



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 05:57 AM UTC

PDB ID : 2H3A / pdb_00002h3a
Title : Structural basis for nucleic acid and toxin recognition of the bacterial antitoxin CcdA
Authors : Madl, T.; Van Melderen, L.; Respondek, M.; Oberer, M.; Keller, W.; Zangger, K.
Deposited on : 2006-05-22

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

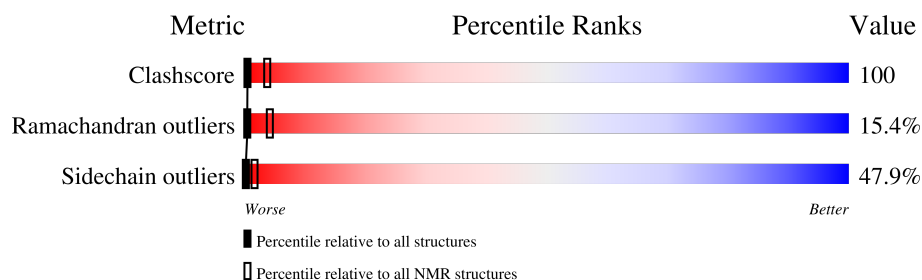
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	C	13	
2	D	13	
3	A	72	
3	B	72	

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:2-A:38, B:102-B:138 (74)	0.67	12

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 1 single-model cluster was found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3159 atoms, of which 1448 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	C	13	Total	C	H	N	O	P	0
			415	127	149	47	79	13	

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

Mol	Chain	Residues	Atoms						Trace
2	D	13	Total	C	H	N	O	P	0
			418	128	149	49	79	13	

- Molecule 3 is a protein called CcdA.

Mol	Chain	Residues	Atoms						Trace
3	A	72	Total	C	H	N	O	S	0
			1163	362	575	105	117	4	
3	B	72	Total	C	H	N	O	S	0
			1163	362	575	105	117	4	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	LYS	ARG	engineered mutation	UNP Q9S0Z5
B	170	LYS	ARG	engineered mutation	UNP Q9S0Z5

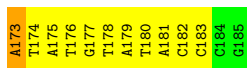
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

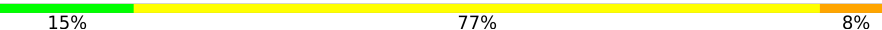
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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.

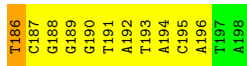
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 



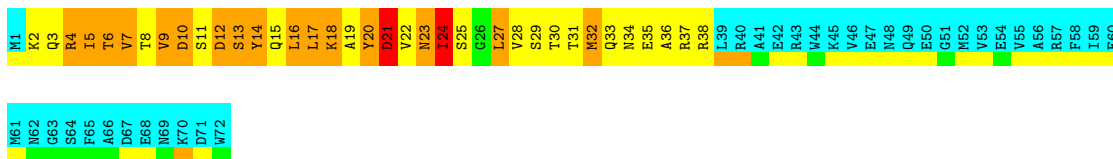
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 



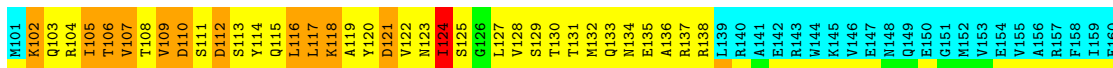
- Molecule 3: CcdA

Chain A: 



- Molecule 3: CcdA

Chain B: 

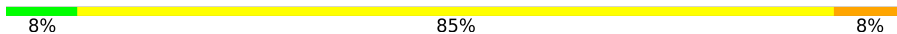


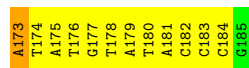
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

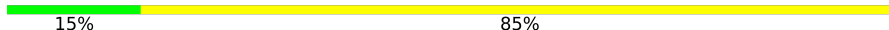
4.2.1 Score per residue for model 1

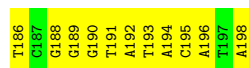
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 



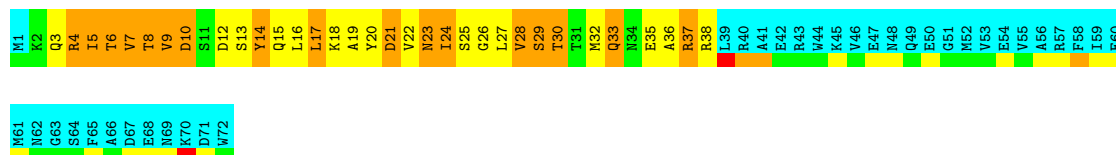
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 

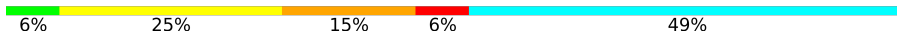


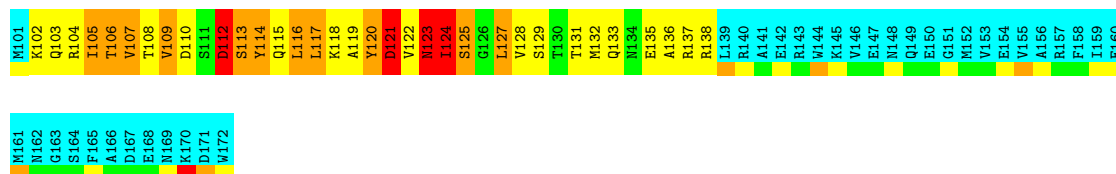
- Molecule 3: CcdA

Chain A: 



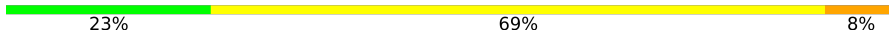
- Molecule 3: CcdA

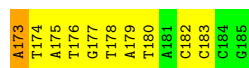
Chain B: 



4.2.2 Score per residue for model 2

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

Chain C: 



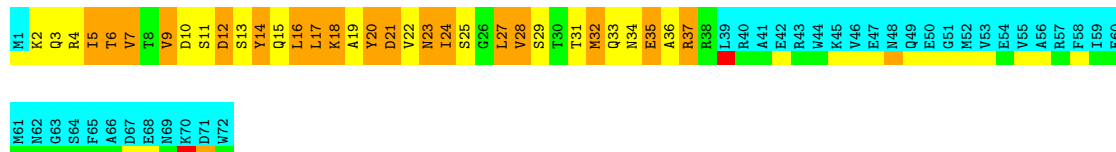
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D:  15% 85%



- Molecule 3: CcdA

Chain A:  6% 21% 25% 49%



- Molecule 3: CcdA

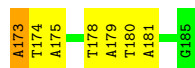
Chain B:  6% 21% 22% 49%



4.2.3 Score per residue for model 3

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

Chain C:  46% 46% 8%



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

Chain D:  23% 69% 8%



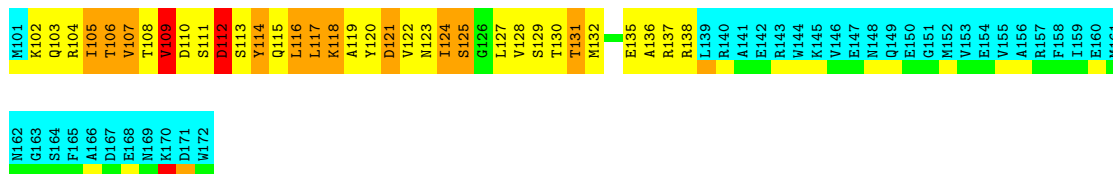
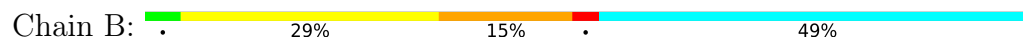
- Molecule 3: CcdA

Chain A:  7% 22% 21% 49%





• Molecule 3: CcdA

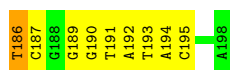


4.2.4 Score per residue for model 4

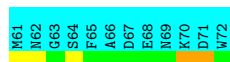
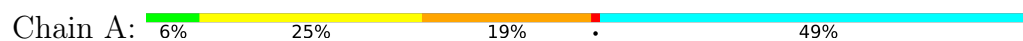
• Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'



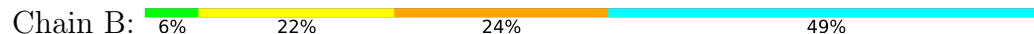
• Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'



• Molecule 3: CcdA

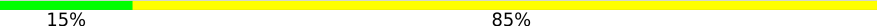


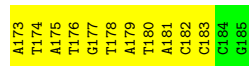
• Molecule 3: CcdA



4.2.5 Score per residue for model 5

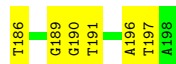
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 



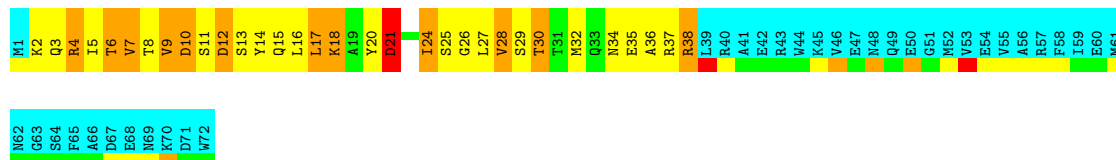
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 



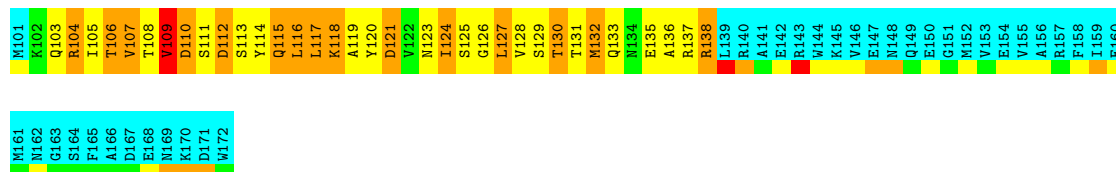
- Molecule 3: CcdA

Chain A: 



- Molecule 3: CcdA

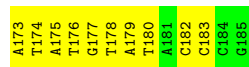
Chain B: 



4.2.6 Score per residue for model 6

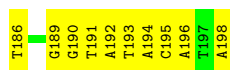
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 

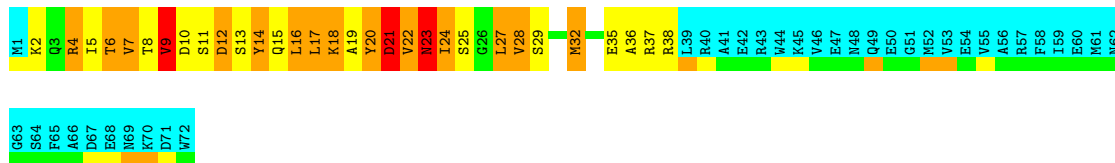


- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

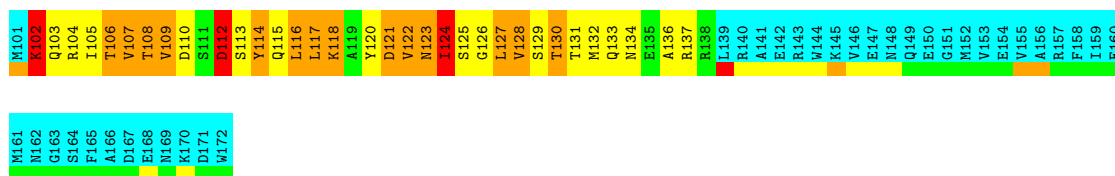
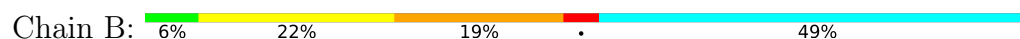
Chain D: 



• Molecule 3: CcdA

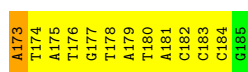


• Molecule 3: CcdA

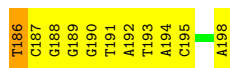


4.2.7 Score per residue for model 7

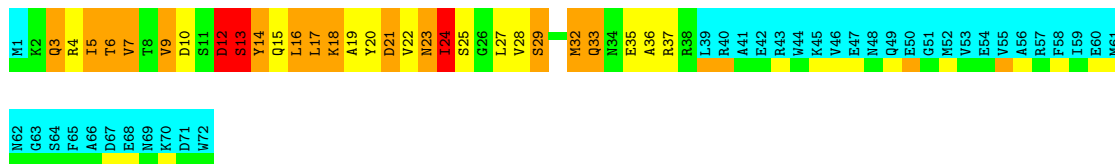
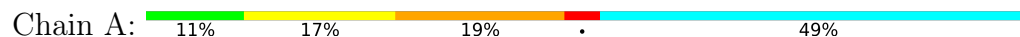
• Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'



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

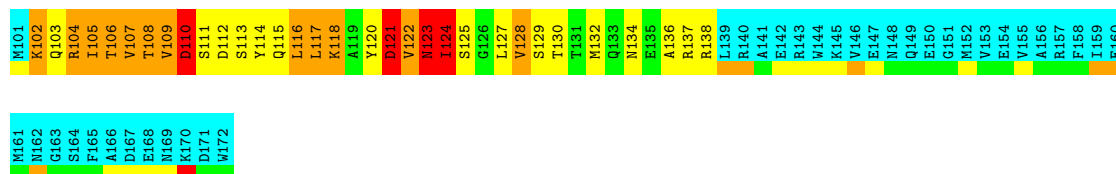


• Molecule 3: CcdA



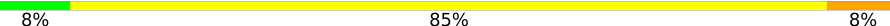
• Molecule 3: CcdA

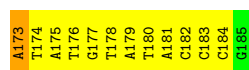
Chain B:  7% 22% 17% 6% 49%



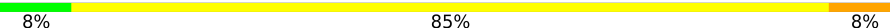
4.2.8 Score per residue for model 8

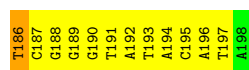
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C:  8% 85% 8%



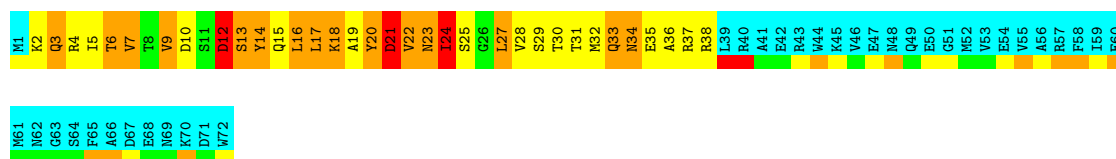
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D:  8% 85% 8%



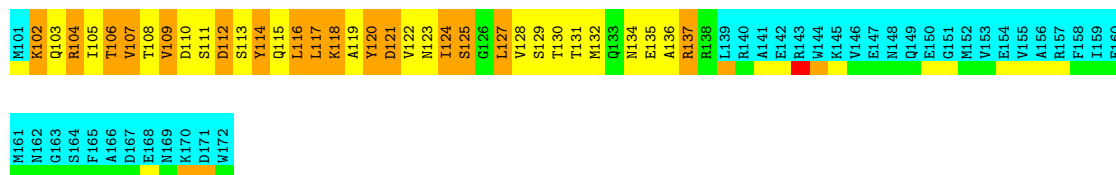
- Molecule 3: CcdA

Chain A:  22% 21% 49%



- Molecule 3: CcdA

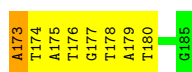
Chain B:  25% 22% 49%



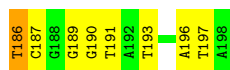
4.2.9 Score per residue for model 9

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

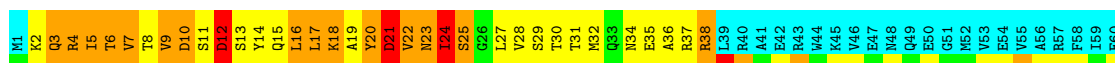
Chain C:  38% 54% 8%



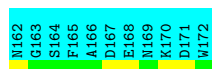
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'



- Molecule 3: CcdA

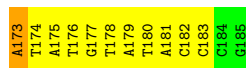


- Molecule 3: CcdA

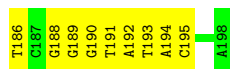


4.2.10 Score per residue for model 10

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



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

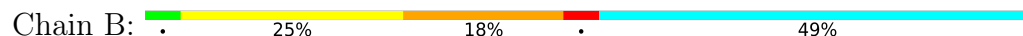


- Molecule 3: CcdA



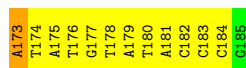


• Molecule 3: CcdA

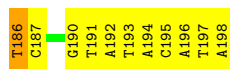
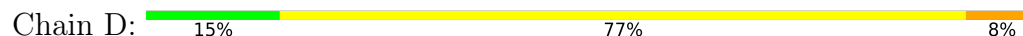


4.2.11 Score per residue for model 11

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



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



• Molecule 3: CcdA

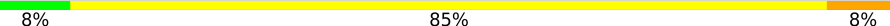


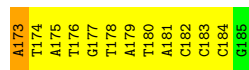
• Molecule 3: CcdA



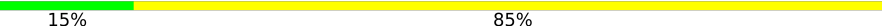
4.2.12 Score per residue for model 12 (medoid)

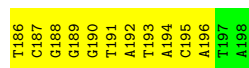
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 



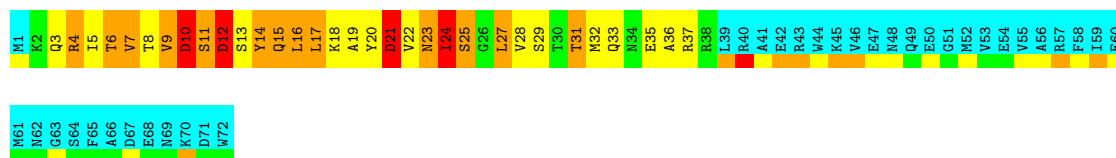
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 



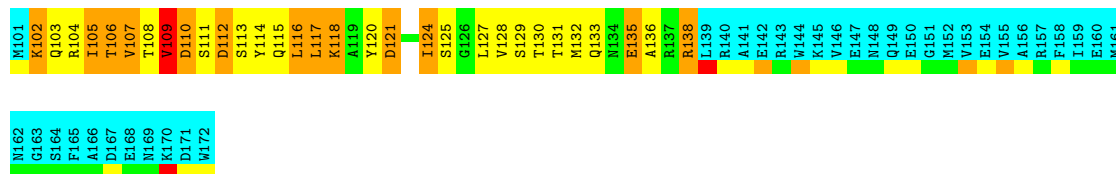
- Molecule 3: CcdA

Chain A: 



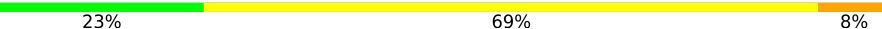
- Molecule 3: CcdA

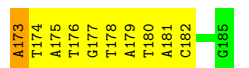
Chain B: 



4.2.13 Score per residue for model 13

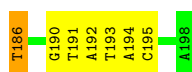
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 

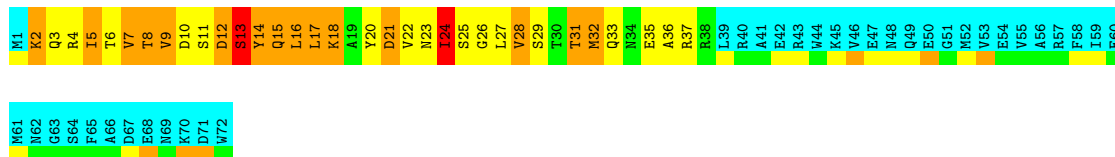
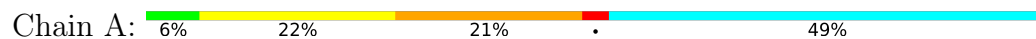


- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

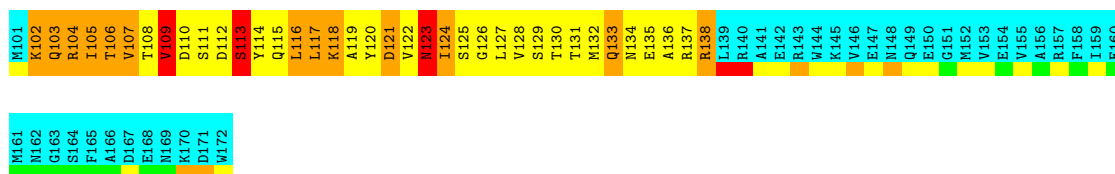
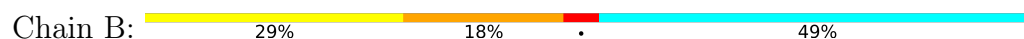
Chain D: 



• Molecule 3: CcdA

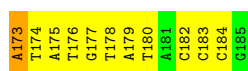


• Molecule 3: CcdA



4.2.14 Score per residue for model 14

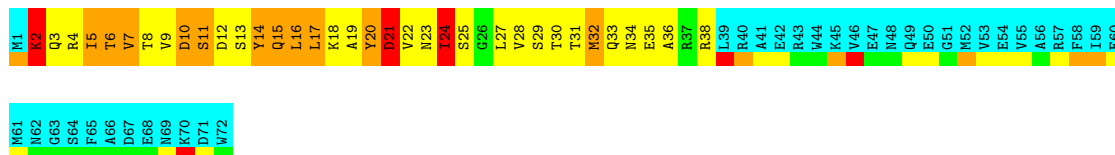
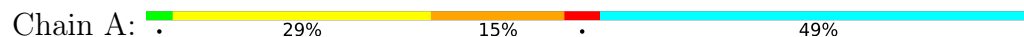
• Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'



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

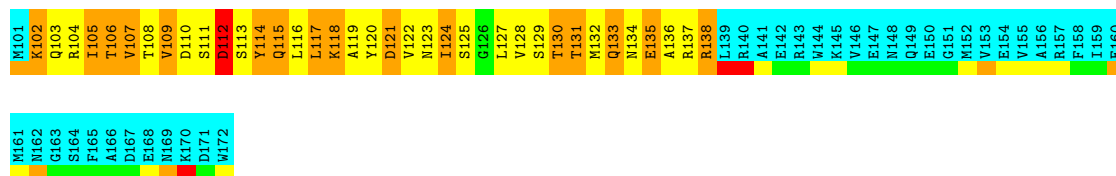


• Molecule 3: CcdA



• Molecule 3: CcdA

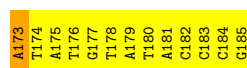
Chain B: 26% 22% 49%



4.2.15 Score per residue for model 15

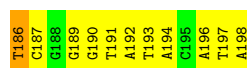
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 92% 8%



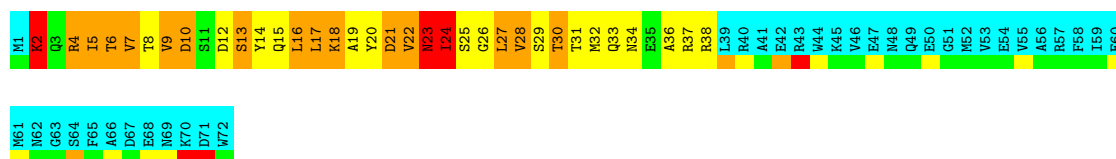
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 15% 77% 8%



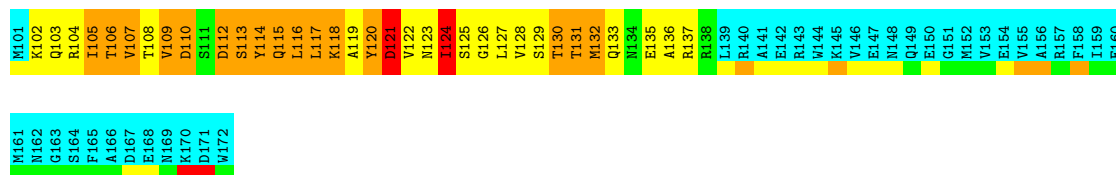
- Molecule 3: CcdA

Chain A: 22% 21% 49%



- Molecule 3: CcdA

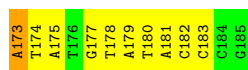
Chain B: 22% 22% 49%



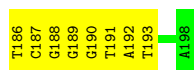
4.2.16 Score per residue for model 16

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

Chain C: 23% 69% 8%



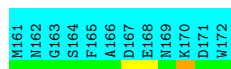
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'



- Molecule 3: CcdA

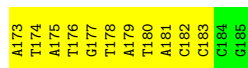


- Molecule 3: CcdA

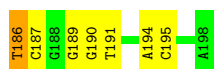


4.2.17 Score per residue for model 17

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

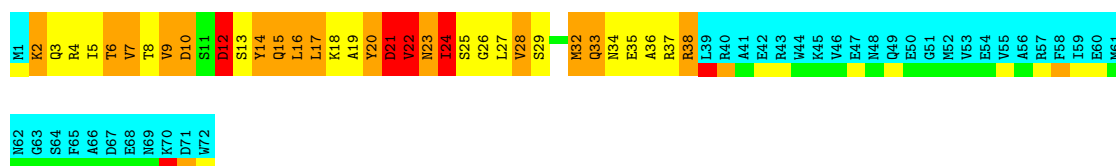


- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'



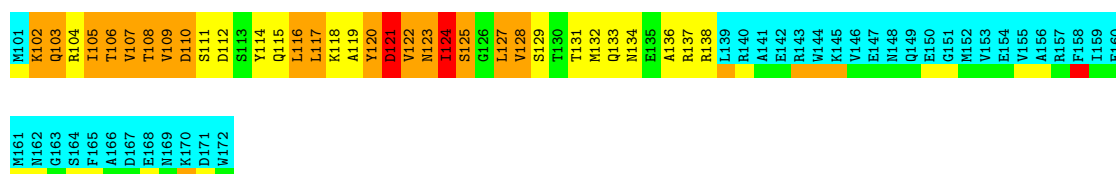
- Molecule 3: CcdA





• Molecule 3: CcdA

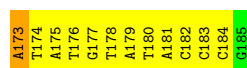
Chain B: 6% 21% 22% . 49%



4.2.18 Score per residue for model 18

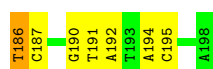
• Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 8% 85% 8%



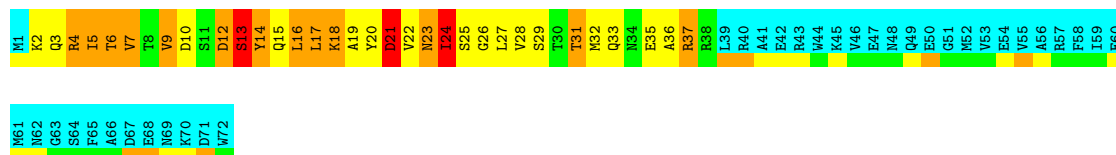
• Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 46% 46% 8%



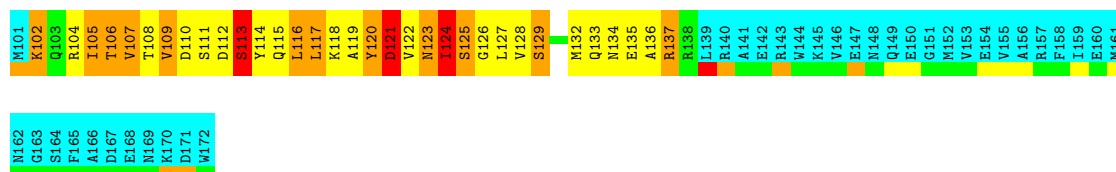
• Molecule 3: CcdA

Chain A: 7% 22% 18% . 49%



• Molecule 3: CcdA

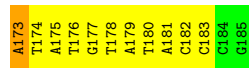
Chain B: 6% 25% 17% . 49%



4.2.19 Score per residue for model 19

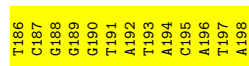
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 15% 77% 8%



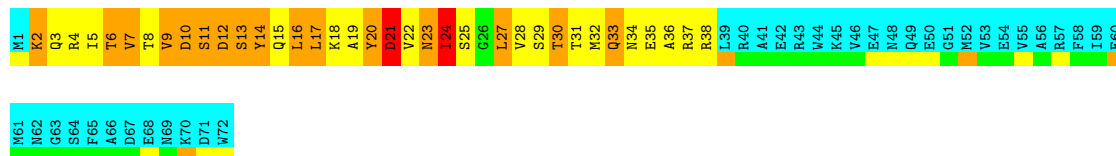
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 100%



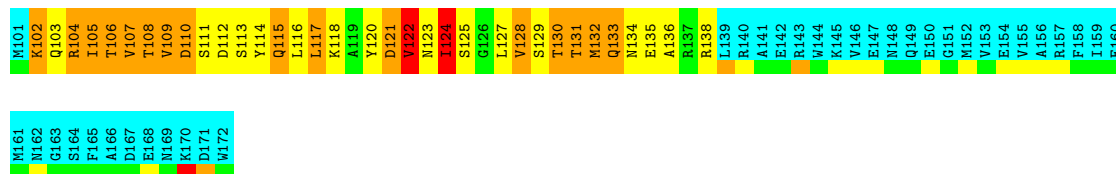
- Molecule 3: CcdA

Chain A: 25% 22% 49%



- Molecule 3: CcdA

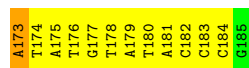
Chain B: 22% 22% 49%



4.2.20 Score per residue for model 20

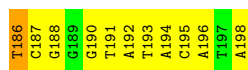
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 8% 85% 8%

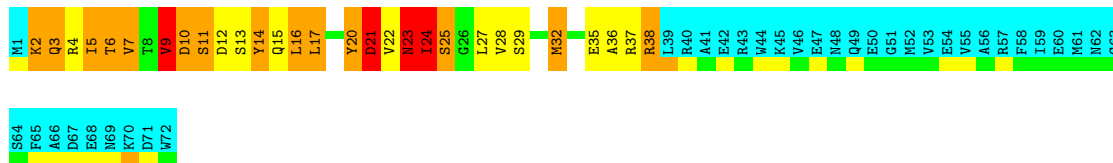


- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

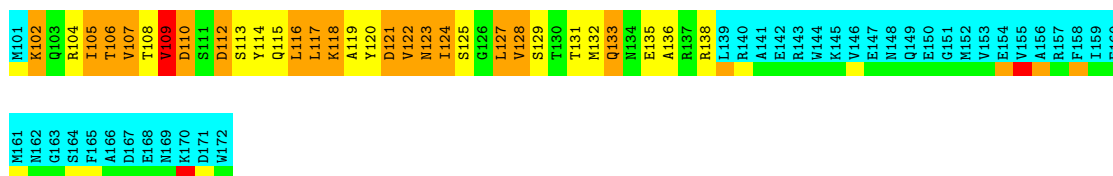
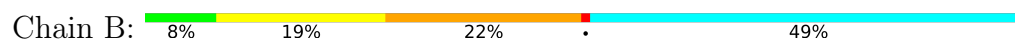
Chain D: 15% 77% 8%



● Molecule 3: CcdA



● Molecule 3: CcdA



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	C	0.42±0.01	1±0/297 (0.3± 0.0%)	0.59±0.02	0±0/454 (0.0± 0.0%)
2	D	0.41±0.00	1±0/301 (0.3± 0.0%)	0.58±0.02	0±0/461 (0.0± 0.0%)
3	A	0.68±0.04	0±0/295 (0.0± 0.0%)	0.90±0.04	0±0/399 (0.0± 0.1%)
3	B	0.66±0.04	0±0/295 (0.0± 0.0%)	0.90±0.05	0±0/399 (0.0± 0.1%)
All	All	0.56	40/23760 (0.2%)	0.75	3/34260 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	173	DA	OP3-P	5.68	1.59	1.48	2	20
2	D	186	DT	OP3-P	5.66	1.59	1.48	4	20

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
3	B	124	ILE	N-CA-C	5.17	120.10	109.34	18	1
3	A	24	ILE	N-CA-C	5.16	120.07	109.34	11	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	C	266	149	148	21±7
2	D	269	149	148	13±4
3	A	293	298	298	127±11
3	B	293	298	298	128±10
All	All	22420	17880	17840	4016

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 100.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:VAL:HG21	3:A:14:TYR:CD2	1.12	1.79	11	1
3:A:9:VAL:HG21	3:A:14:TYR:CD1	1.09	1.81	10	4
3:A:17:LEU:HD12	3:B:132:MET:HA	1.07	1.21	3	2
3:B:124:ILE:CG2	3:B:128:VAL:HG23	1.05	1.81	11	17
3:A:24:ILE:CG2	3:A:28:VAL:HG23	1.03	1.81	15	15
3:A:28:VAL:HG21	3:B:128:VAL:HG22	1.02	1.25	15	1
3:B:109:VAL:HG21	3:B:114:TYR:CB	1.02	1.84	13	15
3:B:109:VAL:HG21	3:B:114:TYR:CD2	1.02	1.89	15	3
3:A:24:ILE:HD11	3:B:105:ILE:HD12	1.02	1.24	12	3
3:A:24:ILE:HG21	3:B:132:MET:HE3	1.01	1.31	11	3
3:A:5:ILE:HG21	3:B:114:TYR:CZ	1.01	1.90	11	9
3:B:124:ILE:HG22	3:B:127:LEU:HD12	1.00	1.29	18	2
3:A:28:VAL:CG2	3:B:128:VAL:HG22	1.00	1.87	15	8
3:A:5:ILE:HG21	3:B:114:TYR:CE1	1.00	1.92	7	14
3:A:5:ILE:HD13	3:B:114:TYR:CD2	0.99	1.92	8	3
3:A:28:VAL:HG22	3:B:124:ILE:HG21	0.99	1.33	8	9
3:A:14:TYR:CD2	3:B:105:ILE:HD13	0.98	1.94	10	3
3:A:32:MET:SD	3:B:117:LEU:HD12	0.98	1.98	6	3
3:A:4:ARG:HG3	3:B:108:THR:HG23	0.97	1.31	19	5
3:A:24:ILE:HG21	3:B:132:MET:SD	0.97	1.99	7	2
3:A:17:LEU:HD12	3:B:132:MET:SD	0.97	2.00	15	3
3:A:24:ILE:HG21	3:A:28:VAL:HG23	0.96	1.31	15	9
3:A:17:LEU:HD22	3:B:132:MET:HA	0.96	1.37	8	1
3:A:28:VAL:HG13	3:A:32:MET:HE3	0.95	1.35	10	6
3:B:123:ASN:O	3:B:124:ILE:HD12	0.95	1.60	15	5
3:B:109:VAL:HG11	3:B:114:TYR:CB	0.95	1.89	4	11
3:A:14:TYR:CZ	3:B:105:ILE:HG21	0.95	1.96	4	5
3:B:124:ILE:HG21	3:B:128:VAL:HG23	0.95	1.33	17	14
3:A:4:ARG:HG2	3:B:106:THR:HG22	0.94	1.39	14	4
3:B:109:VAL:HG21	3:B:114:TYR:CD1	0.94	1.98	8	3
3:A:23:ASN:O	3:A:24:ILE:HD12	0.94	1.62	12	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:35:GLU:HB3	3:B:117:LEU:HD21	0.93	1.36	5	11
3:A:32:MET:HE1	3:B:124:ILE:HG21	0.93	1.40	13	1
3:A:24:ILE:HD11	3:B:105:ILE:CD1	0.93	1.93	12	4
3:B:117:LEU:HD12	3:B:127:LEU:HD22	0.92	1.41	3	1
3:A:5:ILE:CG1	3:B:124:ILE:HD11	0.91	1.94	7	4
3:A:7:VAL:O	3:B:105:ILE:HG23	0.91	1.64	20	4
3:A:9:VAL:HG21	3:A:14:TYR:CB	0.91	1.94	16	9
3:A:14:TYR:CE1	3:B:105:ILE:HD11	0.91	2.00	12	1
3:A:9:VAL:HG11	3:A:14:TYR:CB	0.91	1.96	11	12
3:A:24:ILE:HG21	3:B:132:MET:CE	0.90	1.96	11	5
3:A:32:MET:SD	3:B:117:LEU:HB2	0.90	2.06	18	11
3:B:109:VAL:HG21	3:B:114:TYR:CG	0.89	2.02	16	10
3:A:14:TYR:HA	3:B:132:MET:SD	0.89	2.07	9	10
3:A:24:ILE:HG23	3:B:132:MET:HE2	0.89	1.43	5	5
3:A:17:LEU:HB2	3:B:132:MET:SD	0.89	2.07	14	13
3:B:109:VAL:HG21	3:B:114:TYR:HB3	0.88	1.43	13	6
3:A:14:TYR:CD1	3:B:105:ILE:HD13	0.88	2.03	6	7
3:A:28:VAL:HG22	3:B:128:VAL:CG2	0.87	1.99	20	13
3:B:124:ILE:HB	3:B:128:VAL:HG23	0.87	1.47	18	13
3:A:14:TYR:CE1	3:B:105:ILE:HG21	0.87	2.04	4	6
1:C:177:DG:C8	1:C:178:DT:H72	0.87	2.05	18	6
3:A:28:VAL:HG12	3:A:32:MET:SD	0.87	2.09	17	3
3:A:9:VAL:HG23	3:A:14:TYR:HB3	0.86	1.44	14	1
3:A:5:ILE:HD13	3:B:114:TYR:CD1	0.86	2.06	5	11
3:A:5:ILE:HD11	3:B:107:VAL:HG13	0.86	1.45	11	6
3:B:128:VAL:HG13	3:B:132:MET:SD	0.86	2.10	19	4
3:B:124:ILE:CG2	3:B:127:LEU:HD12	0.86	2.00	18	2
3:A:24:ILE:HG23	3:B:132:MET:HE3	0.85	1.48	9	2
3:A:9:VAL:HG21	3:A:14:TYR:HB3	0.85	1.44	3	7
3:A:32:MET:HE2	3:B:124:ILE:HG23	0.85	1.48	10	8
3:A:9:VAL:HG11	3:A:14:TYR:HB3	0.84	1.49	12	13
3:A:4:ARG:HG3	3:B:108:THR:HG22	0.84	1.46	1	17
3:A:12:ASP:CB	3:B:129:SER:HB2	0.84	2.03	2	9
3:B:109:VAL:HG21	3:B:114:TYR:HB2	0.84	1.47	1	7
3:A:28:VAL:HG22	3:B:128:VAL:HG21	0.84	1.49	16	2
3:A:32:MET:HE2	3:B:124:ILE:HG21	0.84	1.49	18	1
3:A:5:ILE:HG13	3:B:124:ILE:HD11	0.84	1.50	7	4
3:A:25:SER:HA	3:B:107:VAL:HG22	0.84	1.50	18	5
3:B:124:ILE:HG22	3:B:127:LEU:HB3	0.83	1.50	2	14
3:A:24:ILE:HB	3:A:28:VAL:HG23	0.83	1.47	18	14
2:D:190:DG:C8	2:D:191:DT:H72	0.83	2.08	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:24:ILE:HG12	3:B:132:MET:HE1	0.83	1.47	7	5
3:A:9:VAL:HG11	3:A:14:TYR:CG	0.83	2.09	2	4
3:A:27:LEU:HD12	3:B:132:MET:SD	0.83	2.14	2	4
3:A:6:THR:HB	3:B:106:THR:HG23	0.83	1.48	20	4
3:A:24:ILE:HG21	3:B:128:VAL:HG22	0.82	1.51	8	8
3:A:35:GLU:HG2	3:B:127:LEU:HD13	0.82	1.48	9	2
3:B:117:LEU:HD12	3:B:122:VAL:CG1	0.82	2.04	9	4
1:C:180:DT:H2''	1:C:181:DA:N7	0.82	1.90	3	12
3:A:24:ILE:HG22	3:A:27:LEU:HB3	0.81	1.50	16	15
3:B:128:VAL:HG13	3:B:132:MET:CE	0.81	2.05	19	6
3:B:107:VAL:HG23	3:B:109:VAL:HG13	0.81	1.53	19	2
3:B:128:VAL:HG13	3:B:132:MET:HE3	0.81	1.51	14	6
3:A:6:THR:CB	3:B:106:THR:HG23	0.81	2.05	14	4
3:B:117:LEU:HD13	3:B:122:VAL:CG1	0.81	2.06	10	2
2:D:186:DT:H2''	2:D:187:DC:O5'	0.81	1.76	15	4
3:A:32:MET:SD	3:B:114:TYR:HA	0.80	2.16	16	13
3:A:36:ALA:HB1	3:B:116:LEU:HB3	0.80	1.52	7	6
1:C:173:DA:H2''	1:C:174:DT:O5'	0.80	1.75	11	2
3:A:23:ASN:C	3:A:24:ILE:HD12	0.80	2.02	12	8
3:A:17:LEU:HD23	3:A:20:TYR:CE2	0.80	2.11	3	1
1:C:174:DT:H2''	1:C:175:DA:N7	0.80	1.92	17	4
3:A:24:ILE:CD1	3:B:105:ILE:HD12	0.80	2.05	12	3
3:A:16:LEU:HB3	3:B:136:ALA:HB1	0.80	1.52	19	10
3:A:32:MET:HE1	3:B:124:ILE:CG2	0.80	2.07	13	2
3:B:109:VAL:HG11	3:B:114:TYR:HB2	0.80	1.52	15	8
1:C:178:DT:H73	3:A:6:THR:HG23	0.80	1.54	16	3
3:A:4:ARG:HG3	3:B:108:THR:CG2	0.80	2.07	7	20
3:A:17:LEU:HD11	3:A:27:LEU:HD22	0.79	1.53	18	1
3:A:7:VAL:HG23	3:B:124:ILE:HD13	0.79	1.52	20	3
3:B:109:VAL:HG11	3:B:114:TYR:HB3	0.79	1.53	4	7
3:A:23:ASN:O	3:B:132:MET:HE1	0.79	1.78	10	4
3:A:28:VAL:HG13	3:A:32:MET:SD	0.79	2.17	16	1
3:A:6:THR:CG2	3:B:106:THR:HG23	0.78	2.07	14	4
3:A:14:TYR:CE1	3:B:105:ILE:CG1	0.78	2.67	15	2
3:B:107:VAL:HG12	3:B:109:VAL:HG22	0.78	1.56	16	2
3:A:5:ILE:CG1	3:B:107:VAL:HG13	0.78	2.08	1	11
3:A:24:ILE:N	3:A:24:ILE:HD12	0.78	1.94	2	8
3:B:128:VAL:CG1	3:B:132:MET:SD	0.78	2.72	9	4
3:A:28:VAL:CG1	3:A:32:MET:HE2	0.78	2.09	13	1
3:A:12:ASP:HB3	3:B:129:SER:HB2	0.77	1.55	6	10
3:A:14:TYR:CE2	3:B:105:ILE:HG13	0.77	2.15	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:TYR:CD2	3:B:105:ILE:HG21	0.77	2.14	7	8
3:A:17:LEU:HD22	3:A:27:LEU:HD22	0.76	1.56	9	1
3:A:17:LEU:CD1	3:A:27:LEU:HD22	0.76	2.09	18	2
3:A:29:SER:HB3	3:B:112:ASP:CB	0.76	2.11	2	6
3:A:24:ILE:CB	3:A:28:VAL:HG23	0.76	2.11	4	13
3:A:9:VAL:HG11	3:A:14:TYR:HB2	0.76	1.56	11	8
3:A:28:VAL:HG13	3:A:32:MET:HE2	0.76	1.57	13	3
3:A:5:ILE:HD13	3:B:107:VAL:HG13	0.76	1.56	4	1
3:A:32:MET:CE	3:B:124:ILE:HG21	0.76	2.10	13	1
3:B:123:ASN:C	3:B:124:ILE:HD12	0.76	2.06	16	4
3:A:28:VAL:CG1	3:A:32:MET:SD	0.76	2.73	16	4
3:B:124:ILE:HD12	3:B:124:ILE:N	0.75	1.97	2	12
3:A:7:VAL:HG13	3:B:105:ILE:HG12	0.75	1.58	13	7
3:A:32:MET:HA	3:B:117:LEU:HD23	0.75	1.58	8	5
3:A:14:TYR:CE1	3:B:105:ILE:CD1	0.75	2.70	12	1
3:A:17:LEU:HD11	3:B:135:GLU:HB2	0.75	1.57	3	1
3:A:32:MET:HE3	3:B:124:ILE:CG2	0.75	2.12	15	5
3:A:6:THR:CG2	3:B:104:ARG:HG2	0.75	2.11	13	1
3:A:12:ASP:CB	3:B:129:SER:HB3	0.75	2.11	19	9
3:A:5:ILE:HG21	3:B:114:TYR:CD1	0.74	2.16	13	15
3:A:14:TYR:CE1	3:B:105:ILE:HG13	0.74	2.17	15	2
3:A:6:THR:HB	3:B:106:THR:HB	0.74	1.59	8	13
3:A:6:THR:HA	3:B:105:ILE:O	0.74	1.83	15	19
3:A:17:LEU:HG	3:B:132:MET:SD	0.74	2.22	2	4
3:A:7:VAL:HG22	3:A:9:VAL:HG22	0.74	1.56	6	6
3:A:32:MET:HE1	3:B:124:ILE:HG12	0.74	1.58	13	3
3:A:24:ILE:HD13	3:A:28:VAL:HG21	0.74	1.58	1	1
3:B:107:VAL:HG13	3:B:109:VAL:HG13	0.74	1.59	13	1
3:A:24:ILE:HG22	3:A:28:VAL:HG23	0.74	1.59	3	3
3:A:17:LEU:CB	3:B:132:MET:SD	0.74	2.76	2	12
3:A:28:VAL:HG13	3:A:32:MET:CE	0.74	2.13	9	5
3:A:35:GLU:CB	3:B:117:LEU:HD21	0.73	2.14	16	3
3:A:28:VAL:HG22	3:B:128:VAL:HG22	0.73	1.57	1	8
3:A:32:MET:HE3	3:B:124:ILE:HG23	0.73	1.59	1	5
3:A:5:ILE:HD12	3:B:124:ILE:HD11	0.73	1.59	13	3
3:A:9:VAL:HG23	3:A:14:TYR:CB	0.73	2.13	14	1
3:A:12:ASP:HB3	3:B:129:SER:CB	0.73	2.13	6	16
3:A:24:ILE:HD12	3:A:24:ILE:N	0.72	1.99	5	2
1:C:174:DT:H2''	1:C:175:DA:O5'	0.72	1.84	10	9
3:A:17:LEU:HD12	3:A:24:ILE:HG23	0.72	1.59	13	1
3:A:5:ILE:HG12	3:B:107:VAL:HG13	0.72	1.61	1	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:24:ILE:CG2	3:B:132:MET:SD	0.72	2.76	7	2
3:A:24:ILE:CG2	3:A:27:LEU:HD12	0.72	2.13	13	4
2:D:188:DG:H2''	2:D:189:DG:O4'	0.72	1.83	14	1
3:A:5:ILE:CD1	3:B:107:VAL:HG13	0.72	2.14	4	8
3:A:28:VAL:CG1	3:A:32:MET:HE3	0.72	2.14	9	5
3:A:32:MET:HG3	3:B:114:TYR:HA	0.72	1.60	13	7
3:A:14:TYR:CE2	3:B:105:ILE:HG21	0.72	2.20	10	6
3:A:17:LEU:HD12	3:A:22:VAL:CG1	0.72	2.15	12	3
3:A:24:ILE:HG21	3:B:132:MET:HE1	0.72	1.58	1	1
3:A:32:MET:HE1	3:B:123:ASN:O	0.72	1.85	20	5
3:A:16:LEU:HD22	3:B:136:ALA:HB1	0.72	1.60	7	7
2:D:189:DG:H2''	2:D:190:DG:O5'	0.72	1.84	15	1
3:A:7:VAL:HG22	3:B:125:SER:HA	0.71	1.60	20	4
3:B:107:VAL:HG22	3:B:109:VAL:HG22	0.71	1.62	17	5
3:B:114:TYR:CZ	3:B:118:LYS:HD3	0.71	2.20	19	12
3:B:117:LEU:HD13	3:B:122:VAL:HG13	0.71	1.60	10	1
3:A:14:TYR:CD1	3:B:105:ILE:HG13	0.71	2.20	12	2
3:A:24:ILE:HG12	3:B:132:MET:CE	0.71	2.16	13	8
3:A:28:VAL:HG13	3:B:124:ILE:HG21	0.71	1.62	1	3
3:A:29:SER:CB	3:B:112:ASP:HB3	0.71	2.14	3	14
3:A:14:TYR:HA	3:B:132:MET:HG3	0.71	1.62	15	5
3:A:32:MET:HA	3:B:117:LEU:HD12	0.71	1.62	18	2
1:C:178:DT:H72	3:A:6:THR:OG1	0.71	1.86	8	8
3:A:17:LEU:HG	3:A:27:LEU:HD22	0.71	1.61	5	2
3:A:12:ASP:HB2	3:B:129:SER:HB2	0.71	1.61	15	3
3:A:24:ILE:HD13	3:A:28:VAL:CG2	0.71	2.16	1	1
3:A:17:LEU:HD13	3:A:27:LEU:CD1	0.71	2.15	3	1
3:A:24:ILE:HG22	3:A:27:LEU:HD12	0.71	1.63	13	3
3:A:5:ILE:HG21	3:B:114:TYR:CG	0.70	2.21	1	8
3:A:32:MET:CE	3:B:124:ILE:HG12	0.70	2.16	18	3
3:B:107:VAL:CG1	3:B:109:VAL:HG13	0.70	2.15	13	1
3:A:22:VAL:O	3:A:22:VAL:HG13	0.70	1.86	15	7
3:B:124:ILE:N	3:B:124:ILE:HD12	0.70	2.00	7	3
3:A:5:ILE:HG21	3:B:114:TYR:CE2	0.70	2.22	6	5
3:A:24:ILE:CG2	3:B:132:MET:HE3	0.70	2.16	13	5
3:A:36:ALA:HB1	3:B:116:LEU:HD22	0.70	1.62	3	9
3:A:24:ILE:HG13	3:B:132:MET:HE1	0.70	1.63	15	7
3:A:6:THR:CB	3:B:106:THR:HB	0.70	2.16	11	9
1:C:174:DT:C2'	1:C:175:DA:C8	0.70	2.74	13	9
2:D:190:DG:H2'	2:D:191:DT:H71	0.69	1.64	9	7
3:B:104:ARG:NH2	3:B:106:THR:HG21	0.69	2.01	12	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:27:LEU:HD11	3:B:135:GLU:HG2	0.69	1.62	15	1
3:B:117:LEU:HD11	3:B:127:LEU:HD13	0.69	1.63	3	1
3:A:32:MET:SD	3:B:117:LEU:CB	0.69	2.80	8	11
3:B:105:ILE:HD11	3:B:128:VAL:HG11	0.69	1.64	5	8
3:A:32:MET:HE1	3:B:124:ILE:HG23	0.69	1.64	7	3
1:C:174:DT:H2'	1:C:175:DA:C8	0.69	2.23	16	9
3:B:117:LEU:HD13	3:B:120:TYR:CE2	0.69	2.23	16	3
3:A:9:VAL:HG21	3:A:14:TYR:CG	0.69	2.23	18	7
3:B:122:VAL:HG13	3:B:122:VAL:O	0.69	1.87	20	3
3:A:6:THR:HB	3:B:106:THR:CB	0.69	2.18	11	15
3:A:9:VAL:CG2	3:B:105:ILE:HD12	0.69	2.17	4	1
3:A:9:VAL:HG21	3:A:14:TYR:HB2	0.69	1.65	6	5
3:A:4:ARG:CG	3:B:108:THR:HG23	0.69	2.16	19	2
3:A:32:MET:HE1	3:B:123:ASN:C	0.68	2.13	3	1
3:B:124:ILE:HD12	3:B:124:ILE:H	0.68	1.47	4	11
1:C:174:DT:H2''	1:C:175:DA:C8	0.68	2.23	17	16
3:A:29:SER:HB2	3:B:112:ASP:CB	0.68	2.19	15	7
3:A:36:ALA:CB	3:B:116:LEU:HB3	0.68	2.18	7	8
3:B:124:ILE:HG23	3:B:127:LEU:HD23	0.68	1.64	9	3
3:A:17:LEU:HD22	3:A:22:VAL:CG1	0.68	2.18	15	2
2:D:191:DT:H72	3:B:106:THR:OG1	0.68	1.88	10	4
3:A:10:ASP:HB2	3:B:103:GLN:HB3	0.68	1.64	14	6
3:B:105:ILE:O	3:B:105:ILE:HG13	0.68	1.87	11	9
1:C:173:DA:C3'	1:C:174:DT:H5''	0.68	2.19	15	5
1:C:173:DA:H1'	1:C:174:DT:O4'	0.68	1.88	11	1
3:A:5:ILE:HG23	3:B:107:VAL:O	0.68	1.89	13	2
3:A:35:GLU:HG3	3:B:127:LEU:HD21	0.68	1.63	11	1
3:A:14:TYR:CZ	3:B:105:ILE:CG2	0.68	2.77	4	6
3:A:6:THR:HG21	3:B:104:ARG:CZ	0.68	2.18	6	3
3:B:128:VAL:O	3:B:132:MET:HG2	0.67	1.89	12	10
3:B:124:ILE:H	3:B:124:ILE:HD12	0.67	1.49	5	2
3:A:24:ILE:HG22	3:A:27:LEU:CB	0.67	2.18	7	2
3:A:12:ASP:HB3	3:B:129:SER:HB3	0.67	1.66	19	5
3:A:24:ILE:CG2	3:B:132:MET:HE1	0.67	2.19	1	3
3:B:109:VAL:CG1	3:B:114:TYR:HB3	0.67	2.20	4	5
3:A:16:LEU:HB3	3:B:136:ALA:CB	0.67	2.19	9	11
3:A:14:TYR:CD1	3:B:105:ILE:HG21	0.67	2.25	11	9
3:A:32:MET:SD	3:B:127:LEU:HD22	0.67	2.30	3	1
3:A:9:VAL:HG23	3:A:12:ASP:HB2	0.67	1.64	9	2
3:A:32:MET:O	3:B:117:LEU:HD23	0.67	1.89	14	5
3:B:124:ILE:HG22	3:B:127:LEU:CD1	0.67	2.15	18	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:29:SER:HB2	3:B:112:ASP:HB3	0.67	1.67	15	7
3:A:14:TYR:CE2	3:B:105:ILE:CG1	0.67	2.78	2	1
3:A:24:ILE:HG13	3:B:132:MET:CE	0.67	2.18	15	11
3:A:29:SER:HB3	3:B:112:ASP:HB3	0.67	1.66	5	6
3:A:24:ILE:CG1	3:B:132:MET:HE1	0.67	2.19	7	6
3:A:14:TYR:CE2	3:B:105:ILE:CD1	0.67	2.77	2	1
3:B:117:LEU:HD11	3:B:127:LEU:HD12	0.67	1.65	15	1
3:A:17:LEU:CG	3:B:132:MET:SD	0.67	2.83	2	5
3:A:17:LEU:HB3	3:B:132:MET:SD	0.67	2.30	3	3
3:A:24:ILE:HG23	3:B:132:MET:HE1	0.67	1.67	15	2
2:D:187:DC:H2''	2:D:188:DG:N7	0.66	2.04	12	4
2:D:189:DG:H2'	2:D:190:DG:O4'	0.66	1.88	17	4
3:A:32:MET:HE2	3:B:124:ILE:CG2	0.66	2.19	9	2
3:B:128:VAL:HG13	3:B:132:MET:HE2	0.66	1.67	20	7
3:B:117:LEU:CD1	3:B:122:VAL:HG13	0.66	2.19	10	1
2:D:188:DG:H2''	2:D:189:DG:N7	0.66	2.05	8	5
3:A:29:SER:HB3	3:B:112:ASP:HB2	0.66	1.67	2	6
3:B:109:VAL:HG11	3:B:114:TYR:CG	0.66	2.24	4	2
3:A:35:GLU:CG	3:B:127:LEU:HD13	0.66	2.21	9	1
3:A:25:SER:HA	3:B:107:VAL:CG2	0.66	2.21	13	2
3:A:17:LEU:CB	3:B:132:MET:HG2	0.66	2.21	19	1
3:A:24:ILE:HD12	3:A:24:ILE:H	0.66	1.48	2	8
3:B:124:ILE:HG22	3:B:128:VAL:HG23	0.66	1.65	16	3
1:C:178:DT:H72	3:A:6:THR:HG23	0.66	1.67	11	1
3:A:24:ILE:HG12	3:B:105:ILE:HD12	0.66	1.66	20	7
3:A:29:SER:CB	3:B:112:ASP:CB	0.66	2.74	14	9
3:A:28:VAL:CG2	3:B:128:VAL:CG2	0.66	2.74	5	8
3:A:6:THR:HG21	3:B:104:ARG:NH1	0.66	2.05	17	3
1:C:179:DA:H2''	1:C:180:DT:O5'	0.66	1.88	7	9
3:A:4:ARG:CG	3:B:108:THR:HG22	0.66	2.20	7	7
3:A:17:LEU:HD11	3:A:27:LEU:CD2	0.66	2.21	18	2
3:B:124:ILE:CB	3:B:128:VAL:HG23	0.66	2.20	5	15
3:A:17:LEU:HD22	3:A:22:VAL:HB	0.66	1.68	3	2
1:C:176:DT:H2''	1:C:177:DG:O5'	0.66	1.91	13	8
3:A:14:TYR:CE1	3:B:103:GLN:HG2	0.66	2.26	7	3
3:A:20:TYR:O	3:A:21:ASP:HB2	0.65	1.90	5	17
3:A:10:ASP:HB2	3:B:103:GLN:CB	0.65	2.21	14	7
1:C:176:DT:H2'	3:A:8:THR:OG1	0.65	1.92	1	5
3:A:32:MET:HA	3:B:117:LEU:CD1	0.65	2.20	7	1
3:A:24:ILE:HG23	3:A:27:LEU:HD23	0.65	1.68	4	4
3:B:120:TYR:O	3:B:121:ASP:HB2	0.65	1.91	2	16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:TYR:CD2	3:B:105:ILE:HG13	0.65	2.27	2	1
3:A:17:LEU:HB2	3:B:132:MET:HG2	0.65	1.66	19	2
3:B:129:SER:HA	3:B:132:MET:SD	0.65	2.31	11	2
3:A:9:VAL:HG22	3:A:10:ASP:H	0.65	1.51	8	6
3:A:35:GLU:HG2	3:B:127:LEU:HD11	0.65	1.68	12	1
3:B:117:LEU:HD12	3:B:122:VAL:HG11	0.65	1.66	19	1
3:A:9:VAL:HG23	3:B:103:GLN:HB3	0.65	1.69	2	3
3:B:126:GLY:O	3:B:130:THR:HB	0.65	1.92	11	5
3:A:24:ILE:HG22	3:A:27:LEU:CG	0.65	2.20	7	3
3:A:28:VAL:HB	3:B:107:VAL:HG21	0.65	1.68	18	3
1:C:173:DA:C2'	1:C:174:DT:H5''	0.65	2.21	14	8
3:A:14:TYR:CE1	3:B:105:ILE:HB	0.65	2.26	20	2
3:A:4:ARG:NH1	3:B:108:THR:CG2	0.65	2.59	20	2
3:A:24:ILE:CG2	3:A:27:LEU:HB3	0.65	2.22	16	8
3:B:107:VAL:O	3:B:107:VAL:HG12	0.65	1.90	13	1
3:A:17:LEU:HD22	3:A:22:VAL:HG13	0.65	1.69	15	1
3:A:14:TYR:CE2	3:B:105:ILE:HD11	0.65	2.27	2	1
3:A:9:VAL:O	3:A:10:ASP:HB2	0.65	1.92	20	4
3:A:12:ASP:CB	3:B:129:SER:CB	0.65	2.74	17	14
3:A:28:VAL:O	3:A:32:MET:HG2	0.65	1.92	19	10
3:B:127:LEU:HD23	3:B:127:LEU:C	0.64	2.17	4	2
3:A:4:ARG:CB	3:B:108:THR:HG22	0.64	2.22	7	1
3:A:32:MET:HE1	3:B:124:ILE:HG13	0.64	1.68	10	9
3:A:17:LEU:CD2	3:A:27:LEU:HD22	0.64	2.22	9	1
3:A:17:LEU:HD22	3:A:22:VAL:HG11	0.64	1.67	13	1
3:A:32:MET:CE	3:B:124:ILE:HG13	0.64	2.23	20	16
3:B:128:VAL:O	3:B:132:MET:CG	0.64	2.45	2	9
3:A:17:LEU:HD23	3:B:132:MET:HA	0.64	1.69	14	3
1:C:181:DA:C2	2:D:192:DA:C2	0.64	2.86	10	2
3:B:132:MET:O	3:B:136:ALA:N	0.64	2.30	11	19
3:A:9:VAL:O	3:A:10:ASP:HB3	0.64	1.92	8	11
3:B:109:VAL:HG12	3:B:112:ASP:HB2	0.64	1.68	5	3
3:A:35:GLU:HB3	3:B:117:LEU:HD11	0.64	1.69	7	1
3:B:109:VAL:HG21	3:B:112:ASP:HB3	0.64	1.67	11	1
1:C:179:DA:H2'	1:C:180:DT:H71	0.64	1.70	7	9
3:B:117:LEU:HD23	3:B:120:TYR:CE2	0.64	2.28	18	1
3:A:9:VAL:O	3:A:10:ASP:CB	0.64	2.46	20	17
3:A:7:VAL:HG12	3:A:9:VAL:CG1	0.64	2.23	2	2
3:A:17:LEU:CD1	3:B:132:MET:HA	0.64	2.23	9	1
3:A:5:ILE:CD1	3:B:114:TYR:CD1	0.63	2.81	10	11
3:A:31:THR:HB	3:B:127:LEU:HD21	0.63	1.70	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:7:VAL:O	3:A:7:VAL:HG12	0.63	1.93	20	1
2:D:191:DT:H2'	2:D:192:DA:N7	0.63	2.09	19	3
3:B:127:LEU:O	3:B:131:THR:HB	0.63	1.94	2	6
3:A:5:ILE:HG12	3:B:124:ILE:HD11	0.63	1.67	7	3
3:A:32:MET:HE2	3:B:123:ASN:O	0.63	1.94	8	1
3:A:24:ILE:HG23	3:B:132:MET:SD	0.63	2.34	18	1
3:A:5:ILE:O	3:B:106:THR:HA	0.63	1.93	9	14
3:A:6:THR:OG1	3:B:104:ARG:HG2	0.63	1.94	4	11
3:B:109:VAL:O	3:B:110:ASP:CB	0.63	2.47	16	16
3:B:107:VAL:CG2	3:B:109:VAL:HB	0.63	2.24	11	1
3:B:117:LEU:HG	3:B:127:LEU:HD12	0.63	1.70	14	4
3:A:20:TYR:C	3:A:20:TYR:CD1	0.63	2.77	3	1
3:B:120:TYR:O	3:B:121:ASP:HB3	0.63	1.94	13	3
3:A:6:THR:HB	3:B:106:THR:CG2	0.63	2.23	14	8
3:B:105:ILE:CD1	3:B:128:VAL:HG11	0.63	2.24	20	3
3:B:128:VAL:CG1	3:B:132:MET:HE2	0.63	2.24	15	2
3:B:109:VAL:O	3:B:110:ASP:HB3	0.63	1.94	10	8
1:C:180:DT:H71	3:A:4:ARG:HD2	0.63	1.71	12	3
3:A:14:TYR:CZ	3:B:105:ILE:HG22	0.63	2.28	3	2
1:C:182:DC:H2''	1:C:183:DC:O5'	0.62	1.94	11	16
3:A:7:VAL:CG1	3:A:9:VAL:HG22	0.62	2.24	14	2
3:A:17:LEU:HD21	3:B:135:GLU:CG	0.62	2.24	16	2
3:A:17:LEU:HD12	3:A:24:ILE:CG2	0.62	2.25	13	1
3:A:6:THR:HG22	3:B:106:THR:HG23	0.62	1.69	14	1
3:A:32:MET:HE3	3:B:124:ILE:CG1	0.62	2.24	1	2
3:A:24:ILE:CG1	3:B:132:MET:CE	0.62	2.78	13	4
2:D:189:DG:H2'	3:B:108:THR:OG1	0.62	1.94	16	2
1:C:179:DA:H62	3:B:104:ARG:NH1	0.62	1.92	20	1
3:A:17:LEU:HD13	3:A:27:LEU:HD11	0.62	1.72	3	1
3:A:12:ASP:HB2	3:B:129:SER:CB	0.62	2.24	15	3
3:A:32:MET:CG	3:B:117:LEU:HB2	0.62	2.24	16	1
3:A:20:TYR:CD1	3:A:21:ASP:N	0.62	2.68	17	6
3:B:109:VAL:CG2	3:B:114:TYR:CD1	0.62	2.79	6	3
3:A:10:ASP:HB3	3:B:102:LYS:HA	0.62	1.71	17	3
3:A:17:LEU:HD21	3:B:135:GLU:CB	0.61	2.25	1	3
3:A:13:SER:CB	3:B:133:GLN:HB2	0.61	2.25	19	2
3:A:6:THR:CA	3:B:105:ILE:O	0.61	2.47	12	9
3:A:29:SER:HA	3:A:32:MET:SD	0.61	2.34	1	1
3:A:32:MET:CE	3:B:124:ILE:CG1	0.61	2.78	18	6
3:A:7:VAL:HG13	3:B:105:ILE:CG1	0.61	2.25	18	11
3:A:32:MET:O	3:A:36:ALA:N	0.61	2.34	5	19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:117:LEU:HD13	3:B:124:ILE:CG2	0.61	2.25	18	1
3:A:9:VAL:CG2	3:A:12:ASP:HB2	0.61	2.26	1	1
3:A:32:MET:CE	3:B:124:ILE:HG23	0.61	2.26	20	11
3:A:9:VAL:CG1	3:A:14:TYR:CB	0.61	2.79	9	7
3:B:109:VAL:HG23	3:B:110:ASP:N	0.61	2.11	15	4
3:A:9:VAL:CG2	3:A:14:TYR:HB3	0.61	2.25	8	6
3:A:22:VAL:CG1	3:A:27:LEU:HB2	0.61	2.26	3	2
3:A:17:LEU:HD11	3:A:27:LEU:HD13	0.61	1.72	14	1
3:A:5:ILE:HB	3:B:114:TYR:CE1	0.61	2.30	1	3
3:A:9:VAL:HB	3:A:14:TYR:HB3	0.61	1.72	2	2
3:A:7:VAL:HG12	3:B:124:ILE:HD13	0.61	1.71	4	2
3:B:117:LEU:HD12	3:B:123:ASN:O	0.61	1.96	10	3
3:B:109:VAL:CG2	3:B:112:ASP:CB	0.61	2.79	11	1
3:A:7:VAL:HG12	3:A:7:VAL:O	0.61	1.95	14	4
3:B:117:LEU:HD13	3:B:122:VAL:HB	0.61	1.73	14	1
3:A:9:VAL:HG22	3:A:10:ASP:N	0.61	2.11	19	5
3:A:17:LEU:CD1	3:A:24:ILE:HG23	0.61	2.26	13	1
3:B:109:VAL:CB	3:B:114:TYR:HB3	0.61	2.26	2	10
3:A:29:SER:O	3:B:113:SER:HB2	0.61	1.96	13	2
3:A:20:TYR:O	3:A:21:ASP:HB3	0.60	1.95	13	2
3:A:15:GLN:O	3:A:18:LYS:HG3	0.60	1.96	14	11
3:A:14:TYR:HE1	3:B:105:ILE:HD11	0.60	1.52	12	1
3:A:7:VAL:HG22	3:A:9:VAL:CG1	0.60	2.26	18	5
3:A:5:ILE:CG2	3:B:114:TYR:CZ	0.60	2.85	19	11
1:C:173:DA:C3'	1:C:174:DT:C5'	0.60	2.80	12	3
3:A:24:ILE:HG12	3:B:132:MET:HE3	0.60	1.73	13	2
3:A:24:ILE:HG12	3:B:128:VAL:HG13	0.60	1.73	15	1
3:A:15:GLN:HA	3:A:18:LYS:HE2	0.60	1.73	14	9
3:B:117:LEU:HG	3:B:127:LEU:CD1	0.60	2.26	15	6
3:B:104:ARG:NH1	3:B:104:ARG:HB3	0.60	2.11	1	1
3:B:109:VAL:CG2	3:B:114:TYR:HB3	0.60	2.27	14	4
3:B:115:GLN:HA	3:B:118:LYS:HE2	0.60	1.74	9	5
3:A:17:LEU:HD13	3:A:20:TYR:CE2	0.60	2.32	11	5
3:A:13:SER:HB3	3:B:133:GLN:HB3	0.60	1.74	13	1
3:A:10:ASP:CB	3:B:102:LYS:HA	0.60	2.27	17	3
1:C:180:DT:H73	3:A:4:ARG:HD2	0.60	1.73	11	2
3:A:23:ASN:O	3:A:24:ILE:CD1	0.60	2.49	1	1
3:A:9:VAL:CG2	3:A:14:TYR:CD1	0.60	2.74	10	3
3:A:17:LEU:HG	3:B:132:MET:HG3	0.60	1.72	19	1
3:B:124:ILE:CG2	3:B:127:LEU:HB3	0.60	2.24	2	7
3:A:3:GLN:N	3:B:110:ASP:HB2	0.60	2.12	18	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:107:VAL:HG12	3:B:107:VAL:O	0.60	1.97	7	4
3:B:109:VAL:HG22	3:B:110:ASP:H	0.59	1.55	11	3
1:C:177:DG:P	3:B:125:SER:HB3	0.59	2.36	7	3
3:A:5:ILE:HD11	3:A:28:VAL:HG11	0.59	1.74	8	9
3:A:14:TYR:CG	3:B:105:ILE:HG21	0.59	2.32	3	10
3:A:4:ARG:HG2	3:B:106:THR:OG1	0.59	1.96	7	7
1:C:178:DT:H73	3:A:6:THR:HB	0.59	1.73	13	1
3:B:128:VAL:HG13	3:B:132:MET:HE1	0.59	1.73	19	1
3:B:105:ILE:HD13	3:B:128:VAL:HG11	0.59	1.74	20	2
3:A:17:LEU:CD1	3:A:22:VAL:HB	0.59	2.28	19	1
3:A:32:MET:SD	3:B:117:LEU:HG	0.59	2.37	5	2
3:A:27:LEU:C	3:A:27:LEU:HD13	0.59	2.22	7	2
1:C:178:DT:OP2	3:A:5:ILE:HA	0.59	1.98	11	2
3:B:107:VAL:CG1	3:B:107:VAL:O	0.59	2.51	13	1
3:A:7:VAL:CG1	3:A:7:VAL:O	0.59	2.50	14	1
3:A:7:VAL:HG13	3:B:105:ILE:HD11	0.59	1.73	4	3
3:B:104:ARG:NH1	3:B:106:THR:HG21	0.59	2.13	6	1
1:C:175:DA:C8	1:C:176:DT:C7	0.59	2.86	9	2
3:A:32:MET:HE1	3:B:124:ILE:CG1	0.59	2.26	13	4
3:A:9:VAL:CG2	3:A:12:ASP:CB	0.59	2.80	1	1
3:A:5:ILE:HD12	3:B:114:TYR:CD1	0.59	2.32	14	3
3:B:128:VAL:O	3:B:131:THR:HG22	0.59	1.97	17	1
3:A:14:TYR:CZ	3:A:18:LYS:HD3	0.59	2.32	14	11
3:B:115:GLN:O	3:B:118:LYS:HG3	0.59	1.98	19	14
1:C:173:DA:H3'	1:C:174:DT:C5'	0.59	2.27	12	2
3:A:24:ILE:CG2	3:A:27:LEU:HD23	0.59	2.27	4	5
3:A:24:ILE:HG22	3:A:27:LEU:CD1	0.59	2.27	13	3
3:A:10:ASP:HB2	3:B:102:LYS:HA	0.59	1.75	12	2
3:A:31:THR:HG21	3:B:131:THR:HG21	0.59	1.75	19	2
3:A:9:VAL:HG21	3:A:12:ASP:HB3	0.59	1.75	1	1
3:A:14:TYR:CE2	3:A:18:LYS:HD3	0.59	2.32	5	1
2:D:190:DG:N7	2:D:191:DT:H72	0.59	2.12	6	1
3:A:7:VAL:CG1	3:A:9:VAL:HB	0.59	2.28	15	1
3:A:17:LEU:HD23	3:A:22:VAL:O	0.58	1.98	9	1
3:B:109:VAL:CG2	3:B:114:TYR:CD2	0.58	2.81	14	3
1:C:175:DA:C2	2:D:198:DA:C2	0.58	2.90	1	7
3:B:107:VAL:HG22	3:B:109:VAL:CG2	0.58	2.27	1	1
3:A:17:LEU:CD1	3:B:132:MET:SD	0.58	2.88	10	1
3:A:14:TYR:HA	3:B:132:MET:CG	0.58	2.28	15	2
3:B:120:TYR:O	3:B:121:ASP:CB	0.58	2.51	10	20
3:A:29:SER:CB	3:B:112:ASP:O	0.58	2.51	12	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:179:DA:H62	3:B:104:ARG:NE	0.58	1.96	6	2
3:A:9:VAL:CG1	3:A:14:TYR:HB3	0.58	2.29	4	13
3:A:14:TYR:CE1	3:A:18:LYS:HD3	0.58	2.33	18	2
1:C:184:DC:H2''	1:C:185:DG:H5'	0.58	1.76	15	1
3:A:29:SER:HB2	3:B:112:ASP:O	0.58	1.98	20	6
3:A:24:ILE:CG2	3:B:132:MET:CE	0.58	2.80	19	8
3:A:20:TYR:CD1	3:A:20:TYR:C	0.58	2.82	19	7
3:A:3:GLN:CB	3:B:110:ASP:HB2	0.58	2.29	18	5
3:A:17:LEU:HD21	3:B:135:GLU:HB3	0.58	1.75	4	3
3:B:109:VAL:O	3:B:110:ASP:HB2	0.58	1.97	17	4
3:A:4:ARG:CG	3:B:106:THR:HG22	0.58	2.25	14	1
3:B:109:VAL:HB	3:B:114:TYR:HB3	0.58	1.75	20	4
3:B:107:VAL:O	3:B:107:VAL:HG22	0.58	1.98	4	2
3:A:4:ARG:HA	3:B:108:THR:HA	0.58	1.75	19	7
3:A:32:MET:SD	3:B:117:LEU:CD1	0.58	2.90	3	1
3:A:32:MET:HG2	3:B:117:LEU:HB2	0.58	1.75	16	1
3:B:109:VAL:CG1	3:B:114:TYR:CB	0.57	2.82	7	5
3:A:14:TYR:CE2	3:B:103:GLN:HG2	0.57	2.34	17	2
3:A:7:VAL:CG1	3:B:105:ILE:CG2	0.57	2.82	12	1
1:C:183:DC:H2''	1:C:184:DC:C6	0.57	2.34	12	7
3:A:3:GLN:HB3	3:B:110:ASP:HB2	0.57	1.75	4	5
3:A:9:VAL:HG23	3:A:10:ASP:N	0.57	2.14	18	3
3:A:17:LEU:HD12	3:B:132:MET:HG2	0.57	1.75	13	1
1:C:177:DG:OP2	3:A:7:VAL:HA	0.57	1.99	20	3
3:A:6:THR:HB	3:B:106:THR:CA	0.57	2.28	4	3
3:A:31:THR:OG1	3:B:131:THR:HG21	0.57	2.00	8	3
3:A:17:LEU:HD13	3:A:20:TYR:CZ	0.57	2.34	16	3
3:A:24:ILE:HB	3:A:28:VAL:CG2	0.57	2.27	4	5
3:B:124:ILE:HG22	3:B:127:LEU:HD22	0.57	1.76	4	1
3:B:117:LEU:HD12	3:B:122:VAL:HG13	0.57	1.75	9	2
3:A:7:VAL:CG2	3:A:9:VAL:HB	0.57	2.30	5	3
3:A:16:LEU:CB	3:B:136:ALA:HB1	0.57	2.30	2	7
3:A:17:LEU:CD1	3:A:27:LEU:HD11	0.57	2.29	3	1
3:B:120:TYR:CD1	3:B:120:TYR:C	0.57	2.83	18	7
3:B:122:VAL:O	3:B:122:VAL:CG1	0.57	2.52	16	3
3:B:117:LEU:HD11	3:B:127:LEU:HG	0.57	1.75	17	1
3:A:10:ASP:HA	3:A:15:GLN:HG3	0.57	1.76	14	1
3:A:15:GLN:HA	3:A:18:LYS:CE	0.57	2.29	14	1
1:C:173:DA:H2''	1:C:174:DT:H5''	0.57	1.76	10	5
2:D:191:DT:OP2	3:B:105:ILE:HA	0.57	1.98	5	10
3:B:109:VAL:HG13	3:B:112:ASP:HB2	0.57	1.77	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:LEU:HD12	3:A:20:TYR:CE1	0.57	2.34	8	1
1:C:178:DT:H72	3:A:6:THR:CG2	0.57	2.30	2	10
3:A:5:ILE:O	3:A:5:ILE:HG13	0.57	1.98	13	8
2:D:190:DG:C8	2:D:191:DT:C7	0.56	2.88	4	2
2:D:186:DT:H72	2:D:187:DC:C5	0.56	2.35	7	1
3:A:7:VAL:HG12	3:A:9:VAL:HG22	0.56	1.75	20	1
2:D:191:DT:H71	3:B:106:THR:OG1	0.56	1.99	2	1
3:A:9:VAL:CB	3:A:14:TYR:HB3	0.56	2.31	6	8
3:B:105:ILE:O	3:B:105:ILE:HG22	0.56	1.99	2	2
3:A:31:THR:HG22	3:B:127:LEU:HD11	0.56	1.75	9	3
3:B:124:ILE:CG2	3:B:127:LEU:HD23	0.56	2.29	9	4
1:C:173:DA:H1'	1:C:174:DT:H73	0.56	1.76	10	1
2:D:190:DG:C5	2:D:191:DT:C4	0.56	2.93	1	2
3:B:107:VAL:CG2	3:B:109:VAL:HG22	0.56	2.30	17	3
2:D:193:DT:O4	3:B:104:ARG:HD2	0.56	2.00	8	5
3:A:17:LEU:HG	3:A:20:TYR:CE2	0.56	2.35	9	1
1:C:177:DG:N2	2:D:196:DA:C4	0.56	2.73	11	1
3:A:14:TYR:CD1	3:B:105:ILE:CG1	0.56	2.87	12	1
3:A:20:TYR:O	3:A:21:ASP:CB	0.56	2.54	4	18
3:A:17:LEU:HD23	3:A:27:LEU:CD1	0.56	2.30	8	1
3:B:107:VAL:HG22	3:B:109:VAL:CG1	0.56	2.31	15	6
3:A:9:VAL:HG11	3:A:14:TYR:H	0.56	1.59	16	4
2:D:190:DG:OP1	3:A:25:SER:HA	0.56	2.01	17	4
3:B:117:LEU:HD22	3:B:127:LEU:HD22	0.56	1.77	7	1
1:C:180:DT:H2''	1:C:181:DA:C8	0.56	2.35	3	7
3:A:32:MET:SD	3:B:127:LEU:HD12	0.56	2.40	20	2
1:C:174:DT:H71	1:C:174:DT:OP1	0.56	2.00	16	1
3:A:9:VAL:HG13	3:A:10:ASP:N	0.56	2.16	1	1
3:A:32:MET:CG	3:B:114:TYR:HA	0.56	2.31	16	7
3:A:10:ASP:HB2	3:B:103:GLN:HB2	0.56	1.78	15	1
3:A:17:LEU:HD21	3:B:135:GLU:HG2	0.56	1.78	16	1
3:A:9:VAL:HG21	3:A:14:TYR:CE1	0.56	2.36	2	1
3:A:12:ASP:O	3:B:129:SER:HA	0.56	2.01	12	3
3:B:115:GLN:HA	3:B:118:LYS:CE	0.56	2.31	9	1
3:A:6:THR:OG1	3:B:104:ARG:HG3	0.56	2.01	12	3
3:A:22:VAL:CG1	3:A:22:VAL:O	0.56	2.54	17	2
3:A:22:VAL:O	3:A:22:VAL:CG1	0.56	2.53	4	4
1:C:178:DT:H2''	1:C:179:DA:O5'	0.56	2.01	15	8
3:A:5:ILE:HG21	3:B:114:TYR:CD2	0.56	2.36	2	6
3:A:24:ILE:CG1	3:B:105:ILE:HD12	0.56	2.31	9	5
3:A:35:GLU:HB3	3:B:117:LEU:CD2	0.56	2.31	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:VAL:CG2	3:A:14:TYR:CD2	0.56	2.73	11	2
3:A:23:ASN:C	3:B:132:MET:HE1	0.55	2.26	2	3
3:A:28:VAL:CG2	3:B:128:VAL:HG21	0.55	2.27	16	1
3:A:12:ASP:HB2	3:B:129:SER:OG	0.55	2.00	18	2
3:A:9:VAL:N	3:B:103:GLN:O	0.55	2.40	2	6
3:B:128:VAL:CG1	3:B:132:MET:HE3	0.55	2.30	14	4
3:A:32:MET:HA	3:B:117:LEU:CD2	0.55	2.31	9	2
3:A:28:VAL:HG21	3:B:128:VAL:CG2	0.55	2.16	15	1
3:A:22:VAL:C	3:A:24:ILE:H	0.55	2.09	1	3
3:A:25:SER:HA	3:B:107:VAL:HB	0.55	1.77	1	1
3:A:9:VAL:HG22	3:B:103:GLN:O	0.55	2.02	2	2
3:A:14:TYR:CE1	3:B:105:ILE:CG2	0.55	2.89	14	5
3:A:6:THR:HG21	3:B:104:ARG:NH2	0.55	2.15	6	1
2:D:190:DG:N7	3:A:4:ARG:NH1	0.55	2.54	20	1
3:B:109:VAL:HG22	3:B:110:ASP:N	0.55	2.17	11	4
3:A:17:LEU:HD23	3:B:132:MET:CA	0.55	2.32	12	5
2:D:193:DT:H73	3:B:104:ARG:NH1	0.55	2.16	10	2
3:A:4:ARG:CZ	3:B:108:THR:CG2	0.55	2.84	12	2
3:A:16:LEU:HD13	3:B:136:ALA:HB1	0.55	1.78	12	4
3:B:117:LEU:CD2	3:B:127:LEU:HD22	0.55	2.32	7	1
3:A:7:VAL:HG22	3:A:9:VAL:HG13	0.55	1.78	18	3
3:B:109:VAL:CG2	3:B:114:TYR:CB	0.55	2.84	9	6
3:A:24:ILE:HG23	3:B:132:MET:CE	0.55	2.29	4	8
3:A:5:ILE:CG2	3:B:114:TYR:CE1	0.55	2.88	12	9
3:B:114:TYR:CZ	3:B:118:LYS:HG2	0.55	2.36	2	3
1:C:179:DA:C2	1:C:180:DT:C2	0.55	2.95	15	9
3:B:117:LEU:CD1	3:B:127:LEU:HD12	0.55	2.31	15	6
3:B:107:VAL:O	3:B:109:VAL:HG13	0.55	2.01	6	2
3:B:105:ILE:HG21	3:B:128:VAL:HG11	0.55	1.79	15	1
3:A:5:ILE:CD1	3:B:114:TYR:CD2	0.55	2.86	6	2
3:A:32:MET:SD	3:B:124:ILE:HG23	0.55	2.42	20	2
3:A:4:ARG:CG	3:B:106:THR:OG1	0.55	2.55	7	4
3:A:32:MET:SD	3:B:124:ILE:HG21	0.55	2.42	13	1
3:A:7:VAL:N	3:B:105:ILE:O	0.54	2.40	15	5
3:B:117:LEU:CD1	3:B:127:LEU:HD22	0.54	2.25	3	1
2:D:197:DT:H2''	2:D:198:DA:C8	0.54	2.38	11	2
1:C:178:DT:H3'	3:A:4:ARG:O	0.54	2.02	16	1
3:A:36:ALA:HB1	3:B:116:LEU:HD13	0.54	1.79	17	4
3:A:6:THR:HG23	3:B:106:THR:HG22	0.54	1.79	13	1
3:A:9:VAL:HG23	3:A:14:TYR:CD2	0.54	2.36	20	1
3:A:18:LYS:HB3	3:A:23:ASN:HA	0.54	1.79	11	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:109:VAL:HG11	3:B:114:TYR:H	0.54	1.61	10	3
3:A:12:ASP:O	3:B:129:SER:HB2	0.54	2.02	4	4
3:A:32:MET:HB3	3:B:113:SER:O	0.54	2.03	5	3
1:C:175:DA:C5	1:C:176:DT:C4	0.54	2.96	14	12
3:B:120:TYR:CD1	3:B:121:ASP:N	0.54	2.75	16	6
3:B:115:GLN:O	3:B:119:ALA:N	0.54	2.40	15	11
1:C:173:DA:H3'	1:C:174:DT:H5''	0.54	1.80	13	4
3:A:31:THR:HG22	3:B:127:LEU:HD21	0.54	1.78	12	1
3:A:7:VAL:HG22	3:A:9:VAL:HG12	0.54	1.79	1	2
3:B:114:TYR:OH	3:B:118:LYS:HD3	0.54	2.02	1	9
3:A:31:THR:CG2	3:B:127:LEU:HD21	0.54	2.32	14	2
3:A:28:VAL:C	3:A:32:MET:HG2	0.54	2.27	20	3
3:A:29:SER:CB	3:B:112:ASP:HB2	0.54	2.33	20	5
3:B:127:LEU:C	3:B:127:LEU:HD13	0.54	2.28	13	2
1:C:184:DC:C2'	1:C:185:DG:H5'	0.54	2.32	15	1
3:A:28:VAL:O	3:A:32:MET:CG	0.54	2.56	10	6
3:B:117:LEU:CD1	3:B:122:VAL:CG1	0.54	2.86	11	3
2:D:186:DT:H72	2:D:187:DC:C6	0.54	2.37	7	1
3:B:107:VAL:HG12	3:B:109:VAL:HG12	0.54	1.79	7	1
2:D:191:DT:H72	3:B:106:THR:CG2	0.54	2.31	10	3
3:B:109:VAL:HG21	3:B:112:ASP:CB	0.54	2.33	11	1
3:B:109:VAL:CG2	3:B:112:ASP:HB2	0.54	2.32	11	1
1:C:173:DA:H2'	1:C:174:DT:H5''	0.54	1.80	13	2
3:A:32:MET:HE1	3:B:114:TYR:HD1	0.54	1.62	15	1
3:A:23:ASN:O	3:A:24:ILE:HG13	0.54	2.02	1	1
3:B:117:LEU:CD1	3:B:127:LEU:HD13	0.54	2.33	3	1
3:A:32:MET:HB2	3:B:113:SER:HB2	0.54	1.79	13	2
1:C:177:DG:C8	1:C:178:DT:C7	0.54	2.91	6	8
3:A:23:ASN:O	3:A:24:ILE:CG1	0.54	2.56	1	1
1:C:174:DT:H2'	1:C:175:DA:N7	0.54	2.18	16	3
3:A:6:THR:OG1	3:B:104:ARG:CG	0.53	2.56	11	5
3:A:23:ASN:O	3:A:25:SER:N	0.53	2.42	12	9
3:B:117:LEU:HD22	3:B:122:VAL:CG1	0.53	2.32	20	1
3:A:14:TYR:OH	3:A:18:LYS:HD3	0.53	2.03	14	8
3:A:4:ARG:HG3	3:B:106:THR:OG1	0.53	2.02	13	1
3:A:7:VAL:CG2	3:A:9:VAL:HG22	0.53	2.33	16	1
3:A:28:VAL:CG2	3:B:124:ILE:HG21	0.53	2.28	4	2
1:C:178:DT:O4	3:B:104:ARG:HD2	0.53	2.04	19	1
3:B:123:ASN:O	3:B:125:SER:N	0.53	2.42	18	5
3:A:5:ILE:HD12	3:B:124:ILE:CD1	0.53	2.33	13	3
3:A:7:VAL:HG11	3:B:128:VAL:CG1	0.53	2.33	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:4:ARG:HG2	3:B:106:THR:CG2	0.53	2.28	15	2
2:D:193:DT:H2''	2:D:194:DA:C8	0.53	2.39	11	8
3:B:127:LEU:C	3:B:127:LEU:CD2	0.53	2.82	11	3
3:A:32:MET:SD	3:B:117:LEU:CG	0.53	2.97	5	2
3:A:14:TYR:CD2	3:B:105:ILE:CD1	0.53	2.89	8	3
3:A:7:VAL:HG11	3:B:128:VAL:HG11	0.53	1.79	11	3
3:B:129:SER:HA	3:B:132:MET:HG2	0.53	1.81	18	1
2:D:190:DG:H2''	2:D:191:DT:O5'	0.53	2.03	3	3
3:B:124:ILE:HB	3:B:128:VAL:CG2	0.53	2.34	9	5
3:A:7:VAL:O	3:A:9:VAL:HG13	0.53	2.02	11	1
3:A:4:ARG:NH1	3:B:108:THR:HG23	0.53	2.18	20	1
3:A:24:ILE:O	3:A:25:SER:C	0.53	2.51	14	20
3:B:114:TYR:CE2	3:B:118:LYS:HD3	0.53	2.38	20	10
3:A:27:LEU:HD21	3:B:131:THR:HG23	0.53	1.80	4	1
3:B:107:VAL:HG12	3:B:109:VAL:CG1	0.53	2.33	7	1
3:A:6:THR:HG23	3:B:106:THR:CG2	0.53	2.32	13	1
2:D:191:DT:C7	3:B:106:THR:HB	0.53	2.34	15	3
3:B:105:ILE:CG1	3:B:105:ILE:O	0.53	2.56	18	1
3:B:117:LEU:HD12	3:B:122:VAL:O	0.53	2.04	15	2
1:C:177:DG:C4	1:C:178:DT:C5	0.53	2.97	6	8
3:B:104:ARG:HH21	3:B:106:THR:HG21	0.53	1.61	5	2
2:D:190:DG:P	3:A:25:SER:HB3	0.52	2.44	1	2
3:A:17:LEU:HD23	3:B:132:MET:O	0.52	2.04	2	2
3:A:14:TYR:CE2	3:B:105:ILE:CG2	0.52	2.93	19	4
3:B:107:VAL:O	3:B:109:VAL:N	0.52	2.41	4	5
3:A:6:THR:HB	3:B:106:THR:HG22	0.52	1.79	5	3
1:C:173:DA:H3'	1:C:174:DT:H73	0.52	1.80	8	1
3:A:6:THR:HG21	3:B:104:ARG:HG2	0.52	1.81	13	1
2:D:187:DC:C2'	2:D:188:DG:C8	0.52	2.91	16	2
3:B:127:LEU:O	3:B:131:THR:N	0.52	2.42	19	1
3:A:9:VAL:HG21	3:A:12:ASP:CB	0.52	2.33	1	1
3:A:24:ILE:N	3:A:24:ILE:CD1	0.52	2.67	15	5
3:A:35:GLU:HG2	3:B:127:LEU:CD1	0.52	2.34	12	2
3:A:12:ASP:O	3:B:129:SER:CB	0.52	2.57	20	5
3:B:109:VAL:CG2	3:B:114:TYR:CG	0.52	2.87	16	4
3:A:5:ILE:HG12	3:A:5:ILE:O	0.52	2.05	14	2
3:A:5:ILE:O	3:A:5:ILE:CG1	0.52	2.57	18	4
3:A:14:TYR:CE2	3:B:105:ILE:HG22	0.52	2.39	3	1
3:A:17:LEU:CD2	3:A:20:TYR:CE2	0.52	2.89	3	1
3:B:114:TYR:CE1	3:B:118:LYS:HD3	0.52	2.39	8	2
3:A:32:MET:CA	3:B:117:LEU:HD23	0.52	2.35	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:102:LYS:O	3:B:102:LYS:NZ	0.52	2.41	9	1
3:A:9:VAL:HB	3:A:14:TYR:CD2	0.52	2.39	12	1
3:B:110:ASP:O	3:B:115:GLN:HG2	0.52	2.04	19	1
3:A:3:GLN:O	3:B:108:THR:HA	0.52	2.05	13	4
3:A:15:GLN:OE1	3:A:18:LYS:NZ	0.52	2.38	1	6
3:A:15:GLN:HA	3:A:18:LYS:CG	0.52	2.35	7	6
1:C:178:DT:C7	3:A:6:THR:HG23	0.52	2.32	16	4
3:A:8:THR:HA	3:B:103:GLN:O	0.52	2.05	14	3
1:C:178:DT:H73	3:A:6:THR:CG2	0.52	2.32	16	2
3:A:20:TYR:CE1	3:A:22:VAL:HB	0.52	2.40	16	1
1:C:177:DG:OP1	3:B:125:SER:HB3	0.52	2.05	13	7
3:A:7:VAL:HG12	3:A:9:VAL:CG2	0.52	2.35	3	1
3:A:28:VAL:O	3:A:32:MET:N	0.52	2.41	9	3
3:A:2:LYS:HA	3:B:110:ASP:HB3	0.52	1.81	15	2
3:A:17:LEU:CD1	3:A:27:LEU:CD2	0.52	2.88	15	2
3:A:17:LEU:HG	3:B:132:MET:CG	0.52	2.35	19	1
1:C:179:DA:C5	1:C:180:DT:C4	0.52	2.98	4	11
3:B:117:LEU:O	3:B:122:VAL:HG12	0.52	2.05	10	1
3:A:17:LEU:HG	3:B:132:MET:HG2	0.52	1.82	11	2
3:B:128:VAL:HG12	3:B:129:SER:N	0.52	2.18	11	1
3:A:7:VAL:O	3:A:7:VAL:CG1	0.52	2.57	20	3
3:B:117:LEU:HG	3:B:127:LEU:HD22	0.52	1.82	19	3
3:A:32:MET:HB2	3:B:113:SER:CB	0.52	2.34	13	1
2:D:192:DA:H2''	2:D:193:DT:O5'	0.51	2.05	4	4
1:C:181:DA:C2	1:C:182:DC:C2	0.51	2.98	15	6
3:A:2:LYS:HE3	3:A:2:LYS:HA	0.51	1.82	19	1
3:B:105:ILE:O	3:B:105:ILE:CG2	0.51	2.58	2	2
3:A:12:ASP:HB2	3:B:129:SER:HB3	0.51	1.81	17	4
3:B:117:LEU:CG	3:B:127:LEU:HD12	0.51	2.35	14	1
3:A:24:ILE:HG21	3:B:128:VAL:CG2	0.51	2.31	8	2
3:B:118:LYS:HB3	3:B:123:ASN:HA	0.51	1.81	18	2
3:A:32:MET:HG2	3:B:117:LEU:HG	0.51	1.81	15	2
3:A:7:VAL:HG12	3:A:9:VAL:HG13	0.51	1.82	2	1
3:A:32:MET:O	3:A:36:ALA:HB2	0.51	2.05	19	4
1:C:179:DA:C2'	1:C:180:DT:C6	0.51	2.93	20	5
3:B:115:GLN:HA	3:B:118:LYS:CG	0.51	2.36	10	10
1:C:177:DG:H2'	1:C:178:DT:H71	0.51	1.82	10	2
3:A:27:LEU:HD13	3:A:27:LEU:C	0.51	2.30	11	2
3:A:31:THR:CG2	3:B:127:LEU:HD11	0.51	2.35	13	2
3:A:32:MET:SD	3:B:127:LEU:CD2	0.51	2.99	3	2
3:A:13:SER:O	3:B:132:MET:HB3	0.51	2.06	12	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:24:ILE:CG1	3:B:132:MET:HE3	0.51	2.36	13	1
3:A:2:LYS:HE3	3:B:109:VAL:O	0.51	2.05	4	3
2:D:187:DC:O5'	2:D:187:DC:C6	0.51	2.64	8	1
3:B:138:ARG:HA	3:B:138:ARG:NE	0.51	2.20	9	1
1:C:178:DT:C7	3:A:6:THR:HB	0.51	2.36	13	1
3:A:2:LYS:HA	3:B:110:ASP:CB	0.51	2.36	13	1
3:A:27:LEU:CD1	3:B:132:MET:HG3	0.51	2.36	19	1
3:A:5:ILE:HD12	3:B:124:ILE:CG1	0.51	2.36	12	5
3:A:9:VAL:HG11	3:A:12:ASP:HB2	0.51	1.83	20	1
3:A:28:VAL:O	3:A:32:MET:HG3	0.51	2.06	10	6
1:C:178:DT:O4	3:B:104:ARG:NE	0.51	2.43	8	6
3:A:7:VAL:HG22	3:A:9:VAL:CG2	0.51	2.36	16	2
3:A:31:THR:HG21	3:B:131:THR:OG1	0.51	2.06	12	1
3:B:124:ILE:O	3:B:125:SER:C	0.50	2.55	10	20
3:A:27:LEU:CD1	3:B:132:MET:SD	0.50	2.97	2	1
2:D:186:DT:H2''	2:D:187:DC:C5'	0.50	2.36	8	2
3:B:105:ILE:O	3:B:105:ILE:CG1	0.50	2.59	14	5
3:A:14:TYR:CZ	3:B:105:ILE:HG12	0.50	2.41	12	1
3:B:115:GLN:O	3:B:119:ALA:HB2	0.50	2.06	16	2
3:B:122:VAL:HG12	3:B:122:VAL:O	0.50	2.07	1	1
2:D:191:DT:C7	3:B:106:THR:OG1	0.50	2.60	10	3
3:B:120:TYR:CE1	3:B:122:VAL:HB	0.50	2.42	2	1
3:A:6:THR:OG1	3:B:106:THR:HB	0.50	2.06	13	1
3:A:24:ILE:HD13	3:B:107:VAL:HG23	0.50	1.83	16	1
2:D:196:DA:H2'	2:D:197:DT:H71	0.50	1.83	8	2
3:A:32:MET:O	3:A:36:ALA:CB	0.50	2.60	19	7
2:D:189:DG:O3'	3:A:25:SER:OG	0.50	2.26	7	1
3:A:7:VAL:HG21	3:B:124:ILE:O	0.50	2.05	2	2
3:A:14:TYR:CD1	3:A:15:GLN:N	0.50	2.79	10	3
3:B:114:TYR:CE1	3:B:118:LYS:HG2	0.50	2.42	6	2
3:A:24:ILE:CG2	3:B:132:MET:HE2	0.50	2.32	14	2
3:A:7:VAL:O	3:A:7:VAL:HG22	0.50	2.06	8	3
3:B:117:LEU:HD13	3:B:122:VAL:HG11	0.50	1.79	10	1
1:C:173:DA:C2'	1:C:174:DT:O5'	0.50	2.58	1	2
3:A:9:VAL:HG13	3:A:12:ASP:HB2	0.50	1.84	3	4
2:D:192:DA:H62	3:B:104:ARG:CZ	0.50	2.20	12	1
1:C:179:DA:H2''	1:C:180:DT:C6	0.50	2.41	20	1
3:B:132:MET:O	3:B:136:ALA:CB	0.50	2.60	18	8
1:C:175:DA:H2''	1:C:176:DT:C6	0.50	2.42	8	3
3:B:124:ILE:HG21	3:B:128:VAL:CG2	0.50	2.26	11	2
2:D:194:DA:H1'	2:D:195:DC:O4'	0.50	2.07	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:5:ILE:CG2	3:B:114:TYR:CD1	0.49	2.92	13	2
3:A:10:ASP:HB2	3:B:103:GLN:N	0.49	2.22	19	3
3:A:15:GLN:O	3:A:19:ALA:CB	0.49	2.60	3	7
3:A:4:ARG:HA	3:B:108:THR:HG22	0.49	1.84	9	2
3:B:110:ASP:O	3:B:115:GLN:HG3	0.49	2.07	11	1
3:B:111:SER:HA	3:B:115:GLN:CD	0.49	2.31	17	1
2:D:194:DA:C5	2:D:195:DC:C5	0.49	3.00	3	6
3:A:5:ILE:HD11	3:B:107:VAL:CG1	0.49	2.36	6	4
3:A:15:GLN:O	3:A:19:ALA:N	0.49	2.44	16	10
3:B:115:GLN:OE1	3:B:118:LYS:NZ	0.49	2.39	2	2
3:B:117:LEU:CD1	3:B:127:LEU:CD1	0.49	2.90	20	2
3:B:107:VAL:O	3:B:107:VAL:CG1	0.49	2.60	7	2
3:A:10:ASP:HA	3:A:15:GLN:CD	0.49	2.33	19	1
1:C:179:DA:C2	2:D:194:DA:C2	0.49	3.00	8	4
3:A:32:MET:CE	3:B:124:ILE:CG2	0.49	2.89	18	2
3:A:17:LEU:HD21	3:B:135:GLU:HB2	0.49	1.83	1	1
3:A:9:VAL:CG2	3:B:103:GLN:HB3	0.49	2.36	2	2
1:C:178:DT:C7	3:A:6:THR:OG1	0.49	2.61	18	2
3:A:7:VAL:CG1	3:B:105:ILE:HG21	0.49	2.38	12	1
2:D:187:DC:H2''	2:D:188:DG:O5'	0.49	2.07	16	1
2:D:190:DG:OP1	3:A:25:SER:CA	0.49	2.61	17	1
3:A:9:VAL:CG1	3:A:14:TYR:CG	0.49	2.94	9	4
2:D:190:DG:OP1	3:A:25:SER:HB3	0.49	2.08	10	3
3:B:107:VAL:O	3:B:109:VAL:HG23	0.49	2.08	10	1
3:A:2:LYS:HA	3:B:109:VAL:O	0.49	2.08	2	4
2:D:194:DA:C4	2:D:195:DC:C6	0.49	3.01	11	7
3:A:18:LYS:HG3	3:A:19:ALA:N	0.49	2.23	3	4
3:A:6:THR:HG22	3:B:106:THR:HB	0.49	1.82	18	2
3:A:12:ASP:HB3	3:B:129:SER:OG	0.49	2.07	7	1
3:B:124:ILE:N	3:B:124:ILE:CD1	0.49	2.72	10	10
2:D:190:DG:C5	2:D:191:DT:H72	0.49	2.43	6	1
3:A:5:ILE:HG13	3:B:114:TYR:CE1	0.49	2.43	20	2
2:D:191:DT:C7	3:A:4:ARG:HD3	0.49	2.38	18	1
1:C:175:DA:O5'	1:C:175:DA:H8	0.49	1.91	20	1
3:B:123:ASN:C	3:B:124:ILE:CD1	0.49	2.85	16	3
2:D:191:DT:H2''	2:D:192:DA:N7	0.49	2.23	18	2
3:A:7:VAL:HG22	3:A:9:VAL:HB	0.49	1.84	9	2
1:C:173:DA:H1'	1:C:174:DT:OP1	0.49	2.08	9	2
3:B:127:LEU:HD13	3:B:128:VAL:N	0.49	2.23	18	2
3:B:122:VAL:O	3:B:124:ILE:N	0.49	2.42	1	2
3:A:14:TYR:CD1	3:B:105:ILE:CD1	0.49	2.95	9	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:176:DT:H72	3:A:8:THR:HG21	0.49	1.84	10	3
3:B:109:VAL:HG13	3:B:114:TYR:CD2	0.49	2.43	18	1
3:A:22:VAL:O	3:A:24:ILE:N	0.49	2.36	11	7
2:D:190:DG:OP2	3:B:107:VAL:HA	0.49	2.07	2	4
3:A:7:VAL:O	3:A:9:VAL:HG22	0.49	2.07	4	1
3:B:107:VAL:HG22	3:B:107:VAL:O	0.49	2.08	19	3
3:B:105:ILE:CD1	3:B:132:MET:HE1	0.49	2.37	11	2
3:A:7:VAL:HG13	3:A:9:VAL:HG13	0.49	1.84	20	2
3:A:5:ILE:CG1	3:A:5:ILE:O	0.48	2.61	15	8
3:A:23:ASN:O	3:B:132:MET:CE	0.48	2.61	15	4
3:A:6:THR:HG22	3:B:104:ARG:HG2	0.48	1.84	13	1
2:D:192:DA:H62	3:B:104:ARG:NE	0.48	2.05	20	1
1:C:177:DG:C2	2:D:196:DA:C2	0.48	3.01	6	5
1:C:175:DA:C8	1:C:175:DA:O5'	0.48	2.66	8	2
2:D:190:DG:P	3:A:25:SER:HB2	0.48	2.47	9	2
3:A:7:VAL:HG21	3:B:128:VAL:HB	0.48	1.85	15	1
3:B:117:LEU:CG	3:B:127:LEU:CD1	0.48	2.91	15	1
2:D:186:DT:C2'	2:D:187:DC:O5'	0.48	2.57	15	3
3:A:3:GLN:HG2	3:B:114:TYR:CE2	0.48	2.43	7	3
1:C:173:DA:C3'	1:C:174:DT:H73	0.48	2.38	8	1
3:A:28:VAL:CB	3:B:107:VAL:HG11	0.48	2.38	8	2
3:A:5:ILE:O	3:B:107:VAL:N	0.48	2.46	1	2
3:A:14:TYR:CD2	3:B:132:MET:HE3	0.48	2.43	2	2
3:A:28:VAL:HG21	3:B:107:VAL:HG11	0.48	1.85	19	4
1:C:174:DT:OP1	1:C:174:DT:C5	0.48	2.66	10	1
3:A:9:VAL:HG23	3:A:9:VAL:O	0.48	2.09	14	1
2:D:191:DT:H72	3:B:106:THR:HG21	0.48	1.85	15	4
3:B:109:VAL:CG1	3:B:114:TYR:CD2	0.48	2.95	18	1
3:B:109:VAL:CG1	3:B:114:TYR:CG	0.48	2.97	18	1
3:B:128:VAL:O	3:B:132:MET:HB2	0.48	2.08	19	1
3:B:112:ASP:O	3:B:114:TYR:N	0.48	2.45	18	2
3:B:114:TYR:CD2	3:B:115:GLN:N	0.48	2.82	13	4
3:B:122:VAL:C	3:B:124:ILE:H	0.48	2.17	18	2
3:A:26:GLY:O	3:A:30:THR:HB	0.48	2.09	15	3
3:A:32:MET:SD	3:B:114:TYR:CA	0.48	2.97	8	3
2:D:192:DA:C5	2:D:193:DT:C4	0.48	3.02	13	2
3:A:23:ASN:C	3:A:24:ILE:CD1	0.48	2.81	12	4
3:B:102:LYS:O	3:B:102:LYS:HG2	0.48	2.08	14	1
3:A:2:LYS:HA	3:A:2:LYS:HE3	0.48	1.85	15	1
3:A:7:VAL:HG13	3:A:9:VAL:HB	0.48	1.85	15	1
2:D:190:DG:OP2	3:A:25:SER:CB	0.48	2.62	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:121:ASP:O	3:B:122:VAL:CG2	0.48	2.62	17	3
1:C:179:DA:N7	3:A:4:ARG:NH2	0.48	2.62	7	1
3:B:118:LYS:HG3	3:B:119:ALA:N	0.48	2.24	18	2
3:B:117:LEU:CD1	3:B:122:VAL:HB	0.48	2.39	13	2
3:A:21:ASP:O	3:A:22:VAL:HG23	0.48	2.09	16	2
3:A:23:ASN:O	3:B:132:MET:HE2	0.48	2.09	16	2
2:D:192:DA:O5'	2:D:192:DA:H8	0.47	1.92	1	3
3:A:31:THR:CB	3:B:127:LEU:HD21	0.47	2.37	4	1
2:D:189:DG:O3'	3:A:25:SER:HB3	0.47	2.08	14	2
1:C:173:DA:C2'	1:C:174:DT:OP1	0.47	2.62	12	5
3:B:124:ILE:HA	3:B:127:LEU:HB3	0.47	1.85	14	5
1:C:177:DG:OP1	3:B:125:SER:HA	0.47	2.08	15	1
2:D:191:DT:C2	2:D:192:DA:C6	0.47	3.02	18	1
3:B:111:SER:HA	3:B:115:GLN:HG2	0.47	1.86	19	1
3:A:16:LEU:HD22	3:A:20:TYR:CE1	0.47	2.44	1	1
3:A:3:GLN:O	3:B:109:VAL:N	0.47	2.44	5	8
3:A:33:GLN:HB2	3:B:113:SER:OG	0.47	2.09	18	3
3:B:109:VAL:HG12	3:B:112:ASP:OD1	0.47	2.09	16	1
1:C:173:DA:H5'	1:C:173:DA:N3	0.47	2.24	18	1
3:A:7:VAL:HG22	3:A:7:VAL:O	0.47	2.07	5	3
3:A:17:LEU:HD23	3:A:27:LEU:HG	0.47	1.85	8	1
3:B:115:GLN:O	3:B:119:ALA:CB	0.47	2.62	18	3
3:A:29:SER:HA	3:B:112:ASP:O	0.47	2.09	19	1
1:C:177:DG:C8	1:C:178:DT:H71	0.47	2.44	6	3
3:A:32:MET:HE3	3:B:114:TYR:HD1	0.47	1.69	19	2
2:D:192:DA:N7	3:B:104:ARG:HD2	0.47	2.25	15	2
3:A:14:TYR:CA	3:B:132:MET:SD	0.47	2.96	16	5
3:A:27:LEU:HD13	3:A:28:VAL:N	0.47	2.23	11	3
2:D:186:DT:C2'	2:D:187:DC:C5'	0.47	2.93	8	1
3:B:128:VAL:HG12	3:B:132:MET:SD	0.47	2.49	9	2
3:B:128:VAL:CG1	3:B:132:MET:CE	0.47	2.92	17	2
1:C:184:DC:N4	2:D:187:DC:N4	0.47	2.63	12	2
3:A:7:VAL:O	3:B:105:ILE:CG2	0.47	2.53	20	1
3:A:5:ILE:HG12	3:B:107:VAL:O	0.47	2.10	10	2
3:A:14:TYR:CZ	3:B:105:ILE:CG1	0.47	2.97	2	1
3:A:14:TYR:CD2	3:A:15:GLN:N	0.47	2.83	9	5
3:B:128:VAL:O	3:B:132:MET:N	0.47	2.43	4	2
3:B:109:VAL:HG12	3:B:112:ASP:CB	0.47	2.40	5	2
1:C:175:DA:C2	1:C:176:DT:C2	0.47	3.03	6	2
3:A:18:LYS:HB3	3:A:23:ASN:HB3	0.47	1.86	14	2
3:A:5:ILE:HD13	3:A:5:ILE:O	0.47	2.09	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:190:DG:C8	3:A:4:ARG:NH1	0.47	2.83	20	1
3:A:9:VAL:HG13	3:A:10:ASP:H	0.47	1.69	1	1
3:A:15:GLN:O	3:A:19:ALA:HB2	0.47	2.10	11	6
1:C:176:DT:C6	3:A:8:THR:OG1	0.47	2.68	6	1
3:B:107:VAL:O	3:B:109:VAL:HG12	0.47	2.10	7	1
3:A:5:ILE:HD13	3:B:114:TYR:HD2	0.47	1.59	8	1
3:A:5:ILE:O	3:B:106:THR:CA	0.47	2.62	8	2
3:A:9:VAL:HG11	3:A:14:TYR:CD1	0.47	2.44	8	1
2:D:188:DG:H8	2:D:188:DG:O5'	0.47	1.93	12	1
3:A:27:LEU:HD11	3:B:135:GLU:CG	0.47	2.36	15	1
3:A:35:GLU:HB2	3:B:117:LEU:HD21	0.47	1.86	16	1
2:D:186:DT:H2''	2:D:187:DC:O4'	0.47	2.08	20	1
2:D:192:DA:O5'	2:D:192:DA:C8	0.47	2.68	16	4
3:B:107:VAL:HG22	3:B:109:VAL:HG13	0.47	1.86	2	4
3:B:121:ASP:O	3:B:122:VAL:HG23	0.47	2.10	17	3
3:A:17:LEU:CD2	3:B:132:MET:HA	0.47	2.39	12	4
3:A:29:SER:O	3:B:113:SER:HB3	0.47	2.10	10	2
2:D:190:DG:C8	2:D:191:DT:H73	0.47	2.44	4	1
3:A:12:ASP:O	3:B:129:SER:CA	0.47	2.63	4	4
1:C:173:DA:O4'	1:C:174:DT:H72	0.47	2.09	10	1
3:A:9:VAL:HG12	3:A:11:SER:H	0.47	1.68	12	1
3:A:32:MET:HE2	3:B:124:ILE:HG12	0.47	1.87	18	1
3:A:32:MET:HE2	3:B:124:ILE:HG13	0.47	1.86	20	1
1:C:179:DA:H2'	1:C:180:DT:H72	0.47	1.85	12	4
3:B:138:ARG:N	3:B:138:ARG:HD2	0.47	2.25	14	1
3:B:117:LEU:HD13	3:B:120:TYR:CZ	0.46	2.45	15	4
3:A:35:GLU:HG2	3:B:117:LEU:HD21	0.46	1.87	8	1
3:A:21:ASP:O	3:A:22:VAL:CG2	0.46	2.64	16	2
2:D:192:DA:H62	3:B:104:ARG:NH2	0.46	2.08	12	1
3:A:24:ILE:HG12	3:B:128:VAL:CG1	0.46	2.40	15	1
3:A:14:TYR:OH	3:A:18:LYS:NZ	0.46	2.37	3	3
2:D:193:DT:C4	2:D:194:DA:N6	0.46	2.83	10	1
2:D:189:DG:C8	2:D:190:DG:N7	0.46	2.83	12	1
2:D:190:DG:OP1	3:A:25:SER:HB2	0.46	2.10	15	2
3:A:17:LEU:HD12	3:A:22:VAL:HG13	0.46	1.85	12	3
3:A:30:THR:CG2	3:A:31:THR:N	0.46	2.77	15	4
3:A:3:GLN:HB3	3:B:110:ASP:HA	0.46	1.88	19	2
2:D:191:DT:C4	2:D:192:DA:N6	0.46	2.83	8	5
3:A:7:VAL:O	3:A:9:VAL:N	0.46	2.48	1	4
3:A:27:LEU:HD13	3:B:135:GLU:HG2	0.46	1.87	4	1
3:B:105:ILE:O	3:B:105:ILE:HD13	0.46	2.10	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:TYR:CZ	3:A:18:LYS:HG2	0.46	2.44	10	3
2:D:190:DG:OP2	3:A:25:SER:HB2	0.46	2.10	11	2
3:A:23:ASN:C	3:A:24:ILE:HG13	0.46	2.35	1	2
3:B:132:MET:O	3:B:136:ALA:HB2	0.46	2.10	18	3
2:D:189:DG:O3'	3:A:25:SER:CB	0.46	2.63	14	2
1:C:177:DG:OP1	3:B:125:SER:CA	0.46	2.64	15	1
3:A:9:VAL:HG23	3:A:12:ASP:CB	0.46	2.38	9	1
3:A:35:GLU:HB2	3:B:127:LEU:HD11	0.46	1.85	10	1
3:A:3:GLN:N	3:B:109:VAL:O	0.46	2.40	17	3
2:D:190:DG:OP2	3:A:25:SER:HB3	0.46	2.10	1	1
3:B:117:LEU:HD22	3:B:120:TYR:CE2	0.46	2.46	15	2
3:A:17:LEU:HD11	3:B:135:GLU:HG2	0.46	1.88	16	2
2:D:191:DT:H2'	2:D:192:DA:C8	0.46	2.46	12	1
3:A:31:THR:HG22	3:B:127:LEU:CD2	0.46	2.40	12	1
3:B:133:GLN:HG3	3:B:134:ASN:N	0.46	2.25	13	1
3:B:112:ASP:C	3:B:114:TYR:H	0.46	2.18	17	2
3:A:28:VAL:HG11	3:B:107:VAL:HG11	0.46	1.88	1	2
3:A:7:VAL:HG12	3:B:105:ILE:CG2	0.46	2.41	12	1
1:C:179:DA:N3	1:C:180:DT:C2	0.46	2.84	1	4
3:B:117:LEU:HD12	3:B:127:LEU:CD2	0.46	2.28	3	1
3:A:17:LEU:CD1	3:A:22:VAL:CG1	0.46	2.94	7	2
3:A:36:ALA:HB1	3:B:116:LEU:CB	0.46	2.34	7	1
1:C:175:DA:N1	2:D:198:DA:C2	0.46	2.84	19	1
1:C:178:DT:H2''	1:C:179:DA:C8	0.45	2.47	12	4
3:A:14:TYR:CD2	3:A:15:GLN:HG2	0.45	2.46	1	1
3:A:17:LEU:HA	3:A:20:TYR:CE1	0.45	2.46	8	1
3:B:128:VAL:C	3:B:132:MET:HG2	0.45	2.36	18	1
3:A:17:LEU:HD12	3:A:22:VAL:HB	0.45	1.88	19	1
3:A:24:ILE:HA	3:A:27:LEU:CB	0.45	2.41	19	4
3:B:125:SER:OG	3:B:126:GLY:N	0.45	2.50	13	5
3:B:109:VAL:HG23	3:B:112:ASP:HB2	0.45	1.88	4	1
3:A:29:SER:HA	3:A:32:MET:HG2	0.45	1.87	7	1
2:D:195:DC:C2	2:D:196:DA:N7	0.45	2.84	2	2
3:A:32:MET:SD	3:B:114:TYR:O	0.45	2.75	8	4
2:D:189:DG:H2''	2:D:190:DG:C8	0.45	2.47	4	1
2:D:190:DG:P	3:B:107:VAL:HA	0.45	2.50	5	2
3:B:128:VAL:O	3:B:132:MET:HG3	0.45	2.12	16	4
2:D:191:DT:H73	3:A:4:ARG:HD3	0.45	1.88	18	1
3:A:36:ALA:HA	3:B:120:TYR:CE2	0.45	2.46	19	1
1:C:175:DA:C8	1:C:176:DT:C4	0.45	3.05	8	1
2:D:196:DA:C8	2:D:197:DT:H71	0.45	2.46	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:LEU:HD12	3:A:22:VAL:HG11	0.45	1.86	12	1
3:B:117:LEU:HD13	3:B:124:ILE:HG23	0.45	1.89	18	1
3:A:14:TYR:CZ	3:B:105:ILE:HD11	0.45	2.46	2	1
3:A:24:ILE:HA	3:A:27:LEU:HB3	0.45	1.88	3	6
3:A:24:ILE:HD11	3:B:105:ILE:HG12	0.45	1.89	4	1
3:A:6:THR:HG23	3:B:106:THR:CB	0.45	2.42	13	1
3:A:5:ILE:HG23	3:B:109:VAL:HG12	0.45	1.88	4	1
1:C:182:DC:C4	1:C:183:DC:N4	0.45	2.85	16	1
3:A:7:VAL:HG12	3:A:9:VAL:HG12	0.45	1.87	15	1
3:B:137:ARG:HA	3:B:137:ARG:NE	0.45	2.27	18	1
3:A:25:SER:OG	3:A:26:GLY:N	0.45	2.50	17	4
3:A:17:LEU:HD12	3:A:22:VAL:O	0.45	2.12	6	1
3:A:14:TYR:HD2	3:B:132:MET:HE1	0.45	1.72	16	1
3:B:121:ASP:C	3:B:122:VAL:HG23	0.45	2.37	17	3
3:A:32:MET:HE3	3:B:114:TYR:CD1	0.45	2.46	3	1
2:D:189:DG:N7	2:D:190:DG:C5	0.45	2.85	8	1
3:A:3:GLN:HB3	3:B:110:ASP:CB	0.45	2.41	9	1
3:A:10:ASP:O	3:A:15:GLN:CG	0.44	2.65	1	1
1:C:180:DT:O4	3:A:4:ARG:HD2	0.44	2.12	2	1
1:C:177:DG:OP1	3:B:125:SER:HB2	0.44	2.12	5	4
3:B:107:VAL:CG2	3:B:109:VAL:HG13	0.44	2.34	19	3
2:D:186:DT:H1'	2:D:187:DC:OP1	0.44	2.12	8	1
1:C:176:DT:O3'	3:B:125:SER:HB3	0.44	2.11	11	1
3:B:122:VAL:O	3:B:123:ASN:CG	0.44	2.61	11	1
2:D:196:DA:C8	2:D:197:DT:C7	0.44	3.01	9	1
3:B:110:ASP:HA	3:B:115:GLN:HG3	0.44	1.88	9	1
1:C:174:DT:OP1	1:C:174:DT:C6	0.44	2.71	10	1
3:A:17:LEU:CG	3:B:132:MET:HG2	0.44	2.42	11	1
3:B:115:GLN:HA	3:B:118:LYS:HE3	0.44	1.89	18	1
3:B:129:SER:HA	3:B:132:MET:CG	0.44	2.42	18	1
3:A:11:SER:OG	3:B:102:LYS:NZ	0.44	2.35	19	1
2:D:192:DA:H2''	2:D:193:DT:C6	0.44	2.47	16	6
3:A:7:VAL:HG13	3:B:105:ILE:CD1	0.44	2.42	5	3
3:B:130:THR:CG2	3:B:131:THR:N	0.44	2.80	6	5
3:A:17:LEU:HD11	3:B:135:GLU:HB3	0.44	1.90	8	1
3:B:109:VAL:HG11	3:B:114:TYR:N	0.44	2.28	10	1
3:B:111:SER:OG	3:B:112:ASP:N	0.44	2.50	13	1
3:A:9:VAL:C	3:A:11:SER:H	0.44	2.20	14	1
2:D:187:DC:C6	2:D:187:DC:O5'	0.44	2.70	19	2
3:B:107:VAL:CG1	3:B:109:VAL:HB	0.44	2.42	18	1
3:A:22:VAL:C	3:A:24:ILE:N	0.44	2.74	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:LEU:CD1	3:A:20:TYR:CE1	0.44	3.00	8	1
1:C:173:DA:H2''	1:C:174:DT:C5'	0.44	2.42	11	1
2:D:186:DT:H71	2:D:187:DC:C2'	0.44	2.43	11	1
3:A:5:ILE:CB	3:B:114:TYR:CE1	0.44	3.01	18	2
3:A:9:VAL:O	3:B:102:LYS:HA	0.44	2.12	15	2
3:B:117:LEU:HD12	3:B:127:LEU:HD12	0.44	1.89	20	2
3:A:13:SER:O	3:B:132:MET:HB2	0.44	2.12	7	2
1:C:173:DA:H2''	1:C:174:DT:OP1	0.44	2.13	15	6
1:C:173:DA:C1'	1:C:174:DT:H73	0.44	2.42	10	1
1:C:174:DT:H2''	1:C:175:DA:C5'	0.44	2.43	10	2
2:D:191:DT:H3'	3:B:104:ARG:O	0.44	2.13	10	1
1:C:175:DA:OP2	3:B:102:LYS:HD2	0.44	2.12	14	1
2:D:186:DT:C6	2:D:187:DC:C6	0.44	3.06	17	1
3:B:117:LEU:HD11	3:B:127:LEU:CD1	0.44	2.38	3	1
3:A:13:SER:HB2	3:B:129:SER:O	0.44	2.13	19	2
3:A:28:VAL:HB	3:B:107:VAL:HG11	0.44	1.89	8	1
3:A:7:VAL:HG13	3:B:105:ILE:CG2	0.44	2.42	12	1
3:B:107:VAL:CG2	3:B:107:VAL:O	0.44	2.66	19	2
3:A:14:TYR:HD2	3:B:132:MET:HE3	0.44	1.72	2	2
3:B:105:ILE:O	3:B:105:ILE:HG12	0.44	2.13	7	2
3:A:17:LEU:O	3:A:20:TYR:CD1	0.44	2.71	8	1
3:A:17:LEU:HD13	3:B:132:MET:HA	0.44	1.88	9	1
3:A:9:VAL:HB	3:A:14:TYR:HD2	0.44	1.72	12	1
2:D:193:DT:O4	3:B:104:ARG:CD	0.44	2.66	13	1
3:A:5:ILE:HG22	3:B:114:TYR:CZ	0.44	2.48	17	2
1:C:173:DA:C4'	1:C:174:DT:OP1	0.44	2.65	20	1
3:A:7:VAL:HG23	3:B:124:ILE:CD1	0.44	2.36	20	1
3:B:109:VAL:CG1	3:B:112:ASP:HB2	0.44	2.42	16	2
3:B:107:VAL:O	3:B:107:VAL:CG2	0.44	2.65	4	1
3:A:9:VAL:CG2	3:A:14:TYR:CB	0.44	2.93	14	2
3:A:6:THR:CG2	3:B:106:THR:HB	0.44	2.43	18	3
3:A:7:VAL:O	3:A:7:VAL:CG2	0.44	2.66	8	1
2:D:192:DA:H62	3:B:104:ARG:NH1	0.44	2.11	12	1
2:D:186:DT:H4'	2:D:186:DT:OP3	0.44	2.13	13	1
3:A:9:VAL:O	3:B:103:GLN:N	0.43	2.44	1	1
2:D:194:DA:H2''	2:D:195:DC:O5'	0.43	2.13	2	3
3:A:4:ARG:NH1	3:B:108:THR:HG21	0.43	2.28	2	1
3:A:33:GLN:HG3	3:A:34:ASN:N	0.43	2.27	17	2
1:C:182:DC:H2''	1:C:183:DC:C5'	0.43	2.43	14	1
3:A:27:LEU:HD11	3:B:131:THR:CG2	0.43	2.43	17	1
3:A:14:TYR:O	3:B:132:MET:SD	0.43	2.76	5	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:128:VAL:HG13	3:B:132:MET:HG3	0.43	1.89	8	1
3:B:124:ILE:CG2	3:B:127:LEU:HD13	0.43	2.42	11	1
3:A:17:LEU:HG	3:A:27:LEU:CD1	0.43	2.43	12	1
3:B:128:VAL:O	3:B:132:MET:SD	0.43	2.76	19	2
3:A:9:VAL:O	3:A:14:TYR:HB3	0.43	2.13	14	1
3:A:17:LEU:HG	3:A:27:LEU:CD2	0.43	2.43	14	1
2:D:194:DA:C5	2:D:195:DC:C4	0.43	3.06	18	1
3:A:17:LEU:HD22	3:A:22:VAL:CB	0.43	2.44	18	1
2:D:189:DG:C2'	2:D:190:DG:C8	0.43	3.01	4	1
3:B:107:VAL:O	3:B:109:VAL:HG22	0.43	2.13	9	3
2:D:186:DT:C7	2:D:187:DC:C6	0.43	3.01	7	1
3:A:13:SER:OG	3:B:133:GLN:HB2	0.43	2.12	9	2
3:A:25:SER:CA	3:B:107:VAL:HG22	0.43	2.33	18	1
3:A:2:LYS:HE3	3:A:2:LYS:CA	0.43	2.43	19	1
3:A:21:ASP:C	3:A:22:VAL:HG23	0.43	2.39	8	4
3:A:14:TYR:HD1	3:B:105:ILE:HD13	0.43	1.68	11	1
3:A:7:VAL:O	3:B:105:ILE:HB	0.43	2.14	12	1
3:A:6:THR:HG23	3:B:106:THR:HB	0.43	1.89	13	1
1:C:177:DG:C5	1:C:178:DT:C4	0.43	3.06	19	2
3:A:3:GLN:HG2	3:A:5:ILE:CG2	0.43	2.43	11	1
3:B:138:ARG:HD2	3:B:138:ARG:C	0.43	2.38	12	1
3:B:134:ASN:O	3:B:138:ARG:HD3	0.43	2.13	14	1
2:D:193:DT:O4	3:B:104:ARG:HD3	0.43	2.13	19	1
1:C:173:DA:H2''	1:C:174:DT:C6	0.43	2.48	2	4
3:B:127:LEU:O	3:B:128:VAL:C	0.43	2.61	15	1
2:D:196:DA:C5	2:D:197:DT:C4	0.43	3.07	19	2
1:C:179:DA:H62	3:B:104:ARG:CZ	0.43	2.26	6	1
3:A:6:THR:CB	3:B:105:ILE:O	0.43	2.67	12	1
2:D:188:DG:H2''	2:D:189:DG:C8	0.43	2.49	8	4
3:A:5:ILE:CG2	3:B:114:TYR:CE2	0.43	3.02	17	3
3:A:35:GLU:CB	3:B:117:LEU:HD11	0.43	2.43	7	1
1:C:175:DA:H2'	1:C:176:DT:H71	0.43	1.90	10	1
3:A:10:ASP:CA	3:A:15:GLN:HG3	0.43	2.42	14	1
2:D:191:DT:H71	3:B:106:THR:HB	0.43	1.89	15	1
3:B:103:GLN:CD	3:B:103:GLN:C	0.43	2.87	15	1
2:D:191:DT:H73	3:A:4:ARG:HD2	0.43	1.90	19	1
3:A:12:ASP:O	3:A:13:SER:HB2	0.43	2.12	4	2
1:C:177:DG:C6	1:C:178:DT:C4	0.43	3.07	6	1
3:A:7:VAL:O	3:B:105:ILE:HG12	0.43	2.13	14	2
3:A:17:LEU:HA	3:A:20:TYR:CD1	0.43	2.49	8	1
3:B:116:LEU:O	3:B:119:ALA:HB3	0.43	2.14	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:VAL:HG13	3:A:12:ASP:CB	0.43	2.44	12	1
3:A:24:ILE:HG21	3:A:28:VAL:CG2	0.43	2.23	15	1
3:A:7:VAL:HG21	3:B:124:ILE:C	0.43	2.39	20	1
3:A:8:THR:HG23	3:B:104:ARG:HG3	0.43	1.90	1	1
3:A:28:VAL:CG1	3:B:107:VAL:HG11	0.43	2.44	11	2
2:D:186:DT:O2	2:D:186:DT:O4'	0.43	2.37	15	2
3:A:5:ILE:HG12	3:B:124:ILE:CD1	0.43	2.41	7	1
3:A:32:MET:SD	3:B:117:LEU:HB3	0.43	2.53	8	1
3:A:34:ASN:OD1	3:A:38:ARG:NE	0.43	2.50	8	1
3:B:117:LEU:CD1	3:B:127:LEU:HG	0.43	2.41	17	1
3:A:33:GLN:O	3:A:37:ARG:HB2	0.42	2.14	18	2
3:A:7:VAL:CG1	3:A:9:VAL:CG2	0.42	2.97	14	2
3:B:112:ASP:O	3:B:113:SER:HB2	0.42	2.14	12	3
2:D:190:DG:OP1	3:B:107:VAL:HB	0.42	2.13	5	1
3:A:2:LYS:HB3	3:B:109:VAL:O	0.42	2.14	8	1
1:C:173:DA:C4'	1:C:174:DT:H5'	0.42	2.44	11	1
2:D:191:DT:H72	3:B:106:THR:CB	0.42	2.44	15	2
3:A:17:LEU:HD23	3:A:27:LEU:CG	0.42	2.43	8	1
3:A:32:MET:HE1	3:B:114:TYR:CD2	0.42	2.49	8	1
3:A:15:GLN:CA	3:A:18:LYS:HE2	0.42	2.44	9	1
2:D:189:DG:C4	2:D:190:DG:C8	0.42	3.07	10	1
3:A:16:LEU:CB	3:B:136:ALA:CB	0.42	2.97	10	1
3:B:115:GLN:CA	3:B:118:LYS:HE2	0.42	2.44	13	2
3:A:9:VAL:HG12	3:A:10:ASP:N	0.42	2.30	3	1
3:B:114:TYR:CE2	3:B:118:LYS:HG2	0.42	2.49	4	1
3:B:116:LEU:O	3:B:120:TYR:CD2	0.42	2.73	9	1
3:B:138:ARG:NE	3:B:138:ARG:CA	0.42	2.82	9	1
3:A:17:LEU:HG	3:B:132:MET:HA	0.42	1.91	18	1
3:B:117:LEU:HD22	3:B:122:VAL:HG13	0.42	1.90	20	1
3:B:102:LYS:HE3	3:B:102:LYS:HA	0.42	1.92	8	1
3:A:27:LEU:O	3:A:28:VAL:C	0.42	2.62	20	2
3:B:129:SER:CA	3:B:132:MET:HG2	0.42	2.44	18	1
2:D:191:DT:C2'	2:D:192:DA:C8	0.42	3.02	20	1
3:A:32:MET:CE	3:B:123:ASN:O	0.42	2.65	20	1
3:B:109:VAL:HG22	3:B:111:SER:H	0.42	1.74	7	1
1:C:178:DT:C7	3:A:6:THR:CG2	0.42	2.97	12	1
3:A:7:VAL:HG13	3:B:105:ILE:HG13	0.42	1.90	19	1
3:A:14:TYR:CD1	3:B:105:ILE:CG2	0.42	3.03	20	1
3:B:114:TYR:CD1	3:B:115:GLN:N	0.42	2.87	2	1
2:D:188:DG:C2'	2:D:189:DG:N7	0.42	2.80	8	1
3:A:2:LYS:HE3	3:B:108:THR:O	0.42	2.13	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:180:DT:O4	3:B:104:ARG:NH2	0.42	2.53	17	2
1:C:181:DA:OP2	2:D:186:DT:H72	0.42	2.15	8	1
3:A:12:ASP:O	3:A:13:SER:CB	0.42	2.66	15	1
3:B:114:TYR:CG	3:B:115:GLN:N	0.42	2.85	18	1
3:A:20:TYR:CD1	3:A:21:ASP:HB2	0.42	2.49	19	1
3:A:14:TYR:CD1	3:A:14:TYR:C	0.42	2.96	2	1
1:C:180:DT:H71	3:A:4:ARG:CD	0.42	2.45	3	2
3:A:17:LEU:CD1	3:A:22:VAL:HG13	0.42	2.43	4	1
1:C:173:DA:H3'	1:C:174:DT:C7	0.42	2.44	8	1
2:D:187:DC:C2	2:D:188:DG:C6	0.42	3.07	8	1
3:B:107:VAL:HG22	3:B:109:VAL:HB	0.42	1.90	11	1
3:A:35:GLU:CG	3:B:127:LEU:HD11	0.42	2.41	12	1
3:A:24:ILE:HG21	3:A:27:LEU:HD12	0.42	1.91	13	1
3:A:24:ILE:CB	3:A:28:VAL:CG2	0.42	2.97	15	1
3:A:13:SER:C	3:B:132:MET:HB3	0.42	2.40	1	1
3:A:27:LEU:O	3:A:31:THR:HB	0.42	2.15	8	1
3:A:34:ASN:O	3:A:38:ARG:HB2	0.42	2.15	9	1
3:A:14:TYR:HD1	3:B:132:MET:HE3	0.42	1.75	12	1
3:A:17:LEU:HG	3:A:27:LEU:HD12	0.42	1.90	12	1
3:B:138:ARG:C	3:B:138:ARG:CD	0.42	2.93	12	1
3:A:5:ILE:CD1	3:A:28:VAL:HG11	0.42	2.45	14	1
3:A:9:VAL:HG13	3:B:105:ILE:HB	0.42	1.90	2	1
3:A:22:VAL:O	3:A:23:ASN:CG	0.42	2.63	14	1
3:A:15:GLN:HA	3:A:18:LYS:HE3	0.42	1.90	16	1
3:A:24:ILE:O	3:B:107:VAL:HG21	0.42	2.15	16	1
2:D:191:DT:C7	3:A:4:ARG:HD2	0.42	2.44	19	1
2:D:192:DA:N6	3:B:104:ARG:NH2	0.41	2.68	12	1
1:C:178:DT:H71	3:B:104:ARG:HE	0.41	1.74	14	1
3:A:15:GLN:CA	3:A:18:LYS:HE3	0.41	2.45	16	1
3:A:4:ARG:NE	3:B:108:THR:CG2	0.41	2.83	17	1
3:A:5:ILE:HD13	3:B:114:TYR:HD1	0.41	1.73	18	1
3:A:9:VAL:HG13	3:A:14:TYR:CD2	0.41	2.49	19	1
1:C:174:DT:O5'	1:C:174:DT:H6	0.41	1.98	1	1
3:A:9:VAL:CB	3:A:14:TYR:CB	0.41	2.98	4	1
1:C:175:DA:C8	1:C:176:DT:C5	0.41	3.09	13	2
1:C:175:DA:H3'	3:B:102:LYS:HD3	0.41	1.90	12	1
3:B:102:LYS:HD3	3:B:102:LYS:N	0.41	2.31	14	1
2:D:190:DG:C4	2:D:191:DT:C5	0.41	3.08	15	1
3:A:6:THR:HA	3:B:106:THR:HA	0.41	1.92	18	2
1:C:178:DT:H71	3:A:6:THR:OG1	0.41	2.15	18	1
3:A:33:GLN:CB	3:B:113:SER:CB	0.41	2.98	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:124:ILE:O	3:B:128:VAL:N	0.41	2.52	1	1
3:A:5:ILE:O	3:A:5:ILE:HG12	0.41	2.08	4	1
3:A:29:SER:CA	3:B:112:ASP:O	0.41	2.68	16	1
3:A:5:ILE:CG2	3:B:109:VAL:HG12	0.41	2.46	18	1
3:B:118:LYS:CB	3:B:123:ASN:HA	0.41	2.45	18	1
3:A:9:VAL:CG2	3:A:10:ASP:N	0.41	2.82	19	1
2:D:186:DT:C2'	2:D:187:DC:H5''	0.41	2.45	8	1
3:A:4:ARG:CZ	3:B:108:THR:HG21	0.41	2.45	11	2
3:A:13:SER:HB3	3:B:129:SER:O	0.41	2.15	11	1
3:B:109:VAL:C	3:B:111:SER:H	0.41	2.24	13	1
3:B:115:GLN:HA	3:B:118:LYS:HG2	0.41	1.93	19	1
3:A:7:VAL:HG22	3:B:125:SER:CA	0.41	2.39	20	1
3:A:22:VAL:O	3:A:22:VAL:HG12	0.41	2.15	20	2
1:C:175:DA:C8	1:C:176:DT:H71	0.41	2.51	9	1
3:B:115:GLN:HG2	3:B:118:LYS:HE2	0.41	1.92	11	1
1:C:184:DC:C2'	1:C:185:DG:C5'	0.41	2.98	15	1
3:A:13:SER:HB3	3:B:133:GLN:HB2	0.41	1.92	19	1
3:A:17:LEU:HB2	3:B:132:MET:CG	0.41	2.42	19	1
3:A:5:ILE:HG23	3:B:109:VAL:CG2	0.41	2.45	20	1
2:D:192:DA:C2'	2:D:193:DT:C6	0.41	3.04	1	1
2:D:191:DT:C4	2:D:192:DA:C6	0.41	3.08	8	1
3:A:14:TYR:HD1	3:B:132:MET:HE1	0.41	1.75	9	1
3:A:17:LEU:HD13	3:B:132:MET:HG2	0.41	1.93	9	1
3:B:124:ILE:HG22	3:B:127:LEU:CB	0.41	2.45	9	1
2:D:188:DG:O5'	2:D:188:DG:C8	0.41	2.73	12	1
3:A:17:LEU:CD1	3:B:132:MET:HG2	0.41	2.46	13	1
3:A:17:LEU:O	3:A:22:VAL:HG12	0.41	2.15	13	1
3:A:35:GLU:HG2	3:B:127:LEU:HG	0.41	1.92	13	1
3:B:117:LEU:HD22	3:B:117:LEU:HA	0.41	1.75	14	1
3:B:123:ASN:C	3:B:124:ILE:HG13	0.41	2.40	17	1
2:D:192:DA:N7	3:B:104:ARG:NH1	0.41	2.69	1	1
2:D:192:DA:H2'	2:D:193:DT:C5	0.41	2.51	4	1
3:A:24:ILE:HG12	3:B:105:ILE:CD1	0.41	2.46	7	1
3:A:29:SER:CA	3:A:32:MET:HG2	0.41	2.44	7	1
3:B:133:GLN:OE1	3:B:137:ARG:NH2	0.41	2.45	9	1
3:B:109:VAL:HG13	3:B:110:ASP:N	0.41	2.30	11	1
3:B:126:GLY:O	3:B:130:THR:CB	0.41	2.68	13	1
3:A:24:ILE:HG22	3:A:27:LEU:CD2	0.41	2.45	1	1
3:A:33:GLN:O	3:A:37:ARG:CG	0.41	2.69	2	1
3:A:5:ILE:CG1	3:B:124:ILE:CD1	0.41	2.85	7	1
2:D:189:DG:C6	2:D:190:DG:C6	0.41	3.09	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:TYR:CG	3:A:15:GLN:N	0.41	2.87	12	2
3:A:23:ASN:HB2	3:A:24:ILE:HD12	0.41	1.91	15	1
3:A:24:ILE:HG12	3:B:132:MET:HE2	0.41	1.90	18	1
3:A:8:THR:HA	3:B:104:ARG:HA	0.41	1.93	1	1
3:B:104:ARG:CZ	3:B:106:THR:HG21	0.41	2.45	5	1
3:B:110:ASP:HA	3:B:115:GLN:CD	0.41	2.41	6	1
3:B:124:ILE:HA	3:B:127:LEU:CB	0.41	2.46	8	1
3:B:117:LEU:CD1	3:B:122:VAL:HG11	0.41	2.46	11	1
3:B:127:LEU:O	3:B:131:THR:CB	0.41	2.69	11	1
2:D:191:DT:C7	3:B:106:THR:HG23	0.41	2.46	13	1
3:B:109:VAL:CG2	3:B:110:ASP:N	0.41	2.79	14	1
3:A:5:ILE:HD12	3:B:124:ILE:HG12	0.41	1.93	15	1
3:A:18:LYS:NZ	3:B:103:GLN:OE1	0.41	2.51	17	1
3:A:20:TYR:HD1	3:A:21:ASP:N	0.41	2.13	17	1
3:A:36:ALA:HA	3:B:120:TYR:HE2	0.41	1.76	19	1
3:A:5:ILE:CD1	3:B:107:VAL:HG12	0.41	2.46	20	1
3:A:17:LEU:HD21	3:B:135:GLU:HG3	0.41	1.93	2	1
3:A:7:VAL:O	3:A:9:VAL:HG23	0.41	2.15	12	1
3:A:17:LEU:CD1	3:A:24:ILE:CG2	0.41	2.95	13	1
2:D:191:DT:O4	3:A:4:ARG:HD3	0.41	2.16	18	1
2:D:192:DA:N7	3:B:104:ARG:HD3	0.41	2.31	20	1
2:D:186:DT:C7	2:D:188:DG:N7	0.40	2.84	7	1
2:D:195:DC:C2	2:D:196:DA:C8	0.40	3.09	12	1
2:D:190:DG:H5''	3:A:23:ASN:HB3	0.40	1.92	7	1
3:A:17:LEU:HD12	3:A:27:LEU:CD1	0.40	2.46	10	1
3:A:32:MET:SD	3:B:127:LEU:CD1	0.40	3.09	20	1
3:B:129:SER:O	3:B:132:MET:HB2	0.40	2.17	15	1
3:A:27:LEU:HD11	3:B:131:THR:HG23	0.40	1.91	17	1
3:A:24:ILE:HD11	3:B:105:ILE:CG1	0.40	2.46	4	1
1:C:179:DA:H2'	1:C:180:DT:C7	0.40	2.46	12	1
3:A:4:ARG:CG	3:B:108:THR:CG2	0.40	2.93	17	1
3:A:10:ASP:CG	3:B:103:GLN:HB2	0.40	2.41	19	1
3:A:17:LEU:HB2	3:B:132:MET:HB3	0.40	1.94	2	1
1:C:180:DT:C2	1:C:181:DA:C6	0.40	3.09	5	1
2:D:186:DT:H4'	2:D:187:DC:C5'	0.40	2.46	9	1
1:C:178:DT:C4	3:B:104:ARG:HD2	0.40	2.52	19	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	37/72 (51%)	25±1 (66±3%)	6±1 (17±4%)	6±1 (17±3%)	0	3
3	B	37/72 (51%)	25±1 (66±2%)	7±1 (20±4%)	5±1 (14±4%)	0	5
All	All	1480/2880 (51%)	984 (66%)	268 (18%)	228 (15%)	0	4

All 23 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	21	ASP	20
3	B	109	VAL	20
3	B	121	ASP	20
3	A	9	VAL	19
3	A	23	ASN	16
3	A	24	ILE	15
3	A	12	ASP	13
3	A	13	SER	12
3	B	113	SER	11
3	B	124	ILE	11
3	B	122	VAL	10
3	B	112	ASP	9
3	A	22	VAL	9
3	A	10	ASP	8
3	B	110	ASP	8
3	B	123	ASN	7
3	A	28	VAL	4
3	A	11	SER	4
3	A	2	LYS	4
3	B	108	THR	3
3	B	111	SER	2
3	B	102	LYS	2
3	A	8	THR	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	34/64 (53%)	18±2 (53±6%)	16±2 (47±6%)	0	2
3	B	34/64 (53%)	17±2 (51±6%)	17±2 (49±6%)	0	1
All	All	1360/2560 (53%)	709 (52%)	651 (48%)	0	2

All 68 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	7	VAL	20
3	A	17	LEU	20
3	B	106	THR	20
3	B	107	VAL	20
3	B	117	LEU	20
3	A	6	THR	19
3	A	37	ARG	19
3	B	116	LEU	19
3	B	124	ILE	19
3	A	24	ILE	18
3	A	16	LEU	17
3	A	14	TYR	16
3	B	102	LYS	16
3	B	137	ARG	15
3	B	105	ILE	14
3	B	133	GLN	14
3	A	5	ILE	13
3	B	131	THR	13
3	B	118	LYS	13
3	B	130	THR	13
3	A	33	GLN	12
3	A	18	LYS	12
3	A	4	ARG	11
3	B	138	ARG	11
3	A	20	TYR	11
3	A	32	MET	11
3	A	21	ASP	11
3	B	112	ASP	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
3	A	27	LEU	10
3	A	34	ASN	10
3	B	104	ARG	10
3	A	30	THR	9
3	B	127	LEU	9
3	A	12	ASP	9
3	A	2	LYS	9
3	B	114	TYR	8
3	B	125	SER	8
3	A	38	ARG	8
3	B	109	VAL	8
3	B	115	GLN	8
3	B	134	ASN	8
3	B	120	TYR	7
3	B	128	VAL	7
3	B	121	ASP	6
3	B	123	ASN	6
3	A	11	SER	6
3	A	13	SER	6
3	A	3	GLN	6
3	A	31	THR	5
3	A	25	SER	5
3	B	111	SER	5
3	B	135	GLU	5
3	A	15	GLN	5
3	A	28	VAL	4
3	B	132	MET	4
3	A	9	VAL	4
3	A	23	ASN	4
3	B	113	SER	4
3	A	29	SER	3
3	A	10	ASP	3
3	B	103	GLN	3
3	A	8	THR	2
3	B	110	ASP	2
3	B	129	SER	2
3	B	122	VAL	2
3	B	108	THR	2
3	A	35	GLU	1
3	A	22	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided