(1,133)	1:238:A:VAL:C	1:239:A:PHE:N	1:239:A:PHE:CA	1:239:A:PHE:C	7	9.34
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	17	6.26
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	18	6.21
(1,133)	1:238:A:VAL:C	1:239:A:PHE:N	1:239:A:PHE:CA	1:239:A:PHE:C	2	5.39
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	16	5.24
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	8	5.16
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	19	5.14
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	18	4.96
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	1	4.95
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	17	4.9
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	7	4.67
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	15	4.63
(1,38)	1:40:A:ASP:N	1:40:A:ASP:CA	1:40:A:ASP:C	1:41:A:SER:N	5	4.61
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	8	4.43
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	19	4.38
(1,151)	1:267:A:THR:C	1:268:A:ARG:N	1:268:A:ARG:CA	1:268:A:ARG:C	7	4.35
(1,106)	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	1:154:A:GLU:N	11	4.24
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	16	4.2
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	9	4.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	14	4.14
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	12	4.11
(1,151)	1:267:A:THR:C	1:268:A:ARG:N	1:268:A:ARG:CA	1:268:A:ARG:C	2	4.08
(1,93)	1:128:A:VAL:C	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	7	4.0
(1,93)	1:128:A:VAL:C	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	8	4.0
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	4	3.95
(1,53)	1:58:A:VAL:C	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	13	3.93
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	12	3.9
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	1	3.84
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	9	3.77
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	5	3.75
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	3	3.73
(1,53)	1:58:A:VAL:C	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	15	3.7
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	4	3.7
(1,133)	1:238:A:VAL:C	1:239:A:PHE:N	1:239:A:PHE:CA	1:239:A:PHE:C	18	3.69
(1,73)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:GLY:N	20	3.64
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	5	3.6
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	3	3.59
(1,149)	1:266:A:VAL:C	1:267:A:THR:N	1:267:A:THR:CA	1:267:A:THR:C	7	3.57
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	4	3.57
(1,23)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:THR:N	9	3.56
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	19	3.53
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	3	3.52
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	10	3.47
(1,144)	1:264:A:VAL:N	1:264:A:VAL:CA	1:264:A:VAL:C	1:265:A:LYS:N	7	3.45
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	3	3.44
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	2	3.44
(1,97)	1:147:A:GLY:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	6	3.42
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	16	3.37
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	7	3.29
(1,24)	1:25:A:GLN:C	1:26:A:THR:N	1:26:A:THR:CA	1:26:A:THR:C	18	3.26
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	9	3.24
(1,67)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:PRO:N	17	3.21
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	8	3.17
(1,67)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:PRO:N	1	3.15
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	12	3.11
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	9	3.07
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	18	3.07
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	2	3.01
(1,26)	1:26:A:THR:C	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	18	2.99
(1,147)	1:265:A:LYS:C	1:266:A:VAL:N	1:266:A:VAL:CA	1:266:A:VAL:C	3	2.93
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	4	2.9
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ILE:N	11	2.86
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	4	2.85
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	14	2.82
(1,153)	1:268:A:ARG:C	1:269:A:MET:N	1:269:A:MET:CA	1:269:A:MET:C	2	2.8
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	11	2.8
(1,67)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:PRO:N	6	2.76
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	20	2.76
(1,101)	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1:151:A:VAL:N	4	2.75
(1,136)	1:240:A:ALA:N	1:240:A:ALA:CA	1:240:A:ALA:C	1:241:A:LYS:N	2	2.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	11	2.7
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	1	2.7
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	11	2.7
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	5	2.67
(1,55)	1:59:A:SER:C	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	19	2.66
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	14	2.66
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	6	2.65
(1,152)	1:268:A:ARG:N	1:268:A:ARG:CA	1:268:A:ARG:C	1:269:A:MET:N	8	2.62
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	11	2.62
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	2	2.6
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	6	2.57
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	3	2.51
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	18	2.51
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	7	2.49
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	17	2.48
(1,171)	1:290:A:HIS:C	1:291:A:VAL:N	1:291:A:VAL:CA	1:291:A:VAL:C	12	2.47
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	6	2.46
(1,20)	1:23:A:GLU:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	18	2.45
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	3	2.44
(1,164)	1:283:A:LYS:N	1:283:A:LYS:CA	1:283:A:LYS:C	1:284:A:GLY:N	8	2.43
(1,113)	1:161:A:TRP:C	1:162:A:SER:N	1:162:A:SER:CA	1:162:A:SER:C	2	2.43
(1,109)	1:159:A:GLN:C	1:160:A:TRP:N	1:160:A:TRP:CA	1:160:A:TRP:C	15	2.42
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ILE:N	8	2.41
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	19	2.41
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	10	2.4
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	7	2.39
(1,101)	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1:151:A:VAL:N	5	2.36
(1,65)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:LEU:N	15	2.36
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ILE:N	9	2.35
(1,23)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:THR:N	16	2.34
(1,57)	1:60:A:HIS:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	17	2.33
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	6	2.33
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	3	2.31
(1,103)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:ILE:N	20	2.3
(1,15)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:GLN:N	15	2.29
(1,119)	1:169:A:ARG:C	1:170:A:VAL:N	1:170:A:VAL:CA	1:170:A:VAL:C	6	2.28
(1,15)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:GLN:N	14	2.27
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	7	2.26
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	17	2.25
(1,16)	1:21:A:ARG:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	12	2.25
(1,106)	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	1:154:A:GLU:N	10	2.22
(1,106)	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	1:154:A:GLU:N	2	2.18
(1,20)	1:23:A:GLU:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	20	2.14
(1,50)	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	1:54:A:GLU:N	14	2.13
(1,59)	1:61:A:TYR:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	1	2.1
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	2	2.09
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	5	2.08
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	12	2.06
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	6	2.05
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	2	2.05
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	13	2.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,171)	1:290:A:HIS:C	1:291:A:VAL:N	1:291:A:VAL:CA	1:291:A:VAL:C	6	2.04
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	14	2.04
(1,5)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:TRP:N	3	2.03
(1,87)	1:87:A:PHE:N	1:87:A:PHE:CA	1:87:A:PHE:C	1:88:A:TYR:N	16	2.02
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	19	2.02
(1,69)	1:71:A:PHE:N	1:71:A:PHE:CA	1:71:A:PHE:C	1:72:A:LYS:N	15	2.02
(1,56)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:TYR:N	13	2.02
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	16	2.02
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	16	2.02
(1,20)	1:23:A:GLU:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	10	2.01
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	19	2.0
(1,147)	1:265:A:LYS:C	1:266:A:VAL:N	1:266:A:VAL:CA	1:266:A:VAL:C	18	1.99
(1,136)	1:240:A:ALA:N	1:240:A:ALA:CA	1:240:A:ALA:C	1:241:A:LYS:N	18	1.99
(1,101)	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1:151:A:VAL:N	17	1.98
(1,90)	1:127:A:TYR:N	1:127:A:TYR:CA	1:127:A:TYR:C	1:128:A:VAL:N	16	1.97
(1,59)	1:61:A:TYR:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	2	1.97
(1,55)	1:59:A:SER:C	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	16	1.96
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	16	1.96
(1,90)	1:127:A:TYR:N	1:127:A:TYR:CA	1:127:A:TYR:C	1:128:A:VAL:N	15	1.94
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	15	1.94
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	4	1.93
(1,93)	1:128:A:VAL:C	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	10	1.91
(1,73)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:GLY:N	3	1.91
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	11	1.91
(1,20)	1:23:A:GLU:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	5	1.91
(1,101)	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1:151:A:VAL:N	12	1.9
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	10	1.9
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	20	1.88
(1,164)	1:283:A:LYS:N	1:283:A:LYS:CA	1:283:A:LYS:C	1:284:A:GLY:N	20	1.86
(1,114)	1:162:A:SER:N	1:162:A:SER:CA	1:162:A:SER:C	1:163:A:ALA:N	11	1.86
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	11	1.86
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	17	1.86
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	10	1.84
(1,103)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:ILE:N	15	1.82
(1,87)	1:87:A:PHE:N	1:87:A:PHE:CA	1:87:A:PHE:C	1:88:A:TYR:N	14	1.82
(1,106)	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	1:154:A:GLU:N	4	1.8
(1,101)	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1:151:A:VAL:N	9	1.8
(1,101)	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1:151:A:VAL:N	16	1.8
(1,59)	1:61:A:TYR:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	18	1.79
(1,103)	1:151:A:VAL:N	1:151:A:VAL:CA	1:151:A:VAL:C	1:152:A:ILE:N	13	1.77
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	13	1.76
(1,53)	1:58:A:VAL:C	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	6	1.75
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	16	1.75
(1,77)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ALA:N	12	1.72
(1,69)	1:71:A:PHE:N	1:71:A:PHE:CA	1:71:A:PHE:C	1:72:A:LYS:N	1	1.72
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	13	1.72
(1,147)	1:265:A:LYS:C	1:266:A:VAL:N	1:266:A:VAL:CA	1:266:A:VAL:C	9	1.69
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	18	1.69
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	1	1.67
(1,6)	1:13:A:ALA:C	1:14:A:TRP:N	1:14:A:TRP:CA	1:14:A:TRP:C	13	1.67
(1,154)	1:269:A:MET:N	1:269:A:MET:CA	1:269:A:MET:C	1:270:A:ASN:N	7	1.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	7	1.66
(1,12)	1:16:A:MET:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	12	1.66
(1,162)	1:278:A:GLU:N	1:278:A:GLU:CA	1:278:A:GLU:C	1:279:A:VAL:N	5	1.65
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	2	1.65
(1,96)	1:130:A:THR:N	1:130:A:THR:CA	1:130:A:THR:C	1:131:A:LEU:N	10	1.64
(1,87)	1:87:A:PHE:N	1:87:A:PHE:CA	1:87:A:PHE:C	1:88:A:TYR:N	7	1.64
(1,162)	1:278:A:GLU:N	1:278:A:GLU:CA	1:278:A:GLU:C	1:279:A:VAL:N	6	1.63
(1,106)	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	1:154:A:GLU:N	5	1.63
(1,138)	1:241:A:LYS:N	1:241:A:LYS:CA	1:241:A:LYS:C	1:242:A:ALA:N	13	1.62
(1,69)	1:71:A:PHE:N	1:71:A:PHE:CA	1:71:A:PHE:C	1:72:A:LYS:N	6	1.61
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	12	1.6
(1,159)	1:276:A:GLU:C	1:277:A:GLY:N	1:277:A:GLY:CA	1:277:A:GLY:C	2	1.59
(1,8)	1:14:A:TRP:C	1:15:A:TYR:N	1:15:A:TYR:CA	1:15:A:TYR:C	4	1.58
(1,7)	1:14:A:TRP:N	1:14:A:TRP:CA	1:14:A:TRP:C	1:15:A:TYR:N	10	1.57
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	4	1.56
(1,20)	1:23:A:GLU:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	8	1.55
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	10	1.53
(1,171)	1:290:A:HIS:C	1:291:A:VAL:N	1:291:A:VAL:CA	1:291:A:VAL:C	20	1.52
(1,162)	1:278:A:GLU:N	1:278:A:GLU:CA	1:278:A:GLU:C	1:279:A:VAL:N	13	1.52
(1,87)	1:87:A:PHE:N	1:87:A:PHE:CA	1:87:A:PHE:C	1:88:A:TYR:N	10	1.52
(1,20)	1:23:A:GLU:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	17	1.52
(1,162)	1:278:A:GLU:N	1:278:A:GLU:CA	1:278:A:GLU:C	1:279:A:VAL:N	16	1.51
(1,133)	1:238:A:VAL:C	1:239:A:PHE:N	1:239:A:PHE:CA	1:239:A:PHE:C	4	1.51
(1,87)	1:87:A:PHE:N	1:87:A:PHE:CA	1:87:A:PHE:C	1:88:A:TYR:N	12	1.51
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	9	1.5
(1,59)	1:61:A:TYR:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	12	1.49
(1,50)	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	1:54:A:GLU:N	16	1.49
(1,96)	1:130:A:THR:N	1:130:A:THR:CA	1:130:A:THR:C	1:131:A:LEU:N	11	1.48
(1,90)	1:127:A:TYR:N	1:127:A:TYR:CA	1:127:A:TYR:C	1:128:A:VAL:N	9	1.48
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	10	1.47
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	1	1.46
(1,131)	1:178:A:VAL:C	1:179:A:GLU:N	1:179:A:GLU:CA	1:179:A:GLU:C	12	1.45
(1,55)	1:59:A:SER:C	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	14	1.45
(1,119)	1:169:A:ARG:C	1:170:A:VAL:N	1:170:A:VAL:CA	1:170:A:VAL:C	16	1.42
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	14	1.42
(1,146)	1:265:A:LYS:N	1:265:A:LYS:CA	1:265:A:LYS:C	1:266:A:VAL:N	2	1.4
(1,90)	1:127:A:TYR:N	1:127:A:TYR:CA	1:127:A:TYR:C	1:128:A:VAL:N	20	1.4
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	14	1.4
(1,106)	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	1:154:A:GLU:N	17	1.39
(1,89)	1:88:A:TYR:N	1:88:A:TYR:CA	1:88:A:TYR:C	1:89:A:LYS:N	19	1.39
(1,73)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:GLY:N	15	1.37
(1,38)	1:40:A:ASP:N	1:40:A:ASP:CA	1:40:A:ASP:C	1:41:A:SER:N	6	1.37
(1,154)	1:269:A:MET:N	1:269:A:MET:CA	1:269:A:MET:C	1:270:A:ASN:N	13	1.35
(1,93)	1:128:A:VAL:C	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	15	1.35
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	14	1.34
(1,70)	1:71:A:PHE:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	5	1.34
(1,96)	1:130:A:THR:N	1:130:A:THR:CA	1:130:A:THR:C	1:131:A:LEU:N	4	1.33
(1,55)	1:59:A:SER:C	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	13	1.33
(1,20)	1:23:A:GLU:C	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	13	1.33
(1,148)	1:266:A:VAL:N	1:266:A:VAL:CA	1:266:A:VAL:C	1:267:A:THR:N	15	1.32
(1,104)	1:152:A:ILE:N	1:152:A:ILE:CA	1:152:A:ILE:C	1:153:A:ILE:N	15	1.32

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	9	1.32
(1,163)	1:282:A:ARG:C	1:283:A:LYS:N	1:283:A:LYS:CA	1:283:A:LYS:C	2	1.31
(1,7)	1:14:A:TRP:N	1:14:A:TRP:CA	1:14:A:TRP:C	1:15:A:TYR:N	15	1.31
(1,155)	1:274:A:GLN:C	1:275:A:TRP:N	1:275:A:TRP:CA	1:275:A:TRP:C	7	1.3
(1,87)	1:87:A:PHE:N	1:87:A:PHE:CA	1:87:A:PHE:C	1:88:A:TYR:N	4	1.3
(1,69)	1:71:A:PHE:N	1:71:A:PHE:CA	1:71:A:PHE:C	1:72:A:LYS:N	7	1.3
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	1	1.3
(1,13)	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1:18:A:PRO:N	15	1.3
(1,73)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:GLY:N	14	1.29
(1,95)	1:129:A:ARG:C	1:130:A:THR:N	1:130:A:THR:CA	1:130:A:THR:C	7	1.28
(1,27)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:LEU:N	20	1.28
(1,108)	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1:155:A:LYS:N	19	1.27
(1,101)	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1:151:A:VAL:N	13	1.27
(1,89)	1:88:A:TYR:N	1:88:A:TYR:CA	1:88:A:TYR:C	1:89:A:LYS:N	15	1.27
(1,69)	1:71:A:PHE:N	1:71:A:PHE:CA	1:71:A:PHE:C	1:72:A:LYS:N	20	1.27
(1,51)	1:56:A:SER:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	14	1.27
(1,117)	1:163:A:ALA:C	1:164:A:ARG:N	1:164:A:ARG:CA	1:164:A:ARG:C	15	1.25
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ILE:N	10	1.25
(1,73)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:GLY:N	11	1.23
(1,155)	1:274:A:GLN:C	1:275:A:TRP:N	1:275:A:TRP:CA	1:275:A:TRP:C	6	1.22
(1,151)	1:267:A:THR:C	1:268:A:ARG:N	1:268:A:ARG:CA	1:268:A:ARG:C	8	1.22
(1,69)	1:71:A:PHE:N	1:71:A:PHE:CA	1:71:A:PHE:C	1:72:A:LYS:N	10	1.21
(1,15)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:GLN:N	2	1.21
(1,87)	1:87:A:PHE:N	1:87:A:PHE:CA	1:87:A:PHE:C	1:88:A:TYR:N	6	1.2
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	9	1.2
(1,38)	1:40:A:ASP:N	1:40:A:ASP:CA	1:40:A:ASP:C	1:41:A:SER:N	2	1.2
(1,162)	1:278:A:GLU:N	1:278:A:GLU:CA	1:278:A:GLU:C	1:279:A:VAL:N	19	1.19
(1,50)	1:53:A:SER:N	1:53:A:SER:CA	1:53:A:SER:C	1:54:A:GLU:N	17	1.19
(1,16)	1:21:A:ARG:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	9	1.19
(1,104)	1:152:A:ILE:N	1:152:A:ILE:CA	1:152:A:ILE:C	1:153:A:ILE:N	13	1.18
(1,129)	1:177:A:TYR:C	1:178:A:VAL:N	1:178:A:VAL:CA	1:178:A:VAL:C	13	1.17
(1,106)	1:153:A:ILE:N	1:153:A:ILE:CA	1:153:A:ILE:C	1:154:A:GLU:N	8	1.17
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	6	1.16
(1,7)	1:14:A:TRP:N	1:14:A:TRP:CA	1:14:A:TRP:C	1:15:A:TYR:N	20	1.16
(1,87)	1:87:A:PHE:N	1:87:A:PHE:CA	1:87:A:PHE:C	1:88:A:TYR:N	17	1.14
(1,77)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ALA:N	1	1.14
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ILE:N	12	1.13
(1,171)	1:290:A:HIS:C	1:291:A:VAL:N	1:291:A:VAL:CA	1:291:A:VAL:C	18	1.12
(1,138)	1:241:A:LYS:N	1:241:A:LYS:CA	1:241:A:LYS:C	1:242:A:ALA:N	4	1.12
(1,138)	1:241:A:LYS:N	1:241:A:LYS:CA	1:241:A:LYS:C	1:242:A:ALA:N	20	1.12
(1,93)	1:128:A:VAL:C	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	4	1.12
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:ILE:N	5	1.11
(1,171)	1:290:A:HIS:C	1:291:A:VAL:N	1:291:A:VAL:CA	1:291:A:VAL:C	7	1.1
(1,142)	1:263:A:ILE:N	1:263:A:ILE:CA	1:263:A:ILE:C	1:264:A:VAL:N	5	1.1
(1,59)	1:61:A:TYR:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	3	1.1
(1,54)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:HIS:N	1	1.1
(1,85)	1:86:A:GLU:N	1:86:A:GLU:CA	1:86:A:GLU:C	1:87:A:PHE:N	11	1.09
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	8	1.09
(1,10)	1:15:A:TYR:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1	1.09
(1,171)	1:290:A:HIS:C	1:291:A:VAL:N	1:291:A:VAL:CA	1:291:A:VAL:C	13	1.08
(1,132)	1:238:A:VAL:N	1:238:A:VAL:CA	1:238:A:VAL:C	1:239:A:PHE:N	9	1.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,68)	1:70:A:ARG:C	1:71:A:PHE:N	1:71:A:PHE:CA	1:71:A:PHE:C	19	1.08
(1,59)	1:61:A:TYR:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	14	1.08
(1,33)	1:37:A:LEU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	6	1.08
(1,19)	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	1:24:A:ALA:N	15	1.08
(1,169)	1:285:A:LEU:C	1:286:A:PHE:N	1:286:A:PHE:CA	1:286:A:PHE:C	2	1.07
(1,155)	1:274:A:GLN:C	1:275:A:TRP:N	1:275:A:TRP:CA	1:275:A:TRP:C	12	1.06
(1,55)	1:59:A:SER:C	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	18	1.06
(1,153)	1:268:A:ARG:C	1:269:A:MET:N	1:269:A:MET:CA	1:269:A:MET:C	1	1.05
(1,45)	1:50:A:LEU:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	20	1.05
(1,164)	1:283:A:LYS:N	1:283:A:LYS:CA	1:283:A:LYS:C	1:284:A:GLY:N	2	1.04
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	10	1.04
(1,7)	1:14:A:TRP:N	1:14:A:TRP:CA	1:14:A:TRP:C	1:15:A:TYR:N	13	1.04
(1,110)	1:160:A:TRP:N	1:160:A:TRP:CA	1:160:A:TRP:C	1:161:A:TRP:N	10	1.03
(1,78)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	20	1.03
(1,62)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:ASN:N	8	1.03
(1,162)	1:278:A:GLU:N	1:278:A:GLU:CA	1:278:A:GLU:C	1:279:A:VAL:N	9	1.02
(1,110)	1:160:A:TRP:N	1:160:A:TRP:CA	1:160:A:TRP:C	1:161:A:TRP:N	6	1.02
(1,69)	1:71:A:PHE:N	1:71:A:PHE:CA	1:71:A:PHE:C	1:72:A:LYS:N	4	1.02
(1,162)	1:278:A:GLU:N	1:278:A:GLU:CA	1:278:A:GLU:C	1:279:A:VAL:N	18	1.01
(1,109)	1:159:A:GLN:C	1:160:A:TRP:N	1:160:A:TRP:CA	1:160:A:TRP:C	13	1.0