



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:17 PM BST

PDB ID : 2H3A
Title : Structural basis for nucleic acid and toxin recognition of the bacterial antitoxin CcdA
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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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

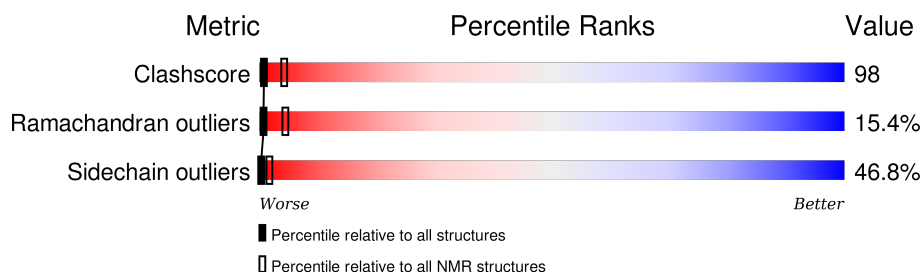
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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)	0.39	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	UNP Q9S0Z5
B	170	LYS	ARG	ENGINEERED	UNP Q9S0Z5

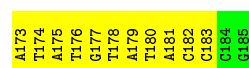
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

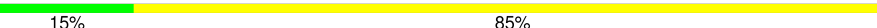
These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain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

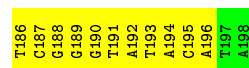
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 




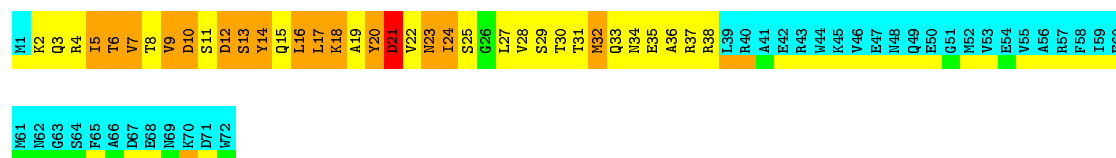
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 




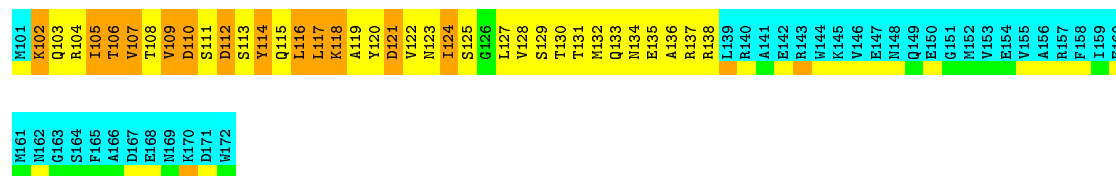
- Molecule 3: CcdA

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: 


A173
T174
A175
T176
G177
T178
A179
T180
A181
C182
C183
C184
G185

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

Chain D: 

T186
C187
G188
G189
G190
T191
A192
T193
A194
C195
A196
T197
A198

- Molecule 3: CcdA

Chain A: 

M1
F2
Q3
R4
I5
T6
V7
T8
V9
D10
S11
D12
S13
Y14
Q15
L16
L17
K18
A19
Y20
D21
V22
N23
I24
S25
Q26
L27
V28
S29
T30
T31
M32
Q33
E34
E35
A36
R37
R38
L39
R40
A41
E42
R43
W44
K45
V46
E47
M48
Q49
E50
G51
M52
V53
E54
V55
A56
R57
F58
I59
E60

- Molecule 3: CcdA

Chain B: 

M101
K102
Q103
R104
T105
T106
V107
T108
V109
D110
S111
D112
S113
Y114
Q115
L116
L117
K118
A119
Y120
D121
V122
N123
I124
S125
Q126
L127
V128
S129
T130
T131
M132
Q133
E134
E135
A136
R137
R138
L139
R140
A141
E142
R143
W144
K145
V146
E147
M148
Q149
E150
G151
M152
V153
E154
V155
A156
R157
F158
I159
E160

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: 


A173
T174
A175
T176
G177
T178
A179
T180
A181
C182
C183
C184
G185

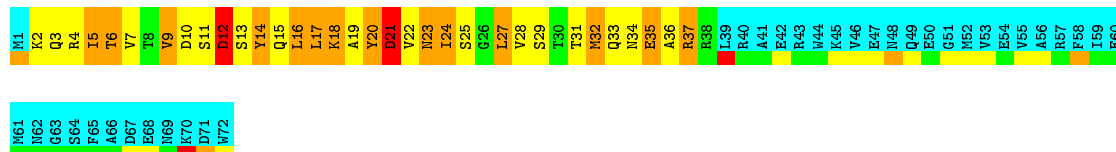
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D:  23% 77%



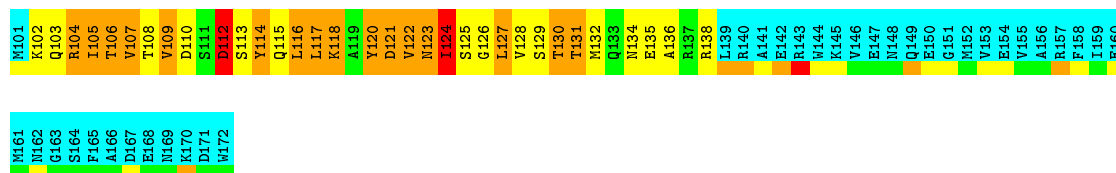
- Molecule 3: CcdA

Chain A:  6% 24% 19% 49%



- Molecule 3: CcdA

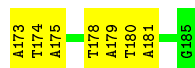
Chain B:  6% 21% 22% 49%



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% 54%




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

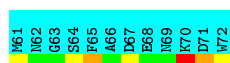
Chain D:  23% 77%



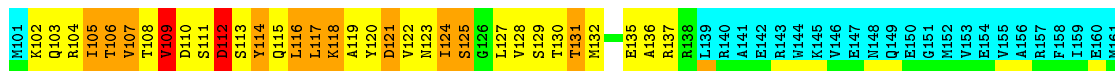
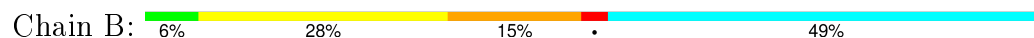
- Molecule 3: CcdA

Chain A:  7% 25% 18% 49%





• Molecule 3: CcdA

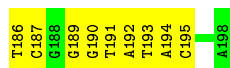


4.2.4 Score per residue for model 4

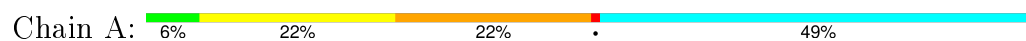
• Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'



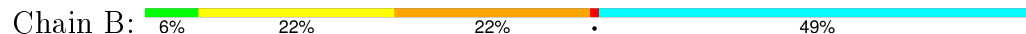
• Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'



• Molecule 3: CcdA




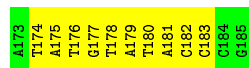
• Molecule 3: CcdA



4.2.5 Score per residue for model 5

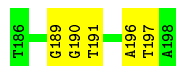
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 



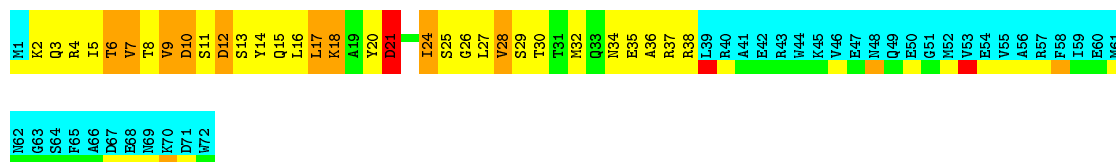
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 




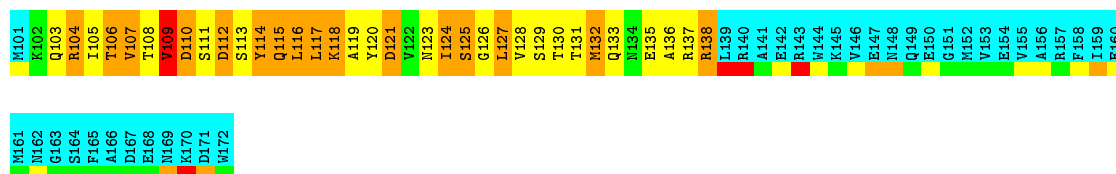
- Molecule 3: CcdA

Chain A: 



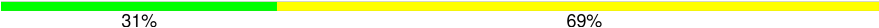
- Molecule 3: CcdA

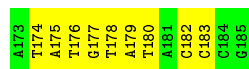
Chain B: 



4.2.6 Score per residue for model 6

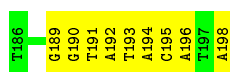
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 

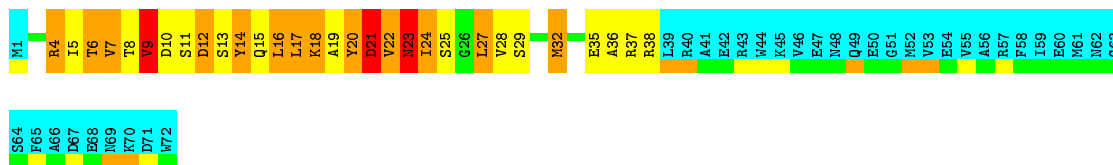
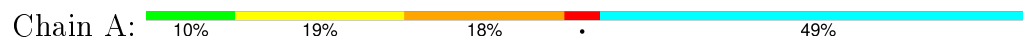


- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

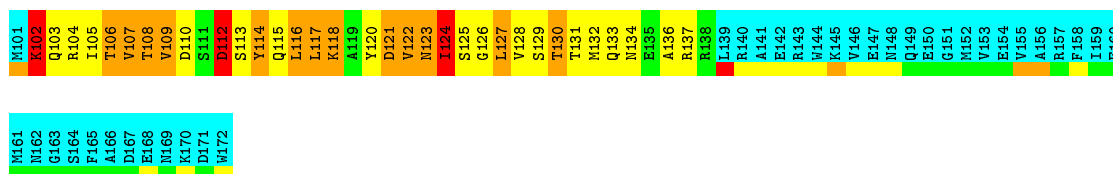
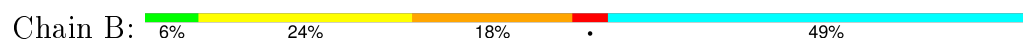
Chain D: 



- Molecule 3: CcdA

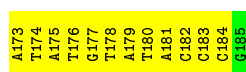


- Molecule 3: CcdA

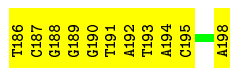


4.2.7 Score per residue for model 7

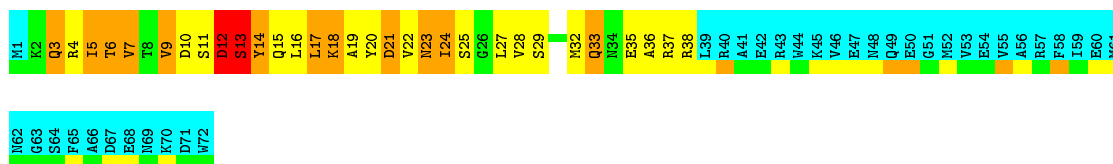
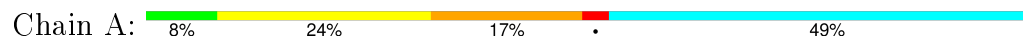
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'




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

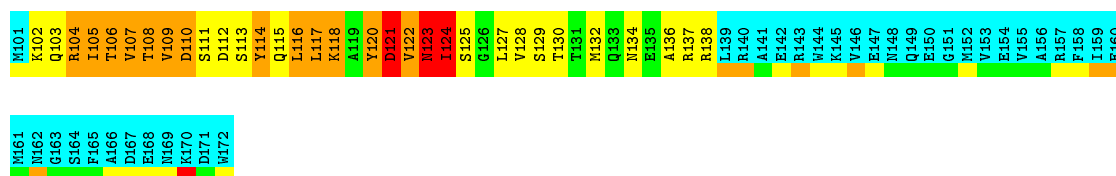


- Molecule 3: CcdA



- Molecule 3: CcdA

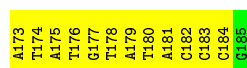
Chain B: 



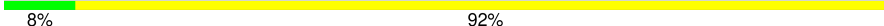
4.2.8 Score per residue for model 8

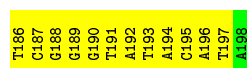
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 




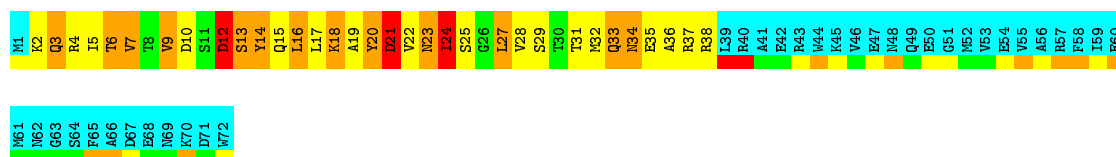
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 



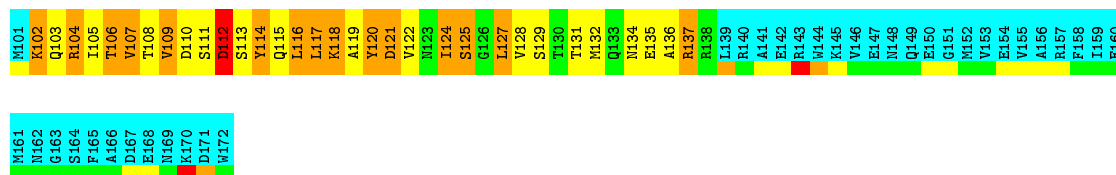
- Molecule 3: CcdA

Chain A: 



- Molecule 3: CcdA

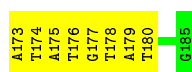
Chain B: 



4.2.9 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: 



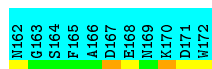
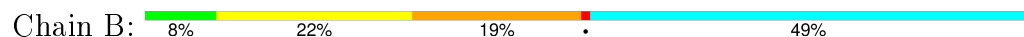
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'



- Molecule 3: CcdA

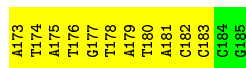


- Molecule 3: CcdA

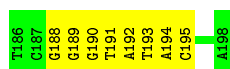


4.2.10 Score per residue for model 10

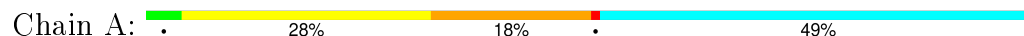
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

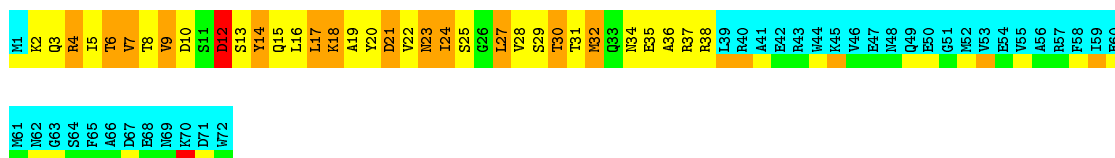


- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'



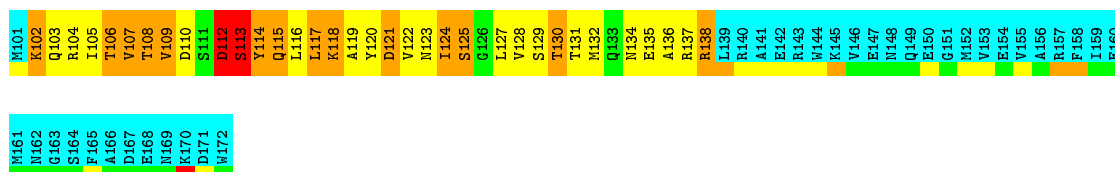
- Molecule 3: CcdA





• Molecule 3: CcdA

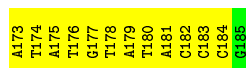
Chain B: . 25% 19% . 49%



4.2.11 Score per residue for model 11

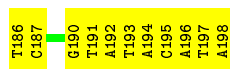
• Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 8% 92%



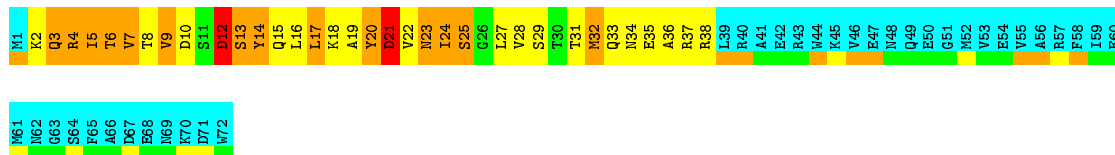
• Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 15% 85%



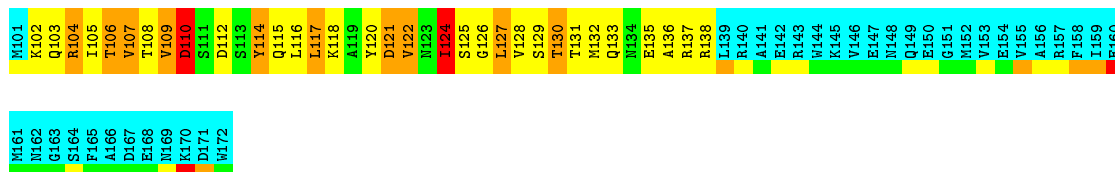
• Molecule 3: CcdA

Chain A: . 25% 19% . 49%




• Molecule 3: CcdA

Chain B: 7% 28% 14% . 49%



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: 

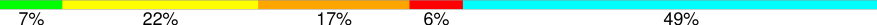
A173
T174
A175
T176
G177
T178
A179
T180
A181
C182
C183
C184
G185

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

Chain D: 


T186
C187
G188
G189
G190
T191
A192
T193
A194
C195
A196
T197
A198

- Molecule 3: CcdA

Chain A: 

M1
R2
Q3
R4
I5
T6
V7
T8
V9
D10
S11
D12
S13
Y14
Q15
L16
L17
K18
A19
Y20
D21
V22
N23
I24
S25
G26
L27
V28
S29
T30
T31
R32
Q33
N34
E35
A36
R37
R38
L39
R40
A41
E42
R43
R44
K45
V46
E47
N48
Q49
E50
G51
M52
V53
V54
V55
A56
R57
F58
T59
E60
M61
M62
G63
S64
F65
A66
D67
E68
M69
K70
D71
W72

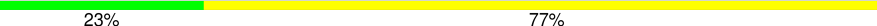
- Molecule 3: CcdA

Chain B: 

M01
K02
Q03
R04
I05
T06
V07
T08
V09
D10
S11
D12
S13
Y14
Q15
L16
L17
K18
A19
Y20
D21
I24
S125
G126
L127
V128
S129
T130
T131
M132
Q133
M134
E135
A136
R137
R138
L139
R140
A141
E142
R143
M144
K145
V146
E147
M148
Q149
E150
G151
M152
V153
V154
V155
A156
R157
F158
T159
E160
M161
M162
G163
S164
F165
A166
D167
E168
M169
D170
M171
M172

4.2.13 Score per residue for model 13

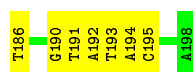
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 

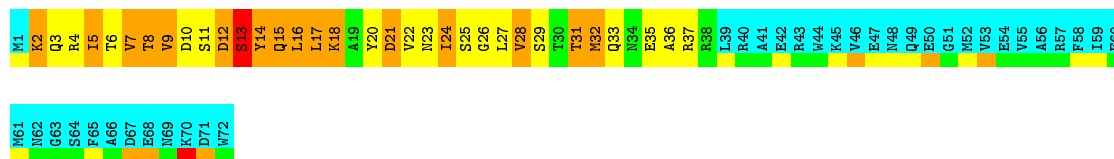
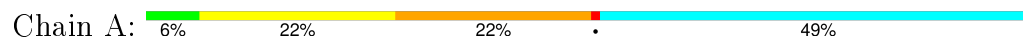
A173
T174
A175
T176
G177
T178
A179
T180
A181
C182
G185

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

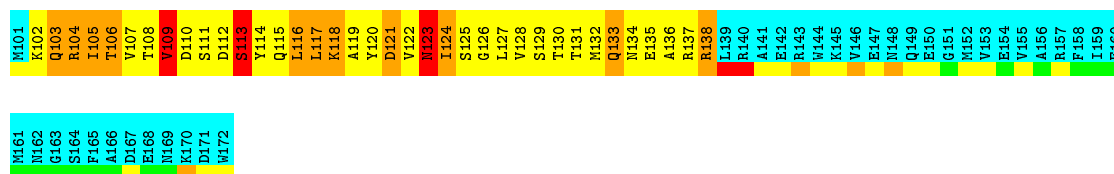
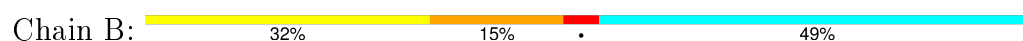
Chain D: 



• Molecule 3: CcdA

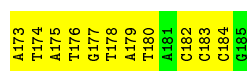
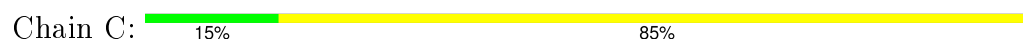


• Molecule 3: CcdA



4.2.14 Score per residue for model 14

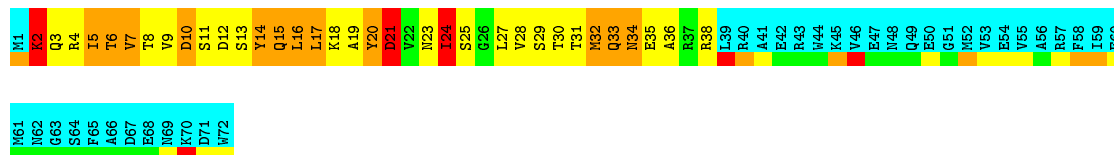
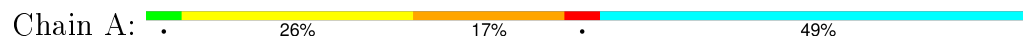
• Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'




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

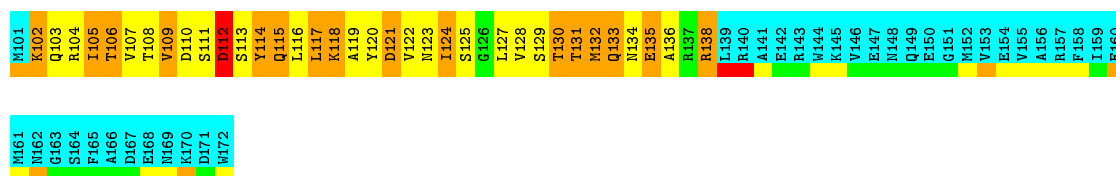


• Molecule 3: CcdA



• Molecule 3: CcdA

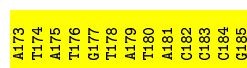
Chain B: 



4.2.15 Score per residue for model 15

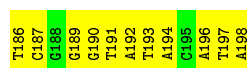
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 



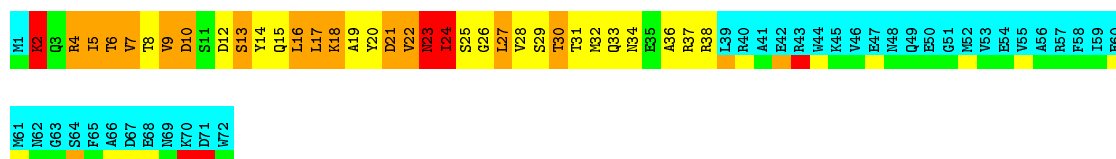
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 



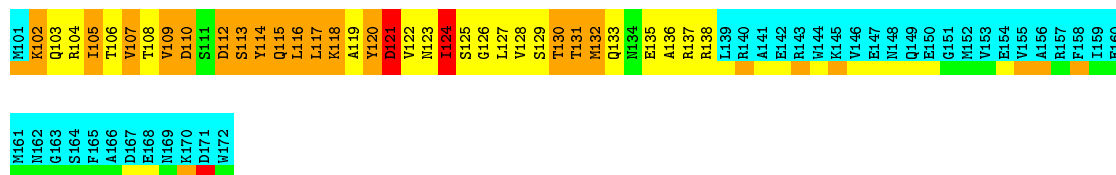
- Molecule 3: CcdA

Chain A: 



- Molecule 3: CcdA

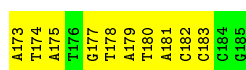
Chain B: 



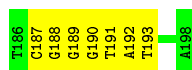
4.2.16 Score per residue for model 16

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

Chain C: 



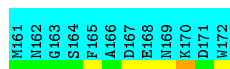
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'



- Molecule 3: CcdA

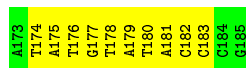


- Molecule 3: CcdA

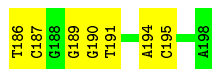


4.2.17 Score per residue for model 17

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

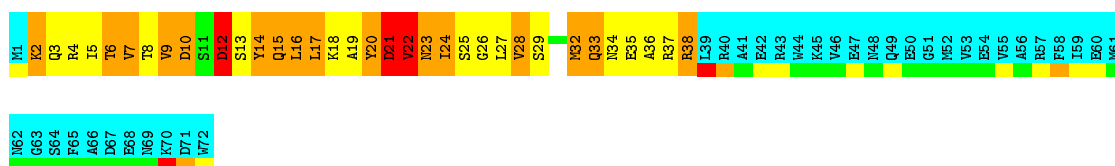


- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'



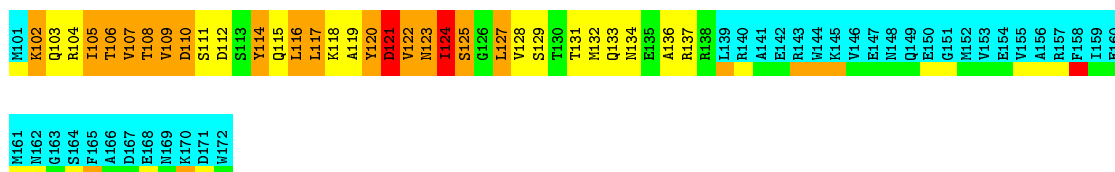
- Molecule 3: CcdA





- Molecule 3: CcdA

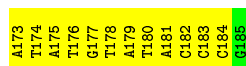
Chain B: 7% 21% 21% • 49%



4.2.18 Score per residue for model 18

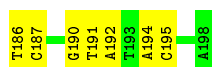
- Molecule 1: 5'-D(P*AP*TP*AP*TP*GP*TP*AP*TP*AP*CP*CP*CP*G)-3'

Chain C: 8% 92%



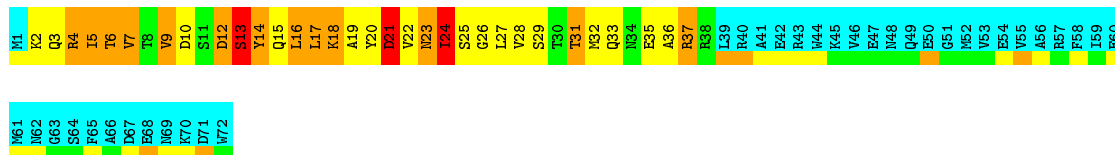
- Molecule 2: 5'-D(P*TP*CP*GP*GP*GP*TP*AP*TP*AP*CP*AP*TP*A)-3'

Chain D: 46% 54%



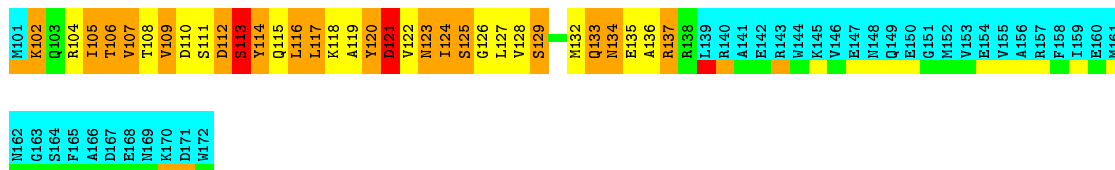
- Molecule 3: CcdA

Chain A: 7% 22% 18% • 49%




- Molecule 3: CcdA

Chain B: 6% 19% 24% • 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% 85%

A173
T174
A175
T176
G177
T178
A179
T180
A181
C182
C183
C184
G185

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

Chain D:  8% 92%

T186
C187
G188
G189
G190
T191
A192
T193
A194
C195
A196
T197
A198

- Molecule 3: CcdA

Chain A:  24% 21% 49%

M1
K2
Q3
R4
T5
T6
V7
T8
V9
D10
S11
D12
S13
Y14
Q15
L16
L17
K18
A19
Y20
D21
V22
N23
I24
S25
G26
L27
V28
S29
T30
T31
T32
Q33
N34
E35
A36
R37
R38
L39
R40
A41
E42
R43
R44
K45
V46
E47
N48
Q49
E50
G51
M52
V53
E54
V55
A56
R57
F58
I59
E60

M61
M62
G63
S64
F65
A66
D67
E68
M69
K70
D71
W72

- Molecule 3: CcdA

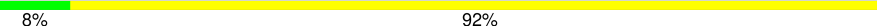
Chain B:  21% 24% 49%

M101
K102
Q103
R104
T105
T106
V107
T108
V109
D110
S111
D112
S113
Y114
Q115
L116
L117
K118
A119
Y120
D121
V122
N123
I124
S125
G126
L127
V128
S129
T130
T131
M132
Q133
N134
E135
A136
R137
R138
L139
R140
A141
E142
R143
R144
K145
V146
E147
N148
Q149
E150
G151
M152
V153
E154
V155
A156
R157
F158
I159
E160

M161
M162
G163
S164
F165
A166
D167
E168
M169
K170
D171
W172

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% 92%

A173
T174
A175
T176
G177
T178
A179
T180
A181
C182
C183
C184
G185

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

Chain D:  15% 85%

T186	C187	G188	G189	G190	T191	A192	T193	A194	C195	A196	T197	A198
------	------	------	------	------	------	------	------	------	------	------	------	------

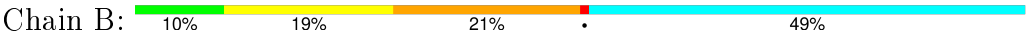
● Molecule 3: CcdA



M1	K2	Q3	R4	I5	T6	M69	K70	D71	T8	V9	D10	S11	D12	S13	Y14	Q15	L16	L17	Y20	D21	V22	N23	I24	S25	G26	L27	V28	S29	M32	E35	A36	R37	R38	L39	R40	A41	E42	R43	W44	K45	V46	E47	N48	Q49	E50	G51	M52	V53	E54	V55	A56	R57	F58	I59	E60	M61	N62	G63
----	----	----	----	----	----	-----	-----	-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

S64	F65	A66	D67	E68	M69	K70	D71	W72
-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 3: CcdA



M101	K102	Q103	R104	I105	T106	V107	T108	V109	D110	S111	D112	S113	Y114	Q115	L116	L117	K118	A119	Y120	D121	V122	N123	I124	S125	G126	L127	V128	S129	T130	T131	M132	Q133	M134	E135	A136	L139	R140	A141	E142	R143	E144	M145	K146	V147	E148	M149	Q149	E150	G151	M152	V153	E154	V155	A156	R157	F158	I159	E160	M161
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

M162	G163	S164	F165	A166	D167	E168	M169	K170	D171	W172
------	------	------	------	------	------	------	------	------	------	------

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	C	266	149	148	21±7
2	D	269	149	148	13±4
3	A	293	298	298	126±10
3	B	293	298	298	126±10
All	All	22420	17880	17840	3951

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 98.

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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:5:ILE:HG21	3:B:114:TYR:CE1	1.00	1.92	7	14
3:A:28:VAL:CG2	3:B:128:VAL:HG22	1.00	1.87	15	8
3:A:24:ILE:HG21	3:B:132:MET:HE3	0.99	1.34	11	3
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:32:MET:HE2	3:B:124:ILE:HG23	0.96	1.37	4	9
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
3:A:35:GLU:HB3	3:B:117:LEU:HD21	0.93	1.36	5	11
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:24:ILE:HG23	3:B:132:MET:HE2	0.91	1.40	5	8
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: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	3
3:A:28:VAL:HG12	3:A:32:MET:SD	0.87	2.09	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:124:ILE:CG2	3:B:127:LEU:HD12	0.86	2.00	18	2
3:B:128:VAL:HG13	3:B:132:MET:SD	0.86	2.10	19	4
3:A:9:VAL:HG21	3:A:14:TYR:HB3	0.85	1.44	3	7
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:A:28:VAL:HG13	3:A:32:MET:HE2	0.84	1.45	9	2
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:25:SER:HA	3:B:107:VAL:HG22	0.84	1.50	18	5
3:A:5:ILE:HG13	3:B:124:ILE:HD11	0.84	1.50	7	4
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
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:B:128:VAL:HG13	3:B:132:MET:HE3	0.83	1.49	4	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:32:MET:HE2	3:B:124:ILE:HG21	0.82	1.51	18	1
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: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:36:ALA:HB1	3:B:116:LEU:HB3	0.80	1.52	7	6
3:A:32:MET:SD	3:B:114:TYR:HA	0.80	2.16	16	13
1:C:173:DA:H2"	1:C:174:DT:O5'	0.80	1.75	11	2
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:B:109:VAL:HG11	3:B:114:TYR:HB2	0.80	1.52	15	8
3:A:4:ARG:HG3	3:B:108:THR:CG2	0.80	2.07	7	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:32:MET:HE1	3:B:124:ILE:CG1	0.79	2.08	1	6
3:B:109:VAL:HG11	3:B:114:TYR:HB3	0.79	1.53	4	7
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:32:MET:HE3	3:B:124:ILE:HG12	0.78	1.52	15	1
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:HD12	3:A:24:ILE:N	0.78	1.94	2	6
3:B:128:VAL:CG1	3:B:132:MET:SD	0.78	2.72	9	4
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
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:32:MET:CE	3:B:124:ILE:HG21	0.76	2.10	13	1
3:A:5:ILE:HD13	3:B:107:VAL:HG13	0.76	1.56	4	1
3:A:23:ASN:C	3:A:24:ILE:HD12	0.76	2.02	12	7
3:A:28:VAL:CG1	3:A:32:MET:SD	0.76	2.73	16	4
3:B:124:ILE:N	3:B:124:ILE:HD12	0.75	1.97	2	10
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: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:B:124:ILE:HD12	3:B:124:ILE:N	0.74	1.97	12	5
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:17:LEU:HG	3:B:132:MET:SD	0.74	2.22	2	4
3:A:6:THR:HA	3:B:105:ILE:O	0.74	1.83	15	19
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	1.56	16	3
3:A:24:ILE:HG23	3:B:132:MET:HE3	0.74	1.59	9	2
3:B:107:VAL:HG13	3:B:109:VAL:HG13	0.74	1.59	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:24:ILE:HD13	3:A:28:VAL:HG21	0.74	1.58	1	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	6
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: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:17:LEU:HD12	3:A:24:ILE:HG23	0.72	1.59	13	1
1:C:174:DT:H2''	1:C:175:DA:O5'	0.72	1.84	10	9
3:A:24:ILE:CG2	3:A:27:LEU:HD12	0.72	2.13	13	4
3:A:24:ILE:CG2	3:B:132:MET:SD	0.72	2.76	7	2
3:A:5:ILE:HG12	3:B:107:VAL:HG13	0.72	1.61	1	10
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: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:16:LEU:HD22	3:B:136:ALA:HB1	0.72	1.60	7	7
3:A:24:ILE:N	3:A:24:ILE:HD12	0.72	2.00	8	4
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:114:TYR:CZ	3:B:118:LYS:HD3	0.71	2.20	19	12
3:B:107:VAL:HG22	3:B:109:VAL:HG22	0.71	1.62	17	5
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	7
3:A:29:SER:CB	3:B:112:ASP:HB3	0.71	2.14	3	14
3:A:28:VAL:HG13	3:B:124:ILE:HG21	0.71	1.62	1	3
3:B:123:ASN:C	3:B:124:ILE:HD12	0.71	2.06	16	3
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:HG22	3:A:27:LEU:HD12	0.71	1.63	13	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:5:ILE:HG21	3:B:114:TYR:CG	0.70	2.21	1	8
3:A:32:MET:HE3	3:B:124:ILE:CG1	0.70	2.16	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:MET:CE	3:B:124:ILE:HG12	0.70	2.16	18	2
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	4
3:A:5:ILE:HG21	3:B:114:TYR:CE2	0.70	2.22	6	5
3:A:36:ALA:HB1	3:B:116:LEU:HD22	0.70	1.62	3	9
3:A:32:MET:HE1	3:B:124:ILE:HG23	0.70	1.62	20	5
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
3:B:104:ARG:NH2	3:B:106:THR:HG21	0.69	2.01	12	4
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
1:C:174:DT:H2'	1:C:175:DA:C8	0.69	2.23	16	9
3:B:105:ILE:HD11	3:B:128:VAL:HG11	0.69	1.64	5	8
3:A:9:VAL:HG21	3:A:14:TYR:CG	0.69	2.23	18	7
3:B:117:LEU:HD13	3:B:120:TYR:CE2	0.69	2.23	16	3
3:B:122:VAL:HG13	3:B:122:VAL:O	0.69	1.87	20	2
3:A:6:THR:HB	3:B:106:THR:CB	0.69	2.18	11	15
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:9:VAL:CG2	3:B:105:ILE:HD12	0.69	2.17	4	1
3:B:124:ILE:H	3:B:124:ILE:HD12	0.68	1.47	4	9
3:A:24:ILE:HG13	3:B:132:MET:HE1	0.68	1.65	15	7
1:C:174:DT:H2''	1:C:175:DA:C8	0.68	2.23	17	16
3:A:32:MET:HE1	3:B:123:ASN:O	0.68	1.88	7	4
3:A:36:ALA:CB	3:B:116:LEU:HB3	0.68	2.18	7	8
3:A:29:SER:HB2	3:B:112:ASP:CB	0.68	2.19	15	7
3:A:17:LEU:HD22	3:A:22:VAL:CG1	0.68	2.18	15	2
3:B:124:ILE:HG23	3:B:127:LEU:HD23	0.68	1.64	9	3
2:D:191:DT:H72	3:B:106:THR:OG1	0.68	1.88	10	4
3:A:5:ILE:HG23	3:B:107:VAL:O	0.68	1.89	13	2
1:C:173:DA:C3'	1:C:174:DT:H5''	0.68	2.19	15	5
3:A:10:ASP:HB2	3:B:103:GLN:HB3	0.68	1.64	14	6
3:B:105:ILE:HG13	3:B:105:ILE:O	0.68	1.87	11	4
1:C:173:DA:H1'	1:C:174:DT:O4'	0.68	1.88	11	1
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:A:24:ILE:HG22	3:A:27:LEU:CB	0.67	2.18	7	2
3:B:128:VAL:O	3:B:132:MET:HG2	0.67	1.89	12	10
3:A:12:ASP:HB3	3:B:129:SER:HB3	0.67	1.66	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:9:VAL:HG23	3:A:12:ASP:HB2	0.67	1.64	9	2
3:A:32:MET:HE3	3:B:124:ILE:HG23	0.67	1.66	11	4
3:A:32:MET:SD	3:B:127:LEU:HD22	0.67	2.30	3	1
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
3:A:24:ILE:HG12	3:B:132:MET:HE3	0.67	1.66	13	2
3:B:124:ILE:HD12	3:B:124:ILE:H	0.67	1.50	14	4
3:A:29:SER:HB2	3:B:112:ASP:HB3	0.67	1.67	15	7
3:A:32:MET:HE1	3:B:124:ILE:HG13	0.67	1.66	20	8
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: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:B:107:VAL:HG12	3:B:107:VAL:O	0.66	1.90	13	3
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: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: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:35:GLU:CG	3:B:127:LEU:HD13	0.66	2.21	9	1
3:A:24:ILE:HD12	3:A:24:ILE:H	0.66	1.48	2	7
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	3
3:A:24:ILE:HG12	3:B:105:ILE:HD12	0.66	1.66	20	7
3:B:122:VAL:O	3:B:122:VAL:HG13	0.66	1.91	16	1
3:A:28:VAL:CG2	3:B:128:VAL:CG2	0.66	2.74	5	8
3:A:29:SER:CB	3:B:112:ASP:CB	0.66	2.74	14	9
3:A:6:THR:HG21	3:B:104:ARG:NH1	0.66	2.05	17	3
3:A:4:ARG:CG	3:B:108:THR:HG22	0.66	2.20	7	7
1:C:179:DA:H2''	1:C:180:DT:O5'	0.66	1.88	7	9
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:LEU:HD22	3:A:22:VAL:HB	0.66	1.68	3	2
3:A:23:ASN:O	3:B:132:MET:HE3	0.66	1.91	15	1
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:32:MET:HE3	3:B:124:ILE:CG2	0.65	2.21	11	2
3:A:24:ILE:HG23	3:A:27:LEU:HD23	0.65	1.68	4	4
3:B:129:SER:HA	3:B:132:MET:SD	0.65	2.31	11	2
3:B:120:TYR:O	3:B:121:ASP:HB2	0.65	1.91	2	16
3:A:17:LEU:HB2	3:B:132:MET:HG2	0.65	1.66	19	2
3:A:14:TYR:CD2	3:B:105:ILE:HG13	0.65	2.27	2	1
3:B:117:LEU:HD12	3:B:122:VAL:HG11	0.65	1.66	19	1
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:A:24:ILE:HG22	3:A:27:LEU:CG	0.65	2.20	7	3
1:C:173:DA:C2'	1:C:174:DT:H5''	0.65	2.21	14	8
3:A:28:VAL:HB	3:B:107:VAL:HG21	0.65	1.68	18	3
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:CG2	3:A:27:LEU:HB3	0.65	2.22	16	8
3:A:4:ARG:NH1	3:B:108:THR:CG2	0.65	2.59	20	2
3:A:14:TYR:CE1	3:B:105:ILE:HB	0.65	2.26	20	2
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:A:4:ARG:CB	3:B:108:THR:HG22	0.64	2.22	7	1
3:A:17:LEU:HD22	3:A:22:VAL:HG11	0.64	1.67	13	1
3:A:17:LEU:CD2	3:A:27:LEU:HD22	0.64	2.22	9	1
3:A:24:ILE:CG1	3:B:132:MET:HE1	0.64	2.22	15	3
1:C:181:DA:C2	2:D:192:DA:C2	0.64	2.86	10	2
3:A:17:LEU:HD23	3:B:132:MET:HA	0.64	1.69	14	3
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:9:VAL:O	3:A:10:ASP:HB3	0.64	1.92	8	11
3:B:132:MET:O	3:B:136:ALA:N	0.64	2.30	11	19
3:B:109:VAL:HG12	3:B:112:ASP:HB2	0.64	1.68	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:35:GLU:HB3	3:B:117:LEU:HD11	0.64	1.69	7	1
1:C:178:DT:H72	3:A:6:THR:CG2	0.64	2.22	14	12
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	8
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
3:A:7:VAL:HG12	3:A:7:VAL:O	0.63	1.93	20	3
2:D:191:DT:H2'	2:D:192:DA:N7	0.63	2.09	19	3
3:A:5:ILE:HG12	3:B:124:ILE:HD11	0.63	1.67	7	3
3:B:127:LEU:O	3:B:131:THR:HB	0.63	1.94	2	6
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:B:109:VAL:O	3:B:110:ASP:CB	0.63	2.47	16	16
3:A:6:THR:OG1	3:B:104:ARG:HG2	0.63	1.94	4	11
3:B:107:VAL:CG2	3:B:109:VAL:HB	0.63	2.24	11	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:117:LEU:HG	3:B:127:LEU:HD12	0.63	1.70	14	4
3:B:105:ILE:CD1	3:B:128:VAL:HG11	0.63	2.24	20	3
3:B:109:VAL:O	3:B:110:ASP:HB3	0.63	1.94	10	8
3:A:14:TYR:CZ	3:B:105:ILE:HG22	0.63	2.28	3	2
1:C:180:DT:H71	3:A:4:ARG:HD2	0.63	1.71	12	3
3:A:24:ILE:HG21	3:B:132:MET:HE2	0.62	1.70	1	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: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:32:MET:HE2	3:B:124:ILE:CG2	0.62	2.23	18	5
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:10:ASP:HB3	3:B:102:LYS:HA	0.62	1.71	17	3
3:A:20:TYR:CD1	3:A:21:ASP:N	0.62	2.68	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:109:VAL:CG2	3:B:114:TYR:CD1	0.62	2.79	6	3
3:A:24:ILE:CG2	3:B:132:MET:HE2	0.62	2.25	3	9
3:A:24:ILE:H	3:A:24:ILE:HD12	0.62	1.55	6	1
3:A:20:TYR:O	3:A:21:ASP:HB3	0.61	1.95	13	2
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:7:VAL:HG13	3:B:105:ILE:CG1	0.61	2.25	18	11
3:A:6:THR:CA	3:B:105:ILE:O	0.61	2.47	12	9
3:A:32:MET:CE	3:B:124:ILE:CG1	0.61	2.78	18	6
3:A:29:SER:HA	3:A:32:MET:SD	0.61	2.34	1	1
3:A:32:MET:O	3:A:36:ALA:N	0.61	2.34	5	19
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: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: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: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:O	3:A:7:VAL:HG12	0.61	1.95	14	2
3:B:117:LEU:HD13	3:B:122:VAL:HB	0.61	1.73	14	1
3:A:17:LEU:CD1	3:A:24:ILE:HG23	0.61	2.26	13	1
3:A:9:VAL:HG22	3:A:10:ASP:N	0.61	2.11	19	5
3:A:29:SER:O	3:B:113:SER:HB2	0.61	1.96	13	2
3:B:109:VAL:CB	3:B:114:TYR:HB3	0.61	2.26	2	10
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
1:C:173:DA:C3'	1:C:174:DT:C5'	0.60	2.80	12	3
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
3:A:24:ILE:CG2	3:B:132:MET:HE1	0.60	2.27	15	1
3:A:24:ILE:HG12	3:B:128:VAL:HG13	0.60	1.73	15	1
3:A:32:MET:CE	3:B:124:ILE:HG23	0.60	2.26	20	10
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:115:GLN:HA	3:B:118:LYS:HE2	0.60	1.74	9	5
3:A:13:SER:HB3	3:B:133:GLN:HB3	0.60	1.74	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:109:VAL:CG2	3:B:114:TYR:HB3	0.60	2.27	14	4
3:A:17:LEU:HD13	3:A:20:TYR:CE2	0.60	2.32	11	5
3:B:104:ARG:HB3	3:B:104:ARG:NH1	0.60	2.11	1	1
3:A:10:ASP:CB	3:B:102:LYS:HA	0.60	2.27	17	3
3:A:17:LEU:HG	3:B:132:MET:HG3	0.60	1.72	19	1
3:A:9:VAL:CG2	3:A:14:TYR:CD1	0.60	2.74	10	3
3:A:23:ASN:O	3:A:24:ILE:CD1	0.60	2.49	1	1
1:C:180:DT:H73	3:A:4:ARG:HD2	0.60	1.73	11	2
3:B:124:ILE:CG2	3:B:127:LEU:HB3	0.60	2.24	2	7
3:B:127:LEU:C	3:B:127:LEU:HD23	0.60	2.17	4	2
3:A:24:ILE:CG2	3:B:132:MET:HE3	0.60	2.26	13	2
3:A:3:GLN:N	3:B:110:ASP:HB2	0.60	2.12	18	4
3:B:107:VAL:O	3:B:107:VAL:HG12	0.60	1.97	7	2
3:A:5:ILE:HD11	3:A:28:VAL:HG11	0.59	1.74	8	9
1:C:177:DG:P	3:B:125:SER:HB3	0.59	2.36	7	3
3:B:109:VAL:HG22	3:B:110:ASP:H	0.59	1.55	11	3
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
3:A:17:LEU:CD1	3:A:22:VAL:HB	0.59	2.28	19	1
3:B:105:ILE:HD13	3:B:128:VAL:HG11	0.59	1.74	20	2
3:B:107:VAL:O	3:B:107:VAL:CG1	0.59	2.51	13	2
3:B:105:ILE:O	3:B:105:ILE:HG13	0.59	1.96	19	5
3:A:32:MET:SD	3:B:117:LEU:HG	0.59	2.37	5	2
1:C:178:DT:OP2	3:A:5:ILE:HA	0.59	1.98	11	2
3:A:7:VAL:CG1	3:A:7:VAL:O	0.59	2.50	14	2
1:C:175:DA:C8	1:C:176:DT:C7	0.59	2.86	9	2
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
3:B:128:VAL:O	3:B:131:THR:HG22	0.59	1.97	17	1
3:A:5:ILE:HD12	3:B:114:TYR:CD1	0.59	2.32	14	3
3:A:9:VAL:CG2	3:A:12:ASP:CB	0.59	2.80	1	1
1:C:173:DA:H3'	1:C:174:DT:C5'	0.59	2.27	12	2
3:B:115:GLN:O	3:B:118:LYS:HG3	0.59	1.98	19	14
3:A:14:TYR:CZ	3:A:18:LYS:HD3	0.59	2.32	14	11
3:A:24:ILE:HG22	3:A:27:LEU:CD1	0.59	2.27	13	3
3:A:31:THR:HG21	3:B:131:THR:HG21	0.59	1.75	19	2
3:A:24:ILE:CG2	3:A:27:LEU:HD23	0.59	2.27	4	5
3:A:10:ASP:HB2	3:B:102:LYS:HA	0.59	1.75	12	2
3:A:9:VAL:HG21	3:A:12:ASP:HB3	0.59	1.75	1	1
2:D:190:DG:N7	2:D:191:DT:H72	0.59	2.12	6	1
3:A:14:TYR:CE2	3:A:18:LYS:HD3	0.59	2.32	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:7:VAL:CG1	3:A:9:VAL:HB	0.59	2.28	15	1
3:A:22:VAL:HG13	3:A:22:VAL:O	0.58	1.98	1	3
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:A:17:LEU:CD1	3:B:132:MET:SD	0.58	2.88	10	1
3:B:107:VAL:HG22	3:B:109:VAL:CG2	0.58	2.27	1	1
3:B:120:TYR:O	3:B:121:ASP:CB	0.58	2.51	10	20
3:A:14:TYR:HA	3:B:132:MET:CG	0.58	2.28	15	2
1:C:179:DA:H62	3:B:104:ARG:NE	0.58	1.96	6	2
3:A:29:SER:CB	3:B:112:ASP:O	0.58	2.51	12	6
3:A:28:VAL:HG13	3:A:32:MET:HE1	0.58	1.75	13	1
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
3:A:20:TYR:CD1	3:A:20:TYR:C	0.58	2.77	3	2
1:C:184:DC:H2"	1:C:185:DG:H5'	0.58	1.76	15	1
3:A:24:ILE:CG2	3:B:132:MET:CE	0.58	2.80	19	8
3:A:29:SER:HB2	3:B:112:ASP:O	0.58	1.98	20	6
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:HG22	3:B:107:VAL:O	0.58	1.98	4	3
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:A:24:ILE:HG12	3:B:132:MET:HE2	0.57	1.75	7	5
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
3:A:17:LEU:HD12	3:B:132:MET:HG2	0.57	1.75	13	1
3:A:9:VAL:HG23	3:A:10:ASP:N	0.57	2.14	18	3
3:A:3:GLN:HB3	3:B:110:ASP:HB2	0.57	1.75	4	5
1:C:183:DC:H2"	1:C:184:DC:C6	0.57	2.34	12	7
1:C:177:DG:OP2	3:A:7:VAL:HA	0.57	1.99	20	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:6:THR:HB	3:B:106:THR:CA	0.57	2.28	4	3
3:B:117:LEU:HD12	3:B:122:VAL:HG13	0.57	1.75	9	2
3:A:24:ILE:HB	3:A:28:VAL:CG2	0.57	2.27	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:124:ILE:HG22	3:B:127:LEU:HD22	0.57	1.76	4	1
3:A:16:LEU:CB	3:B:136:ALA:HB1	0.57	2.30	2	7
3:A:7:VAL:CG2	3:A:9:VAL:HB	0.57	2.30	5	3
3:A:17:LEU:CD1	3:A:27:LEU:HD11	0.57	2.29	3	1
3:A:24:ILE:HG23	3:B:132:MET:CE	0.57	2.29	4	8
3:B:117:LEU:HD11	3:B:127:LEU:HG	0.57	1.75	17	1
3:B:122:VAL:O	3:B:122:VAL:CG1	0.57	2.52	16	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:A:17:LEU:HD12	3:A:20:TYR:CE1	0.57	2.34	8	1
3:B:109:VAL:HG13	3:B:112:ASP:HB2	0.57	1.77	3	2
3:A:5:ILE:HG13	3:A:5:ILE:O	0.57	1.98	13	3
3:A:24:ILE:HG13	3:B:132:MET:HE2	0.57	1.77	2	1
2:D:186:DT:H72	2:D:187:DC:C5	0.56	2.35	7	1
2:D:190:DG:C8	2:D:191:DT:C7	0.56	2.88	4	2
3:A:7:VAL:HG12	3:A:9:VAL:HG22	0.56	1.75	20	1
3:A:9:VAL:CB	3:A:14:TYR:HB3	0.56	2.31	6	8
3:B:124:ILE:CG2	3:B:127:LEU:HD23	0.56	2.29	9	4
3:B:105:ILE:HG22	3:B:105:ILE:O	0.56	1.99	2	2
2:D:191:DT:H71	3:B:106:THR:OG1	0.56	1.99	2	1
3:A:31:THR:HG22	3:B:127:LEU:HD11	0.56	1.75	9	3
1:C:173:DA:H1'	1:C:174:DT:H73	0.56	1.76	10	1
2:D:193:DT:O4	3:B:104:ARG:HD2	0.56	2.00	8	5
3:B:107:VAL:CG2	3:B:109:VAL:HG22	0.56	2.30	17	3
3:A:17:LEU:HG	3:A:20:TYR:CE2	0.56	2.35	9	1
2:D:190:DG:C5	2:D:191:DT:C4	0.56	2.93	1	2
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:117:LEU:HD22	3:B:127:LEU:HD22	0.56	1.77	7	1
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:107:VAL:HG22	3:B:109:VAL:CG1	0.56	2.31	15	6
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
3:A:32:MET:CG	3:B:114:TYR:HA	0.56	2.31	16	7
3:A:9:VAL:HG13	3:A:10:ASP:N	0.56	2.16	1	1
3:A:10:ASP:HB2	3:B:103:GLN:HB2	0.56	1.78	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:22:VAL:CG1	3:A:22:VAL:O	0.56	2.54	17	4
3:B:115:GLN:HA	3:B:118:LYS:CE	0.56	2.31	9	1
3:A:12:ASP:O	3:B:129:SER:HA	0.56	2.01	12	3
3:A:24:ILE:HG23	3:B:132:MET:HE1	0.56	1.77	10	3
3:A:6:THR:OG1	3:B:104:ARG:HG3	0.56	2.01	12	3
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:35:GLU:HB3	3:B:117:LEU:CD2	0.56	2.31	8	1
3:A:24:ILE:CG1	3:B:105:ILE:HD12	0.56	2.31	9	5
3:A:9:VAL:CG2	3:A:14:TYR:CD2	0.56	2.73	11	2
3:A:12:ASP:HB2	3:B:129:SER:OG	0.55	2.00	18	2
3:A:28:VAL:CG2	3:B:128:VAL:HG21	0.55	2.27	16	1
3:A:9:VAL:N	3:B:103:GLN:O	0.55	2.40	2	6
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: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:25:SER:HA	3:B:107:VAL:HB	0.55	1.77	1	1
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:A:17:LEU:HD23	3:B:132:MET:CA	0.55	2.32	12	5
3:B:109:VAL:HG22	3:B:110:ASP:N	0.55	2.17	11	4
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:B:117:LEU:CD2	3:B:127:LEU:HD22	0.55	2.32	7	1
3:A:16:LEU:HD13	3:B:136:ALA:HB1	0.55	1.78	12	4
3:A:7:VAL:HG22	3:A:9:VAL:HG13	0.55	1.78	18	3
3:A:5:ILE:O	3:A:5:ILE:HG13	0.55	2.00	18	5
3:B:109:VAL:CG2	3:B:114:TYR:CB	0.55	2.84	9	6
3:A:5:ILE:CG2	3:B:114:TYR:CE1	0.55	2.88	12	9
1:C:179:DA:C2	1:C:180:DT:C2	0.55	2.95	15	9
3:B:114:TYR:CZ	3:B:118:LYS:HG2	0.55	2.36	2	3
1:C:178:DT:C7	3:A:6:THR:HG23	0.55	2.32	16	5
3:B:107:VAL:O	3:B:109:VAL:HG13	0.55	2.01	6	2
3:B:117:LEU:CD1	3:B:127:LEU:HD12	0.55	2.31	15	6
3:B:105:ILE:HG21	3:B:128:VAL:HG11	0.55	1.79	15	1
3:A:32:MET:SD	3:B:124:ILE:HG21	0.55	2.42	13	1
3:A:4:ARG:CG	3:B:106:THR:OG1	0.55	2.55	7	4
3:A:5:ILE:CD1	3:B:114:TYR:CD2	0.55	2.86	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:MET:SD	3:B:124:ILE:HG23	0.55	2.42	20	2
3:A:27:LEU:C	3:A:27:LEU:HD13	0.55	2.22	7	4
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:6:THR:HG23	3:B:106:THR:HG22	0.54	1.79	13	1
3:A:36:ALA:HB1	3:B:116:LEU:HD13	0.54	1.79	17	4
3:A:9:VAL:HG23	3:A:14:TYR:CD2	0.54	2.36	20	1
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
3:A:18:LYS:HB3	3:A:23:ASN:HA	0.54	1.79	11	3
3:B:109:VAL:HG11	3:B:114:TYR:H	0.54	1.61	10	3
1:C:173:DA:H3'	1:C:174:DT:H5''	0.54	1.80	13	4
1:C:175:DA:C5	1:C:176:DT:C4	0.54	2.96	14	12
3:B:115:GLN:O	3:B:119:ALA:N	0.54	2.40	15	11
3:B:120:TYR:CD1	3:B:121:ASP:N	0.54	2.75	16	6
3:B:122:VAL:CG1	3:B:122:VAL:O	0.54	2.54	6	2
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:A:29:SER:CB	3:B:112:ASP:HB2	0.54	2.33	20	5
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
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
1:C:173:DA:H2'	1:C:174:DT:H5''	0.54	1.80	13	2
3:B:107:VAL:HG12	3:B:109:VAL:HG12	0.54	1.79	7	1
2:D:186:DT:H72	2:D:187:DC:C6	0.54	2.37	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
3:A:32:MET:HB2	3:B:113:SER:HB2	0.54	1.79	13	2
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
1:C:174:DT:H2'	1:C:175:DA:N7	0.54	2.18	16	3
1:C:177:DG:C8	1:C:178:DT:C7	0.54	2.91	6	10
3:A:23:ASN:O	3:A:24:ILE:CG1	0.54	2.56	1	1
3:A:23:ASN:O	3:A:25:SER:N	0.53	2.42	12	9
3:A:6:THR:OG1	3:B:104:ARG:CG	0.53	2.56	11	5
3:B:117:LEU:HD22	3:B:122:VAL:CG1	0.53	2.32	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:4:ARG:HG3	3:B:106:THR:OG1	0.53	2.02	13	1
3:A:14:TYR:OH	3:A:18:LYS:HD3	0.53	2.03	14	8
3:A:7:VAL:CG2	3:A:9:VAL:HG22	0.53	2.33	16	1
3:A:24:ILE:CG1	3:B:132:MET:HE3	0.53	2.33	13	1
3:A:20:TYR:C	3:A:20:TYR:CD1	0.53	2.82	19	6
1:C:178:DT:O4	3:B:104:ARG:HD2	0.53	2.04	19	1
3:A:28:VAL:HG13	3:A:32:MET:HE3	0.53	1.78	8	3
3:A:28:VAL:CG2	3:B:124:ILE:HG21	0.53	2.28	4	2
2:D:190:DG:H2'	2:D:191:DT:H71	0.53	1.78	12	5
3:A:5:ILE:HD12	3:B:124:ILE:CD1	0.53	2.33	13	3
3:B:123:ASN:O	3:B:125:SER:N	0.53	2.42	18	5
3:A:7:VAL:HG11	3:B:128:VAL:CG1	0.53	2.33	11	2
3:A:4:ARG:HG2	3:B:106:THR:CG2	0.53	2.28	15	2
3:A:14:TYR:CD2	3:B:105:ILE:CD1	0.53	2.89	8	3
3:A:32:MET:SD	3:B:117:LEU:CG	0.53	2.97	5	2
3:A:7:VAL:HG11	3:B:128:VAL:HG11	0.53	1.79	11	3
2:D:193:DT:H2''	2:D:194:DA:C8	0.53	2.39	11	8
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:6:THR:HG23	3:B:106:THR:CG2	0.53	2.32	13	1
3:B:107:VAL:HG12	3:B:109:VAL:CG1	0.53	2.33	7	1
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:105:ILE:O	3:B:105:ILE:CG1	0.53	2.56	18	2
2:D:191:DT:C7	3:B:106:THR:HB	0.53	2.34	15	3
3:A:32:MET:CE	3:B:124:ILE:CG2	0.53	2.86	13	2
1:C:177:DG:C4	1:C:178:DT:C5	0.53	2.97	6	8
3:B:117:LEU:HD12	3:B:122:VAL:O	0.53	2.04	15	2
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:6:THR:HG21	3:B:104:ARG:HG2	0.52	1.81	13	1
3:B:107:VAL:O	3:B:109:VAL:N	0.52	2.41	4	5
3:A:14:TYR:CE2	3:B:105:ILE:CG2	0.52	2.93	19	4
3:B:127:LEU:O	3:B:131:THR:N	0.52	2.42	19	1
3:A:6:THR:HB	3:B:106:THR:HG22	0.52	1.79	5	3
3:A:17:LEU:HD23	3:B:132:MET:O	0.52	2.04	2	2
2:D:187:DC:C2'	2:D:188:DG:C8	0.52	2.91	16	2
1:C:173:DA:H3'	1:C:174:DT:H73	0.52	1.80	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:120:TYR:CD1	3:B:120:TYR:C	0.52	2.83	18	3
3:B:109:VAL:CG2	3:B:114:TYR:CG	0.52	2.87	16	4
3:A:5:ILE:O	3:A:5:ILE:HG12	0.52	2.05	14	3
3:A:24:ILE:CD1	3:A:24:ILE:N	0.52	2.67	15	4
3:A:12:ASP:O	3:B:129:SER:CB	0.52	2.57	20	5
3:A:9:VAL:HG21	3:A:12:ASP:CB	0.52	2.33	1	1
3:A:35:GLU:HG2	3:B:127:LEU:CD1	0.52	2.34	12	2
3:A:5:ILE:CG1	3:A:5:ILE:O	0.52	2.57	18	6
3:B:110:ASP:O	3:B:115:GLN:HG2	0.52	2.04	19	1
3:A:32:MET:CA	3:B:117:LEU:HD23	0.52	2.35	9	2
3:B:114:TYR:CE1	3:B:118:LYS:HD3	0.52	2.39	8	2
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:A:9:VAL:HB	3:A:14:TYR:CD2	0.52	2.39	12	1
3:A:3:GLN:O	3:B:108:THR:HA	0.52	2.05	13	4
3:A:15:GLN:HA	3:A:18:LYS:CG	0.52	2.35	7	6
3:A:15:GLN:OE1	3:A:18:LYS:NZ	0.52	2.38	1	6
3:A:8:THR:HA	3:B:103:GLN:O	0.52	2.05	14	3
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:2:LYS:HA	3:B:110:ASP:HB3	0.52	1.81	15	2
3:A:17:LEU:HG	3:B:132:MET:CG	0.52	2.35	19	1
3:A:28:VAL:O	3:A:32:MET:N	0.52	2.41	9	3
3:A:7:VAL:HG12	3:A:9:VAL:CG2	0.52	2.35	3	1
3:A:17:LEU:CD1	3:A:27:LEU:CD2	0.52	2.88	15	2
1:C:179:DA:C5	1:C:180:DT:C4	0.52	2.98	4	11
3:A:17:LEU:HG	3:B:132:MET:HG2	0.52	1.82	11	2
3:B:117:LEU:O	3:B:122:VAL:HG12	0.52	2.05	10	1
3:B:128:VAL:HG12	3:B:129:SER:N	0.52	2.18	11	1
3:A:32:MET:HB2	3:B:113:SER:CB	0.52	2.34	13	1
3:A:32:MET:HE1	3:B:124:ILE:CG2	0.52	2.35	20	3
3:B:117:LEU:HG	3:B:127:LEU:HD22	0.52	1.82	19	3
3:A:7:VAL:O	3:A:7:VAL:CG1	0.52	2.57	20	2
1:C:181:DA:C2	1:C:182:DC:C2	0.51	2.98	15	6
2:D:192:DA:H2''	2:D:193:DT:O5'	0.51	2.05	4	4
3:A:2:LYS:HE3	3:A:2:LYS:HA	0.51	1.82	19	2
3:B:105:ILE:CG2	3:B:105:ILE:O	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:MET:O	3:A:36:ALA:HB2	0.51	2.05	19	4
3:A:7:VAL:HG12	3:A:9:VAL:HG13	0.51	1.82	2	1
3:A:23:ASN:O	3:B:132:MET:HE1	0.51	2.06	14	2
3:A:32:MET:HG2	3:B:117:LEU:HG	0.51	1.81	15	2
3:A:31:THR:CG2	3:B:127:LEU:HD11	0.51	2.35	13	2
1:C:177:DG:H2'	1:C:178:DT:H71	0.51	1.82	10	3
3:B:115:GLN:HA	3:B:118:LYS:CG	0.51	2.36	10	10
1:C:179:DA:C2'	1:C:180:DT:C6	0.51	2.93	20	5
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
1:C:178:DT:C7	3:A:6:THR:HB	0.51	2.36	13	1
2:D:187:DC:O5'	2:D:187:DC:C6	0.51	2.64	8	2
3:A:2:LYS:HE3	3:B:109:VAL:O	0.51	2.05	4	3
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:B:138:ARG:NE	3:B:138:ARG:HA	0.51	2.20	9	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:7:VAL:HG22	3:A:9:VAL:CG2	0.51	2.36	16	2
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:22:VAL:C	3:A:24:ILE:H	0.51	2.09	1	2
3:A:31:THR:HG21	3:B:131:THR:OG1	0.51	2.06	12	1
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:CG1	3:B:105:ILE:O	0.50	2.59	14	4
3:A:24:ILE:CG1	3:B:132:MET:HE2	0.50	2.36	18	1
3:A:14:TYR:CZ	3:B:105:ILE:HG12	0.50	2.41	12	1
3:B:120:TYR:CE1	3:B:122:VAL:HB	0.50	2.42	2	1
2:D:191:DT:C7	3:B:106:THR:OG1	0.50	2.60	10	3
3:B:122:VAL:HG12	3:B:122:VAL:O	0.50	2.07	1	1
3:B:115:GLN:O	3:B:119:ALA:HB2	0.50	2.06	16	2
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
3:A:32:MET:O	3:A:36:ALA:CB	0.50	2.60	19	7
3:A:7:VAL:HG21	3:B:124:ILE:O	0.50	2.05	2	2
3:B:114:TYR:CE1	3:B:118:LYS:HG2	0.50	2.42	6	2
3:A:14:TYR:CD1	3:A:15:GLN:N	0.50	2.79	10	3
3:A:7:VAL:HG22	3:A:7:VAL:O	0.50	2.06	8	4
3:B:117:LEU:HD13	3:B:122:VAL:HG11	0.50	1.79	10	1
3:A:9:VAL:HG13	3:A:12:ASP:HB2	0.50	1.84	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:173:DA:C2'	1:C:174:DT:O5'	0.50	2.58	1	2
1:C:179:DA:H2''	1:C:180:DT:C6	0.50	2.41	20	1
2:D:192:DA:H62	3:B:104:ARG:CZ	0.50	2.20	12	1
3:B:132:MET:O	3:B:136:ALA:CB	0.50	2.60	18	8
2:D:194:DA:H1'	2:D:195:DC:O4'	0.50	2.07	19	1
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
3:A:5:ILE:CG2	3:B:114:TYR:CD1	0.49	2.92	13	2
3:A:4:ARG:HA	3:B:108:THR:HG22	0.49	1.84	9	2
3:A:22:VAL:O	3:A:22:VAL:CG1	0.49	2.60	7	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:B:110:ASP:O	3:B:115:GLN:HG3	0.49	2.07	11	1
3:A:15:GLN:O	3:A:19:ALA:N	0.49	2.44	16	10
2:D:194:DA:C5	2:D:195:DC:C5	0.49	3.00	3	6
3:B:115:GLN:OE1	3:B:118:LYS:NZ	0.49	2.39	2	2
3:A:5:ILE:HD11	3:B:107:VAL:CG1	0.49	2.36	6	4
3:B:117:LEU:CD1	3:B:127:LEU:CD1	0.49	2.90	20	2
3:B:127:LEU:HD13	3:B:127:LEU:C	0.49	2.28	13	2
1:C:179:DA:C2	2:D:194:DA:C2	0.49	3.00	8	4
3:A:28:VAL:C	3:A:32:MET:HG2	0.49	2.27	20	2
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
2:D:190:DG:OP1	3:A:25:SER:CA	0.49	2.61	17	1
3:A:17:LEU:HD21	3:B:135:GLU:HB2	0.49	1.83	1	1
2:D:187:DC:H2''	2:D:188:DG:O5'	0.49	2.07	16	1
3:A:7:VAL:CG1	3:B:105:ILE:HG21	0.49	2.38	12	1
2:D:190:DG:OP1	3:A:25:SER:HB3	0.49	2.08	10	3
3:A:9:VAL:CG1	3:A:14:TYR:CG	0.49	2.94	9	4
3:B:107:VAL:O	3:B:109:VAL:HG23	0.49	2.08	10	1
2:D:194:DA:C4	2:D:195:DC:C6	0.49	3.01	11	7
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:A:18:LYS:HG3	3:A:19:ALA:N	0.49	2.23	3	4
3:A:2:LYS:HA	3:B:109:VAL:O	0.49	2.08	2	4
3:B:124:ILE:CD1	3:B:124:ILE:N	0.49	2.72	10	5
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
1:C:175:DA:H8	1:C:175:DA:O5'	0.49	1.91	20	1
2:D:191:DT:C7	3:A:4:ARG:HD3	0.49	2.38	18	1
3:B:127:LEU:HD13	3:B:128:VAL:N	0.49	2.23	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:D:191:DT:H2''	2:D:192:DA:N7	0.49	2.23	18	2
3:A:14:TYR:CD1	3:B:105:ILE:CD1	0.49	2.95	9	4
1:C:176:DT:H72	3:A:8:THR:HG21	0.49	1.84	10	3
3:B:122:VAL:O	3:B:124:ILE:N	0.49	2.42	1	2
3:B:109:VAL:HG13	3:B:114:TYR:CD2	0.49	2.43	18	1
2:D:190:DG:OP2	3:B:107:VAL:HA	0.49	2.07	2	4
3:A:22:VAL:O	3:A:24:ILE:N	0.49	2.36	11	7
3:B:107:VAL:O	3:B:107:VAL:HG22	0.49	2.08	19	2
3:A:7:VAL:O	3:A:9:VAL:HG22	0.49	2.07	4	1
3:A:7:VAL:HG13	3:A:9:VAL:HG13	0.49	1.84	20	2
3:A:6:THR:HG22	3:B:104:ARG:HG2	0.48	1.84	13	1
3:A:5:ILE:O	3:A:5:ILE:CG1	0.48	2.61	15	7
3:B:105:ILE:CD1	3:B:132:MET:HE1	0.48	2.38	11	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	1
2:D:190:DG:P	3:A:25:SER:HB2	0.48	2.47	9	2
3:B:117:LEU:CG	3:B:127:LEU:CD1	0.48	2.91	15	1
3:A:7:VAL:HG21	3:B:128:VAL:HB	0.48	1.85	15	1
3:A:3:GLN:HG2	3:B:114:TYR:CE2	0.48	2.43	7	3
3:A:28:VAL:CB	3:B:107:VAL:HG11	0.48	2.38	8	2
1:C:173:DA:C3'	1:C:174:DT:H73	0.48	2.38	8	1
2:D:186:DT:C2'	2:D:187:DC:O5'	0.48	2.57	15	3
3:A:5:ILE:O	3:B:107:VAL:N	0.48	2.46	1	2
3:A:28:VAL:HG21	3:B:107:VAL:HG11	0.48	1.85	19	4
3:B:128:VAL:O	3:B:132:MET:HB2	0.48	2.08	19	1
2:D:191:DT:H72	3:B:106:THR:HG21	0.48	1.85	15	4
3:A:32:MET:HE2	3:B:114:TYR:HD1	0.48	1.69	17	1
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
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
1:C:178:DT:H72	3:A:6:THR:HB	0.48	1.83	13	1
3:B:112:ASP:O	3:B:114:TYR:N	0.48	2.45	18	2
3:A:24:ILE:O	3:A:25:SER:C	0.48	2.51	14	18
3:B:114:TYR:CD2	3:B:115:GLN:N	0.48	2.82	13	4
3:B:127:LEU:CD2	3:B:127:LEU:C	0.48	2.82	11	2
3:B:107:VAL:CG1	3:B:107:VAL:O	0.48	2.61	18	2
2:D:192:DA:C5	2:D:193:DT:C4	0.48	3.02	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:MET:SD	3:B:114:TYR:CA	0.48	2.97	8	3
3:A:26:GLY:O	3:A:30:THR:HB	0.48	2.09	15	3
3:A:24:ILE:HG12	3:B:132:MET:HE1	0.48	1.84	7	4
3:B:124:ILE:N	3:B:124:ILE:CD1	0.48	2.67	12	5
3:B:102:LYS:HG2	3:B:102:LYS:O	0.48	2.08	14	1
3:A:7:VAL:HG13	3:A:9:VAL:HB	0.48	1.85	15	1
3:B:117:LEU:CD1	3:B:122:VAL:HB	0.48	2.39	13	2
1:C:179:DA:N7	3:A:4:ARG:NH2	0.48	2.62	7	1
3:B:121:ASP:O	3:B:122:VAL:CG2	0.48	2.62	17	3
3:B:118:LYS:HG3	3:B:119:ALA:N	0.48	2.24	18	2
2:D:190:DG:OP2	3:A:25:SER:CB	0.48	2.62	1	1
3:A:21:ASP:O	3:A:22:VAL:HG23	0.48	2.09	16	2
1:C:173:DA:C2'	1:C:174:DT:OP1	0.47	2.62	12	5
3:B:111:SER:HA	3:B:115:GLN:HG2	0.47	1.86	19	1
2:D:192:DA:H8	2:D:192:DA:O5'	0.47	1.92	1	3
3:A:23:ASN:O	3:B:132:MET:CE	0.47	2.61	15	5
3:A:31:THR:CB	3:B:127:LEU:HD21	0.47	2.37	4	1
3:B:124:ILE:HA	3:B:127:LEU:HB3	0.47	1.85	14	5
2:D:189:DG:O3'	3:A:25:SER:HB3	0.47	2.08	14	2
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:A:16:LEU:HD22	3:A:20:TYR:CE1	0.47	2.44	1	1
3:A:33:GLN:HB2	3:B:113:SER:OG	0.47	2.09	18	3
3:A:3:GLN:O	3:B:109:VAL:N	0.47	2.44	5	8
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:29:SER:HA	3:B:112:ASP:O	0.47	2.09	19	1
3:A:17:LEU:HD23	3:A:27:LEU:HG	0.47	1.85	8	1
3:A:7:VAL:O	3:A:7:VAL:HG22	0.47	2.08	16	2
3:B:115:GLN:O	3:B:119:ALA:CB	0.47	2.62	18	3
3:A:32:MET:HE1	3:B:124:ILE:HG21	0.47	1.86	13	1
3:A:27:LEU:HD13	3:A:28:VAL:N	0.47	2.23	11	3
1:C:177:DG:C8	1:C:178:DT:H71	0.47	2.44	6	3
2:D:186:DT:C2'	2:D:187:DC:C5'	0.47	2.93	8	1
3:B:128:VAL:CG1	3:B:132:MET:CE	0.47	2.92	17	2
3:B:128:VAL:HG12	3:B:132:MET:SD	0.47	2.49	9	2
3:A:14:TYR:CA	3:B:132:MET:SD	0.47	2.96	16	5
2:D:192:DA:N7	3:B:104:ARG:HD2	0.47	2.25	15	2
3:A:7:VAL:O	3:B:105:ILE:CG2	0.47	2.53	20	1
1:C:184:DC:N4	2:D:187:DC:N4	0.47	2.63	12	2
3:A:14:TYR:CZ	3:B:105:ILE:CG1	0.47	2.97	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:5:ILE:HG12	3:B:107:VAL:O	0.47	2.10	10	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	1
3:B:109:VAL:HG12	3:B:112:ASP:CB	0.47	2.40	5	2
2:D:190:DG:C8	3:A:4:ARG:NH1	0.47	2.83	20	1
3:B:107:VAL:O	3:B:109:VAL:HG12	0.47	2.10	7	1
3:A:15:GLN:O	3:A:19:ALA:HB2	0.47	2.10	11	6
3:A:5:ILE:HD13	3:B:114:TYR:HD2	0.47	1.59	8	1
3:A:9:VAL:HG11	3:A:14:TYR:CD1	0.47	2.44	8	1
3:A:5:ILE:O	3:B:106:THR:CA	0.47	2.62	8	2
2:D:196:DA:C8	2:D:197:DT:H72	0.47	2.45	8	1
3:A:24:ILE:N	3:A:24:ILE:CD1	0.47	2.72	4	1
3:A:9:VAL:HG13	3:A:10:ASP:H	0.47	1.69	1	1
1:C:176:DT:C6	3:A:8:THR:OG1	0.47	2.68	6	1
2:D:196:DA:H2'	2:D:197:DT:H71	0.47	1.87	5	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:188:DG:H8	2:D:188:DG:O5'	0.47	1.93	12	1
3:B:121:ASP:O	3:B:122:VAL:HG23	0.47	2.10	17	3
3:B:107:VAL:HG22	3:B:109:VAL:HG13	0.47	1.86	2	4
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:192:DA:C8	2:D:192:DA:O5'	0.47	2.68	16	1
3:A:12:ASP:O	3:B:129:SER:CA	0.47	2.63	4	4
2:D:190:DG:C8	2:D:191:DT:H73	0.47	2.44	4	1
1:C:173:DA:O4'	1:C:174:DT:H72	0.47	2.09	10	1
1:C:174:DT:OP1	1:C:174:DT:H72	0.47	2.09	16	1
3:A:9:VAL:HG12	3:A:11:SER:H	0.47	1.68	12	1
3:B:128:VAL:HG13	3:B:132:MET:HE1	0.47	1.84	19	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
3:A:24:ILE:HG12	3:B:128:VAL:CG1	0.46	2.40	15	1
2:D:192:DA:H62	3:B:104:ARG:NH2	0.46	2.08	12	1
3:A:14:TYR:OH	3:A:18:LYS:NZ	0.46	2.37	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:193:DT:C4	2:D:194:DA:N6	0.46	2.83	10	1
1:C:176:DT:H2'	3:A:8:THR:HG1	0.46	1.69	1	1
2:D:190:DG:OP1	3:A:25:SER:HB2	0.46	2.10	15	2
2:D:189:DG:C8	2:D:190:DG:N7	0.46	2.83	12	1
3:A:17:LEU:HD12	3:A:22:VAL:HG13	0.46	1.85	12	3
3:A:3:GLN:HB3	3:B:110:ASP:HA	0.46	1.88	19	2
3:A:30:THR:CG2	3:A:31:THR:N	0.46	2.77	15	4
3:A:14:TYR:CZ	3:A:18:LYS:HG2	0.46	2.44	10	3
2:D:191:DT:C4	2:D:192:DA:N6	0.46	2.83	8	5
3:A:27:LEU:HD13	3:B:135:GLU:HG2	0.46	1.87	4	1
3:B:105:ILE:HD13	3:B:105:ILE:O	0.46	2.10	4	1
3:A:7:VAL:O	3:A:9:VAL:N	0.46	2.48	1	4
2:D:190:DG:OP2	3:A:25:SER:HB2	0.46	2.10	11	2
2:D:189:DG:O3'	3:A:25:SER:CB	0.46	2.63	14	2
3:B:132:MET:O	3:B:136:ALA:HB2	0.46	2.10	18	3
1:C:177:DG:OP1	3:B:125:SER:CA	0.46	2.64	15	1
3:A:3:GLN:N	3:B:109:VAL:O	0.46	2.40	17	3
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:32:MET:HE2	3:B:124:ILE:HG12	0.46	1.88	18	1
3:B:133:GLN:HG3	3:B:134:ASN:N	0.46	2.25	13	2
3:B:117:LEU:HD22	3:B:120:TYR:CE2	0.46	2.46	15	2
2:D:190:DG:OP2	3:A:25:SER:HB3	0.46	2.10	1	1
2:D:192:DA:O5'	2:D:192:DA:C8	0.46	2.69	3	3
3:A:17:LEU:HD11	3:B:135:GLU:HG2	0.46	1.88	16	2
3:A:31:THR:HG22	3:B:127:LEU:CD2	0.46	2.40	12	1
2:D:191:DT:H2'	2:D:192:DA:C8	0.46	2.46	12	1
3:B:124:ILE:O	3:B:125:SER:C	0.46	2.55	10	19
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
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: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:HD12	3:A:22:VAL:HB	0.45	1.88	19	1
3:A:17:LEU:HA	3:A:20:TYR:CE1	0.45	2.46	8	1
3:A:14:TYR:CD2	3:A:15:GLN:HG2	0.45	2.46	1	1
1:C:178:DT:H2''	1:C:179:DA:C8	0.45	2.47	12	4
3:B:125:SER:OG	3:B:126:GLY:N	0.45	2.50	13	5
3:A:29:SER:HA	3:A:32:MET:HG2	0.45	1.87	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:24:ILE:HA	3:A:27:LEU:CB	0.45	2.41	19	4
3:A:32:MET:HE2	3:B:124:ILE:HG13	0.45	1.88	19	1
3:B:109:VAL:HG23	3:B:112:ASP:HB2	0.45	1.88	4	1
3:B:128:VAL:O	3:B:132:MET:HG3	0.45	2.12	16	4
3:A:36:ALA:HA	3:B:120:TYR:CE2	0.45	2.46	19	1
3:A:32:MET:SD	3:B:114:TYR:O	0.45	2.75	8	4
2:D:195:DC:C2	2:D:196:DA:N7	0.45	2.84	2	2
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
2:D:191:DT:H73	3:A:4:ARG:HD3	0.45	1.88	18	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
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:6:THR:HG23	3:B:106:THR:CB	0.45	2.42	13	1
3:A:24:ILE:HA	3:A:27:LEU:HB3	0.45	1.88	3	6
3:A:14:TYR:CZ	3:B:105:ILE:HD11	0.45	2.46	2	1
3:A:24:ILE:HD11	3:B:105:ILE:HG12	0.45	1.89	4	1
3:A:5:ILE:O	3:A:5:ILE:HD13	0.45	2.11	20	1
3:B:111:SER:HA	3:B:115:GLN:CD	0.45	2.31	17	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:10:ASP:HA	3:A:15:GLN:CD	0.45	2.33	19	1
3:A:7:VAL:HG12	3:A:9:VAL:HG12	0.45	1.87	15	1
3:B:137:ARG:NE	3:B:137:ARG:HA	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:32:MET:CE	3:B:123:ASN:O	0.45	2.65	20	2
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:B:107:VAL:CG2	3:B:109:VAL:HG13	0.44	2.34	19	3
1:C:180:DT:O4	3:A:4:ARG:HD2	0.44	2.12	2	1
2:D:186:DT:H1'	2:D:187:DC:OP1	0.44	2.12	8	1
1:C:177:DG:OP1	3:B:125:SER:HB2	0.44	2.12	5	4
3:A:10:ASP:O	3:A:15:GLN:CG	0.44	2.65	1	1
1:C:176:DT:O3'	3:B:125:SER:HB3	0.44	2.11	11	1
3:A:11:SER:OG	3:B:102:LYS:NZ	0.44	2.35	19	1
3:B:110:ASP:HA	3:B:115:GLN:HG3	0.44	1.88	9	1
2:D:196:DA:C8	2:D:197:DT:C7	0.44	3.01	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:111:SER:OG	3:B:112:ASP:N	0.44	2.50	13	1
3:B:130:THR:CG2	3:B:131:THR:N	0.44	2.80	6	5
2:D:187:DC:C6	2:D:187:DC:O5'	0.44	2.70	19	1
3:A:17:LEU:HD11	3:B:135:GLU:HB3	0.44	1.90	8	1
3:A:7:VAL:HG13	3:B:105:ILE:CD1	0.44	2.42	5	3
3:B:109:VAL:HG11	3:B:114:TYR:N	0.44	2.28	10	1
2:D:192:DA:H2''	2:D:193:DT:C6	0.44	2.47	16	6
3:B:107:VAL:CG1	3:B:109:VAL:HB	0.44	2.42	18	1
3:A:5:ILE:CB	3:B:114:TYR:CE1	0.44	3.01	18	2
3:A:17:LEU:CD1	3:A:20:TYR:CE1	0.44	3.00	8	1
3:A:12:ASP:O	3:A:13:SER:HB2	0.44	2.12	4	2
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:9:VAL:O	3:B:102:LYS:HA	0.44	2.12	15	2
1:C:173:DA:H2''	1:C:174:DT:OP1	0.44	2.13	15	6
3:A:13:SER:O	3:B:132:MET:HB2	0.44	2.12	7	2
2:D:186:DT:C6	2:D:187:DC:C6	0.44	3.06	17	1
2:D:191:DT:H3'	3:B:104:ARG:O	0.44	2.13	10	1
1:C:174:DT:H2''	1:C:175:DA:C5'	0.44	2.43	10	2
1:C:173:DA:C1'	1:C:174:DT:H73	0.44	2.42	10	1
3:B:117:LEU:HD12	3:B:127:LEU:HD12	0.44	1.89	20	2
1:C:175:DA:OP2	3:B:102:LYS:HD2	0.44	2.12	14	1
3:A:23:ASN:C	3:A:24:ILE:CD1	0.44	2.81	12	1
3:B:107:VAL:O	3:B:107:VAL:CG2	0.44	2.66	19	3
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:B:117:LEU:HD11	3:B:127:LEU:CD1	0.44	2.38	3	1
3:A:7:VAL:HG13	3:B:105:ILE:CG2	0.44	2.42	12	1
2:D:193:DT:O4	3:B:104:ARG:CD	0.44	2.66	13	1
3:B:105:ILE:HG12	3:B:105:ILE:O	0.44	2.13	7	2
3:A:17:LEU:O	3:A:20:TYR:CD1	0.44	2.71	8	1
3:A:5:ILE:HG22	3:B:114:TYR:CZ	0.44	2.48	17	2
3:A:17:LEU:HD13	3:B:132:MET:HA	0.44	1.88	9	1
3:A:7:VAL:HG23	3:B:124:ILE:CD1	0.44	2.36	20	1
1:C:173:DA:C4'	1:C:174:DT:OP1	0.44	2.65	20	1
3:A:9:VAL:HB	3:A:14:TYR:HD2	0.44	1.72	12	1
3:B:109:VAL:CG1	3:B:112:ASP:HB2	0.44	2.42	16	2
2:D:186:DT:OP3	2:D:186:DT:H4'	0.44	2.13	13	1
3:A:6:THR:CG2	3:B:106:THR:HB	0.44	2.43	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:7:VAL:CG2	3:A:7:VAL:O	0.44	2.66	8	1
3:A:9:VAL:CG2	3:A:14:TYR:CB	0.44	2.93	14	2
2:D:192:DA:H62	3:B:104:ARG:NH1	0.44	2.11	12	1
3:A:4:ARG:NH1	3:B:108:THR:HG21	0.43	2.28	2	1
2:D:194:DA:H2''	2:D:195:DC:O5'	0.43	2.13	2	3
3:A:33:GLN:HG3	3:A:34:ASN:N	0.43	2.27	17	3
3:A:27:LEU:HD11	3:B:131:THR:CG2	0.43	2.43	17	1
3:A:9:VAL:O	3:B:103:GLN:N	0.43	2.44	1	1
1:C:175:DA:O5'	1:C:175:DA:C8	0.43	2.71	11	1
1:C:182:DC:H2''	1:C:183:DC:C5'	0.43	2.43	14	1
3:B:128:VAL:O	3:B:132:MET:SD	0.43	2.76	19	2
3:B:128:VAL:HG13	3:B:132:MET:HG3	0.43	1.89	8	1
3:A:14:TYR:O	3:B:132:MET:SD	0.43	2.76	5	3
3:B:124:ILE:CG2	3:B:127:LEU:HD13	0.43	2.42	11	1
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
3:A:17:LEU:HG	3:A:27:LEU:CD1	0.43	2.43	12	1
3:A:17:LEU:HD22	3:A:22:VAL:CB	0.43	2.44	18	1
2:D:194:DA:C5	2:D:195:DC:C4	0.43	3.06	18	1
2:D:186:DT:C7	2:D:187:DC:C6	0.43	3.01	7	1
3:A:2:LYS:CA	3:A:2:LYS:HE3	0.43	2.43	19	1
3:B:120:TYR:C	3:B:120:TYR:CD1	0.43	2.92	8	3
3:B:107:VAL:O	3:B:109:VAL:HG22	0.43	2.13	9	3
3:A:13:SER:OG	3:B:133:GLN:HB2	0.43	2.12	9	2
3:B:127:LEU:C	3:B:127:LEU:CD2	0.43	2.86	4	1
2:D:189:DG:C2'	2:D:190:DG:C8	0.43	3.01	4	1
3:A:25:SER:CA	3:B:107:VAL:HG22	0.43	2.33	18	1
3:A:6:THR:HG23	3:B:106:THR:HB	0.43	1.89	13	1
3:B:122:VAL:C	3:B:124:ILE:H	0.43	2.17	18	2
1:C:177:DG:C5	1:C:178:DT:C4	0.43	3.06	19	2
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:B:112:ASP:O	3:B:113:SER:HB2	0.43	2.14	7	3
2:D:193:DT:O4	3:B:104:ARG:HD3	0.43	2.13	19	1
3:A:3:GLN:HG2	3:A:5:ILE:CG2	0.43	2.43	11	1
3:B:134:ASN:O	3:B:138:ARG:HD3	0.43	2.13	14	1
1:C:173:DA:H2''	1:C:174:DT:C6	0.43	2.48	2	4
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
3:A:35:GLU:CB	3:B:117:LEU:HD11	0.43	2.43	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:191:DT:H73	3:A:4:ARG:HD2	0.43	1.90	19	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
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:123:ASN:C	3:B:124:ILE:CD1	0.43	2.85	16	1
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
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:24:ILE:HG21	3:A:28:VAL:CG2	0.43	2.23	15	1
3:A:9:VAL:HG13	3:A:12:ASP:CB	0.43	2.44	12	1
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: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:O4'	2:D:186:DT:O2	0.43	2.37	15	2
3:A:2:LYS:HB3	3:B:109:VAL:O	0.42	2.14	8	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
1:C:173:DA:C4'	1:C:174:DT:H5'	0.42	2.44	11	1
2:D:190:DG:OP1	3:B:107:VAL:HB	0.42	2.13	5	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:15:GLN:CA	3:A:18:LYS:HE2	0.42	2.44	9	1
3:A:16:LEU:CB	3:B:136:ALA:CB	0.42	2.97	10	1
2:D:189:DG:C4	2:D:190:DG:C8	0.42	3.07	10	1
3:B:115:GLN:CA	3:B:118:LYS:HE2	0.42	2.44	13	2
3:B:116:LEU:O	3:B:120:TYR:CD2	0.42	2.73	9	1
3:B:138:ARG:CA	3:B:138:ARG:NE	0.42	2.82	9	1
3:B:114:TYR:CE2	3:B:118:LYS:HG2	0.42	2.49	4	1
3:A:9:VAL:HG12	3:A:10:ASP:N	0.42	2.30	3	1
3:B:117:LEU:HD22	3:B:122:VAL:HG13	0.42	1.90	20	1
3:A:17:LEU:HG	3:B:132:MET:HA	0.42	1.91	18	1
3:B:102:LYS:HE3	3:B:102:LYS:HA	0.42	1.92	8	1
2:D:191:DT:C2'	2:D:192:DA:C8	0.42	3.02	20	1
3:B:129:SER:CA	3:B:132:MET:HG2	0.42	2.44	18	1
3:B:109:VAL:HG22	3:B:111:SER:H	0.42	1.74	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:C:178:DT:C7	3:A:6:THR:CG2	0.42	2.97	12	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:20:TYR:CD1	3:A:21:ASP:HB2	0.42	2.49	19	1
3:A:2:LYS:HE3	3:B:108:THR:O	0.42	2.13	2	1
1:C:181:DA:OP2	2:D:186:DT:H72	0.42	2.15	8	1
1:C:180:DT:O4	3:B:104:ARG:NH2	0.42	2.53	17	2
3:B:114:TYR:CG	3:B:115:GLN:N	0.42	2.85	18	2
3:A:12:ASP:O	3:A:13:SER:CB	0.42	2.66	15	1
3:A:24:ILE:HG21	3:A:27:LEU:HD12	0.42	1.91	13	1
2:D:187:DC:C2	2:D:188:DG:C6	0.42	3.07	8	1
1:C:173:DA:H3'	1:C:174:DT:C7	0.42	2.44	8	1
3:A:17:LEU:CD1	3:A:22:VAL:HG13	0.42	2.43	4	1
1:C:180:DT:H71	3:A:4:ARG:CD	0.42	2.45	3	2
3:B:107:VAL:HG22	3:B:109:VAL:HB	0.42	1.90	11	1
3:A:24:ILE:CB	3:A:28:VAL:CG2	0.42	2.97	15	1
3:A:35:GLU:CG	3:B:127:LEU:HD11	0.42	2.41	12	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:5:ILE:CD1	3:A:28:VAL:HG11	0.42	2.45	14	1
3:A:17:LEU:HG	3:A:27:LEU:HD12	0.42	1.90	12	1
2:D:191:DT:C7	3:A:4:ARG:HD2	0.42	2.44	19	1
3:A:9:VAL:HG13	3:B:105:ILE:HB	0.42	1.90	2	1
3:A:24:ILE:O	3:B:107:VAL:HG21	0.42	2.15	16	1
3:A:15:GLN:HA	3:A:18:LYS:HE3	0.42	1.90	16	1
3:A:9:VAL:HG13	3:A:14:TYR:CD2	0.41	2.49	19	1
3:A:4:ARG:NE	3:B:108:THR:CG2	0.41	2.83	17	1
3:A:32:MET:HE1	3:B:114:TYR:CD1	0.41	2.50	15	1
3:A:15:GLN:CA	3:A:18:LYS:HE3	0.41	2.45	16	1
2:D:192:DA:N6	3:B:104:ARG:NH2	0.41	2.68	12	1
3:A:5:ILE:HD13	3:B:114:TYR:HD1	0.41	1.73	18	1
1:C:175:DA:C8	1:C:176:DT:C5	0.41	3.09	13	2
3:A:9:VAL:CB	3:A:14:TYR:CB	0.41	2.98	4	1
1:C:174:DT:H6	1:C:174:DT:O5'	0.41	1.98	1	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:175:DA:H3'	3:B:102:LYS:HD3	0.41	1.90	12	1
1:C:178:DT:H71	3:A:6:THR:OG1	0.41	2.15	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:VAL:CG2	3:A:10:ASP:N	0.41	2.82	19	1
3:A:23:ASN:C	3:A:24:ILE:HG13	0.41	2.35	1	1
3:B:124:ILE:O	3:B:128:VAL:N	0.41	2.52	1	1
3:A:33:GLN:CB	3:B:113:SER:CB	0.41	2.98	1	1
3:A:28:VAL:HG12	3:A:29:SER:N	0.41	2.30	6	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:B:115:GLN:HA	3:B:118:LYS:HG2	0.41	1.93	19	1
2:D:186:DT:C2'	2:D:187:DC:H5''	0.41	2.45	8	1
1:C:178:DT:H73	3:A:6:THR:HG23	0.41	1.90	4	1
3:A:13:SER:HB3	3:B:129:SER:O	0.41	2.15	11	1
3:A:4:ARG:CZ	3:B:108:THR:HG21	0.41	2.45	11	2
3:A:7:VAL:HG22	3:B:125:SER:CA	0.41	2.39	20	1
3:A:17:LEU:HB2	3:B:132:MET:CG	0.41	2.42	19	1
3:A:13:SER:HB3	3:B:133:GLN:HB2	0.41	1.92	19	1
1:C:175:DA:C8	1:C:176:DT:H71	0.41	2.51	9	1
3:A:22:VAL:O	3:A:22:VAL:HG12	0.41	2.15	20	2
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:5:ILE:HG23	3:B:109:VAL:CG2	0.41	2.45	20	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:A:17:LEU:CD1	3:B:132:MET:HG2	0.41	2.46	13	1
2:D:191:DT:C4	2:D:192:DA:C6	0.41	3.08	8	1
3:B:124:ILE:HG22	3:B:127:LEU:CB	0.41	2.45	9	1
3:A:17:LEU:HD13	3:B:132:MET:HG2	0.41	1.93	9	1
2:D:192:DA:C2'	2:D:193:DT:C6	0.41	3.04	1	1
3:B:117:LEU:HD22	3:B:117:LEU:HA	0.41	1.75	14	1
2:D:188:DG:C8	2:D:188:DG:O5'	0.41	2.73	12	1
3:B:126:GLY:O	3:B:130:THR:CB	0.41	2.68	13	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:112:ASP:C	3:B:114:TYR:H	0.41	2.18	17	1
3:B:133:GLN:OE1	3:B:137:ARG:NH2	0.41	2.45	9	1
2:D:192:DA:H2'	2:D:193:DT:C5	0.41	2.51	4	1
2:D:192:DA:N7	3:B:104:ARG:NH1	0.41	2.69	1	1
3:B:109:VAL:HG13	3:B:110:ASP:N	0.41	2.30	11	1
3:A:5:ILE:CG1	3:B:124:ILE:CD1	0.41	2.85	7	1
3:A:33:GLN:O	3:A:37:ARG:CG	0.41	2.69	2	1
2:D:189:DG:C6	2:D:190:DG:C6	0.41	3.09	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:24:ILE:HG22	3:A:27:LEU:CD2	0.41	2.45	1	1
1:C:179:DA:C8	1:C:180:DT:H72	0.41	2.50	14	1
3:A:23:ASN:HB2	3:A:24:ILE:HD12	0.41	1.91	15	1
3:A:14:TYR:CG	3:A:15:GLN:N	0.41	2.87	12	2
2:D:191:DT:C7	3:B:106:THR:HG23	0.41	2.46	13	1
3:A:36:ALA:HA	3:B:120:TYR:HE2	0.41	1.76	19	1
3:B:124:ILE:HA	3:B:127:LEU:CB	0.41	2.46	8	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:8:THR:HA	3:B:104:ARG:HA	0.41	1.93	1	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
3:B:109:VAL:CG2	3:B:110:ASP:N	0.41	2.79	14	1
3:B:104:ARG:CZ	3:B:106:THR:HG21	0.41	2.45	5	1
3:A:5:ILE:HD12	3:B:124:ILE:HG12	0.41	1.93	15	1
3:A:5:ILE:CD1	3:B:107:VAL:HG12	0.41	2.46	20	1
3:B:128:VAL:C	3:B:132:MET:HG2	0.41	2.36	18	1
3:A:17:LEU:CD1	3:A:24:ILE:CG2	0.41	2.95	13	1
3:A:17:LEU:HD21	3:B:135:GLU:HG3	0.41	1.93	2	1
3:A:28:VAL:CG1	3:A:32:MET:HE1	0.41	2.46	17	1
1:C:174:DT:OP1	1:C:174:DT:C7	0.41	2.68	16	1
2:D:192:DA:N7	3:B:104:ARG:HD3	0.41	2.31	20	1
3:A:7:VAL:O	3:A:9:VAL:HG23	0.41	2.15	12	1
2:D:191:DT:O4	3:A:4:ARG:HD3	0.41	2.16	18	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:A:27:LEU:HD11	3:B:131:THR:HG23	0.40	1.91	17	1
3:B:129:SER:O	3:B:132:MET:HB2	0.40	2.17	15	1
3:A:4:ARG:CG	3:B:108:THR:CG2	0.40	2.93	17	1
3:A:24:ILE:HD11	3:B:105:ILE:CG1	0.40	2.46	4	1
3:B:128:VAL:CG1	3:B:132:MET:HE3	0.40	2.35	4	1
1:C:179:DA:H2'	1:C:180:DT:C7	0.40	2.46	12	1
1:C:178:DT:C4	3:B:104:ARG:HD2	0.40	2.52	19	1
3:A:17:LEU:HB2	3:B:132:MET:HB3	0.40	1.94	2	1
2:D:186:DT:H4'	2:D:187:DC:C5'	0.40	2.46	9	1
1:C:180:DT:C2	1:C:181:DA:C6	0.40	3.09	5	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%)	1	5
All	All	1480/2880 (51%)	984 (66%)	268 (18%)	228 (15%)	1	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	B	121	ASP	20
3	B	109	VAL	20
3	A	21	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	A	22	VAL	9
3	B	112	ASP	9
3	B	110	ASP	8
3	A	10	ASP	8
3	B	123	ASN	7
3	A	2	LYS	4
3	A	28	VAL	4
3	A	11	SER	4
3	B	108	THR	3
3	B	102	LYS	2
3	B	111	SER	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%)	19±2 (55±6%)	15±2 (45±6%)	0	2
3	B	34/64 (53%)	18±2 (52±6%)	16±2 (48±6%)	0	1
All	All	1360/2560 (53%)	724 (53%)	636 (47%)	0	2

All 66 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	B	117	LEU	20
3	A	17	LEU	19
3	B	116	LEU	19
3	A	6	THR	19
3	B	106	THR	19
3	B	114	TYR	18
3	B	107	VAL	18
3	B	124	ILE	18
3	A	14	TYR	18
3	A	37	ARG	17
3	A	7	VAL	17
3	B	137	ARG	16
3	A	24	ILE	15
3	A	16	LEU	14
3	B	105	ILE	14
3	B	133	GLN	14
3	B	102	LYS	14
3	A	5	ILE	13
3	B	112	ASP	13
3	B	118	LYS	13
3	A	18	LYS	12
3	B	131	THR	12
3	A	12	ASP	12
3	B	138	ARG	12
3	A	21	ASP	12
3	A	33	GLN	12
3	A	38	ARG	11
3	A	20	TYR	11

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Mol	Chain	Res	Type	Models (Total)
3	A	32	MET	10
3	A	34	ASN	10
3	B	130	THR	10
3	B	104	ARG	10
3	B	125	SER	9
3	B	115	GLN	9
3	B	127	LEU	9
3	A	4	ARG	9
3	A	27	LEU	9
3	B	120	TYR	8
3	B	134	ASN	8
3	A	2	LYS	8
3	A	13	SER	8
3	A	15	GLN	7
3	B	109	VAL	7
3	A	11	SER	7
3	A	30	THR	6
3	B	123	ASN	6
3	B	121	ASP	6
3	A	3	GLN	6
3	B	111	SER	5
3	A	25	SER	5
3	B	113	SER	5
3	B	132	MET	4
3	B	135	GLU	4
3	A	31	THR	4
3	A	23	ASN	4
3	A	9	VAL	3
3	A	10	ASP	3
3	A	8	THR	2
3	B	108	THR	2
3	B	122	VAL	2
3	B	129	SER	2
3	B	110	ASP	2
3	A	29	SER	2
3	A	35	GLU	1
3	A	22	VAL	1
3	B	103	GLN	1

6.3.3 RNA ⓘ

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 carbohydrates 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