



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 12:30 PM UTC

PDB ID : 1Q6B / pdb_00001q6b
Title : Solution Structure of the C-terminal Domain of Thermosynechococcus elongatus KaiA (ThKaiA180C); Ensemble of 25 Structures
Authors : Vakonakis, I.; Sun, J.; Golden, S.S.; Holzenburg, A.; LiWang, A.C.
Deposited on : 2003-08-13

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

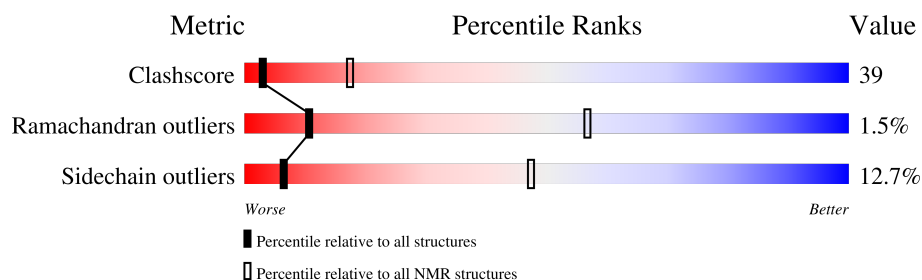
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	107	
1	B	107	

2 Ensemble composition and analysis

This entry contains 25 models. Model 24 is the overall representative, medoid model (most similar to other models). The authors have identified model 13 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:104, B:208-B:304 (194)	0.61	24

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3576 atoms, of which 1810 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Circadian clock protein KaiA homolog.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1788	561	905	151	166	5	
1	B	107	Total	C	H	N	O	S	0
			1788	561	905	151	166	5	

There are 6 discrepancies between the modelled and reference sequences:

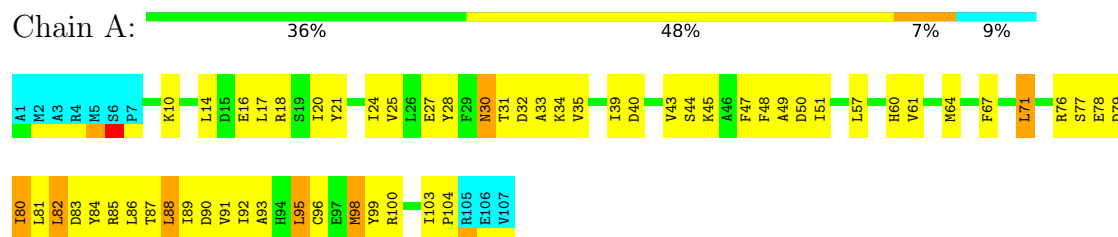
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	cloning artifact	UNP Q8RR35
A	2	MET	-	cloning artifact	UNP Q8RR35
A	3	ALA	-	cloning artifact	UNP Q8RR35
B	201	ALA	-	cloning artifact	UNP Q8RR35
B	202	MET	-	cloning artifact	UNP Q8RR35
B	203	ALA	-	cloning artifact	UNP Q8RR35

4 Residue-property plots

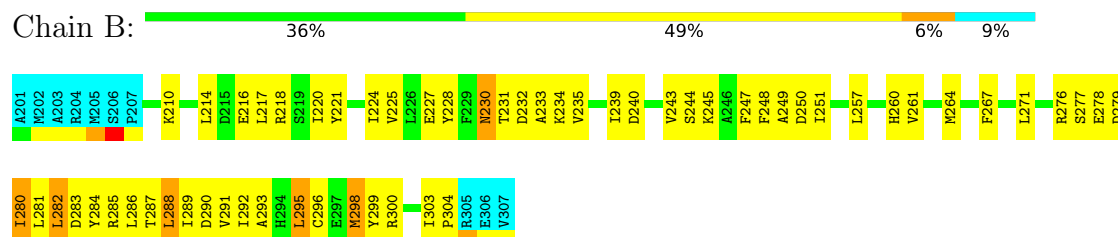
4.1 Average score per residue in the NMR ensemble

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: Circadian clock protein KaiA homolog



- Molecule 1: Circadian clock protein KaiA homolog

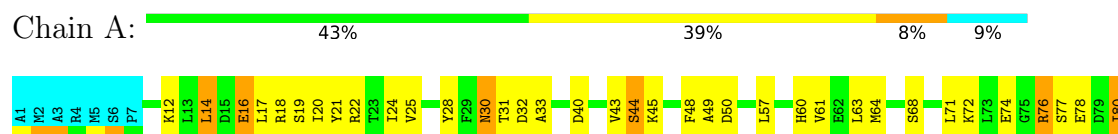


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

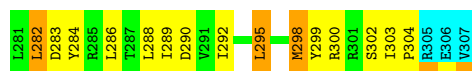
- Molecule 1: Circadian clock protein KaiA homolog





- Molecule 1: Circadian clock protein KaiA homolog

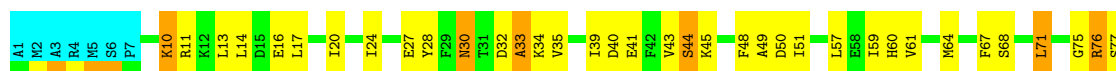
Chain B: 43% 39% 8% 9%



4.2.2 Score per residue for model 2

- Molecule 1: Circadian clock protein KaiA homolog

Chain A: 38% 41% 11% 9%



- Molecule 1: Circadian clock protein KaiA homolog

Chain B: 38% 42% 10% 9%



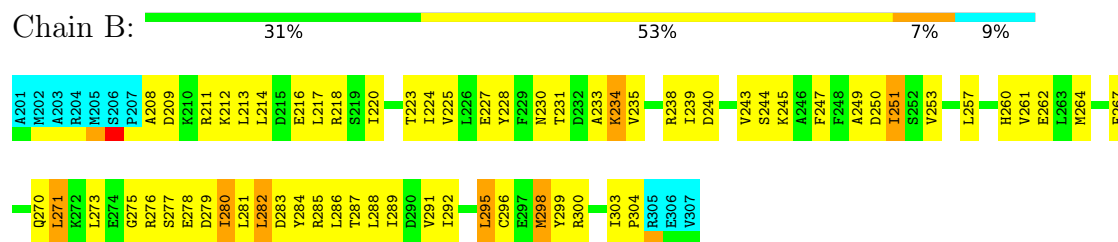
4.2.3 Score per residue for model 3

- Molecule 1: Circadian clock protein KaiA homolog

Chain A: 32% 52% 7% 9%

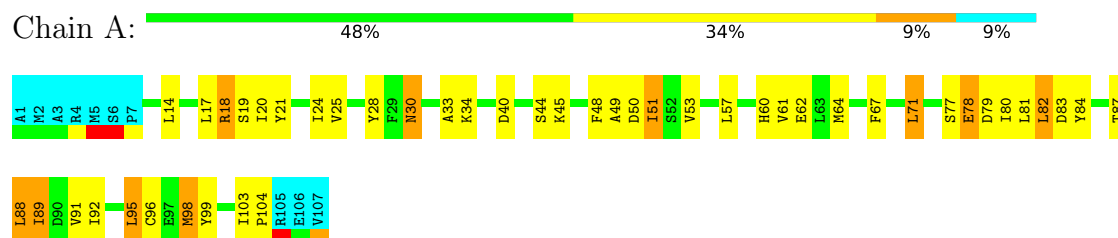


- Molecule 1: Circadian clock protein KaiA homolog

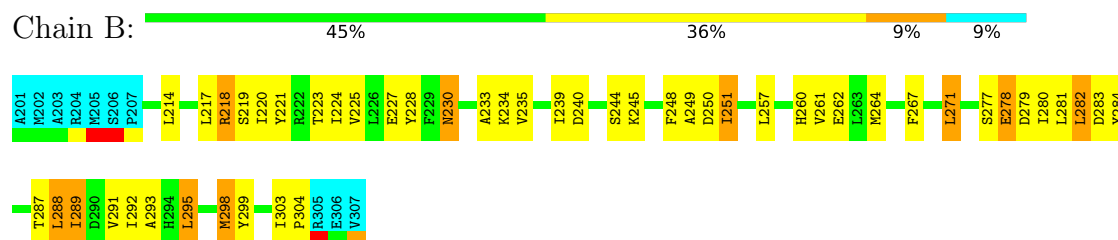


4.2.4 Score per residue for model 4

- Molecule 1: Circadian clock protein KaiA homolog

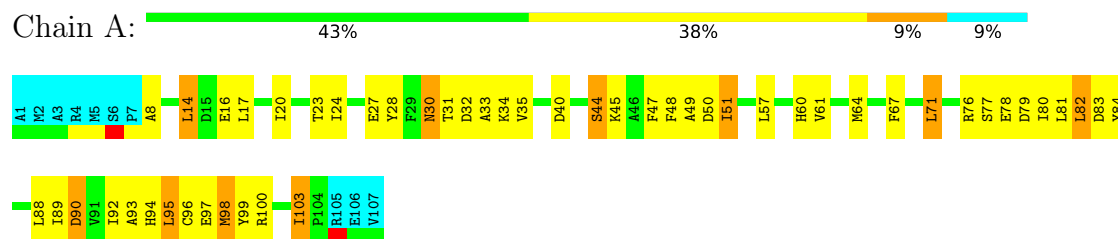


- Molecule 1: Circadian clock protein KaiA homolog

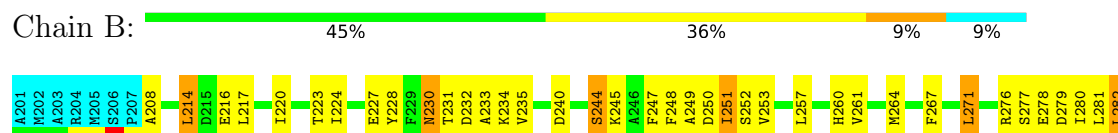


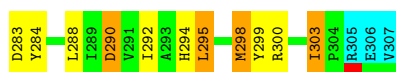
4.2.5 Score per residue for model 5

- Molecule 1: Circadian clock protein KaiA homolog



- Molecule 1: Circadian clock protein KaiA homolog

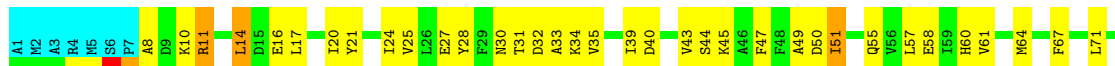




4.2.6 Score per residue for model 6

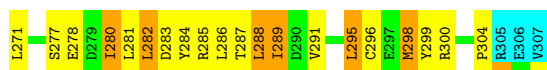
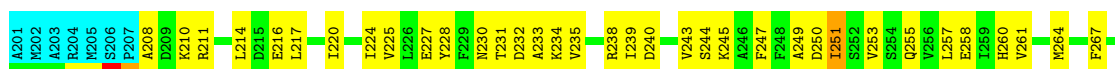
- Molecule 1: Circadian clock protein KaiA homolog

Chain A: 39% 43% 8% 9%



- Molecule 1: Circadian clock protein KaiA homolog

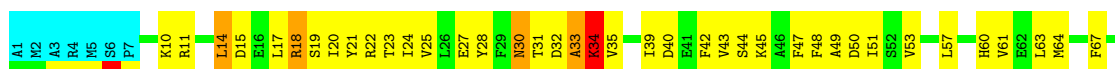
Chain B: 39% 45% 7% 9%



4.2.7 Score per residue for model 7

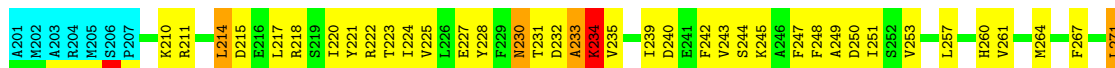
- Molecule 1: Circadian clock protein KaiA homolog

Chain A: 33% 48% 9% 9%



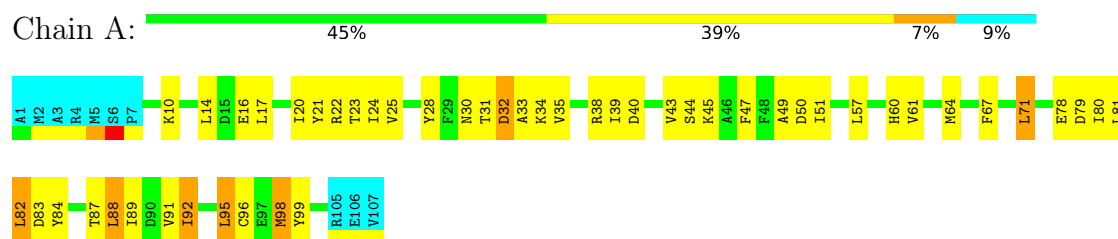
- Molecule 1: Circadian clock protein KaiA homolog

Chain B: 36% 47% 7% 9%

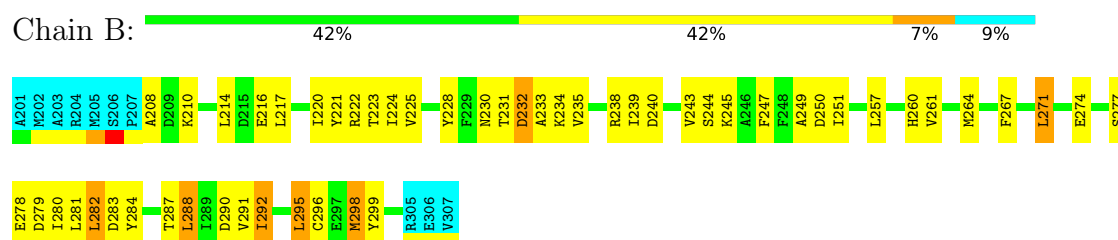


4.2.8 Score per residue for model 8

- Molecule 1: Circadian clock protein KaiA homolog

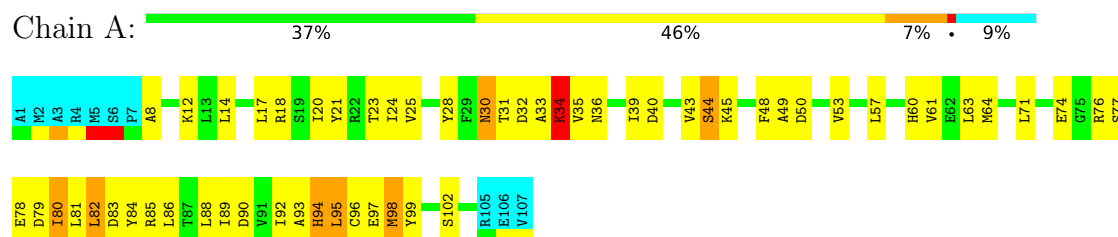


- Molecule 1: Circadian clock protein KaiA homolog

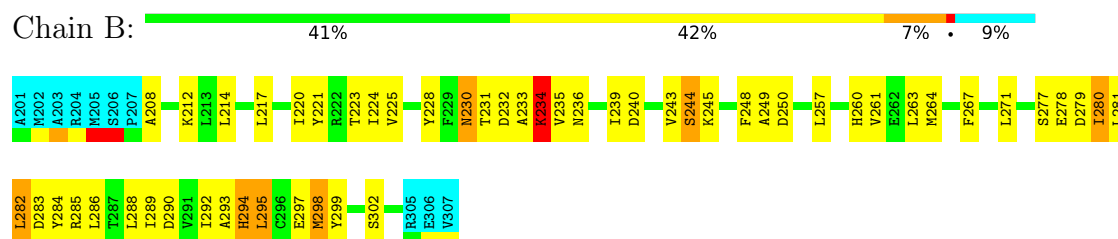


4.2.9 Score per residue for model 9

- Molecule 1: Circadian clock protein KaiA homolog

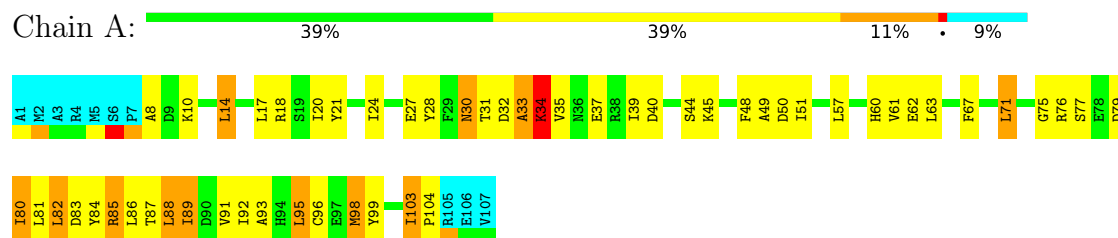


- Molecule 1: Circadian clock protein KaiA homolog

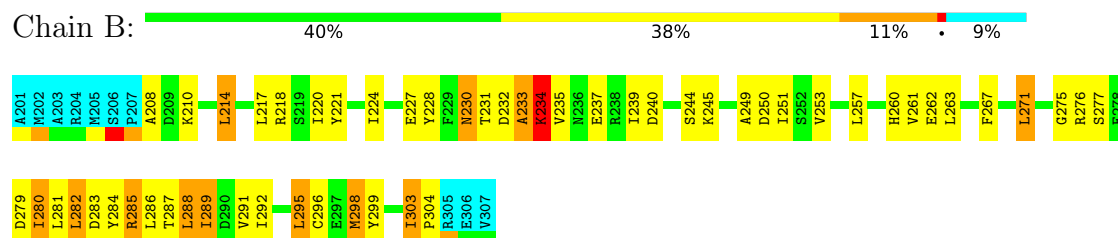


4.2.10 Score per residue for model 10

- Molecule 1: Circadian clock protein KaiA homolog

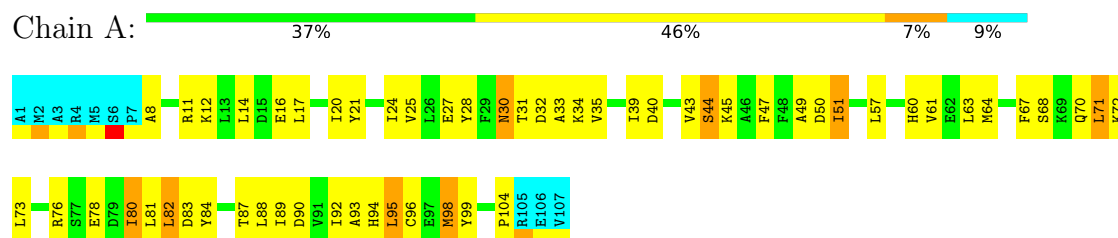


- Molecule 1: Circadian clock protein KaiA homolog

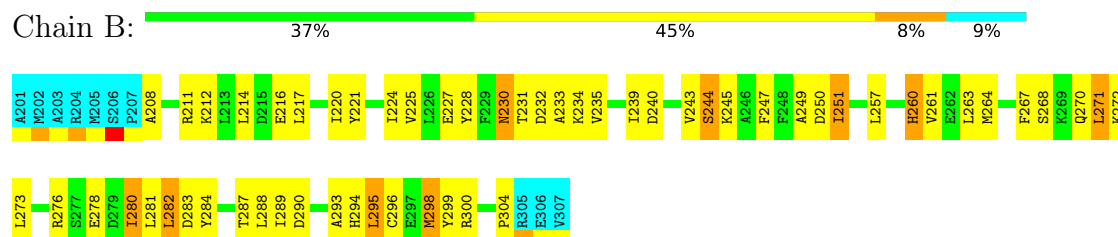


4.2.11 Score per residue for model 11

- Molecule 1: Circadian clock protein KaiA homolog

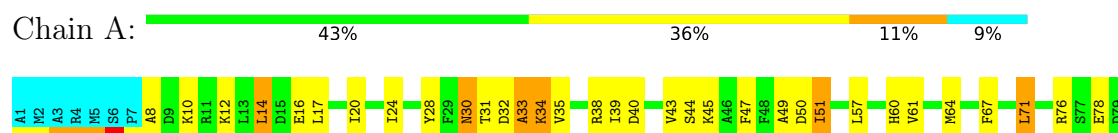


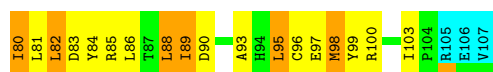
- Molecule 1: Circadian clock protein KaiA homolog



4.2.12 Score per residue for model 12

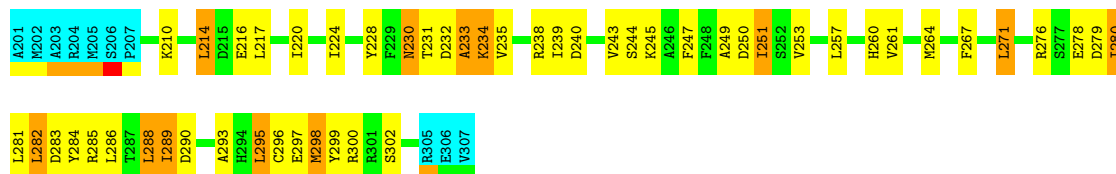
- Molecule 1: Circadian clock protein KaiA homolog





- Molecule 1: Circadian clock protein KaiA homolog

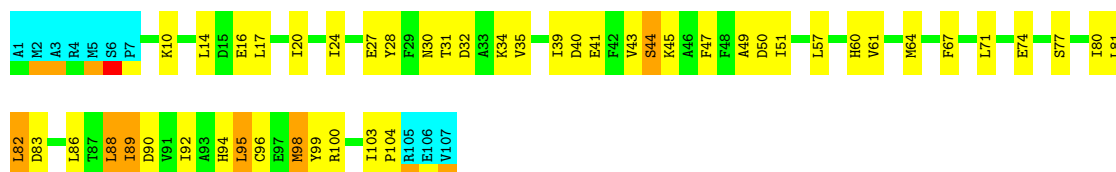
Chain B: 43% 36% 11% 9%



4.2.13 Score per residue for model 13

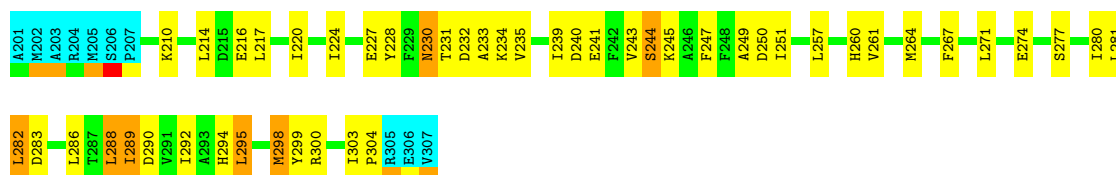
- Molecule 1: Circadian clock protein KaiA homolog

Chain A: 46% 39% 6% 9%



- Molecule 1: Circadian clock protein KaiA homolog

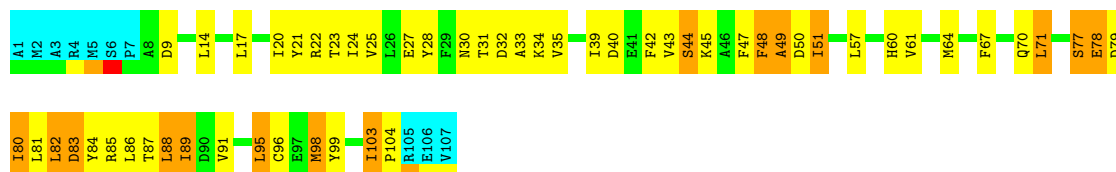
Chain B: 46% 38% 7% 9%



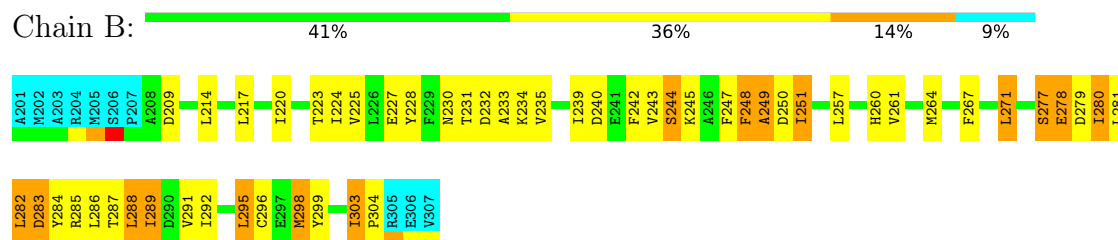
4.2.14 Score per residue for model 14

- Molecule 1: Circadian clock protein KaiA homolog

Chain A: 39% 37% 14% 9%

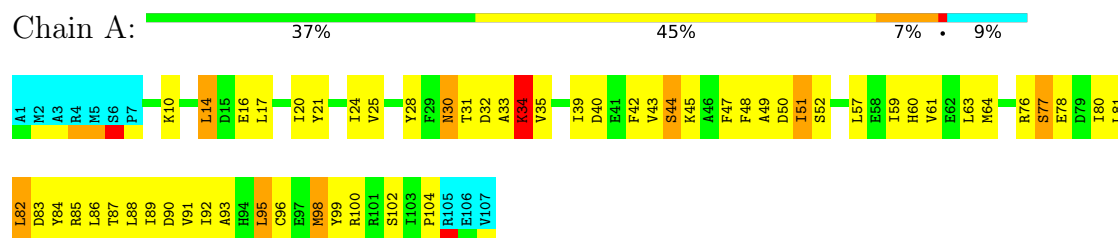


- Molecule 1: Circadian clock protein KaiA homolog

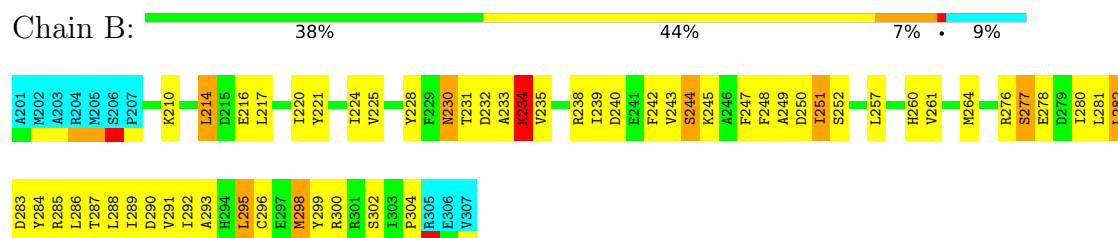


4.2.15 Score per residue for model 15

- Molecule 1: Circadian clock protein KaiA homolog

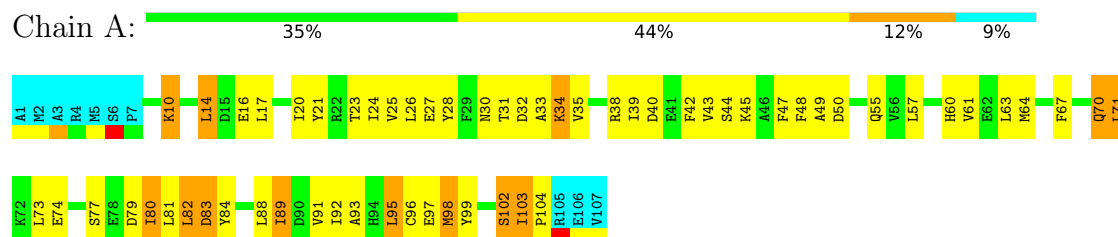


- Molecule 1: Circadian clock protein KaiA homolog

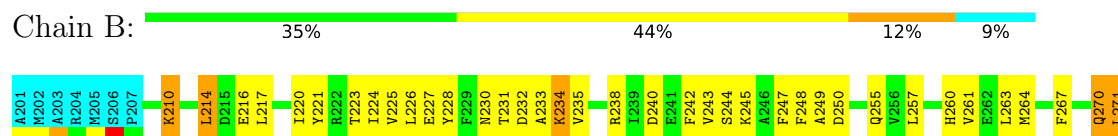


4.2.16 Score per residue for model 16

- Molecule 1: Circadian clock protein KaiA homolog



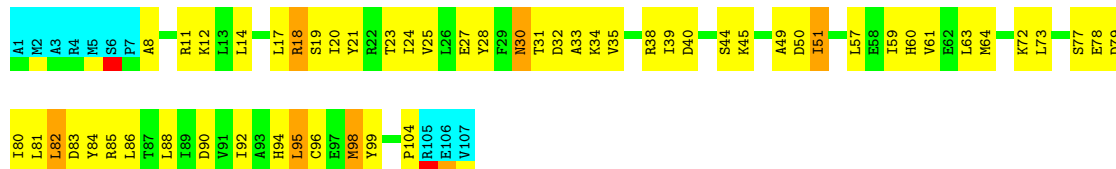
- Molecule 1: Circadian clock protein KaiA homolog



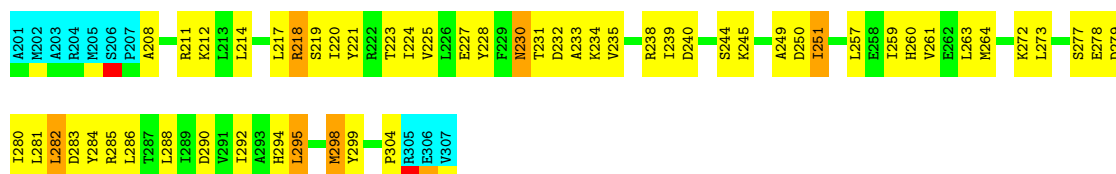


4.2.17 Score per residue for model 17

- Molecule 1: Circadian clock protein KaiA homolog



- Molecule 1: Circadian clock protein KaiA homolog

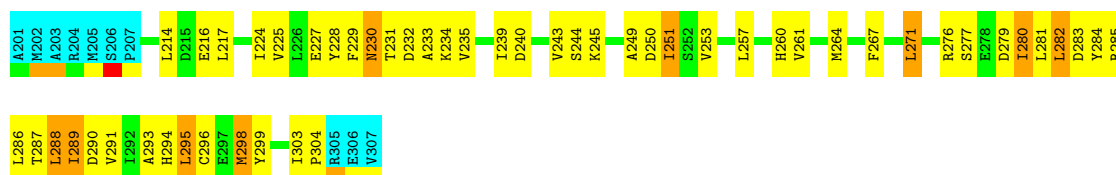


4.2.18 Score per residue for model 18

- Molecule 1: Circadian clock protein KaiA homolog

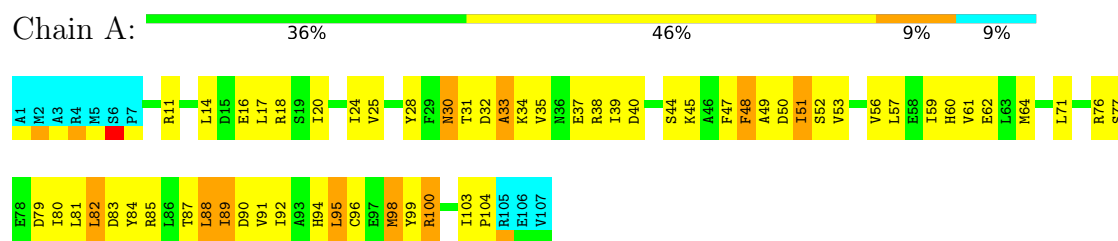


- Molecule 1: Circadian clock protein KaiA homolog

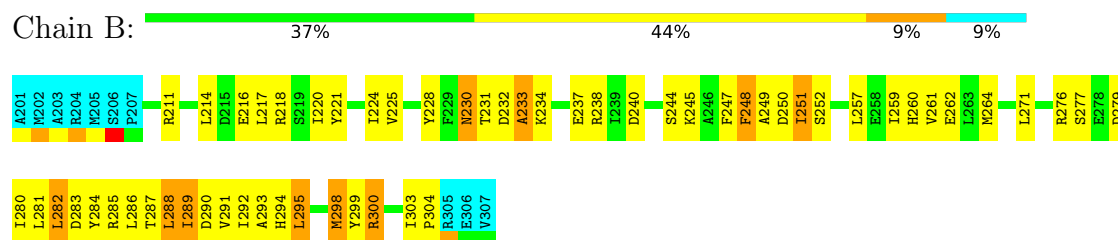


4.2.19 Score per residue for model 19

- Molecule 1: Circadian clock protein KaiA homolog

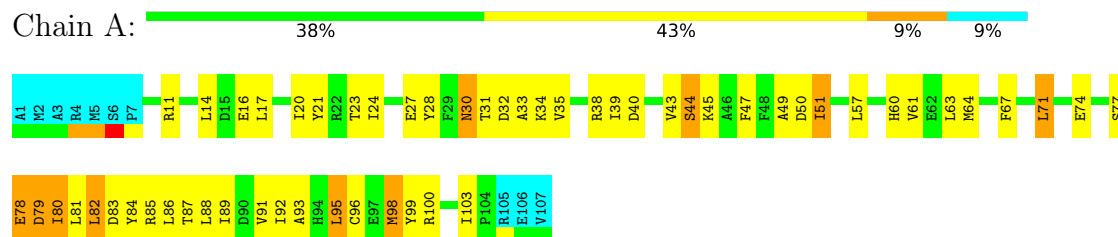


- Molecule 1: Circadian clock protein KaiA homolog

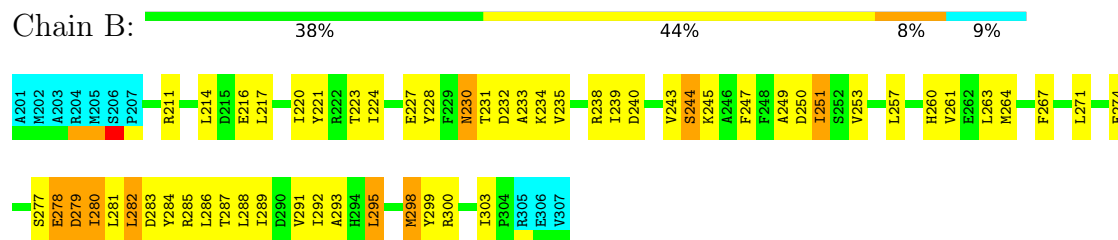


4.2.20 Score per residue for model 20

- Molecule 1: Circadian clock protein KaiA homolog

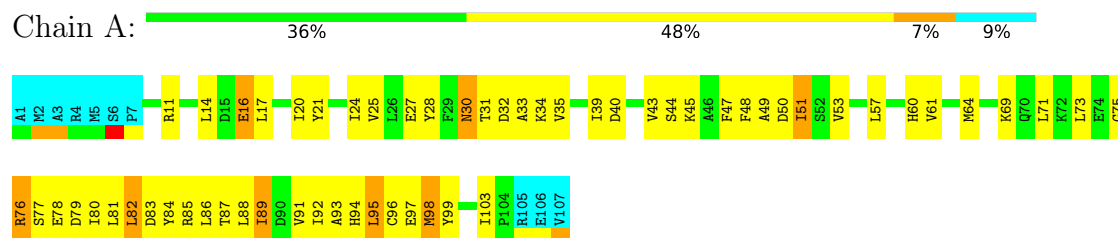


- Molecule 1: Circadian clock protein KaiA homolog

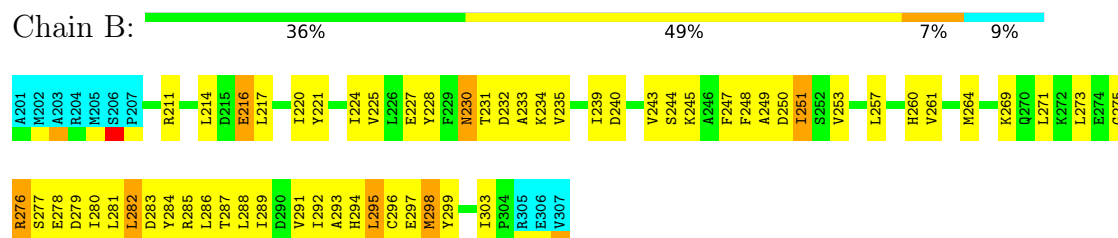


4.2.21 Score per residue for model 21

- Molecule 1: Circadian clock protein KaiA homolog

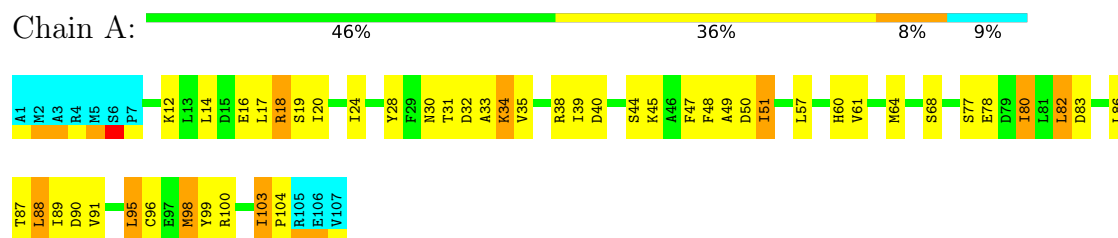


- Molecule 1: Circadian clock protein KaiA homolog

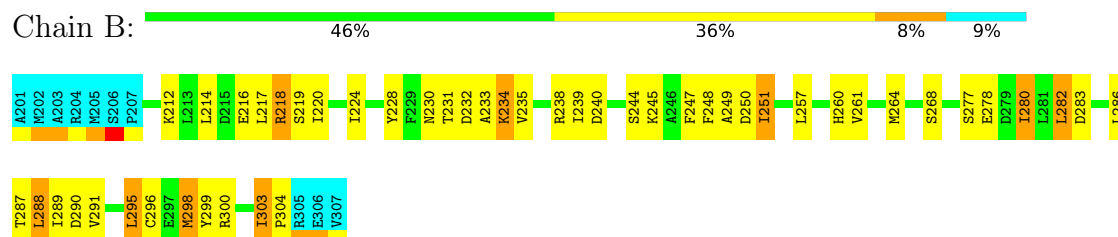


4.2.22 Score per residue for model 22

- Molecule 1: Circadian clock protein KaiA homolog

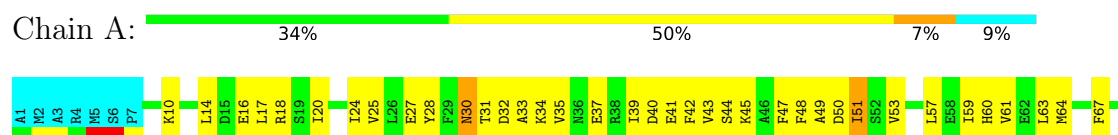


- Molecule 1: Circadian clock protein KaiA homolog



4.2.23 Score per residue for model 23

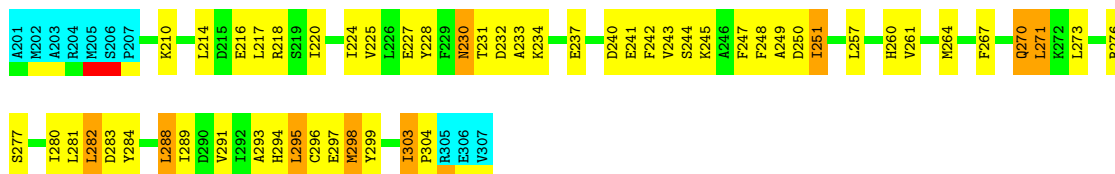
- Molecule 1: Circadian clock protein KaiA homolog





- Molecule 1: Circadian clock protein KaiA homolog

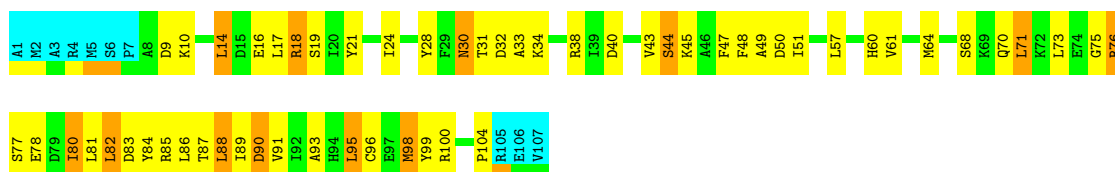
Chain B: 40% 42% 8% 9%



4.2.24 Score per residue for model 24 (medoid)

- Molecule 1: Circadian clock protein KaiA homolog

Chain A: 38% 41% 11% 9%



- Molecule 1: Circadian clock protein KaiA homolog

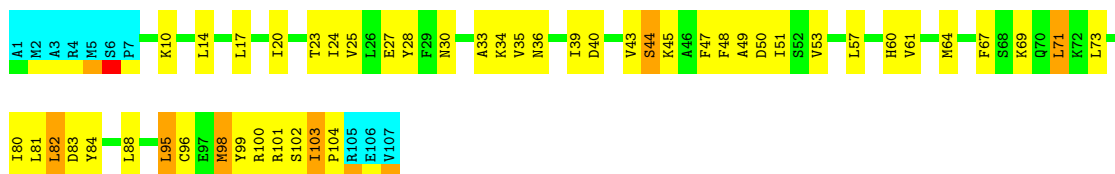
Chain B: 42% 37% 11% 9%



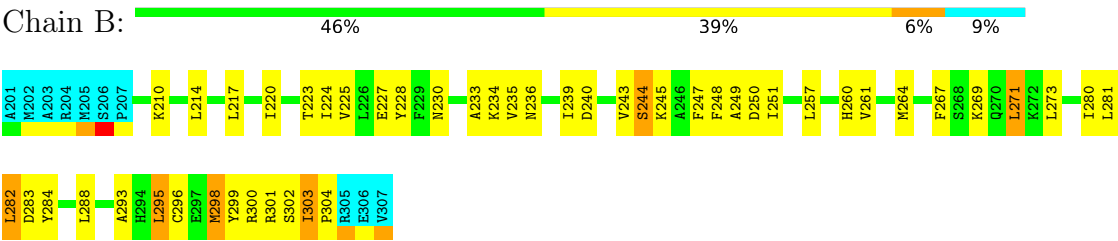
4.2.25 Score per residue for model 25

- Molecule 1: Circadian clock protein KaiA homolog

Chain A: 46% 39% 6% 9%



- Molecule 1: Circadian clock protein KaiA homolog



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Distance geometry, Simulating annealing, Radius-of-gyration, Carbon chemical shift and conformational database potential refinement.*

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	Classification	Version
XPLOR-NIH	structure solution	2.9.1
XPLOR-NIH	refinement	2.9.1

No chemical shift data was provided.

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	0.62±0.01	0±0/817 (0.0± 0.0%)	1.07±0.01	0±0/1101 (0.0± 0.0%)
1	B	0.62±0.01	0±0/817 (0.0± 0.0%)	1.07±0.01	0±0/1101 (0.0± 0.0%)
All	All	0.62	0/40850 (0.0%)	1.07	1/55050 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	260	HIS	CA-CB-CG	-5.02	108.78	113.80	11	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	805	822	820	65±5
1	B	805	822	820	65±5
All	All	40250	41100	41000	3149

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:260:HIS:CD2	1:B:288:LEU:HD12	1.00	1.92	4	14
1:A:60:HIS:CD2	1:A:88:LEU:HD12	0.98	1.92	4	14
1:A:82:LEU:HD12	1:A:82:LEU:O	0.98	1.59	9	19
1:B:282:LEU:O	1:B:282:LEU:HD12	0.98	1.59	9	19
1:A:30:ASN:OD1	1:A:33:ALA:HB3	0.93	1.63	19	8
1:B:230:ASN:OD1	1:B:233:ALA:HB3	0.93	1.63	19	9
1:A:57:LEU:O	1:A:61:VAL:HG23	0.93	1.64	5	25
1:B:257:LEU:O	1:B:261:VAL:HG23	0.91	1.64	5	25
1:B:288:LEU:C	1:B:288:LEU:HD13	0.84	1.98	9	11
1:A:88:LEU:HD13	1:A:88:LEU:C	0.83	1.98	9	11
1:B:225:VAL:HG11	1:B:284:TYR:CE2	0.82	2.10	15	13
1:A:25:VAL:HG11	1:A:84:TYR:CE2	0.82	2.10	15	13
1:A:24:ILE:O	1:A:28:TYR:N	0.80	2.14	24	25
1:A:87:THR:O	1:A:91:VAL:HG23	0.80	1.76	19	14
1:B:287:THR:O	1:B:291:VAL:HG23	0.79	1.76	19	14
1:B:224:ILE:O	1:B:228:TYR:N	0.79	2.16	22	25
1:B:295:LEU:C	1:B:295:LEU:HD12	0.79	2.02	7	14
1:A:47:PHE:CD2	1:A:98:MET:SD	0.79	2.76	7	6
1:B:230:ASN:ND2	1:B:233:ALA:N	0.78	2.31	10	4
1:B:247:PHE:CD2	1:B:298:MET:SD	0.78	2.76	7	6
1:A:95:LEU:HD12	1:A:95:LEU:C	0.78	2.04	21	14
1:B:292:ILE:O	1:B:295:LEU:HD23	0.78	1.79	1	11
1:A:92:ILE:O	1:A:95:LEU:HD23	0.78	1.79	1	11
1:A:30:ASN:HD22	1:A:33:ALA:N	0.77	1.78	24	1
1:A:30:ASN:ND2	1:A:33:ALA:H	0.76	1.78	23	4
1:A:30:ASN:ND2	1:A:33:ALA:N	0.76	2.31	10	4
1:B:230:ASN:ND2	1:B:233:ALA:H	0.76	1.78	23	4
1:B:278:GLU:O	1:B:280:ILE:N	0.75	2.19	20	1
1:B:230:ASN:HD22	1:B:233:ALA:N	0.75	1.78	24	1
1:A:78:GLU:O	1:A:80:ILE:N	0.75	2.19	20	1
1:B:230:ASN:HD22	1:B:232:ASP:N	0.74	1.80	2	3
1:A:95:LEU:CD1	1:A:99:TYR:CZ	0.74	2.71	2	4
1:A:81:LEU:HD12	1:A:84:TYR:CD2	0.74	2.18	3	14
1:B:281:LEU:HD12	1:B:284:TYR:CD2	0.74	2.18	3	13
1:A:30:ASN:HD22	1:A:32:ASP:N	0.73	1.80	2	3
1:A:100:ARG:NH2	1:B:250:ASP:CG	0.73	2.46	1	1
1:B:295:LEU:CD1	1:B:299:TYR:CZ	0.73	2.71	2	4
1:A:64:MET:SD	1:A:81:LEU:HD11	0.72	2.24	5	4
1:A:48:PHE:C	1:A:48:PHE:CD1	0.72	2.67	14	2
1:B:264:MET:SD	1:B:281:LEU:HD11	0.71	2.24	5	4
1:A:89:ILE:HD13	1:B:288:LEU:HD13	0.71	1.63	23	2
1:B:248:PHE:C	1:B:248:PHE:CD1	0.71	2.68	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:230:ASN:OD1	1:B:233:ALA:N	0.71	2.23	11	15
1:A:40:ASP:O	1:A:44:SER:OG	0.71	2.09	13	25
1:A:20:ILE:HD12	1:A:45:LYS:HZ1	0.71	1.45	20	14
1:B:230:ASN:ND2	1:B:230:ASN:C	0.71	2.49	21	9
1:B:277:SER:O	1:B:280:ILE:HG22	0.71	1.86	16	10
1:A:33:ALA:O	1:A:35:VAL:N	0.71	2.24	7	2
1:A:30:ASN:OD1	1:A:33:ALA:N	0.70	2.23	11	14
1:B:295:LEU:HD11	1:B:299:TYR:CE2	0.70	2.22	6	10
1:B:233:ALA:O	1:B:235:VAL:N	0.70	2.24	7	2
1:A:100:ARG:NH1	1:B:299:TYR:OH	0.70	2.24	20	1
1:A:30:ASN:C	1:A:30:ASN:ND2	0.70	2.49	2	8
1:B:240:ASP:O	1:B:244:SER:OG	0.70	2.09	2	25
1:A:88:LEU:HD13	1:B:289:ILE:HD13	0.70	1.60	23	1
1:A:77:SER:O	1:A:79:ASP:N	0.70	2.24	20	7
1:B:277:SER:O	1:B:279:ASP:N	0.70	2.24	20	7
1:A:100:ARG:NH2	1:B:299:TYR:OH	0.69	2.25	5	5
1:A:77:SER:O	1:A:80:ILE:HG22	0.69	1.86	16	9
1:A:95:LEU:HD11	1:A:99:TYR:CE2	0.69	2.22	6	10
1:A:50:ASP:OD1	1:B:300:ARG:NH1	0.69	2.26	24	3
1:A:16:GLU:N	1:A:16:GLU:OE1	0.69	2.26	21	1
1:B:290:ASP:OD1	1:B:294:HIS:NE2	0.68	2.26	18	1
1:A:50:ASP:OD1	1:B:300:ARG:NH2	0.68	2.26	6	5
1:B:244:SER:O	1:B:248:PHE:N	0.68	2.23	15	13
1:B:216:GLU:N	1:B:216:GLU:OE1	0.68	2.26	21	1
1:A:50:ASP:CG	1:B:300:ARG:NH2	0.68	2.52	1	1
1:B:211:ARG:NH1	1:B:215:ASP:OD1	0.68	2.27	7	1
1:A:90:ASP:OD1	1:A:94:HIS:CD2	0.68	2.47	9	3
1:B:290:ASP:OD1	1:B:294:HIS:CD2	0.68	2.47	9	3
1:A:90:ASP:OD1	1:A:94:HIS:NE2	0.68	2.26	18	1
1:B:230:ASN:HD22	1:B:233:ALA:H	0.68	1.31	23	3
1:A:11:ARG:NH1	1:A:15:ASP:OD1	0.68	2.27	7	1
1:A:67:PHE:O	1:A:71:LEU:HD22	0.67	1.90	3	13
1:B:280:ILE:HD11	1:B:284:TYR:OH	0.67	1.90	2	5
1:A:71:LEU:O	1:A:75:GLY:N	0.67	2.26	3	3
1:A:51:ILE:O	1:B:300:ARG:NH2	0.67	2.28	3	1
1:A:82:LEU:O	1:A:82:LEU:CD1	0.67	2.43	4	13
1:A:80:ILE:HD11	1:A:84:TYR:OH	0.67	1.90	2	5
1:A:27:GLU:O	1:A:30:ASN:ND2	0.67	2.26	13	10
1:A:92:ILE:O	1:A:96:CYS:SG	0.67	2.53	5	10
1:A:30:ASN:CG	1:A:33:ALA:HB3	0.67	2.15	16	12
1:B:267:PHE:O	1:B:271:LEU:HD22	0.67	1.89	3	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:ASP:O	1:A:94:HIS:ND1	0.67	2.28	13	1
1:B:223:THR:O	1:B:227:GLU:OE1	0.66	2.13	16	1
1:A:82:LEU:HD12	1:A:82:LEU:C	0.66	2.15	9	16
1:B:282:LEU:HD12	1:B:282:LEU:C	0.66	2.15	9	17
1:A:76:ARG:O	1:A:77:SER:CB	0.66	2.43	15	4
1:A:90:ASP:C	1:A:90:ASP:OD1	0.66	2.39	24	2
1:B:260:HIS:CG	1:B:288:LEU:HD12	0.66	2.25	14	3
1:B:214:LEU:HA	1:B:217:LEU:HD12	0.66	1.67	2	24
1:B:227:GLU:O	1:B:230:ASN:ND2	0.66	2.25	3	10
1:B:247:PHE:C	1:B:247:PHE:CD1	0.66	2.74	5	13
1:A:14:LEU:HA	1:A:17:LEU:HD12	0.66	1.67	2	24
1:A:100:ARG:NH2	1:B:250:ASP:OD1	0.66	2.29	1	4
1:B:230:ASN:CG	1:B:233:ALA:HB3	0.66	2.16	16	12
1:B:282:LEU:O	1:B:282:LEU:CD1	0.66	2.43	7	14
1:B:290:ASP:OD1	1:B:290:ASP:C	0.66	2.38	24	3
1:B:276:ARG:O	1:B:277:SER:CB	0.66	2.43	15	4
1:B:230:ASN:ND2	1:B:231:THR:N	0.66	2.44	23	2
1:A:60:HIS:CG	1:A:88:LEU:HD12	0.66	2.25	14	3
1:A:30:ASN:ND2	1:A:32:ASP:N	0.65	2.43	21	3
1:A:78:GLU:O	1:A:81:LEU:N	0.65	2.28	20	4
1:A:47:PHE:C	1:A:47:PHE:CD1	0.65	2.74	5	13
1:B:290:ASP:O	1:B:294:HIS:ND1	0.65	2.28	13	1
1:B:230:ASN:ND2	1:B:232:ASP:N	0.65	2.43	21	3
1:A:30:ASN:ND2	1:A:31:THR:N	0.65	2.44	23	2
1:A:92:ILE:HD11	1:B:292:ILE:HD11	0.65	1.68	21	1
1:A:44:SER:O	1:A:48:PHE:N	0.65	2.25	24	14
1:A:30:ASN:HD22	1:A:33:ALA:H	0.65	1.31	23	3
1:A:23:THR:O	1:A:27:GLU:OE1	0.65	2.13	16	1
1:B:220:ILE:HD12	1:B:245:LYS:HZ1	0.65	1.52	20	15
1:A:30:ASN:OD1	1:A:33:ALA:CB	0.65	2.44	4	7
1:B:278:GLU:O	1:B:282:LEU:N	0.65	2.28	6	9
1:B:232:ASP:O	1:B:233:ALA:C	0.65	2.40	12	2
1:A:20:ILE:HD12	1:A:45:LYS:NZ	0.64	2.07	20	19
1:A:78:GLU:O	1:A:82:LEU:N	0.64	2.28	6	9
1:B:278:GLU:O	1:B:281:LEU:N	0.64	2.28	20	4
1:B:220:ILE:HD12	1:B:245:LYS:NZ	0.64	2.07	20	19
1:B:230:ASN:OD1	1:B:233:ALA:CB	0.64	2.44	4	7
1:B:288:LEU:HD13	1:B:288:LEU:O	0.64	1.92	16	11
1:A:32:ASP:O	1:A:33:ALA:C	0.64	2.40	12	2
1:B:230:ASN:HD22	1:B:230:ASN:C	0.64	2.01	2	1
1:B:243:VAL:CG1	1:B:298:MET:SD	0.64	2.86	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:LEU:HD13	1:A:88:LEU:O	0.64	1.93	16	11
1:A:30:ASN:HD22	1:A:30:ASN:C	0.64	2.01	2	1
1:A:60:HIS:CE1	1:A:64:MET:CG	0.64	2.81	9	15
1:B:271:LEU:O	1:B:275:GLY:N	0.64	2.26	3	3
1:B:277:SER:O	1:B:278:GLU:C	0.64	2.40	20	1
1:B:260:HIS:CE1	1:B:264:MET:CG	0.63	2.81	9	16
1:A:30:ASN:ND2	1:A:35:VAL:CG2	0.63	2.61	6	5
1:A:43:VAL:CG1	1:A:98:MET:SD	0.63	2.86	25	1
1:B:295:LEU:O	1:B:298:MET:CG	0.63	2.46	10	20
1:A:89:ILE:CD1	1:B:288:LEU:HD13	0.63	2.23	13	10
1:A:88:LEU:HD13	1:B:289:ILE:CD1	0.63	2.23	13	10
1:A:51:ILE:O	1:B:300:ARG:NH1	0.63	2.30	25	1
1:A:77:SER:O	1:A:78:GLU:C	0.63	2.40	20	1
1:B:230:ASN:C	1:B:230:ASN:HD22	0.63	2.02	21	4
1:B:230:ASN:HD22	1:B:233:ALA:CB	0.63	2.07	24	1
1:A:88:LEU:C	1:A:88:LEU:CD1	0.63	2.72	9	11
1:B:249:ALA:O	1:B:250:ASP:C	0.62	2.42	7	25
1:B:230:ASN:ND2	1:B:232:ASP:O	0.62	2.31	2	1
1:B:283:ASP:C	1:B:283:ASP:OD1	0.62	2.42	6	12
1:A:95:LEU:O	1:A:98:MET:CG	0.62	2.46	10	20
1:A:18:ARG:NH2	1:A:62:GLU:OE2	0.62	2.32	4	1
1:A:30:ASN:HD22	1:A:33:ALA:CB	0.62	2.07	24	1
1:B:280:ILE:O	1:B:283:ASP:OD1	0.62	2.17	9	16
1:A:49:ALA:O	1:A:50:ASP:C	0.62	2.42	7	25
1:B:230:ASN:ND2	1:B:235:VAL:CG2	0.62	2.61	6	5
1:A:80:ILE:O	1:A:83:ASP:OD1	0.62	2.18	13	16
1:A:88:LEU:O	1:A:88:LEU:HD23	0.62	1.95	11	11
1:B:288:LEU:HD23	1:B:288:LEU:O	0.62	1.95	11	14
1:B:295:LEU:C	1:B:295:LEU:CD1	0.62	2.71	7	9
1:A:30:ASN:ND2	1:A:32:ASP:O	0.62	2.31	2	1
1:B:218:ARG:NH2	1:B:262:GLU:OE2	0.62	2.32	4	1
1:B:295:LEU:HD12	1:B:295:LEU:O	0.62	1.94	7	11
1:A:16:GLU:CD	1:A:16:GLU:N	0.62	2.58	1	1
1:B:278:GLU:O	1:B:279:ASP:C	0.62	2.42	20	4
1:A:32:ASP:O	1:A:33:ALA:O	0.62	2.18	19	2
1:A:95:LEU:HD12	1:A:95:LEU:O	0.62	1.94	7	10
1:A:30:ASN:OD1	1:A:31:THR:N	0.61	2.33	17	7
1:A:99:TYR:OH	1:B:300:ARG:NH2	0.61	2.32	5	4
1:A:30:ASN:C	1:A:30:ASN:HD22	0.61	2.02	21	4
1:A:83:ASP:OD1	1:A:83:ASP:C	0.61	2.42	20	21
1:A:31:THR:O	1:A:32:ASP:OD1	0.61	2.19	8	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:232:ASP:O	1:B:233:ALA:O	0.61	2.18	19	2
1:A:78:GLU:O	1:A:79:ASP:C	0.61	2.42	20	3
1:B:280:ILE:O	1:B:283:ASP:CG	0.61	2.44	16	15
1:A:50:ASP:CG	1:B:300:ARG:HH21	0.61	2.03	22	1
1:B:231:THR:O	1:B:232:ASP:OD1	0.61	2.19	8	18
1:B:277:SER:C	1:B:279:ASP:H	0.61	2.03	21	8
1:A:39:ILE:O	1:A:43:VAL:HG23	0.61	1.96	2	3
1:B:239:ILE:O	1:B:243:VAL:HG23	0.61	1.96	2	3
1:A:77:SER:C	1:A:79:ASP:H	0.61	2.03	21	8
1:A:80:ILE:O	1:A:83:ASP:CG	0.61	2.44	16	15
1:B:230:ASN:OD1	1:B:231:THR:N	0.61	2.33	17	6
1:B:232:ASP:O	1:B:234:LYS:N	0.61	2.34	7	1
1:B:230:ASN:HD22	1:B:233:ALA:HB3	0.61	1.56	24	1
1:B:288:LEU:C	1:B:288:LEU:CD1	0.61	2.73	3	11
1:B:230:ASN:ND2	1:B:232:ASP:C	0.61	2.59	2	1
1:A:30:ASN:HD22	1:A:33:ALA:HB3	0.61	1.56	24	1
1:B:216:GLU:N	1:B:216:GLU:CD	0.60	2.58	1	2
1:B:233:ALA:O	1:B:234:LYS:C	0.60	2.44	9	2
1:A:16:GLU:HB2	1:A:45:LYS:HZ2	0.60	1.54	13	12
1:B:230:ASN:HD22	1:B:231:THR:N	0.60	1.95	21	1
1:B:279:ASP:O	1:B:282:LEU:N	0.60	2.34	20	1
1:B:216:GLU:HB2	1:B:245:LYS:HZ2	0.60	1.54	13	12
1:A:32:ASP:O	1:A:34:LYS:N	0.60	2.34	7	1
1:A:79:ASP:O	1:A:82:LEU:N	0.60	2.34	20	1
1:B:230:ASN:OD1	1:B:232:ASP:O	0.60	2.19	19	1
1:A:18:ARG:NH2	1:A:62:GLU:OE1	0.60	2.35	3	1
1:B:230:ASN:OD1	1:B:232:ASP:N	0.60	2.35	8	3
1:A:30:ASN:OD1	1:A:32:ASP:O	0.60	2.19	19	1
1:A:30:ASN:ND2	1:A:32:ASP:C	0.60	2.60	2	1
1:B:283:ASP:OD1	1:B:283:ASP:C	0.60	2.44	24	9
1:B:216:GLU:CB	1:B:245:LYS:NZ	0.60	2.65	13	16
1:A:100:ARG:NH2	1:B:247:PHE:O	0.60	2.35	20	1
1:A:35:VAL:O	1:A:39:ILE:N	0.59	2.27	8	20
1:A:27:GLU:O	1:A:30:ASN:OD1	0.59	2.21	23	4
1:B:249:ALA:HB3	1:B:251:ILE:HG13	0.59	1.74	25	12
1:A:30:ASN:HD22	1:A:31:THR:N	0.59	1.95	21	1
1:A:33:ALA:O	1:A:34:LYS:C	0.59	2.44	9	2
1:A:25:VAL:CG1	1:A:84:TYR:CE2	0.59	2.86	16	10
1:A:95:LEU:CD1	1:A:99:TYR:CE2	0.59	2.86	22	9
1:B:295:LEU:CD1	1:B:299:TYR:CE2	0.59	2.86	22	9
1:B:218:ARG:NH2	1:B:262:GLU:OE1	0.59	2.35	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:GLU:CB	1:A:45:LYS:NZ	0.59	2.65	13	15
1:B:227:GLU:O	1:B:230:ASN:OD1	0.59	2.20	23	4
1:A:30:ASN:ND2	1:A:33:ALA:HB3	0.59	2.12	24	5
1:B:288:LEU:HD23	1:B:288:LEU:C	0.59	2.23	11	4
1:A:35:VAL:HG12	1:A:39:ILE:HG13	0.59	1.74	14	12
1:A:88:LEU:CD2	1:A:88:LEU:C	0.59	2.76	12	12
1:A:80:ILE:O	1:A:83:ASP:OD2	0.59	2.21	5	8
1:A:30:ASN:OD1	1:A:32:ASP:N	0.59	2.35	8	4
1:B:277:SER:C	1:B:278:GLU:OE1	0.59	2.45	14	1
1:B:212:LYS:O	1:B:216:GLU:OE2	0.59	2.21	1	1
1:B:225:VAL:CG1	1:B:284:TYR:CE2	0.59	2.86	8	10
1:A:42:PHE:CE2	1:A:91:VAL:CG1	0.59	2.86	7	2
1:A:51:ILE:N	1:B:300:ARG:HH22	0.59	1.95	25	1
1:B:280:ILE:O	1:B:283:ASP:OD2	0.59	2.21	5	8
1:B:269:LYS:O	1:B:273:LEU:HD12	0.59	1.98	21	1
1:B:277:SER:OG	1:B:279:ASP:OD2	0.58	2.21	19	1
1:A:69:LYS:O	1:A:73:LEU:HD12	0.58	1.98	21	1
1:B:242:PHE:CE2	1:B:291:VAL:CG1	0.58	2.86	7	2
1:A:77:SER:C	1:A:78:GLU:OE1	0.58	2.45	14	1
1:B:288:LEU:C	1:B:288:LEU:CD2	0.58	2.76	12	14
1:B:230:ASN:ND2	1:B:233:ALA:HB3	0.58	2.12	24	5
1:B:223:THR:HG21	1:B:238:ARG:NH1	0.58	2.13	3	2
1:B:230:ASN:O	1:B:230:ASN:ND2	0.58	2.36	19	1
1:A:100:ARG:NH2	1:B:251:ILE:O	0.58	2.37	3	1
1:A:30:ASN:OD1	1:A:30:ASN:C	0.58	2.47	8	2
1:A:79:ASP:O	1:A:83:ASP:OD2	0.58	2.22	8	1
1:A:64:MET:O	1:A:81:LEU:HD21	0.58	1.99	9	1
1:A:30:ASN:O	1:A:30:ASN:ND2	0.58	2.36	19	1
1:A:100:ARG:NH1	1:B:250:ASP:OD1	0.58	2.36	24	3
1:A:77:SER:OG	1:A:79:ASP:OD2	0.58	2.21	19	1
1:A:100:ARG:HH21	1:B:250:ASP:CG	0.58	2.07	22	1
1:B:247:PHE:CD1	1:B:247:PHE:O	0.58	2.57	21	6
1:A:10:LYS:NZ	1:A:14:LEU:HD11	0.58	2.14	6	2
1:B:235:VAL:HG12	1:B:239:ILE:HG13	0.58	1.74	14	12
1:A:47:PHE:O	1:A:47:PHE:CD1	0.58	2.57	21	4
1:A:88:LEU:HD23	1:A:88:LEU:C	0.58	2.23	11	3
1:A:10:LYS:NZ	1:A:55:GLN:HE21	0.58	1.97	16	1
1:B:233:ALA:O	1:B:234:LYS:CB	0.57	2.52	15	1
1:A:49:ALA:HB3	1:A:51:ILE:HG13	0.57	1.75	25	10
1:B:279:ASP:O	1:B:283:ASP:OD2	0.57	2.22	8	1
1:B:274:GLU:C	1:B:276:ARG:H	0.57	2.07	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:235:VAL:O	1:B:239:ILE:N	0.57	2.29	14	18
1:A:28:TYR:OH	1:A:90:ASP:OD2	0.57	2.20	13	1
1:B:264:MET:O	1:B:281:LEU:HD21	0.57	1.99	9	2
1:A:60:HIS:CG	1:A:88:LEU:CD1	0.57	2.87	14	4
1:B:210:LYS:NZ	1:B:255:GLN:HE21	0.57	1.97	16	1
1:B:230:ASN:HD22	1:B:233:ALA:CA	0.57	2.11	24	1
1:B:210:LYS:NZ	1:B:214:LEU:HD11	0.57	2.14	6	2
1:B:230:ASN:OD1	1:B:230:ASN:C	0.57	2.47	8	3
1:A:40:ASP:OD1	1:A:44:SER:OG	0.57	2.22	23	2
1:B:240:ASP:OD1	1:B:244:SER:OG	0.57	2.22	23	2
1:B:260:HIS:CG	1:B:288:LEU:CD1	0.57	2.87	14	4
1:A:27:GLU:OE1	1:A:38:ARG:NH1	0.57	2.37	20	1
1:A:12:LYS:O	1:A:16:GLU:OE2	0.57	2.21	1	1
1:B:281:LEU:CD1	1:B:284:TYR:CD2	0.57	2.88	21	2
1:A:30:ASN:HD22	1:A:33:ALA:CA	0.57	2.11	24	1
1:B:264:MET:O	1:B:268:SER:OG	0.57	2.22	24	3
1:A:23:THR:HG21	1:A:38:ARG:NH1	0.57	2.13	3	2
1:A:99:TYR:OH	1:B:300:ARG:CZ	0.57	2.52	25	1
1:A:74:GLU:C	1:A:76:ARG:H	0.57	2.07	1	3
1:A:95:LEU:C	1:A:95:LEU:CD1	0.57	2.76	8	11
1:A:44:SER:O	1:A:48:PHE:CB	0.57	2.53	2	1
1:B:230:ASN:CG	1:B:233:ALA:H	0.57	2.08	8	1
1:A:33:ALA:O	1:A:34:LYS:CG	0.57	2.53	15	1
1:A:34:LYS:H	1:A:34:LYS:CD	0.57	2.13	22	1
1:A:93:ALA:CB	1:B:253:VAL:HG11	0.56	2.30	24	10
1:B:218:ARG:NH1	1:B:262:GLU:OE2	0.56	2.38	10	1
1:B:221:TYR:OH	1:B:260:HIS:ND1	0.56	2.26	11	1
1:A:33:ALA:O	1:A:34:LYS:CB	0.56	2.52	15	1
1:A:81:LEU:CD1	1:A:84:TYR:CD2	0.56	2.88	21	2
1:A:100:ARG:HH22	1:B:251:ILE:N	0.56	1.97	25	1
1:B:244:SER:O	1:B:248:PHE:CB	0.56	2.53	2	1
1:B:227:GLU:OE1	1:B:238:ARG:NH1	0.56	2.37	20	1
1:B:260:HIS:CD2	1:B:288:LEU:CD1	0.56	2.84	12	9
1:A:33:ALA:O	1:A:35:VAL:HG23	0.56	2.01	10	1
1:A:18:ARG:NH1	1:A:62:GLU:OE2	0.56	2.38	10	1
1:A:64:MET:O	1:A:68:SER:OG	0.56	2.21	22	3
1:A:20:ILE:CD1	1:A:45:LYS:HZ3	0.56	2.13	17	3
1:B:210:LYS:HZ2	1:B:214:LEU:HD11	0.56	1.60	6	2
1:B:221:TYR:CD2	1:B:263:LEU:HD22	0.56	2.36	20	4
1:A:30:ASN:CG	1:A:33:ALA:H	0.56	2.08	8	1
1:B:216:GLU:OE1	1:B:216:GLU:CA	0.56	2.54	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:233:ALA:O	1:B:235:VAL:HG23	0.56	2.01	10	1
1:B:285:ARG:CD	1:B:286:LEU:N	0.56	2.69	10	1
1:A:21:TYR:CD2	1:A:63:LEU:HD22	0.56	2.36	20	5
1:A:31:THR:O	1:A:32:ASP:CG	0.56	2.49	8	4
1:B:231:THR:O	1:B:232:ASP:CG	0.55	2.49	8	4
1:A:79:ASP:O	1:A:82:LEU:CB	0.55	2.54	14	6
1:A:85:ARG:CD	1:A:86:LEU:N	0.55	2.69	10	1
1:A:60:HIS:CD2	1:A:88:LEU:CD1	0.55	2.85	12	9
1:B:279:ASP:O	1:B:282:LEU:CB	0.55	2.54	14	6
1:B:228:TYR:OH	1:B:290:ASP:OD2	0.55	2.20	13	2
1:A:99:TYR:OH	1:B:300:ARG:NE	0.55	2.40	15	2
1:B:298:MET:O	1:B:302:SER:OG	0.55	2.24	16	1
1:B:233:ALA:O	1:B:234:LYS:CG	0.55	2.53	15	1
1:B:238:ARG:HA	1:B:238:ARG:NE	0.55	2.17	19	2
1:A:88:LEU:C	1:A:88:LEU:HD23	0.55	2.26	22	10
1:B:230:ASN:OD1	1:B:233:ALA:CA	0.55	2.55	7	2
1:A:14:LEU:HD22	1:A:17:LEU:HD12	0.55	1.79	12	22
1:A:38:ARG:NE	1:A:38:ARG:HA	0.55	2.17	19	3
1:A:80:ILE:CD1	1:A:84:TYR:OH	0.55	2.55	2	2
1:B:225:VAL:HG13	1:B:284:TYR:CE1	0.55	2.37	11	4
1:A:30:ASN:OD1	1:A:33:ALA:CA	0.55	2.55	7	2
1:A:42:PHE:CE1	1:A:91:VAL:CG1	0.55	2.91	15	3
1:A:98:MET:O	1:A:102:SER:OG	0.55	2.24	16	1
1:A:16:GLU:OE1	1:A:16:GLU:CA	0.55	2.54	21	1
1:A:80:ILE:CG1	1:A:84:TYR:OH	0.54	2.55	2	3
1:B:234:LYS:H	1:B:234:LYS:CD	0.54	2.13	22	2
1:A:16:GLU:N	1:A:16:GLU:CD	0.54	2.65	21	1
1:B:280:ILE:CD1	1:B:284:TYR:OH	0.54	2.55	2	2
1:B:220:ILE:CD1	1:B:245:LYS:NZ	0.54	2.71	17	13
1:A:88:LEU:C	1:A:88:LEU:CD2	0.54	2.81	11	2
1:A:70:GLN:O	1:A:73:LEU:N	0.54	2.41	3	4
1:B:270:GLN:O	1:B:273:LEU:N	0.54	2.41	3	4
1:A:10:LYS:HZ2	1:A:14:LEU:HD11	0.54	1.62	6	2
1:A:21:TYR:HH	1:A:60:HIS:CE1	0.54	2.18	11	1
1:A:21:TYR:OH	1:A:60:HIS:ND1	0.54	2.25	11	1
1:A:20:ILE:CD1	1:A:45:LYS:NZ	0.54	2.71	17	14
1:B:242:PHE:CE1	1:B:291:VAL:CG1	0.54	2.90	14	3
1:A:25:VAL:HG13	1:A:84:TYR:CE1	0.54	2.37	11	4
1:A:80:ILE:HG23	1:A:81:LEU:H	0.54	1.63	5	3
1:B:302:SER:O	1:B:302:SER:OG	0.53	2.25	1	2
1:B:237:GLU:OE1	1:B:237:GLU:N	0.53	2.42	23	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:288:LEU:C	1:B:288:LEU:HD23	0.53	2.26	22	9
1:B:223:THR:HG21	1:B:238:ARG:HD2	0.53	1.81	3	2
1:B:208:ALA:O	1:B:212:LYS:N	0.53	2.37	9	3
1:A:88:LEU:HD23	1:A:88:LEU:O	0.53	2.04	22	3
1:B:286:LEU:O	1:B:290:ASP:CG	0.53	2.51	22	6
1:A:86:LEU:O	1:A:90:ASP:CG	0.53	2.51	22	6
1:B:230:ASN:ND2	1:B:230:ASN:O	0.53	2.42	15	3
1:B:280:ILE:CG1	1:B:284:TYR:OH	0.53	2.55	2	3
1:A:43:VAL:HG12	1:A:98:MET:HE3	0.53	1.80	20	5
1:A:30:ASN:ND2	1:A:30:ASN:O	0.53	2.42	15	3
1:A:60:HIS:ND1	1:A:64:MET:HE3	0.53	2.19	17	2
1:B:214:LEU:HD22	1:B:217:LEU:HD12	0.53	1.79	12	22
1:B:243:VAL:HG12	1:B:298:MET:HE3	0.53	1.80	20	4
1:A:64:MET:N	1:A:64:MET:HE2	0.52	2.18	19	2
1:B:264:MET:N	1:B:264:MET:HE2	0.52	2.18	19	2
1:A:85:ARG:CG	1:A:86:LEU:N	0.52	2.72	15	10
1:A:37:GLU:N	1:A:37:GLU:OE1	0.52	2.42	23	2
1:B:260:HIS:ND1	1:B:264:MET:HE3	0.52	2.19	17	2
1:A:102:SER:O	1:A:102:SER:OG	0.52	2.25	1	2
1:A:48:PHE:C	1:A:50:ASP:H	0.52	2.13	14	1
1:B:230:ASN:CG	1:B:231:THR:N	0.52	2.67	23	2
1:A:23:THR:HG21	1:A:38:ARG:HD2	0.52	1.80	3	2
1:A:74:GLU:C	1:A:76:ARG:N	0.52	2.67	1	1
1:A:83:ASP:OD1	1:A:84:TYR:N	0.52	2.43	6	4
1:B:260:HIS:CE1	1:B:264:MET:HE3	0.52	2.40	13	12
1:B:248:PHE:C	1:B:250:ASP:H	0.52	2.13	14	1
1:B:285:ARG:CG	1:B:286:LEU:N	0.52	2.72	15	10
1:A:47:PHE:CD1	1:A:47:PHE:C	0.52	2.86	22	5
1:B:270:GLN:O	1:B:271:LEU:C	0.52	2.53	16	4
1:B:274:GLU:C	1:B:276:ARG:N	0.52	2.67	1	1
1:A:8:ALA:O	1:A:12:LYS:N	0.52	2.37	9	4
1:B:280:ILE:HG23	1:B:281:LEU:H	0.52	1.63	5	4
1:A:21:TYR:CE1	1:A:91:VAL:HG21	0.52	2.40	15	2
1:A:92:ILE:O	1:A:95:LEU:CD2	0.52	2.58	10	11
1:A:77:SER:C	1:A:79:ASP:N	0.52	2.68	5	10
1:B:249:ALA:HB3	1:B:251:ILE:CG1	0.52	2.35	22	16
1:B:295:LEU:HD23	1:B:296:CYS:H	0.52	1.65	10	3
1:B:234:LYS:N	1:B:234:LYS:CD	0.52	2.72	7	1
1:A:59:ILE:O	1:A:63:LEU:N	0.52	2.38	17	3
1:A:25:VAL:CG1	1:A:84:TYR:CZ	0.51	2.93	14	5
1:B:260:HIS:CE1	1:B:264:MET:SD	0.51	3.04	17	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:247:PHE:CD1	1:B:247:PHE:C	0.51	2.85	6	5
1:A:31:THR:C	1:A:32:ASP:OD1	0.51	2.54	24	1
1:A:43:VAL:HG13	1:A:95:LEU:HA	0.51	1.81	8	12
1:A:60:HIS:CE1	1:A:64:MET:SD	0.51	3.04	17	9
1:A:49:ALA:HB3	1:A:51:ILE:CG1	0.51	2.36	22	16
1:A:40:ASP:O	1:A:44:SER:N	0.51	2.42	20	15
1:A:95:LEU:HD23	1:A:96:CYS:H	0.51	1.66	10	3
1:B:299:TYR:O	1:B:302:SER:OG	0.51	2.26	15	1
1:A:99:TYR:OH	1:B:300:ARG:NH1	0.51	2.44	20	1
1:B:283:ASP:OD1	1:B:284:TYR:N	0.51	2.43	6	5
1:B:295:LEU:HG	1:B:296:CYS:N	0.51	2.21	2	14
1:A:51:ILE:C	1:B:300:ARG:HH12	0.51	2.13	25	1
1:A:53:VAL:HG11	1:B:293:ALA:CB	0.51	2.36	4	7
1:B:221:TYR:CE1	1:B:291:VAL:HG21	0.51	2.40	15	3
1:B:229:PHE:CE2	1:B:283:ASP:OD1	0.51	2.64	18	1
1:B:293:ALA:O	1:B:297:GLU:CG	0.51	2.59	2	6
1:B:231:THR:C	1:B:232:ASP:OD1	0.51	2.54	24	1
1:B:243:VAL:HG13	1:B:295:LEU:HA	0.51	1.81	8	14
1:A:93:ALA:O	1:A:97:GLU:CG	0.51	2.59	2	6
1:B:277:SER:C	1:B:279:ASP:N	0.51	2.68	5	10
1:A:29:PHE:CE2	1:A:83:ASP:OD1	0.51	2.64	18	1
1:A:70:GLN:O	1:A:71:LEU:C	0.51	2.54	23	4
1:B:225:VAL:CG1	1:B:284:TYR:CZ	0.51	2.94	14	5
1:B:277:SER:O	1:B:278:GLU:CB	0.51	2.59	24	1
1:B:292:ILE:O	1:B:295:LEU:CD2	0.51	2.58	3	10
1:A:60:HIS:CE1	1:A:64:MET:HE3	0.51	2.40	13	11
1:A:47:PHE:CD2	1:A:99:TYR:CE1	0.51	2.99	23	5
1:B:275:GLY:O	1:B:276:ARG:O	0.50	2.28	2	3
1:B:230:ASN:CG	1:B:233:ALA:CB	0.50	2.85	3	2
1:A:14:LEU:HD23	1:A:14:LEU:N	0.50	2.22	16	18
1:B:214:LEU:HD23	1:B:214:LEU:N	0.50	2.21	19	22
1:A:75:GLY:O	1:A:76:ARG:O	0.50	2.28	2	3
1:B:267:PHE:CB	1:B:281:LEU:HD13	0.50	2.37	25	4
1:A:34:LYS:N	1:A:34:LYS:CD	0.50	2.72	7	1
1:B:233:ALA:C	1:B:234:LYS:CG	0.50	2.84	15	1
1:A:17:LEU:O	1:A:21:TYR:CB	0.50	2.60	15	6
1:B:247:PHE:CD2	1:B:299:TYR:CE1	0.50	2.99	23	5
1:A:33:ALA:C	1:A:34:LYS:CG	0.50	2.84	15	1
1:B:300:ARG:NH1	1:B:300:ARG:CG	0.50	2.74	19	1
1:A:30:ASN:CG	1:A:33:ALA:CB	0.50	2.85	3	2
1:A:89:ILE:CD1	1:B:288:LEU:HD12	0.50	2.37	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LYS:O	1:A:49:ALA:N	0.50	2.33	18	1
1:A:47:PHE:CD1	1:A:47:PHE:O	0.50	2.65	22	2
1:A:79:ASP:O	1:A:80:ILE:C	0.50	2.55	20	1
1:A:77:SER:O	1:A:78:GLU:CB	0.50	2.59	24	1
1:B:223:THR:O	1:B:227:GLU:N	0.50	2.42	17	6
1:B:230:ASN:ND2	1:B:235:VAL:HG21	0.50	2.22	6	3
1:A:95:LEU:O	1:A:98:MET:HG3	0.50	2.07	25	3
1:B:240:ASP:O	1:B:244:SER:N	0.50	2.42	20	11
1:A:30:ASN:CG	1:A:31:THR:N	0.50	2.69	17	3
1:B:280:ILE:HG23	1:B:281:LEU:N	0.50	2.21	13	7
1:B:231:THR:OG1	1:B:232:ASP:N	0.50	2.45	23	3
1:B:281:LEU:HD12	1:B:284:TYR:CE2	0.50	2.42	18	1
1:A:77:SER:O	1:A:78:GLU:HB2	0.50	2.07	24	1
1:A:95:LEU:HG	1:A:96:CYS:N	0.49	2.21	2	14
1:A:23:THR:CG2	1:A:38:ARG:NH1	0.49	2.75	20	2
1:B:223:THR:CG2	1:B:238:ARG:NH1	0.49	2.75	20	2
1:A:67:PHE:CB	1:A:81:LEU:HD13	0.49	2.37	25	4
1:B:295:LEU:O	1:B:298:MET:HG3	0.49	2.07	25	6
1:B:293:ALA:O	1:B:297:GLU:N	0.49	2.43	23	1
1:A:30:ASN:ND2	1:A:35:VAL:HG21	0.49	2.22	6	2
1:B:283:ASP:OD1	1:B:284:TYR:CD1	0.49	2.66	10	4
1:B:217:LEU:O	1:B:221:TYR:CB	0.49	2.60	15	5
1:A:80:ILE:HG23	1:A:81:LEU:N	0.49	2.21	13	7
1:A:93:ALA:O	1:A:97:GLU:N	0.49	2.43	23	1
1:B:220:ILE:HD11	1:B:245:LYS:HZ3	0.49	1.66	3	3
1:A:23:THR:O	1:A:27:GLU:N	0.49	2.42	5	4
1:A:31:THR:OG1	1:A:32:ASP:N	0.49	2.45	17	3
1:B:218:ARG:NE	1:B:262:GLU:OE1	0.49	2.46	19	1
1:A:16:GLU:HB3	1:A:45:LYS:NZ	0.49	2.23	3	4
1:B:300:ARG:CG	1:B:300:ARG:HH11	0.49	2.21	19	1
1:A:83:ASP:OD1	1:A:84:TYR:CD1	0.49	2.66	12	4
1:B:290:ASP:OD1	1:B:290:ASP:O	0.49	2.31	9	1
1:A:95:LEU:HD11	1:A:99:TYR:CZ	0.48	2.42	12	3
1:B:223:THR:HG21	1:B:238:ARG:HE	0.48	1.68	8	1
1:A:88:LEU:HD12	1:B:289:ILE:CD1	0.48	2.36	16	1
1:A:81:LEU:HD12	1:A:84:TYR:CE2	0.48	2.42	18	1
1:A:20:ILE:HD11	1:A:45:LYS:HZ3	0.48	1.67	3	3
1:A:99:TYR:O	1:A:102:SER:OG	0.48	2.26	15	1
1:A:100:ARG:NE	1:B:299:TYR:OH	0.48	2.44	24	1
1:B:222:ARG:NH1	1:B:267:PHE:CE1	0.48	2.81	8	1
1:A:90:ASP:OD1	1:A:90:ASP:O	0.48	2.31	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:277:SER:O	1:B:278:GLU:HB2	0.48	2.07	24	1
1:A:99:TYR:O	1:A:103:ILE:CG1	0.48	2.61	14	5
1:A:77:SER:O	1:A:80:ILE:CG2	0.48	2.62	1	2
1:B:216:GLU:HB3	1:B:245:LYS:NZ	0.48	2.22	3	4
1:B:290:ASP:O	1:B:294:HIS:CD2	0.48	2.67	5	2
1:A:90:ASP:OD1	1:A:90:ASP:C	0.48	2.55	9	1
1:A:30:ASN:OD1	1:A:32:ASP:C	0.48	2.56	12	2
1:B:259:ILE:O	1:B:263:LEU:N	0.48	2.38	17	1
1:B:290:ASP:CG	1:B:294:HIS:NE2	0.48	2.72	18	1
1:B:299:TYR:O	1:B:303:ILE:CG1	0.48	2.62	10	5
1:A:29:PHE:CZ	1:A:83:ASP:OD1	0.48	2.67	18	1
1:A:100:ARG:CG	1:A:100:ARG:HH11	0.48	2.21	19	1
1:A:82:LEU:C	1:A:82:LEU:CD1	0.48	2.86	22	8
1:A:90:ASP:O	1:A:94:HIS:CD2	0.48	2.67	5	2
1:A:23:THR:HG21	1:A:38:ARG:HE	0.48	1.68	8	1
1:B:230:ASN:OD1	1:B:232:ASP:C	0.48	2.56	12	2
1:A:63:LEU:HD11	1:A:67:PHE:CE1	0.48	2.44	10	1
1:A:90:ASP:CG	1:A:94:HIS:NE2	0.48	2.72	18	1
1:B:279:ASP:O	1:B:280:ILE:C	0.48	2.55	20	1
1:B:267:PHE:O	1:B:271:LEU:CD2	0.48	2.62	11	10
1:A:89:ILE:HD13	1:B:288:LEU:HD12	0.48	1.85	5	2
1:A:48:PHE:CG	1:A:49:ALA:N	0.48	2.81	14	1
1:B:277:SER:O	1:B:280:ILE:CG2	0.47	2.62	1	2
1:A:68:SER:HA	1:A:81:LEU:HD22	0.47	1.86	11	1
1:B:248:PHE:CG	1:B:249:ALA:N	0.47	2.81	14	1
1:A:103:ILE:CD1	1:B:302:SER:OG	0.47	2.62	12	1
1:B:264:MET:SD	1:B:284:TYR:CB	0.47	3.03	23	3
1:A:64:MET:SD	1:A:84:TYR:CB	0.47	3.03	23	3
1:B:280:ILE:CG1	1:B:284:TYR:CZ	0.47	2.98	2	3
1:A:60:HIS:CE1	1:A:64:MET:HG3	0.47	2.44	25	3
1:A:47:PHE:CG	1:A:98:MET:SD	0.47	3.07	7	1
1:A:22:ARG:NH1	1:A:67:PHE:CE1	0.47	2.81	8	1
1:B:229:PHE:CZ	1:B:283:ASP:OD1	0.47	2.67	18	1
1:A:79:ASP:O	1:A:83:ASP:N	0.47	2.47	20	1
1:B:282:LEU:C	1:B:282:LEU:CD1	0.47	2.84	23	8
1:A:80:ILE:HG12	1:A:84:TYR:CZ	0.47	2.45	2	5
1:B:280:ILE:HG12	1:B:284:TYR:CZ	0.47	2.45	2	5
1:A:76:ARG:HH21	1:A:80:ILE:HD13	0.47	1.70	10	1
1:B:280:ILE:O	1:B:284:TYR:CD1	0.47	2.68	8	5
1:B:247:PHE:CG	1:B:298:MET:SD	0.47	3.07	7	1
1:B:216:GLU:HB2	1:B:245:LYS:NZ	0.47	2.23	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:PHE:O	1:A:71:LEU:CD2	0.47	2.62	11	10
1:B:263:LEU:HD11	1:B:267:PHE:CE1	0.47	2.44	10	2
1:A:30:ASN:ND2	1:A:35:VAL:HG23	0.47	2.25	22	1
1:A:60:HIS:NE2	1:A:64:MET:HG3	0.47	2.24	19	19
1:B:295:LEU:HD11	1:B:299:TYR:CZ	0.47	2.42	12	3
1:B:230:ASN:ND2	1:B:235:VAL:HG23	0.47	2.25	22	1
1:B:260:HIS:CE1	1:B:264:MET:HG3	0.47	2.44	25	4
1:A:89:ILE:O	1:A:93:ALA:CB	0.47	2.63	11	1
1:A:27:GLU:OE1	1:A:27:GLU:N	0.47	2.48	16	1
1:B:268:SER:HA	1:B:281:LEU:HD22	0.47	1.86	11	1
1:A:80:ILE:O	1:A:84:TYR:CD1	0.46	2.67	8	5
1:B:233:ALA:O	1:B:235:VAL:CG2	0.46	2.63	10	1
1:A:100:ARG:CG	1:A:100:ARG:NH1	0.46	2.74	19	1
1:B:279:ASP:O	1:B:283:ASP:N	0.46	2.47	20	1
1:A:80:ILE:CG1	1:A:84:TYR:CZ	0.46	2.98	2	3
1:B:285:ARG:HD3	1:B:286:LEU:N	0.46	2.25	10	1
1:B:227:GLU:OE1	1:B:227:GLU:N	0.46	2.48	16	1
1:A:18:ARG:NE	1:A:62:GLU:OE1	0.46	2.46	19	1
1:A:98:MET:HG3	1:A:99:TYR:N	0.46	2.25	13	23
1:A:33:ALA:O	1:A:35:VAL:CG2	0.46	2.63	10	1
1:B:289:ILE:O	1:B:293:ALA:CB	0.46	2.63	11	1
1:A:100:ARG:CZ	1:B:250:ASP:OD1	0.46	2.63	1	1
1:A:28:TYR:CE1	1:A:90:ASP:OD2	0.46	2.69	11	1
1:B:221:TYR:HH	1:B:260:HIS:CE1	0.46	2.19	11	1
1:A:88:LEU:HD12	1:B:289:ILE:HD13	0.46	1.86	15	1
1:B:260:HIS:NE2	1:B:264:MET:HG3	0.46	2.24	19	18
1:B:264:MET:SD	1:B:284:TYR:HB3	0.46	2.51	14	4
1:A:85:ARG:HD3	1:A:86:LEU:N	0.46	2.25	10	1
1:B:218:ARG:CG	1:B:219:SER:N	0.46	2.77	24	2
1:B:298:MET:HG3	1:B:299:TYR:N	0.46	2.25	6	23
1:A:16:GLU:HB2	1:A:45:LYS:NZ	0.46	2.26	15	8
1:B:250:ASP:CG	1:B:250:ASP:O	0.46	2.59	6	1
1:B:228:TYR:CE1	1:B:290:ASP:OD2	0.46	2.69	11	1
1:A:18:ARG:CG	1:A:19:SER:N	0.45	2.77	24	2
1:B:278:GLU:O	1:B:280:ILE:CG2	0.45	2.64	20	1
1:A:21:TYR:CE2	1:A:63:LEU:HD22	0.45	2.47	16	4
1:A:89:ILE:HG12	1:B:289:ILE:CD1	0.45	2.41	1	2
1:A:34:LYS:CE	1:A:37:GLU:OE1	0.45	2.64	10	1
1:A:93:ALA:HB1	1:B:253:VAL:HG11	0.45	1.87	24	1
1:B:218:ARG:HG2	1:B:219:SER:N	0.45	2.25	4	5
1:B:234:LYS:CE	1:B:237:GLU:OE1	0.45	2.64	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LYS:CD	1:A:34:LYS:H	0.45	2.21	12	1
1:A:78:GLU:O	1:A:80:ILE:CG2	0.45	2.64	20	1
1:A:30:ASN:HD22	1:A:35:VAL:CG2	0.45	2.24	22	1
1:A:17:LEU:O	1:A:21:TYR:N	0.45	2.39	7	3
1:A:74:GLU:N	1:A:74:GLU:CD	0.45	2.72	16	4
1:B:295:LEU:HD23	1:B:296:CYS:N	0.45	2.26	10	1
1:B:221:TYR:CE2	1:B:263:LEU:HD22	0.45	2.47	16	4
1:B:221:TYR:CD1	1:B:221:TYR:C	0.45	2.93	4	2
1:A:55:GLN:OE1	1:A:58:GLU:OE1	0.45	2.35	6	1
1:A:95:LEU:CD1	1:A:99:TYR:OH	0.45	2.65	1	2
1:B:276:ARG:HH21	1:B:280:ILE:HD13	0.45	1.70	10	1
1:A:14:LEU:N	1:A:14:LEU:HD23	0.45	2.26	2	6
1:A:18:ARG:HG2	1:A:19:SER:N	0.45	2.27	1	6
1:A:64:MET:SD	1:A:84:TYR:HB3	0.45	2.51	14	4
1:A:16:GLU:CB	1:A:45:LYS:HZ2	0.45	2.21	13	1
1:B:230:ASN:ND2	1:B:231:THR:C	0.45	2.75	23	1
1:B:264:MET:SD	1:B:281:LEU:CD1	0.45	3.02	5	2
1:A:85:ARG:HG3	1:A:86:LEU:N	0.45	2.27	24	4
1:A:50:ASP:O	1:A:50:ASP:CG	0.45	2.59	6	1
1:A:69:LYS:O	1:A:73:LEU:CD1	0.45	2.65	25	1
1:B:295:LEU:CD1	1:B:299:TYR:OH	0.45	2.65	1	2
1:B:214:LEU:CD2	1:B:217:LEU:HD12	0.45	2.42	18	3
1:A:95:LEU:HD12	1:A:99:TYR:OH	0.44	2.12	1	2
1:A:92:ILE:CD1	1:B:289:ILE:HG23	0.44	2.43	11	4
1:B:269:LYS:O	1:B:273:LEU:CD1	0.44	2.65	25	2
1:B:301:ARG:C	1:B:303:ILE:H	0.44	2.20	25	1
1:A:9:ASP:O	1:A:13:LEU:N	0.44	2.49	3	1
1:A:51:ILE:O	1:B:300:ARG:CZ	0.44	2.65	3	1
1:B:255:GLN:OE1	1:B:258:GLU:OE1	0.44	2.35	6	1
1:B:236:ASN:OD1	1:B:236:ASN:C	0.44	2.61	25	2
1:A:95:LEU:HD23	1:A:96:CYS:N	0.44	2.26	10	1
1:B:224:ILE:O	1:B:228:TYR:HB2	0.44	2.12	16	4
1:B:230:ASN:HD22	1:B:235:VAL:CG2	0.44	2.24	22	1
1:A:36:ASN:OD1	1:A:36:ASN:C	0.44	2.61	25	2
1:B:264:MET:SD	1:B:284:TYR:HB2	0.44	2.53	11	1
1:A:24:ILE:O	1:A:28:TYR:HB2	0.44	2.12	16	4
1:A:30:ASN:ND2	1:A:31:THR:C	0.44	2.75	23	1
1:B:271:LEU:HD22	1:B:271:LEU:H	0.44	1.72	25	3
1:A:48:PHE:C	1:A:50:ASP:N	0.44	2.76	14	1
1:A:101:ARG:C	1:A:103:ILE:H	0.44	2.20	25	1
1:A:32:ASP:C	1:A:33:ALA:O	0.44	2.60	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:260:HIS:CG	1:B:288:LEU:HG	0.44	2.48	22	9
1:A:98:MET:O	1:A:102:SER:N	0.44	2.47	25	1
1:A:71:LEU:HD22	1:A:71:LEU:H	0.44	1.73	12	2
1:A:64:MET:SD	1:A:84:TYR:HB2	0.44	2.53	11	1
1:A:59:ILE:O	1:A:63:LEU:CB	0.44	2.66	17	1
1:A:82:LEU:CD1	1:A:82:LEU:C	0.44	2.90	25	2
1:B:245:LYS:O	1:B:249:ALA:N	0.44	2.38	3	2
1:B:285:ARG:HG3	1:B:286:LEU:N	0.44	2.27	24	5
1:B:288:LEU:CD2	1:B:292:ILE:HD11	0.44	2.43	8	1
1:B:237:GLU:N	1:B:237:GLU:CD	0.44	2.76	19	1
1:A:82:LEU:CD1	1:A:85:ARG:HH21	0.43	2.26	19	1
1:A:64:MET:SD	1:A:81:LEU:CD1	0.43	3.02	5	2
1:A:14:LEU:O	1:A:18:ARG:N	0.43	2.50	9	1
1:B:295:LEU:CD1	1:B:295:LEU:C	0.43	2.89	22	2
1:A:23:THR:HG21	1:A:38:ARG:CD	0.43	2.43	17	1
1:B:282:LEU:CD1	1:B:285:ARG:HH21	0.43	2.26	19	1
1:A:18:ARG:CG	1:A:18:ARG:HH11	0.43	2.26	22	1
1:B:223:THR:HG21	1:B:238:ARG:CD	0.43	2.43	17	1
1:B:218:ARG:NH1	1:B:218:ARG:CG	0.43	2.80	22	1
1:A:71:LEU:H	1:A:71:LEU:HD22	0.43	1.72	25	1
1:B:295:LEU:HD12	1:B:299:TYR:OH	0.43	2.12	1	1
1:A:60:HIS:CG	1:A:88:LEU:HG	0.43	2.48	22	9
1:A:100:ARG:CZ	1:B:251:ILE:O	0.43	2.66	3	1
1:B:288:LEU:HD22	1:B:292:ILE:HD11	0.43	1.91	8	1
1:B:259:ILE:O	1:B:263:LEU:CB	0.43	2.66	17	1
1:A:43:VAL:HG22	1:A:95:LEU:CA	0.43	2.43	21	1
1:A:87:THR:O	1:A:91:VAL:N	0.43	2.46	4	2
1:B:260:HIS:O	1:B:264:MET:HG2	0.43	2.14	25	2
1:A:37:GLU:N	1:A:37:GLU:CD	0.43	2.76	19	1
1:A:27:GLU:O	1:A:30:ASN:CG	0.43	2.62	20	1
1:B:232:ASP:C	1:B:233:ALA:O	0.43	2.60	19	2
1:B:234:LYS:CB	1:B:234:LYS:NZ	0.43	2.82	3	1
1:A:14:LEU:CD2	1:A:17:LEU:HD12	0.43	2.42	18	4
1:A:88:LEU:HD22	1:A:92:ILE:HD11	0.43	1.90	8	1
1:B:282:LEU:CD1	1:B:282:LEU:C	0.43	2.92	6	1
1:A:60:HIS:O	1:A:64:MET:HG2	0.43	2.14	25	2
1:A:18:ARG:CG	1:A:18:ARG:NH1	0.43	2.80	22	1
1:A:88:LEU:CD2	1:A:92:ILE:HD11	0.43	2.43	8	1
1:A:95:LEU:CD1	1:A:95:LEU:C	0.43	2.88	12	2
1:A:34:LYS:CB	1:A:34:LYS:NZ	0.43	2.82	3	1
1:A:34:LYS:O	1:A:35:VAL:C	0.43	2.62	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ASN:ND2	1:A:30:ASN:C	0.43	2.71	19	1
1:B:220:ILE:CD1	1:B:245:LYS:HZ3	0.42	2.26	4	4
1:B:221:TYR:HE1	1:B:291:VAL:HG21	0.42	1.74	10	1
1:A:99:TYR:CZ	1:B:300:ARG:NE	0.42	2.87	15	1
1:A:30:ASN:CG	1:A:33:ALA:N	0.42	2.76	8	1
1:B:279:ASP:O	1:B:282:LEU:HB3	0.42	2.14	10	1
1:B:248:PHE:C	1:B:250:ASP:N	0.42	2.76	14	1
1:B:210:LYS:HZ1	1:B:255:GLN:HG3	0.42	1.74	6	1
1:B:230:ASN:CG	1:B:233:ALA:N	0.42	2.77	8	1
1:B:260:HIS:CD2	1:B:264:MET:HG3	0.42	2.49	11	1
1:B:227:GLU:O	1:B:230:ASN:CG	0.42	2.61	20	1
1:A:50:ASP:OD1	1:B:300:ARG:CZ	0.42	2.67	1	1
1:A:21:TYR:C	1:A:21:TYR:CD1	0.42	2.97	24	4
1:B:243:VAL:HG22	1:B:295:LEU:CA	0.42	2.43	21	1
1:B:218:ARG:CG	1:B:218:ARG:HH11	0.42	2.26	22	1
1:B:244:SER:O	1:B:248:PHE:HB2	0.42	2.14	2	1
1:B:288:LEU:CD2	1:B:288:LEU:O	0.42	2.67	18	1
1:A:10:LYS:HZ1	1:A:55:GLN:HG3	0.42	1.74	6	1
1:A:81:LEU:HA	1:A:84:TYR:CD2	0.42	2.49	6	1
1:B:282:LEU:O	1:B:282:LEU:CG	0.42	2.66	7	1
1:A:60:HIS:CD2	1:A:64:MET:HG3	0.42	2.49	11	1
1:A:53:VAL:HG11	1:B:293:ALA:HB2	0.42	1.91	23	2
1:A:87:THR:O	1:A:91:VAL:CG2	0.42	2.67	22	1
1:B:281:LEU:HA	1:B:284:TYR:CD2	0.42	2.49	6	1
1:A:25:VAL:HG11	1:A:84:TYR:CD2	0.42	2.50	16	1
1:A:82:LEU:O	1:A:82:LEU:CG	0.42	2.66	7	1
1:A:88:LEU:CD2	1:A:88:LEU:O	0.42	2.67	18	2
1:B:234:LYS:O	1:B:235:VAL:C	0.42	2.62	16	1
1:A:18:ARG:HG2	1:A:59:ILE:HG23	0.42	1.92	19	1
1:B:210:LYS:O	1:B:213:LEU:HB2	0.42	2.15	2	1
1:B:223:THR:CG2	1:B:238:ARG:HH11	0.42	2.28	3	1
1:B:225:VAL:CG1	1:B:284:TYR:CE1	0.42	3.03	4	1
1:B:225:VAL:HG11	1:B:284:TYR:CZ	0.42	2.50	14	1
1:A:100:ARG:NH2	1:B:250:ASP:HA	0.42	2.30	22	1
1:B:267:PHE:HB3	1:B:281:LEU:HD13	0.41	1.92	20	1
1:A:88:LEU:O	1:A:88:LEU:CD2	0.41	2.68	24	1
1:B:274:GLU:N	1:B:274:GLU:CD	0.41	2.72	16	4
1:B:264:MET:HA	1:B:264:MET:HE2	0.41	1.92	9	1
1:B:225:VAL:HG11	1:B:284:TYR:CD2	0.41	2.50	16	1
1:B:217:LEU:O	1:B:221:TYR:N	0.41	2.38	20	1
1:B:288:LEU:O	1:B:288:LEU:CD2	0.41	2.68	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LYS:CB	1:A:34:LYS:HZ2	0.41	2.29	3	1
1:A:85:ARG:HD2	1:A:86:LEU:H	0.41	1.75	10	1
1:B:214:LEU:N	1:B:214:LEU:HD23	0.41	2.30	13	1
1:A:26:LEU:HB2	1:A:27:GLU:OE1	0.41	2.16	16	1
1:B:226:LEU:HB2	1:B:227:GLU:OE1	0.41	2.15	16	1
1:A:56:VAL:O	1:A:60:HIS:N	0.41	2.52	19	1
1:A:38:ARG:HH11	1:A:38:ARG:HG3	0.41	1.76	20	1
1:A:67:PHE:HB3	1:A:81:LEU:HD13	0.41	1.91	20	1
1:A:10:LYS:O	1:A:13:LEU:HB2	0.41	2.15	2	1
1:B:238:ARG:NE	1:B:238:ARG:HA	0.41	2.29	12	3
1:A:84:TYR:O	1:A:87:THR:N	0.41	2.54	11	1
1:A:22:ARG:NH1	1:A:70:GLN:OE1	0.41	2.51	14	1
1:A:11:ARG:HH12	1:A:55:GLN:HE22	0.41	1.57	6	1
1:A:79:ASP:O	1:A:82:LEU:HB3	0.41	2.14	10	1
1:B:260:HIS:CE1	1:B:288:LEU:HB2	0.41	2.50	25	2
1:B:298:MET:O	1:B:302:SER:N	0.41	2.47	25	1
1:B:274:GLU:O	1:B:276:ARG:N	0.41	2.54	1	1
1:A:25:VAL:CG1	1:A:84:TYR:CE1	0.41	3.03	4	1
1:B:230:ASN:OD1	1:B:233:ALA:O	0.41	2.38	12	1
1:B:225:VAL:CG1	1:B:284:TYR:CD2	0.41	3.04	16	1
1:A:74:GLU:O	1:A:76:ARG:N	0.41	2.54	1	1
1:A:21:TYR:HE1	1:A:91:VAL:HG21	0.41	1.74	10	1
1:B:285:ARG:HD2	1:B:286:LEU:H	0.41	1.75	10	1
1:A:70:GLN:HA	1:A:73:LEU:HD12	0.41	1.93	11	1
1:B:264:MET:O	1:B:281:LEU:HD11	0.41	2.16	11	1
1:A:30:ASN:HD22	1:A:31:THR:C	0.41	2.24	21	1
1:A:60:HIS:CE1	1:A:88:LEU:HB2	0.41	2.50	25	1
1:B:209:ASP:O	1:B:213:LEU:N	0.41	2.49	3	1
1:B:276:ARG:O	1:B:277:SER:HB3	0.41	2.15	3	1
1:A:97:GLU:OE2	1:B:252:SER:OG	0.41	2.39	5	1
1:B:267:PHE:CB	1:B:281:LEU:CD1	0.41	2.99	6	1
1:B:284:TYR:O	1:B:287:THR:N	0.41	2.54	11	1
1:A:60:HIS:NE2	1:A:64:MET:CG	0.41	2.84	19	1
1:A:102:SER:O	1:B:303:ILE:HG23	0.41	2.16	23	1
1:A:67:PHE:HB2	1:A:81:LEU:HD13	0.41	1.92	25	1
1:A:89:ILE:CD1	1:B:289:ILE:HG12	0.41	2.46	1	2
1:A:20:ILE:O	1:A:24:ILE:HG12	0.41	2.16	11	1
1:A:64:MET:O	1:A:81:LEU:HD11	0.41	2.16	11	1
1:B:214:LEU:HD22	1:B:217:LEU:CD1	0.41	2.46	12	1
1:B:248:PHE:CD1	1:B:249:ALA:N	0.41	2.89	14	1
1:B:233:ALA:O	1:B:234:LYS:HB3	0.41	2.16	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:218:ARG:HG2	1:B:259:ILE:HG23	0.41	1.92	19	1
1:B:260:HIS:NE2	1:B:264:MET:CG	0.41	2.84	19	1
1:A:50:ASP:HA	1:B:300:ARG:NH2	0.41	2.31	20	1
1:B:230:ASN:HD22	1:B:231:THR:C	0.41	2.24	21	1
1:A:53:VAL:HG11	1:B:293:ALA:HB1	0.41	1.92	9	1
1:A:64:MET:HA	1:A:64:MET:HE2	0.41	1.92	9	1
1:B:292:ILE:HG13	1:B:293:ALA:N	0.41	2.31	15	2
1:A:25:VAL:CG1	1:A:84:TYR:CD2	0.41	3.04	16	1
1:B:230:ASN:OD1	1:B:235:VAL:CG2	0.41	2.69	21	1
1:A:93:ALA:O	1:A:97:GLU:HG2	0.41	2.16	23	1
1:A:30:ASN:OD1	1:A:35:VAL:CG2	0.40	2.70	2	1
1:A:30:ASN:OD1	1:A:33:ALA:O	0.40	2.38	12	1
1:A:92:ILE:HG13	1:A:93:ALA:N	0.40	2.31	15	2
1:A:88:LEU:HD12	1:B:289:ILE:HD12	0.40	1.93	16	1
1:B:274:GLU:CD	1:B:274:GLU:N	0.40	2.77	8	1
1:A:21:TYR:CD1	1:A:63:LEU:HD22	0.40	2.51	11	1
1:A:25:VAL:HG11	1:A:84:TYR:CZ	0.40	2.50	14	1
1:A:89:ILE:HG23	1:B:292:ILE:CD1	0.40	2.46	14	1
1:B:216:GLU:CB	1:B:245:LYS:HZ2	0.40	2.28	3	1
1:A:67:PHE:CB	1:A:81:LEU:CD1	0.40	2.99	6	1
1:B:270:GLN:HA	1:B:273:LEU:HD12	0.40	1.93	11	1
1:B:285:ARG:O	1:B:289:ILE:CG1	0.40	2.70	16	1
1:A:50:ASP:CB	1:B:300:ARG:NH2	0.40	2.84	1	1
1:B:230:ASN:HD22	1:B:230:ASN:N	0.40	2.15	19	1
1:A:85:ARG:O	1:A:89:ILE:CG1	0.40	2.69	21	1
1:B:293:ALA:O	1:B:297:GLU:HG2	0.40	2.16	23	1
1:A:44:SER:O	1:A:48:PHE:HB2	0.40	2.14	2	1
1:A:17:LEU:CD2	1:A:45:LYS:HE3	0.40	2.47	7	2
1:B:221:TYR:CD1	1:B:263:LEU:HD22	0.40	2.51	11	1
1:A:48:PHE:CD1	1:A:49:ALA:N	0.40	2.89	14	1
1:B:267:PHE:HB2	1:B:281:LEU:HD13	0.40	1.92	25	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	97/107 (91%)	90±1 (93±1%)	6±2 (6±2%)	1±1 (2±1%)	11	57
1	B	97/107 (91%)	90±1 (93±1%)	6±2 (6±2%)	2±1 (2±1%)	10	55
All	All	4850/5350 (91%)	4491 (93%)	284 (6%)	75 (2%)	11	57

All 18 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	76	ARG	9
1	B	276	ARG	9
1	B	230	ASN	7
1	A	78	GLU	6
1	B	278	GLU	6
1	A	30	ASN	6
1	A	33	ALA	5
1	B	233	ALA	5
1	A	77	SER	4
1	B	277	SER	4
1	A	34	LYS	4
1	B	234	LYS	4
1	A	32	ASP	1
1	B	232	ASP	1
1	A	49	ALA	1
1	B	249	ALA	1
1	A	79	ASP	1
1	B	279	ASP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/99 (92%)	79±2 (87±2%)	12±2 (13±2%)	6	47
1	B	91/99 (92%)	80±2 (87±2%)	11±2 (13±2%)	6	48
All	All	4550/4950 (92%)	3974 (87%)	576 (13%)	6	47

All 74 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	82	LEU	25
1	A	95	LEU	25
1	A	98	MET	25
1	B	282	LEU	25
1	B	295	LEU	25
1	B	298	MET	25
1	A	34	LYS	24
1	B	234	LYS	24
1	A	51	ILE	21
1	B	251	ILE	21
1	A	71	LEU	20
1	B	271	LEU	19
1	A	103	ILE	15
1	B	303	ILE	15
1	A	89	ILE	15
1	B	289	ILE	15
1	A	80	ILE	14
1	B	280	ILE	14
1	A	88	LEU	13
1	B	288	LEU	13
1	A	30	ASN	11
1	A	44	SER	11
1	B	230	ASN	11
1	B	244	SER	11
1	A	14	LEU	9
1	B	214	LEU	8
1	A	10	LYS	8
1	A	11	ARG	8
1	B	210	LYS	8
1	B	211	ARG	8
1	A	18	ARG	6
1	B	218	ARG	6
1	A	94	HIS	5
1	B	294	HIS	5
1	A	72	LYS	3
1	B	272	LYS	3
1	A	41	GLU	3
1	B	241	GLU	3
1	A	16	GLU	2
1	A	22	ARG	2
1	B	216	GLU	2
1	B	222	ARG	2
1	A	90	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	B	290	ASP	2
1	A	102	SER	2
1	B	302	SER	2
1	A	23	THR	2
1	B	223	THR	2
1	A	48	PHE	2
1	A	83	ASP	2
1	B	248	PHE	2
1	B	283	ASP	2
1	A	52	SER	2
1	B	252	SER	2
1	A	38	ARG	2
1	A	70	GLN	2
1	B	238	ARG	2
1	B	270	GLN	2
1	A	68	SER	1
1	B	268	SER	1
1	A	59	ILE	1
1	B	259	ILE	1
1	A	76	ARG	1
1	B	276	ARG	1
1	A	92	ILE	1
1	B	292	ILE	1
1	A	85	ARG	1
1	B	285	ARG	1
1	A	12	LYS	1
1	B	212	LYS	1
1	A	73	LEU	1
1	B	273	LEU	1
1	A	100	ARG	1
1	B	300	ARG	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 [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided