



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 06:24 PM UTC

PDB ID : 2LP4 / pdb_00002lp4
BMRB ID : 18234
Title : Solution structure of P1-CheY/P2 complex in bacterial chemotaxis
Authors : Dahlquist, F.; Mo, G.; Zhou, H.; Kamamura, T.
Deposited on : 2012-01-31

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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
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

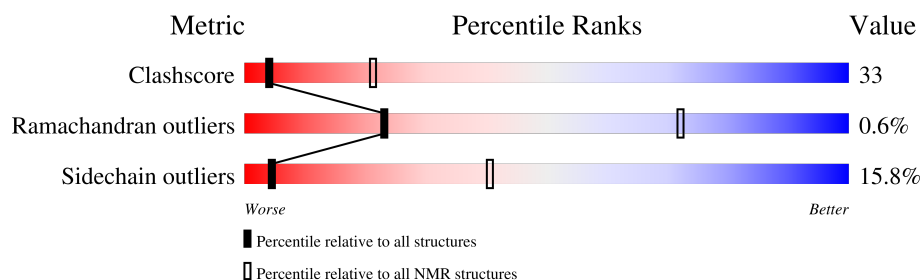
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 5%.

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	225	
2	Y	128	

2 Ensemble composition and analysis

This entry contains 25 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:7-A:132 (126)	0.07	7
2	A:160-A:225, Y:2-Y:129 (194)	0.00	2

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. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5367 atoms, of which 2669 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chemotaxis protein CheA.

Mol	Chain	Residues	Atoms						Trace
1	A	225	Total	C	H	N	O	S	0
			3439	1087	1695	284	365	8	

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ASP	VAL	SEE REMARK 999	UNP P07363
A	31	VAL	GLN	SEE REMARK 999	UNP P07363
A	34	SER	ALA	SEE REMARK 999	UNP P07363
A	60	THR	SER	SEE REMARK 999	UNP P07363
A	61	ILE	VAL	SEE REMARK 999	UNP P07363
A	107	ASN	GLN	SEE REMARK 999	UNP P07363
A	109	GLU	GLN	SEE REMARK 999	UNP P07363
A	117	GLU	ASP	SEE REMARK 999	UNP P07363
A	121	ASN	GLN	SEE REMARK 999	UNP P07363

- Molecule 2 is a protein called Chemotaxis protein CheY.

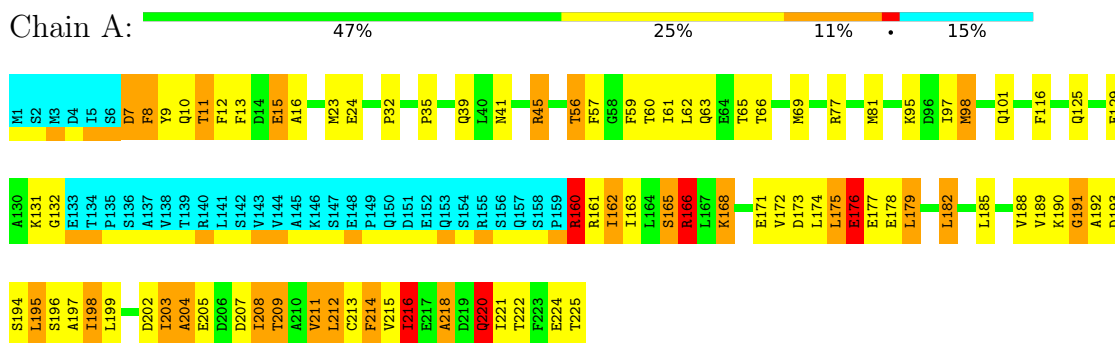
Mol	Chain	Residues	Atoms						Trace
2	Y	128	Total	C	H	N	O	S	0
			1928	612	974	154	182	6	

4 Residue-property plots

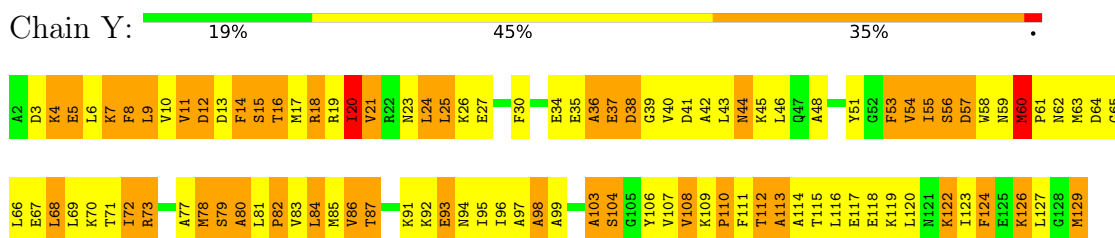
4.1 Average score per residue in the NMR ensemble

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: Chemotaxis protein CheA



• Molecule 2: Chemotaxis protein CheY



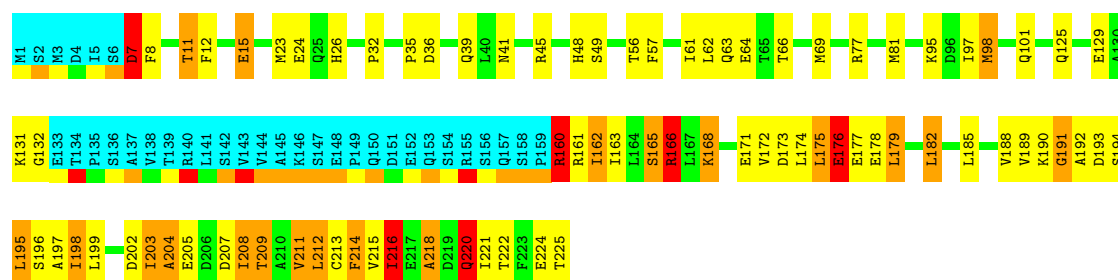
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

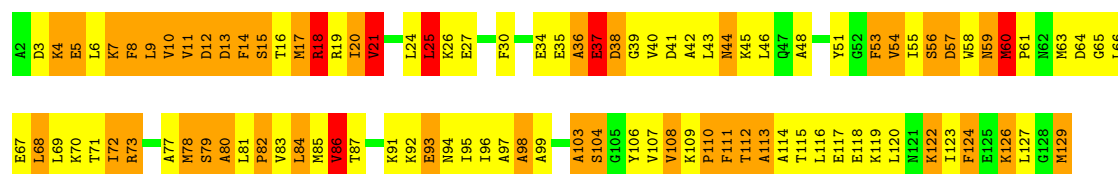
• Molecule 1: Chemotaxis protein CheA





• Molecule 2: Chemotaxis protein CheY

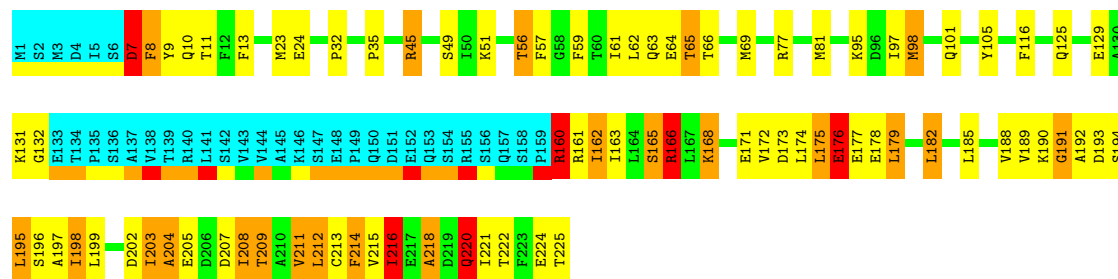
Chain Y: 20% 42% 33% 5%



4.2.2 Score per residue for model 2 (medoid)

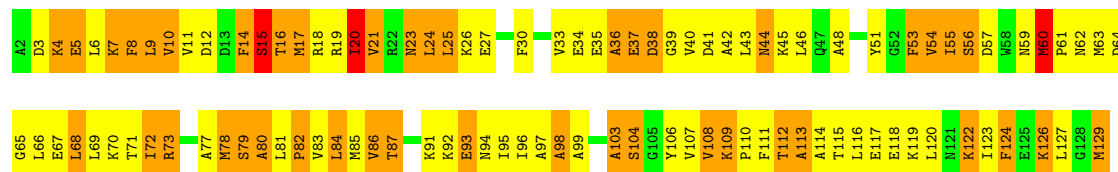
• Molecule 1: Chemotaxis protein CheA

Chain A: 48% 25% 10% 15%



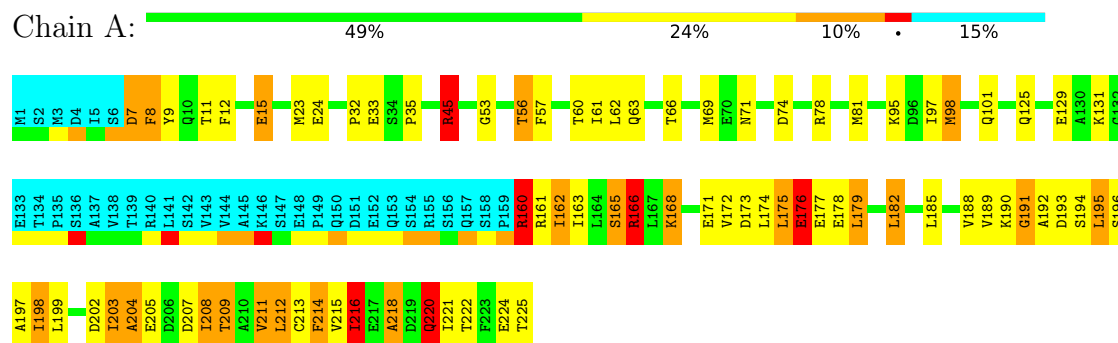
• Molecule 2: Chemotaxis protein CheY

Chain Y: 20% 45% 34%

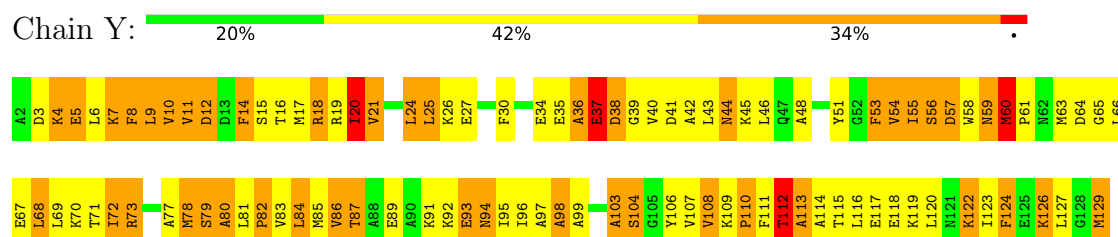


4.2.3 Score per residue for model 3

• Molecule 1: Chemotaxis protein CheA

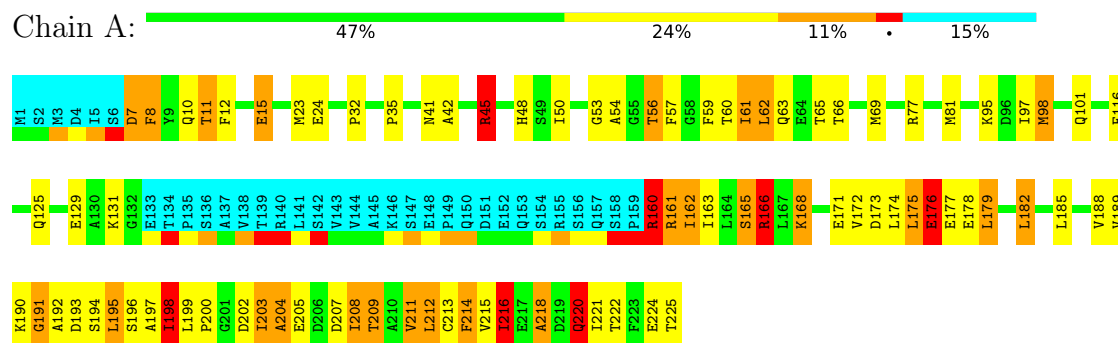


• Molecule 2: Chemotaxis protein CheY

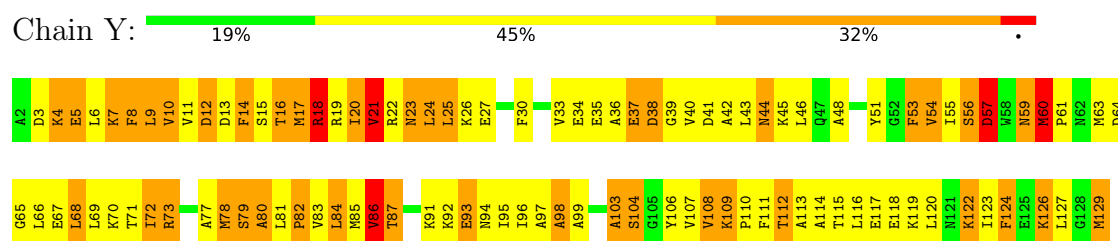


4.2.4 Score per residue for model 4

• Molecule 1: Chemotaxis protein CheA

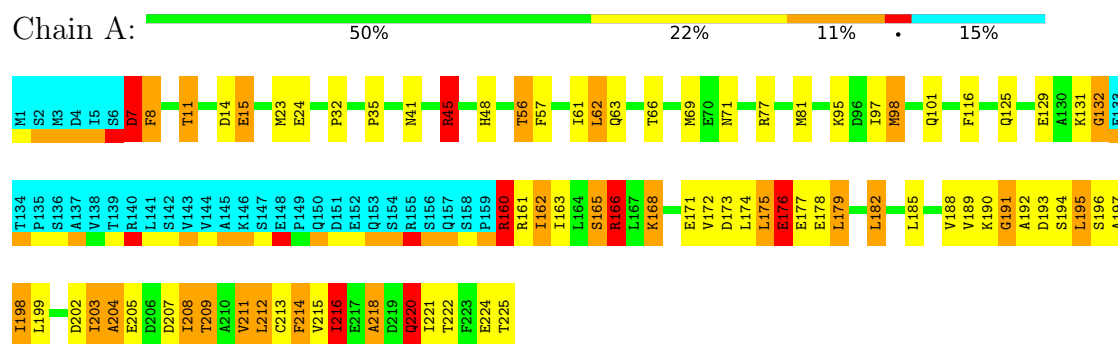


• Molecule 2: Chemotaxis protein CheY

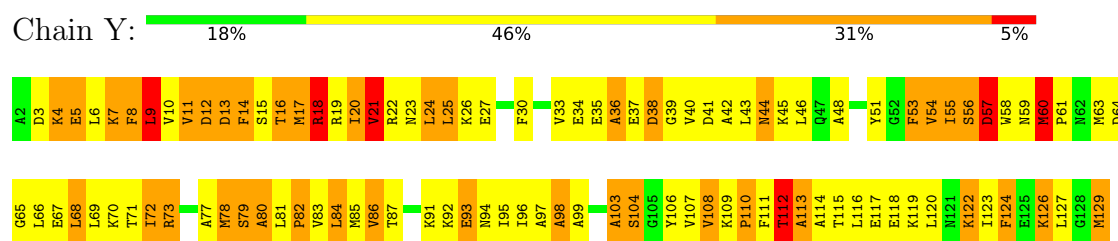


4.2.5 Score per residue for model 5

- Molecule 1: Chemotaxis protein CheA

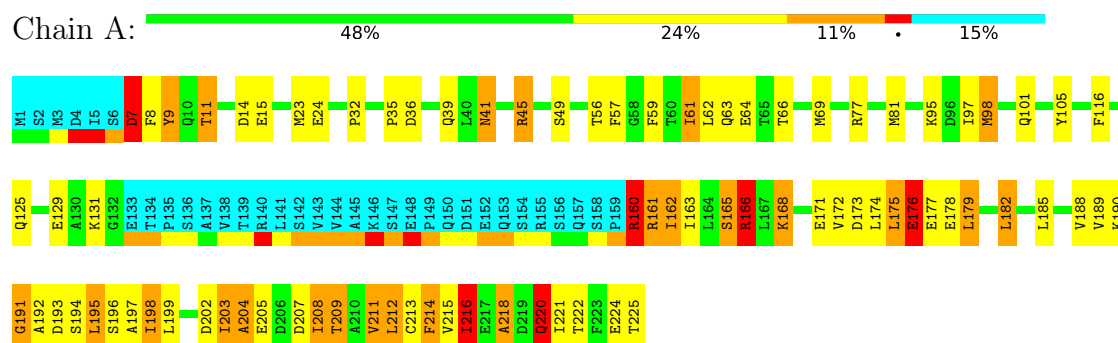


- Molecule 2: Chemotaxis protein CheY

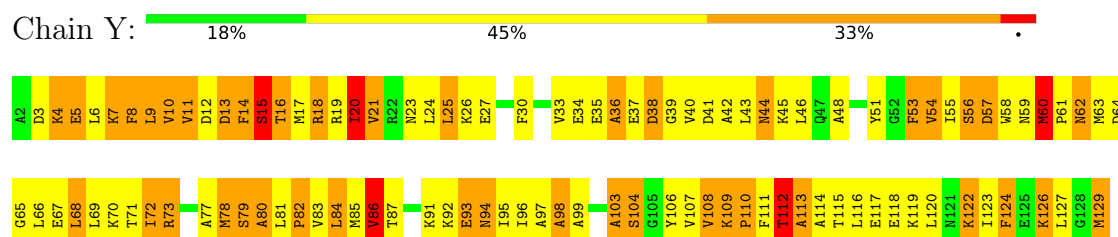


4.2.6 Score per residue for model 6

- Molecule 1: Chemotaxis protein CheA

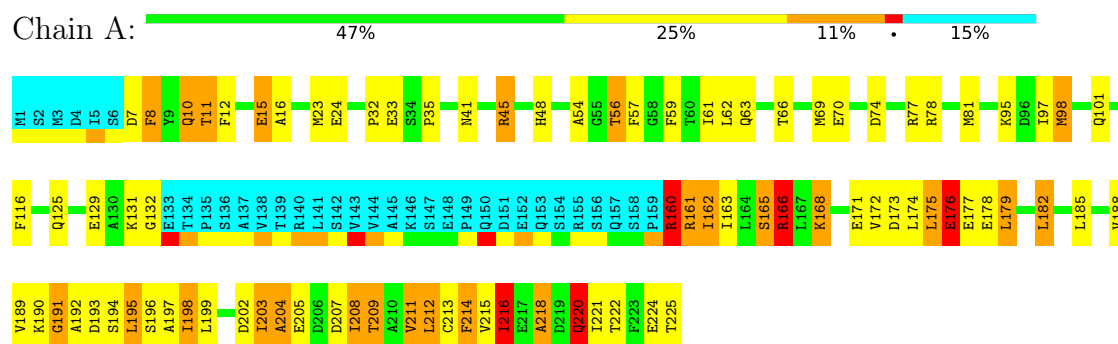


- Molecule 2: Chemotaxis protein CheY

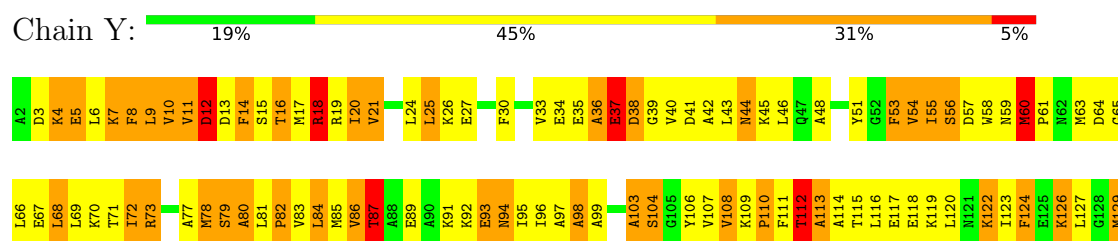


4.2.7 Score per residue for model 7

- Molecule 1: Chemotaxis protein CheA

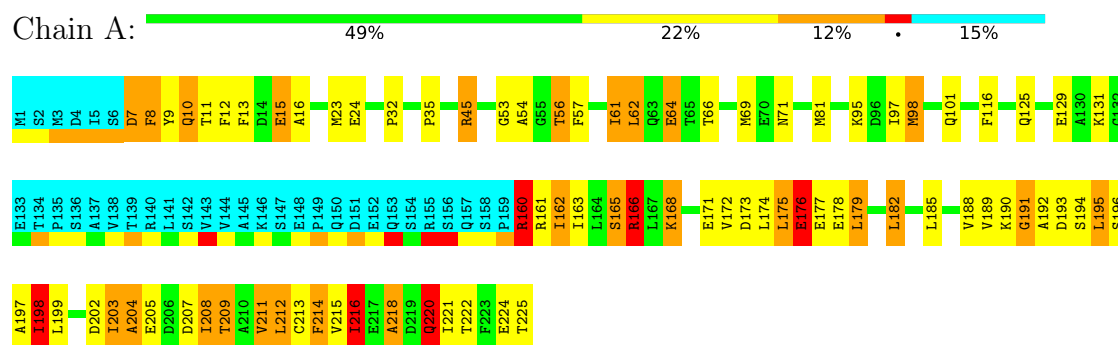


- Molecule 2: Chemotaxis protein CheY

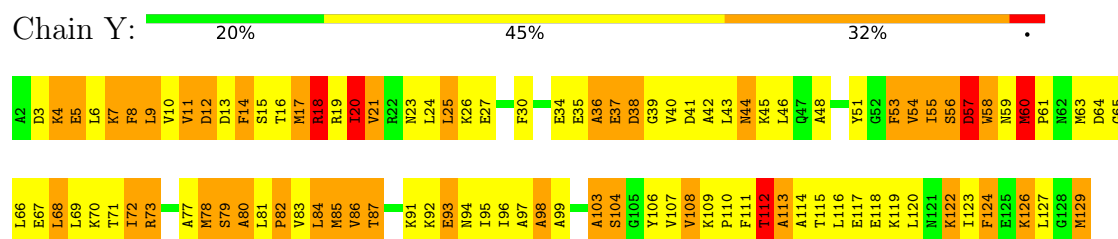


4.2.8 Score per residue for model 8

- Molecule 1: Chemotaxis protein CheA

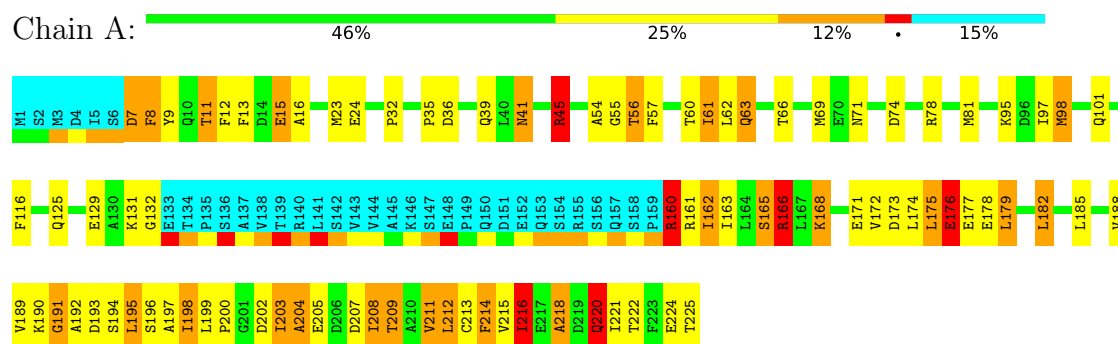


- Molecule 2: Chemotaxis protein CheY

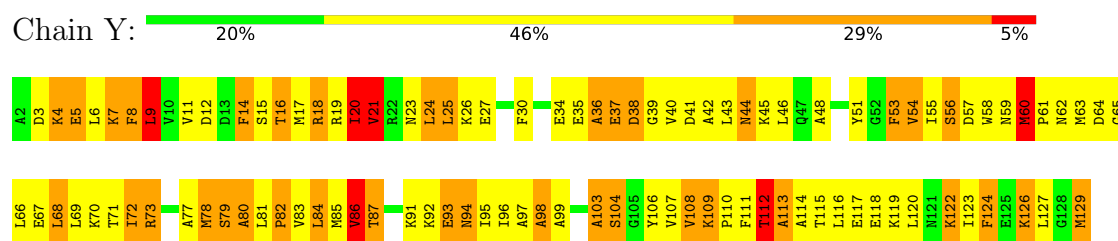


4.2.9 Score per residue for model 9

- Molecule 1: Chemotaxis protein CheA

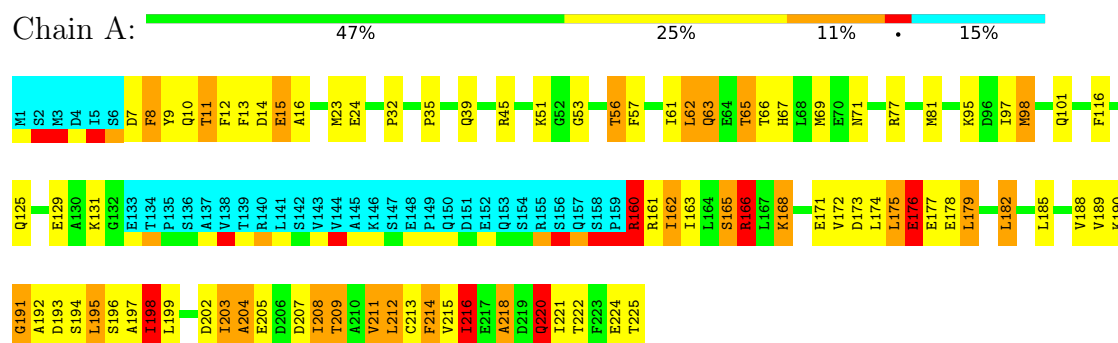


- Molecule 2: Chemotaxis protein CheY

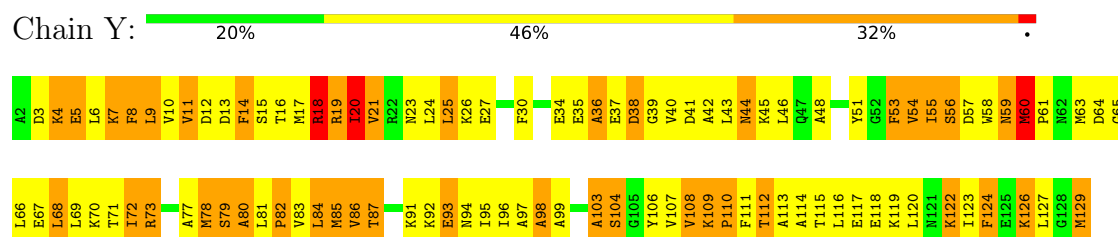


4.2.10 Score per residue for model 10

- Molecule 1: Chemotaxis protein CheA

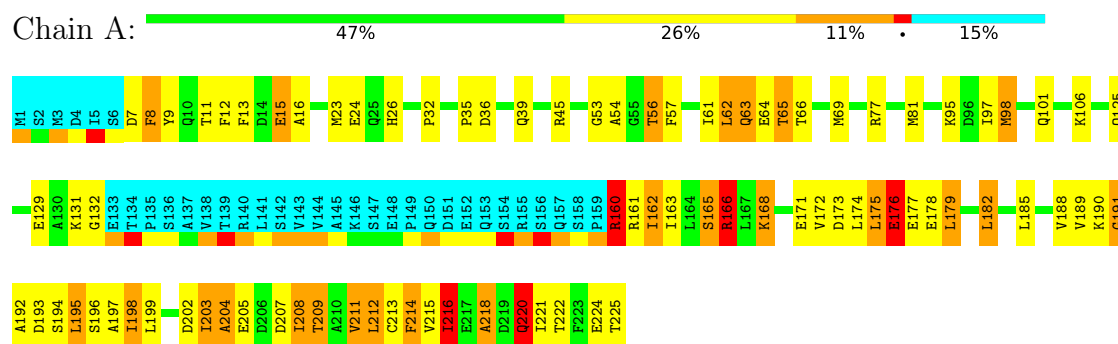


- Molecule 2: Chemotaxis protein CheY

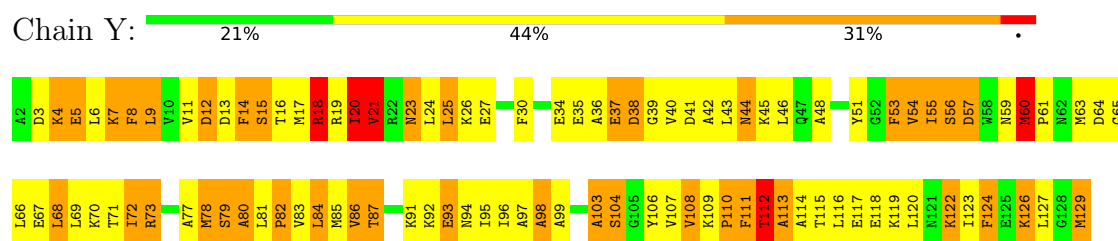


4.2.11 Score per residue for model 11

- Molecule 1: Chemotaxis protein CheA

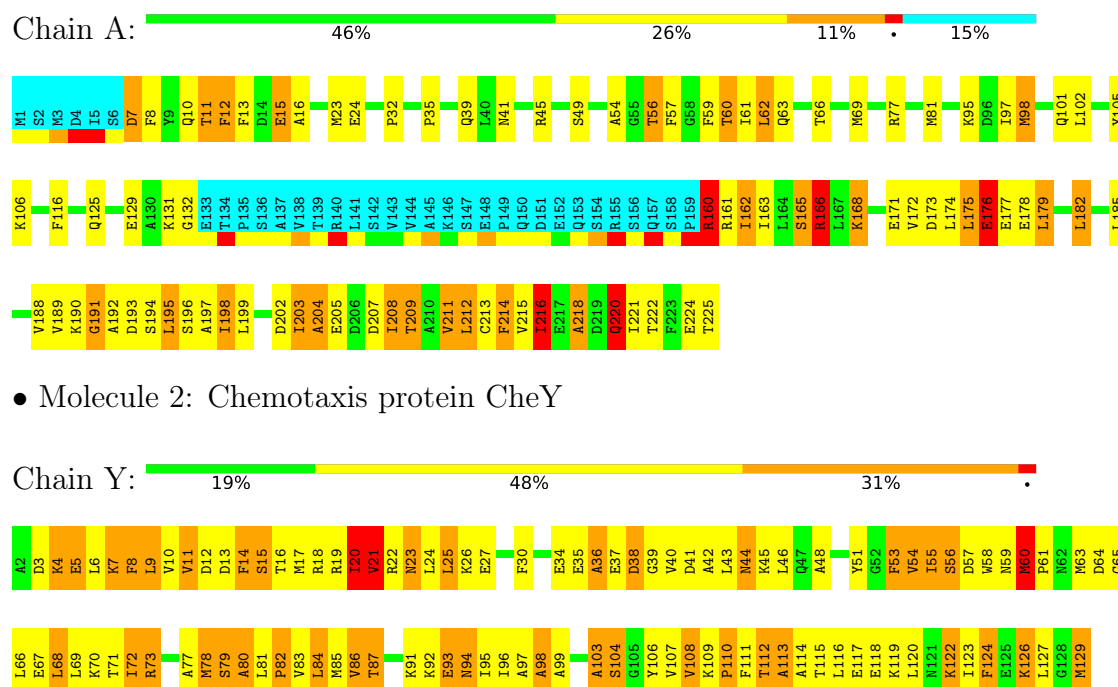


- Molecule 2: Chemotaxis protein CheY



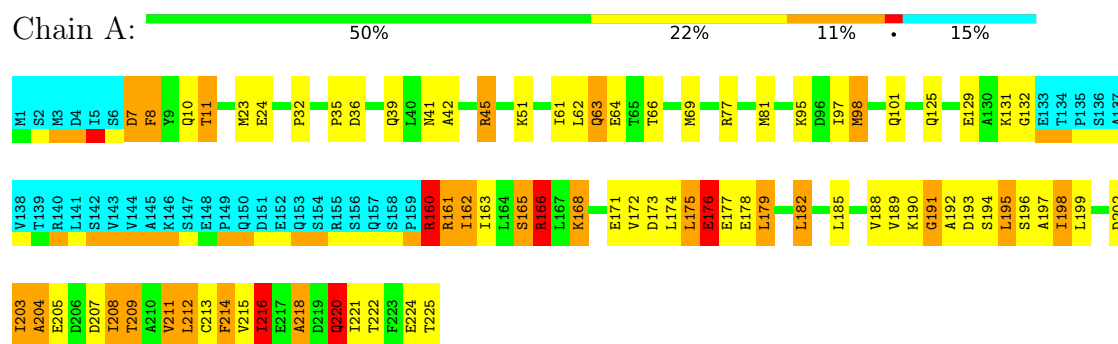
4.2.12 Score per residue for model 12

- Molecule 1: Chemotaxis protein CheA

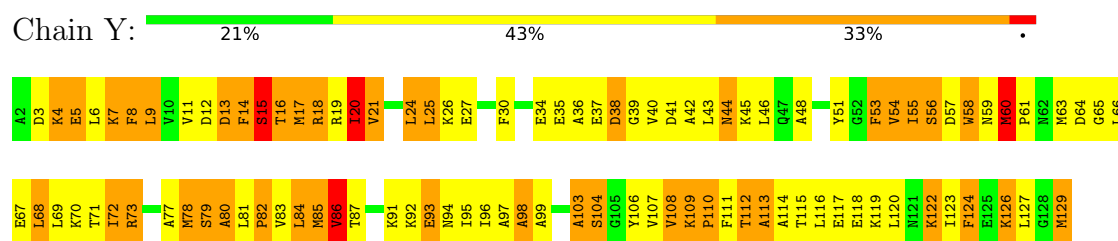


4.2.13 Score per residue for model 13

- Molecule 1: Chemotaxis protein CheA

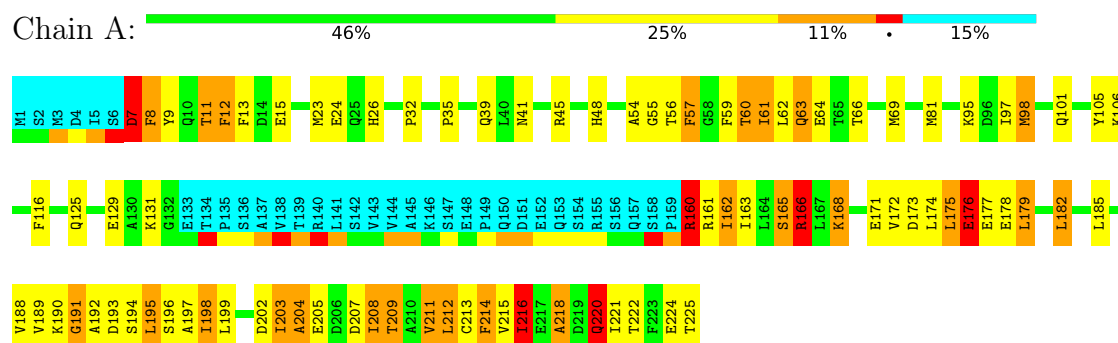


- Molecule 2: Chemotaxis protein CheY

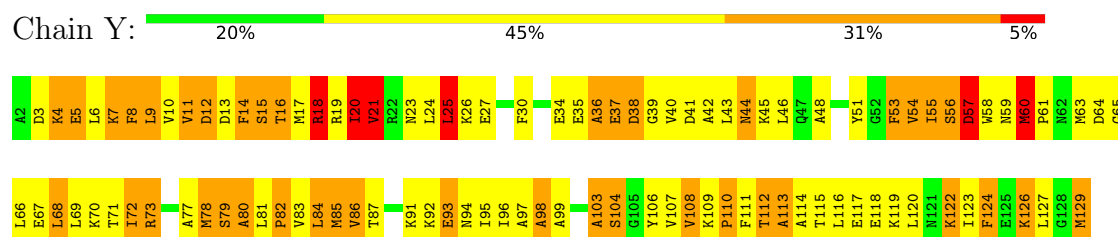


4.2.14 Score per residue for model 14

- Molecule 1: Chemotaxis protein CheA

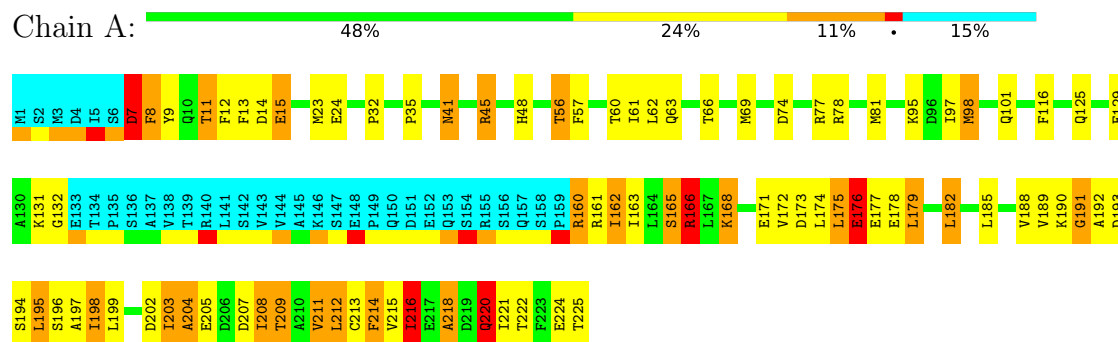


- Molecule 2: Chemotaxis protein CheY

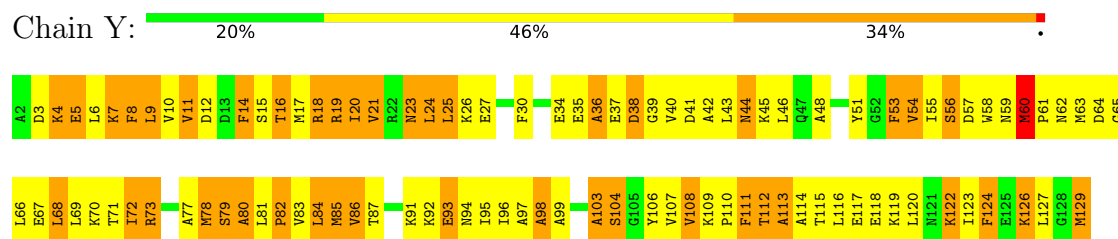


4.2.15 Score per residue for model 15

- Molecule 1: Chemotaxis protein CheA

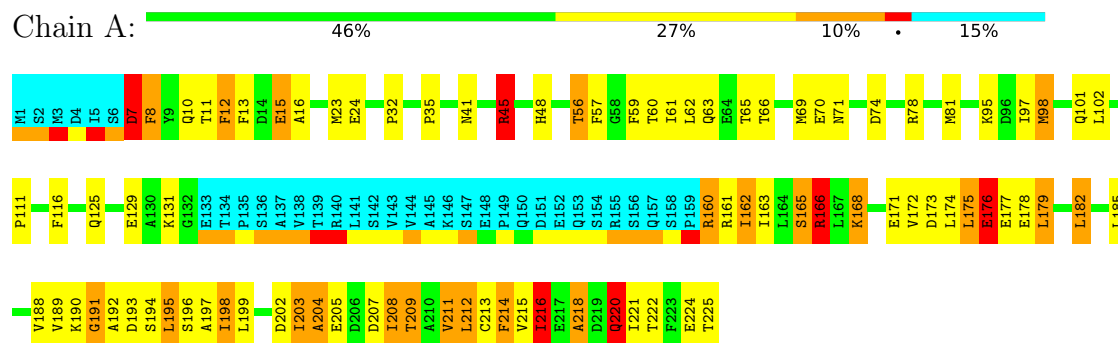


- Molecule 2: Chemotaxis protein CheY

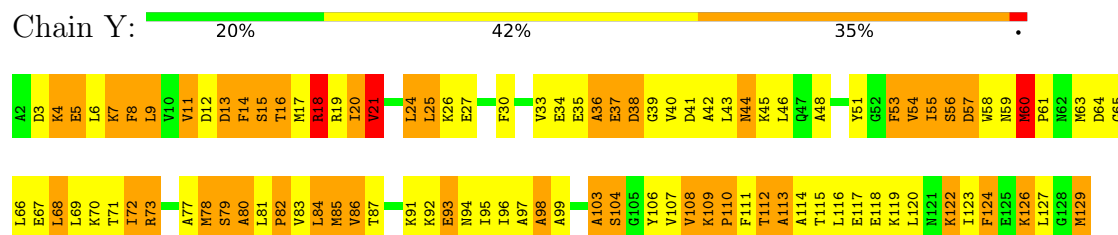


4.2.16 Score per residue for model 16

- Molecule 1: Chemotaxis protein CheA

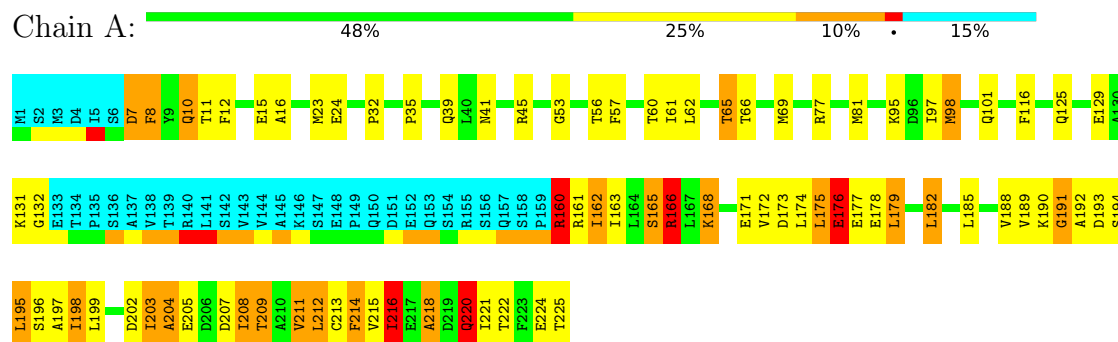


- Molecule 2: Chemotaxis protein CheY

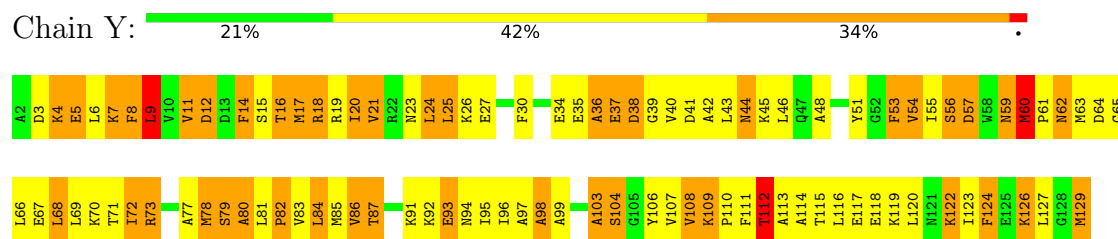


4.2.17 Score per residue for model 17

- Molecule 1: Chemotaxis protein CheA

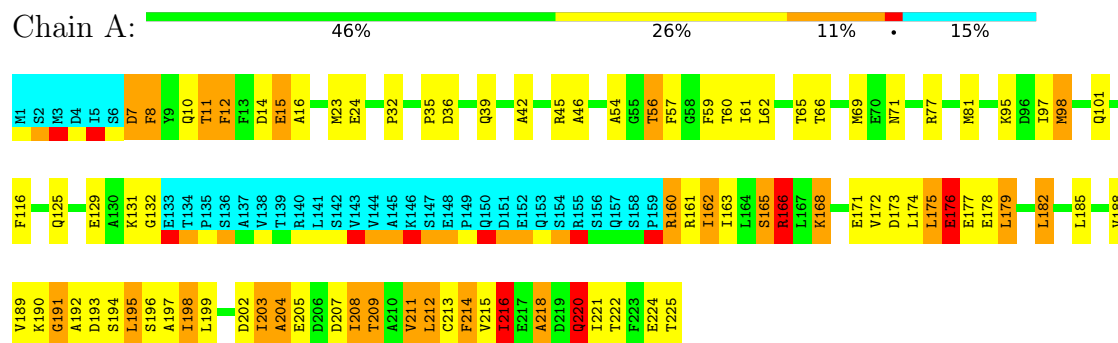


- Molecule 2: Chemotaxis protein CheY

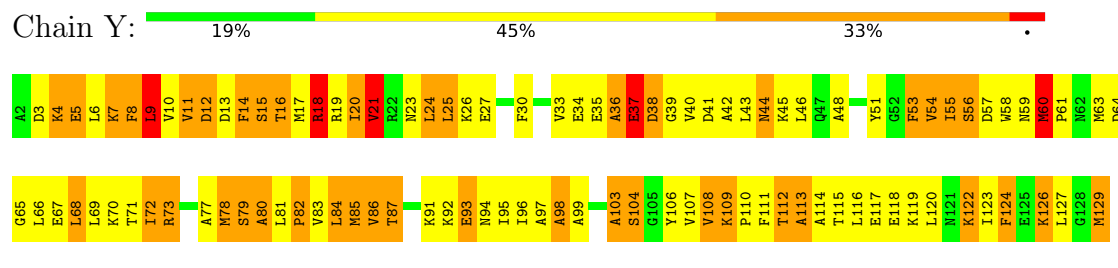


4.2.18 Score per residue for model 18

- Molecule 1: Chemotaxis protein CheA

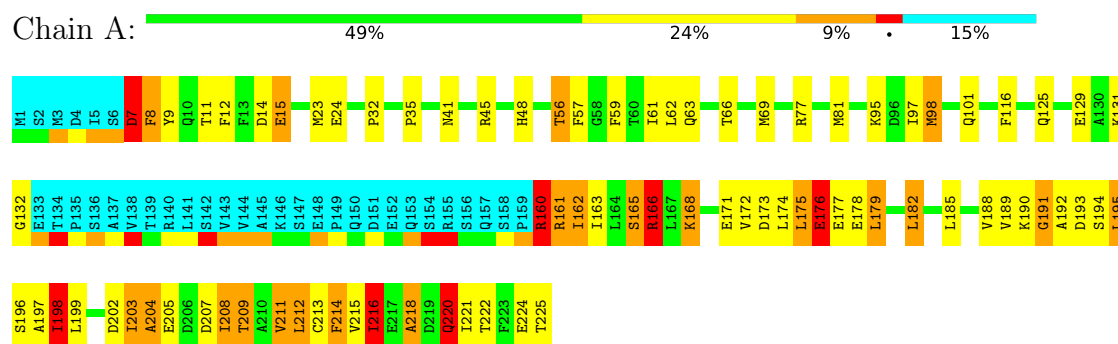


- Molecule 2: Chemotaxis protein CheY

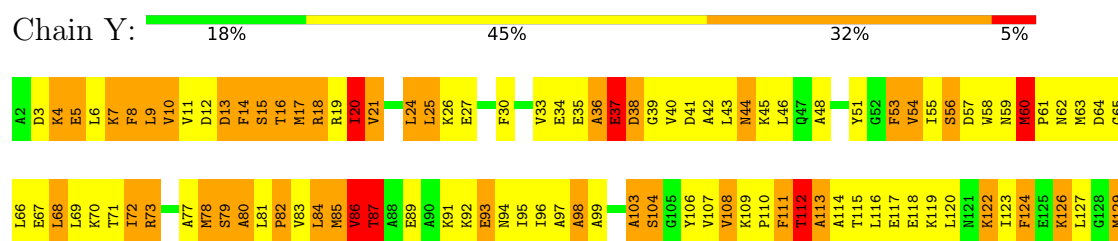


4.2.19 Score per residue for model 19

- Molecule 1: Chemotaxis protein CheA

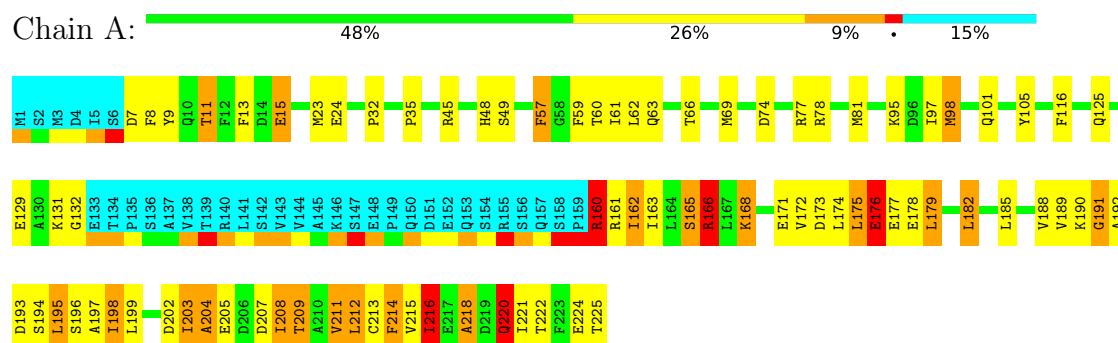


- Molecule 2: Chemotaxis protein CheY

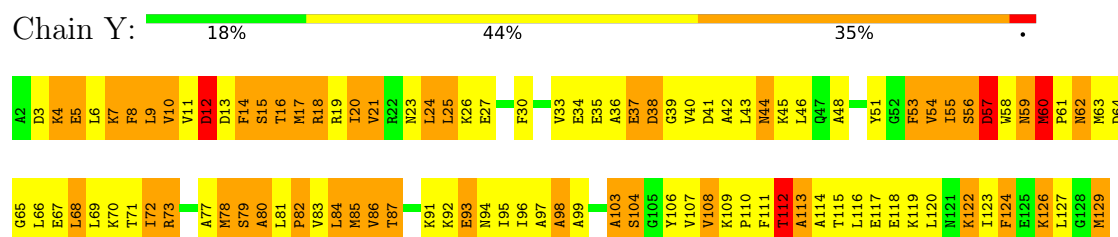


4.2.20 Score per residue for model 20

- Molecule 1: Chemotaxis protein CheA

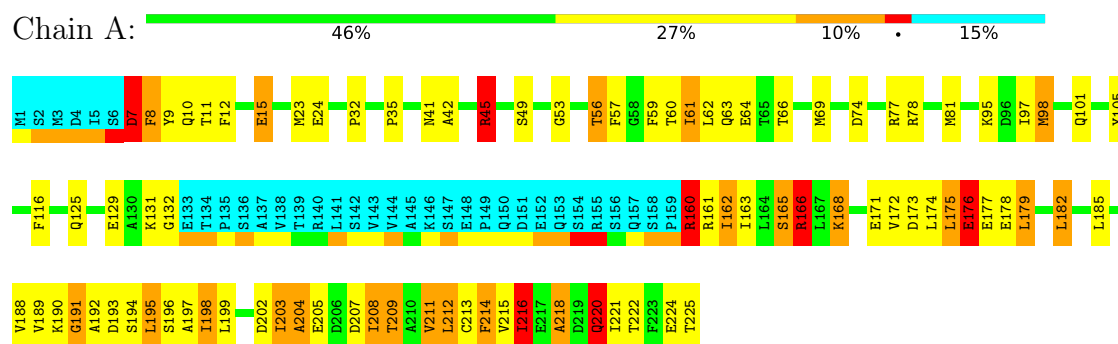


- Molecule 2: Chemotaxis protein CheY

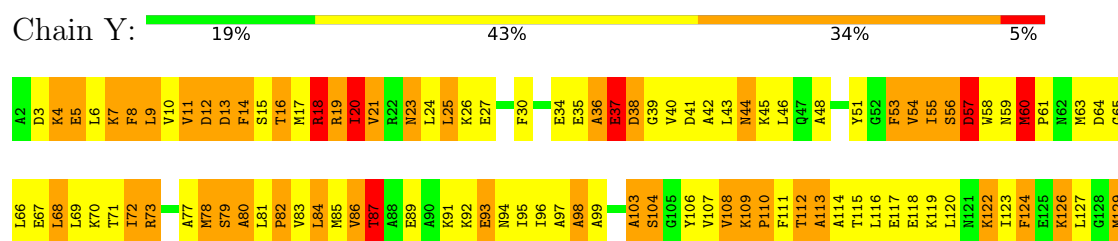


4.2.21 Score per residue for model 21

- Molecule 1: Chemotaxis protein CheA

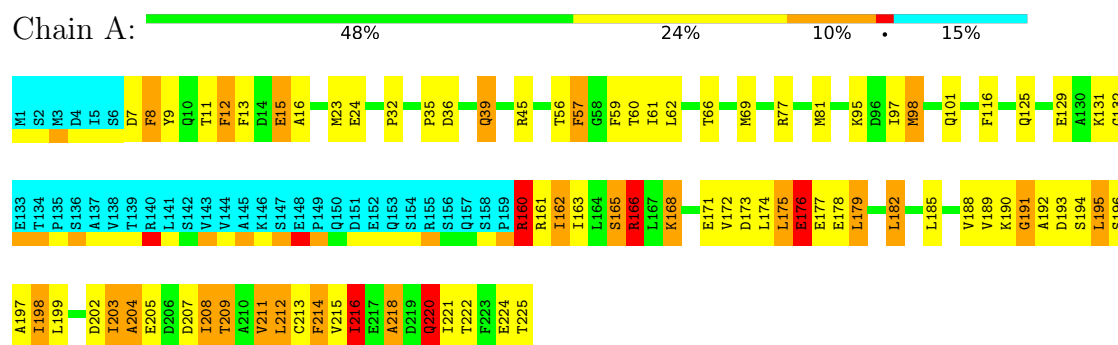


- Molecule 2: Chemotaxis protein CheY

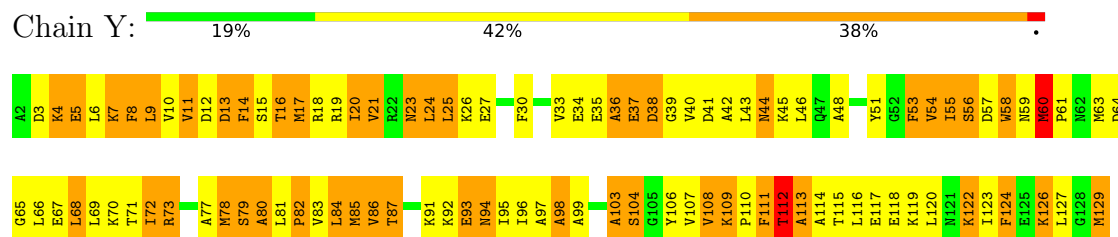


4.2.22 Score per residue for model 22

- Molecule 1: Chemotaxis protein CheA

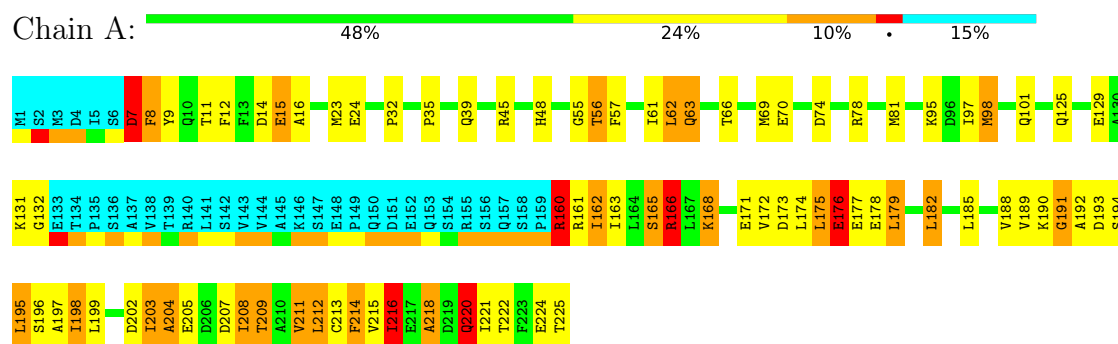


- Molecule 2: Chemotaxis protein CheY

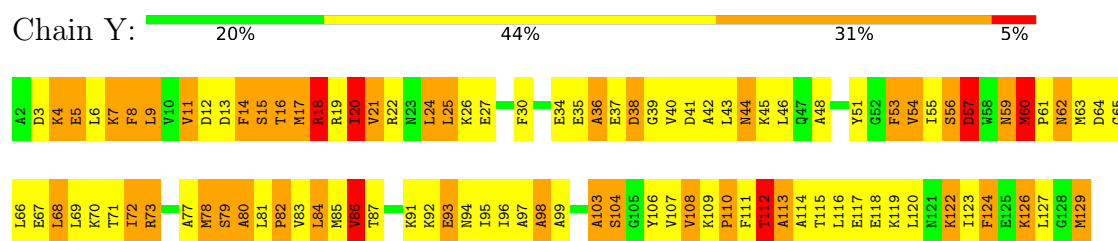


4.2.23 Score per residue for model 23

- Molecule 1: Chemotaxis protein CheA

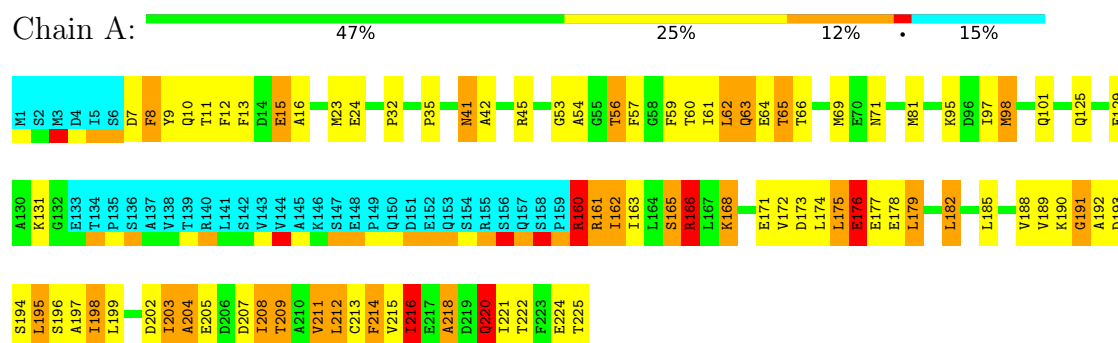


- Molecule 2: Chemotaxis protein CheY

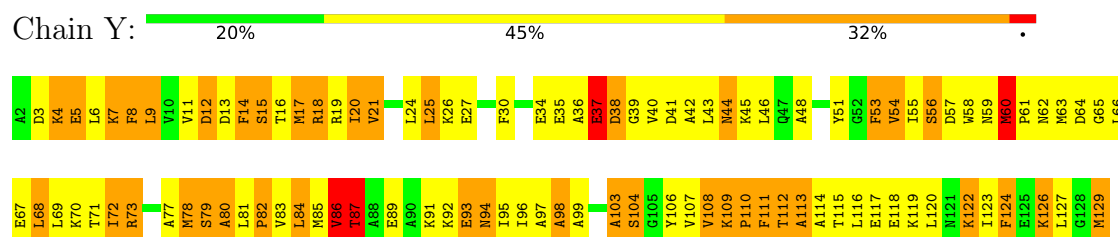


4.2.24 Score per residue for model 24

- Molecule 1: Chemotaxis protein CheA

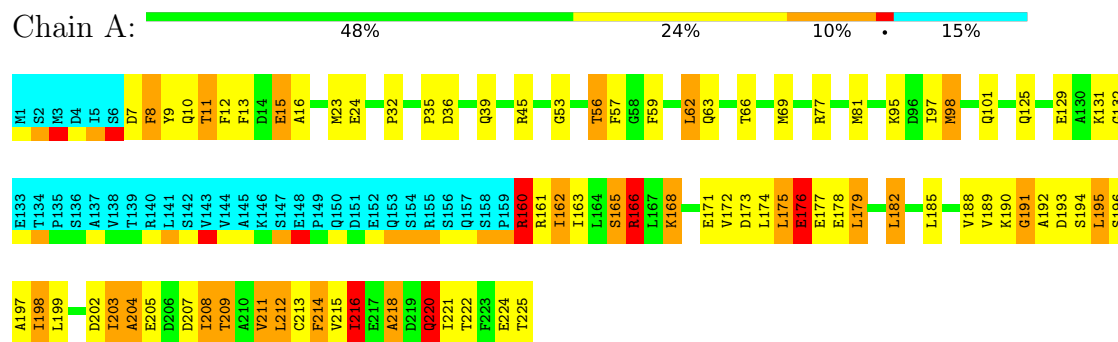


- Molecule 2: Chemotaxis protein CheY

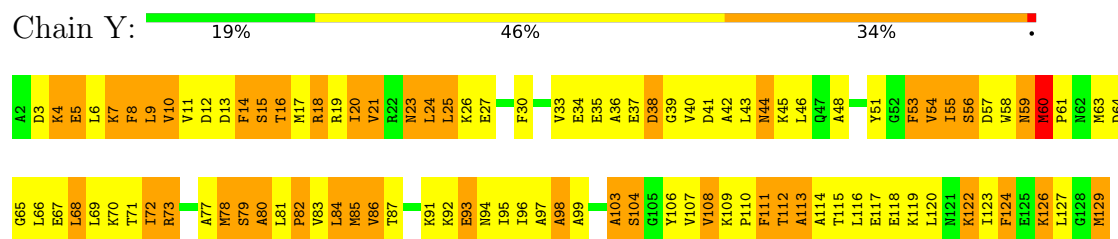


4.2.25 Score per residue for model 25

• Molecule 1: Chemotaxis protein CheA



• Molecule 2: Chemotaxis protein CheY



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 25 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
XPLOR-NIH	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	216
Number of shifts mapped to atoms	216
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	5%

6 Model quality i

6.1 Standard geometry i

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	1.28±0.00	22±1/1517 (1.4± 0.0%)	1.40±0.00	24±0/2054 (1.2± 0.0%)
2	Y	1.97±0.00	35±0/966 (3.6± 0.0%)	2.14±0.00	42±1/1302 (3.2± 0.1%)
All	All	1.59	1418/62075 (2.3%)	1.73	1650/83900 (2.0%)

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	1.3±0.7
2	Y	0.0±0.0	0.8±0.4
All	All	0	54

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	196	SER	CA-C	-8.19	1.42	1.52	1	25
1	A	194	SER	CA-C	-7.69	1.43	1.52	1	25
2	Y	112	THR	CA-C	-7.30	1.42	1.53	1	25
2	Y	82	PRO	C-N	-7.24	1.24	1.33	1	25
2	Y	8	PHE	N-CA	-7.10	1.37	1.46	1	25
2	Y	85	MET	N-CA	-7.01	1.37	1.46	1	25
2	Y	81	LEU	C-N	6.90	1.40	1.33	1	25
2	Y	71	THR	CA-C	-6.71	1.44	1.52	1	25
1	A	23	MET	CG-SD	6.65	1.97	1.80	8	25
1	A	98	MET	SD-CE	6.61	1.96	1.79	16	25
2	Y	56	SER	CA-C	-6.60	1.44	1.52	1	25
2	Y	57	ASP	N-CA	-6.43	1.37	1.45	1	25
2	Y	14	PHE	N-CA	6.41	1.54	1.46	1	25
2	Y	56	SER	N-CA	-6.27	1.38	1.46	1	25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	198	ILE	N-CA	-6.08	1.39	1.46	1	25
1	A	81	MET	CG-SD	6.08	1.96	1.80	2	25
1	A	197	ALA	N-CA	-6.03	1.38	1.46	1	25
2	Y	38	ASP	N-CA	6.02	1.53	1.46	1	25
1	A	165	SER	N-CA	-6.01	1.39	1.45	1	25
1	A	98	MET	CG-SD	5.94	1.95	1.80	19	25
1	A	208	ILE	CA-C	-5.91	1.45	1.52	1	25
2	Y	84	LEU	CA-C	-5.90	1.45	1.53	1	25
2	Y	83	VAL	N-CA	-5.82	1.38	1.46	1	25
2	Y	67	GLU	CA-C	-5.81	1.44	1.52	1	25
2	Y	110	PRO	C-N	-5.79	1.25	1.33	1	25
1	A	69	MET	SD-CE	5.77	1.94	1.79	6	25
1	A	195	LEU	C-N	-5.70	1.25	1.33	1	25
2	Y	103	ALA	N-CA	5.66	1.53	1.45	1	25
2	Y	53	PHE	CA-C	-5.63	1.46	1.52	1	25
2	Y	86	VAL	CA-C	-5.62	1.45	1.52	1	25
2	Y	36	ALA	CA-C	-5.61	1.45	1.52	1	25
2	Y	54	VAL	N-CA	-5.56	1.39	1.46	1	25
1	A	162	ILE	C-N	-5.54	1.26	1.33	1	25
2	Y	12	ASP	C-N	-5.49	1.25	1.33	1	25
2	Y	87	THR	N-CA	-5.48	1.39	1.45	1	25
1	A	222	THR	CA-C	-5.45	1.45	1.52	1	25
1	A	195	LEU	N-CA	-5.38	1.40	1.46	1	25
2	Y	106	TYR	CA-C	5.33	1.59	1.52	1	25
1	A	209	THR	N-CA	-5.32	1.40	1.46	1	25
2	Y	20	ILE	CA-CB	-5.29	1.47	1.54	1	25
2	Y	53	PHE	N-CA	-5.29	1.39	1.46	1	25
1	A	81	MET	SD-CE	5.27	1.92	1.79	19	25
2	Y	56	SER	C-N	-5.26	1.26	1.33	1	25
2	Y	118	GLU	CA-C	5.24	1.59	1.52	1	25
2	Y	124	PHE	N-CA	-5.24	1.40	1.46	1	25
1	A	220	GLN	CA-C	-5.21	1.45	1.52	1	25
2	Y	37	GLU	C-N	5.21	1.40	1.33	1	25
2	Y	69	LEU	CA-C	5.17	1.59	1.52	1	25
1	A	163	ILE	N-CA	-5.17	1.40	1.46	1	25
2	Y	80	ALA	CA-C	5.17	1.59	1.52	1	25
2	Y	113	ALA	N-CA	-5.16	1.40	1.46	1	25
2	Y	99	ALA	CA-C	5.11	1.59	1.52	1	25
1	A	69	MET	CG-SD	5.10	1.93	1.80	11	15
1	A	204	ALA	CA-C	-5.09	1.46	1.52	1	25
2	Y	73	ARG	CA-C	5.07	1.59	1.52	1	25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	23	MET	SD-CE	5.03	1.92	1.79	15	3
2	Y	71	THR	N-CA	-5.02	1.40	1.46	1	25
1	A	189	VAL	N-CA	-5.01	1.40	1.46	1	25

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
2	Y	77	ALA	N-CA-C	10.49	123.78	111.71	1	25
2	Y	82	PRO	N-CA-CB	10.33	110.15	103.23	1	25
2	Y	15	SER	N-CA-C	9.28	122.24	111.11	1	25
1	A	162	ILE	CA-C-N	-9.12	111.27	123.12	1	25
1	A	162	ILE	C-N-CA	-9.12	111.27	123.12	1	25
1	A	176	GLU	N-CA-C	-8.84	101.73	111.36	1	25
2	Y	55	ILE	N-CA-CB	8.32	120.54	111.89	1	25
2	Y	55	ILE	N-CA-C	-7.95	93.52	106.32	1	25
2	Y	118	GLU	N-CA-C	7.74	119.72	111.28	1	25
2	Y	60	MET	N-CA-C	7.70	115.15	108.22	1	25
2	Y	68	LEU	N-CA-C	-7.69	102.59	110.97	1	25
1	A	216	ILE	N-CA-CB	-7.58	103.95	112.45	1	25
2	Y	21	VAL	N-CA-C	-7.33	102.66	110.36	1	25
2	Y	71	THR	N-CA-C	-7.13	102.92	111.69	1	25
1	A	212	LEU	N-CA-C	-7.12	103.52	111.71	1	25
1	A	196	SER	N-CA-C	-6.95	98.53	109.50	1	25
2	Y	25	LEU	N-CA-C	-6.90	102.98	111.33	1	25
2	Y	53	PHE	CA-C-N	-6.88	114.09	122.90	1	25
2	Y	53	PHE	C-N-CA	-6.88	114.09	122.90	1	25
1	A	211	VAL	N-CA-C	6.70	118.68	111.58	1	25
2	Y	73	ARG	N-CA-C	6.62	120.57	112.23	1	25
2	Y	112	THR	N-CA-C	-6.55	101.09	110.59	1	25
2	Y	80	ALA	N-CA-C	6.55	121.21	112.30	1	25
2	Y	14	PHE	N-CA-C	6.52	119.35	108.20	1	25
2	Y	7	LYS	N-CA-CB	6.51	120.06	110.35	1	25
2	Y	82	PRO	CB-CA-C	-6.43	105.55	111.40	1	25
1	A	193	ASP	CA-C-N	-6.40	111.85	122.21	1	25
1	A	193	ASP	C-N-CA	-6.40	111.85	122.21	1	25
2	Y	84	LEU	CA-C-N	-6.39	112.36	121.50	1	25
2	Y	84	LEU	C-N-CA	-6.39	112.36	121.50	1	25
2	Y	72	ILE	N-CA-C	-6.33	104.34	110.42	1	25
1	A	214	PHE	CB-CA-C	-6.23	97.67	110.38	1	25
2	Y	67	GLU	N-CA-C	-6.20	104.63	111.82	1	25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	Y	38	ASP	N-CA-C	6.18	116.73	108.38	1	25
2	Y	124	PHE	N-CA-C	-6.01	103.90	111.11	1	25
1	A	195	LEU	CA-C-O	5.98	127.79	120.25	1	25
2	Y	86	VAL	N-CA-CB	5.90	117.15	110.72	1	25
2	Y	108	VAL	N-CA-C	5.87	116.31	107.80	1	25
2	Y	94	ASN	N-CA-C	-5.87	104.81	111.14	1	25
1	A	208	ILE	O-C-N	5.84	127.53	121.87	1	25
2	Y	19	ARG	N-CA-C	5.83	117.72	111.36	1	25
1	A	208	ILE	N-CA-C	-5.72	104.78	110.62	1	25
2	Y	18	ARG	NE-CZ-NH2	5.67	124.30	119.20	4	9
2	Y	67	GLU	O-C-N	5.63	129.20	122.27	1	25
1	A	166	ARG	N-CA-C	5.61	118.86	111.28	1	25
1	A	160	ARG	CA-C-N	-5.58	114.84	122.93	1	25
1	A	160	ARG	C-N-CA	-5.58	114.84	122.93	1	25
2	Y	112	THR	CB-CA-C	-5.57	99.97	110.51	1	25
2	Y	122	LYS	N-CA-C	5.52	117.38	111.36	1	25
2	Y	38	ASP	CA-C-N	5.50	126.05	120.00	1	25
2	Y	38	ASP	C-N-CA	5.50	126.05	120.00	1	25
2	Y	98	ALA	N-CA-C	-5.46	105.22	111.07	1	25
2	Y	9	LEU	N-CA-C	-5.44	98.42	107.99	1	25
2	Y	84	LEU	N-CA-CB	5.40	119.30	110.39	1	25
2	Y	92	LYS	N-CA-C	5.38	120.19	111.37	1	25
1	A	220	GLN	N-CA-C	-5.29	106.77	113.18	1	25
1	A	218	ALA	N-CA-C	5.29	118.52	111.75	1	25
1	A	182	LEU	CB-CA-C	-5.28	100.14	110.11	1	25
2	Y	126	LYS	N-CA-C	5.27	117.77	111.71	1	25
2	Y	97	ALA	N-CA-C	-5.22	105.59	111.28	1	25
2	Y	96	ILE	CB-CA-C	-5.20	105.28	112.24	1	25
1	A	207	ASP	CA-CB-CG	5.18	117.78	112.60	1	25
1	A	179	LEU	N-CA-C	-5.14	105.80	111.71	1	25
2	Y	57	ASP	CA-CB-CG	-5.09	107.51	112.60	14	16
1	A	191	GLY	CA-C-N	-5.06	113.50	120.28	1	25
1	A	191	GLY	C-N-CA	-5.06	113.50	120.28	1	25
1	A	168	LYS	N-CA-C	5.02	117.89	110.46	1	25

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)
2	Y	18	ARG	Sidechain	21

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	45	ARG	Sidechain	20
1	A	7	ASP	Peptide	13

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	1497	1452	1448	66±9
2	Y	954	974	957	104±9
All	All	61275	60650	60121	3995

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:ASP:HB3	1:A:8:PHE:CD1	1.59	1.26	6	3
1:A:7:ASP:CB	1:A:8:PHE:CE1	1.51	1.90	6	2
1:A:7:ASP:HB3	1:A:8:PHE:CE1	1.45	1.44	6	3
2:Y:17:MET:O	2:Y:21:VAL:HG22	1.26	1.25	12	2
2:Y:17:MET:O	2:Y:21:VAL:CG2	1.23	1.85	14	3
1:A:57:PHE:O	1:A:57:PHE:CD1	1.23	1.92	14	1
1:A:7:ASP:CB	1:A:8:PHE:CD1	1.23	2.16	6	2
2:Y:21:VAL:O	2:Y:25:LEU:HG	1.15	1.39	16	3
2:Y:17:MET:O	2:Y:21:VAL:HG23	1.14	1.39	14	7
2:Y:11:VAL:O	2:Y:12:ASP:OD1	1.13	1.67	5	1
2:Y:10:VAL:HG23	2:Y:34:GLU:O	1.10	1.44	20	3
1:A:41:ASN:O	1:A:45:ARG:HG2	1.07	1.49	13	2
2:Y:38:ASP:OD2	2:Y:62:ASN:OD1	1.06	1.72	6	2
2:Y:11:VAL:HG23	2:Y:56:SER:HA	1.06	1.20	23	1
2:Y:9:LEU:HD23	2:Y:11:VAL:HG22	1.05	1.10	12	2
2:Y:11:VAL:HG22	2:Y:56:SER:HA	1.04	1.25	11	1
1:A:7:ASP:OD2	1:A:10:GLN:NE2	1.04	1.90	25	1
2:Y:14:PHE:O	2:Y:18:ARG:HG3	1.03	1.53	22	8
1:A:7:ASP:HB2	1:A:8:PHE:CE1	1.02	1.88	6	2
2:Y:24:LEU:HD21	2:Y:113:ALA:CB	1.01	1.84	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:17:MET:HG3	2:Y:18:ARG:N	1.01	1.61	24	1
1:A:7:ASP:O	1:A:7:ASP:OD1	1.00	1.78	10	3
1:A:12:PHE:O	1:A:15:GLU:HG3	1.00	1.56	17	1
1:A:7:ASP:CG	1:A:8:PHE:CE1	0.99	2.41	6	1
2:Y:24:LEU:HD21	2:Y:113:ALA:CA	0.99	1.87	7	1
2:Y:61:PRO:O	2:Y:62:ASN:ND2	0.98	1.96	6	2
2:Y:11:VAL:CG2	2:Y:56:SER:HA	0.97	1.89	11	2
2:Y:10:VAL:CG2	2:Y:34:GLU:O	0.97	2.11	19	2
2:Y:24:LEU:HD21	2:Y:113:ALA:HB2	0.97	1.32	7	5
1:A:65:THR:HG21	1:A:101:GLN:HE22	0.97	1.18	18	5
1:A:7:ASP:OD2	1:A:8:PHE:HE1	0.97	1.43	6	2
2:Y:24:LEU:HD11	2:Y:113:ALA:HA	0.97	1.32	7	1
2:Y:20:ILE:O	2:Y:24:LEU:HG	0.96	1.61	4	9
2:Y:9:LEU:HD12	2:Y:51:TYR:CE1	0.96	1.96	15	2
2:Y:9:LEU:CD2	2:Y:11:VAL:HG22	0.95	1.92	15	3
2:Y:9:LEU:HD23	2:Y:11:VAL:CG2	0.94	1.91	12	2
1:A:57:PHE:CD1	1:A:57:PHE:C	0.94	2.45	14	1
1:A:8:PHE:CE1	1:A:57:PHE:CD1	0.94	2.55	2	3
2:Y:18:ARG:O	2:Y:21:VAL:HG23	0.94	1.62	12	1
1:A:77:ARG:HH12	2:Y:61:PRO:HB3	0.94	1.20	13	15
2:Y:18:ARG:O	2:Y:21:VAL:HG12	0.93	1.62	3	3
2:Y:20:ILE:HG12	2:Y:24:LEU:HD21	0.93	1.40	4	1
2:Y:18:ARG:NH2	2:Y:37:GLU:OE2	0.93	2.02	11	2
2:Y:59:ASN:N	2:Y:59:ASN:OD1	0.93	2.01	25	1
1:A:11:THR:HG22	2:Y:16:THR:OG1	0.92	1.65	17	8
1:A:59:PHE:O	1:A:63:GLN:HG3	0.92	1.64	14	1
1:A:7:ASP:OD2	1:A:8:PHE:CE1	0.91	2.23	6	2
2:Y:11:VAL:HG12	2:Y:60:MET:SD	0.91	2.05	19	6
1:A:57:PHE:CE1	1:A:59:PHE:CD1	0.91	2.59	14	1
1:A:56:THR:OG1	2:Y:17:MET:HE1	0.91	1.65	1	1
2:Y:21:VAL:HA	2:Y:24:LEU:HD11	0.90	1.38	17	1
2:Y:14:PHE:O	2:Y:18:ARG:CG	0.90	2.20	2	2
1:A:57:PHE:CE1	1:A:59:PHE:CE1	0.90	2.60	14	1
1:A:41:ASN:O	1:A:45:ARG:CG	0.90	2.19	13	2
1:A:11:THR:OG1	2:Y:16:THR:HG22	0.89	1.66	21	1
1:A:59:PHE:CD1	1:A:105:TYR:CD1	0.88	2.61	14	5
2:Y:10:VAL:HG21	2:Y:33:VAL:CG1	0.88	1.99	6	8
1:A:57:PHE:CZ	1:A:59:PHE:CE1	0.88	2.61	14	1
2:Y:9:LEU:HD12	2:Y:51:TYR:CZ	0.87	2.04	15	2
1:A:56:THR:HG23	1:A:57:PHE:CD1	0.87	2.04	2	2
1:A:59:PHE:O	1:A:63:GLN:CG	0.86	2.23	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLY:O	1:A:57:PHE:CD2	0.86	2.28	21	5
2:Y:13:ASP:OD1	2:Y:60:MET:HG2	0.85	1.71	1	1
2:Y:54:VAL:HG12	2:Y:56:SER:HB2	0.85	1.48	1	25
2:Y:9:LEU:HD13	2:Y:51:TYR:CE1	0.85	2.07	11	14
2:Y:20:ILE:HG22	2:Y:24:LEU:HD12	0.84	1.47	18	1
2:Y:10:VAL:HG22	2:Y:34:GLU:O	0.84	1.72	19	1
1:A:7:ASP:O	1:A:7:ASP:CG	0.84	2.21	16	2
2:Y:11:VAL:HG13	2:Y:60:MET:SD	0.84	2.12	21	2
1:A:166:ARG:NH2	1:A:220:GLN:HA	0.83	1.88	1	25
1:A:59:PHE:CE1	1:A:105:TYR:CD1	0.83	2.66	14	4
1:A:56:THR:HG22	1:A:57:PHE:CD1	0.83	2.08	21	6
1:A:12:PHE:HA	1:A:15:GLU:OE1	0.83	1.74	18	14
2:Y:9:LEU:HG	2:Y:11:VAL:HG22	0.83	1.51	8	12
2:Y:24:LEU:CD2	2:Y:113:ALA:HB2	0.82	2.02	7	8
2:Y:23:ASN:OD1	2:Y:23:ASN:C	0.82	2.22	4	2
2:Y:25:LEU:CD2	2:Y:116:LEU:HD21	0.82	2.05	4	10
2:Y:17:MET:HE2	2:Y:21:VAL:HG13	0.81	1.52	12	1
1:A:8:PHE:HB2	1:A:57:PHE:HZ	0.81	1.32	4	1
2:Y:21:VAL:O	2:Y:25:LEU:CG	0.81	2.26	16	1
1:A:54:ALA:O	1:A:63:GLN:NE2	0.81	2.12	24	1
1:A:8:PHE:CD1	1:A:8:PHE:N	0.81	2.46	9	14
1:A:175:LEU:HD11	1:A:216:ILE:HD13	0.81	1.53	1	25
1:A:42:ALA:HA	1:A:45:ARG:HD2	0.80	1.53	13	1
1:A:9:TYR:CE1	1:A:57:PHE:CD2	0.80	2.68	14	3
2:Y:58:TRP:CE3	2:Y:85:MET:HE2	0.80	2.11	25	7
1:A:8:PHE:N	1:A:8:PHE:CD1	0.80	2.49	22	6
2:Y:9:LEU:CG	2:Y:11:VAL:HG22	0.80	2.07	17	2
2:Y:18:ARG:NH1	2:Y:35:GLU:OE1	0.80	2.14	13	3
1:A:8:PHE:CE1	1:A:57:PHE:CE1	0.80	2.70	2	2
1:A:9:TYR:CE1	1:A:59:PHE:CZ	0.79	2.70	6	5
1:A:12:PHE:O	1:A:15:GLU:OE1	0.79	2.00	3	2
1:A:56:THR:CG2	1:A:57:PHE:CD1	0.79	2.65	21	7
1:A:9:TYR:CE1	1:A:57:PHE:CG	0.79	2.71	6	3
2:Y:18:ARG:O	2:Y:21:VAL:CG1	0.79	2.31	25	2
1:A:15:GLU:HG2	2:Y:16:THR:HG23	0.78	1.52	1	2
1:A:9:TYR:CZ	1:A:59:PHE:CZ	0.78	2.72	6	1
2:Y:11:VAL:HG23	2:Y:56:SER:CA	0.78	2.06	23	1
2:Y:24:LEU:CD1	2:Y:113:ALA:HA	0.78	2.07	7	1
2:Y:58:TRP:CZ3	2:Y:87:THR:HB	0.78	2.14	22	1
2:Y:112:THR:OG1	2:Y:114:ALA:N	0.77	2.17	10	4
1:A:12:PHE:CD1	1:A:15:GLU:OE1	0.77	2.37	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:PHE:CE1	1:A:53:GLY:HA3	0.77	2.15	8	6
2:Y:61:PRO:O	2:Y:62:ASN:CG	0.76	2.28	6	2
2:Y:11:VAL:HG22	2:Y:56:SER:CA	0.76	2.10	11	1
1:A:9:TYR:CZ	1:A:57:PHE:CD1	0.76	2.73	6	2
2:Y:59:ASN:O	2:Y:60:MET:HG3	0.76	1.81	1	25
2:Y:24:LEU:N	2:Y:24:LEU:HD23	0.75	1.96	13	3
1:A:11:THR:O	2:Y:16:THR:HG21	0.75	1.82	21	2
2:Y:11:VAL:CG1	2:Y:60:MET:SD	0.75	2.73	19	3
1:A:63:GLN:O	1:A:63:GLN:NE2	0.75	2.20	10	1
1:A:45:ARG:HD3	2:Y:61:PRO:CG	0.75	2.11	15	1
2:Y:9:LEU:HD22	2:Y:51:TYR:CZ	0.75	2.17	5	3
1:A:57:PHE:HD1	1:A:57:PHE:O	0.75	1.65	6	1
1:A:57:PHE:CZ	1:A:59:PHE:CZ	0.75	2.75	14	1
2:Y:84:LEU:HD13	2:Y:123:ILE:HD11	0.75	1.59	1	25
1:A:8:PHE:HB2	1:A:57:PHE:CZ	0.75	2.17	4	3
2:Y:54:VAL:CG1	2:Y:56:SER:HB2	0.74	2.12	1	25
2:Y:25:LEU:HD22	2:Y:30:PHE:CD1	0.74	2.17	19	4
1:A:77:ARG:NH1	2:Y:61:PRO:HB3	0.74	1.95	20	9
1:A:59:PHE:CE1	1:A:105:TYR:CG	0.74	2.76	14	2
1:A:9:TYR:CZ	1:A:57:PHE:CE1	0.74	2.76	6	2
2:Y:55:ILE:CG2	2:Y:86:VAL:CG2	0.74	2.65	22	15
1:A:15:GLU:OE2	1:A:16:ALA:HB2	0.74	1.83	16	9
2:Y:14:PHE:CZ	2:Y:16:THR:HB	0.74	2.18	3	20
1:A:15:GLU:OE2	2:Y:14:PHE:CZ	0.74	2.41	5	2
1:A:59:PHE:CD1	1:A:105:TYR:CE1	0.74	2.76	14	4
1:A:42:ALA:HA	1:A:45:ARG:CD	0.73	2.13	13	2
1:A:7:ASP:CB	1:A:8:PHE:CZ	0.73	2.67	6	1
2:Y:11:VAL:HG13	2:Y:36:ALA:HB3	0.73	1.59	15	14
1:A:59:PHE:O	1:A:63:GLN:HG2	0.73	1.83	24	2
2:Y:9:LEU:HD11	2:Y:11:VAL:HG13	0.73	1.60	17	1
2:Y:20:ILE:HA	2:Y:23:ASN:CG	0.73	2.09	8	3
2:Y:20:ILE:HG22	2:Y:23:ASN:OD1	0.73	1.83	14	1
1:A:62:LEU:HD12	1:A:66:THR:HG23	0.73	1.59	5	3
2:Y:25:LEU:HD23	2:Y:116:LEU:CD2	0.73	2.13	4	3
2:Y:11:VAL:HG23	2:Y:36:ALA:HB3	0.72	1.60	1	2
2:Y:55:ILE:HG23	2:Y:86:VAL:CG2	0.72	2.14	18	15
2:Y:25:LEU:HB3	2:Y:30:PHE:HB2	0.72	1.61	5	23
2:Y:58:TRP:CZ3	2:Y:85:MET:CB	0.72	2.71	22	4
1:A:56:THR:CG2	1:A:57:PHE:CE1	0.72	2.73	3	7
1:A:60:THR:HA	1:A:63:GLN:OE1	0.72	1.84	24	1
1:A:11:THR:CG2	2:Y:16:THR:HG23	0.72	2.14	14	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLN:HG3	1:A:11:THR:N	0.72	1.98	8	1
2:Y:25:LEU:CD2	2:Y:116:LEU:CD2	0.72	2.67	4	3
2:Y:12:ASP:OD1	2:Y:57:ASP:CB	0.72	2.38	5	1
2:Y:10:VAL:HG21	2:Y:33:VAL:HG12	0.72	1.62	20	3
2:Y:20:ILE:O	2:Y:24:LEU:CG	0.72	2.37	17	2
1:A:57:PHE:O	1:A:57:PHE:CG	0.72	2.43	14	1
2:Y:17:MET:O	2:Y:21:VAL:HG12	0.72	1.84	25	1
2:Y:20:ILE:HA	2:Y:23:ASN:OD1	0.71	1.85	2	3
1:A:7:ASP:HB3	1:A:8:PHE:CG	0.71	2.14	6	1
1:A:59:PHE:HD1	1:A:105:TYR:CE1	0.71	2.02	14	1
1:A:166:ARG:NH1	1:A:220:GLN:HG3	0.71	2.01	1	25
2:Y:11:VAL:HG12	2:Y:36:ALA:HB3	0.71	1.61	23	1
2:Y:18:ARG:O	2:Y:21:VAL:CG2	0.71	2.38	12	1
1:A:8:PHE:CD1	1:A:57:PHE:CE1	0.71	2.79	2	2
1:A:7:ASP:HB2	1:A:8:PHE:CZ	0.71	2.18	6	1
2:Y:11:VAL:CG2	2:Y:56:SER:CA	0.71	2.68	11	2
1:A:9:TYR:CE1	1:A:57:PHE:CD1	0.71	2.79	19	2
1:A:7:ASP:OD1	1:A:7:ASP:N	0.70	2.24	19	2
2:Y:20:ILE:HG23	2:Y:23:ASN:HD21	0.70	1.45	5	1
1:A:11:THR:HG22	2:Y:16:THR:CG2	0.70	2.16	23	3
1:A:9:TYR:CZ	1:A:57:PHE:CE2	0.70	2.79	14	1
2:Y:25:LEU:HD13	2:Y:30:PHE:CB	0.70	2.17	14	1
2:Y:111:PHE:CE2	2:Y:116:LEU:HD13	0.70	2.22	25	3
1:A:56:THR:HG22	1:A:57:PHE:CG	0.70	2.21	21	12
2:Y:111:PHE:CZ	2:Y:116:LEU:HD22	0.70	2.22	14	2
2:Y:111:PHE:CD1	2:Y:116:LEU:HB2	0.70	2.22	7	16
1:A:8:PHE:CZ	1:A:57:PHE:CD1	0.70	2.80	2	1
2:Y:10:VAL:CG2	2:Y:33:VAL:CG1	0.70	2.69	6	8
1:A:15:GLU:OE2	1:A:16:ALA:N	0.69	2.25	9	6
1:A:8:PHE:HB3	2:Y:20:ILE:HD13	0.69	1.64	14	1
2:Y:9:LEU:HG	2:Y:11:VAL:HG23	0.69	1.63	19	1
2:Y:20:ILE:O	2:Y:24:LEU:CD2	0.69	2.41	17	2
1:A:215:VAL:HG12	1:A:216:ILE:HD12	0.69	1.62	1	25
1:A:60:THR:HA	1:A:63:GLN:CD	0.69	2.12	24	1
2:Y:9:LEU:HD22	2:Y:51:TYR:CE1	0.69	2.23	5	3
2:Y:14:PHE:CE1	2:Y:16:THR:HB	0.69	2.23	13	14
1:A:9:TYR:CE1	1:A:59:PHE:CE2	0.69	2.81	6	2
1:A:8:PHE:CE2	2:Y:110:PRO:CG	0.68	2.76	3	1
1:A:77:ARG:HH12	2:Y:61:PRO:CB	0.68	2.01	20	2
2:Y:40:VAL:H	2:Y:62:ASN:ND2	0.68	1.85	20	2
2:Y:9:LEU:CD1	2:Y:51:TYR:CE1	0.68	2.76	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:55:ILE:CG2	2:Y:86:VAL:HG21	0.68	2.19	22	12
2:Y:73:ARG:HD3	2:Y:79:SER:O	0.68	1.88	1	25
1:A:9:TYR:CE2	1:A:57:PHE:CZ	0.68	2.81	6	1
1:A:57:PHE:CD1	1:A:59:PHE:CD2	0.68	2.81	14	1
1:A:162:ILE:HB	1:A:199:LEU:HD22	0.68	1.65	1	25
2:Y:9:LEU:HD13	2:Y:51:TYR:CZ	0.68	2.23	2	10
2:Y:58:TRP:CH2	2:Y:85:MET:HB2	0.68	2.24	22	1
2:Y:11:VAL:HG12	2:Y:56:SER:HA	0.67	1.64	1	1
1:A:8:PHE:HB2	2:Y:20:ILE:HD12	0.67	1.66	3	2
2:Y:12:ASP:OD2	2:Y:17:MET:HE3	0.67	1.89	17	1
2:Y:25:LEU:HD22	2:Y:30:PHE:CG	0.67	2.25	19	1
1:A:42:ALA:HA	1:A:45:ARG:HD3	0.67	1.67	4	1
2:Y:21:VAL:HG12	2:Y:25:LEU:HD11	0.67	1.67	20	1
2:Y:57:ASP:OD2	2:Y:59:ASN:O	0.67	2.13	8	4
1:A:11:THR:OG1	2:Y:16:THR:CG2	0.66	2.43	8	3
1:A:9:TYR:OH	1:A:59:PHE:CE1	0.66	2.48	6	1
1:A:77:ARG:HH22	2:Y:61:PRO:HB3	0.66	1.49	19	5
2:Y:40:VAL:O	2:Y:44:ASN:N	0.66	2.28	1	25
2:Y:24:LEU:HD12	2:Y:111:PHE:CE1	0.66	2.26	23	1
1:A:62:LEU:HD12	1:A:66:THR:CG2	0.66	2.21	5	4
1:A:66:THR:HG22	1:A:98:MET:HE3	0.66	1.68	7	25
2:Y:17:MET:HE2	2:Y:17:MET:HA	0.65	1.68	5	1
1:A:60:THR:HA	1:A:63:GLN:CG	0.65	2.21	24	1
2:Y:126:LYS:O	2:Y:126:LYS:HG3	0.65	1.91	1	25
1:A:11:THR:HG23	2:Y:16:THR:CG2	0.65	2.21	16	8
2:Y:25:LEU:HD22	2:Y:30:PHE:HB2	0.65	1.69	19	4
1:A:8:PHE:CB	2:Y:20:ILE:CD1	0.65	2.75	3	2
2:Y:24:LEU:HD11	2:Y:112:THR:C	0.65	2.16	20	3
2:Y:20:ILE:HA	2:Y:23:ASN:ND2	0.65	2.07	8	6
1:A:51:LYS:HG3	1:A:63:GLN:HE21	0.65	1.50	10	1
2:Y:13:ASP:HA	2:Y:37:GLU:HG2	0.64	1.68	1	2
2:Y:14:PHE:CZ	2:Y:16:THR:OG1	0.64	2.50	1	2
2:Y:10:VAL:CG2	2:Y:33:VAL:HG13	0.64	2.22	2	7
2:Y:24:LEU:HD13	2:Y:24:LEU:C	0.64	2.17	7	1
1:A:11:THR:CG2	2:Y:16:THR:CG2	0.64	2.74	9	8
1:A:41:ASN:O	1:A:45:ARG:CD	0.64	2.45	4	2
2:Y:91:LYS:O	2:Y:95:ILE:HG13	0.64	1.92	1	25
1:A:11:THR:HG23	2:Y:16:THR:HG21	0.64	1.69	3	6
1:A:59:PHE:CZ	1:A:105:TYR:HB3	0.64	2.27	6	1
2:Y:9:LEU:CD1	2:Y:51:TYR:CZ	0.64	2.81	12	2
1:A:60:THR:O	1:A:63:GLN:CG	0.64	2.46	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:9:LEU:HB2	2:Y:51:TYR:CD1	0.64	2.28	14	24
1:A:11:THR:HB	2:Y:16:THR:CG2	0.63	2.23	10	4
2:Y:38:ASP:O	2:Y:42:ALA:N	0.63	2.30	1	25
2:Y:9:LEU:HD11	2:Y:36:ALA:HB2	0.63	1.69	8	6
1:A:9:TYR:CD1	1:A:57:PHE:CD2	0.63	2.86	6	3
2:Y:14:PHE:CD2	2:Y:17:MET:HB2	0.63	2.27	11	9
1:A:77:ARG:NH2	2:Y:61:PRO:HB3	0.63	2.08	19	3
1:A:54:ALA:HB2	1:A:62:LEU:HD23	0.63	1.70	12	3
1:A:9:TYR:CE1	1:A:57:PHE:HD2	0.63	2.06	14	1
2:Y:18:ARG:C	2:Y:21:VAL:HG12	0.63	2.17	25	2
1:A:51:LYS:HG3	1:A:63:GLN:NE2	0.63	2.09	10	1
2:Y:72:ILE:HA	2:Y:78:MET:HE3	0.63	1.70	1	25
2:Y:24:LEU:CD2	2:Y:113:ALA:CB	0.63	2.76	20	6
2:Y:14:PHE:CZ	2:Y:16:THR:HG22	0.62	2.29	5	3
1:A:9:TYR:CE2	1:A:57:PHE:CE1	0.62	2.87	6	2
1:A:57:PHE:CD1	1:A:57:PHE:O	0.62	2.51	6	1
2:Y:25:LEU:HD12	2:Y:33:VAL:HG21	0.62	1.70	16	2
2:Y:12:ASP:OD1	2:Y:57:ASP:HB2	0.62	1.93	5	2
1:A:61:ILE:O	1:A:65:THR:OG1	0.62	2.18	11	2
2:Y:42:ALA:O	2:Y:46:LEU:N	0.62	2.31	1	25
1:A:8:PHE:CE1	1:A:57:PHE:HD1	0.62	2.11	21	2
2:Y:20:ILE:CG2	2:Y:23:ASN:OD1	0.62	2.48	14	1
2:Y:124:PHE:HD1	2:Y:129:MET:HE2	0.62	1.52	1	25
2:Y:14:PHE:O	2:Y:18:ARG:HG2	0.62	1.95	2	1
1:A:42:ALA:HA	1:A:45:ARG:CG	0.62	2.24	4	3
1:A:65:THR:HG22	1:A:66:THR:N	0.62	2.08	10	2
1:A:57:PHE:CD1	1:A:59:PHE:CG	0.62	2.88	14	1
1:A:42:ALA:HA	1:A:45:ARG:HG2	0.62	1.71	21	2
2:Y:37:GLU:OE1	2:Y:41:ASP:CB	0.62	2.48	18	1
2:Y:53:PHE:CE1	2:Y:84:LEU:HB2	0.62	2.29	1	25
2:Y:58:TRP:CZ3	2:Y:85:MET:HB2	0.62	2.30	22	2
2:Y:59:ASN:C	2:Y:60:MET:HG3	0.61	2.19	1	25
2:Y:112:THR:HG22	2:Y:113:ALA:N	0.61	2.11	14	7
2:Y:17:MET:HE3	2:Y:21:VAL:HB	0.61	1.71	3	1
1:A:8:PHE:CD2	2:Y:110:PRO:HB2	0.61	2.29	7	4
1:A:62:LEU:HD22	1:A:101:GLN:HB2	0.61	1.70	5	1
1:A:12:PHE:CE1	1:A:15:GLU:OE2	0.61	2.54	8	2
2:Y:13:ASP:OD1	2:Y:13:ASP:N	0.61	2.34	5	4
2:Y:15:SER:HA	2:Y:18:ARG:NH1	0.61	2.10	13	1
2:Y:25:LEU:HD22	2:Y:116:LEU:CD2	0.61	2.25	17	1
1:A:45:ARG:HD3	2:Y:37:GLU:OE2	0.61	1.96	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:THR:HG22	2:Y:16:THR:HG1	0.61	1.56	25	1
2:Y:58:TRP:CZ3	2:Y:85:MET:HB3	0.60	2.31	22	2
1:A:45:ARG:NH1	2:Y:37:GLU:OE1	0.60	2.34	9	3
1:A:15:GLU:HG3	2:Y:14:PHE:CE1	0.60	2.31	4	8
1:A:173:ASP:OD1	1:A:190:LYS:NZ	0.60	2.29	1	25
2:Y:25:LEU:O	2:Y:30:PHE:N	0.60	2.33	1	25
2:Y:57:ASP:OD1	2:Y:58:TRP:N	0.60	2.34	1	1
1:A:26:HIS:ND1	1:A:39:GLN:OE1	0.60	2.34	11	3
2:Y:10:VAL:CG1	2:Y:18:ARG:HG2	0.60	2.27	1	2
2:Y:15:SER:HA	2:Y:18:ARG:HG3	0.60	1.74	2	1
2:Y:24:LEU:CD2	2:Y:113:ALA:CA	0.60	2.75	7	3
2:Y:15:SER:HA	2:Y:18:ARG:CZ	0.60	2.27	13	2
2:Y:18:ARG:CZ	2:Y:35:GLU:HB3	0.60	2.27	10	3
1:A:42:ALA:O	1:A:45:ARG:HG3	0.60	1.97	21	1
2:Y:55:ILE:HG22	2:Y:86:VAL:HG21	0.60	1.74	13	7
2:Y:14:PHE:C	2:Y:14:PHE:CD1	0.60	2.80	4	16
1:A:36:ASP:OD2	1:A:39:GLN:HG3	0.59	1.97	25	3
2:Y:14:PHE:C	2:Y:18:ARG:NH1	0.59	2.60	14	1
2:Y:13:ASP:HB3	2:Y:37:GLU:HG3	0.59	1.73	19	1
1:A:57:PHE:CD1	1:A:57:PHE:N	0.59	2.70	22	1
1:A:9:TYR:CD1	1:A:57:PHE:CE2	0.59	2.90	20	2
2:Y:12:ASP:HB3	2:Y:18:ARG:HD3	0.59	1.73	18	1
1:A:59:PHE:C	1:A:63:GLN:CD	0.59	2.71	24	1
1:A:56:THR:HG23	1:A:57:PHE:CE1	0.59	2.33	2	1
2:Y:11:VAL:CG2	2:Y:56:SER:CB	0.59	2.80	11	2
1:A:54:ALA:HB2	1:A:62:LEU:CD2	0.59	2.27	4	3
1:A:7:ASP:C	1:A:8:PHE:HD1	0.59	2.06	9	6
1:A:36:ASP:OD2	1:A:39:GLN:HG2	0.59	1.98	9	3
2:Y:112:THR:HG22	2:Y:113:ALA:H	0.59	1.56	14	12
1:A:15:GLU:OE2	1:A:16:ALA:CB	0.59	2.51	16	4
2:Y:24:LEU:HD22	2:Y:113:ALA:CA	0.59	2.28	21	5
2:Y:57:ASP:OD2	2:Y:59:ASN:ND2	0.59	2.36	4	2
2:Y:11:VAL:O	2:Y:12:ASP:CG	0.58	2.46	3	2
2:Y:72:ILE:HG23	2:Y:78:MET:HB3	0.58	1.73	1	25
2:Y:18:ARG:HE	2:Y:35:GLU:HB3	0.58	1.57	14	3
1:A:12:PHE:CD1	1:A:15:GLU:OE2	0.58	2.56	8	3
1:A:60:THR:O	1:A:63:GLN:HG2	0.58	1.98	24	1
1:A:48:HIS:NE2	2:Y:59:ASN:ND2	0.58	2.51	1	2
1:A:12:PHE:CE2	1:A:59:PHE:CE2	0.58	2.91	18	3
1:A:62:LEU:HD12	1:A:101:GLN:OE1	0.58	1.99	1	1
1:A:168:LYS:O	1:A:171:GLU:HB2	0.58	1.98	1	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:55:ILE:HG23	2:Y:86:VAL:HG23	0.58	1.76	2	7
1:A:62:LEU:O	1:A:66:THR:HG23	0.58	1.99	14	25
1:A:62:LEU:HD12	1:A:101:GLN:HB2	0.58	1.75	11	1
2:Y:37:GLU:OE1	2:Y:38:ASP:N	0.58	2.37	18	1
1:A:41:ASN:ND2	1:A:77:ARG:HH11	0.58	1.95	21	2
2:Y:111:PHE:CE1	2:Y:116:LEU:HB2	0.58	2.33	14	5
2:Y:21:VAL:HG13	2:Y:25:LEU:HD11	0.58	1.75	11	2
1:A:61:ILE:O	1:A:65:THR:HG23	0.58	1.99	18	1
1:A:15:GLU:OE2	2:Y:14:PHE:CE2	0.57	2.57	5	1
1:A:8:PHE:CD1	1:A:8:PHE:C	0.57	2.82	2	3
1:A:7:ASP:CG	1:A:8:PHE:CD1	0.57	2.72	6	1
1:A:15:GLU:OE1	2:Y:14:PHE:CZ	0.57	2.57	7	6
1:A:59:PHE:CD1	1:A:105:TYR:CG	0.57	2.92	14	1
1:A:65:THR:HG21	1:A:101:GLN:NE2	0.57	2.02	18	1
2:Y:37:GLU:CD	2:Y:41:ASP:OD2	0.57	2.47	21	1
1:A:61:ILE:HG23	1:A:116:PHE:CD1	0.57	2.35	7	15
2:Y:10:VAL:HG21	2:Y:33:VAL:HG13	0.57	1.76	7	6
2:Y:21:VAL:O	2:Y:25:LEU:HD23	0.57	1.99	17	1
2:Y:114:ALA:O	2:Y:117:GLU:HB3	0.57	1.99	1	25
1:A:56:THR:HG22	1:A:57:PHE:CD2	0.57	2.35	16	7
2:Y:24:LEU:HD21	2:Y:113:ALA:N	0.57	2.14	7	1
1:A:8:PHE:HB2	2:Y:20:ILE:HG21	0.57	1.75	21	1
2:Y:17:MET:HG3	2:Y:18:ARG:H	0.57	1.53	24	1
2:Y:12:ASP:O	2:Y:18:ARG:NH2	0.57	2.37	14	2
2:Y:25:LEU:HD22	2:Y:30:PHE:CB	0.57	2.29	19	3
2:Y:18:ARG:NE	2:Y:35:GLU:HB3	0.57	2.14	7	6
1:A:15:GLU:OE2	1:A:16:ALA:CA	0.57	2.53	9	4
2:Y:57:ASP:OD1	2:Y:60:MET:SD	0.57	2.62	6	3
2:Y:12:ASP:OD1	2:Y:12:ASP:C	0.56	2.48	7	1
2:Y:58:TRP:CH2	2:Y:94:ASN:HB3	0.56	2.34	7	5
1:A:55:GLY:HA2	1:A:63:GLN:NE2	0.56	2.15	14	1
1:A:45:ARG:NH2	2:Y:61:PRO:CG	0.56	2.68	3	1
1:A:7:ASP:C	1:A:8:PHE:CD1	0.56	2.84	22	16
2:Y:14:PHE:CZ	2:Y:16:THR:CG2	0.56	2.88	5	3
2:Y:13:ASP:HA	2:Y:37:GLU:HG3	0.56	1.76	16	4
1:A:213:CYS:O	2:Y:126:LYS:NZ	0.56	2.34	1	25
2:Y:20:ILE:HG12	2:Y:23:ASN:OD1	0.56	2.00	2	1
2:Y:38:ASP:CG	2:Y:62:ASN:OD1	0.56	2.47	6	2
2:Y:18:ARG:CZ	2:Y:37:GLU:OE2	0.56	2.54	11	1
1:A:57:PHE:CE1	1:A:59:PHE:CG	0.56	2.94	14	1
1:A:56:THR:HG21	1:A:57:PHE:CE1	0.56	2.36	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ARG:NH2	2:Y:61:PRO:HG2	0.56	2.16	3	1
2:Y:17:MET:SD	2:Y:21:VAL:HG23	0.56	2.41	6	1
2:Y:57:ASP:OD1	2:Y:57:ASP:N	0.56	2.36	6	1
1:A:57:PHE:CE2	1:A:59:PHE:CZ	0.56	2.94	14	1
2:Y:12:ASP:CG	2:Y:17:MET:HE3	0.56	2.26	17	1
1:A:11:THR:HG22	2:Y:16:THR:HG23	0.56	1.78	23	2
2:Y:93:GLU:CD	2:Y:93:GLU:H	0.55	2.09	1	14
2:Y:93:GLU:H	2:Y:93:GLU:CD	0.55	2.09	2	11
2:Y:14:PHE:CD2	2:Y:17:MET:HB3	0.55	2.35	13	3
2:Y:107:VAL:HG22	2:Y:108:VAL:N	0.55	2.17	1	25
2:Y:18:ARG:HD2	2:Y:35:GLU:HB3	0.55	1.78	21	5
2:Y:10:VAL:CG2	2:Y:33:VAL:HG12	0.55	2.29	20	1
2:Y:17:MET:HE2	2:Y:109:LYS:HD2	0.55	1.79	9	1
1:A:54:ALA:HB3	1:A:63:GLN:HG2	0.55	1.79	11	1
2:Y:45:LYS:O	2:Y:48:ALA:HB3	0.55	2.00	1	25
1:A:7:ASP:O	1:A:8:PHE:HD1	0.55	1.85	13	4
1:A:65:THR:CG2	1:A:66:THR:N	0.55	2.69	10	1
1:A:54:ALA:C	1:A:63:GLN:NE2	0.55	2.64	24	1
1:A:12:PHE:CD1	1:A:15:GLU:CD	0.55	2.85	8	2
2:Y:12:ASP:OD1	2:Y:18:ARG:CD	0.55	2.55	7	1
1:A:48:HIS:NE2	2:Y:59:ASN:HB3	0.55	2.16	5	1
1:A:15:GLU:CD	1:A:16:ALA:N	0.55	2.65	12	2
2:Y:21:VAL:HG12	2:Y:25:LEU:CD1	0.55	2.31	20	1
2:Y:20:ILE:HG23	2:Y:23:ASN:ND2	0.55	2.14	5	1
1:A:8:PHE:HB2	2:Y:20:ILE:CD1	0.55	2.32	3	2
1:A:9:TYR:OH	1:A:57:PHE:CD1	0.55	2.59	6	1
1:A:62:LEU:HD22	1:A:66:THR:HG23	0.55	1.79	23	1
2:Y:15:SER:OG	2:Y:18:ARG:NH2	0.55	2.40	6	1
2:Y:87:THR:HG22	2:Y:89:GLU:H	0.54	1.61	3	1
1:A:54:ALA:HB1	1:A:63:GLN:HG2	0.54	1.77	14	1
2:Y:17:MET:HE3	2:Y:109:LYS:HD2	0.54	1.78	21	1
1:A:172:VAL:CG1	1:A:190:LYS:HG2	0.54	2.33	1	25
1:A:62:LEU:HD23	1:A:101:GLN:OE1	0.54	2.02	23	1
1:A:15:GLU:CG	2:Y:14:PHE:CE1	0.54	2.91	15	2
1:A:8:PHE:C	1:A:8:PHE:HD1	0.54	2.11	21	3
2:Y:9:LEU:C	2:Y:9:LEU:HD12	0.54	2.27	17	1
2:Y:24:LEU:HD21	2:Y:113:ALA:HA	0.54	1.76	7	1
2:Y:15:SER:N	2:Y:18:ARG:NH1	0.54	2.56	14	2
1:A:11:THR:HG1	2:Y:16:THR:HG1	0.54	1.45	16	1
2:Y:55:ILE:HG23	2:Y:86:VAL:HG22	0.54	1.79	13	5
1:A:57:PHE:C	1:A:57:PHE:HD1	0.54	2.05	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:82:PRO:HA	2:Y:104:SER:OG	0.54	2.03	1	25
2:Y:13:ASP:OD2	2:Y:60:MET:HG2	0.54	2.02	5	1
2:Y:12:ASP:OD1	2:Y:18:ARG:HD3	0.54	2.02	7	1
2:Y:18:ARG:NH1	2:Y:37:GLU:OE2	0.54	2.37	17	1
2:Y:18:ARG:NH1	2:Y:37:GLU:OE1	0.53	2.41	19	1
1:A:15:GLU:OE2	2:Y:16:THR:CB	0.53	2.56	20	1
1:A:57:PHE:CE1	1:A:59:PHE:CZ	0.53	2.97	14	1
2:Y:120:LEU:HB3	2:Y:124:PHE:CE2	0.53	2.38	1	25
2:Y:25:LEU:HD13	2:Y:30:PHE:HB2	0.53	1.80	14	1
2:Y:17:MET:CE	2:Y:20:ILE:HD12	0.53	2.34	5	1
1:A:45:ARG:HD3	2:Y:61:PRO:HG2	0.53	1.81	15	1
2:Y:58:TRP:CH2	2:Y:85:MET:CB	0.53	2.92	22	1
1:A:8:PHE:CE2	2:Y:110:PRO:CB	0.53	2.91	3	1
1:A:51:LYS:CG	1:A:63:GLN:NE2	0.53	2.71	10	1
2:Y:19:ARG:O	2:Y:23:ASN:ND2	0.53	2.42	21	1
2:Y:24:LEU:HD13	2:Y:24:LEU:O	0.53	2.04	7	1
1:A:213:CYS:HA	1:A:216:ILE:O	0.53	2.04	1	25
1:A:57:PHE:HB2	1:A:59:PHE:CE2	0.53	2.39	25	6
1:A:45:ARG:HH12	2:Y:37:GLU:HB3	0.53	1.64	8	1
1:A:12:PHE:O	1:A:15:GLU:OE2	0.52	2.26	10	4
1:A:9:TYR:CE2	1:A:57:PHE:HE2	0.52	2.21	14	1
2:Y:24:LEU:O	2:Y:25:LEU:C	0.52	2.52	1	25
2:Y:38:ASP:OD2	2:Y:62:ASN:ND2	0.52	2.42	9	5
2:Y:58:TRP:CD1	2:Y:58:TRP:C	0.52	2.87	21	2
2:Y:111:PHE:CD1	2:Y:111:PHE:N	0.52	2.68	25	1
1:A:56:THR:CG2	1:A:57:PHE:CG	0.52	2.92	3	2
2:Y:87:THR:CG2	2:Y:89:GLU:O	0.52	2.58	3	1
1:A:15:GLU:HG2	1:A:16:ALA:N	0.52	2.11	8	5
1:A:9:TYR:CE1	1:A:57:PHE:CE2	0.52	2.97	14	1
2:Y:14:PHE:CD2	2:Y:17:MET:CB	0.52	2.93	13	3
2:Y:10:VAL:HG12	2:Y:18:ARG:CG	0.52	2.34	15	1
2:Y:53:PHE:HE1	2:Y:84:LEU:CB	0.52	2.17	1	25
2:Y:24:LEU:HD22	2:Y:113:ALA:CB	0.52	2.35	12	7
2:Y:20:ILE:HG22	2:Y:24:LEU:CD1	0.52	2.29	18	1
2:Y:58:TRP:CE3	2:Y:85:MET:HB3	0.52	2.40	22	1
1:A:60:THR:CA	1:A:63:GLN:CG	0.52	2.87	24	1
2:Y:12:ASP:OD1	2:Y:57:ASP:HB3	0.52	2.04	5	1
2:Y:17:MET:HE1	2:Y:109:LYS:CD	0.52	2.35	13	1
1:A:8:PHE:CD2	2:Y:20:ILE:HG21	0.52	2.40	24	1
2:Y:10:VAL:CG1	2:Y:18:ARG:CG	0.52	2.87	1	3
1:A:61:ILE:HG23	1:A:116:PHE:CG	0.52	2.40	6	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:18:ARG:O	2:Y:21:VAL:HG13	0.52	2.05	25	1
1:A:11:THR:HG23	2:Y:16:THR:HB	0.52	1.82	1	1
1:A:12:PHE:CE1	1:A:102:LEU:HD11	0.52	2.40	12	1
2:Y:58:TRP:HE3	2:Y:86:VAL:O	0.52	1.88	22	1
1:A:49:SER:HB3	2:Y:14:PHE:CD1	0.51	2.39	1	6
2:Y:17:MET:O	2:Y:18:ARG:C	0.51	2.52	1	25
2:Y:37:GLU:OE2	2:Y:38:ASP:CG	0.51	2.53	3	2
2:Y:55:ILE:HG22	2:Y:86:VAL:CG2	0.51	2.34	13	6
1:A:9:TYR:HB3	1:A:13:PHE:CZ	0.51	2.40	8	1
1:A:62:LEU:CD1	1:A:66:THR:HG23	0.51	2.35	5	1
2:Y:21:VAL:HA	2:Y:24:LEU:CD1	0.51	2.24	17	1
1:A:12:PHE:C	1:A:12:PHE:CD1	0.51	2.87	9	3
2:Y:39:GLY:O	2:Y:43:LEU:HB2	0.51	2.05	1	25
2:Y:18:ARG:O	2:Y:22:ARG:HG3	0.51	2.06	23	2
1:A:11:THR:CG2	2:Y:16:THR:HG21	0.51	2.35	8	2
1:A:45:ARG:HG3	1:A:46:ALA:N	0.51	2.19	18	1
2:Y:13:ASP:O	2:Y:18:ARG:NH2	0.51	2.44	20	1
1:A:165:SER:C	1:A:166:ARG:HG3	0.51	2.29	1	25
1:A:172:VAL:O	1:A:176:GLU:HB3	0.51	2.05	1	25
2:Y:11:VAL:C	2:Y:12:ASP:CG	0.51	2.79	3	1
1:A:60:THR:C	1:A:63:GLN:HG2	0.51	2.31	24	1
2:Y:10:VAL:HG12	2:Y:18:ARG:HG2	0.51	1.81	15	2
2:Y:4:LYS:HA	2:Y:30:PHE:CD2	0.51	2.41	1	25
2:Y:18:ARG:C	2:Y:21:VAL:CG2	0.51	2.84	12	1
1:A:36:ASP:OD2	1:A:39:GLN:NE2	0.51	2.44	22	1
2:Y:40:VAL:CG2	2:Y:62:ASN:HB3	0.51	2.36	2	2
2:Y:57:ASP:C	2:Y:57:ASP:OD1	0.51	2.53	4	1
1:A:60:THR:CA	1:A:63:GLN:CD	0.51	2.84	24	1
2:Y:14:PHE:CE2	2:Y:17:MET:HB2	0.51	2.41	11	6
1:A:9:TYR:CD1	1:A:57:PHE:HD2	0.51	2.23	14	1
2:Y:54:VAL:HG12	2:Y:56:SER:CB	0.51	2.32	1	25
1:A:56:THR:CG2	1:A:57:PHE:N	0.51	2.72	2	3
1:A:11:THR:CG2	2:Y:16:THR:OG1	0.51	2.55	22	1
2:Y:12:ASP:CG	2:Y:14:PHE:H	0.50	2.14	7	2
1:A:125:GLN:O	1:A:129:GLU:HG3	0.50	2.07	1	25
2:Y:12:ASP:OD2	2:Y:17:MET:HE1	0.50	2.06	18	1
2:Y:58:TRP:CH2	2:Y:94:ASN:CB	0.50	2.95	6	1
1:A:12:PHE:O	1:A:15:GLU:CD	0.50	2.54	25	6
1:A:41:ASN:ND2	1:A:41:ASN:C	0.50	2.70	15	1
1:A:174:LEU:O	1:A:178:GLU:N	0.50	2.44	1	25
2:Y:24:LEU:HD22	2:Y:113:ALA:HB2	0.50	1.81	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LYS:O	1:A:63:GLN:NE2	0.50	2.44	13	1
1:A:59:PHE:CE1	1:A:105:TYR:HB3	0.50	2.42	14	1
2:Y:64:ASP:O	2:Y:68:LEU:HB2	0.50	2.07	1	25
2:Y:9:LEU:HG	2:Y:11:VAL:CG2	0.50	2.35	19	2
2:Y:25:LEU:HD13	2:Y:30:PHE:HB3	0.50	1.84	14	1
2:Y:53:PHE:HE1	2:Y:84:LEU:HB2	0.50	1.63	1	25
2:Y:11:VAL:CG1	2:Y:36:ALA:HB3	0.50	2.35	17	3
1:A:11:THR:HB	2:Y:16:THR:HG21	0.50	1.83	10	2
2:Y:20:ILE:CG2	2:Y:24:LEU:HD11	0.50	2.37	6	1
2:Y:21:VAL:CG1	2:Y:25:LEU:HD11	0.50	2.36	16	1
2:Y:12:ASP:OD1	2:Y:57:ASP:OD2	0.50	2.30	1	1
2:Y:24:LEU:CD2	2:Y:113:ALA:N	0.50	2.75	18	2
2:Y:17:MET:SD	2:Y:109:LYS:HD2	0.50	2.47	2	1
1:A:8:PHE:HB3	2:Y:20:ILE:CD1	0.50	2.36	8	4
2:Y:115:THR:O	2:Y:116:LEU:C	0.50	2.53	1	25
1:A:9:TYR:HB3	1:A:13:PHE:CE2	0.50	2.42	24	7
2:Y:11:VAL:C	2:Y:12:ASP:OD1	0.50	2.55	3	2
2:Y:12:ASP:OD1	2:Y:13:ASP:N	0.50	2.45	21	4
2:Y:57:ASP:OD1	2:Y:57:ASP:C	0.49	2.54	1	2
2:Y:111:PHE:CD1	2:Y:111:PHE:C	0.49	2.90	14	2
2:Y:61:PRO:C	2:Y:62:ASN:CG	0.49	2.80	6	2
1:A:9:TYR:CZ	1:A:57:PHE:HE2	0.49	2.23	14	1
1:A:41:ASN:HD22	1:A:77:ARG:HH11	0.49	1.50	21	2
2:Y:20:ILE:C	2:Y:24:LEU:HD21	0.49	2.32	17	1
2:Y:12:ASP:OD2	2:Y:17:MET:HE2	0.49	2.06	20	1
2:Y:12:ASP:HB3	2:Y:18:ARG:CD	0.49	2.36	1	2
2:Y:40:VAL:HG23	2:Y:62:ASN:HB3	0.49	1.84	2	2
2:Y:23:ASN:OD1	2:Y:24:LEU:HD23	0.49	2.08	4	2
1:A:62:LEU:CD1	1:A:66:THR:CG2	0.49	2.90	5	2
1:A:10:GLN:HG2	1:A:11:THR:N	0.49	2.23	7	1
2:Y:11:VAL:HG22	2:Y:36:ALA:HB3	0.49	1.84	19	1
1:A:224:GLU:O	1:A:225:THR:C	0.49	2.55	1	25
1:A:8:PHE:CZ	1:A:57:PHE:CE1	0.49	2.99	2	1
2:Y:20:ILE:CG2	2:Y:21:VAL:N	0.49	2.75	4	2
1:A:204:ALA:O	1:A:205:GLU:C	0.49	2.56	1	25
2:Y:24:LEU:HD22	2:Y:113:ALA:HA	0.49	1.84	2	5
1:A:15:GLU:CD	2:Y:14:PHE:CZ	0.49	2.91	18	2
1:A:41:ASN:OD1	1:A:45:ARG:HD2	0.49	2.08	16	1
1:A:15:GLU:CG	1:A:16:ALA:N	0.49	2.75	25	9
2:Y:18:ARG:HA	2:Y:21:VAL:CG2	0.49	2.38	12	1
2:Y:65:GLY:O	2:Y:68:LEU:HB3	0.49	2.08	1	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:PHE:CE2	2:Y:110:PRO:HG3	0.49	2.41	3	1
2:Y:14:PHE:CE1	2:Y:16:THR:N	0.49	2.80	4	7
2:Y:20:ILE:CG1	2:Y:24:LEU:HD21	0.49	2.29	4	1
2:Y:18:ARG:HD2	2:Y:35:GLU:HG2	0.49	1.83	16	4
2:Y:73:ARG:NH1	2:Y:80:ALA:HA	0.49	2.23	1	25
2:Y:37:GLU:O	2:Y:37:GLU:HG2	0.49	2.07	22	1
2:Y:66:LEU:O	2:Y:70:LYS:N	0.49	2.45	1	25
2:Y:25:LEU:HD23	2:Y:116:LEU:HD21	0.49	1.85	5	2
2:Y:38:ASP:CG	2:Y:62:ASN:HD21	0.49	2.15	20	2
1:A:12:PHE:CG	1:A:13:PHE:N	0.49	2.80	12	1
2:Y:17:MET:CE	2:Y:109:LYS:HD2	0.49	2.38	21	2
2:Y:20:ILE:CG1	2:Y:21:VAL:N	0.49	2.74	23	2
1:A:8:PHE:CZ	2:Y:110:PRO:HG3	0.48	2.43	3	1
2:Y:12:ASP:OD1	2:Y:18:ARG:CG	0.48	2.61	7	1
1:A:11:THR:HG23	2:Y:16:THR:OG1	0.48	2.08	14	2
1:A:62:LEU:HD22	1:A:66:THR:CG2	0.48	2.37	10	1
1:A:13:PHE:CD1	1:A:106:LYS:CG	0.48	2.96	11	3
2:Y:20:ILE:HG13	2:Y:21:VAL:N	0.48	2.23	16	2
1:A:15:GLU:OE2	2:Y:16:THR:HB	0.48	2.07	20	1
2:Y:58:TRP:CZ3	2:Y:94:ASN:HB3	0.48	2.43	6	2
1:A:11:THR:HG21	2:Y:16:THR:HG23	0.48	1.85	14	1
1:A:11:THR:C	2:Y:16:THR:HG21	0.48	2.32	21	2
1:A:45:ARG:NH2	2:Y:13:ASP:HB3	0.48	2.23	8	1
2:Y:13:ASP:C	2:Y:18:ARG:NH1	0.48	2.71	12	2
2:Y:17:MET:SD	2:Y:109:LYS:CD	0.48	3.01	2	1
1:A:56:THR:HG21	1:A:57:PHE:CZ	0.48	2.44	3	1
2:Y:12:ASP:OD1	2:Y:18:ARG:HG3	0.48	2.08	7	1
2:Y:11:VAL:HG21	2:Y:56:SER:OG	0.48	2.08	11	1
2:Y:7:LYS:HD3	2:Y:51:TYR:CE1	0.48	2.44	1	25
2:Y:87:THR:HG22	2:Y:89:GLU:O	0.48	2.09	3	1
1:A:41:ASN:O	1:A:45:ARG:HD2	0.48	2.09	6	2
2:Y:24:LEU:HD11	2:Y:111:PHE:O	0.48	2.09	21	2
2:Y:124:PHE:HD1	2:Y:129:MET:CE	0.47	2.21	1	25
2:Y:57:ASP:OD1	2:Y:57:ASP:O	0.47	2.31	6	1
1:A:63:GLN:HE22	1:A:67:HIS:HB2	0.47	1.69	10	1
2:Y:13:ASP:OD1	2:Y:37:GLU:O	0.47	2.32	1	1
2:Y:27:GLU:O	2:Y:27:GLU:HG3	0.47	2.09	1	25
2:Y:15:SER:CA	2:Y:18:ARG:HG3	0.47	2.39	2	1
2:Y:24:LEU:CD2	2:Y:111:PHE:O	0.47	2.62	10	1
1:A:45:ARG:CZ	2:Y:61:PRO:HG2	0.47	2.39	16	1
1:A:15:GLU:HG2	2:Y:14:PHE:CE1	0.47	2.45	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:PHE:CD2	2:Y:110:PRO:CB	0.47	2.98	5	2
1:A:9:TYR:CD2	1:A:57:PHE:CZ	0.47	3.02	6	1
2:Y:24:LEU:N	2:Y:24:LEU:CD2	0.47	2.69	23	2
2:Y:25:LEU:CD2	2:Y:30:PHE:CD1	0.47	2.96	19	1
2:Y:11:VAL:CG2	2:Y:36:ALA:HB3	0.47	2.36	21	1
2:Y:13:ASP:OD1	2:Y:37:GLU:OE2	0.47	2.33	22	1
1:A:56:THR:HG22	1:A:57:PHE:N	0.47	2.24	9	16
2:Y:109:LYS:HA	2:Y:111:PHE:CD2	0.47	2.44	10	6
2:Y:23:ASN:N	2:Y:23:ASN:HD22	0.47	2.08	11	1
2:Y:9:LEU:CD1	2:Y:11:VAL:HG22	0.47	2.39	17	1
1:A:59:PHE:C	1:A:63:GLN:NE2	0.47	2.73	24	1
1:A:7:ASP:O	1:A:8:PHE:CD1	0.47	2.68	1	1
1:A:54:ALA:HB2	1:A:62:LEU:HD21	0.47	1.86	4	1
1:A:12:PHE:CD1	1:A:12:PHE:C	0.47	2.91	18	1
2:Y:12:ASP:OD1	2:Y:12:ASP:O	0.47	2.33	7	1
2:Y:87:THR:OG1	2:Y:89:GLU:O	0.47	2.33	7	4
2:Y:18:ARG:HH21	2:Y:35:GLU:HB3	0.47	1.69	11	1
1:A:202:ASP:OD1	1:A:203:ILE:HG22	0.47	2.10	1	25
2:Y:25:LEU:CD2	2:Y:30:PHE:HB2	0.47	2.39	1	1
2:Y:57:ASP:OD1	2:Y:59:ASN:ND2	0.47	2.47	1	1
1:A:45:ARG:NH1	2:Y:37:GLU:HB2	0.47	2.25	2	1
2:Y:14:PHE:CZ	2:Y:16:THR:CB	0.47	2.98	5	7
1:A:179:LEU:CB	1:A:185:LEU:HD11	0.46	2.41	1	25
1:A:11:THR:OG1	2:Y:16:THR:HG23	0.46	2.09	8	2
2:Y:23:ASN:OD1	2:Y:24:LEU:N	0.46	2.49	6	2
1:A:182:LEU:HD11	1:A:211:VAL:CG1	0.46	2.41	1	25
2:Y:58:TRP:C	2:Y:59:ASN:OD1	0.46	2.58	6	2
1:A:166:ARG:CZ	1:A:220:GLN:HG3	0.46	2.39	1	25
2:Y:34:GLU:CG	2:Y:35:GLU:N	0.46	2.78	1	25
2:Y:20:ILE:HG23	2:Y:24:LEU:HD11	0.46	1.87	6	1
2:Y:20:ILE:HG23	2:Y:24:LEU:CD1	0.46	2.40	19	2
2:Y:24:LEU:CD1	2:Y:24:LEU:C	0.46	2.88	7	1
1:A:60:THR:O	1:A:63:GLN:HG3	0.46	2.10	24	1
2:Y:98:ALA:HB1	2:Y:103:ALA:HB3	0.46	1.87	1	25
2:Y:59:ASN:ND2	2:Y:59:ASN:H	0.46	2.09	4	1
1:A:9:TYR:OH	1:A:59:PHE:CZ	0.46	2.68	6	1
2:Y:24:LEU:CD2	2:Y:113:ALA:HA	0.46	2.37	7	1
2:Y:12:ASP:O	2:Y:18:ARG:NE	0.46	2.48	11	1
2:Y:14:PHE:CE2	2:Y:17:MET:CB	0.46	2.99	13	1
1:A:24:GLU:HB2	1:A:95:LYS:HE2	0.46	1.87	7	25
1:A:182:LEU:HD11	1:A:211:VAL:HB	0.46	1.86	1	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:TYR:CE1	1:A:57:PHE:HB3	0.46	2.45	2	1
2:Y:40:VAL:CG2	2:Y:62:ASN:HB2	0.46	2.41	20	2
2:Y:9:LEU:CD2	2:Y:11:VAL:CG2	0.46	2.77	15	1
2:Y:11:VAL:O	2:Y:57:ASP:HB3	0.46	2.11	23	4
2:Y:23:ASN:OD1	2:Y:23:ASN:O	0.46	2.33	4	1
1:A:48:HIS:NE2	2:Y:59:ASN:HB2	0.46	2.25	15	1
1:A:15:GLU:OE2	2:Y:14:PHE:CE1	0.46	2.69	3	1
1:A:9:TYR:CG	1:A:57:PHE:CE2	0.46	3.03	6	1
1:A:41:ASN:OD1	1:A:45:ARG:CZ	0.46	2.64	13	1
2:Y:12:ASP:O	2:Y:18:ARG:CZ	0.45	2.65	20	1
2:Y:124:PHE:CD1	2:Y:129:MET:CE	0.45	3.00	1	25
2:Y:37:GLU:OE2	2:Y:38:ASP:N	0.45	2.49	7	1
1:A:11:THR:OG1	2:Y:16:THR:OG1	0.45	2.19	20	1
1:A:59:PHE:CD2	1:A:105:TYR:CD2	0.45	3.04	21	1
1:A:9:TYR:CE1	1:A:59:PHE:CE1	0.45	3.04	21	1
1:A:8:PHE:N	1:A:8:PHE:HD1	0.45	2.00	9	1
1:A:10:GLN:HG3	1:A:11:THR:H	0.45	1.68	8	1
2:Y:25:LEU:HD12	2:Y:30:PHE:HB2	0.45	1.87	17	1
1:A:39:GLN:HA	1:A:39:GLN:OE1	0.45	2.10	22	1
1:A:191:GLY:O	1:A:192:ALA:C	0.45	2.55	1	25
1:A:60:THR:HG22	1:A:61:ILE:N	0.45	2.26	14	2
2:Y:42:ALA:O	2:Y:46:LEU:HG	0.45	2.12	1	25
2:Y:9:LEU:HD11	2:Y:36:ALA:CB	0.45	2.41	8	1
1:A:50:ILE:CG2	1:A:62:LEU:HD11	0.45	2.42	4	1
2:Y:21:VAL:HG13	2:Y:25:LEU:CD1	0.45	2.41	11	1
2:Y:18:ARG:CA	2:Y:21:VAL:CG2	0.45	2.95	12	1
1:A:218:ALA:HA	1:A:221:ILE:HD12	0.45	1.89	1	25
1:A:8:PHE:CE2	2:Y:110:PRO:HB2	0.45	2.47	7	1
1:A:64:GLU:O	1:A:64:GLU:OE1	0.45	2.35	8	1
1:A:12:PHE:CD1	1:A:13:PHE:N	0.45	2.85	16	2
2:Y:11:VAL:O	2:Y:57:ASP:HB2	0.45	2.12	21	1
2:Y:24:LEU:HD22	2:Y:113:ALA:N	0.44	2.27	1	1
2:Y:24:LEU:CD1	2:Y:111:PHE:O	0.44	2.65	21	2
1:A:48:HIS:CD2	2:Y:13:ASP:OD1	0.44	2.70	14	2
2:Y:18:ARG:C	2:Y:21:VAL:HG23	0.44	2.37	14	1
1:A:57:PHE:N	1:A:57:PHE:HD1	0.44	2.08	22	1
1:A:59:PHE:O	1:A:63:GLN:CD	0.44	2.60	24	1
1:A:60:THR:CA	1:A:63:GLN:OE1	0.44	2.62	24	1
1:A:32:PRO:O	1:A:35:PRO:HD3	0.44	2.13	9	25
2:Y:14:PHE:CD1	2:Y:14:PHE:C	0.44	2.95	19	1
2:Y:107:VAL:CG2	2:Y:108:VAL:N	0.44	2.80	1	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:14:PHE:HZ	2:Y:16:THR:CG2	0.44	2.24	5	1
2:Y:24:LEU:CG	2:Y:113:ALA:HA	0.44	2.43	7	1
1:A:60:THR:C	1:A:63:GLN:CG	0.44	2.91	24	1
2:Y:24:LEU:HD13	2:Y:113:ALA:CA	0.44	2.42	25	1
1:A:41:ASN:ND2	1:A:45:ARG:HD2	0.44	2.28	5	1
1:A:10:GLN:CG	1:A:11:THR:N	0.44	2.80	7	1
2:Y:17:MET:HG3	2:Y:21:VAL:CG2	0.44	2.42	22	1
1:A:42:ALA:CA	1:A:45:ARG:HD3	0.44	2.40	4	1
1:A:61:ILE:HD13	1:A:111:PRO:HD2	0.44	1.89	16	1
2:Y:9:LEU:HG	2:Y:11:VAL:HG13	0.44	1.89	23	1
1:A:12:PHE:CD1	1:A:12:PHE:O	0.44	2.71	9	1
1:A:45:ARG:HD2	2:Y:13:ASP:CB	0.44	2.42	25	1
2:Y:86:VAL:HG22	2:Y:107:VAL:CG1	0.44	2.43	9	7
2:Y:12:ASP:O	2:Y:18:ARG:NH1	0.44	2.51	7	1
2:Y:19:ARG:O	2:Y:23:ASN:OD1	0.44	2.36	10	2
2:Y:15:SER:OG	2:Y:18:ARG:NH1	0.44	2.47	13	1
1:A:77:ARG:CZ	2:Y:61:PRO:HB3	0.44	2.43	20	1
2:Y:24:LEU:HD13	2:Y:113:ALA:N	0.44	2.27	25	1
1:A:11:THR:OG1	2:Y:16:THR:HG21	0.44	2.13	8	1
1:A:36:ASP:OD2	1:A:39:GLN:CG	0.44	2.66	18	1
1:A:8:PHE:HB3	2:Y:20:ILE:HG12	0.44	1.87	24	1
2:Y:25:LEU:HD22	2:Y:116:LEU:HD21	0.44	1.87	4	1
2:Y:112:THR:CG2	2:Y:113:ALA:N	0.44	2.81	13	2
1:A:15:GLU:HG2	2:Y:14:PHE:CZ	0.44	2.48	17	1
1:A:56:THR:O	2:Y:110:PRO:HD3	0.44	2.12	21	1
1:A:62:LEU:HD12	1:A:62:LEU:O	0.43	2.12	5	1
1:A:188:VAL:HG13	1:A:195:LEU:HD11	0.43	1.89	1	25
2:Y:23:ASN:OD1	2:Y:24:LEU:HG	0.43	2.12	6	1
1:A:53:GLY:O	1:A:57:PHE:CE2	0.43	2.71	21	1
1:A:215:VAL:HG12	1:A:216:ILE:CD1	0.43	2.40	1	25
1:A:8:PHE:HE2	2:Y:110:PRO:CG	0.43	2.23	3	1
2:Y:20:ILE:HG23	2:Y:23:ASN:OD1	0.43	2.13	18	1
2:Y:21:VAL:HG22	2:Y:25:LEU:HD12	0.43	1.89	25	1
1:A:77:ARG:HH22	2:Y:61:PRO:CB	0.43	2.23	19	1
2:Y:12:ASP:OD2	2:Y:57:ASP:HB2	0.43	2.12	3	1
1:A:41:ASN:C	1:A:45:ARG:HD3	0.43	2.38	4	1
2:Y:17:MET:CG	2:Y:18:ARG:N	0.43	2.76	17	1
2:Y:93:GLU:CD	2:Y:93:GLU:N	0.43	2.76	1	25
2:Y:14:PHE:C	2:Y:18:ARG:HG3	0.43	2.35	2	1
2:Y:12:ASP:HB3	2:Y:18:ARG:HD2	0.43	1.90	1	1
2:Y:10:VAL:HG13	2:Y:12:ASP:OD1	0.43	2.13	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ARG:NH1	2:Y:61:PRO:CG	0.43	2.81	7	1
1:A:45:ARG:NH1	2:Y:37:GLU:HG2	0.43	2.29	8	1
1:A:15:GLU:HG3	2:Y:14:PHE:CZ	0.43	2.48	9	2
1:A:57:PHE:CD1	1:A:59:PHE:CE2	0.43	3.06	14	1
1:A:45:ARG:CD	2:Y:61:PRO:CG	0.43	2.91	15	1
2:Y:84:LEU:HD13	2:Y:123:ILE:CD1	0.43	2.40	1	25
1:A:45:ARG:HH12	2:Y:61:PRO:CG	0.43	2.27	7	1
2:Y:37:GLU:OE1	2:Y:41:ASP:OD2	0.43	2.36	7	1
2:Y:25:LEU:HD12	2:Y:30:PHE:CB	0.43	2.43	17	1
2:Y:21:VAL:HG22	2:Y:25:LEU:CD1	0.43	2.43	25	1
2:Y:6:LEU:HD21	2:Y:53:PHE:CD2	0.43	2.48	1	25
1:A:56:THR:CG2	1:A:57:PHE:CZ	0.43	3.02	3	1
2:Y:59:ASN:OD1	2:Y:59:ASN:N	0.43	2.48	3	2
2:Y:111:PHE:CE1	2:Y:116:LEU:HD22	0.43	2.49	7	3
2:Y:41:ASP:O	2:Y:45:LYS:HB2	0.43	2.12	1	25
2:Y:37:GLU:O	2:Y:37:GLU:CG	0.43	2.66	4	1
1:A:61:ILE:HG12	1:A:116:PHE:CG	0.43	2.49	8	1
1:A:45:ARG:CG	2:Y:61:PRO:HG3	0.43	2.44	15	1
2:Y:20:ILE:C	2:Y:24:LEU:CD2	0.43	2.92	17	1
2:Y:24:LEU:HD23	2:Y:113:ALA:CA	0.43	2.44	18	1
2:Y:18:ARG:NH2	2:Y:35:GLU:OE1	0.43	2.51	23	1
1:A:97:ILE:O	1:A:101:GLN:HG3	0.42	2.14	21	25
2:Y:24:LEU:HA	2:Y:24:LEU:HD23	0.42	1.50	20	4
1:A:45:ARG:CZ	2:Y:13:ASP:HB2	0.42	2.43	8	1
2:Y:17:MET:HE1	2:Y:109:LYS:CB	0.42	2.44	13	1
1:A:36:ASP:HB3	1:A:39:GLN:HG3	0.42	1.90	18	1
2:Y:17:MET:HE1	2:Y:109:LYS:HD3	0.42	1.90	24	2
2:Y:11:VAL:O	2:Y:11:VAL:CG1	0.42	2.67	1	1
1:A:45:ARG:NH2	2:Y:13:ASP:CB	0.42	2.83	8	1
1:A:10:GLN:CD	1:A:11:THR:N	0.42	2.77	17	1
1:A:62:LEU:O	1:A:62:LEU:HD22	0.42	2.14	23	1
1:A:9:TYR:CZ	1:A:57:PHE:CG	0.42	3.03	6	1
2:Y:38:ASP:CG	2:Y:62:ASN:ND2	0.42	2.78	20	2
2:Y:11:VAL:HG21	2:Y:56:SER:CB	0.42	2.44	11	2
2:Y:9:LEU:HD11	2:Y:11:VAL:CG1	0.42	2.40	17	1
2:Y:17:MET:SD	2:Y:21:VAL:HG21	0.42	2.54	24	1
2:Y:43:LEU:HD22	2:Y:63:MET:SD	0.42	2.55	1	25
2:Y:91:LYS:HG3	2:Y:94:ASN:HB2	0.42	1.90	22	1
2:Y:60:MET:HE3	2:Y:60:MET:HB2	0.42	1.63	1	25
2:Y:21:VAL:CG1	2:Y:22:ARG:N	0.42	2.82	4	1
1:A:57:PHE:CG	1:A:59:PHE:CE2	0.42	3.07	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:111:PHE:O	2:Y:111:PHE:HD1	0.42	1.98	25	1
1:A:212:LEU:C	1:A:214:PHE:N	0.42	2.78	1	25
1:A:33:GLU:OE1	1:A:33:GLU:N	0.42	2.45	3	2
1:A:41:ASN:OD1	1:A:41:ASN:C	0.42	2.63	9	1
2:Y:17:MET:C	2:Y:17:MET:SD	0.42	3.02	10	1
2:Y:24:LEU:C	2:Y:26:LYS:N	0.42	2.77	1	25
1:A:55:GLY:N	1:A:63:GLN:HG3	0.42	2.30	23	2
2:Y:58:TRP:HB3	2:Y:59:ASN:OD1	0.42	2.14	25	2
1:A:12:PHE:CZ	1:A:102:LEU:CD1	0.42	3.03	16	1
2:Y:11:VAL:HG12	2:Y:56:SER:CA	0.42	2.41	1	1
2:Y:20:ILE:O	2:Y:23:ASN:ND2	0.42	2.53	2	1
1:A:61:ILE:HG13	1:A:116:PHE:CG	0.42	2.50	4	1
2:Y:18:ARG:CD	2:Y:35:GLU:HB3	0.42	2.44	7	1
1:A:63:GLN:NE2	1:A:63:GLN:C	0.42	2.76	10	1
1:A:59:PHE:CE1	1:A:105:TYR:CB	0.42	3.03	14	1
1:A:45:ARG:CD	2:Y:61:PRO:HG3	0.42	2.44	15	1
2:Y:108:VAL:O	2:Y:111:PHE:HD2	0.42	1.98	18	1
2:Y:20:ILE:HG22	2:Y:21:VAL:N	0.42	2.30	19	1
1:A:54:ALA:C	1:A:63:GLN:HG3	0.41	2.40	9	1
1:A:61:ILE:CG2	1:A:116:PHE:CG	0.41	3.03	9	1
1:A:13:PHE:CD1	1:A:106:LYS:HG2	0.41	2.50	11	1
1:A:56:THR:O	2:Y:110:PRO:HG3	0.41	2.14	24	1
2:Y:38:ASP:HB2	2:Y:61:PRO:O	0.41	2.15	1	25
2:Y:11:VAL:CG2	2:Y:56:SER:OG	0.41	2.67	11	1
2:Y:17:MET:SD	2:Y:21:VAL:HG22	0.41	2.54	14	1
2:Y:6:LEU:HD23	2:Y:8:PHE:CZ	0.41	2.50	1	25
2:Y:14:PHE:O	2:Y:18:ARG:HD3	0.41	2.15	4	1
1:A:15:GLU:CD	2:Y:14:PHE:CE1	0.41	2.98	15	2
2:Y:108:VAL:O	2:Y:111:PHE:CD2	0.41	2.73	11	1
1:A:12:PHE:CA	1:A:15:GLU:OE1	0.41	2.68	16	2
2:Y:17:MET:HG3	2:Y:21:VAL:HG23	0.41	1.91	22	1
1:A:41:ASN:OD1	1:A:42:ALA:N	0.41	2.52	24	1
2:Y:20:ILE:O	2:Y:21:VAL:C	0.41	2.64	1	25
1:A:11:THR:HB	2:Y:16:THR:OG1	0.41	2.14	15	1
1:A:74:ASP:O	1:A:78:ARG:HG2	0.41	2.16	9	8
1:A:11:THR:HG23	2:Y:16:THR:HG23	0.41	1.89	9	1
2:Y:17:MET:HA	2:Y:17:MET:HE3	0.41	1.91	11	1
1:A:48:HIS:CE1	2:Y:59:ASN:HB3	0.41	2.50	20	1
2:Y:17:MET:HE3	2:Y:109:LYS:CD	0.41	2.46	21	1
1:A:11:THR:HG23	2:Y:16:THR:CB	0.41	2.45	1	1
1:A:195:LEU:HD12	1:A:195:LEU:HA	0.41	1.71	1	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:3:ASP:C	2:Y:5:GLU:H	0.41	2.23	1	25
1:A:45:ARG:HG3	2:Y:61:PRO:HG3	0.41	1.92	15	1
2:Y:86:VAL:HG23	2:Y:107:VAL:CG1	0.41	2.46	24	1
1:A:57:PHE:CB	1:A:59:PHE:CE2	0.41	3.04	25	1
2:Y:3:ASP:C	2:Y:5:GLU:N	0.41	2.79	1	25
1:A:12:PHE:CG	1:A:57:PHE:CE2	0.41	3.09	21	1
1:A:214:PHE:HE2	2:Y:95:ILE:HG23	0.41	1.76	1	25
2:Y:53:PHE:CE1	2:Y:84:LEU:CB	0.41	2.99	1	25
2:Y:22:ARG:HG2	2:Y:23:ASN:N	0.41	2.30	12	1
2:Y:24:LEU:HD23	2:Y:113:ALA:N	0.41	2.31	19	1
2:Y:24:LEU:CD1	2:Y:112:THR:C	0.41	2.92	20	1
2:Y:13:ASP:OD1	2:Y:13:ASP:C	0.41	2.63	21	1
1:A:7:ASP:OD1	1:A:7:ASP:C	0.41	2.63	25	1
1:A:9:TYR:HE1	1:A:57:PHE:HB3	0.41	1.76	2	1
2:Y:24:LEU:HD21	2:Y:111:PHE:O	0.41	2.16	10	1
1:A:209:THR:O	1:A:213:CYS:SG	0.40	2.79	1	25
1:A:62:LEU:HD22	1:A:101:GLN:CB	0.40	2.44	5	1
2:Y:17:MET:HA	2:Y:17:MET:CE	0.40	2.41	5	1
2:Y:37:GLU:OE1	2:Y:41:ASP:HB3	0.40	2.16	18	1
2:Y:123:ILE:O	2:Y:124:PHE:C	0.40	2.62	1	25
1:A:51:LYS:HG2	1:A:63:GLN:NE2	0.40	2.31	2	1
1:A:61:ILE:CG2	1:A:116:PHE:CD1	0.40	3.04	9	1
2:Y:14:PHE:CD1	2:Y:15:SER:N	0.40	2.89	12	1
2:Y:25:LEU:HD21	2:Y:116:LEU:HD21	0.40	1.93	21	1
2:Y:24:LEU:HD12	2:Y:111:PHE:HE1	0.40	1.70	23	1
1:A:211:VAL:C	1:A:213:CYS:N	0.40	2.72	1	25
1:A:13:PHE:CD1	1:A:106:LYS:HG3	0.40	2.52	11	1
2:Y:18:ARG:NH2	2:Y:37:GLU:CG	0.40	2.83	14	1
2:Y:24:LEU:HD12	2:Y:113:ALA:N	0.40	2.31	15	1
2:Y:15:SER:HA	2:Y:18:ARG:CG	0.40	2.45	2	1
1:A:54:ALA:CB	1:A:62:LEU:CD2	0.40	3.00	4	1
1:A:48:HIS:HA	1:A:70:GLU:OE1	0.40	2.17	23	3
2:Y:15:SER:N	2:Y:18:ARG:HH11	0.40	2.14	14	1
1:A:41:ASN:OD1	1:A:45:ARG:CD	0.40	2.69	16	1
1:A:11:THR:HG21	2:Y:20:ILE:HD11	0.40	1.93	20	1
1:A:57:PHE:CE1	2:Y:110:PRO:HG3	0.40	2.51	23	1
1:A:174:LEU:HA	1:A:177:GLU:HB2	0.40	1.94	1	25
2:Y:58:TRP:CH2	2:Y:94:ASN:CA	0.40	3.04	6	1
1:A:8:PHE:HD2	2:Y:110:PRO:CB	0.40	2.29	7	1
1:A:57:PHE:O	1:A:57:PHE:CE1	0.40	2.64	14	1
1:A:12:PHE:HA	1:A:15:GLU:HG2	0.40	1.93	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:Y:12:ASP:OD2	2:Y:17:MET:CE	0.40	2.69	18	1
1:A:60:THR:N	1:A:63:GLN:CD	0.40	2.80	24	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	191/225 (85%)	183±1 (96±0%)	7±1 (4±0%)	1±1 (0±0%)	31	76
2	Y	126/128 (98%)	119±0 (94±0%)	6±0 (5±0%)	1±0 (1±0%)	18	68
All	All	7925/8825 (90%)	7554 (95%)	325 (4%)	46 (1%)	23	72

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	Y	79	SER	25
1	A	7	ASP	10
1	A	160	ARG	7
1	A	132	GLY	4

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	160/193 (83%)	140±2 (88±1%)	20±2 (12±1%)	7	48
2	Y	95/102 (93%)	74±2 (78±2%)	21±2 (22±2%)	2	30
All	All	6375/7375 (86%)	5367 (84%)	1008 (16%)	4	40

All 66 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	131	LYS	25
1	A	160	ARG	25
1	A	161	ARG	25
1	A	166	ARG	25
1	A	175	LEU	25
1	A	176	GLU	25
1	A	198	ILE	25
1	A	203	ILE	25
1	A	208	ILE	25
1	A	216	ILE	25
1	A	220	GLN	25
2	Y	4	LYS	25
2	Y	5	GLU	25
2	Y	44	ASN	25
2	Y	60	MET	25
2	Y	78	MET	25
2	Y	93	GLU	25
2	Y	104	SER	25
2	Y	109	LYS	25
2	Y	119	LYS	25
2	Y	122	LYS	25
2	Y	127	LEU	25
2	Y	129	MET	25
1	A	15	GLU	22
1	A	56	THR	22
1	A	8	PHE	21
1	A	63	GLN	20
2	Y	16	THR	18
2	Y	11	VAL	16
1	A	11	THR	15
2	Y	24	LEU	15
2	Y	112	THR	15
2	Y	10	VAL	14
2	Y	87	THR	14
2	Y	20	ILE	13
2	Y	17	MET	12
1	A	10	GLN	12
1	A	60	THR	12
2	Y	15	SER	11
1	A	7	ASP	10
1	A	41	ASN	10

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Mol	Chain	Res	Type	Models (Total)
1	A	61	ILE	10
2	Y	13	ASP	10
2	Y	86	VAL	10
1	A	64	GLU	9
2	Y	21	VAL	9
1	A	62	LEU	9
2	Y	57	ASP	9
2	Y	37	GLU	8
2	Y	59	ASN	8
2	Y	111	PHE	8
2	Y	23	ASN	8
1	A	71	ASN	8
2	Y	18	ARG	7
1	A	45	ARG	7
1	A	14	ASP	7
1	A	65	THR	5
1	A	39	GLN	5
1	A	12	PHE	5
2	Y	9	LEU	4
2	Y	62	ASN	4
2	Y	58	TRP	3
1	A	57	PHE	3
2	Y	25	LEU	2
2	Y	12	ASP	2
1	A	9	TYR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 5% for the well-defined parts and 5% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	216
Number of shifts mapped to atoms	216
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	108	0.14 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 5%, i.e. 216 atoms were assigned a chemical shift out of a possible 4311. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	216/1606 (13%)	108/653 (17%)	0/640 (0%)	108/313 (35%)
Sidechain	0/2460 (0%)	0/1603 (0%)	0/782 (0%)	0/75 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/245 (0%)	0/122 (0%)	0/118 (0%)	0/5 (0%)
Overall	216/4311 (5%)	108/2378 (5%)	0/1540 (0%)	108/393 (27%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 5%, i.e. 216 atoms were assigned a chemical shift out of a possible 4725. 0 out of 62 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	216/1765 (12%)	108/716 (15%)	0/706 (0%)	108/343 (31%)
Sidechain	0/2715 (0%)	0/1768 (0%)	0/862 (0%)	0/85 (0%)
Aromatic	0/245 (0%)	0/122 (0%)	0/118 (0%)	0/5 (0%)
Overall	216/4725 (5%)	108/2606 (4%)	0/1686 (0%)	108/433 (25%)

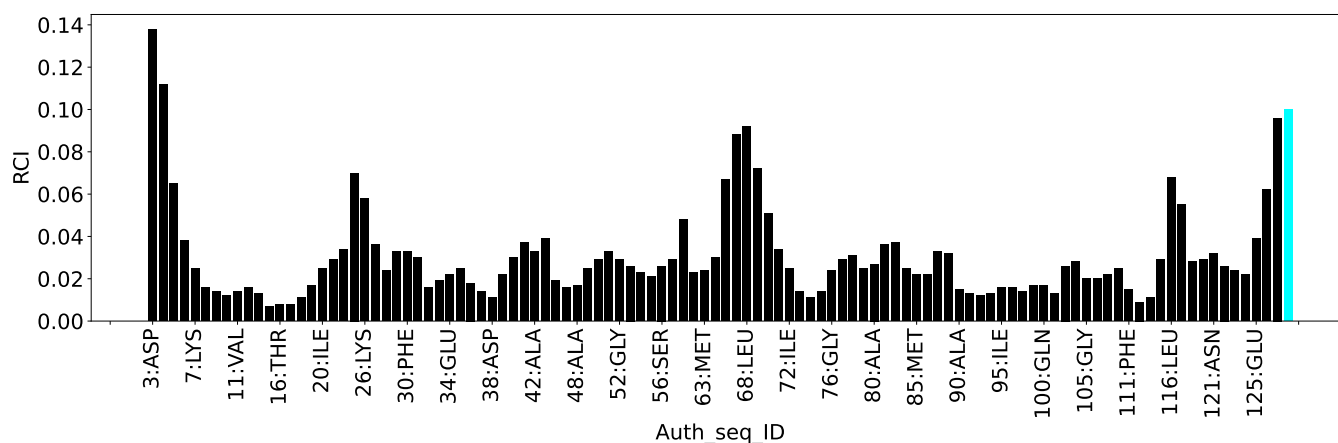
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain Y:



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	81
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	81
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.2
Number of long range restraints per residue ¹	0.0

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)	5.0	0.2
0.2-0.5 (Medium)	5.0	0.49
>0.5 (Large)	1.7	0.84

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

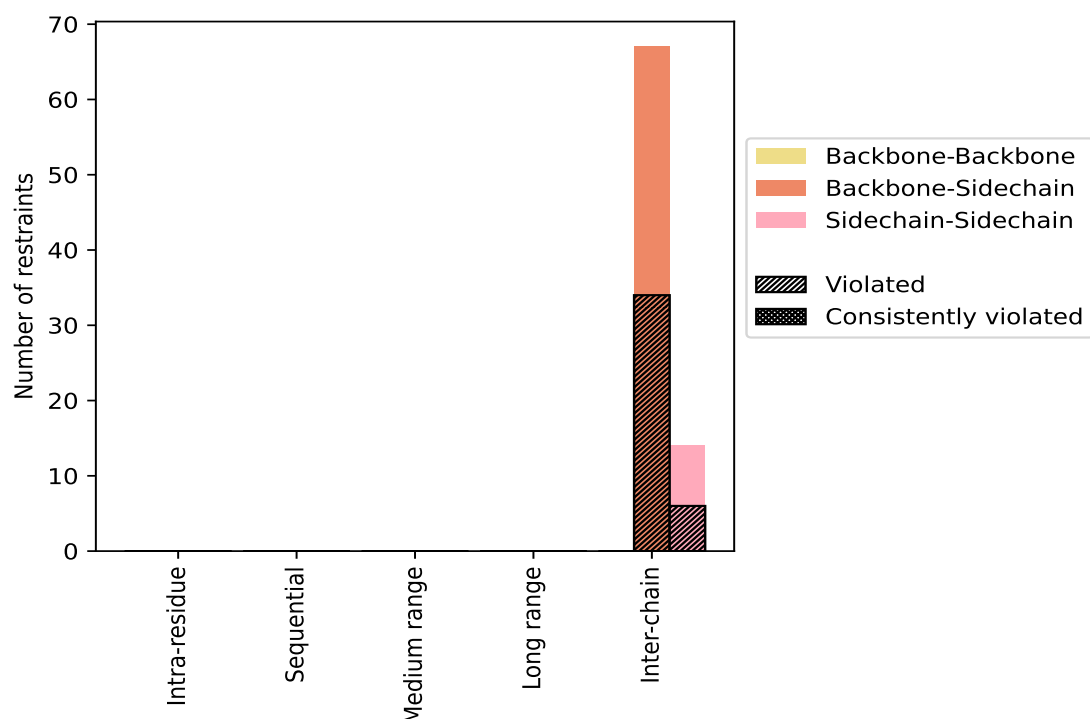
9.1 Summary of distance violations ⓘ

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$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	81	100.0	40	49.4	49.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	67	82.7	34	50.7	42.0	0	0.0	0.0
Sidechain-Sidechain	14	17.3	6	42.9	7.4	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	81	100.0	40	49.4	49.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	67	82.7	34	50.7	42.0	0	0.0	0.0
Sidechain-Sidechain	14	17.3	6	42.9	7.4	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 disulfide bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	14	14	0.22	0.38	0.09	0.2
2	0	0	0	0	6	6	0.19	0.24	0.04	0.19
3	0	0	0	0	12	12	0.25	0.43	0.13	0.2
4	0	0	0	0	14	14	0.21	0.36	0.08	0.18
5	0	0	0	0	16	16	0.38	0.64	0.17	0.32
6	0	0	0	0	10	10	0.21	0.4	0.12	0.14
7	0	0	0	0	8	8	0.29	0.55	0.17	0.24
8	0	0	0	0	20	20	0.29	0.75	0.2	0.22
9	0	0	0	0	12	12	0.41	0.84	0.23	0.34
10	0	0	0	0	6	6	0.45	0.77	0.23	0.3

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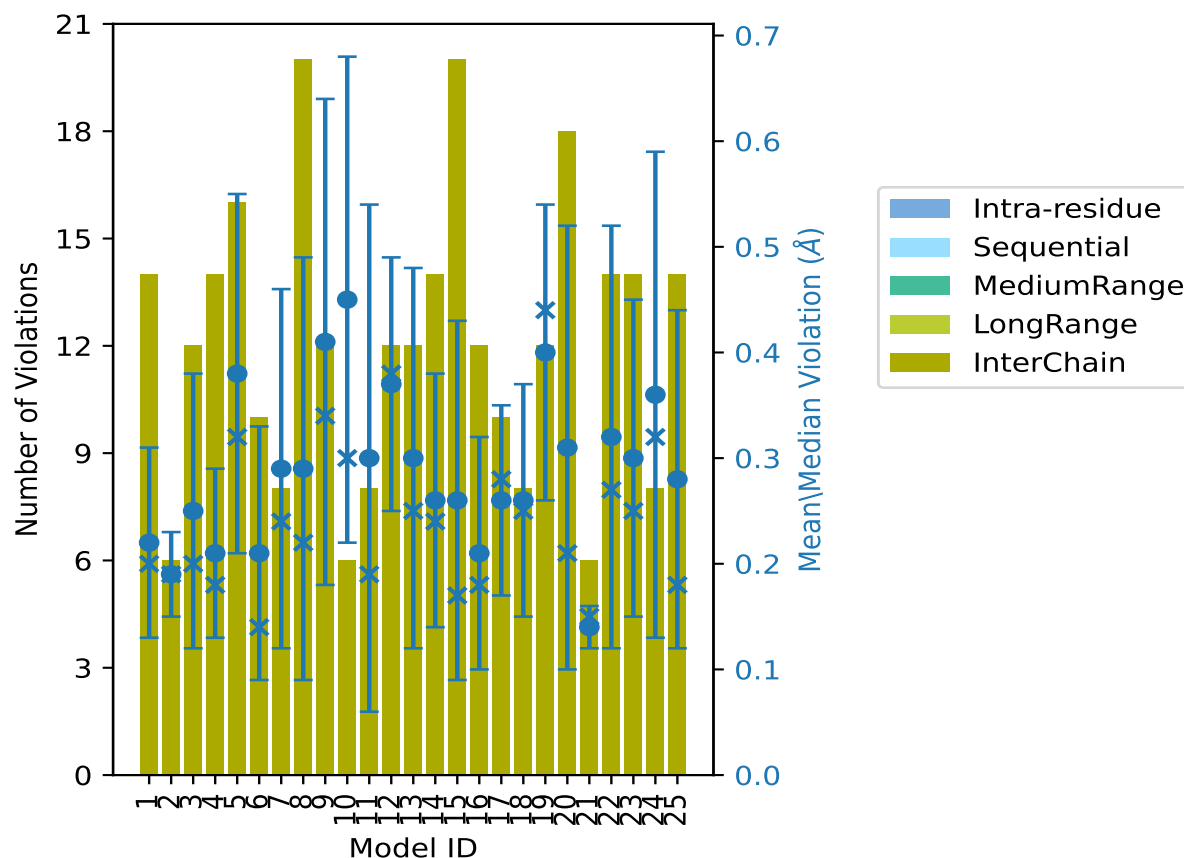
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	8	8	0.3	0.7	0.24	0.19
12	0	0	0	0	12	12	0.37	0.58	0.12	0.38
13	0	0	0	0	12	12	0.3	0.62	0.18	0.25
14	0	0	0	0	14	14	0.26	0.4	0.12	0.24
15	0	0	0	0	20	20	0.26	0.58	0.17	0.17
16	0	0	0	0	12	12	0.21	0.41	0.11	0.18
17	0	0	0	0	10	10	0.26	0.39	0.09	0.28
18	0	0	0	0	8	8	0.26	0.39	0.11	0.25
19	0	0	0	0	12	12	0.4	0.62	0.14	0.44
20	0	0	0	0	18	18	0.31	0.69	0.21	0.21
21	0	0	0	0	6	6	0.14	0.15	0.02	0.15
22	0	0	0	0	14	14	0.32	0.59	0.2	0.27
23	0	0	0	0	14	14	0.3	0.64	0.15	0.25
24	0	0	0	0	8	8	0.36	0.7	0.23	0.32
25	0	0	0	0	14	14	0.28	0.55	0.16	0.18

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 [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 41(IR:0, SQ:0, MR:0, LR:0, IC:41) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	4	4	1	4.0
0	0	0	0	12	12	2	8.0
0	0	0	0	2	2	3	12.0
0	0	0	0	2	2	4	16.0
0	0	0	0	2	2	5	20.0
0	0	0	0	0	0	6	24.0

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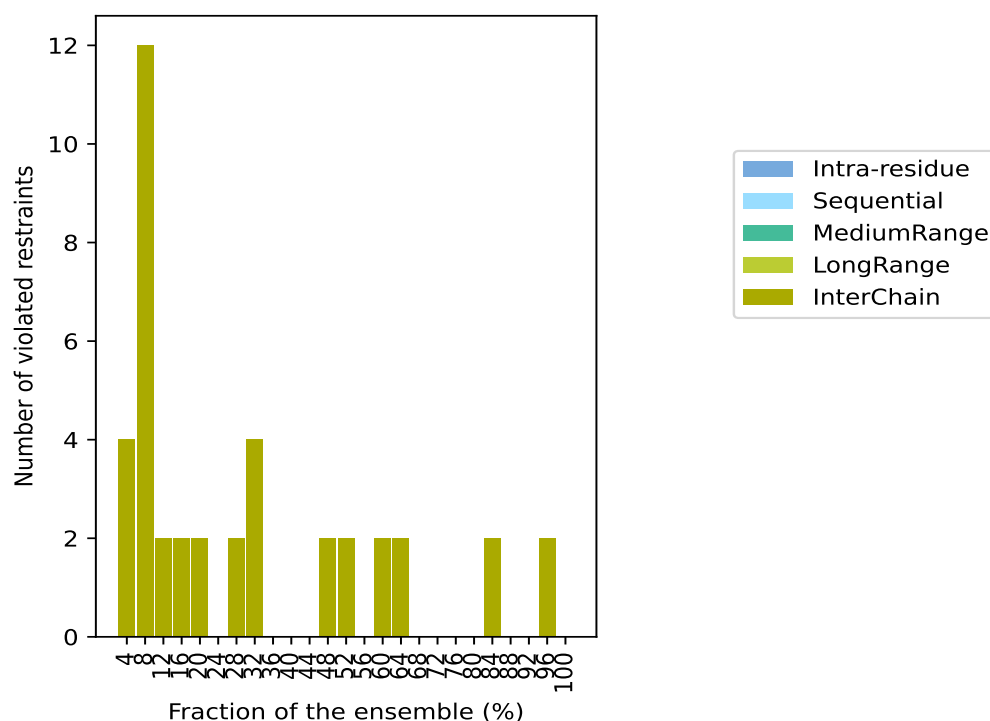
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	2	2	7	28.0
0	0	0	0	4	4	8	32.0
0	0	0	0	0	0	9	36.0
0	0	0	0	0	0	10	40.0
0	0	0	0	0	0	11	44.0
0	0	0	0	2	2	12	48.0
0	0	0	0	2	2	13	52.0
0	0	0	0	0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

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

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

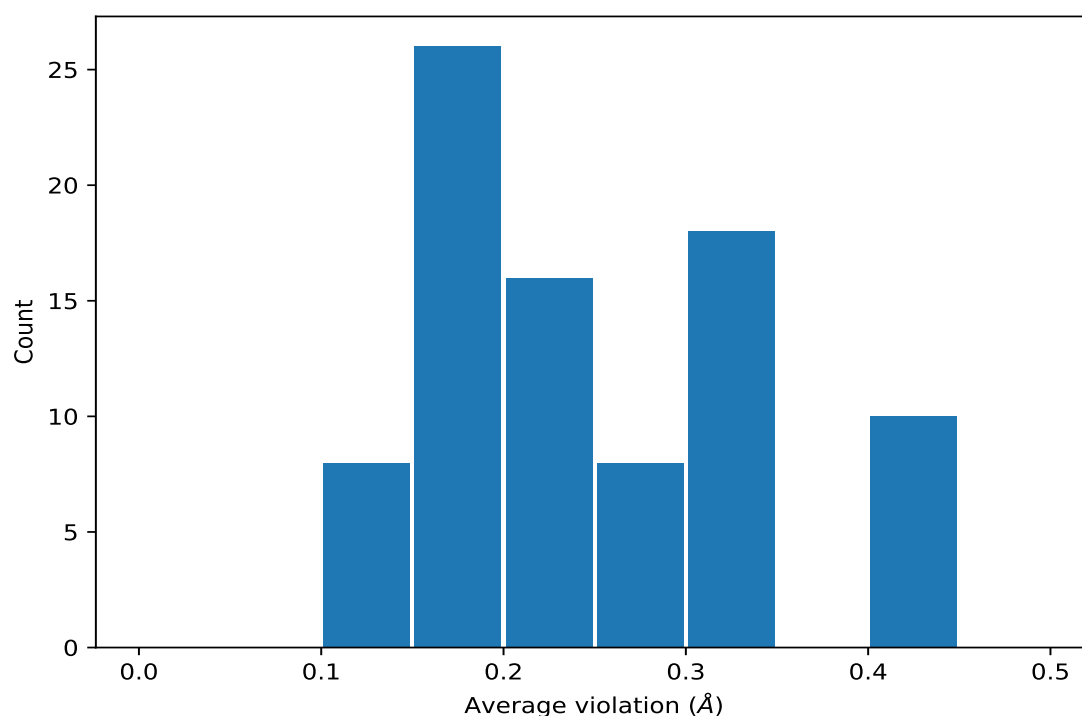
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	24	0.43	0.15	0.42
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	24	0.43	0.15	0.42
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	24	0.43	0.15	0.42
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	24	0.43	0.15	0.42
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	21	0.33	0.15	0.31
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	21	0.33	0.15	0.31
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	21	0.33	0.15	0.31
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	21	0.33	0.15	0.31
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	21	0.33	0.15	0.31
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	21	0.33	0.15	0.31
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	16	0.33	0.22	0.26
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	16	0.33	0.22	0.26
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	16	0.33	0.22	0.26
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	16	0.33	0.22	0.26
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	16	0.33	0.22	0.26
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	16	0.33	0.22	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	15	0.4	0.22	0.38
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	15	0.4	0.22	0.38
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	15	0.4	0.22	0.38
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	15	0.4	0.22	0.38
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	15	0.4	0.22	0.38
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	15	0.4	0.22	0.38
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	13	0.25	0.12	0.24
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	13	0.25	0.12	0.24
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	12	0.18	0.07	0.17
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	12	0.18	0.07	0.17
(1,19)	1:11:A:THR:HG21	2:19:Y:ARG:H	8	0.33	0.16	0.26
(1,19)	1:11:A:THR:HG22	2:19:Y:ARG:H	8	0.33	0.16	0.26
(1,19)	1:11:A:THR:HG23	2:19:Y:ARG:H	8	0.33	0.16	0.26
(1,45)	1:11:A:THR:HG21	2:19:Y:ARG:H	8	0.33	0.16	0.26
(1,45)	1:11:A:THR:HG22	2:19:Y:ARG:H	8	0.33	0.16	0.26
(1,45)	1:11:A:THR:HG23	2:19:Y:ARG:H	8	0.33	0.16	0.26
(2,11)	1:66:A:THR:H	2:89:Y:GLU:CG	8	0.13	0.02	0.13
(2,26)	1:66:A:THR:H	2:89:Y:GLU:CG	8	0.13	0.02	0.13
(2,10)	1:65:A:THR:H	2:89:Y:GLU:CG	7	0.14	0.03	0.13
(2,25)	1:65:A:THR:H	2:89:Y:GLU:CG	7	0.14	0.03	0.13
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD11	5	0.23	0.11	0.2
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD12	5	0.23	0.11	0.2
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD13	5	0.23	0.11	0.2
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD11	5	0.23	0.11	0.2
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD12	5	0.23	0.11	0.2
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD13	5	0.23	0.11	0.2
(1,16)	1:5:A:ILE:HG21	2:111:Y:PHE:H	4	0.18	0.04	0.18
(1,16)	1:5:A:ILE:HG22	2:111:Y:PHE:H	4	0.18	0.04	0.18
(1,16)	1:5:A:ILE:HG23	2:111:Y:PHE:H	4	0.18	0.04	0.18
(1,42)	1:5:A:ILE:HG21	2:111:Y:PHE:H	4	0.18	0.04	0.18
(1,42)	1:5:A:ILE:HG22	2:111:Y:PHE:H	4	0.18	0.04	0.18
(1,42)	1:5:A:ILE:HG23	2:111:Y:PHE:H	4	0.18	0.04	0.18
(1,10)	1:3:A:MET:HE1	2:23:Y:ASN:H	3	0.2	0.03	0.19
(1,10)	1:3:A:MET:HE2	2:23:Y:ASN:H	3	0.2	0.03	0.19
(1,10)	1:3:A:MET:HE3	2:23:Y:ASN:H	3	0.2	0.03	0.19
(1,36)	1:3:A:MET:HE1	2:23:Y:ASN:H	3	0.2	0.03	0.19
(1,36)	1:3:A:MET:HE2	2:23:Y:ASN:H	3	0.2	0.03	0.19
(1,36)	1:3:A:MET:HE3	2:23:Y:ASN:H	3	0.2	0.03	0.19
(1,3)	1:13:A:PHE:H	2:16:Y:THR:HG21	2	0.26	0.0	0.26
(1,3)	1:13:A:PHE:H	2:16:Y:THR:HG22	2	0.26	0.0	0.26
(1,3)	1:13:A:PHE:H	2:16:Y:THR:HG23	2	0.26	0.0	0.26
(1,29)	1:13:A:PHE:H	2:16:Y:THR:HG21	2	0.26	0.0	0.26

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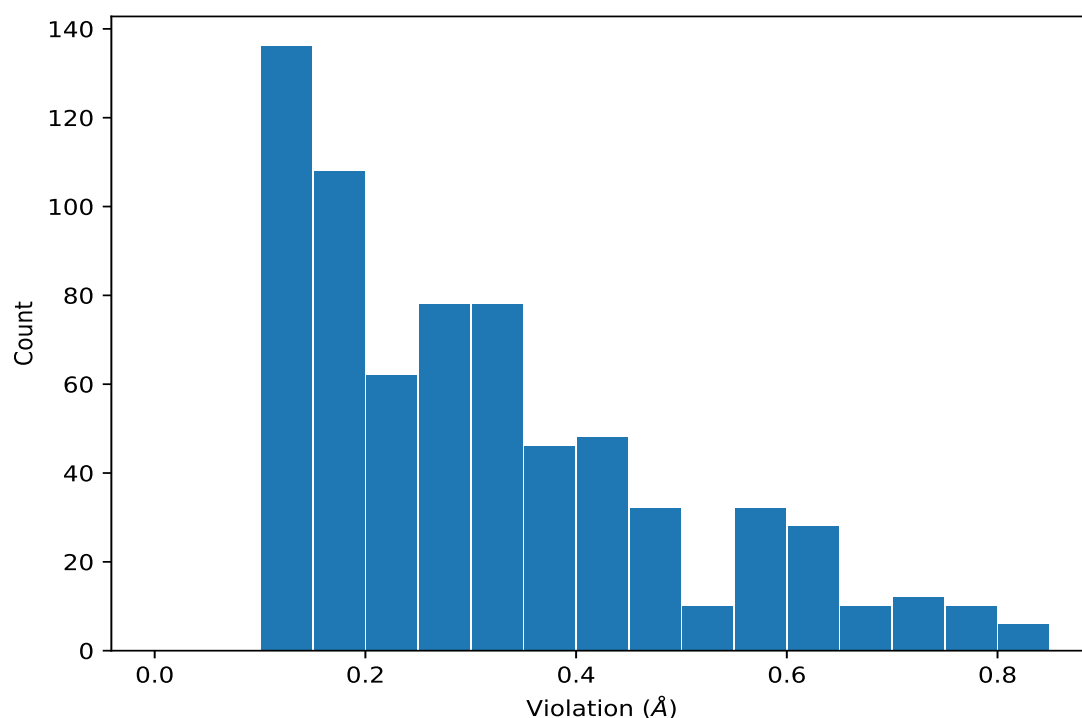
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,29)	1:13:A:PHE:H	2:16:Y:THR:HG22	2	0.26	0.0	0.26
(1,29)	1:13:A:PHE:H	2:16:Y:THR:HG23	2	0.26	0.0	0.26
(2,15)	1:71:A:ASN:HD21	2:91:Y:LYS:CG	2	0.2	0.08	0.2
(2,15)	1:71:A:ASN:HD22	2:91:Y:LYS:CG	2	0.2	0.08	0.2
(2,29)	1:71:A:ASN:HD21	2:91:Y:LYS:CG	2	0.2	0.08	0.2
(2,29)	1:71:A:ASN:HD22	2:91:Y:LYS:CG	2	0.2	0.08	0.2
(1,22)	1:11:A:THR:HG21	2:23:Y:ASN:HD21	2	0.18	0.0	0.18
(1,22)	1:11:A:THR:HG21	2:23:Y:ASN:HD22	2	0.18	0.0	0.18
(1,22)	1:11:A:THR:HG22	2:23:Y:ASN:HD21	2	0.18	0.0	0.18
(1,22)	1:11:A:THR:HG22	2:23:Y:ASN:HD22	2	0.18	0.0	0.18
(1,22)	1:11:A:THR:HG23	2:23:Y:ASN:HD21	2	0.18	0.0	0.18
(1,22)	1:11:A:THR:HG23	2:23:Y:ASN:HD22	2	0.18	0.0	0.18
(1,48)	1:11:A:THR:HG21	2:23:Y:ASN:HD21	2	0.18	0.0	0.18
(1,48)	1:11:A:THR:HG21	2:23:Y:ASN:HD22	2	0.18	0.0	0.18
(1,48)	1:11:A:THR:HG22	2:23:Y:ASN:HD21	2	0.18	0.0	0.18
(1,48)	1:11:A:THR:HG22	2:23:Y:ASN:HD22	2	0.18	0.0	0.18
(1,48)	1:11:A:THR:HG23	2:23:Y:ASN:HD21	2	0.18	0.0	0.18
(1,48)	1:11:A:THR:HG23	2:23:Y:ASN:HD22	2	0.18	0.0	0.18
(1,9)	1:12:A:PHE:H	2:20:Y:ILE:HD11	2	0.18	0.03	0.18
(1,9)	1:12:A:PHE:H	2:20:Y:ILE:HD12	2	0.18	0.03	0.18
(1,9)	1:12:A:PHE:H	2:20:Y:ILE:HD13	2	0.18	0.03	0.18
(1,35)	1:12:A:PHE:H	2:20:Y:ILE:HD11	2	0.18	0.03	0.18
(1,35)	1:12:A:PHE:H	2:20:Y:ILE:HD12	2	0.18	0.03	0.18
(1,35)	1:12:A:PHE:H	2:20:Y:ILE:HD13	2	0.18	0.03	0.18
(1,14)	1:3:A:MET:HB3	2:111:Y:PHE:H	2	0.15	0.04	0.15
(1,40)	1:3:A:MET:HB3	2:111:Y:PHE:H	2	0.15	0.04	0.15
(2,6)	1:61:A:ILE:H	2:89:Y:GLU:CG	2	0.12	0.0	0.12
(2,21)	1:61:A:ILE:H	2:89:Y:GLU:CG	2	0.12	0.0	0.12

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)
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	9	0.84
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	9	0.84
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	9	0.84
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	9	0.84
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	9	0.84
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	9	0.84
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	10	0.77
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	10	0.77
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	10	0.77
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	10	0.77
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	10	0.77
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	10	0.77
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	8	0.75
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	8	0.75
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	8	0.75
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	11	0.7
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	11	0.7
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	11	0.7
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	24	0.7
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	24	0.7
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	24	0.7
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	11	0.7
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	11	0.7
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	11	0.7
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	24	0.7
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	24	0.7
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	24	0.7
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	20	0.69
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	20	0.69
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	20	0.69
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	20	0.69
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	20	0.69
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	20	0.69
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	20	0.66
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	20	0.66
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	20	0.66
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	20	0.66
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	23	0.64
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	23	0.64
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	23	0.64
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	5	0.64
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	5	0.64
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	23	0.64
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	23	0.64
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	23	0.64
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	5	0.64
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	5	0.64
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	13	0.62
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	13	0.62
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	13	0.62
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	19	0.62
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	19	0.62
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	19	0.62
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	13	0.62
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	13	0.62
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	13	0.62
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	19	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	19	0.62
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	19	0.62
(1,45)	1:11:A:THR:HG21	2:19:Y:ARG:H	8	0.6
(1,45)	1:11:A:THR:HG22	2:19:Y:ARG:H	8	0.6
(1,45)	1:11:A:THR:HG23	2:19:Y:ARG:H	8	0.6
(1,19)	1:11:A:THR:HG21	2:19:Y:ARG:H	8	0.6
(1,19)	1:11:A:THR:HG22	2:19:Y:ARG:H	8	0.6
(1,19)	1:11:A:THR:HG23	2:19:Y:ARG:H	8	0.6
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	22	0.59
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	22	0.59
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	22	0.59
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	22	0.59
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	15	0.58
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	15	0.58
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	15	0.58
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	12	0.58
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	12	0.58
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	12	0.58
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	15	0.58
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	15	0.58
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	15	0.58
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	12	0.58
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	12	0.58
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	12	0.58
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	22	0.57
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	22	0.57
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	22	0.57
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	22	0.57
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	22	0.57
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	22	0.57
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	5	0.55
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	5	0.55
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	7	0.55
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	7	0.55
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	25	0.55
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	25	0.55
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	7	0.55
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	7	0.55
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	25	0.55
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	25	0.55
(1,45)	1:11:A:THR:HG21	2:19:Y:ARG:H	5	0.54
(1,45)	1:11:A:THR:HG22	2:19:Y:ARG:H	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:11:A:THR:HG23	2:19:Y:ARG:H	5	0.54
(1,19)	1:11:A:THR:HG21	2:19:Y:ARG:H	5	0.54
(1,19)	1:11:A:THR:HG22	2:19:Y:ARG:H	5	0.54
(1,19)	1:11:A:THR:HG23	2:19:Y:ARG:H	5	0.54
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	9	0.52
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	9	0.52
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	9	0.52
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	9	0.52
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	25	0.49
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	25	0.49
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	25	0.49
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	25	0.49
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	25	0.49
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	25	0.49
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	15	0.48
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	15	0.48
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	15	0.48
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	15	0.48
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	15	0.48
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	15	0.48
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	15	0.48
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	15	0.48
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	15	0.48
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	15	0.48
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	19	0.47
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	19	0.47
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	19	0.47
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	19	0.47
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	19	0.47
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	19	0.47
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	22	0.46
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	22	0.46
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	22	0.46
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	19	0.46
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	19	0.46
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	22	0.46
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	22	0.46
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	22	0.46
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	19	0.46
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	19	0.46
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	13	0.44
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	13	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	24	0.44
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	24	0.44
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	13	0.44
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	13	0.44
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	24	0.44
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	24	0.44
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	3	0.43
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	3	0.43
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	3	0.43
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	3	0.43
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	9	0.42
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	9	0.42
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	9	0.42
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	9	0.42
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	9	0.42
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	9	0.42
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	19	0.41
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	19	0.41
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	19	0.41
(1,45)	1:11:A:THR:HG21	2:19:Y:ARG:H	3	0.41
(1,45)	1:11:A:THR:HG22	2:19:Y:ARG:H	3	0.41
(1,45)	1:11:A:THR:HG23	2:19:Y:ARG:H	3	0.41
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	16	0.41
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	16	0.41
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	19	0.41
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	19	0.41
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	19	0.41
(1,19)	1:11:A:THR:HG21	2:19:Y:ARG:H	3	0.41
(1,19)	1:11:A:THR:HG22	2:19:Y:ARG:H	3	0.41
(1,19)	1:11:A:THR:HG23	2:19:Y:ARG:H	3	0.41
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	16	0.41
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	16	0.41
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	14	0.4
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	14	0.4
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	14	0.4
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	6	0.4
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	6	0.4
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	12	0.4
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	12	0.4
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	14	0.4
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	14	0.4
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	6	0.4
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	6	0.4
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	12	0.4
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	12	0.4
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	18	0.39
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	18	0.39
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	18	0.39
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD11	17	0.39
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD12	17	0.39
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD13	17	0.39
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	14	0.39
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	14	0.39
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	14	0.39
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	18	0.39
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	18	0.39
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	18	0.39
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD11	17	0.39
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD12	17	0.39
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD13	17	0.39
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	14	0.39
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	14	0.39
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	14	0.39
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	20	0.38
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	20	0.38
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	12	0.38
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	12	0.38
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	12	0.38
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	1	0.38
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	1	0.38
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	12	0.38
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	12	0.38
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	12	0.38
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	1	0.38
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	1	0.38
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	12	0.37
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	12	0.37
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	12	0.37
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	12	0.37
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	12	0.37
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	12	0.37
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	4	0.36
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	14	0.36
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	14	0.36
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	4	0.36
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	4	0.36
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	14	0.36
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	14	0.36
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	23	0.35
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	23	0.35
(1,51)	1:56:A:THR:HG21	2:20:Y:ILE:HD11	5	0.33
(1,51)	1:56:A:THR:HG21	2:20:Y:ILE:HD12	5	0.33
(1,51)	1:56:A:THR:HG21	2:20:Y:ILE:HD13	5	0.33
(1,51)	1:56:A:THR:HG22	2:20:Y:ILE:HD11	5	0.33
(1,51)	1:56:A:THR:HG22	2:20:Y:ILE:HD12	5	0.33
(1,51)	1:56:A:THR:HG22	2:20:Y:ILE:HD13	5	0.33
(1,51)	1:56:A:THR:HG23	2:20:Y:ILE:HD11	5	0.33
(1,51)	1:56:A:THR:HG23	2:20:Y:ILE:HD12	5	0.33
(1,51)	1:56:A:THR:HG23	2:20:Y:ILE:HD13	5	0.33
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	18	0.33
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	18	0.33
(1,25)	1:56:A:THR:HG21	2:20:Y:ILE:HD11	5	0.33
(1,25)	1:56:A:THR:HG21	2:20:Y:ILE:HD12	5	0.33
(1,25)	1:56:A:THR:HG21	2:20:Y:ILE:HD13	5	0.33
(1,25)	1:56:A:THR:HG22	2:20:Y:ILE:HD11	5	0.33
(1,25)	1:56:A:THR:HG22	2:20:Y:ILE:HD12	5	0.33
(1,25)	1:56:A:THR:HG22	2:20:Y:ILE:HD13	5	0.33
(1,25)	1:56:A:THR:HG23	2:20:Y:ILE:HD11	5	0.33
(1,25)	1:56:A:THR:HG23	2:20:Y:ILE:HD12	5	0.33
(1,25)	1:56:A:THR:HG23	2:20:Y:ILE:HD13	5	0.33
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	18	0.33
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	18	0.33
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	7	0.32
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	7	0.32
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	5	0.32
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	5	0.32
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	5	0.32
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	4	0.32
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	4	0.32
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	4	0.32
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	5	0.32
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	5	0.32
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	5	0.32
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	4	0.32
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	4	0.32
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	12	0.31
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	12	0.31
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	17	0.31
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	17	0.31
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	17	0.31
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	17	0.31
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	17	0.31
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	17	0.31
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	25	0.3
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	25	0.3
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	25	0.3
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	13	0.3
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	13	0.3
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	13	0.3
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	20	0.3
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	20	0.3
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	20	0.3
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD11	5	0.3
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD12	5	0.3
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD13	5	0.3
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	10	0.3
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	10	0.3
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	6	0.3
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	6	0.3
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	6	0.3
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	25	0.3
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	25	0.3
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	25	0.3
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	13	0.3
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	13	0.3
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	13	0.3
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	20	0.3
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	20	0.3
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	20	0.3
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD11	5	0.3
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD12	5	0.3
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD13	5	0.3
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	10	0.3
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	10	0.3
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	6	0.3
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	6	0.3
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	19	0.29
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	19	0.29
(2,29)	1:71:A:ASN:HD21	2:91:Y:LYS:CG	17	0.28
(2,29)	1:71:A:ASN:HD22	2:91:Y:LYS:CG	17	0.28
(2,15)	1:71:A:ASN:HD21	2:91:Y:LYS:CG	17	0.28
(2,15)	1:71:A:ASN:HD22	2:91:Y:LYS:CG	17	0.28
(1,45)	1:11:A:THR:HG21	2:19:Y:ARG:H	16	0.28
(1,45)	1:11:A:THR:HG22	2:19:Y:ARG:H	16	0.28
(1,45)	1:11:A:THR:HG23	2:19:Y:ARG:H	16	0.28
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	1	0.28
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	1	0.28
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	1	0.28
(1,19)	1:11:A:THR:HG21	2:19:Y:ARG:H	16	0.28
(1,19)	1:11:A:THR:HG22	2:19:Y:ARG:H	16	0.28
(1,19)	1:11:A:THR:HG23	2:19:Y:ARG:H	16	0.28
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	1	0.28
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	1	0.28
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	1	0.28
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	8	0.27
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	8	0.27
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	8	0.27
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	10	0.27
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	10	0.27
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	10	0.27
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	23	0.27
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	23	0.27
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	22	0.27
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	22	0.27
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	22	0.27
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	8	0.27
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	8	0.27
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	8	0.27
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	10	0.27
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	10	0.27
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	10	0.27
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	23	0.27
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	23	0.27
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	22	0.27
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	22	0.27
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	22	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	9	0.26
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	9	0.26
(1,29)	1:13:A:PHE:H	2:16:Y:THR:HG21	8	0.26
(1,29)	1:13:A:PHE:H	2:16:Y:THR:HG22	8	0.26
(1,29)	1:13:A:PHE:H	2:16:Y:THR:HG23	8	0.26
(1,29)	1:13:A:PHE:H	2:16:Y:THR:HG21	9	0.26
(1,29)	1:13:A:PHE:H	2:16:Y:THR:HG22	9	0.26
(1,29)	1:13:A:PHE:H	2:16:Y:THR:HG23	9	0.26
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	1	0.26
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	1	0.26
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	1	0.26
(1,3)	1:13:A:PHE:H	2:16:Y:THR:HG21	8	0.26
(1,3)	1:13:A:PHE:H	2:16:Y:THR:HG22	8	0.26
(1,3)	1:13:A:PHE:H	2:16:Y:THR:HG23	8	0.26
(1,3)	1:13:A:PHE:H	2:16:Y:THR:HG21	9	0.26
(1,3)	1:13:A:PHE:H	2:16:Y:THR:HG22	9	0.26
(1,3)	1:13:A:PHE:H	2:16:Y:THR:HG23	9	0.26
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	1	0.26
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	1	0.26
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	1	0.26
(1,42)	1:5:A:ILE:HG21	2:111:Y:PHE:H	23	0.25
(1,42)	1:5:A:ILE:HG22	2:111:Y:PHE:H	23	0.25
(1,42)	1:5:A:ILE:HG23	2:111:Y:PHE:H	23	0.25
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	5	0.25
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	5	0.25
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	5	0.25
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	23	0.25
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	23	0.25
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	23	0.25
(1,16)	1:5:A:ILE:HG21	2:111:Y:PHE:H	23	0.25
(1,16)	1:5:A:ILE:HG22	2:111:Y:PHE:H	23	0.25
(1,16)	1:5:A:ILE:HG23	2:111:Y:PHE:H	23	0.25
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	5	0.25
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	5	0.25
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	5	0.25
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	23	0.25
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	23	0.25
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	23	0.25
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	3	0.24
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	8	0.24
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	14	0.24
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	8	0.24
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	14	0.24
(1,45)	1:11:A:THR:HG21	2:19:Y:ARG:H	2	0.24
(1,45)	1:11:A:THR:HG22	2:19:Y:ARG:H	2	0.24
(1,45)	1:11:A:THR:HG23	2:19:Y:ARG:H	2	0.24
(1,36)	1:3:A:MET:HE1	2:23:Y:ASN:H	11	0.24
(1,36)	1:3:A:MET:HE2	2:23:Y:ASN:H	11	0.24
(1,36)	1:3:A:MET:HE3	2:23:Y:ASN:H	11	0.24
(1,19)	1:11:A:THR:HG21	2:19:Y:ARG:H	2	0.24
(1,19)	1:11:A:THR:HG22	2:19:Y:ARG:H	2	0.24
(1,19)	1:11:A:THR:HG23	2:19:Y:ARG:H	2	0.24
(1,10)	1:3:A:MET:HE1	2:23:Y:ASN:H	11	0.24
(1,10)	1:3:A:MET:HE2	2:23:Y:ASN:H	11	0.24
(1,10)	1:3:A:MET:HE3	2:23:Y:ASN:H	11	0.24
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	16	0.22
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	16	0.22
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	16	0.22
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	16	0.22
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	16	0.22
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	16	0.22
(1,45)	1:11:A:THR:HG21	2:19:Y:ARG:H	20	0.21
(1,45)	1:11:A:THR:HG22	2:19:Y:ARG:H	20	0.21
(1,45)	1:11:A:THR:HG23	2:19:Y:ARG:H	20	0.21
(1,35)	1:12:A:PHE:H	2:20:Y:ILE:HD11	4	0.21
(1,35)	1:12:A:PHE:H	2:20:Y:ILE:HD12	4	0.21
(1,35)	1:12:A:PHE:H	2:20:Y:ILE:HD13	4	0.21
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	17	0.21
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	17	0.21
(1,19)	1:11:A:THR:HG21	2:19:Y:ARG:H	20	0.21
(1,19)	1:11:A:THR:HG22	2:19:Y:ARG:H	20	0.21
(1,19)	1:11:A:THR:HG23	2:19:Y:ARG:H	20	0.21
(1,9)	1:12:A:PHE:H	2:20:Y:ILE:HD11	4	0.21
(1,9)	1:12:A:PHE:H	2:20:Y:ILE:HD12	4	0.21
(1,9)	1:12:A:PHE:H	2:20:Y:ILE:HD13	4	0.21
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	17	0.21
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	17	0.21
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	1	0.2
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	13	0.2
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	1	0.2
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	13	0.2
(1,45)	1:11:A:THR:HG21	2:19:Y:ARG:H	15	0.2
(1,45)	1:11:A:THR:HG22	2:19:Y:ARG:H	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:11:A:THR:HG23	2:19:Y:ARG:H	15	0.2
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD11	23	0.2
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD12	23	0.2
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD13	23	0.2
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	8	0.2
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	8	0.2
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	8	0.2
(1,19)	1:11:A:THR:HG21	2:19:Y:ARG:H	15	0.2
(1,19)	1:11:A:THR:HG22	2:19:Y:ARG:H	15	0.2
(1,19)	1:11:A:THR:HG23	2:19:Y:ARG:H	15	0.2
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD11	23	0.2
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD12	23	0.2
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD13	23	0.2
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	8	0.2
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	8	0.2
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	8	0.2
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	24	0.19
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	24	0.19
(1,42)	1:5:A:ILE:HG21	2:111:Y:PHE:H	15	0.19
(1,42)	1:5:A:ILE:HG22	2:111:Y:PHE:H	15	0.19
(1,42)	1:5:A:ILE:HG23	2:111:Y:PHE:H	15	0.19
(1,40)	1:3:A:MET:HB3	2:111:Y:PHE:H	20	0.19
(1,36)	1:3:A:MET:HE1	2:23:Y:ASN:H	1	0.19
(1,36)	1:3:A:MET:HE2	2:23:Y:ASN:H	1	0.19
(1,36)	1:3:A:MET:HE3	2:23:Y:ASN:H	1	0.19
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	2	0.19
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	2	0.19
(1,16)	1:5:A:ILE:HG21	2:111:Y:PHE:H	15	0.19
(1,16)	1:5:A:ILE:HG22	2:111:Y:PHE:H	15	0.19
(1,16)	1:5:A:ILE:HG23	2:111:Y:PHE:H	15	0.19
(1,14)	1:3:A:MET:HB3	2:111:Y:PHE:H	20	0.19
(1,10)	1:3:A:MET:HE1	2:23:Y:ASN:H	1	0.19
(1,10)	1:3:A:MET:HE2	2:23:Y:ASN:H	1	0.19
(1,10)	1:3:A:MET:HE3	2:23:Y:ASN:H	1	0.19
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	2	0.19
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	2	0.19
(2,25)	1:65:A:THR:H	2:89:Y:GLU:CG	8	0.18
(2,25)	1:65:A:THR:H	2:89:Y:GLU:CG	25	0.18
(2,10)	1:65:A:THR:H	2:89:Y:GLU:CG	8	0.18
(2,10)	1:65:A:THR:H	2:89:Y:GLU:CG	25	0.18
(1,48)	1:11:A:THR:HG21	2:23:Y:ASN:HD21	4	0.18
(1,48)	1:11:A:THR:HG21	2:23:Y:ASN:HD22	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:11:A:THR:HG22	2:23:Y:ASN:HD21	4	0.18
(1,48)	1:11:A:THR:HG22	2:23:Y:ASN:HD22	4	0.18
(1,48)	1:11:A:THR:HG23	2:23:Y:ASN:HD21	4	0.18
(1,48)	1:11:A:THR:HG23	2:23:Y:ASN:HD22	4	0.18
(1,48)	1:11:A:THR:HG21	2:23:Y:ASN:HD21	12	0.18
(1,48)	1:11:A:THR:HG21	2:23:Y:ASN:HD22	12	0.18
(1,48)	1:11:A:THR:HG22	2:23:Y:ASN:HD21	12	0.18
(1,48)	1:11:A:THR:HG22	2:23:Y:ASN:HD22	12	0.18
(1,48)	1:11:A:THR:HG23	2:23:Y:ASN:HD21	12	0.18
(1,48)	1:11:A:THR:HG23	2:23:Y:ASN:HD22	12	0.18
(1,22)	1:11:A:THR:HG21	2:23:Y:ASN:HD21	4	0.18
(1,22)	1:11:A:THR:HG21	2:23:Y:ASN:HD22	4	0.18
(1,22)	1:11:A:THR:HG22	2:23:Y:ASN:HD21	4	0.18
(1,22)	1:11:A:THR:HG22	2:23:Y:ASN:HD22	4	0.18
(1,22)	1:11:A:THR:HG23	2:23:Y:ASN:HD21	4	0.18
(1,22)	1:11:A:THR:HG23	2:23:Y:ASN:HD22	4	0.18
(1,22)	1:11:A:THR:HG21	2:23:Y:ASN:HD21	12	0.18
(1,22)	1:11:A:THR:HG21	2:23:Y:ASN:HD22	12	0.18
(1,22)	1:11:A:THR:HG22	2:23:Y:ASN:HD21	12	0.18
(1,22)	1:11:A:THR:HG22	2:23:Y:ASN:HD22	12	0.18
(1,22)	1:11:A:THR:HG23	2:23:Y:ASN:HD21	12	0.18
(1,22)	1:11:A:THR:HG23	2:23:Y:ASN:HD22	12	0.18
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	18	0.17
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	25	0.17
(2,26)	1:66:A:THR:H	2:89:Y:GLU:CG	19	0.17
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	18	0.17
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	25	0.17
(2,11)	1:66:A:THR:H	2:89:Y:GLU:CG	19	0.17
(1,42)	1:5:A:ILE:HG21	2:111:Y:PHE:H	3	0.16
(1,42)	1:5:A:ILE:HG22	2:111:Y:PHE:H	3	0.16
(1,42)	1:5:A:ILE:HG23	2:111:Y:PHE:H	3	0.16
(1,36)	1:3:A:MET:HE1	2:23:Y:ASN:H	14	0.16
(1,36)	1:3:A:MET:HE2	2:23:Y:ASN:H	14	0.16
(1,36)	1:3:A:MET:HE3	2:23:Y:ASN:H	14	0.16
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	7	0.16
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	7	0.16
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	7	0.16
(1,16)	1:5:A:ILE:HG21	2:111:Y:PHE:H	3	0.16
(1,16)	1:5:A:ILE:HG22	2:111:Y:PHE:H	3	0.16
(1,16)	1:5:A:ILE:HG23	2:111:Y:PHE:H	3	0.16
(1,10)	1:3:A:MET:HE1	2:23:Y:ASN:H	14	0.16
(1,10)	1:3:A:MET:HE2	2:23:Y:ASN:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:3:A:MET:HE3	2:23:Y:ASN:H	14	0.16
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	7	0.16
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	7	0.16
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	7	0.16
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	2	0.15
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	15	0.15
(2,25)	1:65:A:THR:H	2:89:Y:GLU:CG	15	0.15
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	25	0.15
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	2	0.15
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	15	0.15
(2,10)	1:65:A:THR:H	2:89:Y:GLU:CG	15	0.15
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	25	0.15
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	4	0.15
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	4	0.15
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	4	0.15
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	20	0.15
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	20	0.15
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	20	0.15
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	21	0.15
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	21	0.15
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	21	0.15
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB2	21	0.15
(1,33)	1:15:A:GLU:H	2:19:Y:ARG:HB3	21	0.15
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	3	0.15
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	3	0.15
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	3	0.15
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	4	0.15
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	4	0.15
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	4	0.15
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	20	0.15
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	20	0.15
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	20	0.15
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	21	0.15
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	21	0.15
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	21	0.15
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB2	21	0.15
(1,7)	1:15:A:GLU:H	2:19:Y:ARG:HB3	21	0.15
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	3	0.15
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	3	0.15
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	3	0.15
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	8	0.14
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:11:A:THR:HG21	2:19:Y:ARG:H	9	0.14
(1,45)	1:11:A:THR:HG22	2:19:Y:ARG:H	9	0.14
(1,45)	1:11:A:THR:HG23	2:19:Y:ARG:H	9	0.14
(1,42)	1:5:A:ILE:HG21	2:111:Y:PHE:H	4	0.14
(1,42)	1:5:A:ILE:HG22	2:111:Y:PHE:H	4	0.14
(1,42)	1:5:A:ILE:HG23	2:111:Y:PHE:H	4	0.14
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	6	0.14
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	6	0.14
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	6	0.14
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	11	0.14
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	11	0.14
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	11	0.14
(1,35)	1:12:A:PHE:H	2:20:Y:ILE:HD11	23	0.14
(1,35)	1:12:A:PHE:H	2:20:Y:ILE:HD12	23	0.14
(1,35)	1:12:A:PHE:H	2:20:Y:ILE:HD13	23	0.14
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	18	0.14
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	18	0.14
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	18	0.14
(1,19)	1:11:A:THR:HG21	2:19:Y:ARG:H	9	0.14
(1,19)	1:11:A:THR:HG22	2:19:Y:ARG:H	9	0.14
(1,19)	1:11:A:THR:HG23	2:19:Y:ARG:H	9	0.14
(1,16)	1:5:A:ILE:HG21	2:111:Y:PHE:H	4	0.14
(1,16)	1:5:A:ILE:HG22	2:111:Y:PHE:H	4	0.14
(1,16)	1:5:A:ILE:HG23	2:111:Y:PHE:H	4	0.14
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	6	0.14
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	6	0.14
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	6	0.14
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	11	0.14
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	11	0.14
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	11	0.14
(1,9)	1:12:A:PHE:H	2:20:Y:ILE:HD11	23	0.14
(1,9)	1:12:A:PHE:H	2:20:Y:ILE:HD12	23	0.14
(1,9)	1:12:A:PHE:H	2:20:Y:ILE:HD13	23	0.14
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	18	0.14
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	18	0.14
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	18	0.14
(2,29)	1:71:A:ASN:HD21	2:91:Y:LYS:CG	4	0.13
(2,29)	1:71:A:ASN:HD22	2:91:Y:LYS:CG	4	0.13
(2,26)	1:66:A:THR:H	2:89:Y:GLU:CG	1	0.13
(2,26)	1:66:A:THR:H	2:89:Y:GLU:CG	6	0.13
(2,26)	1:66:A:THR:H	2:89:Y:GLU:CG	8	0.13
(2,26)	1:66:A:THR:H	2:89:Y:GLU:CG	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:65:A:THR:H	2:89:Y:GLU:CG	13	0.13
(2,15)	1:71:A:ASN:HD21	2:91:Y:LYS:CG	4	0.13
(2,15)	1:71:A:ASN:HD22	2:91:Y:LYS:CG	4	0.13
(2,11)	1:66:A:THR:H	2:89:Y:GLU:CG	1	0.13
(2,11)	1:66:A:THR:H	2:89:Y:GLU:CG	6	0.13
(2,11)	1:66:A:THR:H	2:89:Y:GLU:CG	8	0.13
(2,11)	1:66:A:THR:H	2:89:Y:GLU:CG	20	0.13
(2,10)	1:65:A:THR:H	2:89:Y:GLU:CG	13	0.13
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	7	0.13
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	7	0.13
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	7	0.13
(1,46)	1:11:A:THR:HG21	2:20:Y:ILE:H	14	0.13
(1,46)	1:11:A:THR:HG22	2:20:Y:ILE:H	14	0.13
(1,46)	1:11:A:THR:HG23	2:20:Y:ILE:H	14	0.13
(1,43)	1:5:A:ILE:HD11	2:111:Y:PHE:H	16	0.13
(1,43)	1:5:A:ILE:HD12	2:111:Y:PHE:H	16	0.13
(1,43)	1:5:A:ILE:HD13	2:111:Y:PHE:H	16	0.13
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	15	0.13
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	15	0.13
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	15	0.13
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	7	0.13
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	7	0.13
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	7	0.13
(1,20)	1:11:A:THR:HG21	2:20:Y:ILE:H	14	0.13
(1,20)	1:11:A:THR:HG22	2:20:Y:ILE:H	14	0.13
(1,20)	1:11:A:THR:HG23	2:20:Y:ILE:H	14	0.13
(1,17)	1:5:A:ILE:HD11	2:111:Y:PHE:H	16	0.13
(1,17)	1:5:A:ILE:HD12	2:111:Y:PHE:H	16	0.13
(1,17)	1:5:A:ILE:HD13	2:111:Y:PHE:H	16	0.13
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	15	0.13
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	15	0.13
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	15	0.13
(2,26)	1:66:A:THR:H	2:89:Y:GLU:CG	14	0.12
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	15	0.12
(2,21)	1:61:A:ILE:H	2:89:Y:GLU:CG	15	0.12
(2,21)	1:61:A:ILE:H	2:89:Y:GLU:CG	25	0.12
(2,11)	1:66:A:THR:H	2:89:Y:GLU:CG	14	0.12
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	15	0.12
(2,6)	1:61:A:ILE:H	2:89:Y:GLU:CG	15	0.12
(2,6)	1:61:A:ILE:H	2:89:Y:GLU:CG	25	0.12
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD11	13	0.12
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD12	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD13	13	0.12
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD11	16	0.12
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD12	16	0.12
(1,34)	1:8:A:PHE:H	2:20:Y:ILE:HD13	16	0.12
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD11	13	0.12
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD12	13	0.12
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD13	13	0.12
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD11	16	0.12
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD12	16	0.12
(1,8)	1:8:A:PHE:H	2:20:Y:ILE:HD13	16	0.12
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	16	0.11
(2,27)	1:68:A:LEU:H	2:89:Y:GLU:CG	22	0.11
(2,26)	1:66:A:THR:H	2:89:Y:GLU:CG	22	0.11
(2,25)	1:65:A:THR:H	2:89:Y:GLU:CG	5	0.11
(2,25)	1:65:A:THR:H	2:89:Y:GLU:CG	20	0.11
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	22	0.11
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	16	0.11
(2,12)	1:68:A:LEU:H	2:89:Y:GLU:CG	22	0.11
(2,11)	1:66:A:THR:H	2:89:Y:GLU:CG	22	0.11
(2,10)	1:65:A:THR:H	2:89:Y:GLU:CG	5	0.11
(2,10)	1:65:A:THR:H	2:89:Y:GLU:CG	20	0.11
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	22	0.11
(1,40)	1:3:A:MET:HB3	2:111:Y:PHE:H	17	0.11
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	3	0.11
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	3	0.11
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	3	0.11
(1,38)	1:3:A:MET:HE1	2:109:Y:LYS:H	8	0.11
(1,38)	1:3:A:MET:HE2	2:109:Y:LYS:H	8	0.11
(1,38)	1:3:A:MET:HE3	2:109:Y:LYS:H	8	0.11
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG21	21	0.11
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG22	21	0.11
(1,27)	1:11:A:THR:H	2:16:Y:THR:HG23	21	0.11
(1,14)	1:3:A:MET:HB3	2:111:Y:PHE:H	17	0.11
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	3	0.11
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	3	0.11
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	3	0.11
(1,12)	1:3:A:MET:HE1	2:109:Y:LYS:H	8	0.11
(1,12)	1:3:A:MET:HE2	2:109:Y:LYS:H	8	0.11
(1,12)	1:3:A:MET:HE3	2:109:Y:LYS:H	8	0.11
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG21	21	0.11
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG22	21	0.11
(1,1)	1:11:A:THR:H	2:16:Y:THR:HG23	21	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:66:A:THR:H	2:89:Y:GLU:CG	24	0.1
(2,25)	1:65:A:THR:H	2:89:Y:GLU:CG	1	0.1
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	6	0.1
(2,22)	1:62:A:LEU:H	2:89:Y:GLU:CG	11	0.1
(2,11)	1:66:A:THR:H	2:89:Y:GLU:CG	24	0.1
(2,10)	1:65:A:THR:H	2:89:Y:GLU:CG	1	0.1
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	6	0.1
(2,7)	1:62:A:LEU:H	2:89:Y:GLU:CG	11	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found