



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 05:43 AM UTC

PDB ID : 1CO0 / pdb_00001co0
Title : NMR STUDY OF TRP REPRESSOR-MTR OPERATOR DNA COMPLEX
Authors : Zhou, G.P.; Brocchieri, L.; Jardetzky, O.
Deposited on : 1999-05-30

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

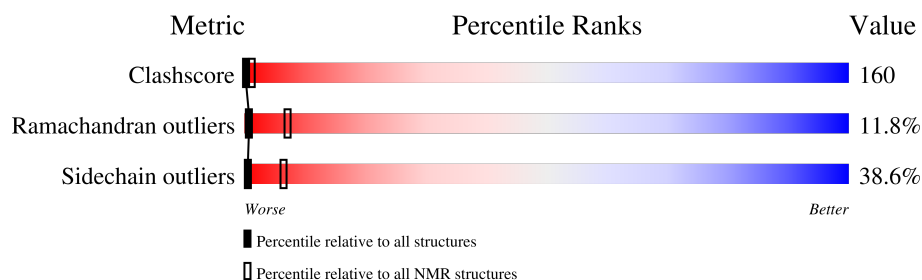
1 Overall quality at a glance

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	E	20	95% 5%
2	F	20	95% 5%
3	A	107	50% 33% 14% .
3	B	107	5% 50% 25% 15% .

2 Ensemble composition and analysis

This entry contains 15 models. Model 4 is the overall representative, medoid model (most similar to other models).

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:17-A:106, B:18-B:106 (179)	1.37	4

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4723 atoms, of which 2189 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*AP*CP*A)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	E	20	636	196	229	71	121	19	0

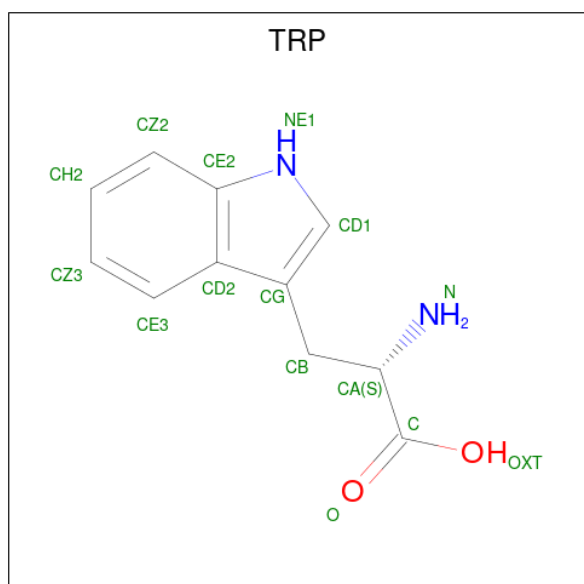
- Molecule 2 is a DNA chain called 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*AP*CP*A)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	F	20	633	195	226	78	115	19	0

- Molecule 3 is a protein called TRP OPERON REPRESSOR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	A	105	1701	528	856	153	161	3	0
3	B	105	1701	528	856	153	161	3	0

- Molecule 4 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



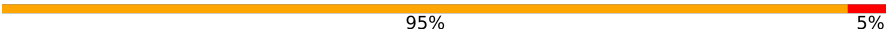
Mol	Chain	Residues	Atoms				
4	B	1	Total	C	H	N	O
			26	11	11	2	2
4	B	1	Total	C	H	N	O
			26	11	11	2	2

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: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E: 

T1 G2 T3 A4 C5 T6 C7 G8 T9 A10 T11 C12 A13 T14 G15 G16 T17 A18 C19 A20

- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*A P*CP*A)-3'

Chain F: 

T1 G2 T3 A4 C5 T6 C7 G8 T9 A10 T11 C12 A13 T14 G15 G16 T17 A18 C19 A20

- Molecule 3: TRP OPERON REPRESSOR

Chain A: 

ALA GLN Q4 S5 S6 Y7 Y8 A9 A10 M11 A12 E13 Q14 R15 H16 Q17 E18 W19 L20 R21 R22 V23 D24 R25 L26 K27 N28 A29 L30 Q31 Q32 D33 L34 L36 E35 E36 P37 P38 L39 M40 L41 E42 M43 L44 T44 P45 P46 D46 E47 E48 E49 A50 A51 L51 G52 T53 R54 V55 V56 R57 V58 E59 L61

L62 R63 G64 E65 S66 M66 Q67 Q68 R69 E70 A71 A72 M73 N74 E75 L76 G77 A78 I79 A80 A81 T81 L82 T83 R84 G85 S86 N87 N88 L89 A90 A91 A92 P93 D94 H95 L96 P97 L98 L99 N100 L101 E102 M103 L104 T105 P106 D107 S107 D108

- Molecule 3: TRP OPERON REPRESSOR

Chain B: 

ALA GLN Q4 S5 S6 Y7 Y8 A9 A10 M11 A12 E13 Q14 R15 H16 Q17 E18 W19 L20 R21 R22 V23 D24 R25 L26 K27 N28 A29 L30 Q31 Q32 D33 L34 H35 L36 P37 L38 L39 N40 L41 E42 M43 L44 T44 P45 P46 D46 E47 E48 E49 A50 A51 L51 G52 T53 R54 V55 V56 R57 V58 E59 L62 R63

G64 E65 S66 M66 Q67 Q68 R69 E70 A71 A72 M73 N74 E75 L76 G77 A78 I79 A80 A81 T81 L82 T83 R84 G85 S86 N87 N88 L89 A90 A91 A92 P93 D94 H95 L96 P97 L98 L99 N100 L101 E102 M103 L104 T105 P106 D107 S107 D108

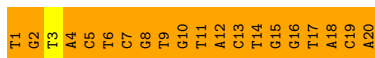
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

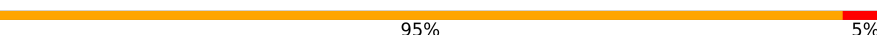
4.2.1 Score per residue for model 1

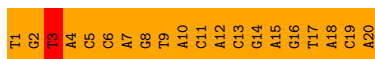
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*AP*CP*A)-3'

Chain E: 



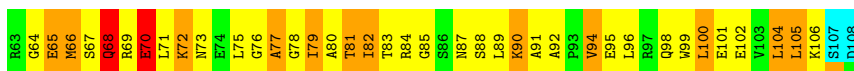
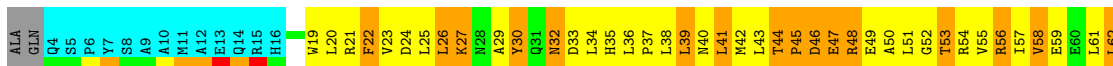
- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*AP*CP*A)-3'

Chain F: 

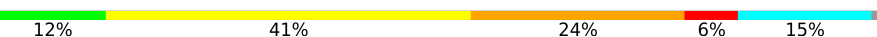


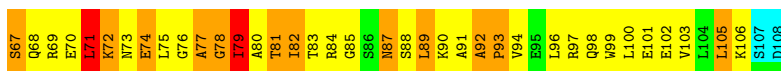
- Molecule 3: TRP OPERON REPRESSOR

Chain A: 



- Molecule 3: TRP OPERON REPRESSOR

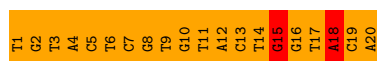
Chain B: 



4.2.2 Score per residue for model 2

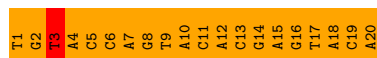
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*AP*CP*A)-3'

Chain E: 



- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*AP*CP*A)-3'

Chain F: 95% 5%



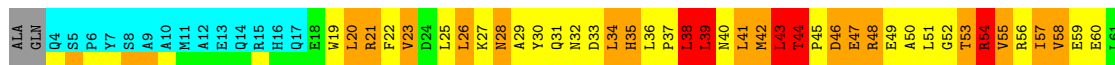
- Molecule 3: TRP OPERON REPRESSOR

Chain A: 7% 40% 28% 8% 14%



- Molecule 3: TRP OPERON REPRESSOR

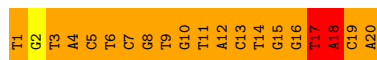
Chain B: 7% 43% 28% 6% 15%



4.2.3 Score per residue for model 3

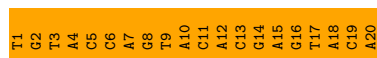
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*AP*CP*A)-3'

Chain E: 5% 85% 10%



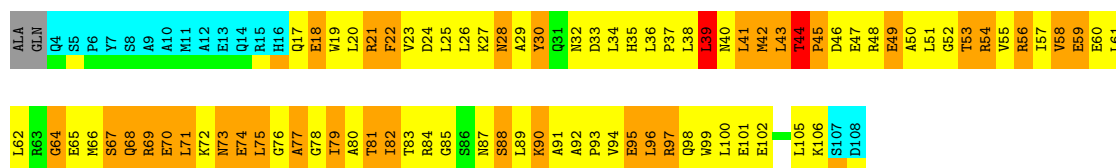
- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*AP*CP*A)-3'

Chain F: 100%



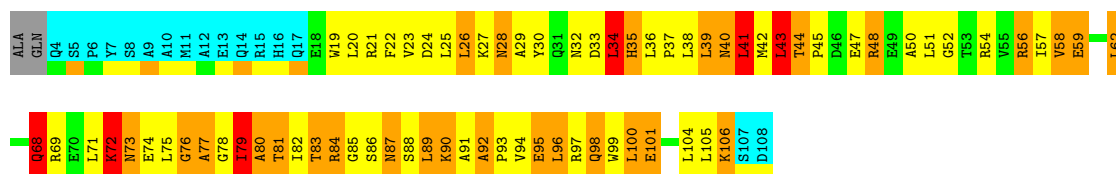
- Molecule 3: TRP OPERON REPRESSOR

Chain A: 5% 47% 31% 14%



• Molecule 3: TRP OPERON REPRESSOR

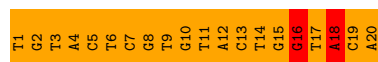
Chain B: 15% 36% 26% 6% 15%



4.2.4 Score per residue for model 4 (medoid)

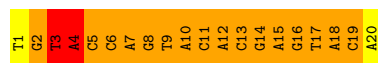
• Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E: 90% 10%



• Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*A P*CP*A)-3'

Chain F: 10% 80% 10%



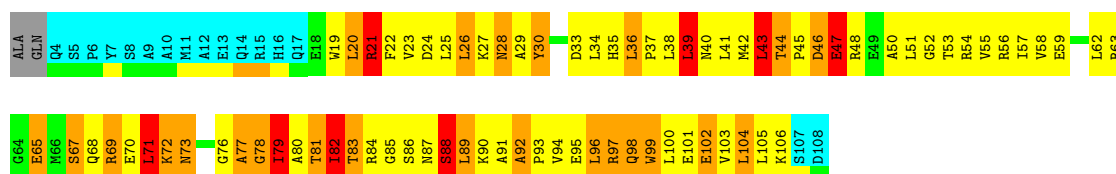
• Molecule 3: TRP OPERON REPRESSOR

Chain A: 5% 51% 19% 9% 14%



• Molecule 3: TRP OPERON REPRESSOR

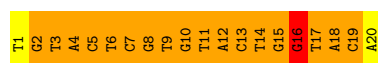
Chain B: 9% 44% 22% 7% 15%



4.2.5 Score per residue for model 5

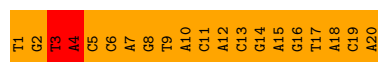
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E: 10% 85% 5%



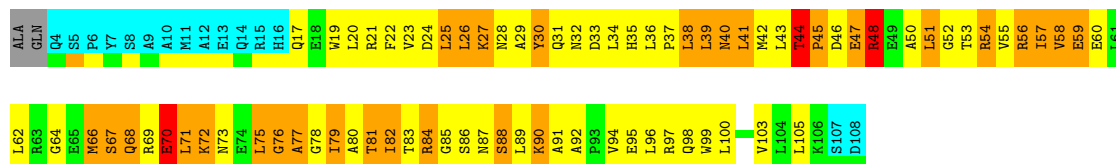
- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*A P*CP*A)-3'

Chain F: 90% 10%



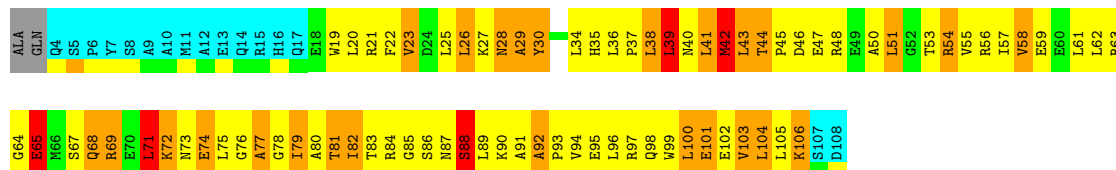
- Molecule 3: TRP OPERON REPRESSOR

Chain A: 10% 43% 28% 14%



- Molecule 3: TRP OPERON REPRESSOR

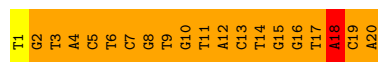
Chain B: 9% 45% 24% 5% 15%



4.2.6 Score per residue for model 6

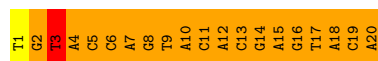
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E: 5% 90% 5%



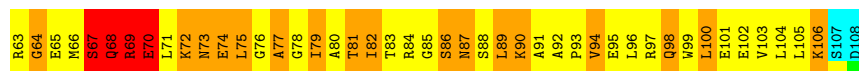
• Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*AP*CP*A)-3'

Chain F: 5% 90% 5%



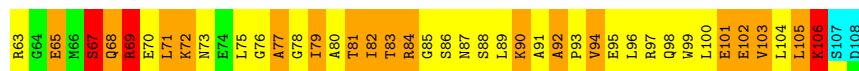
• Molecule 3: TRP OPERON REPRESSOR

Chain A: 5% 41% 33% 6% 14% .



• Molecule 3: TRP OPERON REPRESSOR

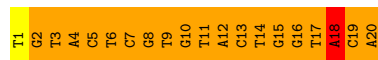
Chain B: 9% 40% 26% 7% 15% .



4.2.7 Score per residue for model 7

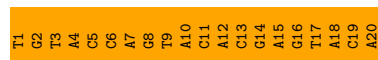
• Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*AP*CP*A)-3'

Chain E: 5% 90% 5%



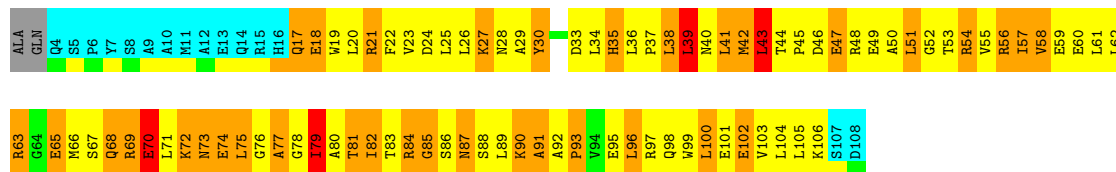
• Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*AP*CP*A)-3'

Chain F: 100%



- Molecule 3: TRP OPERON REPRESSOR

Chain A: 



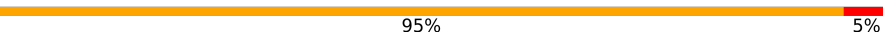
- Molecule 3: TRP OPERON REPRESSOR

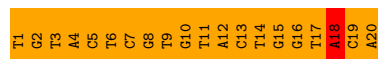
Chain B: 



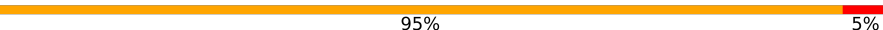
4.2.8 Score per residue for model 8

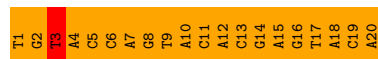
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E: 



- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*A P*CP*A)-3'

Chain F: 



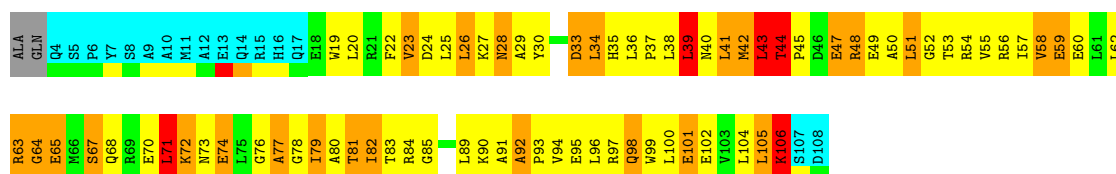
- Molecule 3: TRP OPERON REPRESSOR

Chain A: 



- Molecule 3: TRP OPERON REPRESSOR

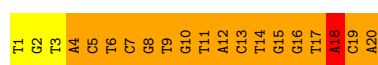
Chain B: 



4.2.9 Score per residue for model 9

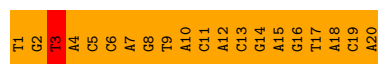
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E: 15% 80% 5%



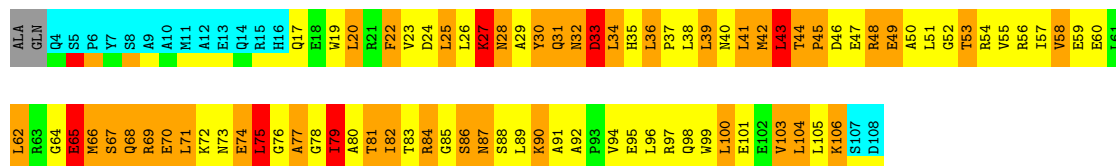
- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*A P*CP*A)-3'

Chain F: 95% 5%



- Molecule 3: TRP OPERON REPRESSOR

Chain A: 6% 38% 35% 6% 14% .



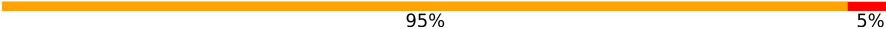
- Molecule 3: TRP OPERON REPRESSOR

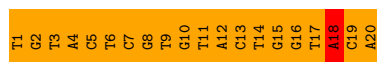
Chain B: 12% 36% 29% 6% 15% .



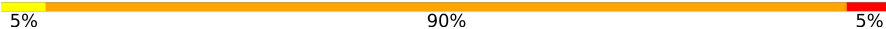
4.2.10 Score per residue for model 10

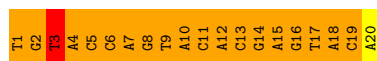
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E:  95% 5%



- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*AP*CP*A)-3'

Chain F:  5% 90% 5%



- Molecule 3: TRP OPERON REPRESSOR

Chain A:  8% 42% 30% 14% 5%



- Molecule 3: TRP OPERON REPRESSOR

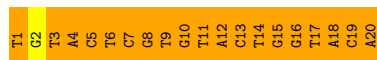
Chain B:  8% 35% 34% 7% 15%



4.2.11 Score per residue for model 11

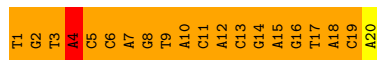
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*AP*CP*A)-3'

Chain E:  5% 95%



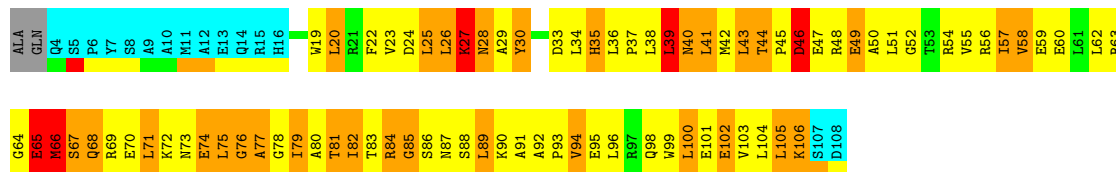
- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*AP*CP*A)-3'

Chain F:  5% 90% 5%



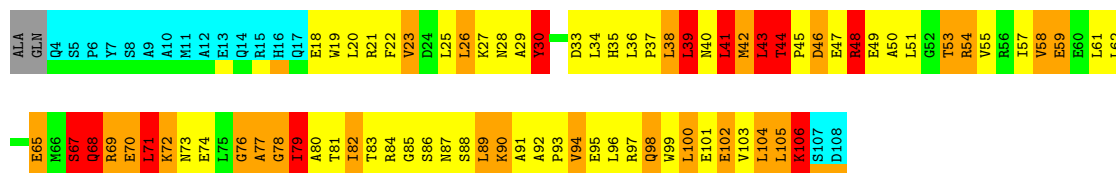
- Molecule 3: TRP OPERON REPRESSOR

Chain A: 



- Molecule 3: TRP OPERON REPRESSOR

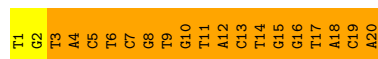
Chain B: 



4.2.12 Score per residue for model 12

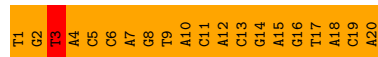
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E: 



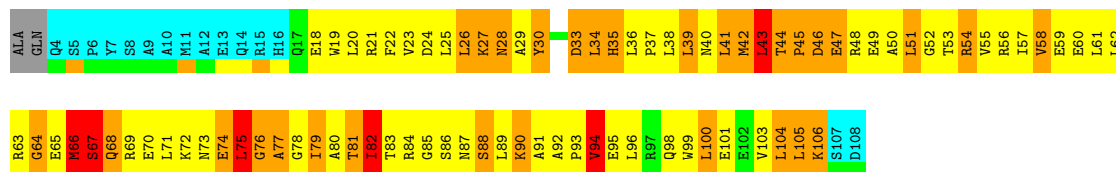
- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*A P*CP*A)-3'

Chain F: 



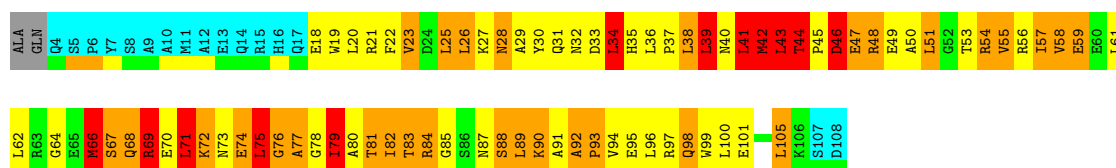
- Molecule 3: TRP OPERON REPRESSOR

Chain A: 



- Molecule 3: TRP OPERON REPRESSOR

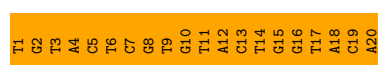
Chain B: 



4.2.13 Score per residue for model 13

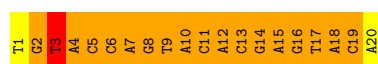
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E: 100%



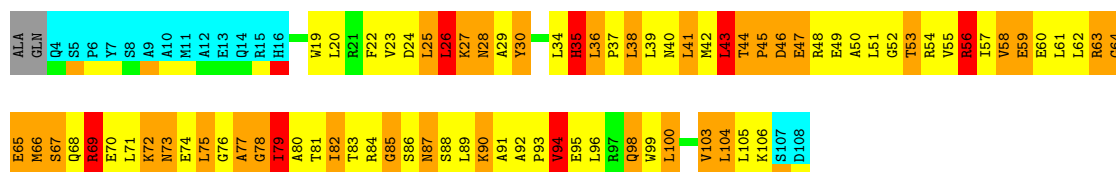
- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*A P*CP*A)-3'

Chain F: 10% 85% 5%



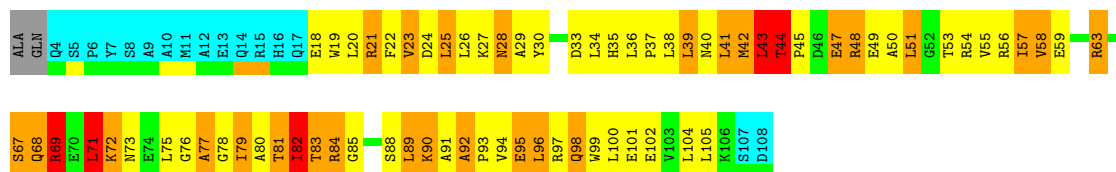
- Molecule 3: TRP OPERON REPRESSOR

Chain A: 8% 39% 30% 7% 14%



- Molecule 3: TRP OPERON REPRESSOR

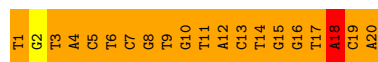
Chain B: 15% 38% 25% 5% 15%



4.2.14 Score per residue for model 14

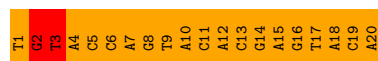
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E:  5% 90% 5%

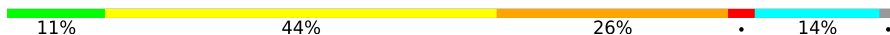


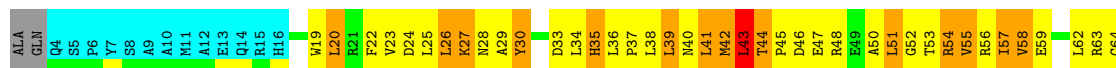
- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*A P*CP*A)-3'

Chain F:  90% 10%



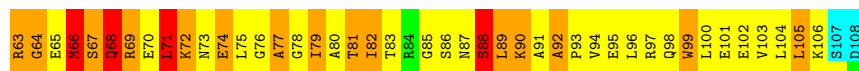
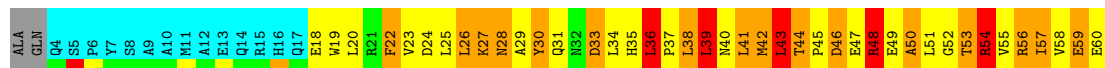
- Molecule 3: TRP OPERON REPRESSOR

Chain A:  11% 44% 26% 14%



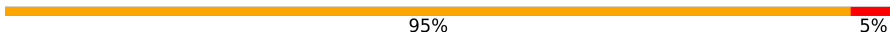
- Molecule 3: TRP OPERON REPRESSOR

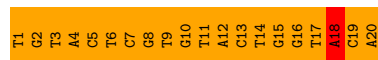
Chain B:  5% 41% 29% 8% 15%



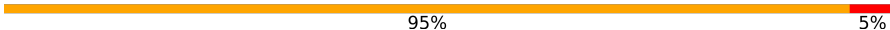
4.2.15 Score per residue for model 15

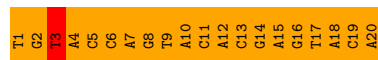
- Molecule 1: 5'-D(*TP*GP*TP*AP*CP*TP*CP*GP*TP*GP*TP*AP*CP*TP*GP*GP*TP*A P*CP*A)-3'

Chain E:  95% 5%

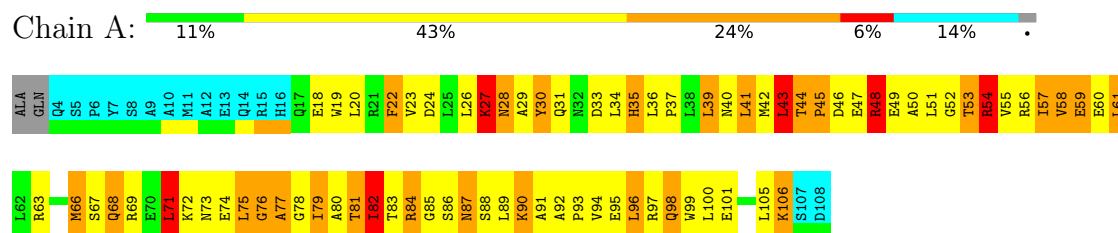


- Molecule 2: 5'-D(*TP*GP*TP*AP*CP*CP*AP*GP*TP*AP*CP*AP*CP*GP*AP*GP*TP*A P*CP*A)-3'

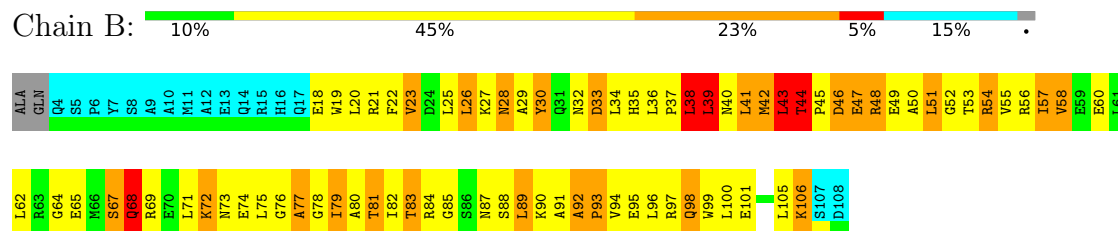
Chain F:  95% 5%



● Molecule 3: TRP OPERON REPRESSOR



● Molecule 3: TRP OPERON REPRESSOR



5 Refinement protocol and experimental data overview

Of the 30 calculated structures, 15 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	

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	E	1.60±0.00	21±1/455 (4.5± 0.3%)	1.88±0.00	20±0/701 (2.9± 0.0%)
2	F	1.59±0.00	20±1/457 (4.4± 0.2%)	1.86±0.00	20±0/703 (2.8± 0.0%)
3	A	1.48±0.01	0±0/738 (0.0± 0.1%)	1.60±0.03	4±3/998 (0.4± 0.3%)
3	B	1.46±0.01	1±0/729 (0.1± 0.0%)	1.62±0.02	5±2/986 (0.5± 0.2%)
All	All	1.52	629/35685 (1.8%)	1.72	728/50820 (1.4%)

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	E	0.0±0.0	0.9±0.7
2	F	0.0±0.0	1.1±0.6
3	A	0.0±0.0	1.1±0.9
3	B	0.0±0.0	0.7±0.7
All	All	0	56

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
3	B	43	LEU	N-CA	6.30	1.54	1.46	15	12
1	E	12	DA	C3'-C2'	-6.15	1.40	1.52	15	15
2	F	13	DC	C3'-C2'	-6.04	1.40	1.52	11	15
3	A	44	THR	C-N	-5.94	1.27	1.34	3	1
2	F	3	DT	C2'-C1'	-5.65	1.41	1.52	10	14
2	F	12	DA	C3'-C2'	-5.64	1.41	1.52	5	15
1	E	13	DC	C3'-C2'	-5.63	1.41	1.52	12	15
1	E	17	DT	C3'-C2'	-5.61	1.41	1.52	3	15
2	F	11	DC	C3'-C2'	-5.57	1.41	1.52	5	15
1	E	16	DG	C3'-C2'	-5.51	1.42	1.52	15	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	F	5	DC	C3'-C2'	-5.50	1.42	1.52	14	15
1	E	6	DT	C3'-C2'	-5.47	1.42	1.52	13	15
1	E	11	DT	C3'-C2'	-5.46	1.42	1.52	11	15
2	F	4	DA	C3'-C2'	-5.44	1.42	1.52	5	15
1	E	7	DC	C3'-C2'	-5.43	1.42	1.52	11	15
2	F	7	DA	C3'-C2'	-5.42	1.42	1.52	5	15
1	E	3	DT	C3'-C2'	-5.40	1.42	1.52	6	15
2	F	17	DT	C3'-C2'	-5.40	1.42	1.52	5	15
1	E	5	DC	C3'-C2'	-5.38	1.42	1.52	15	15
2	F	16	DG	C3'-C2'	-5.38	1.42	1.52	3	15
1	E	8	DG	C3'-C2'	-5.37	1.42	1.52	14	15
3	B	44	THR	C-N	-5.37	1.29	1.33	7	1
1	E	1	DT	C3'-C2'	-5.37	1.42	1.52	2	15
2	F	19	DC	C3'-C2'	-5.37	1.42	1.52	5	15
1	E	20	DA	C3'-C2'	-5.36	1.42	1.52	8	15
1	E	10	DG	C3'-C2'	-5.36	1.42	1.52	1	15
2	F	1	DT	C3'-C2'	-5.36	1.42	1.52	4	15
2	F	9	DT	C3'-C2'	-5.36	1.42	1.52	7	15
1	E	2	DG	C3'-C2'	-5.36	1.42	1.52	14	15
1	E	9	DT	C3'-C2'	-5.36	1.42	1.52	15	15
2	F	20	DA	C3'-C2'	-5.36	1.42	1.52	7	15
1	E	12	DA	C2'-C1'	-5.35	1.42	1.52	10	14
1	E	19	DC	C3'-C2'	-5.35	1.42	1.52	4	15
2	F	10	DA	C3'-C2'	-5.35	1.42	1.52	4	15
1	E	4	DA	C3'-C2'	-5.34	1.42	1.52	15	15
2	F	15	DA	C3'-C2'	-5.34	1.42	1.52	9	15
2	F	18	DA	C3'-C2'	-5.34	1.42	1.52	14	15
3	A	77	ALA	C-N	-5.33	1.28	1.33	4	1
2	F	6	DC	C3'-C2'	-5.31	1.42	1.52	1	13
2	F	2	DG	C3'-C2'	-5.28	1.42	1.52	3	15
3	A	43	LEU	N-CA	5.28	1.52	1.46	8	1
2	F	14	DG	C3'-C2'	-5.24	1.42	1.52	14	15
1	E	15	DG	C3'-C2'	-5.21	1.42	1.52	3	10
2	F	8	DG	C3'-C2'	-5.21	1.42	1.52	1	14
1	E	18	DA	C3'-C2'	-5.19	1.42	1.52	11	15
1	E	16	DG	C2'-C1'	-5.18	1.42	1.52	4	8
2	F	3	DT	C3'-C2'	-5.10	1.42	1.52	9	1
1	E	15	DG	C2'-C1'	-5.09	1.42	1.52	1	3
1	E	14	DT	C3'-C2'	-5.07	1.42	1.52	12	3
2	F	8	DG	C2'-C1'	-5.04	1.42	1.52	13	4
2	F	12	DA	C2'-C1'	-5.04	1.42	1.52	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	27	LYS	N-CA	5.02	1.52	1.46	2	2
1	E	13	DC	C2'-C1'	-5.02	1.43	1.52	14	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	E	12	DA	C3'-C2'-C1'	9.51	115.86	101.60	3	15
1	E	11	DT	C3'-C2'-C1'	9.49	115.83	101.60	11	15
2	F	11	DC	C3'-C2'-C1'	9.40	115.71	101.60	5	15
2	F	12	DA	C3'-C2'-C1'	9.39	115.69	101.60	15	15
2	F	10	DA	C3'-C2'-C1'	9.34	115.61	101.60	11	15
1	E	8	DG	C3'-C2'-C1'	9.34	115.61	101.60	14	15
1	E	6	DT	C3'-C2'-C1'	9.32	115.58	101.60	10	15
1	E	5	DC	C3'-C2'-C1'	9.29	115.54	101.60	6	15
2	F	4	DA	C3'-C2'-C1'	9.29	115.54	101.60	6	15
1	E	10	DG	C3'-C2'-C1'	9.28	115.52	101.60	8	15
1	E	7	DC	C3'-C2'-C1'	9.28	115.51	101.60	8	15
2	F	5	DC	C3'-C2'-C1'	9.28	115.51	101.60	8	15
1	E	4	DA	C3'-C2'-C1'	9.27	115.51	101.60	6	15
1	E	1	DT	C3'-C2'-C1'	9.27	115.50	101.60	6	15
1	E	3	DT	C3'-C2'-C1'	9.27	115.50	101.60	6	15
2	F	9	DT	C3'-C2'-C1'	9.26	115.49	101.60	14	15
2	F	16	DG	C3'-C2'-C1'	9.26	115.49	101.60	4	15
2	F	17	DT	C3'-C2'-C1'	9.26	115.49	101.60	6	15
1	E	2	DG	C3'-C2'-C1'	9.26	115.49	101.60	2	15
2	F	18	DA	C3'-C2'-C1'	9.25	115.48	101.60	12	15
2	F	19	DC	C3'-C2'-C1'	9.24	115.47	101.60	1	15
2	F	2	DG	C3'-C2'-C1'	9.24	115.46	101.60	10	15
2	F	20	DA	C3'-C2'-C1'	9.24	115.46	101.60	7	15
1	E	13	DC	C3'-C2'-C1'	9.24	115.46	101.60	12	15
1	E	9	DT	C3'-C2'-C1'	9.23	115.45	101.60	8	15
1	E	19	DC	C3'-C2'-C1'	9.23	115.45	101.60	7	15
1	E	20	DA	C3'-C2'-C1'	9.23	115.45	101.60	7	15
1	E	18	DA	C3'-C2'-C1'	9.23	115.44	101.60	11	15
2	F	15	DA	C3'-C2'-C1'	9.23	115.44	101.60	5	15
1	E	17	DT	C3'-C2'-C1'	9.22	115.43	101.60	1	15
1	E	16	DG	C3'-C2'-C1'	9.22	115.42	101.60	8	15
2	F	1	DT	C3'-C2'-C1'	9.21	115.42	101.60	11	15
2	F	6	DC	C3'-C2'-C1'	9.18	115.37	101.60	6	15
2	F	7	DA	C3'-C2'-C1'	9.18	115.36	101.60	1	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	F	14	DG	C3'-C2'-C1'	9.13	115.30	101.60	8	15
2	F	13	DC	C3'-C2'-C1'	9.12	115.27	101.60	8	15
2	F	8	DG	C3'-C2'-C1'	9.01	115.12	101.60	11	15
1	E	14	DT	C3'-C2'-C1'	8.97	115.06	101.60	7	15
1	E	15	DG	C3'-C2'-C1'	8.69	114.64	101.60	14	15
2	F	3	DT	C3'-C2'-C1'	8.38	114.17	101.60	13	15
3	B	57	ILE	N-CA-CB	-7.14	105.78	111.64	15	1
3	B	46	ASP	N-CA-C	-6.99	105.56	112.97	15	2
3	A	82	ILE	N-CA-C	-6.97	105.81	111.81	7	2
3	A	58	VAL	N-CA-C	-6.77	106.42	111.90	10	3
3	A	38	LEU	N-CA-C	-6.77	103.93	112.93	8	2
3	B	23	VAL	N-CA-CB	-6.65	103.37	110.62	8	10
3	B	82	ILE	N-CA-C	-6.58	106.59	112.12	6	7
3	A	42	MET	N-CA-CB	-6.55	102.82	110.35	8	1
3	B	39	LEU	N-CA-C	-6.50	105.65	112.93	15	9
3	A	79	ILE	N-CA-CB	-6.40	100.67	111.23	13	1
3	A	39	LEU	N-CA-C	-6.38	105.49	113.20	9	6
3	A	78	GLY	N-CA-C	-6.36	106.14	115.30	13	1
3	B	41	LEU	N-CA-CB	-6.30	102.53	110.90	9	4
3	A	82	ILE	N-CA-CB	-6.20	103.62	110.51	15	2
3	A	46	ASP	N-CA-C	-6.16	104.86	112.38	11	5
3	A	103	VAL	N-CA-CB	-6.12	105.23	112.39	10	7
3	A	94	VAL	N-CA-CB	-5.99	105.20	112.33	3	3
3	B	56	ARG	N-CA-CB	-5.96	102.37	110.95	9	2
3	B	38	LEU	N-CA-C	-5.94	105.28	113.18	15	4
3	B	103	VAL	N-CA-CB	-5.92	105.46	112.39	2	4
3	B	42	MET	N-CA-CB	-5.90	102.63	111.25	14	5
3	B	55	VAL	N-CA-CB	-5.74	105.67	112.39	11	1
3	A	38	LEU	N-CA-CB	-5.71	102.99	110.59	6	2
3	A	77	ALA	N-CA-C	-5.71	106.45	113.41	13	1
3	A	45	PRO	CB-CA-C	5.70	119.65	111.04	3	1
3	A	86	SER	N-CA-C	-5.63	105.15	111.28	8	2
3	A	48	ARG	N-CA-C	-5.50	105.39	111.71	15	2
3	A	81	THR	N-CA-CB	-5.47	102.33	110.10	8	2
3	A	85	GLY	N-CA-C	-5.46	106.03	112.64	13	4
3	B	79	ILE	N-CA-CB	-5.43	102.28	111.23	12	2
3	B	81	THR	N-CA-CB	-5.35	103.50	110.88	15	4
3	A	37	PRO	N-CA-C	-5.29	109.17	114.68	8	1
3	A	35	HIS	CA-CB-CG	-5.27	108.53	113.80	13	2
3	A	80	ALA	N-CA-C	-5.26	105.60	112.23	8	1
3	B	40	ASN	N-CA-C	-5.25	106.19	113.18	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	82	ILE	N-CA-CB	-5.25	102.57	111.23	9	1
3	B	22	PHE	N-CA-CB	-5.25	102.22	110.30	10	1
3	B	29	ALA	N-CA-CB	-5.25	102.81	110.47	9	2
3	A	106	LYS	N-CA-CB	-5.24	104.47	112.28	6	1
3	B	50	ALA	N-CA-C	-5.22	107.08	113.50	14	1
3	B	106	LYS	N-CA-CB	-5.22	104.50	112.28	11	2
3	B	19	TRP	N-CA-CB	-5.21	104.11	110.98	7	1
3	A	75	LEU	N-CA-C	-5.17	107.11	113.41	7	1
3	B	45	PRO	N-CA-C	-5.16	107.44	114.98	10	1
3	B	30	TYR	N-CA-CB	-5.16	103.50	110.67	11	1
3	B	58	VAL	N-CA-C	-5.15	106.66	111.45	3	3
3	A	91	ALA	N-CA-C	-5.14	106.11	112.38	7	1
3	B	80	ALA	N-CA-C	-5.12	106.72	113.12	3	1
3	A	89	LEU	N-CA-C	-5.05	105.29	111.75	4	1
3	B	52	GLY	N-CA-C	-5.05	107.53	113.99	14	1
3	A	72	LYS	N-CA-CB	-5.04	101.98	110.49	6	1
3	A	60	GLU	N-CA-CB	-5.01	102.76	110.42	4	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	F	3	DT	Sidechain	12
1	E	18	DA	Sidechain	10
3	A	56	ARG	Sidechain	6
3	B	54	ARG	Sidechain	6
3	A	54	ARG	Sidechain	4
3	A	84	ARG	Sidechain	4
2	F	4	DA	Sidechain	3
1	E	16	DG	Sidechain	2
3	B	21	ARG	Sidechain	2
1	E	15	DG	Sidechain	1
1	E	17	DT	Sidechain	1
3	A	21	ARG	Sidechain	1
3	B	97	ARG	Sidechain	1
3	B	84	ARG	Sidechain	1
3	A	69	ARG	Sidechain	1
2	F	2	DG	Sidechain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	E	407	229	229	78±11
2	F	407	226	226	98±4
3	A	728	755	755	365±20
3	B	719	747	747	304±19
4	B	30	22	18	49±12
All	All	34365	29685	29625	10236

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 160.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:43:LEU:C	3:B:45:PRO:HD3	1.47	1.33	6	13
1:E:16:DG:N3	1:E:17:DT:O4	1.32	1.60	3	1
3:A:51:LEU:HD13	3:B:22:PHE:CZ	1.29	1.62	6	1
3:A:72:LYS:HB2	3:A:78:GLY:O	1.24	1.31	13	1
1:E:16:DG:C2	2:F:4:DA:N6	1.23	2.05	3	1
3:A:78:GLY:O	3:A:82:ILE:N	1.22	1.72	10	14
3:B:43:LEU:O	3:B:45:PRO:HD3	1.19	1.28	6	3
3:A:55:VAL:HG21	3:B:22:PHE:CZ	1.17	1.74	10	4
3:A:79:ILE:O	3:A:83:THR:HG22	1.15	1.42	13	15
3:A:54:ARG:O	3:A:57:ILE:CD1	1.10	1.99	8	9
3:B:43:LEU:C	3:B:45:PRO:HD2	1.10	1.71	13	4
3:A:43:LEU:HD13	3:B:50:ALA:HB1	1.10	1.10	3	1
3:B:41:LEU:HD23	3:B:41:LEU:C	1.10	1.71	6	9
3:A:51:LEU:HD23	3:B:19:TRP:CH2	1.10	1.80	4	5
3:B:44:THR:HG1	4:B:109:TRP:N	1.10	1.45	6	1
3:A:57:ILE:HD12	3:A:58:VAL:N	1.09	1.62	1	12
3:A:77:ALA:O	3:A:81:THR:OG1	1.08	1.70	6	11
3:B:43:LEU:C	3:B:45:PRO:CD	1.08	2.26	6	13
3:A:57:ILE:HD13	3:A:58:VAL:N	1.08	1.62	4	5
3:B:57:ILE:HG22	3:B:82:ILE:HG22	1.08	1.18	3	7
3:B:26:LEU:HD13	3:B:38:LEU:HD13	1.07	1.22	8	11
3:A:51:LEU:C	3:A:51:LEU:HD12	1.07	1.73	6	1
3:A:42:MET:HE2	3:B:58:VAL:HG11	1.05	1.27	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:42:MET:HE2	3:B:58:VAL:HG21	1.05	1.27	10	4
3:A:54:ARG:O	3:A:57:ILE:HG13	1.04	1.49	5	11
3:B:57:ILE:HD12	3:B:58:VAL:N	1.04	1.67	13	14
3:A:58:VAL:HG11	3:B:41:LEU:HD21	1.04	1.06	3	4
3:B:57:ILE:HG21	3:B:81:THR:HG22	1.03	1.23	10	12
3:A:54:ARG:O	3:A:57:ILE:HD12	1.03	1.53	4	6
1:E:15:DG:O6	3:A:80:ALA:HB2	1.03	1.53	4	15
3:A:42:MET:HE3	3:B:58:VAL:HG11	1.03	1.14	14	3
3:B:41:LEU:HD23	3:B:42:MET:N	1.02	1.69	15	4
3:A:57:ILE:CD1	3:A:58:VAL:HG22	1.02	1.84	2	14
2:F:13:DC:OP1	3:A:43:LEU:O	1.02	1.76	11	2
3:A:40:ASN:HB3	3:B:91:ALA:HB1	1.02	1.32	15	7
3:A:34:LEU:HD13	3:A:34:LEU:C	1.00	1.82	6	2
3:A:96:LEU:C	3:A:96:LEU:HD22	1.00	1.80	3	1
3:A:39:LEU:HD22	3:B:19:TRP:CZ2	1.00	1.90	6	12
3:A:51:LEU:HD13	3:B:22:PHE:CE2	1.00	1.91	6	1
3:A:41:LEU:HD13	3:A:41:LEU:C	0.99	1.82	12	9
3:B:41:LEU:HD23	3:B:41:LEU:O	0.99	1.54	9	6
3:A:51:LEU:CD1	3:A:55:VAL:HG21	0.99	1.85	7	3
3:A:19:TRP:CH2	3:B:39:LEU:HD13	0.99	1.92	9	13
3:B:38:LEU:HA	3:B:41:LEU:HD23	0.98	1.35	7	1
3:A:29:ALA:HB3	3:A:34:LEU:HD12	0.98	1.33	6	2
3:B:93:PRO:O	3:B:97:ARG:N	0.98	1.96	3	10
3:A:22:PHE:O	3:A:26:LEU:HD23	0.98	1.59	13	13
3:A:37:PRO:O	3:A:41:LEU:HD12	0.97	1.56	12	12
3:A:72:LYS:HD2	3:A:79:ILE:CG1	0.97	1.89	2	11
3:A:34:LEU:O	3:A:34:LEU:HD22	0.97	1.57	6	1
3:B:26:LEU:O	3:B:34:LEU:HD22	0.97	1.59	14	1
3:A:91:ALA:HB1	3:B:40:ASN:HB3	0.97	1.34	10	6
3:A:51:LEU:HG	3:B:22:PHE:CZ	0.97	1.94	11	10
3:A:78:GLY:HA2	3:A:81:THR:HB	0.97	1.31	8	13
1:E:16:DG:O6	3:A:79:ILE:HG21	0.96	1.60	2	6
3:B:40:ASN:HA	3:B:45:PRO:CB	0.96	1.89	6	1
3:A:29:ALA:HB2	3:B:99:TRP:CE2	0.96	1.94	12	15
3:B:57:ILE:HG21	3:B:81:THR:CG2	0.96	1.90	14	15
3:A:72:LYS:CD	3:A:79:ILE:HG12	0.96	1.90	2	11
3:A:43:LEU:O	3:A:45:PRO:HD3	0.96	1.58	8	1
3:A:41:LEU:HD22	3:A:41:LEU:O	0.95	1.61	9	13
1:E:16:DG:N7	3:A:79:ILE:HG21	0.95	1.76	3	2
1:E:12:DA:H5''	4:B:109:TRP:OXT	0.95	1.60	10	1
3:A:78:GLY:HA2	3:A:81:THR:CB	0.95	1.91	15	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:51:LEU:HD12	3:A:55:VAL:CG2	0.95	1.91	7	3
3:A:78:GLY:C	3:A:82:ILE:HG12	0.95	1.87	7	13
3:A:91:ALA:CB	3:B:40:ASN:C	0.95	2.39	10	8
1:E:15:DG:C8	3:A:79:ILE:HD13	0.95	1.95	12	2
3:A:26:LEU:HD22	3:A:35:HIS:CE1	0.95	1.97	13	1
3:A:87:ASN:O	3:A:90:LYS:N	0.94	1.99	13	15
3:A:19:TRP:CE2	3:B:39:LEU:HD22	0.94	1.97	7	6
1:E:15:DG:C8	3:A:79:ILE:HD12	0.94	1.97	5	4
2:F:5:DC:H41	3:A:83:THR:HG21	0.94	1.22	3	2
3:B:38:LEU:CD2	3:B:42:MET:HE1	0.94	1.92	3	3
3:A:72:LYS:CB	3:A:78:GLY:O	0.94	2.15	13	1
3:B:54:ARG:O	3:B:57:ILE:HG13	0.94	1.62	1	5
3:B:43:LEU:O	3:B:45:PRO:CD	0.94	2.15	6	9
3:A:36:LEU:HA	3:A:39:LEU:HD23	0.93	1.37	10	9
3:A:100:LEU:HD12	3:B:41:LEU:HD11	0.93	1.35	5	3
3:B:26:LEU:HD13	3:B:34:LEU:HD21	0.93	1.38	14	1
3:A:19:TRP:CE3	3:B:51:LEU:HD12	0.93	1.98	13	6
2:F:3:DT:H71	3:A:82:ILE:HD11	0.93	1.40	2	3
3:B:57:ILE:HG22	3:B:82:ILE:CG2	0.93	1.94	3	12
3:A:55:VAL:CG2	3:B:22:PHE:CZ	0.93	2.51	10	11
3:B:96:LEU:HD13	3:B:96:LEU:N	0.93	1.79	13	1
2:F:4:DA:H8	3:A:83:THR:HG1	0.92	0.97	3	2
3:A:51:LEU:HD23	3:B:22:PHE:CD2	0.92	1.97	12	1
3:A:30:TYR:CD1	3:B:23:VAL:HG13	0.92	2.00	12	7
3:A:51:LEU:HD12	3:A:55:VAL:HG21	0.92	0.95	7	2
1:E:16:DG:H2'	1:E:17:DT:H72	0.92	1.42	11	4
3:A:57:ILE:HD13	3:A:57:ILE:C	0.92	1.88	4	2
1:E:12:DA:H5'	3:B:44:THR:HG21	0.92	1.40	7	3
3:A:93:PRO:O	3:A:94:VAL:HG22	0.91	1.64	13	4
3:B:81:THR:HA	4:B:201:TRP:CZ2	0.91	2.01	9	12
3:A:51:LEU:HD12	3:A:52:GLY:N	0.91	1.80	6	1
3:A:26:LEU:HD13	3:A:35:HIS:CD2	0.91	2.01	14	1
3:A:88:SER:OG	3:B:41:LEU:C	0.91	2.13	9	2
3:A:43:LEU:HB2	3:B:54:ARG:HG3	0.91	1.37	10	2
3:A:43:LEU:CA	4:B:201:TRP:HB2	0.90	1.96	6	9
3:B:30:TYR:CE1	3:B:34:LEU:HD23	0.90	2.01	14	1
3:A:55:VAL:O	3:A:59:GLU:HG3	0.90	1.65	2	12
3:A:91:ALA:HB3	3:B:40:ASN:HA	0.90	1.43	1	1
3:A:72:LYS:HE2	3:A:79:ILE:CG1	0.90	1.96	1	2
3:B:57:ILE:HA	3:B:82:ILE:HG22	0.90	1.42	14	9
3:B:72:LYS:HG3	3:B:79:ILE:HA	0.90	1.41	3	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:54:ARG:HG3	3:B:42:MET:HE2	0.90	1.43	3	1
3:A:40:ASN:CB	3:B:91:ALA:HB1	0.90	1.96	4	13
3:B:72:LYS:HB2	3:B:82:ILE:HG12	0.90	1.43	11	6
3:A:51:LEU:O	3:A:55:VAL:HB	0.90	1.67	4	4
3:A:34:LEU:HD13	3:A:35:HIS:N	0.90	1.80	9	2
3:A:54:ARG:O	3:A:57:ILE:CG1	0.90	2.19	5	13
3:A:51:LEU:HD22	3:B:19:TRP:CH2	0.90	2.01	10	10
3:A:72:LYS:NZ	3:A:79:ILE:HD13	0.90	1.82	6	6
3:B:78:GLY:O	3:B:82:ILE:N	0.90	2.05	9	15
3:A:91:ALA:HB1	3:B:40:ASN:CB	0.89	1.97	10	8
3:B:71:LEU:HD22	3:B:71:LEU:O	0.89	1.66	11	2
1:E:16:DG:O6	3:A:79:ILE:HG22	0.89	1.66	3	4
3:A:51:LEU:HD22	3:B:19:TRP:CZ3	0.89	2.03	10	2
3:A:58:VAL:CG1	3:B:41:LEU:HD21	0.89	1.97	3	3
3:A:43:LEU:CB	3:B:54:ARG:HG3	0.89	1.96	10	3
3:A:99:TRP:CE2	3:B:29:ALA:HB2	0.89	2.02	12	14
3:A:43:LEU:HB2	3:B:54:ARG:HB3	0.89	1.41	9	2
3:A:55:VAL:HB	3:B:22:PHE:CZ	0.88	2.03	3	11
3:A:72:LYS:CE	3:A:79:ILE:HG23	0.88	1.98	1	2
3:A:72:LYS:CD	3:A:79:ILE:CG1	0.88	2.51	2	7
1:E:16:DG:H2'	1:E:17:DT:H71	0.88	1.45	2	9
3:A:29:ALA:HB2	3:B:99:TRP:CZ2	0.88	2.04	4	8
3:A:72:LYS:HD2	3:A:79:ILE:HG12	0.88	1.42	2	9
3:B:44:THR:HG22	3:B:44:THR:O	0.88	1.67	14	11
1:E:1:DT:HO5'	1:E:1:DT:H6	0.88	1.09	10	5
3:A:30:TYR:CD2	3:B:23:VAL:HG13	0.88	2.04	15	4
3:A:43:LEU:HD22	3:B:50:ALA:HA	0.88	1.44	10	2
1:E:15:DG:N7	3:A:79:ILE:HB	0.88	1.84	6	13
3:A:96:LEU:HD13	3:A:97:ARG:N	0.88	1.84	3	1
3:A:99:TRP:NE1	3:B:29:ALA:HB2	0.88	1.84	14	14
3:B:41:LEU:CD2	3:B:42:MET:HG2	0.88	1.99	2	5
3:A:19:TRP:CZ2	3:B:39:LEU:HD22	0.88	2.03	3	6
3:A:26:LEU:HD11	3:B:30:TYR:CE2	0.88	2.04	3	1
3:A:58:VAL:HG11	3:B:41:LEU:CD2	0.87	1.98	9	2
3:B:40:ASN:C	3:B:45:PRO:HG2	0.87	1.94	10	2
3:A:41:LEU:HD11	3:A:42:MET:HE3	0.87	1.44	13	2
3:A:26:LEU:HD12	3:A:30:TYR:CZ	0.87	2.05	5	8
2:F:13:DC:OP1	3:A:43:LEU:HD23	0.87	1.68	10	2
3:B:95:GLU:C	3:B:96:LEU:HD22	0.87	1.94	8	1
3:A:29:ALA:HB1	3:A:34:LEU:HB3	0.87	1.47	6	5
2:F:3:DT:H72	3:A:79:ILE:HD13	0.86	1.45	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:39:LEU:HD12	3:B:45:PRO:O	0.86	1.69	9	3
3:A:57:ILE:C	3:A:57:ILE:HD13	0.86	1.94	10	2
3:A:68:GLN:CG	3:A:82:ILE:HD13	0.86	2.00	14	1
3:A:23:VAL:HG13	3:B:30:TYR:CD2	0.86	2.05	3	12
3:A:29:ALA:HB3	3:A:34:LEU:CD1	0.86	2.00	9	2
3:A:30:TYR:CG	3:B:23:VAL:HG13	0.86	2.03	3	13
2:F:2:DG:H1'	2:F:3:DT:O4'	0.86	1.70	7	9
3:A:75:LEU:O	3:A:75:LEU:HD22	0.86	1.70	2	1
3:B:57:ILE:CD1	3:B:58:VAL:HG13	0.86	2.01	4	8
3:B:78:GLY:O	3:B:81:THR:N	0.86	2.08	4	15
3:A:23:VAL:HG13	3:B:30:TYR:CD1	0.86	2.03	9	2
3:A:57:ILE:HD11	3:A:58:VAL:HG22	0.86	1.44	3	12
3:A:34:LEU:C	3:A:37:PRO:HD2	0.86	1.96	6	5
3:A:87:ASN:O	3:A:90:LYS:CG	0.86	2.24	15	15
3:B:57:ILE:CD1	3:B:58:VAL:HG22	0.86	2.00	2	2
3:A:54:ARG:CD	3:B:42:MET:HE3	0.86	2.01	1	3
3:A:72:LYS:HE2	3:A:79:ILE:HG12	0.85	1.45	5	2
3:B:19:TRP:C	3:B:20:LEU:HD22	0.85	1.96	14	2
1:E:14:DT:H3'	3:A:76:GLY:O	0.85	1.71	5	8
3:B:49:GLU:O	3:B:53:THR:HG22	0.85	1.71	9	2
3:B:51:LEU:HD22	3:B:54:ARG:NE	0.85	1.87	12	1
3:B:41:LEU:C	3:B:41:LEU:CD2	0.85	2.48	6	8
3:B:69:ARG:HA	3:B:79:ILE:HD11	0.85	1.46	13	3
3:B:97:ARG:CD	3:B:100:LEU:HD12	0.85	2.00	10	2
3:A:26:LEU:HD12	3:A:30:TYR:CE1	0.85	2.07	2	8
3:A:85:GLY:O	3:A:88:SER:HB2	0.85	1.72	14	5
3:A:67:SER:HB2	3:A:82:ILE:HD13	0.85	1.48	13	4
3:B:26:LEU:CD1	3:B:38:LEU:HD13	0.84	2.02	13	8
3:A:44:THR:HB	3:A:47:GLU:HB2	0.84	1.47	5	4
3:B:44:THR:N	3:B:45:PRO:HD3	0.84	1.87	8	13
3:A:43:LEU:CD1	3:B:50:ALA:HB1	0.84	1.99	3	1
3:B:26:LEU:CD1	3:B:34:LEU:HD21	0.84	2.01	14	1
3:A:78:GLY:O	3:A:82:ILE:HG12	0.84	1.72	7	12
3:A:41:LEU:HD21	3:B:58:VAL:HG12	0.84	1.49	4	2
3:A:29:ALA:HB3	3:A:34:LEU:CG	0.84	2.02	9	2
2:F:15:DA:H62	3:B:80:ALA:HB2	0.84	1.31	11	2
3:A:19:TRP:CH2	3:B:39:LEU:HD12	0.84	2.06	4	3
3:A:52:GLY:O	3:A:56:ARG:HB3	0.84	1.71	6	6
3:A:51:LEU:HD11	3:B:22:PHE:CG	0.84	2.07	4	1
3:A:29:ALA:HB1	3:A:34:LEU:C	0.84	1.98	2	10
3:A:52:GLY:O	3:A:56:ARG:CG	0.84	2.26	9	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:26:LEU:HD13	3:B:38:LEU:CD1	0.84	2.03	6	7
3:B:29:ALA:HB1	3:B:34:LEU:O	0.84	1.73	9	9
3:B:44:THR:N	4:B:109:TRP:O	0.83	2.11	15	2
3:A:23:VAL:HG13	3:B:30:TYR:CE2	0.83	2.08	3	3
3:B:35:HIS:C	3:B:36:LEU:HD23	0.83	1.97	14	1
3:A:51:LEU:CD1	3:B:22:PHE:CZ	0.83	2.57	6	2
3:A:34:LEU:HD23	3:B:99:TRP:CZ3	0.83	2.07	6	2
1:E:13:DC:OP2	4:B:109:TRP:O	0.83	1.96	10	1
3:B:36:LEU:N	3:B:37:PRO:CD	0.83	2.41	9	15
3:B:29:ALA:HB1	3:B:34:LEU:HB3	0.83	1.47	7	7
2:F:12:DA:O3'	3:A:44:THR:HG21	0.83	1.73	8	1
1:E:15:DG:H3'	3:A:73:ASN:OD1	0.83	1.74	9	6
3:A:19:TRP:O	3:A:23:VAL:HG23	0.83	1.71	4	14
3:A:40:ASN:CG	3:B:91:ALA:HB1	0.83	1.99	13	6
3:A:23:VAL:HG22	3:B:30:TYR:CE1	0.83	2.07	9	1
3:A:42:MET:CE	3:B:58:VAL:HG21	0.83	2.04	15	4
3:A:42:MET:CE	3:B:58:VAL:HG11	0.83	2.03	14	5
3:A:52:GLY:O	3:A:56:ARG:CB	0.83	2.27	12	10
3:A:55:VAL:CG1	3:B:22:PHE:CE1	0.83	2.61	7	3
3:B:78:GLY:C	3:B:82:ILE:HG23	0.83	1.98	3	5
3:B:81:THR:O	4:B:201:TRP:CZ2	0.83	2.32	2	14
3:B:38:LEU:HD23	3:B:41:LEU:CD2	0.83	2.04	11	2
3:A:51:LEU:C	3:A:51:LEU:CD1	0.83	2.48	6	1
3:B:44:THR:N	3:B:45:PRO:CD	0.82	2.42	13	15
3:A:57:ILE:CD1	3:A:58:VAL:N	0.82	2.42	10	12
3:B:57:ILE:HG21	3:B:81:THR:HG23	0.82	1.50	2	6
3:A:55:VAL:HG11	3:B:26:LEU:HD21	0.82	1.47	7	2
2:F:3:DT:C7	3:A:82:ILE:HD11	0.82	2.03	2	5
3:B:22:PHE:HB3	3:B:26:LEU:HG	0.82	1.52	4	2
3:A:78:GLY:HA3	3:A:82:ILE:HG23	0.82	1.50	8	13
1:E:13:DC:H2''	1:E:14:DT:O5'	0.82	1.75	14	15
2:F:5:DC:H2''	2:F:6:DC:O5'	0.82	1.73	3	14
3:A:34:LEU:C	3:A:34:LEU:HD22	0.82	2.00	9	2
3:A:84:ARG:CG	3:B:43:LEU:HD13	0.82	2.04	2	3
3:A:43:LEU:C	4:B:201:TRP:HB2	0.82	1.99	14	9
3:A:39:LEU:HD22	3:B:19:TRP:CE2	0.81	2.10	2	5
3:A:55:VAL:HG12	3:A:59:GLU:HG2	0.81	1.52	3	4
3:A:100:LEU:HD12	3:B:41:LEU:CD1	0.81	2.05	14	6
1:E:12:DA:C5'	3:B:44:THR:HG21	0.81	2.05	7	12
3:A:41:LEU:HD22	3:A:41:LEU:C	0.81	2.00	4	5
3:B:57:ILE:HG22	3:B:82:ILE:HG23	0.81	1.49	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:LEU:HD12	3:B:54:ARG:N	0.81	1.90	13	2
3:A:57:ILE:CD1	3:A:57:ILE:C	0.81	2.54	10	10
3:B:78:GLY:HA3	3:B:82:ILE:HG23	0.81	1.53	10	12
2:F:4:DA:N6	3:A:79:ILE:HD12	0.81	1.90	13	1
3:A:23:VAL:O	3:A:27:LYS:HG2	0.81	1.76	15	7
3:B:23:VAL:O	3:B:27:LYS:NZ	0.81	2.14	14	1
3:A:72:LYS:HG3	3:A:79:ILE:HG12	0.81	1.50	1	7
3:A:72:LYS:HZ1	3:A:79:ILE:HD13	0.81	1.34	1	2
3:A:66:MET:O	3:A:67:SER:O	0.81	1.97	8	4
3:A:96:LEU:HD13	3:B:37:PRO:HB2	0.81	1.50	10	1
3:A:55:VAL:C	3:A:59:GLU:HG3	0.81	2.00	10	4
3:B:97:ARG:NH1	3:B:100:LEU:HD22	0.81	1.91	6	2
3:B:54:ARG:O	3:B:57:ILE:HD12	0.81	1.76	2	1
2:F:3:DT:C7	3:A:79:ILE:HG23	0.81	2.05	3	1
3:A:36:LEU:HD22	3:A:48:ARG:NH2	0.81	1.91	12	2
3:B:81:THR:HA	4:B:201:TRP:NE1	0.80	1.91	3	8
3:B:29:ALA:HB1	3:B:34:LEU:CB	0.80	2.06	7	7
3:A:72:LYS:CE	3:A:79:ILE:HG12	0.80	2.05	5	4
3:B:41:LEU:HD22	3:B:42:MET:SD	0.80	2.17	12	5
3:A:43:LEU:HD13	3:B:50:ALA:CB	0.80	2.02	3	1
3:A:73:ASN:CB	3:A:79:ILE:HD11	0.80	2.06	12	7
3:A:43:LEU:HA	4:B:201:TRP:HB2	0.80	1.52	9	7
3:A:29:ALA:HB3	3:A:35:HIS:CD2	0.80	2.11	13	1
3:A:72:LYS:HB2	3:A:78:GLY:C	0.80	2.01	13	1
3:A:55:VAL:O	3:A:59:GLU:CG	0.80	2.30	8	12
2:F:15:DA:H62	3:B:80:ALA:HB1	0.80	1.34	10	5
3:B:40:ASN:HA	3:B:45:PRO:HB3	0.80	1.52	6	1
1:E:15:DG:OP2	3:A:76:GLY:HA2	0.80	1.75	7	1
3:B:29:ALA:HB1	3:B:34:LEU:C	0.80	2.01	8	4
1:E:14:DT:H2''	1:E:15:DG:O5'	0.80	1.77	7	13
3:A:78:GLY:CA	3:A:82:ILE:HG23	0.80	2.06	7	14
3:A:35:HIS:CE1	3:A:36:LEU:HD23	0.80	2.11	2	1
3:A:24:ASP:HA	3:A:27:LYS:HD3	0.80	1.54	14	15
3:B:78:GLY:CA	3:B:82:ILE:HG23	0.80	2.06	12	13
3:A:96:LEU:HB2	3:B:37:PRO:HA	0.80	1.53	3	1
3:B:44:THR:HB	4:B:109:TRP:O	0.80	1.77	1	3
3:B:81:THR:HA	4:B:201:TRP:CE2	0.80	2.12	9	13
3:A:26:LEU:HD21	3:A:38:LEU:HD22	0.80	1.52	4	5
3:B:72:LYS:HD3	3:B:82:ILE:HD11	0.80	1.53	12	4
3:B:53:THR:O	3:B:57:ILE:HG23	0.80	1.77	8	4
3:A:52:GLY:O	3:A:56:ARG:HB2	0.80	1.75	12	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:29:ALA:CB	3:A:34:LEU:HB3	0.80	2.07	9	2
3:A:43:LEU:HB2	3:B:54:ARG:HB2	0.80	1.53	13	2
3:B:49:GLU:O	3:B:53:THR:OG1	0.80	1.99	14	5
3:B:35:HIS:O	3:B:36:LEU:HD23	0.80	1.76	14	1
3:A:36:LEU:N	3:A:37:PRO:CD	0.79	2.45	10	15
3:A:36:LEU:N	3:A:37:PRO:HD2	0.79	1.93	7	15
3:A:96:LEU:CA	3:B:37:PRO:HB3	0.79	2.07	13	9
3:A:72:LYS:HZ2	3:A:79:ILE:HD13	0.79	1.34	6	4
3:A:96:LEU:HD23	3:B:41:LEU:HD13	0.79	1.53	10	1
3:A:96:LEU:HB3	3:B:37:PRO:HA	0.79	1.53	1	8
3:B:38:LEU:HA	3:B:41:LEU:HD22	0.79	1.53	8	5
3:A:53:THR:O	3:A:57:ILE:HG23	0.79	1.78	2	14
3:B:72:LYS:CB	3:B:82:ILE:HG21	0.79	2.07	13	8
3:A:36:LEU:HD22	3:B:19:TRP:CD1	0.79	2.12	10	2
3:B:41:LEU:HD21	3:B:42:MET:SD	0.79	2.18	8	3
3:A:44:THR:HB	3:A:47:GLU:HG2	0.79	1.54	1	1
3:B:57:ILE:CG2	3:B:81:THR:HG22	0.79	2.08	10	12
3:B:39:LEU:C	3:B:45:PRO:HB2	0.79	2.03	11	12
2:F:5:DC:N4	3:A:83:THR:HG21	0.79	1.92	3	1
2:F:3:DT:C4	2:F:4:DA:C6	0.79	2.71	12	5
3:A:45:PRO:HD3	4:B:201:TRP:CA	0.79	2.08	12	4
3:A:45:PRO:HD3	4:B:201:TRP:HA	0.79	1.55	12	5
3:A:45:PRO:HB2	3:B:91:ALA:HB2	0.79	1.53	3	1
3:A:55:VAL:HG22	3:B:42:MET:HE1	0.79	1.51	12	2
3:B:97:ARG:HD2	3:B:100:LEU:HD12	0.79	1.54	10	2
3:A:39:LEU:HD11	3:A:48:ARG:CB	0.78	2.07	15	5
3:A:81:THR:O	4:B:109:TRP:CZ2	0.78	2.36	4	15
3:A:56:ARG:O	3:A:60:GLU:HB2	0.78	1.78	4	8
3:A:43:LEU:HB2	3:B:54:ARG:CB	0.78	2.08	13	3
1:E:16:DG:C2'	1:E:17:DT:H71	0.78	2.08	6	5
3:A:42:MET:HE3	3:B:58:VAL:HG21	0.78	1.55	2	2
3:B:53:THR:HG23	3:B:75:LEU:CD1	0.78	2.08	15	1
3:B:72:LYS:HG3	3:B:79:ILE:CA	0.78	2.07	3	12
3:A:91:ALA:HB3	3:B:40:ASN:CA	0.78	2.09	1	2
3:A:41:LEU:HB3	3:B:91:ALA:HB3	0.78	1.54	15	3
3:A:39:LEU:O	3:A:39:LEU:HD12	0.78	1.78	9	10
3:B:38:LEU:HD23	3:B:42:MET:HE1	0.78	1.53	3	2
3:B:36:LEU:HD23	3:B:39:LEU:HD21	0.78	1.54	7	1
2:F:2:DG:H3'	3:A:68:GLN:OE1	0.78	1.79	12	2
3:B:38:LEU:O	3:B:42:MET:HE3	0.78	1.78	10	2
3:A:34:LEU:HD23	3:B:99:TRP:HB2	0.78	1.53	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:62:LEU:CD1	3:A:100:LEU:HD22	0.78	2.08	13	7
2:F:12:DA:O3'	3:A:44:THR:HG23	0.78	1.79	6	9
3:A:34:LEU:HB2	3:B:99:TRP:CE3	0.78	2.13	9	2
3:A:43:LEU:HA	3:B:54:ARG:CG	0.78	2.09	7	1
3:B:57:ILE:HD13	3:B:58:VAL:HG13	0.78	1.56	14	3
3:A:42:MET:HE2	3:B:58:VAL:CG1	0.78	2.08	13	3
3:A:81:THR:HA	4:B:109:TRP:CE2	0.78	2.14	7	5
3:B:57:ILE:CG2	3:B:82:ILE:HG22	0.77	2.07	3	3
3:B:30:TYR:CZ	3:B:34:LEU:HD23	0.77	2.14	14	1
3:B:55:VAL:O	3:B:59:GLU:HG3	0.77	1.80	5	4
3:A:88:SER:HB2	3:B:41:LEU:C	0.77	2.04	15	2
3:B:62:LEU:HD21	3:B:97:ARG:CZ	0.77	2.09	15	1
2:F:2:DG:H2''	2:F:3:DT:O5'	0.77	1.77	13	14
2:F:8:DG:H2''	2:F:9:DT:O5'	0.77	1.79	15	15
3:A:78:GLY:O	3:A:82:ILE:CG1	0.77	2.32	1	14
3:B:100:LEU:HD22	3:B:100:LEU:O	0.77	1.80	10	2
3:A:41:LEU:HD12	3:A:41:LEU:O	0.77	1.78	1	1
1:E:16:DG:C4	1:E:17:DT:O4	0.77	2.37	3	1
3:A:99:TRP:CB	3:B:34:LEU:HD22	0.77	2.09	4	1
3:A:51:LEU:HD22	3:B:22:PHE:CE2	0.77	2.13	6	1
2:F:12:DA:H2''	2:F:13:DC:O5'	0.77	1.79	7	9
2:F:3:DT:C7	3:A:79:ILE:HD13	0.77	2.10	13	5
3:B:42:MET:O	3:B:44:THR:N	0.77	2.17	6	7
3:A:72:LYS:HE3	3:A:82:ILE:HD11	0.77	1.55	5	1
3:B:95:GLU:C	3:B:96:LEU:HD12	0.77	2.05	10	4
3:A:78:GLY:O	3:A:79:ILE:HG12	0.77	1.79	13	1
2:F:3:DT:H2''	3:A:83:THR:OG1	0.77	1.79	14	7
2:F:13:DC:H2''	2:F:14:DG:O5'	0.77	1.80	15	15
3:A:51:LEU:HG	3:B:22:PHE:CE1	0.77	2.14	8	4
3:A:54:ARG:HG2	4:B:109:TRP:HB2	0.77	1.55	7	4
3:B:72:LYS:HB3	3:B:82:ILE:HG21	0.77	1.57	3	5
3:A:51:LEU:CD2	3:B:22:PHE:CD2	0.77	2.68	7	4
1:E:15:DG:N7	3:A:77:ALA:HB1	0.77	1.93	13	1
2:F:1:DT:HO5'	2:F:1:DT:H6	0.77	1.18	15	8
3:A:42:MET:HB3	3:B:54:ARG:CG	0.77	2.10	11	4
3:A:50:ALA:HB1	3:A:54:ARG:NE	0.76	1.95	8	2
3:B:103:VAL:O	3:B:104:LEU:HD22	0.76	1.80	7	1
3:B:38:LEU:O	3:B:42:MET:HE2	0.76	1.80	14	3
3:A:43:LEU:C	3:A:45:PRO:HD3	0.76	2.05	8	1
3:A:99:TRP:CH2	3:B:38:LEU:HD11	0.76	2.15	7	7
3:B:47:GLU:O	3:B:49:GLU:HG3	0.76	1.79	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:72:LYS:HB2	3:B:82:ILE:HG21	0.76	1.57	2	7
3:A:39:LEU:HA	3:A:43:LEU:HD11	0.76	1.57	7	1
3:B:30:TYR:CD1	3:B:34:LEU:HB3	0.76	2.16	14	1
1:E:13:DC:H5'	3:A:47:GLU:OE2	0.76	1.80	15	1
3:A:39:LEU:CA	3:A:43:LEU:HD11	0.76	2.11	7	1
3:A:93:PRO:O	3:A:94:VAL:HG13	0.76	1.80	12	1
3:A:26:LEU:HD12	3:A:27:LYS:N	0.76	1.95	3	1
3:A:39:LEU:HD11	3:A:48:ARG:HB3	0.76	1.57	14	2
3:A:96:LEU:HD13	3:B:37:PRO:CB	0.76	2.09	10	1
3:A:78:GLY:C	3:A:82:ILE:HG23	0.76	2.06	10	12
3:A:55:VAL:HG12	3:B:22:PHE:CE1	0.76	2.15	12	3
3:A:72:LYS:HD2	3:A:73:ASN:N	0.76	1.95	15	2
2:F:4:DA:OP2	3:A:83:THR:OG1	0.76	2.03	14	13
3:A:34:LEU:HD22	3:B:99:TRP:HB2	0.76	1.56	7	4
3:A:51:LEU:HD23	3:B:19:TRP:CZ2	0.76	2.16	4	2
3:A:68:GLN:O	3:A:70:GLU:HG3	0.76	1.81	11	1
3:A:68:GLN:HG3	3:A:82:ILE:HD13	0.76	1.57	14	1
3:B:27:LYS:HA	3:B:30:TYR:HB2	0.75	1.57	11	14
3:B:78:GLY:O	3:B:82:ILE:HG23	0.75	1.81	15	3
3:A:43:LEU:HD13	3:B:53:THR:OG1	0.75	1.82	10	1
2:F:3:DT:C7	3:A:72:LYS:HD3	0.75	2.11	9	7
1:E:14:DT:OP2	3:A:53:THR:HG21	0.75	1.80	10	3
3:A:96:LEU:CB	3:B:37:PRO:HB3	0.75	2.11	6	8
1:E:16:DG:N3	2:F:4:DA:N6	0.75	2.33	3	1
3:B:39:LEU:HD12	3:B:39:LEU:O	0.75	1.81	7	3
3:B:19:TRP:O	3:B:23:VAL:HG21	0.75	1.81	14	1
3:A:88:SER:HB3	3:B:41:LEU:C	0.75	2.06	1	1
3:A:57:ILE:HD12	3:A:58:VAL:HG22	0.75	1.59	13	8
3:B:76:GLY:O	3:B:77:ALA:HB2	0.75	1.82	3	14
2:F:13:DC:P	3:A:44:THR:HG23	0.75	2.21	11	7
3:A:68:GLN:O	3:A:72:LYS:HG2	0.75	1.82	3	1
3:A:79:ILE:O	3:A:82:ILE:HG13	0.75	1.80	1	8
3:A:81:THR:HG22	4:B:109:TRP:CD2	0.75	2.15	3	9
3:A:23:VAL:HG11	3:B:34:LEU:CD1	0.75	2.10	3	1
3:B:95:GLU:C	3:B:96:LEU:HD13	0.75	2.06	13	1
3:A:51:LEU:HD21	3:B:22:PHE:CD2	0.75	2.17	7	2
3:A:30:TYR:O	3:B:23:VAL:HG11	0.74	1.81	15	8
3:A:72:LYS:CG	3:A:79:ILE:HG12	0.74	2.12	1	9
3:A:96:LEU:CD2	3:B:41:LEU:HD13	0.74	2.11	10	1
3:A:34:LEU:HD23	3:A:36:LEU:CD1	0.74	2.12	12	1
3:A:35:HIS:HE2	3:B:19:TRP:CD1	0.74	1.98	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:44:THR:O	3:A:47:GLU:HG3	0.74	1.82	1	1
3:A:72:LYS:HB2	3:A:82:ILE:HG12	0.74	1.59	5	9
3:A:76:GLY:O	3:A:77:ALA:CB	0.74	2.35	5	14
3:A:53:THR:HG23	3:A:76:GLY:O	0.74	1.81	12	1
3:A:72:LYS:HD3	3:A:79:ILE:CG1	0.74	2.12	15	3
3:A:22:PHE:CE1	3:B:51:LEU:HD21	0.74	2.16	4	3
3:B:47:GLU:O	3:B:49:GLU:N	0.74	2.20	6	4
3:A:55:VAL:HG22	3:B:42:MET:HE2	0.74	1.56	4	2
3:A:72:LYS:HZ2	3:A:79:ILE:HG23	0.74	1.42	4	2
2:F:13:DC:H3'	3:A:43:LEU:HD11	0.74	1.56	11	1
3:B:42:MET:O	4:B:109:TRP:CD2	0.74	2.40	15	13
2:F:3:DT:H73	3:A:68:GLN:HA	0.74	1.58	15	4
1:E:16:DG:H1'	1:E:17:DT:O4	0.74	1.82	3	1
1:E:13:DC:OP2	4:B:109:TRP:HB3	0.74	1.81	7	2
3:A:54:ARG:O	3:A:57:ILE:HD13	0.74	1.82	8	1
3:A:19:TRP:CZ3	3:B:39:LEU:HD12	0.74	2.18	4	1
3:A:57:ILE:HD12	3:A:58:VAL:H	0.74	1.40	11	4
3:A:80:ALA:HB1	3:A:84:ARG:CZ	0.74	2.11	7	3
3:B:57:ILE:HD13	4:B:201:TRP:CZ3	0.74	2.17	8	1
3:B:50:ALA:O	3:B:54:ARG:HB3	0.74	1.82	13	4
3:A:51:LEU:HD11	3:B:22:PHE:CD1	0.74	2.18	4	1
3:A:39:LEU:HD13	3:B:19:TRP:CH2	0.74	2.18	15	2
3:A:43:LEU:O	3:A:43:LEU:HD13	0.74	1.82	11	2
3:A:92:ALA:HB3	3:A:96:LEU:HD21	0.74	1.57	8	3
3:A:72:LYS:HE2	3:A:79:ILE:HA	0.74	1.59	5	1
3:A:67:SER:HB3	3:A:82:ILE:HD13	0.74	1.59	15	2
2:F:6:DC:H2''	2:F:7:DA:O5'	0.73	1.83	8	15
3:A:55:VAL:O	3:A:58:VAL:HG23	0.73	1.82	5	4
3:A:73:ASN:HB3	3:A:79:ILE:HD11	0.73	1.59	12	5
3:A:26:LEU:O	3:A:30:TYR:CG	0.73	2.41	4	2
3:B:35:HIS:CE1	3:B:36:LEU:HD13	0.73	2.18	4	1
3:A:80:ALA:O	3:A:84:ARG:HB2	0.73	1.83	2	15
3:A:90:LYS:HG3	3:A:91:ALA:N	0.73	1.98	6	15
2:F:11:DC:H2''	2:F:12:DA:O5'	0.73	1.83	11	10
3:B:30:TYR:CD1	3:B:34:LEU:O	0.73	2.41	3	1
3:A:35:HIS:CE1	3:B:23:VAL:HG11	0.73	2.18	12	1
3:B:61:LEU:HD12	3:B:82:ILE:O	0.73	1.83	12	1
3:A:58:VAL:O	3:A:62:LEU:HD12	0.73	1.83	12	3
1:E:18:DA:C2	2:F:4:DA:C2	0.73	2.76	3	2
3:A:41:LEU:HD22	3:B:58:VAL:HG11	0.73	1.57	3	3
3:A:91:ALA:HB1	3:B:40:ASN:C	0.73	2.07	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:F:3:DT:P	3:A:82:ILE:HD12	0.73	2.24	10	4
3:A:96:LEU:HD23	3:B:37:PRO:HA	0.73	1.58	11	3
3:B:44:THR:HB	4:B:109:TRP:HA	0.73	1.59	12	9
3:A:40:ASN:CA	3:B:91:ALA:HB1	0.73	2.12	7	6
3:A:57:ILE:C	3:A:57:ILE:HD12	0.73	2.08	14	1
3:A:51:LEU:HD21	3:B:22:PHE:CE1	0.73	2.19	2	4
3:B:44:THR:O	3:B:44:THR:CG2	0.73	2.37	10	14
2:F:3:DT:H71	3:A:79:ILE:HG23	0.73	1.61	3	1
3:A:57:ILE:C	3:A:57:ILE:CD1	0.73	2.61	4	2
3:A:34:LEU:C	3:A:34:LEU:CD1	0.73	2.57	6	1
2:F:7:DA:H2''	2:F:8:DG:O5'	0.73	1.83	2	15
3:A:36:LEU:HD21	3:B:19:TRP:CD1	0.73	2.17	15	9
3:A:67:SER:O	3:A:68:GLN:CB	0.73	2.36	12	11
3:A:26:LEU:HD21	3:A:38:LEU:CD2	0.73	2.14	4	2
2:F:13:DC:H6	2:F:13:DC:O5'	0.73	1.67	15	9
3:A:89:LEU:O	3:A:92:ALA:O	0.73	2.06	2	13
3:A:41:LEU:C	3:A:41:LEU:CD1	0.73	2.61	6	8
3:A:72:LYS:NZ	3:A:79:ILE:HG23	0.73	1.99	5	2
3:A:34:LEU:HD22	3:B:99:TRP:HB3	0.73	1.61	11	2
3:A:55:VAL:HG21	3:B:22:PHE:CE1	0.72	2.19	3	9
3:A:92:ALA:CB	3:A:96:LEU:HD12	0.72	2.14	3	1
3:B:42:MET:C	3:B:45:PRO:HG3	0.72	2.09	8	5
3:A:72:LYS:NZ	3:A:79:ILE:HG13	0.72	1.98	15	2
3:A:96:LEU:C	3:A:96:LEU:CD2	0.72	2.58	3	1
1:E:15:DG:O6	3:A:80:ALA:CB	0.72	2.36	3	8
3:A:90:LYS:HG3	3:A:91:ALA:H	0.72	1.44	8	15
3:B:36:LEU:N	3:B:37:PRO:HD2	0.72	1.99	7	7
3:A:58:VAL:HG21	3:B:41:LEU:HD11	0.72	1.60	11	4
3:A:57:ILE:HG12	4:B:109:TRP:CZ3	0.72	2.20	6	11
3:B:42:MET:HB3	4:B:109:TRP:HA	0.72	1.59	8	3
3:B:54:ARG:O	3:B:57:ILE:HD11	0.72	1.84	14	2
3:A:92:ALA:CB	3:A:96:LEU:HD11	0.72	2.14	4	1
3:A:29:ALA:CB	3:A:34:LEU:HD12	0.72	2.13	6	2
3:A:72:LYS:CE	3:A:79:ILE:HG13	0.72	2.14	8	2
3:A:22:PHE:CZ	3:B:51:LEU:HD21	0.72	2.19	4	3
1:E:9:DT:OP2	1:E:9:DT:H71	0.72	1.85	9	3
3:A:76:GLY:O	3:A:77:ALA:HB3	0.72	1.85	14	3
3:B:38:LEU:CA	3:B:41:LEU:HD22	0.72	2.15	8	1
1:E:11:DT:H2''	1:E:12:DA:N7	0.72	1.99	14	13
3:A:54:ARG:HG3	3:B:42:MET:HE3	0.72	1.62	9	4
3:A:19:TRP:CZ3	3:B:51:LEU:HB3	0.72	2.19	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:30:TYR:CE1	3:B:23:VAL:HG22	0.72	2.19	8	5
3:A:79:ILE:O	3:A:83:THR:CG2	0.72	2.38	7	13
3:A:34:LEU:HD22	3:B:99:TRP:CB	0.72	2.15	11	3
3:A:75:LEU:HD13	3:A:75:LEU:N	0.72	1.99	15	1
3:B:85:GLY:O	3:B:88:SER:N	0.72	2.23	4	11
3:A:17:GLN:N	3:A:17:GLN:CD	0.72	2.45	3	1
3:A:48:ARG:HA	3:B:19:TRP:CH2	0.72	2.19	4	3
3:A:19:TRP:CZ2	3:B:39:LEU:HD13	0.72	2.20	14	7
3:A:78:GLY:O	3:A:82:ILE:HG23	0.72	1.83	5	9
3:B:26:LEU:HD22	3:B:38:LEU:HD11	0.72	1.61	11	5
3:B:35:HIS:C	3:B:37:PRO:HD2	0.72	2.09	7	12
3:B:43:LEU:HD13	3:B:44:THR:N	0.72	1.98	13	9
3:A:40:ASN:O	4:B:201:TRP:N	0.72	2.22	2	7
4:B:201:TRP:O	4:B:201:TRP:CD2	0.72	2.43	2	1
3:B:39:LEU:HA	3:B:45:PRO:HB2	0.71	1.61	12	9
3:A:91:ALA:HB1	3:B:40:ASN:CA	0.71	2.14	12	12
3:A:57:ILE:HD11	4:B:109:TRP:HZ3	0.71	1.43	4	6
3:A:99:TRP:HB2	3:B:34:LEU:HD22	0.71	1.62	1	3
3:B:36:LEU:O	3:B:40:ASN:HB2	0.71	1.84	2	9
3:A:36:LEU:HD23	3:A:39:LEU:CD2	0.71	2.15	15	3
3:A:42:MET:O	3:A:43:LEU:HD22	0.71	1.85	1	1
3:A:51:LEU:HD22	3:B:19:TRP:CZ2	0.71	2.20	13	9
3:A:72:LYS:HE2	3:A:79:ILE:HG23	0.71	1.60	1	1
3:B:72:LYS:HG3	3:B:82:ILE:HG12	0.71	1.62	15	9
3:A:62:LEU:HD21	3:A:97:ARG:CZ	0.71	2.14	14	2
3:B:38:LEU:HD23	3:B:41:LEU:HD22	0.71	1.61	11	1
3:A:36:LEU:HD22	3:A:48:ARG:CZ	0.71	2.16	12	1
3:A:22:PHE:CZ	3:A:26:LEU:HD21	0.71	2.21	13	1
3:A:72:LYS:O	3:A:77:ALA:N	0.71	2.21	8	4
1:E:16:DG:H2''	1:E:17:DT:O5'	0.71	1.85	7	9
3:A:88:SER:CB	3:B:41:LEU:O	0.71	2.39	13	12
3:A:91:ALA:HB1	3:B:40:ASN:HA	0.71	1.62	11	9
3:A:72:LYS:HG2	3:A:73:ASN:N	0.71	2.00	7	1
2:F:3:DT:H2''	2:F:4:DA:C8	0.71	2.21	10	9
3:A:20:LEU:N	3:A:20:LEU:HD22	0.71	2.01	3	10
3:A:76:GLY:O	3:A:77:ALA:HB2	0.71	1.85	1	11
2:F:3:DT:C4	2:F:4:DA:N6	0.71	2.59	4	12
3:A:40:ASN:HA	3:A:45:PRO:HB3	0.71	1.63	6	7
3:A:42:MET:HE1	3:B:100:LEU:HD11	0.71	1.62	15	4
3:A:92:ALA:CB	3:A:96:LEU:HD21	0.71	2.15	4	3
2:F:3:DT:H2'	3:A:83:THR:HB	0.71	1.63	1	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:57:ILE:CG2	3:B:81:THR:HG23	0.71	2.16	2	1
3:A:18:GLU:N	3:A:21:ARG:HG3	0.71	2.01	3	1
3:A:41:LEU:HD21	3:B:58:VAL:CG1	0.71	2.16	4	3
3:A:96:LEU:HD13	3:B:37:PRO:HG2	0.71	1.62	10	1
2:F:4:DA:H2''	2:F:5:DC:C6	0.71	2.20	5	9
3:A:34:LEU:HD22	3:A:34:LEU:O	0.71	1.86	9	1
3:A:42:MET:CG	3:B:58:VAL:HG21	0.71	2.16	7	2
3:A:72:LYS:HZ1	3:A:79:ILE:HG23	0.71	1.43	5	1
3:A:44:THR:HG22	3:A:44:THR:O	0.71	1.84	8	1
3:A:67:SER:O	3:A:68:GLN:HB3	0.71	1.86	12	4
3:A:33:ASP:O	3:A:34:LEU:HD12	0.71	1.86	12	1
3:B:55:VAL:O	3:B:59:GLU:HG2	0.71	1.86	14	2
3:B:81:THR:HG1	4:B:201:TRP:CD1	0.70	2.02	1	8
3:A:41:LEU:HD13	3:A:42:MET:N	0.70	1.99	8	7
3:A:62:LEU:HD13	3:A:100:LEU:HD22	0.70	1.60	2	6
3:A:55:VAL:HG21	3:B:22:PHE:CE2	0.70	2.20	6	2
3:A:42:MET:CB	3:B:54:ARG:HG2	0.70	2.16	10	2
3:A:43:LEU:CD2	3:B:51:LEU:HD23	0.70	2.17	15	1
3:B:78:GLY:O	3:B:82:ILE:HG13	0.70	1.86	10	14
1:E:14:DT:H3'	3:A:77:ALA:HB2	0.70	1.61	14	4
3:B:44:THR:OG1	4:B:109:TRP:N	0.70	2.23	6	1
2:F:4:DA:OP2	3:A:83:THR:HA	0.70	1.87	3	2
3:A:70:GLU:O	3:A:71:LEU:HD22	0.70	1.85	3	1
3:A:26:LEU:HD22	3:A:38:LEU:HD13	0.70	1.63	8	3
3:A:32:ASN:ND2	3:A:34:LEU:HD22	0.70	2.02	8	1
3:A:96:LEU:HD13	3:B:37:PRO:CG	0.70	2.16	10	1
3:B:57:ILE:HD12	3:B:57:ILE:C	0.70	2.10	13	11
3:A:72:LYS:O	3:A:78:GLY:N	0.70	2.24	4	10
3:B:72:LYS:CE	3:B:82:ILE:HD13	0.70	2.16	15	7
3:A:47:GLU:HA	3:A:50:ALA:HB3	0.70	1.62	8	8
3:A:57:ILE:CD1	4:B:109:TRP:HZ3	0.70	2.00	9	7
3:A:40:ASN:O	3:B:91:ALA:HB3	0.70	1.87	8	2
3:B:50:ALA:O	3:B:54:ARG:HG3	0.70	1.85	7	5
3:B:22:PHE:O	3:B:26:LEU:N	0.70	2.23	7	3
3:B:39:LEU:HD23	3:B:40:ASN:OD1	0.70	1.85	14	3
1:E:13:DC:P	4:B:109:TRP:HB3	0.70	2.26	15	3
3:A:51:LEU:CD2	3:B:19:TRP:CH2	0.70	2.71	4	12
3:A:56:ARG:O	3:A:60:GLU:CB	0.70	2.40	4	3
3:B:41:LEU:HD22	3:B:42:MET:CG	0.70	2.16	12	2
3:A:26:LEU:HD22	3:A:38:LEU:CD1	0.70	2.17	8	1
3:A:55:VAL:CG2	3:B:42:MET:HE1	0.70	2.16	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:F:4:DA:H2''	2:F:5:DC:O5'	0.70	1.87	7	9
3:A:55:VAL:CB	3:B:22:PHE:CZ	0.70	2.74	3	10
3:A:91:ALA:HB3	3:B:40:ASN:C	0.70	2.12	8	6
3:B:100:LEU:HD23	3:B:100:LEU:O	0.70	1.85	14	11
3:A:29:ALA:HB1	3:A:34:LEU:O	0.70	1.87	10	6
3:A:96:LEU:HD22	3:A:96:LEU:O	0.70	1.86	3	1
2:F:12:DA:H5'	3:A:46:ASP:OD2	0.70	1.87	5	1
3:A:56:ARG:HG3	3:A:75:LEU:HD13	0.70	1.62	7	1
3:A:43:LEU:O	3:B:54:ARG:NH1	0.70	2.24	1	2
1:E:16:DG:C2	2:F:4:DA:C6	0.69	2.79	3	1
3:A:57:ILE:HD12	3:A:57:ILE:C	0.69	2.12	1	7
3:A:57:ILE:CG1	4:B:109:TRP:CZ3	0.69	2.74	2	11
3:B:72:LYS:HE2	3:B:82:ILE:HD13	0.69	1.63	3	5
2:F:3:DT:H2''	2:F:4:DA:O5'	0.69	1.86	11	6
3:B:96:LEU:N	3:B:96:LEU:CD1	0.69	2.52	13	4
3:B:78:GLY:O	3:B:82:ILE:CG1	0.69	2.41	9	15
3:A:26:LEU:HD13	3:A:30:TYR:CZ	0.69	2.22	3	1
3:A:27:LYS:HG3	3:A:28:ASN:N	0.69	2.01	8	7
3:A:42:MET:HB3	3:B:54:ARG:HB2	0.69	1.64	9	1
2:F:4:DA:OP2	3:A:83:THR:O	0.69	2.10	11	15
2:F:3:DT:H71	3:A:82:ILE:CD1	0.69	2.15	2	4
1:E:16:DG:H2'	1:E:17:DT:C7	0.69	2.17	12	11
3:A:96:LEU:HD23	3:B:36:LEU:O	0.69	1.87	12	4
3:A:96:LEU:HA	3:B:37:PRO:HB3	0.69	1.63	11	6
2:F:5:DC:H41	3:A:83:THR:CG2	0.69	1.99	3	1
3:A:92:ALA:HB3	3:A:96:LEU:HD11	0.69	1.64	4	1
3:B:71:LEU:HD22	3:B:71:LEU:C	0.69	2.11	5	1
3:A:37:PRO:HD3	3:B:96:LEU:HD22	0.69	1.64	15	3
3:B:41:LEU:HD22	3:B:42:MET:HG2	0.69	1.62	6	2
3:A:91:ALA:HB3	3:B:41:LEU:HA	0.69	1.65	10	2
3:A:96:LEU:HD13	3:A:97:ARG:H	0.69	1.43	3	1
3:A:44:THR:HG23	3:B:54:ARG:NH2	0.69	2.03	5	1
2:F:17:DT:OP2	2:F:17:DT:H71	0.69	1.87	9	3
3:B:76:GLY:O	3:B:77:ALA:CB	0.69	2.41	15	14
3:A:43:LEU:HB2	3:B:54:ARG:CG	0.69	2.18	12	3
3:A:43:LEU:HD13	3:B:50:ALA:HA	0.69	1.61	13	3
3:B:73:ASN:HB2	3:B:79:ILE:HD11	0.69	1.64	9	1
3:A:43:LEU:O	3:A:44:THR:OG1	0.69	2.10	5	3
3:A:39:LEU:C	3:A:43:LEU:HD11	0.69	2.12	7	1
3:A:99:TRP:CB	3:B:34:LEU:HD23	0.69	2.18	10	1
3:A:27:LYS:HA	3:A:30:TYR:HB2	0.69	1.62	6	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:36:LEU:O	3:B:40:ASN:OD1	0.69	2.11	1	1
3:A:51:LEU:HG	3:B:22:PHE:CE2	0.69	2.23	4	5
3:A:84:ARG:HD2	3:B:43:LEU:HD22	0.69	1.63	14	1
3:A:96:LEU:HD23	3:B:37:PRO:O	0.69	1.88	4	2
3:B:68:GLN:O	3:B:69:ARG:CB	0.69	2.40	7	6
4:B:109:TRP:CD1	4:B:109:TRP:C	0.69	2.70	6	2
3:A:29:ALA:HB3	3:A:35:HIS:HD2	0.69	1.45	13	1
3:A:84:ARG:CD	3:B:43:LEU:HD13	0.69	2.18	14	1
1:E:11:DT:H1'	1:E:12:DA:N7	0.68	2.03	14	12
3:B:44:THR:N	3:B:45:PRO:HD2	0.68	2.00	1	2
2:F:4:DA:C8	2:F:5:DC:N4	0.68	2.61	3	3
2:F:13:DC:OP1	3:A:44:THR:HG23	0.68	1.89	11	5
2:F:3:DT:C7	3:A:72:LYS:CD	0.68	2.72	9	10
3:A:72:LYS:HE2	3:A:79:ILE:CG2	0.68	2.18	1	1
3:A:26:LEU:CD2	3:A:38:LEU:HD22	0.68	2.18	5	2
3:A:50:ALA:O	3:A:54:ARG:HG3	0.68	1.88	4	2
3:A:78:GLY:O	3:A:82:ILE:HG13	0.68	1.89	14	3
3:A:22:PHE:HB2	3:B:55:VAL:HG21	0.68	1.65	5	4
3:A:100:LEU:CD1	3:B:41:LEU:HD11	0.68	2.18	9	4
3:B:67:SER:HB3	3:B:82:ILE:HG21	0.68	1.65	9	1
3:A:96:LEU:CD1	3:B:37:PRO:HG2	0.68	2.18	10	1
1:E:9:DT:H73	1:E:9:DT:OP2	0.68	1.88	8	3
1:E:12:DA:H4'	3:B:44:THR:HG21	0.68	1.65	9	9
3:A:34:LEU:O	3:A:37:PRO:HD2	0.68	1.87	6	2
3:A:62:LEU:HD22	3:A:97:ARG:NH1	0.68	2.04	7	1
3:A:72:LYS:CG	3:A:79:ILE:HG13	0.68	2.18	12	2
3:B:29:ALA:HB3	3:B:34:LEU:HD13	0.68	1.65	14	1
2:F:11:DC:H4'	3:A:46:ASP:OD2	0.68	1.88	1	1
3:B:57:ILE:HD12	3:B:58:VAL:H	0.68	1.47	9	11
1:E:15:DG:O5'	3:A:73:ASN:ND2	0.68	2.27	4	3
3:A:36:LEU:HD23	3:A:39:LEU:HD23	0.68	1.66	15	4
3:A:43:LEU:CD2	3:B:81:THR:HG21	0.68	2.19	11	1
3:A:43:LEU:HD12	3:B:53:THR:OG1	0.68	1.89	14	1
3:A:44:THR:O	3:A:47:GLU:CG	0.68	2.42	1	6
3:A:91:ALA:HB3	3:B:40:ASN:O	0.68	1.89	4	8
3:B:68:GLN:HA	3:B:79:ILE:HD11	0.68	1.64	2	1
3:B:57:ILE:CA	3:B:82:ILE:HG22	0.68	2.19	14	3
3:A:99:TRP:HB3	3:B:34:LEU:HD12	0.68	1.63	7	1
3:A:44:THR:HG23	4:B:201:TRP:N	0.68	2.04	1	1
3:A:85:GLY:O	3:A:88:SER:CB	0.68	2.41	13	13
3:B:80:ALA:O	3:B:84:ARG:CB	0.68	2.42	1	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:37:PRO:O	3:A:41:LEU:HB3	0.68	1.89	5	1
3:B:53:THR:HG21	3:B:77:ALA:HB3	0.68	1.66	5	3
3:B:78:GLY:C	3:B:82:ILE:HG12	0.68	2.14	14	7
3:B:56:ARG:HA	3:B:59:GLU:HG2	0.68	1.66	10	4
3:A:41:LEU:O	3:A:41:LEU:HD13	0.67	1.89	5	1
3:A:51:LEU:CD2	3:B:22:PHE:CE2	0.67	2.77	14	3
3:A:51:LEU:HD23	3:B:22:PHE:CZ	0.67	2.23	14	1
1:E:18:DA:O5'	1:E:18:DA:H8	0.67	1.73	11	13
3:A:42:MET:HG2	3:B:58:VAL:HG21	0.67	1.65	7	2
3:A:55:VAL:HG12	3:A:59:GLU:CG	0.67	2.18	1	3
3:B:51:LEU:HD13	3:B:51:LEU:C	0.67	2.14	13	12
4:B:201:TRP:CE3	4:B:201:TRP:C	0.67	2.73	2	1
3:A:26:LEU:HA	3:A:35:HIS:CD2	0.67	2.23	13	1
3:A:39:LEU:HD11	3:A:48:ARG:CA	0.67	2.18	14	1
3:B:51:LEU:HD13	3:B:52:GLY:N	0.67	2.05	15	1
3:B:53:THR:HG23	3:B:75:LEU:HD11	0.67	1.65	15	1
1:E:13:DC:C4	1:E:14:DT:H73	0.67	2.24	6	12
2:F:3:DT:H73	3:A:68:GLN:C	0.67	2.15	7	1
3:A:36:LEU:HD23	3:A:39:LEU:HD21	0.67	1.65	12	2
3:A:34:LEU:HD23	3:A:36:LEU:HD12	0.67	1.65	12	1
3:A:36:LEU:HD22	3:B:19:TRP:NE1	0.67	2.04	13	1
3:A:54:ARG:HD2	3:B:42:MET:HE3	0.67	1.64	1	1
3:B:30:TYR:CE1	3:B:35:HIS:CE1	0.67	2.82	8	4
3:A:39:LEU:O	3:A:45:PRO:HB2	0.67	1.88	8	1
3:A:43:LEU:HD23	3:B:51:LEU:HB3	0.67	1.66	2	1
3:A:57:ILE:HG13	4:B:109:TRP:CZ3	0.67	2.25	8	4
3:A:51:LEU:HD13	3:B:22:PHE:CE1	0.67	2.21	6	1
3:A:58:VAL:HG21	3:B:41:LEU:HD21	0.67	1.65	12	2
3:A:71:LEU:O	3:A:72:LYS:C	0.67	2.37	2	6
3:A:43:LEU:CB	3:B:54:ARG:HD3	0.67	2.19	14	1
2:F:3:DT:H72	3:A:79:ILE:CD1	0.67	2.20	8	5
1:E:11:DT:C2'	1:E:12:DA:C8	0.67	2.77	11	1
3:A:72:LYS:HE2	3:A:79:ILE:CB	0.67	2.19	1	2
3:A:96:LEU:HB3	3:B:37:PRO:CA	0.67	2.20	5	6
1:E:15:DG:C2	1:E:16:DG:C6	0.67	2.83	7	7
3:A:51:LEU:O	3:B:22:PHE:CZ	0.67	2.47	4	5
3:A:22:PHE:CZ	3:A:43:LEU:HD13	0.67	2.23	5	1
3:B:72:LYS:HG3	3:B:79:ILE:N	0.67	2.03	15	6
3:A:62:LEU:HD13	3:A:104:LEU:HD23	0.67	1.64	12	1
3:A:55:VAL:CG1	3:B:38:LEU:HD21	0.67	2.20	6	1
3:B:67:SER:OG	3:B:83:THR:HG23	0.67	1.89	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:41:LEU:HD11	3:A:42:MET:CE	0.67	2.20	13	1
3:A:81:THR:HG22	4:B:109:TRP:CE2	0.67	2.24	9	6
3:B:42:MET:HA	4:B:109:TRP:CZ3	0.67	2.25	8	5
3:A:40:ASN:CA	3:A:45:PRO:HB3	0.66	2.19	14	10
3:A:79:ILE:CA	3:A:82:ILE:HG12	0.66	2.20	10	11
3:A:61:LEU:HD12	3:A:66:MET:HA	0.66	1.68	6	1
3:A:38:LEU:HG	3:A:42:MET:HE2	0.66	1.67	11	1
3:B:78:GLY:HA2	3:B:82:ILE:HG23	0.66	1.68	12	2
3:A:41:LEU:CD1	3:A:42:MET:HE3	0.66	2.20	13	2
3:A:55:VAL:HA	3:A:58:VAL:HG23	0.66	1.67	10	7
3:A:19:TRP:CZ3	3:B:39:LEU:HD13	0.66	2.25	12	6
3:A:51:LEU:HD12	3:A:55:VAL:CB	0.66	2.21	4	1
3:A:43:LEU:N	3:A:43:LEU:HD12	0.66	2.05	7	1
3:A:51:LEU:HD23	3:B:19:TRP:CZ3	0.66	2.24	7	1
3:B:57:ILE:HG21	3:B:81:THR:CB	0.66	2.19	11	5
3:A:43:LEU:HD13	3:B:53:THR:CB	0.66	2.20	10	1
1:E:15:DG:C8	3:A:79:ILE:CD1	0.66	2.78	14	2
3:B:45:PRO:HD3	4:B:109:TRP:O	0.66	1.91	1	3
3:A:72:LYS:HD2	3:A:79:ILE:HG13	0.66	1.67	2	3
2:F:5:DC:C4	2:F:6:DC:C4	0.66	2.83	9	14
1:E:17:DT:H2''	1:E:18:DA:C8	0.66	2.26	1	10
3:A:36:LEU:CD2	3:B:19:TRP:CD1	0.66	2.79	9	6
3:A:51:LEU:CD2	3:B:22:PHE:CE1	0.66	2.78	2	6
3:A:91:ALA:C	3:B:40:ASN:HB3	0.66	2.15	1	1
2:F:3:DT:OP2	3:A:82:ILE:HD12	0.66	1.91	8	3
3:A:35:HIS:C	3:A:37:PRO:HD2	0.66	2.16	15	12
3:B:53:THR:OG1	3:B:77:ALA:HB3	0.66	1.90	1	2
3:B:43:LEU:HB3	4:B:109:TRP:NE1	0.66	2.04	4	4
3:A:72:LYS:HE2	3:A:79:ILE:CA	0.66	2.20	5	1
3:B:39:LEU:O	3:B:45:PRO:O	0.66	2.14	7	2
3:B:72:LYS:CG	3:B:79:ILE:HD13	0.66	2.20	9	1
3:A:35:HIS:CD2	3:B:99:TRP:CZ2	0.66	2.84	13	1
2:F:12:DA:H2'	2:F:13:DC:C5	0.66	2.26	6	14
3:A:44:THR:HB	3:A:47:GLU:CG	0.66	2.20	1	3
3:A:34:LEU:HD13	3:B:96:LEU:HB3	0.66	1.67	4	2
3:A:56:ARG:HA	3:A:59:GLU:CG	0.66	2.21	6	12
3:A:26:LEU:HD21	3:A:38:LEU:HD13	0.66	1.67	6	1
3:B:42:MET:CA	3:B:45:PRO:HG3	0.66	2.19	8	4
3:A:99:TRP:HB2	3:B:34:LEU:HD23	0.66	1.68	10	1
1:E:18:DA:H2''	1:E:19:DC:O5'	0.66	1.89	11	11
3:A:84:ARG:O	3:A:87:ASN:N	0.66	2.29	14	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:37:PRO:CG	3:B:96:LEU:HB2	0.66	2.21	3	4
1:E:12:DA:C5'	4:B:109:TRP:OXT	0.66	2.41	10	1
3:B:57:ILE:CD1	3:B:58:VAL:N	0.66	2.59	14	9
2:F:2:DG:H2'	3:A:68:GLN:NE2	0.66	2.04	2	1
3:A:81:THR:O	4:B:109:TRP:CH2	0.66	2.48	14	8
1:E:16:DG:H1'	1:E:17:DT:C7	0.66	2.21	3	1
3:A:51:LEU:HD22	3:B:22:PHE:CD2	0.66	2.25	6	1
3:A:36:LEU:N	3:A:36:LEU:HD23	0.66	2.06	10	3
3:B:33:ASP:O	3:B:37:PRO:CG	0.66	2.43	14	1
3:A:91:ALA:CB	3:B:40:ASN:HB3	0.65	2.19	13	6
3:B:22:PHE:CD1	3:B:26:LEU:HD23	0.65	2.25	9	3
3:A:34:LEU:C	3:A:35:HIS:CG	0.65	2.74	12	1
3:A:36:LEU:HD21	3:B:19:TRP:CG	0.65	2.25	15	1
2:F:12:DA:O5'	2:F:12:DA:H8	0.65	1.74	2	7
3:A:35:HIS:NE2	3:B:23:VAL:HG21	0.65	2.06	12	3
3:B:62:LEU:HD22	3:B:97:ARG:NH2	0.65	2.06	2	3
3:A:97:ARG:O	3:A:101:GLU:HB2	0.65	1.90	8	4
3:B:57:ILE:HB	3:B:81:THR:O	0.65	1.91	8	2
3:A:57:ILE:O	3:A:61:LEU:HD12	0.65	1.90	15	1
2:F:5:DC:H2'	2:F:6:DC:C6	0.65	2.27	2	5
3:B:67:SER:CB	3:B:83:THR:HG23	0.65	2.20	8	1
1:E:17:DT:C4	1:E:18:DA:N6	0.65	2.65	6	8
3:A:87:ASN:O	3:A:90:LYS:HG3	0.65	1.90	11	14
3:B:39:LEU:O	3:B:39:LEU:HG	0.65	1.89	11	10
3:B:41:LEU:CD2	3:B:42:MET:CG	0.65	2.74	2	3
2:F:4:DA:C8	2:F:5:DC:C4	0.65	2.85	3	3
3:A:63:ARG:HB2	3:A:104:LEU:HD11	0.65	1.67	6	1
3:A:26:LEU:O	3:A:30:TYR:HB2	0.65	1.91	14	3
3:A:29:ALA:HB1	3:A:34:LEU:CB	0.65	2.22	8	6
3:A:35:HIS:CE1	3:B:23:VAL:HG21	0.65	2.26	2	2
3:A:37:PRO:O	3:A:41:LEU:CD1	0.65	2.45	6	9
3:B:50:ALA:O	3:B:54:ARG:HG2	0.65	1.91	2	1
3:A:92:ALA:HB3	3:A:96:LEU:HD12	0.65	1.68	3	1
3:A:41:LEU:O	3:A:41:LEU:CD2	0.65	2.42	11	9
3:A:82:ILE:HD12	3:A:83:THR:N	0.65	2.07	4	2
3:A:68:GLN:HG3	3:A:68:GLN:O	0.65	1.90	15	2
3:B:40:ASN:HA	3:B:45:PRO:HB2	0.65	1.67	6	1
3:B:44:THR:CB	4:B:109:TRP:O	0.65	2.44	1	3
3:A:39:LEU:HD11	3:A:48:ARG:HB2	0.65	1.67	6	3
3:A:58:VAL:HB	3:A:100:LEU:HD11	0.65	1.69	12	2
3:B:42:MET:O	4:B:109:TRP:HB2	0.65	1.91	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:57:ILE:CG1	4:B:109:TRP:CH2	0.65	2.80	10	2
2:F:4:DA:H62	3:A:79:ILE:HD12	0.65	1.50	13	1
3:B:85:GLY:HA3	4:B:201:TRP:CZ2	0.65	2.27	3	1
3:B:22:PHE:HB2	3:B:26:LEU:HD23	0.65	1.68	14	1
2:F:6:DC:C2	2:F:7:DA:N7	0.65	2.65	1	13
3:A:62:LEU:HD12	3:A:100:LEU:HD22	0.65	1.67	10	4
3:A:96:LEU:CB	3:B:37:PRO:HA	0.65	2.22	3	5
3:B:78:GLY:O	3:B:79:ILE:C	0.65	2.39	1	15
3:B:42:MET:H	3:B:45:PRO:HG3	0.65	1.50	14	6
3:A:41:LEU:HD22	3:B:58:VAL:CG1	0.65	2.21	3	1
3:A:78:GLY:CA	3:A:81:THR:HB	0.65	2.17	15	2
1:E:13:DC:C5	1:E:14:DT:H73	0.65	2.27	2	14
3:B:47:GLU:O	3:B:51:LEU:N	0.65	2.30	8	5
3:A:79:ILE:HG22	3:A:80:ALA:N	0.65	2.05	13	3
3:B:57:ILE:CD1	3:B:57:ILE:C	0.65	2.70	14	6
3:B:69:ARG:CA	3:B:79:ILE:HD11	0.65	2.19	13	2
3:B:50:ALA:O	3:B:54:ARG:HD3	0.65	1.92	11	2
2:F:3:DT:C2'	3:A:83:THR:OG1	0.65	2.45	7	12
3:A:27:LYS:CA	3:A:30:TYR:HB2	0.65	2.22	2	11
3:A:38:LEU:HA	3:A:41:LEU:CD1	0.65	2.22	10	2
3:A:57:ILE:CD1	3:A:58:VAL:CG2	0.65	2.72	2	2
3:B:36:LEU:HA	3:B:39:LEU:HD23	0.65	1.67	3	3
3:B:43:LEU:HB2	4:B:109:TRP:CD2	0.65	2.27	6	1
3:A:42:MET:O	3:A:44:THR:N	0.65	2.30	8	1
3:A:78:GLY:C	3:A:79:ILE:HG12	0.65	2.17	13	1
3:A:55:VAL:HG11	3:B:22:PHE:CE2	0.65	2.27	14	1
2:F:7:DA:N3	2:F:8:DG:C8	0.64	2.66	8	15
3:A:22:PHE:CE1	3:A:43:LEU:HD11	0.64	2.26	1	1
3:A:79:ILE:C	3:A:83:THR:HG22	0.64	2.15	13	2
3:A:60:GLU:OE1	3:A:71:LEU:HD11	0.64	1.92	11	1
2:F:5:DC:C2	2:F:6:DC:C5	0.64	2.85	11	7
3:B:54:ARG:O	3:B:57:ILE:CD1	0.64	2.45	14	3
3:B:85:GLY:CA	4:B:201:TRP:CH2	0.64	2.80	7	11
3:A:17:GLN:HB3	3:A:20:LEU:HD23	0.64	1.68	3	1
3:A:55:VAL:HG22	3:B:38:LEU:HD21	0.64	1.69	11	3
3:A:30:TYR:CG	3:B:27:LYS:NZ	0.64	2.66	14	1
3:B:34:LEU:HA	3:B:37:PRO:HG3	0.64	1.67	1	4
3:B:55:VAL:O	3:B:59:GLU:CG	0.64	2.44	14	6
3:B:57:ILE:HD13	3:B:58:VAL:HG22	0.64	1.66	2	1
3:B:42:MET:N	3:B:45:PRO:HG3	0.64	2.06	14	7
3:A:72:LYS:HZ1	3:A:79:ILE:CG2	0.64	2.04	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:74:GLU:O	3:B:75:LEU:CB	0.64	2.44	12	1
3:A:23:VAL:HG13	3:B:30:TYR:CG	0.64	2.27	1	5
3:A:91:ALA:CB	3:B:40:ASN:HA	0.64	2.20	1	8
2:F:2:DG:C2'	3:A:68:GLN:NE2	0.64	2.60	2	1
3:A:22:PHE:CG	3:B:51:LEU:HD21	0.64	2.26	11	2
3:A:29:ALA:HB2	3:B:99:TRP:NE1	0.64	2.08	13	6
3:A:51:LEU:CD1	3:B:22:PHE:CE2	0.64	2.78	6	1
2:F:3:DT:C5	3:A:79:ILE:HD13	0.64	2.28	13	5
3:B:57:ILE:HD13	3:B:57:ILE:C	0.64	2.17	2	1
3:A:54:ARG:CG	4:B:109:TRP:HB2	0.64	2.23	15	3
3:B:49:GLU:O	3:B:50:ALA:C	0.64	2.41	11	3
3:A:22:PHE:CE1	3:A:26:LEU:HD21	0.64	2.28	13	2
3:B:81:THR:HG23	4:B:201:TRP:CD2	0.64	2.28	15	1
3:A:68:GLN:O	3:A:68:GLN:CG	0.64	2.44	15	2
3:A:72:LYS:CG	3:A:73:ASN:N	0.64	2.61	13	3
3:A:99:TRP:CH2	3:B:38:LEU:HD12	0.64	2.27	5	1
3:A:96:LEU:HD12	3:A:96:LEU:N	0.64	2.07	11	1
2:F:6:DC:C2	2:F:7:DA:C8	0.64	2.85	7	14
1:E:16:DG:H1'	1:E:17:DT:H73	0.64	1.70	3	1
3:A:55:VAL:HG22	3:B:42:MET:CE	0.64	2.23	12	2
3:B:72:LYS:HG2	3:B:73:ASN:N	0.64	2.08	12	3
3:A:33:ASP:HA	3:A:36:LEU:HD12	0.64	1.69	15	2
2:F:14:DG:OP2	3:B:77:ALA:HB1	0.64	1.93	1	1
3:B:27:LYS:O	3:B:30:TYR:HB2	0.64	1.93	4	11
3:A:30:TYR:CE1	3:A:35:HIS:CE1	0.64	2.85	14	1
3:A:36:LEU:O	3:A:40:ASN:HB2	0.64	1.93	15	5
3:A:42:MET:HE3	3:B:100:LEU:HD11	0.64	1.70	7	1
3:A:91:ALA:HB3	3:B:41:LEU:CA	0.64	2.22	10	2
3:A:35:HIS:CE1	3:A:38:LEU:HD13	0.64	2.28	13	1
3:B:20:LEU:HA	3:B:23:VAL:HB	0.64	1.67	14	1
3:A:54:ARG:CG	3:B:42:MET:HE3	0.64	2.22	9	4
1:E:12:DA:O3'	4:B:109:TRP:OXT	0.64	2.15	2	4
3:B:43:LEU:HD12	4:B:109:TRP:NE1	0.64	2.08	6	1
3:B:51:LEU:HA	3:B:54:ARG:HB2	0.64	1.70	7	4
3:A:57:ILE:HG13	4:B:109:TRP:CH2	0.64	2.28	8	1
1:E:9:DT:H2''	1:E:10:DG:O5'	0.63	1.92	13	13
3:B:81:THR:O	4:B:201:TRP:CH2	0.63	2.51	12	11
1:E:15:DG:C6	3:A:80:ALA:HB2	0.63	2.29	3	1
3:A:51:LEU:CG	3:B:22:PHE:CD2	0.63	2.81	4	1
3:A:25:LEU:HG	3:B:103:VAL:HG11	0.63	1.70	5	1
3:A:35:HIS:O	3:A:39:LEU:HB3	0.63	1.93	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:F:12:DA:C3'	3:A:44:THR:HG21	0.63	2.22	8	1
3:A:55:VAL:HG22	3:B:38:LEU:HD22	0.63	1.66	8	1
3:B:43:LEU:C	3:B:43:LEU:HD13	0.63	2.18	7	10
3:A:67:SER:O	3:A:68:GLN:HB2	0.63	1.93	3	2
2:F:17:DT:H73	2:F:17:DT:OP2	0.63	1.92	8	5
3:B:42:MET:HA	4:B:109:TRP:CE3	0.63	2.28	6	2
3:A:72:LYS:CD	3:A:78:GLY:O	0.63	2.46	13	1
3:A:81:THR:HA	4:B:109:TRP:CZ2	0.63	2.28	9	14
3:A:43:LEU:HD13	3:A:44:THR:OG1	0.63	1.93	2	1
1:E:16:DG:C1'	1:E:17:DT:O4	0.63	2.46	3	1
3:A:17:GLN:CB	3:A:20:LEU:HD23	0.63	2.22	3	1
3:B:39:LEU:O	3:B:45:PRO:C	0.63	2.41	7	6
3:B:71:LEU:O	3:B:72:LYS:C	0.63	2.41	3	2
3:A:96:LEU:HD23	3:B:37:PRO:C	0.63	2.18	4	2
3:B:36:LEU:H	3:B:37:PRO:CD	0.63	2.06	14	1
2:F:4:DA:C4	2:F:5:DC:C4	0.63	2.87	9	13
3:A:67:SER:HB2	3:A:82:ILE:CD1	0.63	2.23	13	1
3:A:85:GLY:HA2	3:A:88:SER:OG	0.63	1.93	1	3
2:F:4:DA:C4	2:F:5:DC:C5	0.63	2.87	2	6
3:B:57:ILE:HD13	3:B:58:VAL:N	0.63	2.08	2	1
3:A:27:LYS:O	3:A:31:GLN:HG2	0.63	1.94	10	2
3:A:51:LEU:CG	3:B:22:PHE:CZ	0.63	2.82	3	7
3:B:78:GLY:HA3	3:B:82:ILE:CG2	0.63	2.24	8	9
3:A:38:LEU:O	3:A:42:MET:HB2	0.63	1.94	9	5
3:A:81:THR:HG1	4:B:109:TRP:CD1	0.63	2.12	14	2
3:A:92:ALA:HB2	3:B:40:ASN:O	0.63	1.93	14	2
3:A:38:LEU:O	3:A:42:MET:HG3	0.63	1.93	10	1
3:B:76:GLY:O	3:B:77:ALA:HB3	0.63	1.93	15	1
3:A:37:PRO:O	3:A:41:LEU:HD23	0.63	1.94	1	1
1:E:16:DG:C2'	1:E:17:DT:H72	0.63	2.21	4	4
3:A:73:ASN:HB2	3:A:79:ILE:HD11	0.63	1.69	5	4
3:B:71:LEU:CD1	3:B:71:LEU:N	0.63	2.61	11	2
3:B:106:LYS:CD	3:B:106:LYS:O	0.63	2.47	6	1
3:A:40:ASN:C	3:B:91:ALA:CB	0.63	2.71	6	13
3:B:72:LYS:CB	3:B:82:ILE:HG12	0.63	2.19	11	6
3:A:42:MET:SD	3:B:58:VAL:HG11	0.63	2.34	11	2
3:A:43:LEU:O	4:B:201:TRP:HB2	0.63	1.94	14	4
3:A:54:ARG:CD	4:B:109:TRP:HB2	0.63	2.24	14	2
3:A:96:LEU:HD22	3:B:41:LEU:HB2	0.63	1.70	4	2
3:B:51:LEU:O	3:B:55:VAL:HG23	0.63	1.94	2	1
3:A:43:LEU:HA	3:B:51:LEU:HD23	0.63	1.70	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:34:LEU:HA	3:A:37:PRO:CG	0.63	2.24	9	2
1:E:12:DA:H5''	4:B:109:TRP:O	0.63	1.93	7	1
3:A:79:ILE:N	3:A:82:ILE:HG12	0.63	2.08	7	2
3:B:96:LEU:H	3:B:96:LEU:HD22	0.63	1.53	13	1
3:A:74:GLU:C	3:A:75:LEU:HD13	0.63	2.18	15	1
1:E:6:DT:H2''	1:E:7:DC:O5'	0.62	1.94	12	15
3:B:73:ASN:O	3:B:75:LEU:N	0.62	2.33	9	1
3:A:19:TRP:CD1	3:B:35:HIS:CB	0.62	2.81	14	1
3:A:19:TRP:CH2	3:B:51:LEU:HB3	0.62	2.29	14	1
3:A:43:LEU:HD12	3:B:53:THR:CB	0.62	2.24	14	1
3:A:44:THR:HB	3:A:47:GLU:CB	0.62	2.23	2	3
3:A:78:GLY:O	3:A:79:ILE:C	0.62	2.40	4	13
1:E:16:DG:O6	3:A:79:ILE:CG2	0.62	2.47	15	7
3:A:88:SER:OG	3:B:41:LEU:O	0.62	2.17	8	5
1:E:13:DC:OP1	3:A:50:ALA:HB1	0.62	1.94	11	2
3:A:96:LEU:CA	3:B:37:PRO:HB2	0.62	2.24	15	2
3:A:34:LEU:HD23	3:B:96:LEU:HB3	0.62	1.70	10	2
2:F:2:DG:C8	3:A:68:GLN:HG2	0.62	2.29	11	1
3:B:27:LYS:HG3	3:B:28:ASN:N	0.62	2.09	4	14
3:B:34:LEU:C	3:B:37:PRO:CD	0.62	2.72	2	8
3:B:72:LYS:CG	3:B:82:ILE:HG12	0.62	2.24	3	10
3:B:26:LEU:HD22	3:B:38:LEU:CD1	0.62	2.25	2	3
3:A:19:TRP:CZ2	3:B:35:HIS:CE1	0.62	2.87	5	2
3:B:104:LEU:O	3:B:105:LEU:HD12	0.62	1.93	8	1
3:B:30:TYR:CE1	3:B:35:HIS:CG	0.62	2.88	7	6
3:A:57:ILE:CD1	4:B:109:TRP:CZ3	0.62	2.82	13	12
3:A:90:LYS:CG	3:A:91:ALA:N	0.62	2.62	14	15
3:A:88:SER:HB2	3:B:41:LEU:O	0.62	1.94	3	4
1:E:13:DC:O5'	1:E:13:DC:H6	0.62	1.76	10	3
3:A:43:LEU:O	4:B:201:TRP:CB	0.62	2.48	12	7
2:F:3:DT:C5	2:F:4:DA:N6	0.62	2.67	9	2
3:B:27:LYS:N	3:B:27:LYS:HE2	0.62	2.10	14	1
3:A:41:LEU:CD1	3:A:41:LEU:C	0.62	2.72	15	1
3:A:85:GLY:O	3:A:88:SER:HB3	0.62	1.94	13	6
3:B:38:LEU:O	3:B:41:LEU:HD22	0.62	1.94	15	2
3:B:36:LEU:N	3:B:37:PRO:HD3	0.62	2.09	1	10
3:B:42:MET:O	4:B:109:TRP:CG	0.62	2.53	9	10
2:F:3:DT:H3'	3:A:83:THR:HA	0.62	1.72	12	5
3:A:43:LEU:HD12	3:B:54:ARG:CA	0.62	2.24	6	2
3:B:39:LEU:HD12	3:B:46:ASP:HA	0.62	1.70	10	1
1:E:15:DG:OP2	3:A:76:GLY:O	0.62	2.18	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:14:DT:H72	3:A:77:ALA:O	0.62	1.95	4	2
3:B:72:LYS:HB2	3:B:78:GLY:HA3	0.62	1.70	7	5
3:A:91:ALA:CB	3:B:40:ASN:O	0.62	2.47	10	5
3:A:96:LEU:HA	3:B:37:PRO:HB2	0.62	1.70	15	2
3:A:35:HIS:CE1	3:A:38:LEU:CD1	0.62	2.82	13	1
3:A:23:VAL:HG21	3:B:35:HIS:CE1	0.62	2.29	14	1
3:A:43:LEU:HA	3:B:54:ARG:CD	0.62	2.25	7	2
3:A:79:ILE:HA	3:A:82:ILE:CG1	0.62	2.25	13	12
3:A:72:LYS:HD3	3:A:79:ILE:HG12	0.62	1.72	2	2
3:B:41:LEU:HD23	3:B:42:MET:CG	0.62	2.25	2	2
3:A:42:MET:C	3:B:54:ARG:HG2	0.62	2.19	3	2
3:A:88:SER:HA	3:B:41:LEU:O	0.62	1.94	10	3
3:A:19:TRP:CE3	3:B:51:LEU:HD21	0.62	2.30	2	1
1:E:16:DG:N7	3:A:79:ILE:CG2	0.62	2.60	3	1
3:A:51:LEU:HD11	3:B:22:PHE:CE1	0.62	2.29	3	1
3:A:44:THR:CB	3:A:47:GLU:HB2	0.62	2.24	5	2
1:E:15:DG:C5	3:A:79:ILE:CG2	0.62	2.83	15	2
3:B:42:MET:CB	3:B:45:PRO:HG3	0.62	2.24	8	1
3:A:26:LEU:HD12	3:A:30:TYR:CE2	0.61	2.28	5	3
3:A:42:MET:C	3:A:43:LEU:HD22	0.61	2.19	1	1
3:A:52:GLY:O	3:A:56:ARG:HG3	0.61	1.93	9	6
3:A:80:ALA:O	3:A:84:ARG:CD	0.61	2.48	11	5
4:B:201:TRP:O	4:B:201:TRP:CG	0.61	2.53	2	1
3:B:50:ALA:HB1	3:B:54:ARG:NH1	0.61	2.10	15	2
3:A:51:LEU:CD2	3:B:19:TRP:CZ3	0.61	2.83	10	2
3:B:54:ARG:HD3	4:B:201:TRP:C	0.61	2.20	8	1
3:A:68:GLN:HG2	3:A:82:ILE:HD13	0.61	1.69	14	1
3:A:40:ASN:O	3:A:45:PRO:HB3	0.61	1.94	13	4
3:A:29:ALA:CB	3:A:34:LEU:CG	0.61	2.78	6	2
2:F:3:DT:H73	3:A:68:GLN:O	0.61	1.95	7	1
3:B:38:LEU:O	3:B:42:MET:CE	0.61	2.48	13	3
3:B:62:LEU:HD21	3:B:97:ARG:NH2	0.61	2.10	12	2
3:A:34:LEU:HD23	3:B:96:LEU:CB	0.61	2.25	10	1
2:F:15:DA:N6	3:B:80:ALA:HB2	0.61	2.08	11	1
3:A:57:ILE:HD11	4:B:109:TRP:CZ3	0.61	2.30	7	7
3:B:93:PRO:O	3:B:97:ARG:HB2	0.61	1.95	13	2
3:B:24:ASP:OD1	3:B:25:LEU:HD12	0.61	1.94	6	1
1:E:15:DG:H8	3:A:73:ASN:OD1	0.61	1.78	8	1
3:A:43:LEU:CB	4:B:201:TRP:CE2	0.61	2.84	8	1
3:B:81:THR:CA	4:B:201:TRP:CZ2	0.61	2.80	9	3
1:E:7:DC:H2''	1:E:8:DG:O5'	0.61	1.96	9	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:F:19:DC:O5'	2:F:19:DC:H6	0.61	1.78	11	15
3:B:34:LEU:C	3:B:37:PRO:HD2	0.61	2.20	6	10
1:E:16:DG:C6	2:F:4:DA:N6	0.61	2.68	4	4
3:A:35:HIS:O	3:A:39:LEU:HD23	0.61	1.94	6	3
1:E:11:DT:H2'	1:E:12:DA:C8	0.61	2.30	11	1
1:E:15:DG:C8	3:A:77:ALA:O	0.61	2.54	13	1
3:A:24:ASP:HA	3:A:27:LYS:CD	0.61	2.25	9	8
3:B:57:ILE:CG2	3:B:81:THR:CG2	0.61	2.78	2	2
2:F:2:DG:N7	3:A:69:ARG:NH1	0.61	2.48	14	3
3:B:38:LEU:HD23	3:B:41:LEU:HD23	0.61	1.72	4	1
3:A:60:GLU:OE1	3:A:71:LEU:HD13	0.61	1.96	5	1
3:B:43:LEU:CB	4:B:109:TRP:CG	0.61	2.83	6	1
3:B:70:GLU:O	3:B:71:LEU:HD23	0.61	1.96	7	1
3:A:99:TRP:CZ3	3:B:38:LEU:HG	0.61	2.31	15	10
2:F:3:DT:OP2	3:A:68:GLN:N	0.61	2.34	3	2
3:A:43:LEU:HB2	3:B:54:ARG:HG2	0.61	1.71	4	2
2:F:11:DC:O2	2:F:12:DA:N7	0.61	2.33	15	1
3:B:47:GLU:O	3:B:48:ARG:C	0.61	2.43	6	7
3:B:72:LYS:HG2	3:B:79:ILE:HG12	0.61	1.73	14	10
3:A:43:LEU:C	3:A:44:THR:OG1	0.61	2.43	5	3
3:A:37:PRO:HB3	3:B:96:LEU:HB2	0.61	1.70	12	4
3:A:56:ARG:CZ	3:A:75:LEU:HD21	0.61	2.26	5	1
3:B:72:LYS:HE2	3:B:72:LYS:N	0.61	2.11	7	1
3:A:34:LEU:HD13	3:A:35:HIS:H	0.61	1.53	9	1
3:A:44:THR:HG21	3:A:47:GLU:OE2	0.61	1.96	13	1
2:F:13:DC:O5'	2:F:13:DC:H6	0.61	1.77	3	3
3:A:78:GLY:C	3:A:82:ILE:H	0.61	2.01	4	6
3:B:50:ALA:HB1	3:B:54:ARG:CZ	0.61	2.25	5	2
3:B:70:GLU:O	3:B:71:LEU:HD12	0.61	1.95	14	2
2:F:3:DT:OP2	3:A:68:GLN:CG	0.61	2.48	14	1
3:A:35:HIS:CE1	3:A:39:LEU:HD22	0.61	2.30	14	1
3:A:72:LYS:HB3	3:A:82:ILE:HD13	0.61	1.72	10	4
3:B:39:LEU:CA	3:B:45:PRO:HB2	0.61	2.25	12	9
2:F:4:DA:H8	3:A:83:THR:OG1	0.61	1.78	11	9
3:B:51:LEU:HD12	3:B:51:LEU:C	0.61	2.20	2	2
3:A:23:VAL:HG11	3:B:34:LEU:HD13	0.61	1.71	3	1
3:B:35:HIS:O	3:B:39:LEU:HB3	0.61	1.95	14	2
2:F:14:DG:OP2	3:B:77:ALA:HB2	0.61	1.96	5	1
3:A:26:LEU:HA	3:A:35:HIS:CG	0.61	2.31	13	1
3:B:26:LEU:HD12	3:B:35:HIS:CE1	0.61	2.30	15	1
3:A:72:LYS:HB2	3:A:79:ILE:N	0.61	2.11	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:51:LEU:HA	3:A:54:ARG:HB2	0.61	1.71	6	4
3:B:36:LEU:HA	3:B:39:LEU:HD22	0.61	1.73	2	2
3:B:54:ARG:CD	4:B:201:TRP:O	0.61	2.49	2	1
1:E:15:DG:C2	1:E:16:DG:C4	0.61	2.89	3	1
3:A:99:TRP:CB	3:B:34:LEU:HD12	0.61	2.25	7	1
3:B:72:LYS:HG3	3:B:79:ILE:CG1	0.61	2.25	9	2
3:A:55:VAL:HG21	3:B:22:PHE:HZ	0.61	1.50	10	1
3:A:41:LEU:CD2	3:B:58:VAL:HG11	0.60	2.26	3	3
3:A:42:MET:O	3:B:57:ILE:CG1	0.60	2.49	14	4
2:F:4:DA:C2'	2:F:5:DC:C6	0.60	2.84	11	6
3:B:72:LYS:CG	3:B:79:ILE:HA	0.60	2.25	2	1
3:A:55:VAL:CG2	3:B:22:PHE:CE1	0.60	2.84	3	4
3:A:54:ARG:C	3:B:42:MET:HG2	0.60	2.22	9	2
1:E:19:DC:H6	1:E:19:DC:O5'	0.60	1.79	7	6
3:A:33:ASP:O	3:B:96:LEU:HD22	0.60	1.96	1	4
3:A:41:LEU:C	3:A:41:LEU:CD2	0.60	2.74	4	3
3:B:19:TRP:O	3:B:19:TRP:CD1	0.60	2.55	14	1
2:F:7:DA:C2	2:F:8:DG:C5	0.60	2.90	12	15
3:B:27:LYS:CG	3:B:28:ASN:N	0.60	2.65	4	14
3:A:37:PRO:HB3	3:B:96:LEU:HD13	0.60	1.72	4	5
3:A:72:LYS:HD3	3:A:79:ILE:CB	0.60	2.26	15	2
3:A:26:LEU:HD12	3:A:30:TYR:HE1	0.60	1.56	15	1
2:F:11:DC:H2''	2:F:12:DA:C8	0.60	2.31	5	8
3:B:72:LYS:HB2	3:B:82:ILE:CG2	0.60	2.26	2	5
3:A:42:MET:HB3	3:B:54:ARG:HG2	0.60	1.71	11	2
3:A:43:LEU:HD13	3:B:50:ALA:CA	0.60	2.27	13	2
3:A:22:PHE:CE1	3:A:43:LEU:HD23	0.60	2.31	7	1
2:F:14:DG:OP2	3:B:77:ALA:HB3	0.60	1.96	8	1
2:F:15:DA:O5'	2:F:15:DA:H8	0.60	1.80	8	1
3:A:42:MET:CB	4:B:201:TRP:HA	0.60	2.25	8	1
3:A:25:LEU:HG	3:B:103:VAL:HG21	0.60	1.72	14	1
3:A:75:LEU:C	3:A:75:LEU:HD13	0.60	2.22	1	1
3:A:87:ASN:O	3:A:90:LYS:HG2	0.60	1.96	15	11
1:E:8:DG:H2'	1:E:9:DT:C6	0.60	2.32	14	5
3:A:29:ALA:CB	3:A:34:LEU:CB	0.60	2.78	9	2
3:A:62:LEU:HD22	3:A:97:ARG:CZ	0.60	2.27	7	1
3:B:45:PRO:C	3:B:47:GLU:H	0.60	2.04	13	13
3:A:57:ILE:HB	3:A:82:ILE:HG22	0.60	1.74	15	3
3:B:53:THR:HA	3:B:56:ARG:HB3	0.60	1.74	12	6
3:A:19:TRP:CH2	3:B:39:LEU:CD1	0.60	2.85	11	8
3:B:27:LYS:C	3:B:29:ALA:N	0.60	2.56	6	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:13:DC:OP1	3:A:50:ALA:CB	0.60	2.50	7	1
1:E:16:DG:O5'	1:E:16:DG:H8	0.60	1.80	7	2
3:A:37:PRO:HG3	3:B:96:LEU:CB	0.60	2.27	14	9
3:A:87:ASN:HB3	3:B:43:LEU:HD12	0.60	1.71	2	2
3:A:91:ALA:CB	3:B:40:ASN:CA	0.60	2.80	12	9
3:B:27:LYS:HA	3:B:30:TYR:CD1	0.60	2.32	8	4
3:A:54:ARG:HD3	4:B:109:TRP:HB2	0.60	1.72	4	2
2:F:16:DG:O5'	2:F:16:DG:H8	0.60	1.80	8	1
3:A:42:MET:HB3	4:B:201:TRP:C	0.60	2.20	8	1
3:A:51:LEU:HD13	3:B:19:TRP:CH2	0.60	2.31	10	1
3:A:44:THR:OG1	3:B:54:ARG:NH1	0.60	2.35	1	1
1:E:3:DT:OP2	1:E:3:DT:H73	0.60	1.96	15	7
3:B:82:ILE:HG13	3:B:83:THR:H	0.60	1.57	12	10
3:A:67:SER:HB3	3:A:82:ILE:HG21	0.60	1.73	3	2
3:A:81:THR:O	4:B:109:TRP:HZ2	0.60	1.80	8	2
3:A:43:LEU:HA	3:B:54:ARG:HG2	0.60	1.72	7	1
3:A:29:ALA:HB3	3:A:34:LEU:HG	0.60	1.72	9	1
3:A:67:SER:OG	3:A:82:ILE:HG21	0.60	1.97	15	1
3:A:81:THR:O	3:A:82:ILE:C	0.59	2.45	9	10
3:A:91:ALA:HB3	3:B:40:ASN:CB	0.59	2.27	1	1
3:B:72:LYS:O	3:B:77:ALA:N	0.59	2.35	8	7
1:E:15:DG:H2''	1:E:16:DG:C8	0.59	2.32	2	1
3:A:38:LEU:HD23	3:A:38:LEU:O	0.59	1.96	12	5
3:A:43:LEU:HD23	3:B:54:ARG:CZ	0.59	2.26	3	1
3:A:106:LYS:O	3:A:106:LYS:CG	0.59	2.50	10	5
2:F:3:DT:O4	3:A:79:ILE:HD11	0.59	1.96	15	2
3:A:46:ASP:O	3:A:49:GLU:N	0.59	2.35	8	3
3:A:72:LYS:HZ3	3:A:79:ILE:HG23	0.59	1.57	12	2
2:F:12:DA:H2''	2:F:13:DC:C6	0.59	2.33	11	12
3:A:34:LEU:N	3:A:34:LEU:HD22	0.59	2.11	2	2
3:B:34:LEU:N	3:B:34:LEU:HD22	0.59	2.12	7	2
3:B:54:ARG:CD	4:B:201:TRP:C	0.59	2.75	2	1
3:B:37:PRO:O	3:B:41:LEU:HD12	0.59	1.96	5	3
3:B:42:MET:HB3	4:B:109:TRP:CE3	0.59	2.32	14	5
3:A:48:ARG:O	3:B:19:TRP:CZ3	0.59	2.55	7	5
3:B:97:ARG:NH1	3:B:100:LEU:HD13	0.59	2.11	9	3
3:A:26:LEU:CD2	3:A:38:LEU:HD13	0.59	2.27	6	3
2:F:14:DG:N7	3:B:80:ALA:HB3	0.59	2.12	8	1
3:A:74:GLU:HB3	3:A:75:LEU:HD23	0.59	1.73	9	1
2:F:5:DC:C2	2:F:6:DC:C6	0.59	2.91	5	8
3:A:51:LEU:HD21	3:B:22:PHE:CD1	0.59	2.32	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:201:TRP:O	4:B:201:TRP:CE3	0.59	2.56	2	1
3:A:30:TYR:O	3:B:23:VAL:HG12	0.59	1.97	4	1
3:A:78:GLY:HA3	3:A:81:THR:HG22	0.59	1.74	4	1
3:A:54:ARG:HB2	4:B:109:TRP:HB2	0.59	1.74	12	3
3:A:96:LEU:HB3	3:B:37:PRO:CB	0.59	2.28	7	2
3:A:50:ALA:C	3:A:54:ARG:HD3	0.59	2.23	15	1
1:E:18:DA:H2''	1:E:19:DC:C6	0.59	2.33	12	14
3:A:95:GLU:O	3:A:98:GLN:CB	0.59	2.50	14	11
1:E:11:DT:H2''	1:E:12:DA:OP2	0.59	1.97	4	12
2:F:15:DA:N7	3:B:80:ALA:HB2	0.59	2.12	15	2
1:E:12:DA:H2'	1:E:13:DC:C6	0.59	2.32	3	7
3:A:40:ASN:C	3:B:91:ALA:HB1	0.59	2.22	11	6
3:A:45:PRO:HD3	4:B:201:TRP:C	0.59	2.22	11	6
3:A:65:GLU:O	3:A:66:MET:C	0.59	2.46	4	1
3:A:66:MET:O	3:A:71:LEU:HD13	0.59	1.97	4	1
3:A:60:GLU:OE1	3:A:71:LEU:HD22	0.59	1.97	5	1
3:B:53:THR:O	3:B:57:ILE:HG13	0.59	1.97	7	3
3:A:42:MET:HA	3:B:57:ILE:HD11	0.59	1.75	11	2
1:E:12:DA:C8	1:E:12:DA:O5'	0.59	2.56	4	13
3:B:106:LYS:CG	3:B:106:LYS:O	0.59	2.49	8	5
3:A:44:THR:CG2	3:A:47:GLU:HG2	0.59	2.28	2	1
1:E:18:DA:C6	2:F:4:DA:N1	0.59	2.70	3	1
3:B:100:LEU:HD13	3:B:100:LEU:C	0.59	2.22	3	1
3:A:29:ALA:HB2	3:B:99:TRP:CH2	0.59	2.32	14	2
3:B:51:LEU:O	3:B:51:LEU:HD22	0.59	1.98	5	1
3:B:38:LEU:HA	3:B:41:LEU:HD13	0.59	1.73	6	1
3:A:85:GLY:O	3:A:88:SER:N	0.59	2.35	13	3
3:B:71:LEU:O	3:B:71:LEU:CD2	0.59	2.48	11	1
3:A:34:LEU:HD23	3:B:99:TRP:CB	0.59	2.26	8	2
3:A:68:GLN:HB2	3:A:71:LEU:HD12	0.59	1.73	1	1
3:A:87:ASN:CB	3:B:43:LEU:HD23	0.59	2.27	12	4
3:A:43:LEU:HD23	3:B:51:LEU:CB	0.59	2.27	2	1
1:E:16:DG:N1	2:F:4:DA:N6	0.59	2.49	3	1
3:B:44:THR:CB	4:B:109:TRP:HA	0.59	2.27	11	4
3:B:41:LEU:HG	3:B:42:MET:N	0.59	2.11	7	2
3:A:24:ASP:OD1	3:A:25:LEU:HD12	0.59	1.97	9	2
3:B:50:ALA:C	3:B:54:ARG:HD3	0.59	2.23	11	1
3:B:26:LEU:HD13	3:B:34:LEU:CD2	0.59	2.22	14	1
3:B:78:GLY:O	3:B:80:ALA:N	0.59	2.35	1	9
3:A:99:TRP:CH2	3:B:38:LEU:CD1	0.59	2.85	7	6
3:B:90:LYS:HE2	3:B:91:ALA:HB2	0.59	1.73	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:99:TRP:CD1	3:B:34:LEU:HD22	0.59	2.32	5	1
3:B:67:SER:CB	3:B:82:ILE:HD12	0.59	2.28	13	1
2:F:3:DT:C7	3:A:72:LYS:CE	0.59	2.81	5	7
2:F:3:DT:C7	3:A:79:ILE:CD1	0.59	2.81	8	5
3:A:67:SER:CB	3:A:82:ILE:HD13	0.59	2.28	15	4
3:A:34:LEU:O	3:A:35:HIS:CG	0.59	2.55	12	1
3:A:100:LEU:HD12	3:B:41:LEU:HD12	0.59	1.75	1	1
3:B:38:LEU:HA	3:B:41:LEU:CD2	0.59	2.28	1	5
3:B:21:ARG:O	3:B:25:LEU:HD13	0.59	1.98	7	3
3:A:58:VAL:CG2	3:B:42:MET:HE3	0.59	2.28	4	2
3:A:51:LEU:HD13	3:A:55:VAL:HG21	0.59	1.74	4	1
3:A:54:ARG:O	3:A:57:ILE:HD11	0.59	1.97	11	3
3:A:72:LYS:HG3	3:A:73:ASN:N	0.59	2.12	12	7
3:A:34:LEU:HD23	3:B:99:TRP:CH2	0.59	2.32	9	1
3:A:67:SER:HB2	3:A:82:ILE:HB	0.59	1.75	13	1
3:A:34:LEU:HA	3:B:96:LEU:HD23	0.59	1.74	14	2
2:F:3:DT:H73	3:A:72:LYS:HE3	0.59	1.74	5	2
3:B:42:MET:CA	4:B:109:TRP:CE3	0.59	2.86	8	6
1:E:15:DG:C2	1:E:16:DG:N3	0.59	2.71	3	1
3:A:55:VAL:CG2	3:B:42:MET:HE2	0.59	2.27	4	1
3:A:19:TRP:CH2	3:B:35:HIS:CE1	0.59	2.91	8	2
3:B:39:LEU:O	3:B:45:PRO:HA	0.59	1.98	6	1
3:A:81:THR:O	3:A:85:GLY:N	0.58	2.35	3	10
3:B:82:ILE:HG13	3:B:83:THR:N	0.58	2.13	12	5
3:B:78:GLY:HA2	3:B:81:THR:HG22	0.58	1.74	8	3
3:A:26:LEU:HA	3:A:34:LEU:HD11	0.58	1.73	9	2
3:B:43:LEU:CB	4:B:109:TRP:CD1	0.58	2.86	6	2
3:A:72:LYS:CB	3:A:82:ILE:HD13	0.58	2.28	7	2
3:A:72:LYS:HB3	3:A:82:ILE:HG21	0.58	1.73	8	1
3:A:41:LEU:C	3:A:41:LEU:HD12	0.58	2.23	15	1
1:E:17:DT:H2''	1:E:18:DA:O5'	0.58	1.97	10	4
3:A:34:LEU:CD1	3:A:34:LEU:N	0.58	2.66	8	2
3:B:96:LEU:HD12	3:B:96:LEU:N	0.58	2.13	10	6
3:A:56:ARG:CG	3:A:75:LEU:HD13	0.58	2.27	7	1
3:B:40:ASN:CA	3:B:45:PRO:HG2	0.58	2.27	10	2
3:A:87:ASN:CG	3:B:43:LEU:HD23	0.58	2.23	8	2
3:B:41:LEU:HD23	3:B:42:MET:HG2	0.58	1.73	11	1
3:A:53:THR:HG21	3:A:76:GLY:O	0.58	1.97	14	1
1:E:11:DT:O2	1:E:12:DA:N7	0.58	2.36	15	14
2:F:19:DC:H2''	2:F:20:DA:O5'	0.58	1.98	9	11
3:A:84:ARG:HG2	3:B:43:LEU:HD13	0.58	1.75	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:45:PRO:C	3:A:47:GLU:N	0.58	2.59	8	4
3:B:85:GLY:CA	4:B:201:TRP:CE2	0.58	2.87	3	1
3:A:85:GLY:O	3:A:88:SER:OG	0.58	2.21	8	4
3:B:92:ALA:HB1	3:B:94:VAL:HG22	0.58	1.74	8	1
3:A:38:LEU:HD12	3:B:99:TRP:CH2	0.58	2.33	12	2
3:A:25:LEU:O	3:A:35:HIS:CD2	0.58	2.56	13	1
3:B:81:THR:C	4:B:201:TRP:CZ2	0.58	2.81	13	9
3:A:25:LEU:CD2	3:B:103:VAL:HG21	0.58	2.29	14	2
3:B:22:PHE:O	3:B:26:LEU:HD23	0.58	1.98	8	6
3:B:44:THR:HB	4:B:109:TRP:HB3	0.58	1.75	8	1
2:F:4:DA:N3	2:F:5:DC:C4	0.58	2.72	9	2
3:A:37:PRO:CB	3:B:96:LEU:CD2	0.58	2.81	13	1
1:E:12:DA:H4'	4:B:109:TRP:OXT	0.58	1.97	14	1
2:F:4:DA:H2'	2:F:5:DC:C5	0.58	2.32	3	5
3:B:39:LEU:O	3:B:45:PRO:HB2	0.58	1.98	15	8
3:A:27:LYS:CG	3:A:28:ASN:N	0.58	2.66	6	5
3:B:85:GLY:HA3	4:B:201:TRP:CE2	0.58	2.34	3	1
3:B:42:MET:O	4:B:109:TRP:HA	0.58	1.99	8	1
3:B:72:LYS:HB2	3:B:82:ILE:CG1	0.58	2.28	9	2
3:B:71:LEU:HD23	3:B:74:GLU:HB2	0.58	1.74	10	2
2:F:3:DT:H2'	3:A:83:THR:CB	0.58	2.28	5	11
2:F:15:DA:H2''	2:F:16:DG:O5'	0.58	1.97	2	12
3:A:50:ALA:O	3:A:54:ARG:N	0.58	2.36	8	9
3:A:87:ASN:O	3:A:88:SER:C	0.58	2.44	13	10
3:B:67:SER:O	3:B:68:GLN:C	0.58	2.46	14	5
3:A:55:VAL:CG2	3:B:22:PHE:CE2	0.58	2.86	6	2
3:A:42:MET:HE2	3:B:58:VAL:CG2	0.58	2.28	12	2
3:A:68:GLN:H	3:A:72:LYS:HB3	0.58	1.58	14	1
2:F:4:DA:OP2	3:A:83:THR:C	0.58	2.46	5	11
2:F:5:DC:C4	2:F:6:DC:N4	0.58	2.72	10	12
2:F:7:DA:C4	2:F:8:DG:C8	0.58	2.92	1	13
3:A:82:ILE:HG13	3:A:83:THR:N	0.58	2.13	8	11
3:B:20:LEU:N	3:B:20:LEU:HD22	0.58	2.14	6	10
1:E:16:DG:C2	1:E:17:DT:C2	0.58	2.92	7	6
3:A:41:LEU:HD11	3:A:42:MET:SD	0.58	2.38	2	2
3:B:42:MET:SD	3:B:45:PRO:HB3	0.58	2.39	2	1
3:A:40:ASN:HA	3:B:91:ALA:HB1	0.58	1.73	3	1
3:A:43:LEU:C	4:B:201:TRP:CB	0.58	2.76	6	8
3:B:53:THR:O	3:B:57:ILE:N	0.58	2.35	5	1
3:A:91:ALA:HB2	3:B:40:ASN:O	0.58	1.98	7	2
3:A:43:LEU:CD1	3:B:53:THR:HB	0.58	2.29	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:51:LEU:HG	3:B:22:PHE:CD2	0.58	2.33	4	1
3:A:72:LYS:CE	3:A:82:ILE:HD11	0.58	2.28	5	1
3:A:42:MET:O	4:B:201:TRP:HA	0.58	1.98	8	1
3:A:55:VAL:HG21	3:B:26:LEU:HD21	0.58	1.74	8	1
3:B:100:LEU:HD22	3:B:100:LEU:C	0.58	2.24	10	1
3:A:58:VAL:CB	3:A:100:LEU:HD11	0.58	2.29	12	1
3:A:50:ALA:HB1	3:A:54:ARG:NH1	0.58	2.14	14	1
3:A:19:TRP:CZ3	3:B:51:LEU:CB	0.58	2.87	10	6
3:A:79:ILE:HA	3:A:82:ILE:HG12	0.58	1.76	1	9
3:A:38:LEU:HD23	3:A:38:LEU:C	0.58	2.23	11	8
3:B:72:LYS:O	3:B:78:GLY:N	0.58	2.37	7	4
3:A:65:GLU:C	3:A:66:MET:HE3	0.58	2.23	6	1
3:A:51:LEU:HD11	3:B:26:LEU:CG	0.58	2.28	7	1
3:A:43:LEU:CB	3:B:54:ARG:HB3	0.58	2.25	9	1
3:A:68:GLN:HA	3:A:72:LYS:HE2	0.58	1.75	11	1
3:A:60:GLU:CD	3:A:71:LEU:HD21	0.58	2.24	15	2
2:F:3:DT:H71	3:A:72:LYS:CD	0.58	2.29	1	2
3:A:75:LEU:N	3:A:75:LEU:CD1	0.58	2.67	2	2
3:A:51:LEU:CD2	3:B:19:TRP:CZ2	0.58	2.87	3	5
2:F:3:DT:H72	3:A:72:LYS:CD	0.58	2.29	6	6
2:F:14:DG:O6	3:B:80:ALA:HB1	0.58	1.99	5	3
3:B:22:PHE:O	3:B:25:LEU:N	0.58	2.37	7	2
3:B:22:PHE:CD1	3:B:26:LEU:CD2	0.58	2.87	7	3
3:A:39:LEU:C	3:A:45:PRO:HB2	0.58	2.24	8	1
3:A:100:LEU:HD12	3:B:41:LEU:HD13	0.58	1.74	11	1
3:A:53:THR:CG2	3:A:76:GLY:CA	0.58	2.82	13	2
1:E:10:DG:H2''	1:E:11:DT:O5'	0.57	1.98	4	12
2:F:4:DA:C2'	2:F:5:DC:C5	0.57	2.87	5	7
1:E:8:DG:H2''	1:E:9:DT:O5'	0.57	1.98	15	6
3:A:81:THR:O	3:A:84:ARG:N	0.57	2.36	3	6
3:B:27:LYS:HA	3:B:30:TYR:CG	0.57	2.34	8	9
3:B:78:GLY:HA2	3:B:81:THR:HB	0.57	1.76	14	4
3:A:27:LYS:O	3:A:31:GLN:CG	0.57	2.52	4	2
3:A:55:VAL:HG12	3:B:22:PHE:HE1	0.57	1.59	7	3
3:A:81:THR:OG1	4:B:109:TRP:NE1	0.57	2.37	4	2
3:A:54:ARG:HB3	3:B:42:MET:HE2	0.57	1.75	6	1
3:A:72:LYS:HD2	3:A:73:ASN:CB	0.57	2.29	15	2
3:A:38:LEU:HD12	3:B:100:LEU:HG	0.57	1.76	10	1
3:B:44:THR:O	3:B:44:THR:HG22	0.57	1.98	15	1
3:B:101:GLU:O	3:B:105:LEU:N	0.57	2.35	9	13
3:A:93:PRO:O	3:A:94:VAL:CG2	0.57	2.52	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:54:ARG:O	3:B:57:ILE:N	0.57	2.28	2	1
3:A:55:VAL:HB	3:B:22:PHE:HZ	0.57	1.59	6	1
3:B:26:LEU:CD2	3:B:38:LEU:HD11	0.57	2.28	11	1
2:F:7:DA:C2	2:F:8:DG:C8	0.57	2.92	7	13
2:F:13:DC:C2	2:F:14:DG:C8	0.57	2.92	13	12
3:A:27:LYS:HA	3:A:30:TYR:CB	0.57	2.28	6	6
3:A:38:LEU:HD23	3:A:42:MET:CB	0.57	2.29	1	1
3:A:55:VAL:CG2	3:B:22:PHE:HZ	0.57	2.12	5	7
3:A:62:LEU:HD13	3:A:104:LEU:HG	0.57	1.75	1	1
3:B:27:LYS:O	3:B:30:TYR:N	0.57	2.37	3	13
3:B:54:ARG:C	3:B:57:ILE:HG13	0.57	2.23	8	2
3:B:57:ILE:HD12	3:B:58:VAL:HG22	0.57	1.76	12	4
3:A:51:LEU:HB3	3:B:22:PHE:CE2	0.57	2.34	12	1
1:E:11:DT:C1'	1:E:12:DA:N7	0.57	2.67	14	12
3:A:91:ALA:HB3	3:B:40:ASN:HB3	0.57	1.77	1	1
3:B:95:GLU:CB	3:B:96:LEU:HD12	0.57	2.29	11	5
3:A:17:GLN:O	3:A:18:GLU:C	0.57	2.46	4	3
3:A:54:ARG:O	3:A:57:ILE:HG23	0.57	1.99	4	1
3:B:87:ASN:O	3:B:89:LEU:N	0.57	2.37	10	6
3:A:19:TRP:CZ3	3:B:51:LEU:HD12	0.57	2.34	14	3
3:A:41:LEU:HD13	3:A:41:LEU:O	0.57	1.98	12	3
3:A:57:ILE:HG21	3:A:81:THR:HB	0.57	1.76	7	3
1:E:15:DG:C5	3:A:79:ILE:HG22	0.57	2.34	15	2
3:A:21:ARG:CB	3:B:55:VAL:HG11	0.57	2.28	12	1
3:B:26:LEU:HB2	3:B:27:LYS:CE	0.57	2.29	14	1
2:F:3:DT:C7	3:A:72:LYS:HE3	0.57	2.29	1	2
2:F:3:DT:OP2	3:A:82:ILE:CD1	0.57	2.52	10	6
2:F:7:DA:C4	2:F:8:DG:N7	0.57	2.73	3	13
3:B:49:GLU:OE2	3:B:50:ALA:HB2	0.57	1.99	1	1
3:A:53:THR:HG23	3:A:76:GLY:CA	0.57	2.29	4	1
3:A:84:ARG:CB	3:B:43:LEU:HD13	0.57	2.29	5	1
3:B:82:ILE:CD1	3:B:83:THR:OG1	0.57	2.52	8	2
3:B:45:PRO:CG	4:B:109:TRP:OXT	0.57	2.52	15	1
3:B:72:LYS:CG	3:B:79:ILE:N	0.57	2.68	5	4
3:B:37:PRO:O	3:B:41:LEU:HB3	0.57	2.00	15	4
3:A:51:LEU:CG	3:A:55:VAL:HG21	0.57	2.30	12	1
3:B:26:LEU:HA	3:B:34:LEU:CD1	0.57	2.30	14	1
3:A:38:LEU:HD12	3:B:99:TRP:CZ3	0.57	2.33	1	4
3:A:84:ARG:O	3:A:87:ASN:CB	0.57	2.53	8	6
3:A:37:PRO:HG3	3:B:96:LEU:HD23	0.57	1.74	8	1
3:B:34:LEU:CD1	3:B:34:LEU:N	0.57	2.68	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:34:LEU:O	3:B:99:TRP:CZ3	0.57	2.57	10	1
3:B:106:LYS:O	3:B:106:LYS:HG3	0.57	1.99	11	1
2:F:4:DA:C2	2:F:5:DC:C2	0.57	2.93	15	7
3:B:99:TRP:CE3	3:B:100:LEU:N	0.57	2.72	11	8
3:B:102:GLU:HA	3:B:106:LYS:CB	0.57	2.29	6	1
3:B:43:LEU:O	3:B:45:PRO:HD2	0.57	2.00	15	1
1:E:5:DC:H6	1:E:5:DC:O5'	0.57	1.82	9	4
2:F:3:DT:C7	3:A:72:LYS:NZ	0.57	2.68	3	1
3:A:38:LEU:O	3:A:38:LEU:HD23	0.57	1.99	6	1
3:A:69:ARG:HA	3:A:72:LYS:HE2	0.57	1.76	7	2
3:B:45:PRO:HD3	4:B:109:TRP:C	0.57	2.25	1	2
3:A:80:ALA:C	3:A:83:THR:HG22	0.57	2.24	3	5
3:A:86:SER:O	3:A:89:LEU:HB2	0.57	2.00	7	4
3:A:72:LYS:CE	3:A:79:ILE:CG1	0.56	2.83	15	3
3:B:35:HIS:C	3:B:37:PRO:CD	0.56	2.77	9	7
2:F:2:DG:H2'	3:A:68:GLN:CD	0.56	2.25	2	1
3:B:81:THR:HG1	4:B:201:TRP:NE1	0.56	1.97	2	4
1:E:16:DG:N2	2:F:4:DA:C6	0.56	2.73	3	1
3:B:41:LEU:O	3:B:41:LEU:CD2	0.56	2.50	3	2
3:A:90:LYS:HE3	3:A:91:ALA:HB2	0.56	1.75	4	3
1:E:20:DA:O5'	1:E:20:DA:H8	0.56	1.83	8	3
3:B:95:GLU:HB3	3:B:96:LEU:HD12	0.56	1.76	6	2
3:A:39:LEU:HD21	3:A:48:ARG:HG3	0.56	1.76	7	1
3:B:22:PHE:CE1	3:B:26:LEU:HD23	0.56	2.35	9	2
3:B:57:ILE:HG21	3:B:81:THR:HB	0.56	1.77	9	2
1:E:6:DT:C2	1:E:7:DC:C5	0.56	2.94	2	9
2:F:1:DT:H2''	2:F:2:DG:O5'	0.56	2.00	2	6
2:F:15:DA:N6	3:B:80:ALA:HB1	0.56	2.10	10	4
3:A:34:LEU:HD12	3:B:99:TRP:HB3	0.56	1.76	2	1
3:A:41:LEU:CB	3:B:91:ALA:HB3	0.56	2.30	15	4
3:A:23:VAL:HA	3:A:26:LEU:HD21	0.56	1.76	3	1
3:A:44:THR:O	3:A:47:GLU:HG2	0.56	1.99	4	2
3:A:57:ILE:HG21	3:A:81:THR:HG22	0.56	1.76	4	1
3:A:60:GLU:CD	3:A:71:LEU:HD22	0.56	2.25	5	1
3:B:81:THR:O	3:B:85:GLY:N	0.56	2.37	9	1
3:B:42:MET:O	4:B:109:TRP:N	0.56	2.39	11	1
3:B:103:VAL:HG23	3:B:104:LEU:CD2	0.56	2.30	11	1
3:B:22:PHE:CE1	3:B:26:LEU:HD21	0.56	2.36	15	7
3:B:41:LEU:HD23	3:B:41:LEU:N	0.56	2.15	1	1
3:A:34:LEU:N	3:A:34:LEU:CD2	0.56	2.69	4	2
3:A:34:LEU:O	3:B:99:TRP:CE3	0.56	2.58	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:LEU:C	3:A:43:LEU:HD12	0.56	2.26	3	1
3:B:72:LYS:CG	3:B:79:ILE:HG12	0.56	2.29	11	8
3:A:41:LEU:HG	3:B:93:PRO:HB3	0.56	1.76	4	1
3:A:37:PRO:HB3	3:B:96:LEU:CD1	0.56	2.30	7	1
3:A:91:ALA:HB3	3:B:41:LEU:N	0.56	2.15	10	2
3:A:68:GLN:O	3:A:72:LYS:HG3	0.56	2.00	8	1
1:E:12:DA:H5''	3:B:44:THR:CG2	0.56	2.30	11	1
2:F:11:DC:H2''	2:F:12:DA:N7	0.56	2.15	15	1
3:B:51:LEU:C	3:B:51:LEU:HD22	0.56	2.24	15	1
2:F:12:DA:C2'	2:F:13:DC:C5	0.56	2.88	6	8
3:B:42:MET:C	3:B:45:PRO:HD3	0.56	2.26	3	6
3:A:60:GLU:O	3:A:64:GLY:N	0.56	2.39	6	6
3:B:30:TYR:CE1	3:B:35:HIS:CD2	0.56	2.93	7	2
3:B:71:LEU:HD22	3:B:74:GLU:HG2	0.56	1.77	9	1
3:A:74:GLU:CB	3:A:75:LEU:HD13	0.56	2.31	15	1
2:F:14:DG:C6	3:B:80:ALA:HB1	0.56	2.36	9	4
3:A:82:ILE:HG13	3:A:83:THR:H	0.56	1.60	8	8
3:B:49:GLU:CD	3:B:50:ALA:N	0.56	2.63	1	2
3:B:78:GLY:C	3:B:82:ILE:CG1	0.56	2.79	11	8
2:F:4:DA:C2	2:F:5:DC:N3	0.56	2.73	2	4
3:A:55:VAL:HG22	3:B:38:LEU:CD2	0.56	2.30	8	7
3:A:91:ALA:CB	3:B:41:LEU:N	0.56	2.68	10	2
2:F:14:DG:N2	2:F:15:DA:C2	0.56	2.74	8	1
3:B:23:VAL:HG12	3:B:27:LYS:HE2	0.56	1.78	13	1
3:A:37:PRO:C	3:A:41:LEU:HD23	0.56	2.25	1	1
3:A:40:ASN:HB2	3:B:91:ALA:HB1	0.56	1.77	2	3
3:A:41:LEU:N	3:B:91:ALA:CB	0.56	2.69	1	6
2:F:9:DT:H2''	2:F:10:DA:O5'	0.56	2.00	13	5
3:B:78:GLY:CA	3:B:81:THR:HG22	0.56	2.30	2	2
3:B:47:GLU:HB3	3:B:50:ALA:HB3	0.56	1.76	3	2
2:F:13:DC:OP1	3:A:43:LEU:HD12	0.56	2.00	9	2
3:A:51:LEU:CD1	3:A:55:VAL:HG11	0.56	2.31	4	1
2:F:2:DG:H2'	3:A:68:GLN:HA	0.56	1.76	7	1
1:E:14:DT:C6	3:A:77:ALA:HB2	0.56	2.36	13	1
3:A:93:PRO:C	3:A:94:VAL:HG13	0.56	2.25	13	1
1:E:16:DG:H2''	1:E:17:DT:C6	0.56	2.36	12	6
2:F:12:DA:O3'	3:A:44:THR:CG2	0.56	2.53	14	8
3:A:19:TRP:HA	3:B:51:LEU:HD11	0.56	1.76	2	1
3:B:44:THR:HB	4:B:109:TRP:CA	0.56	2.31	10	2
1:E:12:DA:H4'	4:B:109:TRP:O	0.56	2.01	4	2
2:F:8:DG:N2	2:F:9:DT:C2	0.56	2.73	12	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:37:PRO:CB	3:B:96:LEU:HB2	0.56	2.30	3	5
3:A:51:LEU:CB	3:B:19:TRP:CZ3	0.56	2.89	12	3
3:A:56:ARG:O	3:A:60:GLU:CG	0.56	2.53	5	2
3:A:70:GLU:O	3:A:74:GLU:N	0.56	2.39	6	1
3:B:72:LYS:HD3	3:B:82:ILE:CD1	0.56	2.31	7	5
3:A:41:LEU:C	3:A:41:LEU:HD13	0.56	2.26	10	1
3:A:62:LEU:HD13	3:A:104:LEU:CD2	0.56	2.31	12	1
3:B:42:MET:C	3:B:45:PRO:CD	0.56	2.79	13	2
3:B:54:ARG:HD2	4:B:201:TRP:C	0.56	2.25	2	1
3:A:40:ASN:C	3:A:42:MET:H	0.56	2.09	8	1
3:A:54:ARG:HG2	3:A:55:VAL:HG23	0.56	1.77	12	1
2:F:14:DG:C2	2:F:15:DA:C5	0.56	2.94	2	9
3:A:30:TYR:CD1	3:A:35:HIS:CG	0.56	2.94	15	5
3:A:92:ALA:HB2	3:B:40:ASN:CB	0.56	2.30	1	1
3:B:43:LEU:HB3	4:B:109:TRP:CD1	0.56	2.36	7	4
3:B:22:PHE:HA	3:B:25:LEU:HB2	0.56	1.77	14	1
2:F:13:DC:OP1	3:B:54:ARG:CZ	0.56	2.53	15	1
2:F:4:DA:H62	3:A:79:ILE:HG23	0.55	1.62	2	1
3:B:19:TRP:O	3:B:23:VAL:HG23	0.55	2.01	2	1
3:A:51:LEU:HG	3:B:19:TRP:CZ3	0.55	2.36	6	2
3:A:72:LYS:CB	3:A:82:ILE:HG21	0.55	2.31	4	4
3:A:81:THR:OG1	4:B:109:TRP:CD1	0.55	2.59	14	2
2:F:12:DA:O3'	3:B:54:ARG:NH2	0.55	2.39	5	1
3:B:47:GLU:O	3:B:49:GLU:CG	0.55	2.54	11	4
3:A:84:ARG:HD2	3:B:43:LEU:HD13	0.55	1.77	14	1
3:A:78:GLY:O	3:A:82:ILE:CG2	0.55	2.54	5	2
3:A:53:THR:HA	3:A:56:ARG:HG2	0.55	1.78	2	3
3:A:67:SER:O	3:A:68:GLN:CG	0.55	2.54	12	2
3:A:78:GLY:O	3:A:81:THR:N	0.55	2.40	15	6
3:A:57:ILE:HD13	3:A:58:VAL:H	0.55	1.60	8	1
1:E:18:DA:N3	1:E:19:DC:C2	0.55	2.74	10	1
1:E:8:DG:C6	2:F:14:DG:C2	0.55	2.94	4	10
2:F:11:DC:C2'	2:F:12:DA:C8	0.55	2.90	1	8
3:B:72:LYS:HD2	3:B:72:LYS:N	0.55	2.16	5	2
3:A:51:LEU:HB3	3:B:19:TRP:CZ3	0.55	2.37	13	8
3:B:42:MET:CB	4:B:109:TRP:CE3	0.55	2.89	2	7
3:A:30:TYR:CD1	3:A:35:HIS:HB3	0.55	2.36	4	1
3:B:106:LYS:O	3:B:106:LYS:CG	0.55	2.54	11	4
3:A:56:ARG:HG2	3:A:75:LEU:HD22	0.55	1.77	7	1
3:A:96:LEU:HB3	3:B:37:PRO:HG3	0.55	1.78	7	1
1:E:15:DG:H8	3:A:77:ALA:O	0.55	1.83	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:22:PHE:N	3:B:22:PHE:CD1	0.55	2.75	14	1
1:E:12:DA:C6	2:F:10:DA:C2	0.55	2.94	5	12
3:A:47:GLU:O	3:A:48:ARG:C	0.55	2.50	3	7
3:A:79:ILE:CA	3:A:82:ILE:CG1	0.55	2.84	13	6
3:A:87:ASN:HB3	3:B:43:LEU:HD23	0.55	1.77	9	6
3:B:42:MET:O	4:B:109:TRP:CE2	0.55	2.60	15	2
1:E:16:DG:N2	2:F:4:DA:N6	0.55	2.49	3	1
3:A:35:HIS:ND1	3:A:36:LEU:HG	0.55	2.17	6	1
3:A:35:HIS:CE1	3:A:36:LEU:HD21	0.55	2.36	10	1
1:E:14:DT:C5	3:A:77:ALA:HB2	0.55	2.36	13	1
3:B:50:ALA:O	3:B:54:ARG:N	0.55	2.35	7	3
3:A:27:LYS:HA	3:A:30:TYR:CG	0.55	2.37	6	2
3:B:68:GLN:CA	3:B:82:ILE:HD11	0.55	2.30	3	1
3:B:51:LEU:N	3:B:54:ARG:HD2	0.55	2.17	7	1
3:B:47:GLU:C	3:B:49:GLU:N	0.55	2.64	14	6
3:B:51:LEU:HA	3:B:54:ARG:HG2	0.55	1.79	9	2
3:A:100:LEU:HD12	3:B:41:LEU:HG	0.55	1.78	12	1
1:E:10:DG:C2	2:F:12:DA:C2	0.55	2.95	10	11
3:A:87:ASN:O	3:A:90:LYS:CB	0.55	2.54	1	10
3:B:39:LEU:O	3:B:45:PRO:HG2	0.55	2.00	1	1
3:B:57:ILE:CB	3:B:82:ILE:HG22	0.55	2.32	1	1
3:A:103:VAL:O	3:A:104:LEU:HD22	0.55	2.02	2	3
3:B:44:THR:HB	4:B:109:TRP:OXT	0.55	2.01	10	2
3:A:51:LEU:CG	3:B:22:PHE:CE1	0.55	2.88	8	2
3:A:34:LEU:C	3:A:34:LEU:CD2	0.55	2.72	9	1
3:A:47:GLU:HA	3:A:50:ALA:CB	0.55	2.32	12	7
3:B:73:ASN:HB2	3:B:79:ILE:HB	0.55	1.78	7	6
1:E:16:DG:C1'	1:E:17:DT:C7	0.55	2.85	3	1
3:A:38:LEU:HA	3:A:41:LEU:HD11	0.55	1.79	10	2
3:A:51:LEU:CD1	3:B:22:PHE:CE1	0.55	2.90	3	2
3:A:29:ALA:CB	3:A:34:LEU:CD1	0.55	2.81	6	1
3:B:43:LEU:HB2	4:B:109:TRP:CG	0.55	2.36	6	1
3:A:50:ALA:HB1	3:A:54:ARG:CZ	0.55	2.31	8	1
3:B:72:LYS:HG2	3:B:79:ILE:HD13	0.55	1.79	9	1
1:E:13:DC:P	4:B:109:TRP:O	0.55	2.64	11	1
3:A:72:LYS:C	3:A:78:GLY:HA3	0.55	2.27	13	1
3:A:30:TYR:CD1	3:A:35:HIS:CD2	0.55	2.95	15	1
2:F:6:DC:O2	2:F:7:DA:C8	0.55	2.60	15	12
3:B:39:LEU:O	3:B:39:LEU:CG	0.55	2.55	15	8
3:B:87:ASN:O	3:B:88:SER:C	0.55	2.48	10	8
1:E:19:DC:H2'	1:E:20:DA:N7	0.55	2.17	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:F:5:DC:C6	2:F:6:DC:C5	0.55	2.94	2	6
3:A:39:LEU:HD12	3:A:39:LEU:C	0.55	2.26	9	5
3:B:50:ALA:O	3:B:54:ARG:CG	0.55	2.55	2	2
1:E:18:DA:C6	2:F:4:DA:C2	0.55	2.95	11	5
2:F:3:DT:H73	3:A:79:ILE:HG23	0.55	1.77	3	1
3:A:50:ALA:C	3:A:54:ARG:CG	0.55	2.80	4	1
3:A:70:GLU:O	3:A:74:GLU:CG	0.55	2.54	6	1
3:A:30:TYR:CD1	3:B:23:VAL:HG22	0.55	2.36	8	3
3:B:72:LYS:CG	3:B:79:ILE:CD1	0.55	2.85	9	1
3:B:73:ASN:CB	3:B:79:ILE:HD11	0.55	2.31	9	1
2:F:5:DC:N3	2:F:6:DC:C4	0.55	2.75	11	6
2:F:9:DT:C4	2:F:10:DA:C6	0.55	2.94	8	7
3:A:57:ILE:HD12	3:A:58:VAL:CA	0.55	2.32	1	3
3:B:44:THR:CA	4:B:109:TRP:O	0.55	2.55	15	2
3:B:56:ARG:NH1	3:B:71:LEU:HD22	0.55	2.17	2	1
3:A:19:TRP:CE3	3:B:51:LEU:HG	0.55	2.36	9	6
3:A:66:MET:CB	3:A:71:LEU:HD22	0.55	2.32	4	1
3:B:103:VAL:O	3:B:104:LEU:HD23	0.55	2.01	4	1
2:F:4:DA:C5	2:F:5:DC:N4	0.55	2.75	9	3
3:A:89:LEU:HD21	3:A:97:ARG:CZ	0.55	2.32	2	1
3:A:73:ASN:HB2	3:A:79:ILE:CD1	0.55	2.32	4	3
3:A:80:ALA:HB1	3:A:84:ARG:NH1	0.55	2.17	7	1
3:A:68:GLN:CA	3:A:72:LYS:HG2	0.55	2.32	8	1
3:B:68:GLN:N	3:B:72:LYS:NZ	0.55	2.55	14	1
3:A:38:LEU:HD23	3:A:42:MET:HB3	0.54	1.77	1	1
3:B:100:LEU:C	3:B:100:LEU:HD23	0.54	2.27	1	1
3:B:85:GLY:CA	4:B:201:TRP:HH2	0.54	2.15	2	6
3:A:19:TRP:CD2	3:B:51:LEU:HD12	0.54	2.36	6	3
3:A:91:ALA:HB1	3:B:45:PRO:HB2	0.54	1.80	6	1
3:A:66:MET:HA	3:A:71:LEU:CB	0.54	2.32	9	1
3:B:72:LYS:HG2	3:B:79:ILE:CD1	0.54	2.32	9	1
3:A:72:LYS:CD	3:A:79:ILE:HG13	0.54	2.32	12	2
3:A:43:LEU:HB2	3:B:54:ARG:HD3	0.54	1.79	14	1
3:A:75:LEU:C	3:A:75:LEU:CD2	0.54	2.80	15	1
2:F:3:DT:C2'	2:F:4:DA:C8	0.54	2.91	9	4
3:A:78:GLY:HA2	3:A:81:THR:OG1	0.54	2.02	15	8
1:E:16:DG:C6	2:F:4:DA:C6	0.54	2.95	4	5
3:A:65:GLU:O	3:A:67:SER:N	0.54	2.41	4	2
3:A:88:SER:CA	3:B:41:LEU:O	0.54	2.56	10	3
3:B:79:ILE:HA	3:B:82:ILE:CG1	0.54	2.31	15	2
3:A:33:ASP:CA	3:A:36:LEU:HD12	0.54	2.32	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:34:LEU:O	3:A:36:LEU:HG	0.54	2.01	12	1
3:B:26:LEU:CB	3:B:27:LYS:HE2	0.54	2.32	14	1
1:E:4:DA:H2''	1:E:5:DC:O5'	0.54	2.03	2	15
2:F:3:DT:C2'	3:A:83:THR:CB	0.54	2.84	5	9
3:A:84:ARG:O	3:A:88:SER:N	0.54	2.40	14	8
3:A:43:LEU:C	3:A:43:LEU:HD22	0.54	2.26	2	1
3:B:39:LEU:HD23	3:B:40:ASN:CG	0.54	2.27	12	3
3:A:29:ALA:O	3:A:32:ASN:N	0.54	2.40	9	2
3:A:34:LEU:CD2	3:B:99:TRP:CZ3	0.54	2.87	6	1
3:A:96:LEU:HB3	3:B:37:PRO:CG	0.54	2.32	7	1
1:E:15:DG:C2	1:E:16:DG:C5	0.54	2.95	10	2
3:A:51:LEU:HD12	3:A:54:ARG:NE	0.54	2.17	13	1
1:E:11:DT:C2'	1:E:12:DA:N7	0.54	2.70	14	12
3:A:47:GLU:OE1	3:A:54:ARG:NH2	0.54	2.41	1	2
3:B:50:ALA:O	3:B:54:ARG:NE	0.54	2.40	9	5
3:B:51:LEU:C	3:B:51:LEU:CD1	0.54	2.80	4	10
2:F:5:DC:C5	2:F:6:DC:N4	0.54	2.75	2	2
3:A:36:LEU:O	3:A:40:ASN:ND2	0.54	2.40	5	3
3:B:95:GLU:HB2	3:B:96:LEU:HD12	0.54	1.79	12	3
3:A:54:ARG:CB	3:B:42:MET:HE2	0.54	2.33	6	1
3:A:55:VAL:O	3:A:58:VAL:N	0.54	2.35	10	2
3:A:54:ARG:CD	3:B:42:MET:CE	0.54	2.85	13	3
3:B:25:LEU:N	3:B:25:LEU:HD12	0.54	2.18	1	3
1:E:17:DT:N3	1:E:18:DA:N6	0.54	2.56	7	8
3:A:93:PRO:O	3:A:94:VAL:HG23	0.54	2.01	2	1
1:E:19:DC:H2''	1:E:20:DA:C8	0.54	2.37	6	8
3:A:48:ARG:HA	3:B:19:TRP:CZ3	0.54	2.38	10	9
3:A:93:PRO:C	3:A:94:VAL:HG22	0.54	2.28	12	4
3:A:39:LEU:HD11	3:A:48:ARG:N	0.54	2.18	14	1
3:B:35:HIS:CD2	3:B:36:LEU:HD21	0.54	2.38	14	1
3:B:51:LEU:HD13	3:B:51:LEU:O	0.54	2.03	7	8
1:E:15:DG:O5'	3:A:73:ASN:OD1	0.54	2.25	8	3
1:E:15:DG:N2	2:F:7:DA:C4	0.54	2.75	3	6
2:F:3:DT:H72	3:A:82:ILE:HD11	0.54	1.76	7	2
3:A:51:LEU:CD1	3:B:26:LEU:HD11	0.54	2.33	7	1
3:B:68:GLN:HA	3:B:72:LYS:CD	0.54	2.33	7	1
3:A:34:LEU:HD13	3:B:99:TRP:HB2	0.54	1.80	11	1
3:A:30:TYR:CG	3:B:23:VAL:CG1	0.54	2.91	5	7
3:A:84:ARG:CB	4:B:109:TRP:HZ2	0.54	2.15	11	5
3:A:73:ASN:CB	3:A:79:ILE:CD1	0.54	2.86	3	1
3:B:72:LYS:HE3	3:B:82:ILE:HG21	0.54	1.78	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:30:TYR:CD1	3:A:35:HIS:CB	0.54	2.90	4	4
3:B:41:LEU:HD23	3:B:42:MET:CA	0.54	2.32	6	1
3:A:44:THR:OG1	3:B:54:ARG:NH2	0.54	2.41	7	1
3:A:41:LEU:N	3:B:91:ALA:HB1	0.54	2.18	15	4
3:A:61:LEU:C	3:A:61:LEU:HD23	0.54	2.28	7	2
3:B:26:LEU:HD22	3:B:38:LEU:HD13	0.54	1.80	10	3
3:B:57:ILE:HD12	3:B:57:ILE:H	0.54	1.63	2	1
2:F:15:DA:OP2	3:B:73:ASN:ND2	0.54	2.40	3	2
3:B:58:VAL:HB	3:B:62:LEU:HD12	0.54	1.79	3	1
1:E:19:DC:O5'	1:E:19:DC:H6	0.54	1.85	12	2
3:A:40:ASN:O	3:A:42:MET:N	0.54	2.40	8	1
3:A:43:LEU:HB3	4:B:201:TRP:CE2	0.54	2.37	8	1
3:A:44:THR:H	4:B:201:TRP:CG	0.54	2.20	8	1
3:B:97:ARG:HH11	3:B:100:LEU:HD13	0.54	1.63	8	2
3:A:51:LEU:HG	3:A:55:VAL:HG21	0.54	1.78	12	1
3:A:72:LYS:HZ3	3:A:79:ILE:CG2	0.54	2.16	12	1
3:B:57:ILE:HA	3:B:82:ILE:CG2	0.54	2.26	14	1
3:A:47:GLU:O	3:A:50:ALA:N	0.54	2.41	5	10
3:A:20:LEU:N	3:A:20:LEU:CD2	0.54	2.71	15	7
3:A:45:PRO:HD2	3:A:46:ASP:H	0.54	1.62	12	5
3:A:39:LEU:HA	3:A:43:LEU:CD1	0.54	2.32	7	1
3:B:106:LYS:O	3:B:106:LYS:HG2	0.54	2.02	10	1
3:A:68:GLN:CG	3:A:68:GLN:O	0.54	2.56	12	1
3:A:43:LEU:HG	3:B:81:THR:HG21	0.54	1.79	14	1
1:E:11:DT:H2''	1:E:12:DA:C8	0.54	2.38	6	15
3:B:22:PHE:CE1	3:B:26:LEU:CD2	0.54	2.91	8	5
3:B:54:ARG:O	3:B:57:ILE:CG1	0.54	2.47	1	2
2:F:3:DT:H71	3:A:68:GLN:NE2	0.54	2.18	2	1
3:A:75:LEU:HD22	3:A:75:LEU:C	0.54	2.28	2	1
3:A:23:VAL:HG11	3:B:34:LEU:HD11	0.54	1.76	3	1
3:A:58:VAL:HG21	3:B:42:MET:HE3	0.54	1.80	3	1
3:A:96:LEU:HB2	3:B:37:PRO:CA	0.54	2.32	3	1
4:B:201:TRP:HA	4:B:201:TRP:CE3	0.54	2.37	6	3
1:E:17:DT:C2	1:E:18:DA:N6	0.54	2.76	4	4
3:A:55:VAL:HG13	3:B:38:LEU:HD21	0.54	1.80	6	1
3:A:72:LYS:CD	3:A:73:ASN:N	0.54	2.71	15	2
3:A:19:TRP:CH2	3:B:35:HIS:CD2	0.54	2.95	12	1
1:E:18:DA:N6	3:A:69:ARG:NH2	0.53	2.56	1	4
3:A:80:ALA:O	3:A:84:ARG:CB	0.53	2.56	1	9
3:B:38:LEU:O	3:B:41:LEU:CD2	0.53	2.56	1	2
3:B:78:GLY:C	3:B:82:ILE:CG2	0.53	2.81	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:33:ASP:C	3:A:34:LEU:HD22	0.53	2.28	4	1
2:F:14:DG:H3'	3:B:77:ALA:HB1	0.53	1.80	6	1
1:E:15:DG:H2''	1:E:16:DG:OP2	0.53	2.03	7	2
3:A:39:LEU:C	3:A:39:LEU:HD12	0.53	2.29	13	1
3:A:71:LEU:O	3:A:74:GLU:CG	0.53	2.57	13	1
3:B:27:LYS:CA	3:B:30:TYR:HB2	0.53	2.33	15	8
1:E:3:DT:H2''	1:E:4:DA:O5'	0.53	2.03	5	9
3:A:22:PHE:CD1	3:A:22:PHE:C	0.53	2.86	2	6
3:A:51:LEU:HD11	3:B:22:PHE:CD2	0.53	2.38	4	1
2:F:13:DC:C4	2:F:14:DG:C5	0.53	2.96	15	7
3:A:54:ARG:HG2	4:B:109:TRP:C	0.53	2.27	8	1
2:F:3:DT:OP2	3:A:67:SER:OG	0.53	2.26	13	1
3:A:25:LEU:C	3:A:35:HIS:NE2	0.53	2.66	13	1
2:F:12:DA:C2'	2:F:13:DC:C6	0.53	2.91	5	9
3:A:79:ILE:O	3:A:80:ALA:C	0.53	2.50	5	4
1:E:18:DA:C2'	1:E:19:DC:C6	0.53	2.90	11	7
3:A:73:ASN:HB3	3:A:79:ILE:CD1	0.53	2.33	3	3
3:A:81:THR:HG1	4:B:109:TRP:NE1	0.53	2.00	4	2
3:B:30:TYR:CE1	3:B:35:HIS:ND1	0.53	2.76	9	4
3:A:66:MET:HB2	3:A:71:LEU:HD13	0.53	1.79	7	1
3:B:50:ALA:HB1	3:B:54:ARG:NE	0.53	2.18	7	1
3:A:73:ASN:ND2	3:A:77:ALA:HA	0.53	2.18	8	2
3:B:79:ILE:C	3:B:81:THR:H	0.53	2.10	9	1
3:A:42:MET:HB3	3:B:54:ARG:CB	0.53	2.34	11	3
3:A:43:LEU:CA	3:B:54:ARG:HG3	0.53	2.34	2	1
3:A:100:LEU:HD23	3:A:100:LEU:O	0.53	2.04	5	2
2:F:15:DA:H2''	2:F:16:DG:C8	0.53	2.38	8	1
3:A:29:ALA:O	3:A:33:ASP:N	0.53	2.41	9	1
3:B:67:SER:O	3:B:68:GLN:CB	0.53	2.54	9	2
3:A:42:MET:SD	3:B:58:VAL:HG21	0.53	2.43	15	1
3:A:37:PRO:HG3	3:B:96:LEU:HB2	0.53	1.81	3	12
1:E:18:DA:N1	2:F:4:DA:C2	0.53	2.76	4	5
3:A:42:MET:N	4:B:201:TRP:HA	0.53	2.18	3	1
3:A:89:LEU:HA	3:A:92:ALA:O	0.53	2.03	7	6
3:A:42:MET:O	3:B:57:ILE:HG12	0.53	2.04	10	3
3:B:99:TRP:O	3:B:103:VAL:HG23	0.53	2.03	5	1
3:A:33:ASP:C	3:B:96:LEU:HD23	0.53	2.28	6	1
3:A:43:LEU:HG	3:B:50:ALA:O	0.53	2.03	9	1
3:A:30:TYR:CE1	3:A:35:HIS:CD2	0.53	2.97	15	1
4:B:109:TRP:O	4:B:109:TRP:CG	0.53	2.62	15	2
1:E:13:DC:C4	1:E:14:DT:C7	0.53	2.92	14	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:18:DA:H2'	1:E:19:DC:C5	0.53	2.38	12	5
3:A:27:LYS:O	3:A:30:TYR:HB2	0.53	2.04	3	1
3:B:81:THR:O	4:B:201:TRP:CE2	0.53	2.62	3	1
2:F:11:DC:C2	2:F:12:DA:C8	0.53	2.96	13	4
3:A:48:ARG:O	3:B:19:TRP:HZ3	0.53	1.87	13	4
3:B:38:LEU:HD23	3:B:42:MET:SD	0.53	2.44	5	1
2:F:4:DA:N6	3:A:79:ILE:CD1	0.53	2.71	15	3
3:A:53:THR:HG21	3:A:76:GLY:CA	0.53	2.34	13	1
3:B:23:VAL:C	3:B:27:LYS:HE3	0.53	2.28	14	1
2:F:18:DA:H2''	2:F:19:DC:O5'	0.53	2.02	8	15
3:A:51:LEU:HA	3:A:54:ARG:NE	0.53	2.19	1	3
3:A:72:LYS:CE	3:A:79:ILE:CG2	0.53	2.81	1	1
3:A:72:LYS:HG3	3:A:79:ILE:CG1	0.53	2.31	1	4
3:B:75:LEU:HD23	3:B:75:LEU:O	0.53	2.04	1	2
3:B:105:LEU:O	3:B:106:LYS:C	0.53	2.51	6	5
2:F:10:DA:C2'	2:F:11:DC:C6	0.53	2.91	11	5
1:E:12:DA:C2	1:E:13:DC:C2	0.53	2.97	11	3
3:A:106:LYS:O	3:A:106:LYS:HG3	0.53	2.03	6	1
1:E:13:DC:H3'	3:A:53:THR:HG21	0.53	1.79	12	1
1:E:7:DC:C2	1:E:8:DG:N7	0.53	2.77	2	13
1:E:8:DG:H2'	1:E:9:DT:C5	0.53	2.39	6	8
2:F:3:DT:H71	3:A:72:LYS:CE	0.53	2.33	1	2
2:F:16:DG:H2''	2:F:17:DT:O5'	0.53	2.03	14	11
3:A:43:LEU:O	3:B:54:ARG:CD	0.53	2.57	5	2
3:A:89:LEU:O	3:A:92:ALA:C	0.53	2.51	12	8
3:A:58:VAL:HG21	3:B:41:LEU:CG	0.53	2.33	15	3
1:E:14:DT:H6	3:A:77:ALA:HB1	0.53	1.62	3	5
2:F:3:DT:C2	2:F:4:DA:C8	0.53	2.97	3	1
3:A:56:ARG:HA	3:A:59:GLU:HG3	0.53	1.80	6	6
3:A:68:GLN:C	3:A:72:LYS:HG2	0.53	2.29	3	1
3:B:72:LYS:O	3:B:76:GLY:N	0.53	2.41	3	1
3:A:66:MET:HE2	3:A:71:LEU:CD2	0.53	2.34	4	1
3:A:99:TRP:HD1	3:B:34:LEU:HD22	0.53	1.62	5	1
3:A:91:ALA:CB	3:B:45:PRO:HB2	0.53	2.34	6	1
3:A:30:TYR:CE1	3:A:35:HIS:HB2	0.53	2.39	9	1
3:A:40:ASN:HA	3:A:45:PRO:HA	0.53	1.80	10	4
3:B:51:LEU:HA	3:B:54:ARG:HD3	0.53	1.80	11	1
3:A:34:LEU:O	3:A:35:HIS:CD2	0.53	2.62	12	1
3:B:71:LEU:HD13	3:B:71:LEU:O	0.53	2.04	13	1
3:A:19:TRP:NE1	3:B:35:HIS:CB	0.53	2.72	14	1
3:A:26:LEU:O	3:A:30:TYR:N	0.53	2.41	11	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:88:SER:HB3	3:B:41:LEU:CA	0.53	2.34	1	1
3:B:96:LEU:O	3:B:97:ARG:C	0.53	2.49	13	13
1:E:15:DG:P	3:A:73:ASN:O	0.53	2.67	2	2
1:E:18:DA:C2	2:F:4:DA:N3	0.53	2.76	3	1
2:F:2:DG:C3'	3:A:68:GLN:HG2	0.53	2.34	3	2
3:A:42:MET:O	3:B:54:ARG:HA	0.53	2.04	11	3
3:A:69:ARG:HA	3:A:72:LYS:CE	0.53	2.34	6	3
3:A:99:TRP:CE2	3:B:29:ALA:CB	0.53	2.92	11	4
3:B:38:LEU:HD23	3:B:41:LEU:HD13	0.53	1.80	6	2
3:A:38:LEU:C	3:A:38:LEU:CD2	0.53	2.82	8	3
3:A:55:VAL:HG12	3:A:59:GLU:HG3	0.53	1.81	14	1
2:F:13:DC:OP1	3:B:54:ARG:NH1	0.53	2.41	15	1
3:A:51:LEU:CD2	3:B:22:PHE:CZ	0.53	2.90	14	5
3:A:67:SER:HA	3:A:71:LEU:HB3	0.53	1.80	3	2
3:B:58:VAL:HG23	3:B:59:GLU:N	0.53	2.18	4	5
3:A:45:PRO:HG3	4:B:201:TRP:C	0.53	2.29	7	3
3:A:55:VAL:HG11	3:B:22:PHE:CE1	0.53	2.39	4	2
2:F:3:DT:C3'	3:A:83:THR:OG1	0.53	2.57	13	2
3:A:38:LEU:HD12	3:B:100:LEU:CG	0.53	2.34	10	1
1:E:5:DC:H2''	1:E:6:DT:O5'	0.52	2.04	2	13
2:F:14:DG:H2''	2:F:15:DA:O5'	0.52	2.04	15	8
3:B:54:ARG:O	3:B:55:VAL:C	0.52	2.52	2	1
3:B:57:ILE:HD12	3:B:57:ILE:N	0.52	2.19	2	2
2:F:10:DA:C2	2:F:11:DC:C2	0.52	2.97	4	6
3:A:51:LEU:O	3:A:51:LEU:HD12	0.52	2.04	4	1
3:A:87:ASN:CB	3:B:43:LEU:HD12	0.52	2.34	5	1
3:B:30:TYR:CZ	3:B:35:HIS:CE1	0.52	2.97	5	2
3:A:43:LEU:HG	3:B:53:THR:HG23	0.52	1.80	9	1
3:A:42:MET:HB2	3:B:54:ARG:HG2	0.52	1.80	10	1
3:B:26:LEU:N	3:B:27:LYS:HE2	0.52	2.19	14	1
1:E:13:DC:C5	1:E:14:DT:C7	0.52	2.92	12	11
2:F:2:DG:C6	3:A:69:ARG:NH2	0.52	2.76	1	1
2:F:3:DT:C2	2:F:4:DA:C6	0.52	2.97	1	3
2:F:5:DC:C5	2:F:6:DC:C4	0.52	2.97	2	3
3:A:81:THR:CA	4:B:109:TRP:CZ2	0.52	2.92	9	8
3:A:85:GLY:HA2	4:B:109:TRP:CH2	0.52	2.40	6	4
3:B:93:PRO:O	3:B:97:ARG:CA	0.52	2.57	13	2
3:B:85:GLY:CA	4:B:201:TRP:CZ2	0.52	2.92	3	1
4:B:201:TRP:CE3	4:B:201:TRP:CA	0.52	2.92	7	3
3:B:40:ASN:CA	3:B:45:PRO:HB3	0.52	2.29	6	1
3:B:51:LEU:CA	3:B:54:ARG:HD2	0.52	2.34	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:LEU:CG	3:B:103:VAL:HG21	0.52	2.33	14	1
1:E:11:DT:O2	1:E:12:DA:N6	0.52	2.43	8	5
2:F:8:DG:C2	2:F:9:DT:C2	0.52	2.98	1	7
3:A:25:LEU:O	3:B:99:TRP:CZ2	0.52	2.63	3	10
3:B:27:LYS:C	3:B:29:ALA:H	0.52	2.12	5	11
3:B:72:LYS:O	3:B:77:ALA:C	0.52	2.52	2	1
3:B:73:ASN:HB2	3:B:79:ILE:HG13	0.52	1.80	3	1
3:A:35:HIS:NE2	3:B:20:LEU:HD11	0.52	2.19	4	1
3:A:35:HIS:O	3:A:39:LEU:CB	0.52	2.57	9	1
1:E:10:DG:C2	2:F:12:DA:N3	0.52	2.78	11	2
3:A:71:LEU:C	3:A:71:LEU:HD13	0.52	2.29	13	1
2:F:3:DT:O4	3:A:69:ARG:NH1	0.52	2.42	14	1
3:A:42:MET:O	3:A:43:LEU:HB2	0.52	2.05	14	1
3:B:73:ASN:CG	3:B:79:ILE:HD12	0.52	2.28	15	1
3:A:85:GLY:CA	4:B:109:TRP:CH2	0.52	2.93	4	5
3:B:44:THR:HB	4:B:109:TRP:C	0.52	2.30	2	2
3:B:54:ARG:O	3:B:56:ARG:N	0.52	2.42	2	1
3:B:38:LEU:HD23	3:B:42:MET:CE	0.52	2.31	3	1
3:A:88:SER:HB3	3:B:41:LEU:O	0.52	2.04	11	3
1:E:15:DG:N3	1:E:16:DG:C6	0.52	2.77	7	1
3:A:45:PRO:HD3	4:B:201:TRP:N	0.52	2.19	7	2
3:A:80:ALA:O	3:A:84:ARG:HG3	0.52	2.05	10	3
3:A:65:GLU:C	3:A:67:SER:H	0.52	2.11	9	1
2:F:4:DA:P	3:A:83:THR:OG1	0.52	2.68	10	11
2:F:4:DA:C2	2:F:5:DC:C4	0.52	2.98	13	3
3:B:27:LYS:O	3:B:29:ALA:N	0.52	2.43	6	11
2:F:10:DA:H2''	2:F:11:DC:O5'	0.52	2.04	4	10
3:A:96:LEU:O	3:A:97:ARG:C	0.52	2.53	15	6
3:A:22:PHE:CD2	3:B:51:LEU:HD21	0.52	2.40	5	2
3:A:30:TYR:CE1	3:A:35:HIS:HB3	0.52	2.40	6	1
3:B:43:LEU:HB3	4:B:109:TRP:CG	0.52	2.40	7	2
3:A:56:ARG:CD	3:A:60:GLU:HG3	0.52	2.34	7	1
1:E:12:DA:H2''	1:E:13:DC:O5'	0.52	2.04	11	2
2:F:4:DA:H2''	2:F:5:DC:C5	0.52	2.40	12	2
2:F:7:DA:N1	2:F:8:DG:C5	0.52	2.78	6	13
3:A:34:LEU:N	3:A:34:LEU:HD12	0.52	2.20	8	3
3:B:80:ALA:O	3:B:84:ARG:HB2	0.52	2.04	6	5
1:E:12:DA:O3'	4:B:109:TRP:C	0.52	2.53	2	1
3:A:83:THR:HG23	3:A:84:ARG:N	0.52	2.19	7	12
2:F:3:DT:H72	3:A:72:LYS:CE	0.52	2.34	3	1
3:A:70:GLU:OE2	3:A:71:LEU:HD23	0.52	2.05	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:67:SER:OG	3:A:82:ILE:HD13	0.52	2.04	4	1
3:A:84:ARG:HD2	3:B:43:LEU:HG	0.52	1.80	10	2
3:A:95:GLU:HG3	3:A:96:LEU:HG	0.52	1.81	4	1
3:A:96:LEU:CD2	3:B:37:PRO:O	0.52	2.58	4	1
1:E:2:DG:H2'	1:E:3:DT:C6	0.52	2.40	7	3
2:F:13:DC:N4	2:F:14:DG:C6	0.52	2.78	15	3
3:A:85:GLY:HA2	3:A:88:SER:HB3	0.52	1.82	5	1
1:E:8:DG:C6	2:F:14:DG:N2	0.52	2.78	6	1
3:A:43:LEU:CD1	3:B:50:ALA:HA	0.52	2.35	14	3
3:B:85:GLY:N	4:B:201:TRP:CH2	0.52	2.78	13	4
3:A:57:ILE:HG12	4:B:109:TRP:CH2	0.52	2.39	10	3
3:A:40:ASN:C	3:A:42:MET:N	0.52	2.67	8	1
3:A:66:MET:HG3	3:A:71:LEU:HD13	0.52	1.81	14	1
1:E:10:DG:N2	2:F:12:DA:C6	0.52	2.78	15	1
1:E:14:DT:O5'	3:A:77:ALA:HB2	0.52	2.05	3	6
4:B:201:TRP:CD1	4:B:201:TRP:C	0.52	2.87	1	1
3:A:85:GLY:CA	4:B:109:TRP:HH2	0.52	2.17	4	5
3:A:41:LEU:CD2	3:B:58:VAL:HG12	0.52	2.29	4	2
2:F:4:DA:C5	2:F:5:DC:C4	0.52	2.98	6	3
1:E:12:DA:C5'	3:B:44:THR:CG2	0.52	2.85	7	1
3:A:55:VAL:HB	3:B:22:PHE:CE1	0.52	2.40	7	1
1:E:16:DG:N9	1:E:17:DT:H72	0.52	2.18	10	1
3:A:27:LYS:HA	3:A:30:TYR:CD2	0.52	2.40	10	1
1:E:16:DG:H2'	1:E:17:DT:C5	0.52	2.40	11	3
2:F:8:DG:C4	2:F:9:DT:H72	0.52	2.40	11	1
3:A:21:ARG:HB3	3:B:55:VAL:HG11	0.52	1.81	12	1
3:A:34:LEU:HB2	3:B:96:LEU:HD23	0.52	1.80	12	1
3:A:42:MET:CG	3:B:54:ARG:O	0.52	2.58	14	2
3:A:35:HIS:CE1	3:A:39:LEU:CB	0.52	2.93	14	1
3:B:24:ASP:CA	3:B:27:LYS:HE3	0.52	2.34	14	1
1:E:1:DT:H2''	1:E:2:DG:O5'	0.52	2.05	2	4
3:B:79:ILE:O	3:B:83:THR:HG22	0.52	2.05	3	4
1:E:19:DC:C2'	1:E:20:DA:C8	0.52	2.93	12	10
3:A:40:ASN:OD1	3:B:91:ALA:HA	0.52	2.05	5	1
3:A:85:GLY:HA2	4:B:109:TRP:HH2	0.52	1.63	14	2
2:F:2:DG:P	3:A:68:GLN:NE2	0.52	2.83	8	1
3:B:30:TYR:CD1	3:B:35:HIS:CG	0.52	2.98	15	3
3:B:62:LEU:HD22	3:B:101:GLU:OE2	0.52	2.04	10	1
3:A:72:LYS:HG3	3:A:79:ILE:HG13	0.52	1.80	12	2
3:A:49:GLU:O	3:A:53:THR:OG1	0.52	2.27	13	1
3:B:27:LYS:O	3:B:31:GLN:HG2	0.52	2.04	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:88:SER:CB	3:B:41:LEU:C	0.52	2.80	15	2
3:B:46:ASP:C	3:B:48:ARG:H	0.52	2.13	4	6
3:A:84:ARG:CB	4:B:109:TRP:CZ2	0.52	2.92	7	6
3:B:85:GLY:HA2	4:B:201:TRP:CH2	0.52	2.39	13	7
3:A:40:ASN:HA	3:A:45:PRO:CB	0.52	2.34	14	3
2:F:4:DA:C8	3:A:83:THR:OG1	0.52	2.63	9	4
3:B:99:TRP:C	3:B:99:TRP:CD2	0.52	2.87	6	2
3:A:84:ARG:HA	3:A:87:ASN:HB3	0.52	1.81	7	1
3:B:99:TRP:CD2	3:B:100:LEU:N	0.52	2.78	10	1
3:A:60:GLU:OE1	3:A:71:LEU:HD21	0.52	2.05	11	1
3:A:99:TRP:HD1	3:B:34:LEU:HD13	0.52	1.65	1	1
2:F:12:DA:H5'	3:A:47:GLU:OE2	0.52	2.05	5	1
1:E:15:DG:C8	3:A:73:ASN:OD1	0.52	2.63	8	1
3:A:54:ARG:HG3	4:B:109:TRP:HB2	0.52	1.81	15	1
3:B:75:LEU:HD23	3:B:75:LEU:N	0.52	2.20	15	1
2:F:13:DC:O5'	2:F:13:DC:C6	0.51	2.62	6	5
3:A:26:LEU:HD13	3:A:30:TYR:CE2	0.51	2.39	3	1
3:A:51:LEU:HD12	3:A:55:VAL:HB	0.51	1.80	4	1
3:A:34:LEU:O	3:A:34:LEU:CD2	0.51	2.46	6	1
3:A:53:THR:O	3:A:57:ILE:CG2	0.51	2.57	10	3
3:B:30:TYR:CE1	3:B:35:HIS:HB2	0.51	2.40	13	5
3:A:89:LEU:HD13	3:A:93:PRO:O	0.51	2.05	7	1
3:A:42:MET:HB3	4:B:201:TRP:HA	0.51	1.80	8	1
3:B:54:ARG:HG2	4:B:201:TRP:N	0.51	2.20	8	1
3:A:36:LEU:N	3:A:36:LEU:CD2	0.51	2.71	10	1
3:A:22:PHE:O	3:A:26:LEU:HG	0.51	2.05	14	1
3:A:64:GLY:O	3:A:65:GLU:HB2	0.51	2.06	14	1
3:B:81:THR:HG23	4:B:201:TRP:CE2	0.51	2.40	15	1
1:E:6:DT:C2	1:E:7:DC:C6	0.51	2.98	4	6
3:A:68:GLN:O	3:A:69:ARG:HG2	0.51	2.05	2	1
1:E:15:DG:C2	1:E:16:DG:C2	0.51	2.98	3	1
2:F:14:DG:N7	3:B:80:ALA:CB	0.51	2.74	8	3
1:E:12:DA:H5'	3:B:44:THR:OG1	0.51	2.05	4	1
3:A:55:VAL:HG21	3:B:22:PHE:HE2	0.51	1.62	6	2
3:A:55:VAL:HG11	3:B:22:PHE:CD1	0.51	2.40	7	2
1:E:16:DG:C2	1:E:17:DT:N3	0.51	2.78	10	1
3:A:26:LEU:HD13	3:A:35:HIS:ND1	0.51	2.20	11	1
3:B:72:LYS:HG3	3:B:79:ILE:HG12	0.51	1.82	11	2
1:E:10:DG:C2	2:F:12:DA:C6	0.51	2.98	15	1
3:B:78:GLY:O	3:B:82:ILE:CG2	0.51	2.58	15	1
1:E:17:DT:C2'	1:E:18:DA:C8	0.51	2.93	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:F:4:DA:P	3:A:83:THR:HG1	0.51	2.28	13	8
3:A:58:VAL:HG11	3:B:41:LEU:CG	0.51	2.36	1	1
1:E:15:DG:C6	1:E:16:DG:C6	0.51	2.98	3	1
3:B:85:GLY:N	4:B:201:TRP:CE2	0.51	2.79	3	1
4:B:201:TRP:HA	4:B:201:TRP:HE3	0.51	1.65	6	3
3:A:96:LEU:CD2	3:B:41:LEU:HB2	0.51	2.34	4	1
3:B:82:ILE:HD12	3:B:83:THR:N	0.51	2.20	4	6
1:E:16:DG:C4	1:E:17:DT:C4	0.51	2.99	6	2
3:A:30:TYR:CD2	3:B:27:LYS:HB3	0.51	2.39	15	3
3:A:42:MET:HE1	3:B:100:LEU:HD21	0.51	1.82	7	1
2:F:3:DT:C4	3:A:79:ILE:CD1	0.51	2.94	15	3
2:F:4:DA:N6	3:A:79:ILE:CG2	0.51	2.73	9	1
3:B:29:ALA:CB	3:B:34:LEU:HB3	0.51	2.33	13	3
3:B:42:MET:HB2	4:B:109:TRP:CE3	0.51	2.41	15	2
3:A:51:LEU:HD23	3:B:22:PHE:CG	0.51	2.41	12	1
3:B:26:LEU:O	3:B:34:LEU:CD2	0.51	2.48	14	1
3:A:40:ASN:HB3	3:B:91:ALA:CB	0.51	2.34	10	5
3:A:50:ALA:O	3:A:54:ARG:CG	0.51	2.57	4	2
1:E:13:DC:C4	1:E:14:DT:C4	0.51	2.98	3	1
3:A:34:LEU:HB3	3:B:99:TRP:CG	0.51	2.41	3	3
3:B:81:THR:HA	4:B:201:TRP:CD1	0.51	2.41	3	1
3:B:53:THR:O	3:B:54:ARG:C	0.51	2.54	14	2
3:A:42:MET:HG3	3:B:54:ARG:C	0.51	2.31	6	1
3:A:96:LEU:HB3	3:B:37:PRO:HB3	0.51	1.82	6	2
3:B:34:LEU:N	3:B:34:LEU:CD2	0.51	2.73	7	1
2:F:18:DA:H2'	2:F:19:DC:C5	0.51	2.40	11	4
3:B:82:ILE:HD11	3:B:83:THR:OG1	0.51	2.05	8	1
2:F:9:DT:C2'	2:F:10:DA:C8	0.51	2.94	11	1
3:A:26:LEU:HD13	3:A:35:HIS:CG	0.51	2.39	13	1
1:E:8:DG:N1	2:F:14:DG:C2	0.51	2.79	13	12
1:E:9:DT:H6	1:E:9:DT:O5'	0.51	1.89	9	5
1:E:10:DG:C2	1:E:11:DT:C2	0.51	2.99	15	4
3:A:43:LEU:CA	3:B:54:ARG:HD2	0.51	2.36	1	1
3:A:47:GLU:OE2	3:A:47:GLU:C	0.51	2.53	1	1
3:A:55:VAL:HA	3:A:58:VAL:CG2	0.51	2.36	1	2
3:A:43:LEU:CB	3:B:54:ARG:CG	0.51	2.88	12	2
2:F:19:DC:H2'	2:F:20:DA:C8	0.51	2.41	8	1
2:F:4:DA:C4	2:F:5:DC:N4	0.51	2.78	9	2
3:A:68:GLN:O	3:A:69:ARG:HB2	0.51	2.04	12	3
3:A:92:ALA:CB	3:A:96:LEU:HB2	0.51	2.36	13	5
1:E:14:DT:C6	3:A:77:ALA:HB1	0.51	2.40	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:66:MET:HB3	3:A:71:LEU:HD22	0.51	1.81	4	1
1:E:5:DC:H2'	1:E:6:DT:C6	0.51	2.40	6	1
3:A:23:VAL:HG22	3:B:35:HIS:HD2	0.51	1.65	7	1
3:B:70:GLU:O	3:B:71:LEU:CG	0.51	2.58	8	1
1:E:18:DA:C2	1:E:19:DC:C2	0.51	2.98	10	1
2:F:3:DT:H71	3:A:72:LYS:HD3	0.51	1.82	11	2
3:B:24:ASP:N	3:B:27:LYS:HE3	0.51	2.19	14	1
3:B:62:LEU:HD21	3:B:97:ARG:NH1	0.51	2.20	15	1
3:A:23:VAL:HG11	3:B:35:HIS:CD2	0.51	2.41	1	1
3:B:93:PRO:C	3:B:97:ARG:HB2	0.51	2.30	14	5
1:E:16:DG:C2'	1:E:17:DT:C5	0.51	2.94	11	4
2:F:11:DC:C2	2:F:12:DA:N7	0.51	2.79	4	9
3:A:66:MET:O	3:A:67:SER:C	0.51	2.54	12	2
1:E:13:DC:OP2	4:B:109:TRP:OXT	0.51	2.29	6	1
2:F:3:DT:N3	2:F:4:DA:N6	0.51	2.59	6	5
3:A:45:PRO:C	3:A:47:GLU:H	0.51	2.13	8	1
3:A:72:LYS:HD2	3:A:73:ASN:ND2	0.51	2.21	8	1
3:A:26:LEU:HD22	3:A:34:LEU:HD21	0.51	1.82	9	1
3:A:86:SER:O	3:A:89:LEU:HD13	0.51	2.06	9	2
3:A:35:HIS:N	3:A:35:HIS:CD2	0.51	2.78	10	1
3:B:67:SER:OG	3:B:68:GLN:N	0.51	2.44	12	1
3:A:68:GLN:HA	3:A:72:LYS:HD3	0.51	1.82	14	1
2:F:12:DA:O5'	2:F:12:DA:C8	0.51	2.64	15	4
3:A:80:ALA:O	3:A:84:ARG:CG	0.51	2.59	1	4
3:A:81:THR:HG22	4:B:109:TRP:CE3	0.51	2.41	2	8
3:A:50:ALA:C	3:A:54:ARG:HD2	0.51	2.31	2	1
3:A:81:THR:C	4:B:109:TRP:CZ2	0.51	2.88	11	9
3:B:94:VAL:HA	3:B:97:ARG:CB	0.51	2.35	13	6
1:E:12:DA:O3'	4:B:109:TRP:O	0.51	2.29	4	3
3:A:36:LEU:O	3:A:40:ASN:CB	0.51	2.59	9	3
3:B:67:SER:O	3:B:69:ARG:N	0.51	2.43	5	2
3:B:71:LEU:C	3:B:71:LEU:CD2	0.51	2.84	5	1
1:E:8:DG:C2	2:F:14:DG:C2	0.51	2.99	9	3
2:F:8:DG:C2	2:F:9:DT:C4	0.51	2.98	11	1
3:A:22:PHE:CD1	3:B:51:LEU:HD21	0.51	2.40	12	2
3:A:41:LEU:H	3:A:41:LEU:CD1	0.51	2.18	11	1
3:B:29:ALA:O	3:B:34:LEU:C	0.51	2.53	11	1
3:A:34:LEU:O	3:A:36:LEU:N	0.51	2.44	12	1
3:A:35:HIS:CD2	3:B:99:TRP:CH2	0.51	2.98	13	1
3:B:26:LEU:HB2	3:B:27:LYS:HE2	0.51	1.80	14	1
3:A:24:ASP:O	3:A:27:LYS:HG3	0.51	2.05	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:F:18:DA:H2''	2:F:19:DC:C6	0.51	2.40	11	14
3:A:30:TYR:CD1	3:B:23:VAL:CG1	0.51	2.93	9	4
3:A:51:LEU:HB3	3:B:19:TRP:CH2	0.51	2.41	3	7
2:F:5:DC:C2'	2:F:6:DC:C6	0.51	2.94	7	4
2:F:4:DA:N7	2:F:5:DC:N4	0.51	2.59	3	2
3:B:80:ALA:O	3:B:84:ARG:N	0.51	2.44	3	1
3:B:81:THR:C	4:B:201:TRP:CE2	0.51	2.88	3	1
3:B:96:LEU:N	3:B:96:LEU:HD12	0.51	2.21	3	2
3:A:45:PRO:CG	4:B:201:TRP:C	0.51	2.83	4	6
2:F:13:DC:C4	2:F:14:DG:C6	0.51	2.99	6	2
3:A:70:GLU:O	3:A:74:GLU:HG2	0.51	2.06	6	1
2:F:4:DA:H62	3:A:79:ILE:CD1	0.51	2.18	15	3
2:F:13:DC:OP1	3:A:44:THR:HA	0.51	2.05	11	1
3:A:43:LEU:HB3	3:B:54:ARG:HD2	0.51	1.83	11	1
3:B:26:LEU:HD13	3:B:38:LEU:HD22	0.51	1.83	12	1
3:B:77:ALA:O	3:B:81:THR:HB	0.51	2.05	15	2
1:E:19:DC:H2''	1:E:20:DA:O5'	0.51	2.05	9	7
2:F:17:DT:H2''	2:F:18:DA:O5'	0.51	2.06	7	11
3:A:62:LEU:HD21	3:A:101:GLU:OE1	0.51	2.06	1	1
1:E:12:DA:N1	2:F:10:DA:C2	0.51	2.79	6	4
3:A:96:LEU:HD23	3:B:37:PRO:CA	0.51	2.36	15	2
3:A:55:VAL:HA	3:B:42:MET:HE2	0.51	1.82	4	1
3:B:70:GLU:C	3:B:71:LEU:HD23	0.51	2.31	7	1
3:B:37:PRO:O	3:B:41:LEU:HB2	0.51	2.05	13	2
3:B:57:ILE:HG22	3:B:78:GLY:HA2	0.51	1.83	14	2
3:A:96:LEU:HD22	3:B:36:LEU:HB2	0.51	1.83	14	1
3:A:90:LYS:CG	3:A:91:ALA:H	0.50	2.17	1	2
3:B:54:ARG:HD2	4:B:201:TRP:O	0.50	2.05	2	1
3:A:43:LEU:HG	3:A:44:THR:N	0.50	2.21	3	1
3:A:35:HIS:CD2	3:A:36:LEU:HG	0.50	2.40	8	2
3:A:99:TRP:CZ3	3:B:38:LEU:HD12	0.50	2.41	5	1
3:A:96:LEU:HD23	3:B:37:PRO:HB3	0.50	1.83	7	1
2:F:16:DG:C2'	2:F:17:DT:C6	0.50	2.95	8	1
3:A:29:ALA:HB1	3:A:34:LEU:HB2	0.50	1.82	13	3
3:A:66:MET:HA	3:A:71:LEU:HB3	0.50	1.83	9	1
3:A:18:GLU:O	3:B:55:VAL:HG21	0.50	2.06	12	1
1:E:13:DC:P	4:B:109:TRP:CB	0.50	2.99	13	2
3:B:19:TRP:O	3:B:19:TRP:CG	0.50	2.65	14	1
1:E:11:DT:O2	1:E:12:DA:C5	0.50	2.63	10	14
3:A:45:PRO:O	3:A:48:ARG:HB3	0.50	2.06	10	2
3:B:81:THR:OG1	4:B:201:TRP:NE1	0.50	2.43	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:12:DA:C4'	3:B:44:THR:HG21	0.50	2.36	4	5
3:B:22:PHE:HD1	3:B:22:PHE:O	0.50	1.89	10	2
3:B:42:MET:C	4:B:109:TRP:CE3	0.50	2.90	8	3
1:E:15:DG:C6	3:A:79:ILE:HG22	0.50	2.41	8	2
3:B:22:PHE:O	3:B:26:LEU:HB2	0.50	2.05	8	1
3:B:53:THR:CG2	3:B:77:ALA:HB3	0.50	2.36	11	1
3:A:30:TYR:CE1	3:A:35:HIS:ND1	0.50	2.80	14	1
3:A:37:PRO:O	3:A:41:LEU:CD2	0.50	2.60	1	1
3:A:88:SER:OG	3:B:43:LEU:N	0.50	2.34	4	2
3:B:54:ARG:CG	3:B:55:VAL:N	0.50	2.74	1	3
3:B:57:ILE:C	3:B:57:ILE:CD1	0.50	2.82	13	2
3:A:27:LYS:C	3:A:30:TYR:HB2	0.50	2.32	15	4
3:A:90:LYS:CE	3:B:43:LEU:O	0.50	2.60	2	1
3:B:39:LEU:C	3:B:39:LEU:HD23	0.50	2.31	2	1
3:A:41:LEU:HD12	3:A:41:LEU:N	0.50	2.21	3	1
2:F:14:DG:N2	2:F:15:DA:C4	0.50	2.79	4	2
3:A:41:LEU:CD2	3:B:58:VAL:CG1	0.50	2.90	4	2
3:B:102:GLU:N	3:B:106:LYS:HB3	0.50	2.20	7	3
3:B:98:GLN:O	3:B:101:GLU:HG2	0.50	2.07	6	1
3:A:96:LEU:O	3:A:100:LEU:N	0.50	2.42	8	1
3:B:51:LEU:CA	3:B:54:ARG:HB2	0.50	2.37	8	1
3:A:36:LEU:CA	3:A:39:LEU:HD23	0.50	2.25	10	1
3:A:43:LEU:HD13	3:B:53:THR:HB	0.50	1.83	10	1
2:F:10:DA:H2''	2:F:11:DC:C6	0.50	2.42	5	9
3:A:24:ASP:CA	3:A:27:LYS:HD3	0.50	2.36	9	5
1:E:18:DA:H2''	1:E:19:DC:C5	0.50	2.42	6	4
3:B:56:ARG:O	3:B:60:GLU:HB2	0.50	2.07	2	1
2:F:4:DA:OP2	3:A:83:THR:CA	0.50	2.60	3	6
3:A:56:ARG:O	3:A:60:GLU:N	0.50	2.43	5	2
3:A:38:LEU:HA	3:A:41:LEU:HD12	0.50	1.83	6	3
3:A:50:ALA:O	3:A:54:ARG:CB	0.50	2.59	8	2
3:A:19:TRP:CZ3	3:B:39:LEU:CD1	0.50	2.95	12	2
3:B:22:PHE:CD1	3:B:26:LEU:HG	0.50	2.41	8	1
3:A:27:LYS:HA	3:B:27:LYS:HG2	0.50	1.82	14	1
3:A:55:VAL:HG21	3:B:22:PHE:CD2	0.50	2.41	14	1
3:B:42:MET:SD	4:B:109:TRP:OXT	0.50	2.69	15	1
3:B:72:LYS:HB2	3:B:78:GLY:CA	0.50	2.36	15	1
1:E:18:DA:H2''	1:E:19:DC:OP2	0.50	2.07	2	3
2:F:13:DC:P	3:A:44:THR:CG2	0.50	3.00	2	1
3:B:93:PRO:C	3:B:97:ARG:CB	0.50	2.85	5	5
3:B:99:TRP:O	3:B:102:GLU:CB	0.50	2.60	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:101:GLU:HG3	3:B:106:LYS:CA	0.50	2.36	6	1
3:A:56:ARG:HD2	3:A:60:GLU:HG3	0.50	1.83	7	1
3:A:54:ARG:HB3	3:B:42:MET:HE3	0.50	1.83	8	1
3:A:34:LEU:HD23	3:A:38:LEU:HD12	0.50	1.83	9	1
1:E:16:DG:C2	1:E:17:DT:C4	0.50	2.99	10	1
3:A:92:ALA:HB2	3:A:96:LEU:HD22	0.50	1.83	11	1
3:B:29:ALA:O	3:B:34:LEU:HB2	0.50	2.05	13	1
3:A:39:LEU:HD22	3:B:19:TRP:CH2	0.50	2.37	15	1
3:A:57:ILE:CG1	4:B:109:TRP:HZ3	0.50	2.18	2	4
3:A:35:HIS:H	3:A:35:HIS:CD2	0.50	2.23	2	1
3:B:93:PRO:O	3:B:97:ARG:CB	0.50	2.59	13	3
2:F:3:DT:OP2	3:A:82:ILE:HD13	0.50	2.06	3	3
3:B:85:GLY:N	4:B:201:TRP:CZ2	0.50	2.79	3	8
1:E:13:DC:OP1	3:A:54:ARG:CD	0.50	2.60	7	1
3:A:19:TRP:CD2	3:B:51:LEU:HG	0.50	2.42	7	1
3:A:30:TYR:CE1	3:A:35:HIS:CG	0.50	3.00	15	3
3:A:23:VAL:HG22	3:B:30:TYR:HE1	0.50	1.61	9	1
3:A:30:TYR:CE1	3:A:35:HIS:CB	0.50	2.94	9	1
3:A:54:ARG:O	3:A:58:VAL:HG22	0.50	2.07	9	1
3:A:94:VAL:HG22	3:A:94:VAL:O	0.50	2.06	11	1
3:A:35:HIS:CE1	3:A:39:LEU:HB3	0.50	2.41	14	2
3:A:55:VAL:HG23	3:B:42:MET:SD	0.50	2.47	14	1
2:F:7:DA:C2	2:F:8:DG:N7	0.50	2.80	7	12
3:A:22:PHE:CE1	3:A:43:LEU:HD21	0.50	2.42	1	1
1:E:4:DA:C2	2:F:18:DA:C2	0.50	3.00	6	4
3:A:73:ASN:O	3:A:74:GLU:C	0.50	2.54	6	9
3:B:43:LEU:C	3:B:43:LEU:CD1	0.50	2.85	4	5
3:B:56:ARG:HA	3:B:59:GLU:HG3	0.50	1.84	5	1
3:A:43:LEU:N	3:A:43:LEU:CD1	0.50	2.70	7	1
3:A:72:LYS:HA	3:A:82:ILE:HG21	0.50	1.83	13	2
3:A:29:ALA:CB	3:B:99:TRP:CE2	0.50	2.89	13	3
3:A:55:VAL:CG2	3:B:38:LEU:HD21	0.50	2.36	11	1
3:A:80:ALA:HB1	3:A:84:ARG:HH21	0.50	1.66	13	1
3:B:95:GLU:CB	3:B:96:LEU:HD13	0.50	2.36	13	1
3:A:81:THR:CG2	4:B:109:TRP:CE2	0.50	2.93	9	4
3:B:58:VAL:HG23	3:B:59:GLU:H	0.50	1.67	8	3
3:A:70:GLU:OE1	3:A:71:LEU:HD12	0.50	2.07	5	2
4:B:201:TRP:CE3	4:B:201:TRP:HA	0.50	2.42	7	2
1:E:1:DT:H2'	1:E:2:DG:N7	0.50	2.22	8	1
3:A:104:LEU:HD13	3:A:104:LEU:O	0.50	2.07	8	1
2:F:13:DC:H3'	3:A:43:LEU:CD1	0.50	2.36	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:19:TRP:CZ2	3:B:39:LEU:CD1	0.50	2.93	14	1
3:B:19:TRP:C	3:B:23:VAL:HG21	0.50	2.31	14	1
3:A:35:HIS:NE2	3:B:19:TRP:NE1	0.50	2.56	15	1
3:A:26:LEU:O	3:A:27:LYS:C	0.50	2.54	5	8
3:B:41:LEU:CD2	3:B:41:LEU:N	0.50	2.75	1	1
3:B:81:THR:OG1	4:B:201:TRP:CD1	0.50	2.65	1	6
3:B:88:SER:O	3:B:89:LEU:C	0.50	2.55	12	12
3:B:32:ASN:HB3	3:B:34:LEU:CD2	0.50	2.37	2	1
3:A:30:TYR:CD2	3:B:23:VAL:HA	0.50	2.41	4	1
3:A:88:SER:O	3:A:91:ALA:N	0.50	2.45	4	2
3:B:65:GLU:O	3:B:66:MET:HB2	0.50	2.07	7	1
3:A:42:MET:C	3:B:54:ARG:CG	0.50	2.85	10	1
3:B:78:GLY:C	3:B:81:THR:H	0.50	2.11	13	2
3:A:43:LEU:HD23	3:B:51:LEU:HD23	0.50	1.80	15	1
3:A:72:LYS:CE	3:A:73:ASN:HB2	0.50	2.36	15	1
1:E:15:DG:C5	3:A:79:ILE:HB	0.49	2.42	10	4
3:A:30:TYR:HD1	3:A:35:HIS:CG	0.49	2.25	5	4
1:E:12:DA:C2	1:E:13:DC:C1'	0.49	2.95	8	7
3:A:22:PHE:CG	3:B:51:LEU:HD13	0.49	2.41	2	1
3:A:68:GLN:CD	3:A:68:GLN:N	0.49	2.66	2	1
3:A:85:GLY:N	4:B:109:TRP:CH2	0.49	2.81	9	3
1:E:15:DG:N2	1:E:16:DG:N3	0.49	2.60	3	1
3:A:30:TYR:CB	3:B:23:VAL:HG13	0.49	2.36	3	2
2:F:3:DT:C2	2:F:4:DA:C5	0.49	3.00	5	3
3:A:72:LYS:HD2	3:A:79:ILE:HA	0.49	1.83	4	1
3:A:17:GLN:O	3:A:20:LEU:N	0.49	2.31	7	1
3:A:96:LEU:N	3:A:96:LEU:CD1	0.49	2.75	11	4
2:F:14:DG:P	3:B:77:ALA:HB3	0.49	2.47	8	1
3:A:34:LEU:HD23	3:B:99:TRP:CG	0.49	2.42	5	2
3:A:92:ALA:HB1	3:A:96:LEU:HB2	0.49	1.82	13	5
1:E:16:DG:N2	2:F:6:DC:O2	0.49	2.45	3	1
3:A:30:TYR:HA	3:A:35:HIS:HB3	0.49	1.82	4	1
3:A:99:TRP:HB3	3:B:34:LEU:HD22	0.49	1.79	4	1
3:A:22:PHE:CZ	3:A:43:LEU:HD23	0.49	2.42	7	1
3:A:43:LEU:HD13	3:A:43:LEU:C	0.49	2.32	11	1
3:A:68:GLN:NE2	3:A:69:ARG:NH2	0.49	2.61	11	1
3:A:72:LYS:CG	3:A:78:GLY:O	0.49	2.59	13	1
3:A:45:PRO:O	3:A:48:ARG:CG	0.49	2.60	14	1
1:E:12:DA:O3'	4:B:109:TRP:HB3	0.49	2.07	15	1
3:A:37:PRO:CD	3:B:96:LEU:HD22	0.49	2.36	15	1
3:B:80:ALA:O	3:B:84:ARG:HB3	0.49	2.07	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:109:TRP:O	4:B:109:TRP:CD1	0.49	2.66	1	2
1:E:2:DG:H2''	1:E:3:DT:O5'	0.49	2.07	2	5
3:A:43:LEU:CB	3:B:54:ARG:HG2	0.49	2.38	4	1
3:B:82:ILE:CG1	3:B:83:THR:N	0.49	2.75	9	8
3:A:96:LEU:C	3:A:98:GLN:N	0.49	2.69	8	3
3:B:26:LEU:CD1	3:B:38:LEU:HD22	0.49	2.37	12	1
3:A:37:PRO:HG3	3:B:96:LEU:CG	0.49	2.37	13	1
3:A:53:THR:HG21	3:A:76:GLY:HA2	0.49	1.84	13	1
3:A:43:LEU:HD12	3:B:53:THR:HB	0.49	1.84	14	1
3:A:66:MET:HE2	3:A:71:LEU:HD13	0.49	1.83	14	1
1:E:16:DG:C2'	1:E:17:DT:C7	0.49	2.87	6	6
3:A:57:ILE:HD13	3:A:58:VAL:HG22	0.49	1.79	2	2
3:A:72:LYS:HZ2	3:A:79:ILE:CG2	0.49	2.16	4	2
3:B:37:PRO:O	3:B:41:LEU:N	0.49	2.45	4	2
2:F:11:DC:N3	2:F:12:DA:N6	0.49	2.60	5	1
3:A:34:LEU:CB	3:B:99:TRP:CE3	0.49	2.94	6	2
3:A:40:ASN:O	3:B:91:ALA:CB	0.49	2.59	8	3
3:B:68:GLN:HA	3:B:82:ILE:CD1	0.49	2.38	9	1
2:F:2:DG:C8	3:A:68:GLN:HG3	0.49	2.43	10	1
3:A:100:LEU:O	3:A:104:LEU:HD22	0.49	2.07	12	1
3:A:37:PRO:HG3	3:B:96:LEU:HG	0.49	1.85	13	1
3:B:29:ALA:HB3	3:B:34:LEU:CD1	0.49	2.37	14	1
1:E:14:DT:H2''	3:A:73:ASN:ND2	0.49	2.22	15	1
3:A:47:GLU:O	3:A:50:ALA:HB3	0.49	2.07	15	1
3:A:88:SER:HB3	3:B:40:ASN:O	0.49	2.08	1	1
3:B:42:MET:O	3:B:45:PRO:HD3	0.49	2.07	13	2
3:B:45:PRO:C	3:B:47:GLU:N	0.49	2.70	13	10
1:E:18:DA:N3	1:E:19:DC:C4	0.49	2.81	2	1
3:A:42:MET:CA	4:B:201:TRP:OXT	0.49	2.60	2	1
3:A:90:LYS:HE2	3:B:43:LEU:O	0.49	2.08	11	2
3:A:19:TRP:CD1	3:B:36:LEU:HD11	0.49	2.43	4	1
3:A:54:ARG:CZ	4:B:109:TRP:OXT	0.49	2.60	11	2
3:B:35:HIS:CE1	3:B:36:LEU:HG	0.49	2.42	10	3
3:B:70:GLU:HB2	3:B:71:LEU:HD12	0.49	1.83	11	1
3:B:78:GLY:CA	3:B:82:ILE:CG2	0.49	2.87	12	1
3:B:79:ILE:CA	3:B:82:ILE:CG1	0.49	2.90	15	1
3:A:105:LEU:O	3:A:106:LYS:C	0.49	2.55	10	6
3:B:54:ARG:HG3	3:B:55:VAL:N	0.49	2.21	9	3
3:A:51:LEU:O	3:A:52:GLY:C	0.49	2.55	15	5
1:E:18:DA:C6	2:F:4:DA:C6	0.49	3.00	3	1
3:A:22:PHE:CZ	3:B:51:LEU:CD2	0.49	2.94	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:21:ARG:O	3:B:25:LEU:HB2	0.49	2.07	4	1
2:F:14:DG:C5	3:B:80:ALA:CB	0.49	2.96	9	3
3:A:40:ASN:HA	3:A:45:PRO:CA	0.49	2.37	10	5
3:B:101:GLU:HB3	3:B:106:LYS:HA	0.49	1.85	10	2
3:B:39:LEU:O	3:B:39:LEU:CD1	0.49	2.60	13	2
3:A:51:LEU:HD12	3:A:54:ARG:CZ	0.49	2.37	13	1
3:A:68:GLN:N	3:A:72:LYS:HB3	0.49	2.23	13	1
3:A:26:LEU:HD13	3:A:35:HIS:NE2	0.49	2.21	14	1
1:E:19:DC:C4	1:E:20:DA:N6	0.49	2.81	15	1
3:A:22:PHE:CG	3:A:22:PHE:O	0.49	2.65	15	1
2:F:13:DC:N3	2:F:14:DG:C5	0.49	2.80	5	9
3:A:44:THR:HB	3:A:47:GLU:HB3	0.49	1.83	7	4
3:A:69:ARG:CA	3:A:72:LYS:HE2	0.49	2.38	6	2
3:A:33:ASP:CB	3:A:36:LEU:HD12	0.49	2.38	5	4
3:A:50:ALA:O	3:A:53:THR:N	0.49	2.45	4	1
3:B:100:LEU:CD2	3:B:104:LEU:HD11	0.49	2.38	4	1
1:E:8:DG:C2'	1:E:9:DT:C6	0.49	2.96	11	2
3:A:99:TRP:HB2	3:B:34:LEU:HG	0.49	1.85	8	2
3:B:71:LEU:O	3:B:74:GLU:CG	0.49	2.61	9	1
1:E:10:DG:N1	2:F:12:DA:C2	0.49	2.80	11	2
3:A:40:ASN:OD1	3:A:41:LEU:N	0.49	2.46	13	1
3:A:22:PHE:CE1	3:A:26:LEU:HD11	0.49	2.41	14	1
3:A:23:VAL:CG1	3:B:30:TYR:CD2	0.49	2.94	10	5
1:E:11:DT:H1'	1:E:12:DA:C8	0.49	2.43	2	5
3:A:17:GLN:O	3:A:19:TRP:N	0.49	2.46	3	1
3:B:70:GLU:O	3:B:71:LEU:CB	0.49	2.58	8	4
3:A:96:LEU:C	3:B:37:PRO:HB3	0.49	2.33	14	4
3:B:30:TYR:OH	3:B:35:HIS:CE1	0.49	2.66	5	1
3:B:35:HIS:N	3:B:37:PRO:HD2	0.49	2.23	6	3
1:E:4:DA:O5'	1:E:4:DA:H8	0.49	1.90	7	2
3:A:96:LEU:HD23	3:B:41:LEU:HB3	0.49	1.85	8	1
3:A:36:LEU:O	3:A:40:ASN:CG	0.49	2.55	9	1
3:A:78:GLY:HA2	3:A:82:ILE:CG2	0.49	2.38	13	1
3:A:79:ILE:CA	3:A:82:ILE:HG13	0.49	2.38	13	1
3:B:26:LEU:CD1	3:B:35:HIS:CE1	0.49	2.95	15	1
3:B:41:LEU:CD2	3:B:42:MET:SD	0.49	3.01	1	1
3:B:44:THR:C	3:B:46:ASP:H	0.49	2.16	1	1
3:A:78:GLY:CA	3:A:81:THR:OG1	0.49	2.61	12	5
3:B:36:LEU:HD23	3:B:39:LEU:CD2	0.49	2.37	3	2
3:B:41:LEU:HB3	3:B:42:MET:SD	0.49	2.47	3	1
2:F:3:DT:O4	2:F:4:DA:N6	0.49	2.46	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:101:GLU:C	3:A:106:LYS:HB2	0.49	2.32	10	6
3:B:51:LEU:O	3:B:54:ARG:HB2	0.49	2.07	14	3
3:A:23:VAL:HA	3:B:30:TYR:CE2	0.49	2.43	11	3
3:A:91:ALA:C	3:B:40:ASN:O	0.49	2.56	14	2
4:B:109:TRP:C	4:B:109:TRP:HD1	0.49	2.11	6	1
3:A:51:LEU:HD11	3:B:26:LEU:HG	0.49	1.83	7	1
3:B:79:ILE:HA	3:B:82:ILE:HG12	0.49	1.84	9	1
3:A:62:LEU:CD1	3:A:104:LEU:HD23	0.49	2.36	12	1
3:B:85:GLY:O	3:B:86:SER:C	0.49	2.53	10	10
3:B:84:ARG:O	3:B:87:ASN:OD1	0.49	2.31	3	1
3:B:88:SER:HB2	3:B:93:PRO:CD	0.49	2.38	14	2
3:A:97:ARG:NH1	3:A:100:LEU:HD13	0.49	2.23	5	1
3:B:30:TYR:CD1	3:B:35:HIS:CB	0.49	2.96	10	4
3:A:51:LEU:HD21	3:B:22:PHE:CG	0.49	2.43	7	1
3:B:72:LYS:HG3	3:B:79:ILE:CB	0.49	2.38	9	1
3:A:68:GLN:CD	3:A:69:ARG:CZ	0.49	2.85	11	1
1:E:16:DG:C2'	1:E:17:DT:C6	0.49	2.95	14	2
3:A:26:LEU:CA	3:A:35:HIS:CD2	0.49	2.96	13	1
3:A:90:LYS:HD2	3:B:43:LEU:HD22	0.49	1.85	13	1
3:B:51:LEU:HD22	3:B:51:LEU:O	0.49	2.07	15	1
3:A:41:LEU:HD12	3:A:41:LEU:C	0.48	2.33	1	1
3:A:47:GLU:C	3:A:49:GLU:N	0.48	2.70	1	4
3:A:99:TRP:NE1	3:B:29:ALA:CB	0.48	2.74	1	4
3:A:43:LEU:CD2	3:B:54:ARG:CZ	0.48	2.91	3	1
3:A:39:LEU:HD13	3:B:19:TRP:CZ2	0.48	2.42	5	1
3:A:56:ARG:O	3:A:57:ILE:C	0.48	2.56	5	1
2:F:19:DC:C2'	2:F:20:DA:C8	0.48	2.96	8	3
3:A:55:VAL:CB	3:B:22:PHE:CE1	0.48	2.95	7	1
2:F:17:DT:H2''	2:F:18:DA:C8	0.48	2.43	8	1
3:A:19:TRP:CZ3	3:B:51:LEU:HD22	0.48	2.43	8	1
3:A:57:ILE:HD12	3:A:58:VAL:CG2	0.48	2.38	9	2
3:A:42:MET:C	3:B:54:ARG:HG3	0.48	2.33	11	1
3:B:67:SER:HB2	3:B:82:ILE:HD12	0.48	1.85	13	1
3:A:55:VAL:CB	3:B:22:PHE:CE2	0.48	2.96	14	1
3:A:75:LEU:C	3:A:75:LEU:HD22	0.48	2.33	15	1
3:A:66:MET:O	3:A:72:LYS:HA	0.48	2.08	1	1
3:A:100:LEU:CD1	3:B:41:LEU:HD12	0.48	2.38	1	1
3:B:39:LEU:HD23	3:B:40:ASN:ND2	0.48	2.22	1	2
3:B:58:VAL:O	3:B:59:GLU:C	0.48	2.54	5	3
3:A:81:THR:CG2	4:B:109:TRP:CD2	0.48	2.93	10	4
3:A:85:GLY:N	4:B:109:TRP:CZ2	0.48	2.82	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:41:LEU:CD1	3:A:41:LEU:N	0.48	2.76	3	4
3:A:29:ALA:CB	3:B:99:TRP:CH2	0.48	2.96	14	2
3:B:41:LEU:CD2	3:B:42:MET:CB	0.48	2.91	6	1
2:F:11:DC:O2	2:F:12:DA:C8	0.48	2.66	13	1
3:A:42:MET:HE2	3:B:58:VAL:CB	0.48	2.38	1	1
1:E:14:DT:C7	3:A:77:ALA:O	0.48	2.61	4	2
3:A:47:GLU:O	3:A:51:LEU:N	0.48	2.44	8	3
3:A:51:LEU:CG	3:B:22:PHE:CE2	0.48	2.96	14	2
3:B:22:PHE:CB	3:B:26:LEU:HG	0.48	2.34	4	1
3:B:43:LEU:HD22	4:B:109:TRP:NE1	0.48	2.23	5	1
3:B:35:HIS:CE1	3:B:36:LEU:HD21	0.48	2.44	10	2
3:A:42:MET:HB3	4:B:201:TRP:CA	0.48	2.38	8	1
3:A:42:MET:O	3:A:43:LEU:CD2	0.48	2.62	9	1
3:A:43:LEU:CD2	3:B:53:THR:HB	0.48	2.38	11	1
3:B:72:LYS:HG2	3:B:73:ASN:H	0.48	1.67	11	1
3:A:65:GLU:O	3:A:66:MET:HB2	0.48	2.08	13	1
3:A:42:MET:CE	3:B:100:LEU:HD11	0.48	2.39	1	2
3:A:58:VAL:HG11	3:B:41:LEU:HD12	0.48	1.84	1	1
2:F:7:DA:C6	2:F:8:DG:N7	0.48	2.82	6	5
3:A:61:LEU:HA	3:A:66:MET:HA	0.48	1.85	3	1
3:A:68:GLN:C	3:A:70:GLU:N	0.48	2.69	3	1
3:A:99:TRP:HB2	3:B:34:LEU:HD13	0.48	1.84	4	1
3:A:99:TRP:CZ3	3:B:38:LEU:CD1	0.48	2.97	14	2
3:A:58:VAL:HG21	3:B:41:LEU:CD2	0.48	2.38	6	2
3:B:36:LEU:HA	3:B:39:LEU:CD2	0.48	2.39	7	1
3:A:42:MET:HG2	4:B:201:TRP:CA	0.48	2.39	8	1
3:A:71:LEU:O	3:A:73:ASN:N	0.48	2.47	8	1
3:A:80:ALA:HB1	3:A:84:ARG:NH2	0.48	2.23	9	2
3:A:69:ARG:H	3:A:72:LYS:CE	0.48	2.22	12	1
3:A:39:LEU:HD12	3:A:39:LEU:O	0.48	2.09	13	1
3:A:43:LEU:O	3:A:43:LEU:HD22	0.48	2.07	14	1
3:B:32:ASN:HB3	3:B:34:LEU:CD1	0.48	2.38	15	1
3:B:50:ALA:O	3:B:54:ARG:CD	0.48	2.61	14	3
3:A:27:LYS:O	3:A:30:TYR:N	0.48	2.46	4	2
3:A:35:HIS:CD2	3:A:36:LEU:CD1	0.48	2.96	4	1
3:A:96:LEU:CD1	3:A:96:LEU:H	0.48	2.22	4	1
3:B:29:ALA:CA	3:B:34:LEU:HB2	0.48	2.39	5	2
3:B:72:LYS:CG	3:B:79:ILE:CG1	0.48	2.91	9	1
3:A:51:LEU:HB2	3:B:19:TRP:CZ3	0.48	2.43	12	1
1:E:14:DT:C3'	3:A:76:GLY:O	0.48	2.61	13	1
3:A:37:PRO:HB3	3:B:96:LEU:CD2	0.48	2.39	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:90:LYS:HD2	3:B:43:LEU:HA	0.48	1.85	13	1
3:A:19:TRP:NE1	3:B:35:HIS:HB3	0.48	2.24	14	1
2:F:4:DA:N3	2:F:5:DC:C2	0.48	2.81	6	3
3:B:30:TYR:CD1	3:B:35:HIS:HB3	0.48	2.44	1	5
3:B:48:ARG:O	3:B:52:GLY:HA3	0.48	2.09	4	3
1:E:16:DG:C6	3:A:79:ILE:HG22	0.48	2.42	3	1
3:A:26:LEU:CD1	3:A:27:LYS:N	0.48	2.74	3	1
3:A:57:ILE:HD12	3:A:57:ILE:H	0.48	1.69	4	1
3:A:90:LYS:CE	3:A:91:ALA:HB2	0.48	2.38	4	2
3:A:45:PRO:O	3:A:48:ARG:N	0.48	2.40	5	3
3:B:87:ASN:O	3:B:90:LYS:HG2	0.48	2.08	11	4
3:A:51:LEU:HA	3:A:55:VAL:HG23	0.48	1.85	12	1
3:B:23:VAL:O	3:B:27:LYS:HD3	0.48	2.09	12	1
3:A:43:LEU:HB3	3:B:54:ARG:HD3	0.48	1.85	14	1
3:B:26:LEU:HA	3:B:34:LEU:HD13	0.48	1.85	14	1
1:E:11:DT:C2'	1:E:12:DA:OP2	0.48	2.61	4	14
1:E:15:DG:C2	2:F:7:DA:C6	0.48	3.02	5	2
2:F:11:DC:H2'	2:F:12:DA:N7	0.48	2.23	5	2
3:A:54:ARG:CG	3:A:55:VAL:N	0.48	2.76	13	6
3:B:73:ASN:CB	3:B:79:ILE:CG1	0.48	2.92	14	6
3:A:56:ARG:NH1	3:A:71:LEU:HD23	0.48	2.22	2	1
3:B:19:TRP:O	3:B:22:PHE:HB3	0.48	2.09	2	1
3:A:19:TRP:CZ3	3:B:51:LEU:HG	0.48	2.44	4	5
3:A:33:ASP:HB3	3:B:96:LEU:HD23	0.48	1.85	3	1
3:B:68:GLN:C	3:B:82:ILE:HD11	0.48	2.33	3	1
3:B:30:TYR:HA	3:B:35:HIS:CB	0.48	2.39	4	1
3:B:43:LEU:HB3	4:B:109:TRP:CE2	0.48	2.44	11	4
3:A:38:LEU:HD12	3:B:99:TRP:HZ3	0.48	1.68	5	1
3:A:96:LEU:O	3:B:37:PRO:CB	0.48	2.62	14	3
3:A:99:TRP:CZ2	3:B:29:ALA:HB2	0.48	2.43	5	1
3:B:99:TRP:O	3:B:102:GLU:HB2	0.48	2.09	6	1
3:B:57:ILE:CG2	3:B:81:THR:HB	0.48	2.38	9	1
3:A:41:LEU:HD21	3:B:58:VAL:HG11	0.48	1.85	10	1
3:A:36:LEU:O	3:A:40:ASN:OD1	0.48	2.32	12	1
2:F:4:DA:H62	3:A:79:ILE:HD13	0.48	1.68	15	1
3:B:35:HIS:CE1	3:B:36:LEU:HD12	0.48	2.43	1	1
3:A:51:LEU:O	3:B:22:PHE:CE2	0.48	2.67	11	7
3:A:41:LEU:O	3:A:41:LEU:CD1	0.48	2.61	5	1
3:A:41:LEU:HD13	3:A:42:MET:HB2	0.48	1.85	5	1
3:A:34:LEU:HA	3:A:37:PRO:CD	0.48	2.39	6	1
3:A:45:PRO:O	3:A:47:GLU:N	0.48	2.47	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:51:LEU:CA	3:A:54:ARG:HB2	0.48	2.39	8	1
3:B:21:ARG:O	3:B:25:LEU:HD12	0.48	2.09	12	1
3:B:19:TRP:O	3:B:23:VAL:CG2	0.48	2.57	14	1
1:E:7:DC:N4	3:B:84:ARG:NH2	0.48	2.61	15	1
1:E:14:DT:C2'	3:A:73:ASN:ND2	0.48	2.77	15	1
3:B:45:PRO:CD	4:B:109:TRP:O	0.48	2.60	1	1
3:B:91:ALA:O	3:B:92:ALA:C	0.48	2.56	13	13
2:F:3:DT:OP2	3:A:68:GLN:OE1	0.48	2.32	2	1
3:B:20:LEU:N	3:B:20:LEU:CD2	0.48	2.77	6	8
3:A:54:ARG:O	3:A:55:VAL:C	0.48	2.56	4	6
3:B:100:LEU:O	3:B:103:VAL:CG2	0.48	2.62	10	2
3:A:43:LEU:C	3:B:54:ARG:HD3	0.48	2.34	5	1
3:B:94:VAL:HG23	3:B:95:GLU:N	0.48	2.24	13	5
3:A:97:ARG:HD2	3:A:97:ARG:N	0.48	2.22	8	1
3:A:106:LYS:O	3:A:106:LYS:HG2	0.48	2.08	11	1
1:E:5:DC:O5'	1:E:5:DC:H6	0.48	1.91	12	1
3:A:34:LEU:CB	3:B:96:LEU:CD2	0.48	2.91	12	1
3:A:42:MET:HG3	3:B:54:ARG:O	0.48	2.08	12	1
3:A:37:PRO:C	3:A:40:ASN:OD1	0.48	2.56	13	1
3:A:67:SER:CB	3:A:82:ILE:HB	0.48	2.39	13	1
1:E:18:DA:C8	1:E:18:DA:O5'	0.48	2.66	9	6
3:A:19:TRP:CE3	3:B:51:LEU:CD1	0.48	2.96	11	2
3:A:58:VAL:HG11	3:B:41:LEU:HB2	0.48	1.86	1	1
3:B:39:LEU:HG	3:B:45:PRO:O	0.48	2.09	1	4
3:B:90:LYS:HG3	3:B:91:ALA:H	0.48	1.69	3	3
3:B:39:LEU:O	3:B:45:PRO:CA	0.48	2.62	6	1
3:A:81:THR:HG23	4:B:109:TRP:CG	0.48	2.44	7	1
4:B:201:TRP:C	4:B:201:TRP:CE3	0.48	2.91	7	1
2:F:18:DA:C2'	2:F:19:DC:C6	0.48	2.97	8	4
3:A:43:LEU:CB	4:B:201:TRP:CD2	0.48	2.97	8	1
3:B:99:TRP:CZ3	3:B:100:LEU:HB2	0.48	2.44	10	1
3:B:73:ASN:HB3	3:B:79:ILE:CG1	0.48	2.39	13	3
3:A:24:ASP:O	3:A:27:LYS:CD	0.48	2.62	13	1
3:A:38:LEU:HG	3:A:42:MET:SD	0.48	2.49	14	1
2:F:2:DG:P	3:A:68:GLN:HG3	0.47	2.49	4	1
3:A:51:LEU:CD1	3:B:22:PHE:CD2	0.47	2.97	4	1
3:B:30:TYR:CZ	3:B:35:HIS:CD2	0.47	3.02	7	1
3:B:73:ASN:CA	3:B:79:ILE:HD11	0.47	2.40	9	1
3:A:54:ARG:HB2	4:B:109:TRP:CB	0.47	2.38	12	1
3:A:55:VAL:CG1	3:A:59:GLU:HG3	0.47	2.39	14	1
3:B:26:LEU:CA	3:B:27:LYS:HE2	0.47	2.38	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:22:PHE:O	3:A:22:PHE:CG	0.47	2.67	9	3
3:A:33:ASP:O	3:A:37:PRO:HD3	0.47	2.10	1	1
3:B:91:ALA:O	3:B:92:ALA:O	0.47	2.32	9	5
3:B:100:LEU:C	3:B:100:LEU:CD2	0.47	2.87	5	4
3:A:67:SER:C	3:A:68:GLN:HG2	0.47	2.34	2	1
3:B:78:GLY:HA2	3:B:81:THR:CG2	0.47	2.40	8	2
2:F:2:DG:H3'	3:A:68:GLN:HG2	0.47	1.86	3	1
3:A:40:ASN:CA	3:B:91:ALA:CB	0.47	2.91	3	1
3:A:96:LEU:CD2	3:B:37:PRO:HA	0.47	2.36	11	2
1:E:18:DA:O5'	1:E:18:DA:C8	0.47	2.63	4	4
3:B:34:LEU:HA	3:B:37:PRO:CG	0.47	2.39	6	1
3:B:41:LEU:HD23	3:B:42:MET:CB	0.47	2.39	6	1
3:B:51:LEU:HG	3:B:52:GLY:N	0.47	2.23	8	1
3:B:100:LEU:O	3:B:104:LEU:CD2	0.47	2.62	10	1
3:A:96:LEU:CD2	3:B:40:ASN:HB2	0.47	2.40	11	1
3:A:22:PHE:CG	3:B:51:LEU:HD11	0.47	2.44	12	1
3:A:100:LEU:HD12	3:B:41:LEU:CG	0.47	2.39	12	1
2:F:3:DT:C7	3:A:72:LYS:HD2	0.47	2.39	5	2
3:A:37:PRO:O	3:A:41:LEU:CG	0.47	2.62	1	2
3:A:54:ARG:NE	4:B:109:TRP:N	0.47	2.62	1	1
3:B:27:LYS:HA	3:B:30:TYR:CB	0.47	2.38	10	5
1:E:1:DT:H6	1:E:1:DT:O5'	0.47	1.91	11	2
3:A:39:LEU:O	3:A:45:PRO:HA	0.47	2.09	11	3
3:A:72:LYS:CB	3:A:82:ILE:HG12	0.47	2.38	14	3
3:B:22:PHE:CD2	3:B:26:LEU:HD21	0.47	2.44	6	1
3:A:72:LYS:O	3:A:78:GLY:HA3	0.47	2.09	13	2
3:A:38:LEU:O	3:A:41:LEU:CD1	0.47	2.62	8	1
3:A:43:LEU:HG	3:B:50:ALA:HA	0.47	1.86	9	1
1:E:10:DG:C6	2:F:12:DA:C2	0.47	3.02	14	2
2:F:10:DA:H1'	2:F:11:DC:O4'	0.47	2.10	11	1
3:A:22:PHE:CD1	3:A:22:PHE:O	0.47	2.68	11	1
3:A:54:ARG:HG2	3:A:55:VAL:N	0.47	2.23	12	1
3:B:34:LEU:O	3:B:38:LEU:HB2	0.47	2.10	14	1
2:F:3:DT:C4	3:A:79:ILE:HD11	0.47	2.44	15	1
3:A:66:MET:HG3	3:A:75:LEU:HD23	0.47	1.85	1	1
3:B:26:LEU:O	3:B:30:TYR:CD1	0.47	2.67	11	6
3:B:79:ILE:O	3:B:83:THR:CG2	0.47	2.62	2	2
3:A:20:LEU:HD22	3:A:20:LEU:H	0.47	1.69	9	4
3:A:42:MET:HA	4:B:201:TRP:OXT	0.47	2.10	2	1
3:A:73:ASN:C	3:A:75:LEU:N	0.47	2.72	8	3
1:E:5:DC:C5	3:B:69:ARG:CD	0.47	2.97	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:17:DT:O5'	1:E:17:DT:C6	0.47	2.68	3	1
3:A:44:THR:O	3:A:47:GLU:HB2	0.47	2.10	3	2
3:B:35:HIS:CD2	3:B:35:HIS:O	0.47	2.67	15	4
3:A:22:PHE:O	3:A:26:LEU:CG	0.47	2.62	14	3
3:A:84:ARG:HD3	3:B:43:LEU:CD1	0.47	2.39	6	1
2:F:13:DC:P	3:A:44:THR:HG21	0.47	2.48	8	1
3:A:72:LYS:CA	3:A:78:GLY:CA	0.47	2.92	13	1
3:A:72:LYS:HD2	3:A:73:ASN:OD1	0.47	2.09	15	1
3:A:40:ASN:ND2	3:A:48:ARG:NH1	0.47	2.62	2	2
3:A:44:THR:CG2	3:A:47:GLU:CG	0.47	2.93	15	2
3:A:43:LEU:O	4:B:201:TRP:HB3	0.47	2.09	3	2
4:B:201:TRP:CE3	4:B:201:TRP:OXT	0.47	2.67	3	1
1:E:1:DT:O5'	1:E:1:DT:H6	0.47	1.92	13	2
3:A:57:ILE:CB	3:A:82:ILE:HG22	0.47	2.38	4	2
3:B:43:LEU:CB	4:B:109:TRP:CE2	0.47	2.97	4	1
3:A:37:PRO:HG3	3:B:96:LEU:HB3	0.47	1.85	6	4
1:E:17:DT:O4	2:F:3:DT:O4	0.47	2.32	6	1
3:A:34:LEU:CD2	3:A:38:LEU:HB2	0.47	2.40	6	1
2:F:14:DG:P	3:B:77:ALA:CB	0.47	3.01	8	1
3:A:96:LEU:CD2	3:B:41:LEU:HB3	0.47	2.39	8	1
3:B:24:ASP:CG	3:B:25:LEU:HD12	0.47	2.34	8	1
3:B:33:ASP:CA	3:B:36:LEU:HD12	0.47	2.40	9	1
3:B:79:ILE:CA	3:B:82:ILE:HG12	0.47	2.39	9	2
2:F:13:DC:H3'	3:A:43:LEU:HD21	0.47	1.87	10	1
3:B:68:GLN:O	3:B:69:ARG:HB3	0.47	2.09	15	2
1:E:9:DT:C4	1:E:10:DG:C6	0.47	3.03	15	1
3:A:21:ARG:O	3:A:25:LEU:HD13	0.47	2.10	3	2
3:A:22:PHE:CZ	3:A:26:LEU:CD2	0.47	2.98	3	1
3:A:70:GLU:HA	3:A:74:GLU:HG3	0.47	1.86	3	1
2:F:3:DT:N3	2:F:4:DA:C6	0.47	2.82	4	3
2:F:14:DG:C6	3:B:80:ALA:CB	0.47	2.98	9	3
3:B:71:LEU:N	3:B:71:LEU:HD13	0.47	2.25	5	1
3:A:34:LEU:HA	3:A:37:PRO:HG3	0.47	1.86	6	1
3:A:17:GLN:HB2	3:A:20:LEU:HB2	0.47	1.86	7	1
3:B:68:GLN:HB3	3:B:79:ILE:CD1	0.47	2.38	7	1
3:A:43:LEU:HB2	4:B:201:TRP:CE2	0.47	2.44	8	1
3:B:41:LEU:HD23	3:B:42:MET:H	0.47	1.67	8	1
3:B:101:GLU:O	3:B:106:LYS:N	0.47	2.48	10	2
2:F:3:DT:OP2	2:F:3:DT:H71	0.47	2.10	9	1
3:A:26:LEU:N	3:A:26:LEU:CD2	0.47	2.78	15	3
1:E:16:DG:C8	1:E:17:DT:H72	0.47	2.45	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:3:DT:H71	1:E:3:DT:OP2	0.47	2.09	14	1
3:A:22:PHE:CE1	3:A:26:LEU:CG	0.47	2.98	14	1
3:B:24:ASP:C	3:B:27:LYS:HE3	0.47	2.34	14	1
2:F:3:DT:H72	3:A:79:ILE:CG1	0.47	2.40	15	1
2:F:7:DA:C5	2:F:8:DG:N7	0.47	2.83	13	9
3:A:39:LEU:CD2	3:B:19:TRP:CZ2	0.47	2.94	5	3
3:A:80:ALA:HA	3:A:83:THR:CG2	0.47	2.40	5	7
3:A:91:ALA:CB	3:B:40:ASN:CB	0.47	2.92	15	5
3:B:27:LYS:O	3:B:28:ASN:C	0.47	2.57	6	11
3:B:72:LYS:HD2	3:B:72:LYS:H	0.47	1.70	1	1
3:A:73:ASN:HA	3:A:77:ALA:N	0.47	2.25	2	1
1:E:15:DG:C8	3:A:79:ILE:HB	0.47	2.44	3	1
3:A:90:LYS:HD3	3:A:91:ALA:N	0.47	2.24	15	4
1:E:19:DC:H2'	1:E:20:DA:C8	0.47	2.45	15	4
2:F:5:DC:N4	2:F:6:DC:N4	0.47	2.63	11	3
3:A:61:LEU:HD12	3:A:66:MET:CA	0.47	2.37	6	1
2:F:3:DT:C4	3:A:79:ILE:HD13	0.47	2.44	7	1
3:A:96:LEU:CG	3:B:37:PRO:HG3	0.47	2.40	7	1
3:B:32:ASN:HB3	3:B:34:LEU:HD23	0.47	1.85	7	1
3:A:42:MET:C	4:B:201:TRP:CE3	0.47	2.93	8	1
3:A:44:THR:C	4:B:201:TRP:HB3	0.47	2.35	8	1
3:B:93:PRO:O	3:B:96:LEU:N	0.47	2.43	8	1
3:B:41:LEU:HD21	3:B:42:MET:HG2	0.47	1.87	15	2
1:E:10:DG:N2	1:E:11:DT:C2	0.47	2.83	11	1
3:A:36:LEU:HA	3:A:39:LEU:CD2	0.47	2.39	13	2
3:A:55:VAL:HG12	3:A:59:GLU:HB3	0.47	1.87	11	2
3:A:35:HIS:NE2	3:B:99:TRP:CZ2	0.47	2.82	13	1
3:B:23:VAL:C	3:B:27:LYS:NZ	0.47	2.73	14	1
3:B:20:LEU:HD22	3:B:20:LEU:H	0.47	1.70	1	2
3:A:58:VAL:HG21	3:B:41:LEU:CD1	0.47	2.39	15	2
4:B:201:TRP:N	4:B:201:TRP:CE3	0.47	2.83	2	2
1:E:10:DG:C2'	1:E:11:DT:C6	0.47	2.98	8	2
1:E:15:DG:N1	1:E:16:DG:C2	0.47	2.83	3	1
1:E:17:DT:H2'	1:E:18:DA:C8	0.47	2.45	3	1
2:F:2:DG:H3'	3:A:68:GLN:CG	0.47	2.40	3	1
3:A:92:ALA:HB3	3:A:96:LEU:CD1	0.47	2.39	3	2
3:B:68:GLN:O	3:B:69:ARG:CG	0.47	2.63	3	2
3:B:68:GLN:O	3:B:83:THR:HB	0.47	2.08	3	1
3:A:50:ALA:O	3:A:51:LEU:C	0.47	2.55	4	2
3:A:57:ILE:HD13	3:A:58:VAL:HG13	0.47	1.87	6	1
2:F:3:DT:OP2	3:A:67:SER:CB	0.47	2.62	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:LEU:HD12	3:A:43:LEU:H	0.47	1.69	7	1
3:A:96:LEU:CB	3:B:37:PRO:CB	0.47	2.92	7	2
3:B:42:MET:N	3:B:45:PRO:CG	0.47	2.77	10	2
3:A:38:LEU:C	3:A:40:ASN:H	0.47	2.18	8	1
3:A:35:HIS:O	3:A:39:LEU:CG	0.47	2.62	9	1
3:A:58:VAL:HG21	3:B:41:LEU:HD22	0.47	1.86	9	1
3:A:24:ASP:O	3:A:27:LYS:CG	0.47	2.63	14	3
3:A:22:PHE:CE1	3:A:26:LEU:CD2	0.47	2.98	13	1
3:A:73:ASN:CG	3:A:77:ALA:HA	0.47	2.35	15	1
2:F:15:DA:N7	3:B:80:ALA:CB	0.47	2.77	2	3
3:A:67:SER:CB	3:A:68:GLN:OE1	0.47	2.63	2	1
3:B:44:THR:H	4:B:109:TRP:HA	0.47	1.69	7	2
4:B:201:TRP:CD2	4:B:201:TRP:C	0.47	2.93	2	2
3:B:71:LEU:O	3:B:74:GLU:N	0.47	2.48	3	1
3:A:27:LYS:O	3:A:28:ASN:C	0.47	2.57	10	3
3:A:81:THR:HG1	4:B:109:TRP:CG	0.47	2.27	14	2
3:A:56:ARG:CD	3:A:75:LEU:HD11	0.47	2.40	5	1
3:B:72:LYS:HZ2	3:B:72:LYS:HB3	0.47	1.69	5	1
3:B:82:ILE:HD12	3:B:83:THR:OG1	0.47	2.10	7	2
2:F:3:DT:OP2	3:A:68:GLN:CD	0.47	2.58	14	1
3:A:99:TRP:CD1	3:B:34:LEU:HD23	0.47	2.45	15	1
2:F:3:DT:H73	3:A:82:ILE:HD11	0.47	1.86	5	2
3:B:40:ASN:C	3:B:42:MET:N	0.47	2.73	1	2
2:F:11:DC:H2"	2:F:12:DA:H8	0.47	1.69	6	5
3:A:51:LEU:CD2	3:B:22:PHE:CD1	0.47	2.98	8	2
3:B:36:LEU:O	3:B:40:ASN:CB	0.47	2.63	6	2
1:E:17:DT:O2	1:E:18:DA:C8	0.47	2.68	3	1
3:A:41:LEU:HD12	3:A:41:LEU:H	0.47	1.70	3	1
3:A:82:ILE:CD1	3:A:83:THR:N	0.47	2.78	4	1
3:B:99:TRP:O	3:B:102:GLU:N	0.47	2.48	13	3
1:E:15:DG:N7	3:A:79:ILE:CB	0.47	2.70	6	2
3:A:91:ALA:HB1	3:B:40:ASN:CG	0.47	2.34	7	1
3:B:93:PRO:CA	3:B:97:ARG:HB2	0.47	2.40	10	2
3:B:54:ARG:HA	4:B:201:TRP:N	0.47	2.25	8	1
2:F:13:DC:P	3:A:43:LEU:O	0.47	2.73	10	3
3:B:62:LEU:HD21	3:B:97:ARG:HH22	0.47	1.70	9	1
3:A:50:ALA:O	3:A:54:ARG:CD	0.47	2.62	10	1
3:A:65:GLU:O	3:A:66:MET:CB	0.47	2.63	13	2
3:B:42:MET:O	3:B:43:LEU:HB3	0.47	2.10	13	1
2:F:2:DG:C5	3:A:69:ARG:NH1	0.47	2.83	14	1
3:B:42:MET:HG3	3:B:45:PRO:HG3	0.47	1.86	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:9:DT:C2'	1:E:10:DG:C8	0.46	2.98	7	2
3:A:57:ILE:O	3:A:61:LEU:HB2	0.46	2.10	4	3
3:A:88:SER:C	3:A:90:LYS:N	0.46	2.68	9	4
3:A:54:ARG:NE	3:B:42:MET:SD	0.46	2.88	6	1
3:B:84:ARG:HB3	4:B:201:TRP:CZ2	0.46	2.45	6	1
2:F:3:DT:OP2	3:A:67:SER:C	0.46	2.58	7	1
2:F:3:DT:OP2	3:A:67:SER:HB3	0.46	2.10	7	1
3:B:33:ASP:HA	3:B:36:LEU:HD12	0.46	1.86	8	3
3:B:71:LEU:HD22	3:B:74:GLU:HB2	0.46	1.86	8	1
3:B:95:GLU:O	3:B:96:LEU:HD22	0.46	2.08	8	1
2:F:5:DC:O5'	2:F:5:DC:H6	0.46	1.93	9	3
3:A:99:TRP:CE3	3:A:100:LEU:N	0.46	2.82	12	1
1:E:14:DT:C2'	3:A:76:GLY:O	0.46	2.63	13	1
3:A:30:TYR:CE2	3:B:23:VAL:HG22	0.46	2.45	13	1
3:A:43:LEU:HA	3:B:54:ARG:NE	0.46	2.25	1	1
3:A:78:GLY:O	3:A:82:ILE:CB	0.46	2.62	5	5
3:B:42:MET:HB2	3:B:45:PRO:HG3	0.46	1.87	1	2
3:B:54:ARG:HD3	4:B:201:TRP:O	0.46	2.10	2	1
1:E:5:DC:C5	3:B:69:ARG:HD2	0.46	2.44	3	1
1:E:15:DG:P	3:A:73:ASN:OD1	0.46	2.73	3	2
3:A:55:VAL:O	3:A:56:ARG:C	0.46	2.58	10	2
3:A:68:GLN:O	3:A:70:GLU:N	0.46	2.48	3	1
3:A:51:LEU:CG	3:B:19:TRP:CZ3	0.46	2.98	4	2
3:A:78:GLY:CA	3:A:81:THR:HG22	0.46	2.38	4	2
3:A:84:ARG:HB3	3:B:43:LEU:HD13	0.46	1.87	5	1
3:B:102:GLU:HA	3:B:106:LYS:HB3	0.46	1.87	5	2
3:A:50:ALA:O	3:A:54:ARG:HB2	0.46	2.09	8	2
3:A:43:LEU:HA	3:B:54:ARG:HD3	0.46	1.87	7	1
3:B:35:HIS:O	3:B:39:LEU:HD23	0.46	2.10	7	1
3:B:68:GLN:O	3:B:69:ARG:HB2	0.46	2.08	7	1
3:B:63:ARG:O	3:B:65:GLU:N	0.46	2.49	8	1
3:A:38:LEU:O	3:A:42:MET:CB	0.46	2.63	12	1
3:A:34:LEU:CA	3:B:96:LEU:HD23	0.46	2.40	14	1
3:A:72:LYS:HZ2	3:A:79:ILE:HG12	0.46	1.69	14	1
3:B:44:THR:O	3:B:46:ASP:N	0.46	2.48	1	1
1:E:13:DC:P	4:B:109:TRP:C	0.46	2.98	2	1
1:E:15:DG:C2	2:F:7:DA:C2	0.46	3.03	4	4
3:A:67:SER:HB3	3:A:72:LYS:HB3	0.46	1.87	6	2
3:B:62:LEU:HD11	3:B:100:LEU:HD11	0.46	1.88	3	1
3:B:72:LYS:CD	3:B:72:LYS:N	0.46	2.78	3	1
3:A:22:PHE:CE2	3:A:38:LEU:CD2	0.46	2.98	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:40:ASN:ND2	3:B:91:ALA:HB1	0.46	2.24	5	1
3:B:45:PRO:CD	4:B:109:TRP:OXT	0.46	2.64	15	1
3:B:39:LEU:HD23	3:B:39:LEU:C	0.46	2.36	1	1
3:B:49:GLU:O	3:B:53:THR:HB	0.46	2.11	13	3
3:B:99:TRP:CD2	3:B:99:TRP:C	0.46	2.93	14	5
3:A:66:MET:O	3:A:70:GLU:CG	0.46	2.63	14	2
3:A:80:ALA:O	3:A:84:ARG:NE	0.46	2.48	2	1
3:A:43:LEU:CD1	3:A:44:THR:OG1	0.46	2.64	3	1
3:A:53:THR:HG23	3:A:76:GLY:C	0.46	2.34	4	1
3:A:69:ARG:CA	3:A:72:LYS:CE	0.46	2.94	4	1
3:A:81:THR:OG1	4:B:109:TRP:CE2	0.46	2.68	4	1
3:A:96:LEU:HD23	3:B:37:PRO:HB2	0.46	1.86	4	1
3:A:23:VAL:HG21	3:B:35:HIS:ND1	0.46	2.26	6	1
3:A:78:GLY:C	3:A:82:ILE:CG2	0.46	2.88	7	1
3:B:38:LEU:C	3:B:41:LEU:HD22	0.46	2.35	8	1
3:B:92:ALA:CB	3:B:94:VAL:HG22	0.46	2.41	8	1
2:F:3:DT:H73	3:A:68:GLN:NE2	0.46	2.25	11	1
3:A:58:VAL:CG1	3:A:100:LEU:HD11	0.46	2.41	12	1
3:A:40:ASN:O	3:A:45:PRO:CB	0.46	2.63	13	1
3:B:94:VAL:HA	3:B:97:ARG:HB2	0.46	1.87	13	1
3:A:43:LEU:N	3:B:54:ARG:HD2	0.46	2.25	14	1
3:A:84:ARG:CD	3:B:43:LEU:HD22	0.46	2.38	14	1
2:F:3:DT:H72	3:A:79:ILE:HG12	0.46	1.87	15	1
3:B:96:LEU:C	3:B:98:GLN:N	0.46	2.73	1	14
3:A:84:ARG:HG3	3:B:43:LEU:HD13	0.46	1.86	2	1
3:B:85:GLY:C	3:B:87:ASN:N	0.46	2.71	10	5
3:A:30:TYR:HD1	3:A:35:HIS:CB	0.46	2.23	7	2
3:B:82:ILE:HD12	3:B:82:ILE:C	0.46	2.34	3	1
3:B:53:THR:HG21	3:B:77:ALA:CB	0.46	2.39	5	1
3:A:51:LEU:HD12	3:A:52:GLY:CA	0.46	2.41	6	1
3:B:100:LEU:HD23	3:B:100:LEU:C	0.46	2.34	7	5
3:A:96:LEU:HA	3:B:37:PRO:CB	0.46	2.40	8	1
3:A:41:LEU:CD1	3:A:41:LEU:H	0.46	2.23	9	1
3:A:23:VAL:O	3:A:27:LYS:CD	0.46	2.64	10	1
3:B:35:HIS:CE1	3:B:36:LEU:CG	0.46	2.99	10	1
3:B:71:LEU:N	3:B:71:LEU:HD12	0.46	2.25	11	1
3:A:96:LEU:CD2	3:B:36:LEU:O	0.46	2.63	13	2
3:B:33:ASP:O	3:B:34:LEU:CB	0.46	2.64	12	1
1:E:14:DT:H2'	3:A:77:ALA:HA	0.46	1.87	13	1
3:A:35:HIS:NE2	3:B:99:TRP:CH2	0.46	2.83	13	1
3:A:72:LYS:O	3:A:78:GLY:CA	0.46	2.64	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:LEU:O	3:B:99:TRP:CH2	0.46	2.69	14	1
1:E:10:DG:N2	2:F:12:DA:C5	0.46	2.83	15	1
1:E:16:DG:C4	1:E:17:DT:C5	0.46	3.04	10	2
3:A:19:TRP:CZ2	3:B:35:HIS:ND1	0.46	2.84	3	1
3:A:79:ILE:C	3:A:81:THR:N	0.46	2.71	13	4
3:A:55:VAL:CB	3:B:42:MET:HE2	0.46	2.41	4	1
3:A:64:GLY:O	3:A:65:GLU:CB	0.46	2.64	10	3
3:A:26:LEU:HD21	3:A:38:LEU:CD1	0.46	2.39	6	1
3:B:43:LEU:CD1	4:B:109:TRP:CD1	0.46	2.99	6	1
3:B:63:ARG:O	3:B:64:GLY:C	0.46	2.57	8	2
1:E:19:DC:O5'	1:E:19:DC:C6	0.46	2.68	9	1
3:B:47:GLU:HB2	3:B:50:ALA:HB3	0.46	1.87	9	1
3:B:24:ASP:O	3:B:28:ASN:HB2	0.46	2.11	10	1
3:A:68:GLN:HA	3:A:72:LYS:CE	0.46	2.41	11	1
3:A:72:LYS:CB	3:A:78:GLY:CA	0.46	2.94	13	1
3:A:26:LEU:CD1	3:A:35:HIS:NE2	0.46	2.78	14	1
3:B:27:LYS:HE2	3:B:27:LYS:H	0.46	1.68	14	1
3:B:63:ARG:O	3:B:64:GLY:O	0.46	2.33	14	1
3:A:51:LEU:HA	3:A:54:ARG:HG2	0.46	1.88	9	2
3:A:26:LEU:O	3:A:30:TYR:CD1	0.46	2.69	4	3
1:E:7:DC:C2	2:F:15:DA:C2	0.46	3.04	7	2
1:E:16:DG:O6	2:F:4:DA:N6	0.46	2.49	14	3
3:A:35:HIS:NE2	3:A:36:LEU:CD1	0.46	2.79	4	1
3:A:33:ASP:O	3:A:37:PRO:CD	0.46	2.64	14	4
1:E:3:DT:H6	1:E:3:DT:O5'	0.46	1.94	10	4
1:E:13:DC:OP1	3:A:50:ALA:HA	0.46	2.10	6	1
3:B:43:LEU:HB2	4:B:109:TRP:CE2	0.46	2.45	6	1
1:E:15:DG:OP2	3:A:77:ALA:N	0.46	2.48	7	1
3:A:54:ARG:CG	4:B:109:TRP:N	0.46	2.79	8	1
3:B:100:LEU:O	3:B:104:LEU:HD21	0.46	2.11	10	1
2:F:2:DG:H3'	3:A:68:GLN:HB3	0.46	1.87	12	1
3:B:43:LEU:CA	3:B:45:PRO:HD2	0.46	2.39	13	1
3:A:56:ARG:CA	3:A:59:GLU:HG3	0.46	2.41	11	5
3:B:72:LYS:HE3	3:B:82:ILE:CD1	0.46	2.40	1	2
1:E:15:DG:N9	3:A:79:ILE:HD12	0.46	2.23	5	1
3:A:41:LEU:HB2	3:B:91:ALA:HB3	0.46	1.88	5	1
3:A:42:MET:HG3	3:B:54:ARG:CB	0.46	2.40	6	1
3:A:43:LEU:HD11	3:B:53:THR:HB	0.46	1.87	6	1
3:A:39:LEU:HA	3:A:43:LEU:HD21	0.46	1.88	7	1
2:F:17:DT:C2'	2:F:18:DA:C8	0.46	2.99	8	1
3:B:42:MET:C	3:B:45:PRO:CG	0.46	2.87	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:F:3:DT:P	3:A:82:ILE:CD1	0.46	3.03	9	1
3:A:34:LEU:HD23	3:A:38:LEU:CD1	0.46	2.41	9	1
3:A:42:MET:HB3	3:B:54:ARG:CA	0.46	2.41	10	1
3:A:25:LEU:O	3:A:35:HIS:NE2	0.46	2.49	13	1
3:B:34:LEU:CD1	3:B:38:LEU:HD12	0.46	2.40	14	1
2:F:3:DT:H73	3:A:68:GLN:CA	0.46	2.35	15	1
3:B:77:ALA:O	3:B:81:THR:CB	0.46	2.64	15	1
3:A:35:HIS:CE1	3:A:36:LEU:CD2	0.46	2.98	10	2
3:A:92:ALA:HB1	3:A:96:LEU:HD12	0.46	1.87	3	1
2:F:3:DT:P	3:A:82:ILE:HD13	0.46	2.50	4	1
3:A:84:ARG:HB3	3:B:43:LEU:HG	0.46	1.88	4	1
3:B:46:ASP:O	3:B:48:ARG:N	0.46	2.49	10	3
3:A:96:LEU:O	3:B:37:PRO:HB3	0.46	2.11	9	3
3:B:39:LEU:O	3:B:45:PRO:CB	0.46	2.64	5	1
3:A:41:LEU:O	3:B:58:VAL:HG11	0.46	2.11	7	1
3:A:81:THR:HG23	4:B:109:TRP:CD2	0.46	2.46	7	1
3:A:33:ASP:C	3:A:34:LEU:HD12	0.46	2.36	8	1
3:B:37:PRO:O	3:B:41:LEU:HD13	0.46	2.11	8	1
3:A:68:GLN:O	3:A:71:LEU:N	0.46	2.41	13	1
3:B:22:PHE:N	3:B:22:PHE:HD1	0.46	2.08	14	1
3:A:35:HIS:NE2	3:B:19:TRP:CD1	0.46	2.83	3	1
3:A:34:LEU:CD1	3:B:96:LEU:O	0.46	2.64	4	1
1:E:16:DG:C5	1:E:17:DT:C4	0.46	3.04	9	2
3:A:19:TRP:CZ2	3:B:39:LEU:CB	0.46	2.99	10	1
3:A:19:TRP:CZ3	3:B:51:LEU:CG	0.46	2.99	11	1
2:F:4:DA:H62	3:A:79:ILE:CG2	0.46	2.24	12	1
3:A:87:ASN:OD1	3:B:43:LEU:HD23	0.46	2.11	13	1
2:F:9:DT:H2'	2:F:10:DA:C8	0.46	2.46	14	1
3:A:62:LEU:HD21	3:A:97:ARG:NH1	0.46	2.25	14	1
3:B:35:HIS:C	3:B:35:HIS:CD2	0.46	2.94	15	1
1:E:15:DG:OP2	3:A:76:GLY:C	0.45	2.59	5	4
3:A:69:ARG:N	3:A:72:LYS:HD3	0.45	2.26	1	1
3:A:96:LEU:HD23	3:B:36:LEU:C	0.45	2.35	1	1
3:A:73:ASN:O	3:A:75:LEU:N	0.45	2.49	2	4
3:A:89:LEU:HD21	3:A:97:ARG:NH2	0.45	2.26	2	1
3:B:53:THR:O	3:B:56:ARG:HB2	0.45	2.11	2	1
3:A:27:LYS:C	3:A:29:ALA:N	0.45	2.73	10	2
3:A:55:VAL:HG13	3:B:42:MET:HE2	0.45	1.86	4	1
3:A:55:VAL:HG22	3:B:42:MET:HE3	0.45	1.88	6	1
1:E:8:DG:C4	2:F:14:DG:N2	0.45	2.84	9	1
3:A:66:MET:O	3:A:66:MET:CG	0.45	2.64	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:54:ARG:HG3	3:B:55:VAL:HG23	0.45	1.87	9	1
3:A:34:LEU:C	3:A:35:HIS:ND1	0.45	2.75	12	1
3:A:34:LEU:CB	3:B:96:LEU:HD23	0.45	2.41	12	1
3:A:68:GLN:O	3:A:68:GLN:HG3	0.45	2.11	12	1
3:A:62:LEU:HB3	3:A:104:LEU:HD23	0.45	1.88	14	1
3:A:84:ARG:CD	3:B:43:LEU:CD1	0.45	2.93	14	1
3:B:42:MET:O	4:B:109:TRP:O	0.45	2.34	15	1
3:A:90:LYS:CE	3:A:91:ALA:N	0.45	2.79	1	1
2:F:17:DT:O5'	2:F:17:DT:H6	0.45	1.94	6	5
3:A:35:HIS:NE2	3:A:36:LEU:HD11	0.45	2.26	4	1
3:B:37:PRO:O	3:B:40:ASN:C	0.45	2.59	4	1
3:B:93:PRO:C	3:B:94:VAL:HG13	0.45	2.37	11	2
3:A:44:THR:OG1	3:B:54:ARG:CZ	0.45	2.64	7	1
3:A:54:ARG:HG2	4:B:109:TRP:N	0.45	2.26	8	1
3:B:61:LEU:C	3:B:61:LEU:HD23	0.45	2.36	9	1
3:B:67:SER:HB3	3:B:82:ILE:CG2	0.45	2.40	9	1
3:A:35:HIS:ND1	3:A:36:LEU:CD2	0.45	2.79	10	1
3:A:38:LEU:HD13	3:B:99:TRP:CH2	0.45	2.46	10	1
3:A:38:LEU:HD12	3:B:99:TRP:HH2	0.45	1.70	11	1
3:A:20:LEU:CD1	3:B:34:LEU:CD2	0.45	2.95	12	1
3:A:54:ARG:HG3	3:A:55:VAL:N	0.45	2.26	13	1
3:B:84:ARG:O	3:B:87:ASN:CG	0.45	2.60	15	1
1:E:17:DT:C2	1:E:18:DA:C6	0.45	3.05	1	1
3:A:22:PHE:CD1	3:A:43:LEU:HD21	0.45	2.46	1	1
3:A:83:THR:CG2	3:A:84:ARG:N	0.45	2.78	7	4
3:B:79:ILE:HG22	3:B:80:ALA:N	0.45	2.25	2	1
3:A:43:LEU:HG	3:B:53:THR:OG1	0.45	2.12	4	1
3:B:35:HIS:CE1	3:B:36:LEU:CD2	0.45	2.99	6	2
3:B:42:MET:C	3:B:44:THR:H	0.45	2.13	6	1
3:A:57:ILE:HD13	3:A:57:ILE:N	0.45	2.26	8	1
3:A:97:ARG:O	3:A:101:GLU:CB	0.45	2.61	8	1
3:A:60:GLU:CB	3:A:66:MET:HB2	0.45	2.41	9	1
3:A:51:LEU:HD23	3:B:22:PHE:CE2	0.45	2.45	10	1
2:F:14:DG:OP2	3:B:53:THR:HG21	0.45	2.11	14	1
3:A:60:GLU:OE2	3:A:71:LEU:HD21	0.45	2.10	15	1
3:A:90:LYS:CD	3:A:91:ALA:N	0.45	2.80	1	2
3:A:96:LEU:HG	3:B:37:PRO:HB3	0.45	1.88	15	3
3:A:99:TRP:CD1	3:B:34:LEU:HB3	0.45	2.46	13	4
3:A:84:ARG:HB3	4:B:109:TRP:CZ2	0.45	2.46	7	2
3:A:55:VAL:CG2	3:B:42:MET:CE	0.45	2.95	3	2
3:B:71:LEU:O	3:B:73:ASN:N	0.45	2.50	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:45:PRO:CD	4:B:201:TRP:C	0.45	2.88	11	6
3:A:34:LEU:HD23	3:B:99:TRP:CD1	0.45	2.46	5	1
3:B:43:LEU:HD23	3:B:44:THR:OG1	0.45	2.11	5	1
3:B:72:LYS:HE3	3:B:82:ILE:HD11	0.45	1.88	5	1
3:A:72:LYS:HD2	3:A:79:ILE:HG23	0.45	1.88	14	2
3:A:42:MET:O	4:B:201:TRP:CA	0.45	2.64	8	1
3:A:48:ARG:HG3	3:A:49:GLU:N	0.45	2.27	15	2
1:E:11:DT:H73	1:E:11:DT:OP2	0.45	2.10	11	1
3:B:46:ASP:O	3:B:47:GLU:C	0.45	2.56	14	2
3:B:97:ARG:O	3:B:98:GLN:C	0.45	2.57	3	6
1:E:18:DA:C2'	1:E:19:DC:C5	0.45	3.00	12	7
3:A:54:ARG:NH2	4:B:109:TRP:O	0.45	2.50	2	1
3:A:67:SER:C	3:A:68:GLN:CG	0.45	2.88	2	1
3:A:57:ILE:HD13	4:B:109:TRP:HZ3	0.45	1.72	3	2
3:A:88:SER:O	3:A:89:LEU:C	0.45	2.58	9	4
3:A:101:GLU:O	3:A:105:LEU:N	0.45	2.50	12	7
3:A:59:GLU:OE2	3:A:60:GLU:CG	0.45	2.64	9	1
3:A:22:PHE:O	3:A:26:LEU:HB2	0.45	2.11	10	1
3:A:57:ILE:HG12	4:B:109:TRP:CE3	0.45	2.46	11	1
2:F:3:DT:OP2	3:A:68:GLN:CB	0.45	2.65	14	1
3:A:96:LEU:HD22	3:B:36:LEU:CB	0.45	2.41	14	1
3:B:22:PHE:HB2	3:B:26:LEU:CD2	0.45	2.38	14	1
3:B:23:VAL:C	3:B:27:LYS:CE	0.45	2.89	14	1
3:B:35:HIS:C	3:B:36:LEU:CD2	0.45	2.83	14	1
1:E:9:DT:H2''	1:E:10:DG:C8	0.45	2.46	1	2
3:B:43:LEU:C	3:B:43:LEU:HD22	0.45	2.37	11	4
3:B:72:LYS:NZ	3:B:72:LYS:HB3	0.45	2.26	1	1
3:B:93:PRO:O	3:B:94:VAL:C	0.45	2.58	10	4
1:E:7:DC:O2	1:E:8:DG:C8	0.45	2.70	3	5
3:B:56:ARG:HA	3:B:59:GLU:OE2	0.45	2.12	2	1
3:A:45:PRO:CB	3:B:91:ALA:HB2	0.45	2.32	3	1
3:A:23:VAL:HG11	3:B:30:TYR:O	0.45	2.12	5	1
1:E:17:DT:H2'	1:E:18:DA:N7	0.45	2.26	6	2
3:A:62:LEU:HD21	3:A:97:ARG:HH21	0.45	1.70	6	1
3:A:81:THR:HA	4:B:109:TRP:NE1	0.45	2.26	6	1
1:E:12:DA:C2'	1:E:13:DC:O5'	0.45	2.64	10	3
3:A:52:GLY:HA2	3:B:22:PHE:CE2	0.45	2.47	15	2
2:F:17:DT:H6	2:F:17:DT:O5'	0.45	1.95	9	3
3:A:72:LYS:HD2	3:A:73:ASN:HB2	0.45	1.86	15	2
3:B:19:TRP:O	3:B:20:LEU:HD22	0.45	2.09	14	2
3:A:19:TRP:CZ2	3:B:35:HIS:HB3	0.45	2.47	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:F:3:DT:C4	3:A:69:ARG:NH1	0.45	2.84	14	1
3:A:84:ARG:O	3:A:85:GLY:C	0.45	2.60	1	5
3:B:72:LYS:CG	3:B:79:ILE:CA	0.45	2.94	1	2
3:A:96:LEU:CG	3:B:37:PRO:HB2	0.45	2.42	4	1
3:B:59:GLU:O	3:B:63:ARG:CG	0.45	2.65	5	1
3:B:103:VAL:C	3:B:104:LEU:HD23	0.45	2.37	5	1
3:A:96:LEU:CB	3:B:37:PRO:HG3	0.45	2.42	7	1
3:A:30:TYR:HA	3:A:35:HIS:ND1	0.45	2.27	8	2
3:A:42:MET:C	4:B:201:TRP:HA	0.45	2.35	8	1
2:F:3:DT:P	3:A:67:SER:OG	0.45	2.75	11	1
2:F:3:DT:H2'	3:A:83:THR:OG1	0.45	2.12	13	1
3:A:79:ILE:O	3:A:81:THR:N	0.45	2.50	13	1
3:B:48:ARG:C	3:B:49:GLU:CG	0.45	2.90	14	2
3:A:55:VAL:CG1	3:B:22:PHE:CE2	0.45	2.98	14	1
3:A:84:ARG:HD2	3:B:43:LEU:CD2	0.45	2.39	14	1
3:B:71:LEU:HD13	3:B:74:GLU:HB2	0.45	1.89	1	1
3:A:55:VAL:CG2	3:B:38:LEU:CD2	0.45	2.95	2	1
2:F:3:DT:H72	3:A:72:LYS:NZ	0.45	2.26	3	1
3:A:55:VAL:CG1	3:B:22:PHE:CD1	0.45	2.99	12	2
1:E:13:DC:OP2	4:B:109:TRP:HB2	0.45	2.11	8	1
3:A:34:LEU:CD2	3:B:99:TRP:CH2	0.45	3.00	9	1
3:A:43:LEU:CG	3:B:53:THR:HG23	0.45	2.41	9	1
3:A:54:ARG:C	3:A:57:ILE:HG13	0.45	2.36	9	1
3:B:55:VAL:HG12	3:B:55:VAL:O	0.45	2.12	15	2
1:E:12:DA:C4'	4:B:109:TRP:OXT	0.45	2.64	14	1
3:A:54:ARG:HG3	3:B:42:MET:HG2	0.45	1.88	1	1
3:B:38:LEU:O	3:B:41:LEU:HD21	0.45	2.11	1	1
3:B:56:ARG:C	3:B:82:ILE:HG22	0.45	2.36	2	1
3:A:55:VAL:HA	3:B:42:MET:CE	0.45	2.41	4	1
3:A:78:GLY:C	3:A:80:ALA:N	0.45	2.74	14	2
3:B:22:PHE:C	3:B:24:ASP:N	0.45	2.75	7	2
3:B:67:SER:O	3:B:68:GLN:HB3	0.45	2.11	13	2
3:B:22:PHE:CD1	3:B:26:LEU:HD21	0.45	2.46	7	1
3:A:34:LEU:HG	3:B:99:TRP:CZ2	0.45	2.47	9	1
3:A:30:TYR:C	3:B:23:VAL:HG11	0.45	2.36	15	2
3:A:51:LEU:HA	3:A:55:VAL:CG2	0.45	2.42	12	1
3:A:72:LYS:HA	3:A:78:GLY:HA2	0.45	1.88	13	1
3:A:74:GLU:O	3:A:75:LEU:CD2	0.45	2.65	13	1
3:B:67:SER:CB	3:B:82:ILE:CD1	0.45	2.95	13	1
3:A:19:TRP:CD1	3:B:35:HIS:CG	0.45	3.05	14	1
3:B:38:LEU:HD23	3:B:41:LEU:CD1	0.45	2.42	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:17:DT:C2	1:E:18:DA:C5	0.45	3.05	1	1
3:B:73:ASN:O	3:B:74:GLU:C	0.45	2.58	3	3
1:E:15:DG:H2'	3:A:73:ASN:ND2	0.45	2.27	2	1
3:A:60:GLU:O	3:A:64:GLY:CA	0.45	2.65	3	1
2:F:3:DT:H73	3:A:72:LYS:CE	0.45	2.40	5	4
1:E:16:DG:N7	3:A:79:ILE:HD13	0.45	2.27	5	1
3:A:27:LYS:O	3:A:31:GLN:NE2	0.45	2.49	15	2
2:F:2:DG:C5	3:A:69:ARG:NH2	0.45	2.85	7	1
3:A:72:LYS:HA	3:A:78:GLY:HA3	0.45	1.89	7	1
1:E:3:DT:H2''	1:E:4:DA:C8	0.45	2.47	8	1
3:B:22:PHE:CE1	3:B:26:LEU:HG	0.45	2.47	8	1
4:B:201:TRP:CA	4:B:201:TRP:CE3	0.45	3.00	8	1
3:A:26:LEU:O	3:A:28:ASN:N	0.45	2.50	9	4
3:A:71:LEU:HD23	3:A:71:LEU:C	0.45	2.37	10	1
3:B:20:LEU:HD22	3:B:20:LEU:N	0.45	2.25	10	2
3:A:62:LEU:CB	3:A:104:LEU:HD21	0.45	2.41	11	1
3:A:25:LEU:CD2	3:B:103:VAL:CG2	0.45	2.95	14	1
3:A:38:LEU:CD2	3:A:42:MET:SD	0.45	3.05	14	1
3:A:30:TYR:HA	3:A:35:HIS:CG	0.44	2.47	2	3
3:A:84:ARG:HB3	3:B:43:LEU:CB	0.44	2.41	1	1
3:B:39:LEU:HA	3:B:45:PRO:CB	0.44	2.40	1	1
3:A:69:ARG:N	3:A:72:LYS:HE3	0.44	2.27	3	1
3:B:43:LEU:O	3:B:43:LEU:CD2	0.44	2.65	6	1
1:E:12:DA:N3	1:E:13:DC:O4'	0.44	2.50	8	4
3:A:42:MET:C	3:A:43:LEU:HG	0.44	2.36	7	1
3:A:43:LEU:N	3:B:54:ARG:CG	0.44	2.80	10	1
3:A:74:GLU:O	3:A:75:LEU:HD12	0.44	2.13	12	1
3:A:56:ARG:NH1	3:A:60:GLU:HG3	0.44	2.26	13	1
3:A:39:LEU:CD1	3:A:48:ARG:HB3	0.44	2.35	14	1
3:A:57:ILE:CD1	4:B:109:TRP:CH2	0.44	3.00	14	1
3:B:30:TYR:CD1	3:B:35:HIS:ND1	0.44	2.85	15	1
3:A:40:ASN:CB	3:B:91:ALA:CB	0.44	2.93	2	2
3:B:87:ASN:C	3:B:89:LEU:N	0.44	2.75	10	3
3:A:23:VAL:HG21	3:B:34:LEU:CD1	0.44	2.42	3	1
3:A:45:PRO:O	3:A:48:ARG:CB	0.44	2.65	5	2
3:A:62:LEU:HD11	3:A:97:ARG:CZ	0.44	2.42	5	1
3:A:34:LEU:HD21	3:A:38:LEU:CD1	0.44	2.41	6	1
3:B:96:LEU:HD12	3:B:96:LEU:H	0.44	1.71	7	1
3:A:96:LEU:CA	3:B:37:PRO:CB	0.44	2.95	8	2
3:A:47:GLU:CD	3:A:50:ALA:CB	0.44	2.90	9	1
3:A:103:VAL:HG23	3:A:104:LEU:HD13	0.44	1.89	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:40:ASN:C	3:A:45:PRO:HB3	0.44	2.37	13	1
3:A:29:ALA:CB	3:B:99:TRP:CZ2	0.44	2.96	14	1
3:B:45:PRO:HG3	4:B:109:TRP:OXT	0.44	2.11	15	1
1:E:17:DT:C2'	1:E:18:DA:N7	0.44	2.80	6	2
3:A:30:TYR:CB	3:B:23:VAL:CG1	0.44	2.96	11	4
3:A:96:LEU:H	3:A:96:LEU:HD12	0.44	1.72	4	1
3:B:35:HIS:CA	3:B:37:PRO:HD2	0.44	2.42	9	2
3:A:29:ALA:CB	3:A:34:LEU:HG	0.44	2.41	6	1
3:A:57:ILE:HG12	3:A:81:THR:O	0.44	2.12	7	1
3:A:67:SER:HA	3:A:71:LEU:CB	0.44	2.43	8	2
3:A:96:LEU:HD23	3:B:41:LEU:CD1	0.44	2.37	10	1
2:F:3:DT:H73	3:A:68:GLN:CD	0.44	2.37	11	1
3:A:73:ASN:CA	3:A:79:ILE:HD11	0.44	2.42	14	2
3:A:39:LEU:HD21	3:A:48:ARG:CB	0.44	2.43	14	1
1:E:13:DC:N3	1:E:14:DT:C4	0.44	2.85	3	4
3:B:45:PRO:O	3:B:47:GLU:N	0.44	2.49	1	2
2:F:12:DA:H2'	2:F:13:DC:C6	0.44	2.47	2	2
3:A:58:VAL:HG21	3:B:41:LEU:HG	0.44	1.88	2	2
3:A:69:ARG:N	3:A:72:LYS:HE2	0.44	2.26	2	2
3:B:19:TRP:CD1	3:B:19:TRP:C	0.44	2.95	15	3
3:B:50:ALA:HA	3:B:54:ARG:CZ	0.44	2.42	2	1
3:B:94:VAL:HG13	3:B:95:GLU:N	0.44	2.26	4	4
3:A:43:LEU:CD1	3:A:43:LEU:C	0.44	2.88	3	1
3:A:45:PRO:CD	4:B:201:TRP:HA	0.44	2.42	5	1
3:B:44:THR:N	4:B:109:TRP:HA	0.44	2.26	6	1
1:E:12:DA:OP1	4:B:109:TRP:O	0.44	2.36	7	1
1:E:5:DC:O5'	1:E:5:DC:C6	0.44	2.70	8	2
3:A:57:ILE:HG21	3:A:81:THR:CG2	0.44	2.42	8	1
1:E:18:DA:N6	3:A:69:ARG:NH1	0.44	2.66	9	1
3:A:99:TRP:HB3	3:B:37:PRO:CG	0.44	2.43	9	1
3:A:62:LEU:HB3	3:A:104:LEU:HD21	0.44	1.88	11	1
3:A:68:GLN:O	3:A:68:GLN:CD	0.44	2.60	15	1
3:A:43:LEU:C	3:B:54:ARG:NH1	0.44	2.75	1	1
3:B:78:GLY:C	3:B:80:ALA:N	0.44	2.74	7	4
1:E:12:DA:C2	1:E:13:DC:H1'	0.44	2.47	14	4
3:A:72:LYS:NZ	3:A:73:ASN:ND2	0.44	2.65	2	1
3:A:75:LEU:O	3:A:75:LEU:CD2	0.44	2.55	2	1
3:A:34:LEU:HD13	3:B:96:LEU:CB	0.44	2.41	4	1
3:A:72:LYS:CG	3:A:79:ILE:CG1	0.44	2.95	4	2
3:A:55:VAL:HG13	3:B:38:LEU:CD2	0.44	2.42	6	1
2:F:3:DT:C7	3:A:68:GLN:HA	0.44	2.42	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:96:LEU:O	3:A:98:GLN:N	0.44	2.50	8	1
3:A:43:LEU:CD2	3:B:53:THR:HG23	0.44	2.42	9	1
1:E:12:DA:H2''	1:E:13:DC:H5'	0.44	1.90	13	1
3:A:78:GLY:HA2	3:A:82:ILE:HG21	0.44	1.90	13	1
3:B:93:PRO:HA	3:B:96:LEU:HD21	0.44	1.89	13	1
3:A:96:LEU:CB	3:B:37:PRO:HB2	0.44	2.43	15	1
3:A:96:LEU:HD22	3:B:41:LEU:CB	0.44	2.42	15	1
3:A:47:GLU:CA	3:A:50:ALA:HB3	0.44	2.42	1	1
1:E:18:DA:C4	2:F:4:DA:C2	0.44	3.06	3	1
3:A:91:ALA:O	3:B:40:ASN:HB3	0.44	2.12	4	1
3:B:37:PRO:O	3:B:41:LEU:CD1	0.44	2.65	5	1
1:E:12:DA:O3'	4:B:109:TRP:N	0.44	2.51	6	1
1:E:16:DG:O5'	1:E:16:DG:C8	0.44	2.66	7	1
3:A:96:LEU:HG	3:B:34:LEU:HD13	0.44	1.89	7	1
3:B:94:VAL:HG23	3:B:95:GLU:OE1	0.44	2.13	9	1
3:A:84:ARG:HD2	3:B:43:LEU:CG	0.44	2.43	10	1
3:A:99:TRP:HB2	3:B:34:LEU:CD2	0.44	2.42	10	1
3:A:82:ILE:CG1	3:A:83:THR:N	0.44	2.81	13	1
3:A:43:LEU:CD1	3:B:53:THR:CB	0.44	2.96	14	1
3:B:42:MET:O	4:B:109:TRP:C	0.44	2.60	15	1
3:A:38:LEU:CD2	3:A:42:MET:HB3	0.44	2.43	1	1
3:A:29:ALA:HB2	3:B:99:TRP:CD2	0.44	2.45	2	1
3:B:20:LEU:N	3:B:20:LEU:HD13	0.44	2.28	2	1
3:A:35:HIS:O	3:A:38:LEU:HB3	0.44	2.13	3	2
3:B:73:ASN:HB2	3:B:79:ILE:CG1	0.44	2.42	3	5
3:A:19:TRP:CE3	3:B:51:LEU:CG	0.44	3.01	10	2
3:B:29:ALA:HA	3:B:34:LEU:HB2	0.44	1.89	5	1
1:E:14:DT:P	3:A:76:GLY:O	0.44	2.76	10	2
3:A:44:THR:CB	3:A:47:GLU:HB3	0.44	2.43	7	1
3:B:97:ARG:O	3:B:100:LEU:N	0.44	2.50	7	1
3:A:39:LEU:O	3:A:44:THR:O	0.44	2.36	1	3
3:A:43:LEU:HA	3:B:54:ARG:HD2	0.44	1.90	1	1
3:B:53:THR:CG2	3:B:54:ARG:N	0.44	2.80	1	1
1:E:14:DT:OP2	3:A:76:GLY:O	0.44	2.36	12	5
3:A:93:PRO:O	3:A:95:GLU:N	0.44	2.51	4	3
2:F:11:DC:C2'	2:F:12:DA:N7	0.44	2.81	5	1
3:B:41:LEU:CD2	3:B:42:MET:N	0.44	2.71	6	1
3:B:22:PHE:O	3:B:23:VAL:C	0.44	2.61	7	1
3:B:22:PHE:CA	3:B:26:LEU:HD23	0.44	2.43	7	1
3:A:81:THR:O	3:A:83:THR:N	0.44	2.51	9	2
3:B:97:ARG:CZ	3:B:97:ARG:HA	0.44	2.43	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:73:ASN:CG	3:A:79:ILE:HD11	0.44	2.38	11	1
2:F:2:DG:N7	3:A:69:ARG:CZ	0.44	2.80	3	1
3:A:26:LEU:CD1	3:A:30:TYR:CE2	0.44	3.01	3	1
3:A:92:ALA:CB	3:A:96:LEU:HB3	0.44	2.43	3	1
3:A:101:GLU:HB3	3:A:106:LYS:CA	0.44	2.43	4	2
3:B:51:LEU:O	3:B:52:GLY:C	0.44	2.61	4	1
3:B:39:LEU:HG	3:B:40:ASN:N	0.44	2.25	6	1
3:A:54:ARG:O	3:A:57:ILE:N	0.44	2.44	7	1
3:A:84:ARG:O	3:A:87:ASN:ND2	0.44	2.47	7	1
1:E:20:DA:O5'	1:E:20:DA:C8	0.44	2.69	8	1
3:B:61:LEU:N	3:B:61:LEU:HD23	0.44	2.28	10	1
3:A:68:GLN:O	3:A:72:LYS:N	0.44	2.51	13	1
1:E:13:DC:OP1	4:B:109:TRP:CB	0.43	2.66	1	1
2:F:3:DT:H73	3:A:72:LYS:HD2	0.43	1.90	1	1
1:E:13:DC:C6	1:E:14:DT:C7	0.43	3.01	3	1
2:F:5:DC:C2	2:F:6:DC:C2	0.43	3.06	3	1
2:F:15:DA:OP2	3:B:73:ASN:OD1	0.43	2.35	11	2
3:B:69:ARG:H	3:B:79:ILE:HD11	0.43	1.73	4	1
3:A:96:LEU:HD23	3:B:37:PRO:CB	0.43	2.43	7	1
2:F:3:DT:C5	3:A:79:ILE:CD1	0.43	3.01	15	3
3:A:42:MET:O	3:A:43:LEU:HD23	0.43	2.12	9	1
3:A:68:GLN:OE1	3:A:69:ARG:HD2	0.43	2.13	10	1
3:B:57:ILE:HG12	3:B:81:THR:HG22	0.43	1.89	11	1
3:B:72:LYS:N	3:B:72:LYS:HE3	0.43	2.28	11	1
1:E:14:DT:O5'	3:A:77:ALA:CB	0.43	2.66	14	1
3:B:101:GLU:CB	3:B:106:LYS:HB2	0.43	2.43	14	2
1:E:13:DC:P	4:B:109:TRP:OXT	0.43	2.76	2	2
3:B:57:ILE:HG22	3:B:82:ILE:N	0.43	2.28	2	1
3:B:48:ARG:O	3:B:52:GLY:N	0.43	2.51	3	2
3:B:72:LYS:HE3	3:B:82:ILE:CG2	0.43	2.44	3	1
3:A:99:TRP:CD1	3:B:29:ALA:HB2	0.43	2.47	4	1
3:B:67:SER:HA	3:B:72:LYS:NZ	0.43	2.28	4	1
3:B:19:TRP:O	3:B:22:PHE:CB	0.43	2.66	6	1
3:A:44:THR:O	3:A:44:THR:CG2	0.43	2.56	8	1
3:A:42:MET:HE1	3:B:100:LEU:CD1	0.43	2.41	11	1
3:A:84:ARG:HA	3:A:87:ASN:HB2	0.43	1.89	13	2
3:A:32:ASN:O	3:A:35:HIS:CE1	0.43	2.71	8	5
3:B:29:ALA:CB	3:B:34:LEU:O	0.43	2.65	1	2
3:A:39:LEU:C	3:A:39:LEU:CD1	0.43	2.91	2	1
3:A:42:MET:O	3:B:54:ARG:HG2	0.43	2.13	3	1
2:F:5:DC:C4	2:F:6:DC:C5	0.43	3.05	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:26:LEU:CD1	3:A:30:TYR:CZ	0.43	2.91	5	2
3:B:39:LEU:HG	3:B:40:ASN:OD1	0.43	2.13	6	1
3:A:32:ASN:O	3:A:33:ASP:CB	0.43	2.67	9	1
3:A:34:LEU:CD2	3:A:38:LEU:CD1	0.43	2.95	9	1
3:A:65:GLU:C	3:A:67:SER:N	0.43	2.75	9	1
1:E:17:DT:H2''	1:E:18:DA:OP2	0.43	2.12	11	2
3:B:58:VAL:HB	3:B:62:LEU:HD11	0.43	1.89	11	1
3:B:60:GLU:N	3:B:60:GLU:CD	0.43	2.77	14	1
1:E:12:DA:N6	2:F:10:DA:C2	0.43	2.86	1	2
3:A:84:ARG:HD3	3:B:43:LEU:HD12	0.43	1.89	1	1
3:B:37:PRO:HA	3:B:40:ASN:OD1	0.43	2.13	1	1
3:B:83:THR:CG2	3:B:84:ARG:N	0.43	2.81	6	4
1:E:13:DC:N4	1:E:14:DT:O4	0.43	2.51	13	2
3:A:20:LEU:CD1	3:B:34:LEU:HG	0.43	2.42	3	1
3:A:67:SER:HB3	3:A:82:ILE:CG2	0.43	2.44	3	1
3:B:94:VAL:O	3:B:95:GLU:C	0.43	2.62	12	3
2:F:3:DT:H73	3:A:72:LYS:HE2	0.43	1.90	4	1
3:A:91:ALA:HB1	3:B:40:ASN:HD22	0.43	1.72	4	1
1:E:12:DA:H3'	4:B:109:TRP:OXT	0.43	2.13	6	1
3:A:55:VAL:HG11	3:B:38:LEU:HD21	0.43	1.88	6	1
1:E:13:DC:OP1	3:A:54:ARG:HD3	0.43	2.14	7	1
3:A:77:ALA:O	3:A:81:THR:CB	0.43	2.66	7	1
3:A:40:ASN:C	3:B:91:ALA:HB3	0.43	2.35	8	1
3:A:51:LEU:HD22	3:B:19:TRP:CE3	0.43	2.45	10	1
3:B:54:ARG:O	3:B:58:VAL:HG22	0.43	2.14	11	1
3:A:71:LEU:C	3:A:71:LEU:CD1	0.43	2.92	13	1
3:A:35:HIS:NE2	3:A:36:LEU:HG	0.43	2.28	8	2
3:B:57:ILE:HD12	3:B:58:VAL:CA	0.43	2.43	1	1
3:A:18:GLU:CA	3:A:21:ARG:HG3	0.43	2.41	3	1
3:A:92:ALA:HB1	3:A:96:LEU:HB3	0.43	1.89	3	1
3:B:100:LEU:HD22	3:B:104:LEU:HD11	0.43	1.90	4	1
3:A:72:LYS:CE	3:A:79:ILE:HA	0.43	2.39	5	1
3:A:26:LEU:CD2	3:A:26:LEU:N	0.43	2.81	7	2
3:A:40:ASN:O	3:B:91:ALA:HB2	0.43	2.13	6	1
3:A:83:THR:C	3:A:85:GLY:N	0.43	2.75	6	2
3:A:39:LEU:C	3:A:43:LEU:CD1	0.43	2.90	7	1
3:A:61:LEU:HD12	3:A:67:SER:OG	0.43	2.14	7	1
2:F:16:DG:H2''	2:F:17:DT:C6	0.43	2.48	8	1
3:A:72:LYS:HD2	3:A:73:ASN:HD22	0.43	1.73	8	1
3:A:44:THR:HB	3:A:47:GLU:HG3	0.43	1.91	9	1
2:F:13:DC:OP1	3:A:44:THR:CG2	0.43	2.66	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:42:MET:CB	3:B:54:ARG:CG	0.43	2.95	10	1
2:F:9:DT:H2''	2:F:10:DA:C8	0.43	2.49	11	1
3:A:41:LEU:O	4:B:201:TRP:CE3	0.43	2.71	11	1
3:A:45:PRO:CG	4:B:201:TRP:O	0.43	2.67	11	1
3:A:34:LEU:HB3	3:B:96:LEU:CD2	0.43	2.43	12	1
1:E:14:DT:OP2	3:A:76:GLY:HA2	0.43	2.13	13	1
2:F:2:DG:N7	3:A:68:GLN:HG3	0.43	2.29	13	1
3:A:72:LYS:HD3	3:A:79:ILE:CD1	0.43	2.44	2	1
3:A:80:ALA:O	3:A:84:ARG:HD3	0.43	2.14	7	3
3:A:37:PRO:HA	3:A:40:ASN:HB2	0.43	1.89	3	1
3:B:106:LYS:O	3:B:106:LYS:CD	0.43	2.67	3	2
3:A:35:HIS:CG	3:A:36:LEU:N	0.43	2.86	5	1
3:A:17:GLN:HB2	3:A:20:LEU:HD23	0.43	1.90	7	1
3:A:51:LEU:CD1	3:B:26:LEU:CD1	0.43	2.97	7	1
3:B:51:LEU:HA	3:B:54:ARG:HD2	0.43	1.89	7	1
3:B:101:GLU:HG3	3:B:106:LYS:HB2	0.43	1.90	7	1
3:A:37:PRO:HG3	3:B:96:LEU:CD2	0.43	2.42	8	1
3:A:54:ARG:CG	4:B:109:TRP:C	0.43	2.92	8	1
3:A:63:ARG:CG	3:A:104:LEU:CD2	0.43	2.97	8	1
3:A:96:LEU:CD2	3:B:41:LEU:CB	0.43	2.97	8	2
3:B:96:LEU:HD22	3:B:96:LEU:N	0.43	2.27	8	1
4:B:109:TRP:CE3	4:B:109:TRP:CA	0.43	3.02	8	1
2:F:13:DC:OP2	3:A:43:LEU:O	0.43	2.37	10	1
3:A:22:PHE:O	3:A:22:PHE:CD1	0.43	2.72	10	2
3:A:35:HIS:CE1	3:B:20:LEU:CD1	0.43	3.02	12	1
3:A:84:ARG:O	3:A:87:ASN:HB2	0.43	2.14	12	1
3:A:63:ARG:HD2	3:A:104:LEU:HD21	0.43	1.89	13	1
3:A:87:ASN:C	3:A:89:LEU:N	0.43	2.76	13	1
3:A:53:THR:CG2	3:A:76:GLY:O	0.43	2.66	14	1
3:A:44:THR:HG21	3:A:47:GLU:CG	0.43	2.44	15	1
3:A:52:GLY:O	3:A:56:ARG:HG2	0.43	2.13	2	1
3:A:41:LEU:HD13	3:A:42:MET:SD	0.43	2.53	11	2
3:B:73:ASN:HA	3:B:77:ALA:N	0.43	2.28	3	1
3:A:26:LEU:CD1	3:A:30:TYR:CE1	0.43	3.01	4	1
3:A:106:LYS:O	3:A:106:LYS:CD	0.43	2.67	6	1
1:E:14:DT:OP2	3:A:77:ALA:HB3	0.43	2.13	7	1
3:B:56:ARG:HA	3:B:59:GLU:CG	0.43	2.42	10	2
3:A:67:SER:O	3:A:70:GLU:CG	0.43	2.67	9	1
3:A:35:HIS:CD2	3:A:35:HIS:H	0.43	2.31	10	1
3:B:51:LEU:HD22	3:B:54:ARG:HE	0.43	1.73	10	1
3:A:42:MET:HG2	3:B:54:ARG:CB	0.43	2.44	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:71:LEU:O	3:A:74:GLU:N	0.43	2.38	13	1
3:B:63:ARG:NH1	3:B:104:LEU:HD21	0.43	2.28	13	1
3:B:53:THR:HG23	3:B:75:LEU:HD12	0.43	1.89	15	1
3:B:32:ASN:O	3:B:35:HIS:CD2	0.43	2.72	1	1
3:A:33:ASP:O	3:B:96:LEU:CD2	0.43	2.67	4	2
3:B:94:VAL:HA	3:B:97:ARG:HB3	0.43	1.90	2	1
2:F:3:DT:OP1	3:A:67:SER:HB2	0.43	2.14	3	1
3:A:19:TRP:CZ2	3:B:39:LEU:CD2	0.43	2.95	9	4
3:B:62:LEU:CD2	3:B:97:ARG:NH2	0.43	2.81	5	2
3:B:88:SER:O	3:B:92:ALA:N	0.43	2.51	3	1
3:B:46:ASP:C	3:B:48:ARG:N	0.43	2.76	4	3
3:A:96:LEU:HD21	3:B:36:LEU:CB	0.43	2.44	6	1
3:A:66:MET:O	3:A:70:GLU:CD	0.43	2.62	7	1
3:A:67:SER:HB3	3:A:82:ILE:HD12	0.43	1.89	7	1
4:B:201:TRP:C	4:B:201:TRP:CD2	0.43	2.91	7	1
1:E:10:DG:C6	2:F:12:DA:N1	0.43	2.87	14	3
2:F:16:DG:O5'	2:F:16:DG:C8	0.43	2.68	8	1
3:B:33:ASP:O	3:B:37:PRO:HD3	0.43	2.13	8	1
3:A:41:LEU:CA	3:B:91:ALA:HB3	0.43	2.44	12	3
3:A:58:VAL:CG2	3:B:41:LEU:HD21	0.43	2.41	12	1
3:B:96:LEU:N	3:B:96:LEU:HD22	0.43	2.23	13	1
3:A:54:ARG:HG3	3:B:42:MET:SD	0.43	2.53	14	1
3:A:58:VAL:HG11	3:B:41:LEU:HG	0.43	1.90	15	1
2:F:3:DT:C7	2:F:3:DT:OP2	0.43	2.67	1	2
3:B:71:LEU:HD11	3:B:75:LEU:CB	0.43	2.44	1	1
1:E:13:DC:C2'	1:E:14:DT:O5'	0.43	2.62	12	4
3:A:36:LEU:HD22	3:A:39:LEU:HD23	0.43	1.91	2	1
3:B:72:LYS:CE	3:B:82:ILE:CD1	0.43	2.97	3	1
3:B:68:GLN:HA	3:B:72:LYS:HE2	0.43	1.90	5	1
3:A:34:LEU:C	3:A:37:PRO:CD	0.43	2.83	6	1
3:B:50:ALA:O	3:B:54:ARG:HB2	0.43	2.13	8	1
3:A:59:GLU:OE2	3:A:60:GLU:HG2	0.43	2.14	9	1
3:A:60:GLU:CB	3:A:66:MET:CB	0.43	2.97	9	1
3:A:35:HIS:ND1	3:B:23:VAL:HG21	0.43	2.29	10	1
3:A:39:LEU:CD2	3:B:19:TRP:CE2	0.43	3.00	10	1
3:A:99:TRP:HA	3:A:102:GLU:HB2	0.43	1.90	10	1
3:B:26:LEU:HD12	3:B:30:TYR:CE1	0.43	2.49	10	1
3:B:59:GLU:O	3:B:63:ARG:HG2	0.43	2.13	10	1
3:B:73:ASN:OD1	3:B:73:ASN:O	0.43	2.36	11	1
3:B:66:MET:O	3:B:67:SER:HB2	0.43	2.13	12	1
3:A:22:PHE:CE2	3:B:51:LEU:CD2	0.43	3.02	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:57:ILE:HD11	4:B:109:TRP:CH2	0.43	2.49	14	1
3:A:40:ASN:OD1	3:A:45:PRO:CB	0.43	2.67	15	1
1:E:12:DA:C3'	4:B:109:TRP:OXT	0.43	2.67	2	2
3:B:32:ASN:HB3	3:B:34:LEU:HD22	0.43	1.90	2	1
2:F:5:DC:N3	2:F:6:DC:C5	0.43	2.86	4	2
3:A:66:MET:O	3:A:71:LEU:CD1	0.43	2.67	4	1
3:A:50:ALA:O	3:A:54:ARG:HB3	0.43	2.14	14	2
2:F:19:DC:H2''	2:F:20:DA:C8	0.43	2.49	6	1
3:A:40:ASN:ND2	3:A:45:PRO:CB	0.43	2.82	6	1
3:B:70:GLU:O	3:B:71:LEU:HB3	0.43	2.14	7	1
3:B:53:THR:O	3:B:57:ILE:CG2	0.43	2.61	8	1
3:A:54:ARG:O	3:B:42:MET:HG2	0.43	2.13	9	1
2:F:3:DT:H72	3:A:79:ILE:HG23	0.43	1.89	10	2
3:A:64:GLY:O	3:A:65:GLU:HB3	0.43	2.13	10	1
3:B:61:LEU:HD11	3:B:82:ILE:O	0.43	2.13	10	1
2:F:3:DT:C4	3:A:68:GLN:NE2	0.43	2.87	11	1
3:A:43:LEU:HB3	3:B:54:ARG:CD	0.43	2.43	11	1
1:E:13:DC:OP1	4:B:109:TRP:HB2	0.43	2.14	13	1
3:A:38:LEU:HG	3:A:42:MET:HE1	0.43	1.89	13	1
3:A:68:GLN:HB3	3:A:70:GLU:CG	0.43	2.44	13	1
3:B:94:VAL:C	3:B:96:LEU:N	0.43	2.76	13	1
2:F:15:DA:P	3:B:73:ASN:ND2	0.43	2.92	14	1
3:A:34:LEU:O	3:A:37:PRO:HG2	0.43	2.13	14	1
1:E:15:DG:C5	3:A:79:ILE:HG21	0.43	2.49	15	1
3:B:45:PRO:CD	4:B:109:TRP:C	0.42	2.92	1	1
3:B:101:GLU:C	3:B:106:LYS:HB2	0.42	2.38	11	5
3:A:23:VAL:HA	3:A:26:LEU:CD2	0.42	2.44	3	1
3:A:50:ALA:C	3:A:54:ARG:HG3	0.42	2.37	4	1
3:A:96:LEU:HD21	3:B:36:LEU:HB2	0.42	1.91	6	1
3:B:29:ALA:HB1	3:B:34:LEU:HB2	0.42	1.90	6	1
1:E:12:DA:H3'	4:B:109:TRP:C	0.42	2.39	7	1
3:A:63:ARG:HD2	3:A:104:LEU:HD13	0.42	1.89	7	1
3:A:30:TYR:CD1	3:B:23:VAL:CG2	0.42	3.01	8	1
1:E:15:DG:C8	3:A:79:ILE:HG13	0.42	2.49	10	1
1:E:10:DG:N2	1:E:11:DT:O2	0.42	2.52	11	1
3:A:26:LEU:HA	3:A:35:HIS:CE1	0.42	2.48	13	1
3:A:19:TRP:CD1	3:B:35:HIS:HB3	0.42	2.49	14	1
3:A:42:MET:HB3	3:B:54:ARG:CD	0.42	2.43	14	1
3:A:43:LEU:O	3:B:54:ARG:HD3	0.42	2.15	15	1
3:B:33:ASP:CG	3:B:36:LEU:HD12	0.42	2.39	15	1
3:A:47:GLU:HB2	3:A:54:ARG:NH2	0.42	2.29	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:67:SER:N	3:A:71:LEU:HB2	0.42	2.30	1	1
3:A:90:LYS:CE	3:A:90:LYS:C	0.42	2.92	1	1
3:B:72:LYS:HG3	3:B:82:ILE:CG1	0.42	2.42	1	2
3:A:43:LEU:N	3:B:54:ARG:HG3	0.42	2.29	2	2
3:A:68:GLN:O	3:A:69:ARG:CG	0.42	2.66	2	1
3:B:57:ILE:CD1	3:B:57:ILE:N	0.42	2.82	2	1
3:A:45:PRO:HB2	3:B:91:ALA:CB	0.42	2.35	3	1
3:B:22:PHE:O	3:B:26:LEU:CG	0.42	2.67	14	2
3:A:55:VAL:CA	3:B:42:MET:HE2	0.42	2.44	4	1
3:B:72:LYS:HB3	3:B:72:LYS:HE2	0.42	1.60	4	1
3:B:55:VAL:O	3:B:58:VAL:HG23	0.42	2.13	13	2
3:A:41:LEU:HA	4:B:201:TRP:O	0.42	2.14	6	2
2:F:14:DG:OP2	3:B:77:ALA:CB	0.42	2.66	12	3
3:A:30:TYR:CE2	3:B:23:VAL:HA	0.42	2.49	7	1
3:A:37:PRO:CB	3:B:96:LEU:HD13	0.42	2.44	7	1
3:B:40:ASN:O	3:B:45:PRO:HG2	0.42	2.13	7	1
3:A:22:PHE:CE1	3:B:30:TYR:OH	0.42	2.72	9	1
3:A:66:MET:O	3:A:70:GLU:HG2	0.42	2.14	10	1
3:B:97:ARG:HB2	3:B:97:ARG:NH2	0.42	2.29	10	1
3:A:93:PRO:O	3:A:94:VAL:CG1	0.42	2.62	12	1
3:A:41:LEU:CD1	3:A:42:MET:SD	0.42	3.08	14	3
1:E:16:DG:C4	2:F:4:DA:N6	0.42	2.87	3	1
2:F:5:DC:O2	2:F:6:DC:N1	0.42	2.52	3	1
3:A:35:HIS:NE2	3:B:20:LEU:CD1	0.42	2.82	4	1
3:B:54:ARG:HA	3:B:57:ILE:CG1	0.42	2.44	5	1
3:B:101:GLU:CB	3:B:106:LYS:HA	0.42	2.44	5	1
3:B:42:MET:C	3:B:44:THR:N	0.42	2.76	6	1
1:E:15:DG:C4	1:E:16:DG:C6	0.42	3.07	7	1
3:A:55:VAL:C	3:A:59:GLU:CG	0.42	2.91	8	1
3:B:22:PHE:HE1	3:B:26:LEU:CD2	0.42	2.28	9	2
3:B:72:LYS:HB3	3:B:82:ILE:HD13	0.42	1.90	9	1
3:B:93:PRO:CB	3:B:97:ARG:HB2	0.42	2.44	10	1
3:B:26:LEU:CD1	3:B:38:LEU:CD1	0.42	2.98	11	1
3:B:51:LEU:HD22	3:B:54:ARG:CZ	0.42	2.40	12	1
3:A:40:ASN:HB2	3:A:45:PRO:HB3	0.42	1.92	13	1
3:B:27:LYS:CE	3:B:27:LYS:H	0.42	2.27	14	1
3:A:94:VAL:HG12	3:A:94:VAL:O	0.42	2.14	1	1
3:B:40:ASN:O	3:B:42:MET:N	0.42	2.52	12	2
1:E:18:DA:H1'	1:E:19:DC:C6	0.42	2.50	2	1
3:B:49:GLU:O	3:B:53:THR:CB	0.42	2.68	2	1
4:B:201:TRP:N	4:B:201:TRP:HE3	0.42	2.12	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:16:DG:N2	2:F:6:DC:C2	0.42	2.88	3	1
3:A:41:LEU:HA	4:B:201:TRP:OXT	0.42	2.14	3	1
3:A:99:TRP:O	3:A:102:GLU:N	0.42	2.53	11	2
3:B:72:LYS:HE3	3:B:82:ILE:CB	0.42	2.44	3	1
2:F:13:DC:N4	2:F:14:DG:O6	0.42	2.53	5	1
3:A:42:MET:SD	3:B:58:VAL:CG2	0.42	3.07	6	1
3:B:47:GLU:O	3:B:49:GLU:CB	0.42	2.67	6	2
3:B:22:PHE:HA	3:B:26:LEU:HD23	0.42	1.91	7	1
3:B:87:ASN:OD1	3:B:87:ASN:C	0.42	2.62	7	1
3:A:51:LEU:CB	3:B:19:TRP:CH2	0.42	3.02	13	2
3:A:84:ARG:CD	3:B:43:LEU:HG	0.42	2.44	8	1
2:F:13:DC:OP1	3:A:43:LEU:CD1	0.42	2.66	9	1
3:B:54:ARG:C	3:B:56:ARG:H	0.42	2.23	9	1
3:B:83:THR:HG22	3:B:84:ARG:N	0.42	2.29	12	2
1:E:18:DA:C2	1:E:19:DC:N3	0.42	2.88	10	1
3:B:41:LEU:C	3:B:43:LEU:H	0.42	2.23	10	1
3:B:51:LEU:CA	3:B:54:ARG:HD3	0.42	2.43	11	1
3:A:53:THR:HG23	3:A:75:LEU:HD12	0.42	1.90	13	1
3:B:23:VAL:O	3:B:27:LYS:CE	0.42	2.68	14	1
3:B:56:ARG:HA	3:B:60:GLU:OE2	0.42	2.14	14	1
1:E:15:DG:N7	3:A:79:ILE:CG2	0.42	2.83	15	1
3:A:96:LEU:HG	3:B:37:PRO:CB	0.42	2.44	15	1
3:A:99:TRP:HB2	3:B:34:LEU:CG	0.42	2.44	15	1
3:B:36:LEU:C	3:B:38:LEU:H	0.42	2.22	15	1
3:A:99:TRP:CZ2	3:B:25:LEU:O	0.42	2.72	2	5
3:B:32:ASN:O	3:B:35:HIS:CE1	0.42	2.72	2	1
3:A:40:ASN:HA	3:B:91:ALA:CB	0.42	2.42	3	1
3:A:68:GLN:C	3:A:70:GLU:H	0.42	2.22	3	1
1:E:6:DT:O2	1:E:7:DC:C6	0.42	2.72	4	1
1:E:8:DG:C5	2:F:14:DG:N2	0.42	2.87	4	1
1:E:17:DT:O2	1:E:18:DA:C5	0.42	2.73	11	3
3:A:56:ARG:CZ	3:A:75:LEU:CD2	0.42	2.97	5	1
2:F:3:DT:C7	3:A:68:GLN:C	0.42	2.90	7	1
3:A:29:ALA:HA	3:A:34:LEU:HB2	0.42	1.92	7	1
3:B:50:ALA:O	3:B:53:THR:OG1	0.42	2.37	7	1
3:A:43:LEU:HB2	4:B:201:TRP:CZ2	0.42	2.49	8	1
3:A:50:ALA:HB1	3:A:54:ARG:HE	0.42	1.70	8	1
3:B:43:LEU:CA	3:B:45:PRO:HD3	0.42	2.42	8	1
2:F:7:DA:C2	2:F:8:DG:C4	0.42	3.08	9	1
3:A:54:ARG:CB	3:B:42:MET:HG2	0.42	2.45	9	1
3:B:72:LYS:CB	3:B:82:ILE:HD13	0.42	2.45	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:79:ILE:C	3:B:81:THR:N	0.42	2.77	9	1
3:B:82:ILE:CG1	3:B:83:THR:H	0.42	2.28	9	1
3:A:68:GLN:HA	3:A:72:LYS:CD	0.42	2.45	11	1
3:A:37:PRO:CG	3:B:96:LEU:HG	0.42	2.44	13	1
3:A:51:LEU:HA	3:A:54:ARG:HE	0.42	1.72	13	1
3:B:37:PRO:O	3:B:41:LEU:CB	0.42	2.67	13	1
3:A:24:ASP:O	3:A:27:LYS:HG2	0.42	2.14	14	1
3:A:54:ARG:HD3	3:B:42:MET:SD	0.42	2.53	2	1
3:A:36:LEU:HB2	3:B:96:LEU:HD22	0.42	1.89	3	1
3:A:43:LEU:CB	3:B:54:ARG:CD	0.42	2.94	14	2
3:A:57:ILE:HB	3:A:82:ILE:HA	0.42	1.92	4	1
3:A:100:LEU:HD23	3:A:100:LEU:C	0.42	2.39	5	1
3:A:54:ARG:C	3:A:56:ARG:N	0.42	2.77	7	1
3:B:93:PRO:C	3:B:97:ARG:HB3	0.42	2.40	7	2
3:B:72:LYS:NZ	3:B:82:ILE:HD13	0.42	2.30	8	1
3:B:67:SER:N	3:B:70:GLU:CD	0.42	2.78	9	1
3:A:22:PHE:CE2	3:B:51:LEU:HD21	0.42	2.49	10	2
3:A:35:HIS:CD2	3:B:23:VAL:HG21	0.42	2.50	12	1
3:A:62:LEU:CB	3:A:104:LEU:HD23	0.42	2.44	12	1
3:A:72:LYS:C	3:A:78:GLY:CA	0.42	2.92	13	1
3:A:72:LYS:CA	3:A:78:GLY:HA2	0.42	2.45	13	1
3:A:42:MET:C	3:B:54:ARG:HD2	0.42	2.39	14	1
3:B:48:ARG:O	3:B:49:GLU:HG2	0.42	2.14	14	1
3:A:101:GLU:CB	3:A:106:LYS:HB2	0.42	2.44	1	3
3:B:73:ASN:HB2	3:B:79:ILE:CB	0.42	2.44	1	1
3:B:19:TRP:CD1	3:B:23:VAL:HG23	0.42	2.50	2	1
2:F:2:DG:P	3:A:68:GLN:HG2	0.42	2.55	6	1
3:B:97:ARG:O	3:B:100:LEU:CB	0.42	2.68	7	1
3:A:78:GLY:CA	3:A:82:ILE:H	0.42	2.28	8	1
3:A:97:ARG:O	3:A:101:GLU:CG	0.42	2.67	8	1
1:E:9:DT:C2	1:E:10:DG:N7	0.42	2.88	11	1
2:F:4:DA:C4	2:F:5:DC:N3	0.42	2.87	11	1
3:A:79:ILE:HD12	3:A:79:ILE:H	0.42	1.74	12	1
3:A:71:LEU:O	3:A:74:GLU:HG3	0.42	2.15	13	1
3:B:96:LEU:O	3:B:98:GLN:N	0.42	2.53	13	1
1:E:13:DC:N3	1:E:14:DT:C5	0.42	2.88	14	1
3:A:38:LEU:O	3:A:42:MET:SD	0.42	2.78	14	1
3:A:54:ARG:CG	3:B:42:MET:SD	0.42	3.08	14	1
3:A:72:LYS:HZ3	3:A:79:ILE:HG13	0.42	1.71	15	1
2:F:3:DT:C7	3:A:68:GLN:NE2	0.42	2.83	2	1
3:A:39:LEU:HD22	3:B:19:TRP:CD2	0.42	2.49	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:78:GLY:HA3	3:B:81:THR:HG22	0.42	1.91	2	1
3:A:18:GLU:N	3:A:21:ARG:CG	0.42	2.80	3	1
3:A:55:VAL:HA	3:B:42:MET:HE3	0.42	1.91	3	1
3:A:55:VAL:HG13	3:B:42:MET:CE	0.42	2.43	4	1
3:A:56:ARG:HA	3:A:59:GLU:OE2	0.42	2.15	4	1
3:A:71:LEU:C	3:A:73:ASN:N	0.42	2.78	4	1
3:B:50:ALA:CB	3:B:54:ARG:NH1	0.42	2.82	5	1
3:A:42:MET:HB3	3:B:54:ARG:HD3	0.42	1.90	6	1
3:A:55:VAL:CB	3:B:22:PHE:HZ	0.42	2.24	6	1
3:A:95:GLU:O	3:A:98:GLN:HB2	0.42	2.13	6	1
3:A:55:VAL:C	3:A:57:ILE:N	0.42	2.78	10	1
3:B:85:GLY:O	3:B:87:ASN:N	0.42	2.52	10	1
3:B:66:MET:O	3:B:67:SER:CB	0.42	2.67	12	1
3:A:56:ARG:NH1	3:A:56:ARG:HB2	0.42	2.29	13	1
3:A:35:HIS:NE2	3:A:39:LEU:CB	0.42	2.82	14	1
3:A:69:ARG:C	3:A:70:GLU:HG2	0.42	2.39	14	1
3:A:81:THR:HG22	4:B:109:TRP:CZ3	0.42	2.50	15	1
3:A:45:PRO:HD3	4:B:201:TRP:HB3	0.42	1.91	2	1
3:A:72:LYS:CE	3:A:73:ASN:ND2	0.42	2.83	2	1
3:A:84:ARG:HG2	3:B:43:LEU:HD22	0.42	1.90	2	1
3:B:59:GLU:CD	3:B:60:GLU:HG2	0.42	2.40	2	1
2:F:5:DC:C2	2:F:6:DC:N1	0.42	2.88	3	1
3:B:72:LYS:HG2	3:B:79:ILE:CG1	0.42	2.44	3	1
3:B:22:PHE:HB3	3:B:26:LEU:CG	0.42	2.36	4	1
3:B:55:VAL:O	3:B:59:GLU:HB3	0.42	2.15	4	1
3:B:58:VAL:CG2	3:B:59:GLU:N	0.42	2.82	4	1
3:B:43:LEU:HD22	4:B:109:TRP:HE1	0.42	1.73	5	1
3:B:101:GLU:CG	3:B:106:LYS:HB2	0.42	2.45	7	1
1:E:6:DT:O5'	1:E:6:DT:H6	0.42	1.98	8	1
1:E:6:DT:OP2	1:E:6:DT:C7	0.42	2.68	8	1
3:A:42:MET:O	3:A:43:LEU:C	0.42	2.62	8	1
3:A:55:VAL:C	3:A:59:GLU:HG2	0.42	2.39	8	1
3:A:63:ARG:O	3:A:64:GLY:O	0.42	2.38	8	1
3:A:90:LYS:NZ	3:B:43:LEU:O	0.42	2.52	8	1
3:B:92:ALA:HB1	3:B:95:GLU:OE1	0.42	2.15	9	1
3:A:78:GLY:O	3:A:81:THR:C	0.42	2.54	12	1
3:B:43:LEU:CD1	3:B:44:THR:N	0.42	2.78	13	1
3:B:42:MET:HE3	3:B:42:MET:HB2	0.42	1.71	14	1
3:A:54:ARG:CD	4:B:109:TRP:HA	0.42	2.44	15	1
2:F:3:DT:C7	3:A:69:ARG:H	0.42	2.28	1	1
3:A:90:LYS:C	3:A:90:LYS:HE3	0.42	2.39	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:62:LEU:HD13	3:A:100:LEU:CD2	0.42	2.39	2	1
1:E:15:DG:N3	1:E:16:DG:C4	0.42	2.88	3	1
3:A:43:LEU:CB	3:B:54:ARG:NE	0.42	2.83	3	1
3:A:56:ARG:CA	3:A:59:GLU:CG	0.42	2.98	3	1
3:A:102:GLU:HA	3:A:106:LYS:HB3	0.42	1.92	7	2
2:F:12:DA:C5'	3:A:47:GLU:OE2	0.42	2.68	5	1
1:E:16:DG:H2''	1:E:17:DT:H71	0.42	1.85	6	1
3:A:93:PRO:O	3:A:94:VAL:HB	0.42	2.15	6	1
3:B:48:ARG:O	3:B:49:GLU:CG	0.42	2.68	14	2
3:A:35:HIS:C	3:A:35:HIS:ND1	0.42	2.77	7	2
3:A:99:TRP:CB	3:B:34:LEU:CD1	0.42	2.98	7	1
3:B:41:LEU:HD12	3:B:41:LEU:C	0.42	2.40	7	1
3:B:101:GLU:C	3:B:106:LYS:HB3	0.42	2.40	7	1
3:A:43:LEU:HB2	4:B:201:TRP:CD2	0.42	2.50	8	1
3:A:84:ARG:HB2	4:B:109:TRP:CZ2	0.42	2.50	8	1
3:A:97:ARG:N	3:A:97:ARG:CD	0.42	2.81	8	1
3:A:30:TYR:OH	3:A:35:HIS:CD2	0.42	2.72	9	1
3:A:36:LEU:CD2	3:B:19:TRP:NE1	0.42	2.83	14	2
3:A:50:ALA:C	3:A:54:ARG:CD	0.42	2.93	10	1
2:F:2:DG:OP1	3:A:68:GLN:NE2	0.42	2.52	12	1
3:A:22:PHE:HB2	3:B:55:VAL:HG22	0.42	1.92	12	1
3:A:65:GLU:C	3:A:70:GLU:OE2	0.42	2.63	13	1
3:B:96:LEU:H	3:B:96:LEU:CD2	0.42	2.27	13	1
2:F:3:DT:OP2	3:A:68:GLN:HG2	0.42	2.15	14	1
1:E:13:DC:OP1	3:A:54:ARG:NE	0.41	2.50	2	1
3:B:24:ASP:HA	3:B:27:LYS:CE	0.41	2.45	3	2
3:A:34:LEU:CD1	3:B:99:TRP:HB3	0.41	2.45	4	1
2:F:10:DA:H2''	2:F:11:DC:H6	0.41	1.73	5	1
3:A:62:LEU:HD11	3:A:97:ARG:NH2	0.41	2.29	5	1
3:B:90:LYS:HD2	4:B:201:TRP:O	0.41	2.15	6	1
1:E:6:DT:H2''	1:E:7:DC:C6	0.41	2.49	8	1
3:A:26:LEU:O	3:A:30:TYR:CB	0.41	2.68	8	1
3:A:35:HIS:O	3:A:39:LEU:CD2	0.41	2.68	9	1
3:B:78:GLY:HA2	3:B:81:THR:CB	0.41	2.45	9	1
3:B:82:ILE:CD1	3:B:83:THR:N	0.41	2.83	9	2
3:A:38:LEU:HA	3:A:42:MET:SD	0.41	2.55	11	1
3:A:68:GLN:OE1	3:A:72:LYS:HE2	0.41	2.15	11	1
1:E:13:DC:OP2	4:B:109:TRP:CB	0.41	2.68	13	1
3:B:48:ARG:C	3:B:49:GLU:HG3	0.41	2.39	13	1
3:A:45:PRO:O	3:A:48:ARG:HG3	0.41	2.15	14	1
1:E:15:DG:C6	3:A:79:ILE:CG2	0.41	3.03	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:58:VAL:HG11	3:B:41:LEU:CD1	0.41	2.45	1	1
3:A:66:MET:N	3:A:71:LEU:HB3	0.41	2.29	1	1
3:B:54:ARG:C	3:B:56:ARG:N	0.41	2.76	2	1
3:A:43:LEU:HD23	3:B:54:ARG:NH2	0.41	2.30	3	1
3:B:53:THR:O	3:B:56:ARG:N	0.41	2.53	14	2
3:B:74:GLU:CB	3:B:75:LEU:HD23	0.41	2.44	5	1
3:A:22:PHE:O	3:A:26:LEU:CD2	0.41	2.68	6	1
3:B:51:LEU:HD22	3:B:54:ARG:CD	0.41	2.44	6	1
3:A:19:TRP:CZ3	3:B:51:LEU:HB2	0.41	2.49	7	1
3:A:30:TYR:HD2	3:B:27:LYS:HB3	0.41	1.75	7	1
3:A:38:LEU:C	3:A:38:LEU:HD23	0.41	2.39	8	1
3:B:71:LEU:CD2	3:B:74:GLU:HB2	0.41	2.45	8	1
3:A:66:MET:CA	3:A:71:LEU:HB3	0.41	2.45	9	1
3:B:81:THR:O	3:B:82:ILE:C	0.41	2.64	9	1
3:B:26:LEU:CD2	3:B:38:LEU:HD13	0.41	2.45	10	1
3:B:93:PRO:O	3:B:95:GLU:N	0.41	2.53	10	1
3:A:36:LEU:HD13	3:B:19:TRP:CD1	0.41	2.50	13	1
3:A:54:ARG:CB	4:B:109:TRP:N	0.41	2.84	13	1
3:B:41:LEU:HD23	3:B:42:MET:SD	0.41	2.55	14	1
3:B:53:THR:HA	3:B:56:ARG:CB	0.41	2.45	14	1
3:A:84:ARG:CG	3:B:43:LEU:HG	0.41	2.46	15	1
3:A:42:MET:HG2	3:B:57:ILE:HD11	0.41	1.91	2	1
3:A:55:VAL:HG23	3:B:42:MET:HE2	0.41	1.92	2	1
3:A:100:LEU:HD11	3:B:41:LEU:HD12	0.41	1.92	2	1
3:A:43:LEU:CD2	3:B:54:ARG:NH2	0.41	2.83	3	1
3:A:99:TRP:HB3	3:B:37:PRO:CB	0.41	2.45	3	1
3:A:57:ILE:O	3:A:61:LEU:CB	0.41	2.67	4	1
3:A:54:ARG:HB3	3:B:42:MET:CE	0.41	2.45	6	1
3:B:44:THR:CG2	4:B:109:TRP:N	0.41	2.84	6	1
3:B:50:ALA:O	3:B:54:ARG:CB	0.41	2.68	8	1
3:B:19:TRP:CD1	3:B:23:VAL:CG2	0.41	3.04	10	1
3:A:39:LEU:HD21	3:A:48:ARG:HE	0.41	1.75	11	1
3:A:69:ARG:C	3:A:70:GLU:CG	0.41	2.92	14	2
3:B:23:VAL:O	3:B:27:LYS:HG2	0.41	2.15	11	1
3:B:73:ASN:C	3:B:75:LEU:H	0.41	2.22	12	1
1:E:10:DG:N2	2:F:12:DA:C4	0.41	2.89	13	1
3:A:71:LEU:HD22	3:A:74:GLU:HG3	0.41	1.93	13	1
3:A:55:VAL:CG2	3:B:22:PHE:HE2	0.41	2.28	14	1
3:B:33:ASP:O	3:B:37:PRO:HG3	0.41	2.13	14	1
3:B:56:ARG:O	3:B:60:GLU:OE2	0.41	2.38	14	1
3:A:50:ALA:O	3:A:54:ARG:HD3	0.41	2.16	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:68:GLN:OE1	3:A:69:ARG:CZ	0.41	2.69	15	1
3:A:78:GLY:C	3:A:82:ILE:CG1	0.41	2.93	15	1
3:B:50:ALA:HA	3:B:54:ARG:NH2	0.41	2.30	15	1
3:A:69:ARG:O	3:A:70:GLU:CG	0.41	2.69	1	1
3:A:86:SER:O	3:A:89:LEU:HD12	0.41	2.16	2	1
3:B:19:TRP:CD1	3:B:19:TRP:O	0.41	2.73	7	2
3:B:52:GLY:O	3:B:56:ARG:CG	0.41	2.68	3	1
3:A:34:LEU:CD1	3:B:96:LEU:HB3	0.41	2.40	4	1
2:F:12:DA:C5'	3:A:46:ASP:OD2	0.41	2.64	5	1
2:F:13:DC:C2	2:F:14:DG:C4	0.41	3.09	6	1
3:B:24:ASP:N	3:B:24:ASP:OD1	0.41	2.53	8	1
1:E:15:DG:OP2	3:A:73:ASN:ND2	0.41	2.53	9	1
3:B:67:SER:O	3:B:70:GLU:OE2	0.41	2.38	9	1
3:A:41:LEU:O	4:B:201:TRP:CZ3	0.41	2.72	11	1
3:B:34:LEU:N	3:B:34:LEU:HD12	0.41	2.30	11	1
3:A:87:ASN:O	3:A:89:LEU:N	0.41	2.53	13	1
3:A:91:ALA:O	3:B:40:ASN:O	0.41	2.39	14	1
3:B:49:GLU:O	3:B:53:THR:CG2	0.41	2.68	1	1
3:A:32:ASN:O	3:A:35:HIS:NE2	0.41	2.51	2	1
3:B:82:ILE:C	4:B:201:TRP:HZ2	0.41	2.22	3	1
1:E:3:DT:O5'	1:E:3:DT:H6	0.41	1.98	4	2
3:A:62:LEU:HD21	3:A:97:ARG:HH12	0.41	1.76	4	1
1:E:15:DG:N2	2:F:7:DA:C5	0.41	2.89	5	1
1:E:8:DG:H2''	1:E:9:DT:C6	0.41	2.51	8	1
3:A:27:LYS:HG3	3:A:28:ASN:H	0.41	1.72	8	2
3:A:60:GLU:HB3	3:A:66:MET:HB2	0.41	1.93	9	1
3:B:30:TYR:O	3:B:31:GLN:C	0.41	2.62	9	1
3:B:34:LEU:O	3:B:37:PRO:HD2	0.41	2.16	9	1
3:B:47:GLU:OE1	3:B:54:ARG:NH1	0.41	2.54	9	1
3:B:78:GLY:O	3:B:81:THR:CB	0.41	2.68	9	1
3:B:99:TRP:CE3	3:B:100:LEU:CA	0.41	3.03	11	1
3:A:68:GLN:O	3:A:69:ARG:CB	0.41	2.65	12	1
3:B:39:LEU:CD2	3:B:40:ASN:OD1	0.41	2.69	12	1
3:B:53:THR:CA	3:B:56:ARG:HB3	0.41	2.44	12	1
3:A:42:MET:HB3	3:B:54:ARG:HD2	0.41	1.92	14	1
3:A:84:ARG:HG2	3:B:43:LEU:CD1	0.41	2.45	2	1
3:A:39:LEU:CD1	3:A:47:GLU:CG	0.41	2.98	4	1
3:A:54:ARG:HG3	3:A:55:VAL:H	0.41	1.76	4	1
3:A:57:ILE:CD1	3:A:57:ILE:N	0.41	2.84	4	2
3:A:80:ALA:O	3:A:83:THR:CG2	0.41	2.69	8	2
1:E:15:DG:OP2	3:A:76:GLY:CA	0.41	2.69	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:47:GLU:OE1	3:B:48:ARG:N	0.41	2.53	6	1
3:A:43:LEU:C	4:B:201:TRP:N	0.41	2.78	7	1
1:E:6:DT:OP2	1:E:6:DT:H73	0.41	2.15	8	1
3:B:59:GLU:OE2	3:B:60:GLU:CG	0.41	2.68	8	1
2:F:13:DC:P	3:A:43:LEU:HD23	0.41	2.52	10	1
3:A:73:ASN:HB3	3:A:79:ILE:CG1	0.41	2.45	10	1
3:A:93:PRO:C	3:A:95:GLU:N	0.41	2.79	10	2
3:A:102:GLU:CG	3:A:106:LYS:CD	0.41	2.98	10	1
3:A:22:PHE:CB	3:B:51:LEU:HD11	0.41	2.46	12	1
3:A:54:ARG:CB	4:B:109:TRP:HB2	0.41	2.45	12	1
3:A:84:ARG:HD2	4:B:109:TRP:HE1	0.41	1.75	13	1
3:B:93:PRO:HA	3:B:96:LEU:CD2	0.41	2.45	13	1
1:E:16:DG:O6	2:F:4:DA:C6	0.41	2.73	14	1
3:A:66:MET:O	3:A:71:LEU:HB2	0.41	2.16	14	1
3:B:25:LEU:C	3:B:27:LYS:N	0.41	2.78	14	1
3:B:41:LEU:CD2	3:B:42:MET:HG3	0.41	2.46	14	1
3:B:69:ARG:C	3:B:70:GLU:CG	0.41	2.93	14	1
3:B:102:GLU:N	3:B:106:LYS:HB2	0.41	2.31	2	3
3:A:93:PRO:O	3:A:94:VAL:CB	0.41	2.69	2	1
1:E:10:DG:H2'	1:E:11:DT:C6	0.41	2.50	3	1
1:E:16:DG:H1'	1:E:17:DT:C4	0.41	2.47	3	1
2:F:2:DG:C3'	3:A:68:GLN:CG	0.41	2.98	3	1
3:A:25:LEU:N	3:A:25:LEU:CD1	0.41	2.84	4	1
3:B:97:ARG:HD3	3:B:100:LEU:HB3	0.41	1.92	4	1
3:A:26:LEU:O	3:A:29:ALA:N	0.41	2.54	5	1
3:A:32:ASN:O	3:A:35:HIS:ND1	0.41	2.53	5	1
3:A:40:ASN:HB2	3:A:45:PRO:CB	0.41	2.46	13	2
3:A:56:ARG:O	3:A:58:VAL:N	0.41	2.54	5	1
3:A:80:ALA:CA	3:A:83:THR:CG2	0.41	2.99	5	1
3:A:85:GLY:O	3:A:86:SER:C	0.41	2.62	13	2
1:E:13:DC:P	3:A:54:ARG:HD2	0.41	2.55	7	1
3:B:42:MET:O	4:B:109:TRP:CA	0.41	2.67	8	1
3:A:36:LEU:HD22	3:B:19:TRP:CG	0.41	2.50	10	1
3:A:41:LEU:CD1	3:A:42:MET:HG3	0.41	2.45	10	1
3:A:20:LEU:HD13	3:A:20:LEU:N	0.41	2.30	11	1
3:A:44:THR:HA	3:A:45:PRO:HD3	0.41	1.75	11	1
3:A:47:GLU:OE2	3:A:54:ARG:NH1	0.41	2.54	11	1
3:B:34:LEU:O	3:B:35:HIS:HB3	0.41	2.16	12	1
3:A:72:LYS:HB2	3:A:78:GLY:CA	0.41	2.46	13	1
2:F:11:DC:O2	2:F:12:DA:C5	0.41	2.73	15	1
3:A:24:ASP:O	3:A:27:LYS:HD3	0.41	2.15	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:58:VAL:HG11	3:B:41:LEU:CB	0.41	2.45	1	1
3:A:58:VAL:O	3:A:59:GLU:C	0.41	2.62	10	2
1:E:16:DG:C6	3:A:79:ILE:CG2	0.41	3.04	3	1
1:E:19:DC:H42	2:F:2:DG:H1	0.41	1.58	3	1
3:A:19:TRP:CH2	3:B:39:LEU:HB2	0.41	2.51	3	1
3:A:19:TRP:O	3:A:23:VAL:CG2	0.41	2.67	3	1
3:A:22:PHE:CE1	3:A:26:LEU:HG	0.41	2.51	14	3
3:A:57:ILE:HD12	3:A:57:ILE:N	0.41	2.30	4	1
3:B:62:LEU:HD21	3:B:97:ARG:NE	0.41	2.31	4	1
3:A:40:ASN:ND2	3:A:41:LEU:N	0.41	2.69	5	1
3:A:46:ASP:OD1	3:A:46:ASP:N	0.41	2.53	5	1
3:A:43:LEU:HD13	3:B:50:ALA:C	0.41	2.40	6	1
3:A:99:TRP:CG	3:B:34:LEU:HB3	0.41	2.51	6	1
3:B:63:ARG:NH2	3:B:104:LEU:HD11	0.41	2.31	6	1
3:A:37:PRO:CA	3:B:96:LEU:HD13	0.41	2.46	7	1
3:B:59:GLU:CD	3:B:59:GLU:C	0.41	2.89	7	1
3:B:80:ALA:C	3:B:84:ARG:HB2	0.41	2.41	7	1
3:B:54:ARG:CA	4:B:201:TRP:N	0.41	2.84	8	1
3:A:47:GLU:OE1	3:A:54:ARG:CZ	0.41	2.69	11	1
3:A:102:GLU:HG3	3:A:103:VAL:N	0.41	2.30	11	1
3:B:75:LEU:HD23	3:B:75:LEU:H	0.41	1.75	15	1
1:E:11:DT:C2	1:E:12:DA:N6	0.41	2.89	1	1
3:A:87:ASN:CB	3:B:43:LEU:CD2	0.41	2.98	1	1
3:A:68:GLN:C	3:A:69:ARG:CD	0.41	2.94	2	1
3:A:87:ASN:HB3	3:B:43:LEU:CD1	0.41	2.45	2	1
3:A:89:LEU:CD2	3:A:97:ARG:NH2	0.41	2.84	2	1
1:E:14:DT:O4	3:A:80:ALA:CB	0.41	2.69	3	1
2:F:5:DC:H1'	2:F:6:DC:O4'	0.41	2.16	3	1
3:B:73:ASN:H	3:B:79:ILE:HG13	0.41	1.75	3	1
3:A:50:ALA:C	3:A:54:ARG:HG2	0.41	2.40	4	1
3:A:68:GLN:O	3:A:69:ARG:C	0.41	2.64	5	1
3:B:54:ARG:HG2	4:B:201:TRP:HB2	0.41	1.92	5	1
2:F:13:DC:OP1	3:A:43:LEU:CD2	0.41	2.69	6	1
3:A:33:ASP:O	3:B:96:LEU:HB3	0.41	2.16	6	1
3:A:34:LEU:HD22	3:A:38:LEU:HB2	0.41	1.92	6	1
3:A:55:VAL:CG2	3:B:42:MET:HE3	0.41	2.46	6	1
3:A:72:LYS:CE	3:A:79:ILE:HD13	0.41	2.45	6	1
3:A:103:VAL:HG23	3:A:104:LEU:HD23	0.41	1.92	6	1
3:B:36:LEU:O	3:B:40:ASN:N	0.41	2.43	6	1
1:E:15:DG:C2'	1:E:16:DG:OP2	0.41	2.69	7	2
2:F:2:DG:N7	3:A:69:ARG:NH2	0.41	2.69	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:38:LEU:C	3:A:40:ASN:N	0.41	2.78	7	1
3:A:54:ARG:HB3	3:B:42:MET:HG2	0.41	1.93	7	1
1:E:1:DT:H2'	1:E:2:DG:C8	0.41	2.51	8	1
1:E:15:DG:H2'	3:A:72:LYS:NZ	0.41	2.30	8	1
3:A:29:ALA:O	3:A:35:HIS:HB3	0.41	2.16	8	1
3:A:30:TYR:HB3	3:B:23:VAL:CG1	0.41	2.46	8	1
3:A:44:THR:O	4:B:201:TRP:HB3	0.41	2.15	8	1
3:B:67:SER:C	3:B:68:GLN:CG	0.41	2.94	8	1
3:B:67:SER:CB	3:B:72:LYS:HA	0.41	2.46	9	1
3:B:72:LYS:CB	3:B:82:ILE:CD1	0.41	2.98	9	1
3:A:43:LEU:HD22	3:B:50:ALA:CA	0.41	2.33	10	1
3:B:45:PRO:N	4:B:109:TRP:N	0.41	2.69	12	2
3:B:71:LEU:O	3:B:71:LEU:HD13	0.41	2.16	11	1
3:B:90:LYS:CD	4:B:201:TRP:O	0.41	2.68	11	1
2:F:1:DT:H6	2:F:1:DT:O5'	0.41	1.99	12	1
3:A:58:VAL:CG1	3:A:100:LEU:CD1	0.41	2.99	12	1
4:B:201:TRP:OXT	4:B:201:TRP:CE3	0.41	2.74	12	1
1:E:18:DA:C2	2:F:3:DT:O2	0.41	2.74	13	1
3:A:98:GLN:CG	3:A:106:LYS:CD	0.41	2.99	13	1
3:B:44:THR:C	4:B:109:TRP:N	0.41	2.79	14	1
3:A:72:LYS:CD	3:A:73:ASN:HB2	0.41	2.46	15	1
3:B:26:LEU:HD12	3:B:35:HIS:HE1	0.41	1.73	15	1
2:F:15:DA:H62	3:B:80:ALA:CB	0.41	2.29	1	1
3:A:35:HIS:NE2	3:A:36:LEU:CD2	0.41	2.84	1	1
3:B:78:GLY:CA	3:B:81:THR:CG2	0.41	2.99	2	1
3:B:81:THR:O	4:B:201:TRP:HZ2	0.41	1.88	2	1
3:A:27:LYS:CG	3:A:28:ASN:H	0.41	2.28	3	1
2:F:3:DT:C7	3:A:72:LYS:HE2	0.41	2.46	4	1
3:A:41:LEU:N	3:A:41:LEU:CD1	0.41	2.83	4	1
3:B:43:LEU:CB	4:B:109:TRP:NE1	0.41	2.81	4	1
3:B:54:ARG:HA	3:B:57:ILE:HG12	0.41	1.93	5	1
3:A:43:LEU:CD1	3:B:54:ARG:N	0.41	2.80	6	1
3:B:24:ASP:CG	3:B:25:LEU:N	0.41	2.79	6	1
3:A:43:LEU:HA	3:B:54:ARG:CB	0.41	2.47	7	1
3:A:87:ASN:ND2	3:A:87:ASN:C	0.41	2.78	7	1
2:F:2:DG:H2'	3:A:68:GLN:HG2	0.41	1.91	8	1
3:A:69:ARG:O	3:A:74:GLU:CG	0.41	2.68	8	1
3:A:20:LEU:HD22	3:A:20:LEU:N	0.41	2.31	9	1
3:A:46:ASP:O	3:A:49:GLU:HG3	0.41	2.16	9	1
2:F:3:DT:OP2	3:A:67:SER:HB2	0.41	2.16	10	1
3:A:41:LEU:HD13	3:A:42:MET:HG3	0.41	1.93	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:51:LEU:HD13	3:B:19:TRP:HH2	0.41	1.75	10	1
1:E:3:DT:H3'	3:B:68:GLN:OE1	0.41	2.16	12	1
3:A:100:LEU:CD1	3:B:41:LEU:CD1	0.41	2.99	12	1
3:B:36:LEU:O	3:B:40:ASN:ND2	0.41	2.55	15	1
3:B:100:LEU:O	3:B:100:LEU:HD23	0.41	2.16	15	1
3:B:68:GLN:N	3:B:72:LYS:HE2	0.40	2.31	1	1
3:A:35:HIS:N	3:A:37:PRO:HD2	0.40	2.31	2	1
3:A:43:LEU:CD2	3:B:51:LEU:HB3	0.40	2.43	2	1
1:E:3:DT:H73	1:E:3:DT:OP2	0.40	2.17	3	1
3:A:19:TRP:CH2	3:B:39:LEU:CB	0.40	3.04	3	1
3:B:40:ASN:O	3:B:41:LEU:C	0.40	2.64	3	1
2:F:3:DT:OP2	3:A:68:GLN:HA	0.40	2.15	4	1
3:A:17:GLN:HA	3:A:20:LEU:HB2	0.40	1.93	4	1
3:B:88:SER:HB3	3:B:93:PRO:CG	0.40	2.46	4	1
3:B:56:ARG:HD3	3:B:71:LEU:HD21	0.40	1.92	5	1
3:A:72:LYS:HB2	3:A:82:ILE:CD1	0.40	2.46	7	1
3:A:54:ARG:NE	4:B:109:TRP:O	0.40	2.54	8	1
3:A:68:GLN:OE1	3:A:69:ARG:NE	0.40	2.55	11	1
3:A:40:ASN:OD1	3:B:91:ALA:HB1	0.40	2.14	13	1
3:B:55:VAL:O	3:B:58:VAL:CG2	0.40	2.69	13	1
3:B:95:GLU:CA	3:B:96:LEU:HD13	0.40	2.47	13	1
3:B:36:LEU:H	3:B:37:PRO:HD2	0.40	1.74	14	1
3:B:59:GLU:OE1	3:B:60:GLU:OE1	0.40	2.39	14	1
3:A:91:ALA:O	3:B:40:ASN:ND2	0.40	2.53	1	1
3:B:68:GLN:CA	3:B:72:LYS:HE2	0.40	2.47	1	1
3:A:28:ASN:O	3:A:31:GLN:HG2	0.40	2.17	2	1
1:E:18:DA:N6	2:F:4:DA:C6	0.40	2.89	3	1
3:A:55:VAL:HB	3:B:22:PHE:CE2	0.40	2.47	3	1
3:A:65:GLU:CB	3:A:70:GLU:OE2	0.40	2.69	3	1
3:B:29:ALA:O	3:B:35:HIS:CA	0.40	2.69	4	1
3:B:38:LEU:CD2	3:B:41:LEU:HD23	0.40	2.43	4	1
3:A:44:THR:HG23	3:B:54:ARG:CZ	0.40	2.46	5	1
3:B:43:LEU:O	3:B:43:LEU:HD23	0.40	2.15	6	1
3:A:17:GLN:CB	3:A:20:LEU:HB2	0.40	2.45	7	1
3:B:22:PHE:O	3:B:24:ASP:N	0.40	2.54	7	1
3:B:65:GLU:O	3:B:66:MET:CB	0.40	2.69	7	1
1:E:9:DT:OP2	1:E:9:DT:C7	0.40	2.66	8	1
2:F:15:DA:C2'	2:F:16:DG:C8	0.40	3.03	8	1
3:A:54:ARG:O	3:B:42:MET:CG	0.40	2.69	9	1
3:B:77:ALA:O	3:B:81:THR:OG1	0.40	2.29	9	1
1:E:12:DA:H2''	1:E:13:DC:C5'	0.40	2.45	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:90:LYS:CE	4:B:201:TRP:O	0.40	2.69	13	1
3:A:51:LEU:HG	3:B:22:PHE:HE2	0.40	1.73	14	1
3:A:40:ASN:HB3	3:A:45:PRO:HB3	0.40	1.94	1	1
3:A:87:ASN:HB3	3:B:43:LEU:CD2	0.40	2.46	1	1
3:B:38:LEU:C	3:B:41:LEU:CD2	0.40	2.95	1	1
3:B:50:ALA:O	3:B:54:ARG:CZ	0.40	2.70	1	1
3:A:72:LYS:NZ	3:A:79:ILE:HD11	0.40	2.32	2	1
3:A:20:LEU:CD1	3:B:34:LEU:CD1	0.40	3.00	3	1
3:A:57:ILE:HD13	4:B:109:TRP:CZ3	0.40	2.51	3	1
3:A:72:LYS:NZ	3:A:79:ILE:CD1	0.40	2.84	3	1
3:B:52:GLY:O	3:B:56:ARG:HG2	0.40	2.16	3	1
3:B:72:LYS:CE	3:B:82:ILE:CG1	0.40	2.99	3	1
3:A:39:LEU:HD21	3:A:48:ARG:HB2	0.40	1.93	4	1
3:A:30:TYR:HB3	3:B:27:LYS:HD3	0.40	1.93	6	1
3:A:40:ASN:ND2	3:A:48:ARG:CZ	0.40	2.84	6	1
3:A:29:ALA:O	3:A:32:ASN:OD1	0.40	2.38	8	1
3:A:34:LEU:CD2	3:B:99:TRP:HB2	0.40	2.37	8	1
3:A:38:LEU:CA	3:A:41:LEU:HD12	0.40	2.46	8	1
3:A:67:SER:O	3:A:68:GLN:CD	0.40	2.64	9	1
3:B:62:LEU:CD2	3:B:97:ARG:CZ	0.40	2.99	11	1
3:B:106:LYS:O	3:B:106:LYS:HD2	0.40	2.17	11	1
3:B:90:LYS:HB2	3:B:90:LYS:NZ	0.40	2.32	13	1
2:F:13:DC:C2	2:F:14:DG:N9	0.40	2.89	14	1
3:A:43:LEU:CD1	3:B:53:THR:OG1	0.40	2.68	14	1
3:B:55:VAL:O	3:B:58:VAL:HG22	0.40	2.17	14	1
3:A:27:LYS:CE	3:A:28:ASN:N	0.40	2.85	2	1
1:E:18:DA:C5	2:F:4:DA:N1	0.40	2.90	3	1
3:A:78:GLY:CA	3:A:81:THR:CG2	0.40	2.99	4	1
3:A:23:VAL:O	3:A:27:LYS:CG	0.40	2.68	5	1
3:B:61:LEU:HD13	3:B:82:ILE:O	0.40	2.16	5	1
3:B:43:LEU:HD12	4:B:109:TRP:CD1	0.40	2.51	6	1
2:F:2:DG:OP2	3:A:68:GLN:NE2	0.40	2.55	7	1
3:A:72:LYS:CA	3:A:78:GLY:HA3	0.40	2.46	7	1
3:B:55:VAL:O	3:B:55:VAL:HG12	0.40	2.17	9	1
3:B:25:LEU:N	3:B:25:LEU:CD1	0.40	2.84	10	1
3:A:54:ARG:NE	4:B:109:TRP:C	0.40	2.79	11	1
3:B:44:THR:HB	4:B:109:TRP:CD1	0.40	2.51	11	1
3:B:83:THR:O	3:B:84:ARG:C	0.40	2.64	11	1
3:A:47:GLU:OE1	3:A:47:GLU:CA	0.40	2.67	13	1
3:A:78:GLY:HA2	3:A:81:THR:CG2	0.40	2.47	14	1
3:B:66:MET:HA	3:B:66:MET:HE3	0.40	1.93	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:GLN:O	3:A:21:ARG:CG	0.40	2.70	4	1
3:A:21:ARG:CZ	3:A:21:ARG:CB	0.40	2.99	4	1
3:A:67:SER:O	3:A:68:GLN:HG3	0.40	2.16	5	1
3:B:64:GLY:O	3:B:65:GLU:HB3	0.40	2.17	5	1
3:A:42:MET:HG3	3:B:54:ARG:CG	0.40	2.47	6	1
1:E:15:DG:N3	1:E:16:DG:C5	0.40	2.90	7	1
3:B:49:GLU:O	3:B:53:THR:HG23	0.40	2.17	7	1
1:E:10:DG:C2	1:E:11:DT:O2	0.40	2.74	8	1
2:F:16:DG:H2'	2:F:17:DT:C6	0.40	2.52	8	1
3:A:41:LEU:N	3:B:91:ALA:O	0.40	2.54	8	1
3:A:55:VAL:O	3:A:57:ILE:N	0.40	2.54	10	1
3:B:41:LEU:CG	3:B:42:MET:N	0.40	2.83	10	1
3:B:102:GLU:HG3	3:B:103:VAL:N	0.40	2.32	11	1
3:B:31:GLN:CG	3:B:32:ASN:N	0.40	2.84	12	1
3:A:69:ARG:HA	3:A:72:LYS:HE3	0.40	1.92	13	1
3:B:21:ARG:HA	3:B:24:ASP:OD2	0.40	2.17	13	1
3:B:84:ARG:CB	4:B:201:TRP:CZ2	0.40	3.05	13	1
3:B:34:LEU:HD11	3:B:38:LEU:CD1	0.40	2.47	14	1
3:B:72:LYS:HB2	3:B:78:GLY:C	0.40	2.42	15	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	
3	A	90/107 (84%)	63±4 (70±4%)	17±4 (19±5%)	10±2 (11±2%)	1	8
3	B	89/107 (83%)	54±3 (61±4%)	24±3 (27±4%)	11±3 (13±3%)	1	6
All	All	2685/3210 (84%)	1752 (65%)	615 (23%)	318 (12%)	1	7

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

Mol	Chain	Res	Type	Models (Total)
3	B	77	ALA	15
3	B	92	ALA	15

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Mol	Chain	Res	Type	Models (Total)
3	B	43	LEU	14
3	A	77	ALA	13
3	B	44	THR	13
3	B	71	LEU	13
3	A	43	LEU	12
3	A	94	VAL	11
3	B	69	ARG	11
3	A	68	GLN	10
3	A	79	ILE	10
3	A	45	PRO	9
3	B	67	SER	9
3	B	65	GLU	9
3	A	65	GLU	8
3	A	66	MET	8
3	A	76	GLY	8
3	A	75	LEU	8
3	B	68	GLN	8
3	A	70	GLU	7
3	A	67	SER	7
3	A	64	GLY	6
3	B	47	GLU	6
3	B	88	SER	6
3	B	79	ILE	5
3	B	93	PRO	5
3	A	93	PRO	5
3	B	66	MET	4
3	A	106	LYS	4
3	B	48	ARG	4
3	B	64	GLY	4
3	A	27	LYS	4
3	B	36	LEU	3
3	B	78	GLY	3
3	B	76	GLY	3
3	A	69	ARG	3
3	B	94	VAL	3
3	A	44	THR	2
3	A	54	ARG	2
3	A	72	LYS	2
3	A	18	GLU	2
3	B	34	LEU	2
3	A	33	ASP	2
3	A	82	ILE	2

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Mol	Chain	Res	Type	Models (Total)
3	B	74	GLU	2
3	B	75	LEU	2
3	B	18	GLU	1
3	B	45	PRO	1
3	B	55	VAL	1
3	B	35	HIS	1
3	B	72	LYS	1
3	A	57	ILE	1
3	B	106	LYS	1
3	A	41	LEU	1
3	B	70	GLU	1
3	A	35	HIS	1
3	B	41	LEU	1
3	A	26	LEU	1
3	B	33	ASP	1
3	A	71	LEU	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	
3	A	79/92 (86%)	49±3 (62±4%)	30±3 (38±4%)	0	7
3	B	78/92 (85%)	48±4 (61±5%)	30±4 (39±5%)	0	6
All	All	2355/2760 (85%)	1445 (61%)	910 (39%)	0	6

All 141 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)
3	A	41	LEU	15
3	A	58	VAL	15
3	B	72	LYS	15
3	B	90	LYS	15
3	A	81	THR	14
3	B	28	ASN	14
3	B	39	LEU	14
3	B	71	LEU	14

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Mol	Chain	Res	Type	Models (Total)
3	A	44	THR	13
3	A	100	LEU	13
3	B	26	LEU	13
3	B	41	LEU	13
3	A	30	TYR	12
3	A	39	LEU	12
3	A	90	LYS	12
3	B	48	ARG	12
3	B	79	ILE	12
3	B	89	LEU	12
3	A	43	LEU	12
3	B	33	ASP	11
3	A	75	LEU	11
3	B	98	GLN	11
3	A	27	LYS	10
3	A	70	GLU	10
3	B	21	ARG	10
3	B	38	LEU	10
3	B	42	MET	10
3	B	44	THR	10
3	B	105	LEU	10
3	A	71	LEU	10
3	A	28	ASN	10
3	B	18	GLU	9
3	B	58	VAL	9
3	B	81	THR	9
3	A	57	ILE	9
3	B	47	GLU	9
3	B	75	LEU	9
3	B	82	ILE	9
3	B	59	GLU	9
3	B	106	LYS	9
3	A	26	LEU	8
3	A	53	THR	8
3	A	66	MET	8
3	A	82	ILE	8
3	A	105	LEU	8
3	B	74	GLU	8
3	A	42	MET	8
3	A	51	LEU	8
3	A	63	ARG	8
3	B	83	THR	8

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Mol	Chain	Res	Type	Models (Total)
3	A	47	GLU	7
3	A	65	GLU	7
3	B	46	ASP	7
3	B	54	ARG	7
3	B	57	ILE	7
3	A	33	ASP	7
3	A	74	GLU	7
3	A	79	ILE	7
3	B	68	GLN	7
3	B	104	LEU	7
3	A	22	PHE	6
3	A	46	ASP	6
3	A	48	ARG	6
3	A	68	GLN	6
3	A	102	GLU	6
3	A	104	LEU	6
3	B	53	THR	6
3	A	69	ARG	6
3	A	88	SER	6
3	A	106	LYS	6
3	B	88	SER	6
3	A	67	SER	6
3	A	54	ARG	6
3	A	98	GLN	6
3	B	30	TYR	6
3	B	65	GLU	6
3	B	51	LEU	6
3	A	21	ARG	5
3	A	72	LYS	5
3	B	70	GLU	5
3	A	56	ARG	5
3	A	73	ASN	5
3	A	84	ARG	5
3	B	67	SER	5
3	B	100	LEU	5
3	B	101	GLU	5
3	A	49	GLU	5
3	A	59	GLU	5
3	A	96	LEU	5
3	B	25	LEU	5
3	B	56	ARG	5
3	B	84	ARG	5

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Mol	Chain	Res	Type	Models (Total)
3	A	20	LEU	5
3	B	63	ARG	5
3	A	25	LEU	5
3	A	87	ASN	5
3	A	35	HIS	5
3	A	17	GLN	4
3	A	36	LEU	4
3	B	34	LEU	4
3	B	43	LEU	4
3	B	96	LEU	4
3	A	40	ASN	4
3	B	99	TRP	4
3	B	102	GLU	4
3	A	89	LEU	4
3	B	69	ARG	4
3	B	66	MET	3
3	A	94	VAL	3
3	B	20	LEU	3
3	B	95	GLU	3
3	B	97	ARG	3
3	A	86	SER	3
3	A	34	LEU	3
3	A	55	VAL	3
3	B	61	LEU	3
3	A	61	LEU	3
3	A	32	ASN	2
3	A	62	LEU	2
3	B	40	ASN	2
3	B	87	ASN	2
3	A	95	GLU	2
3	B	73	ASN	2
3	A	31	GLN	2
3	A	38	LEU	2
3	A	24	ASP	1
3	B	31	GLN	1
3	B	35	HIS	1
3	A	97	ARG	1
3	B	32	ASN	1
3	B	62	LEU	1
3	A	60	GLU	1
3	B	103	VAL	1
3	B	86	SER	1

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Mol	Chain	Res	Type	Models (Total)
3	A	99	TRP	1
3	B	55	VAL	1
3	B	22	PHE	1
3	B	27	LYS	1
3	B	36	LEU	1
3	A	18	GLU	1
3	B	60	GLU	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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	TRP	B	109	-	15,16,16	0.94±0.06	1±0 (7±2%)
4	TRP	B	201	-	15,16,16	1.13±0.22	2±1 (12±6%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types,

if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
4	TRP	B	109	-	18,22,22	1.53±0.04	3±0 (18±2%)
4	TRP	B	201	-	18,22,22	1.69±0.21	4±1 (22±6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRP	B	109	-	-	0±0,8,8,8	0±0,2,2,2
4	TRP	B	201	-	-	0±0,8,8,8	0±0,2,2,2

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
4	B	201	TRP	CB-CG	3.33	1.43	1.50	10	7
4	B	109	TRP	OXT-C	2.97	1.21	1.30	15	15
4	B	201	TRP	CD1-CG	2.84	1.32	1.36	14	6
4	B	201	TRP	OXT-C	2.78	1.21	1.30	2	15
4	B	109	TRP	CD1-CG	2.19	1.33	1.36	8	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	201	TRP	CD2-CE2-NE1	4.48	103.78	107.52	10	15
4	B	109	TRP	CD2-CE2-NE1	4.09	104.11	107.52	7	15
4	B	201	TRP	CA-CB-CG	4.01	105.88	113.49	10	8
4	B	201	TRP	CZ2-CE2-NE1	3.07	135.65	130.74	10	14
4	B	201	TRP	CE2-NE1-CD1	2.96	111.71	109.08	2	12
4	B	109	TRP	CE2-NE1-CD1	2.74	111.51	109.08	1	15
4	B	109	TRP	CZ2-CE2-NE1	2.69	135.06	130.74	9	15
4	B	201	TRP	CG-CD1-NE1	2.34	107.74	110.31	13	7
4	B	201	TRP	CD2-CG-CD1	2.28	108.49	106.16	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	109	TRP	CE2-CD2-CG	2.18	109.37	107.17	9	6
4	B	201	TRP	CE2-CD2-CG	2.07	109.25	107.17	13	3

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided