



# Full wwPDB NMR Structure Validation Report ⓘ

Sep 30, 2021 – 04:18 PM JST

PDB ID : 7D3V  
Title : Non-specific and specific interactions work cooperatively to promote cytidine deamination catalyzed by APOBEC3A  
Authors : Cao, C.Y.; Liu, Y.P.; Lan, W.X.  
Deposited on : 2020-09-21

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

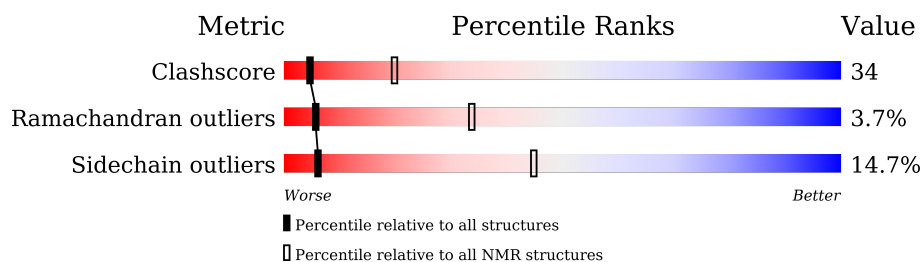
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 75%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	199	
1	B	199	
2	C	10	
2	D	10	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:199, B:204-B:246, B:250-B:300, B:305-B:398 (382)	0.55	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6978 atoms, of which 3326 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA dC->dU-editing enzyme APOBEC-3A.

Mol	Chain	Residues	Atoms						Trace
1	A	199	Total	C	H	N	O	S	0
			3172	1029	1546	295	293	9	
1	B	199	Total	C	H	N	O	S	0
			3172	1029	1546	295	293	9	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ASN	LEU	engineered mutation	UNP P31941
A	64	SER	CYS	engineered mutation	UNP P31941
A	72	GLN	GLU	engineered mutation	UNP P31941
A	171	GLN	CYS	engineered mutation	UNP P31941
B	262	ASN	LEU	engineered mutation	UNP P31941
B	263	SER	CYS	engineered mutation	UNP P31941
B	271	GLN	GLU	engineered mutation	UNP P31941
B	370	GLN	CYS	engineered mutation	UNP P31941

- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3').

Mol	Chain	Residues	Atoms						Trace
2	C	10	Total	C	H	N	O	P	0
			316	99	117	30	61	9	
2	D	10	Total	C	H	N	O	P	0
			316	99	117	30	61	9	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

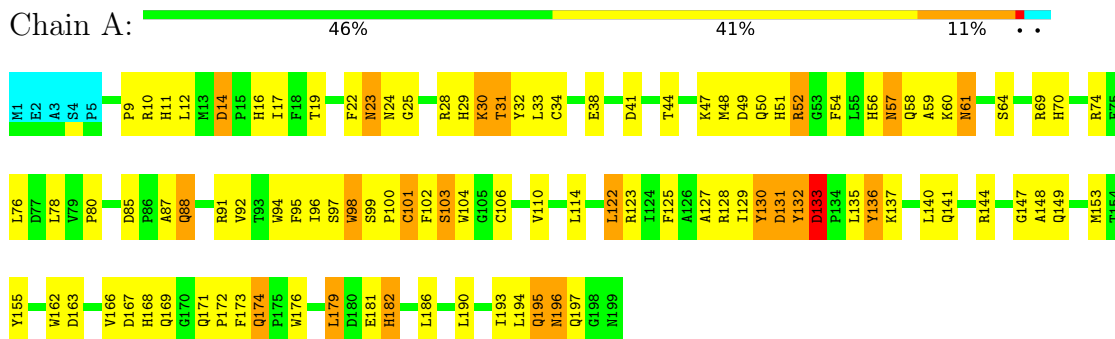
Mol	Chain	Residues	Atoms	
3	A	1	Total	Zn
			1	1
3	B	1	Total	Zn
			1	1

## 4 Residue-property plots

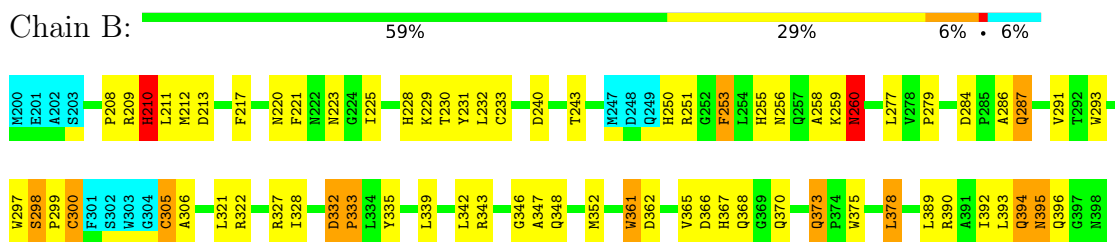
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



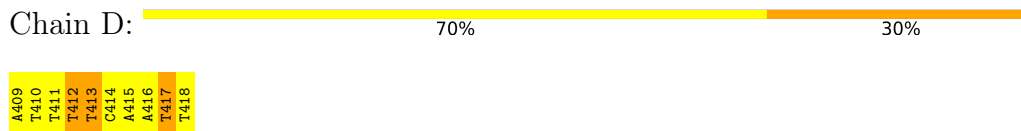
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

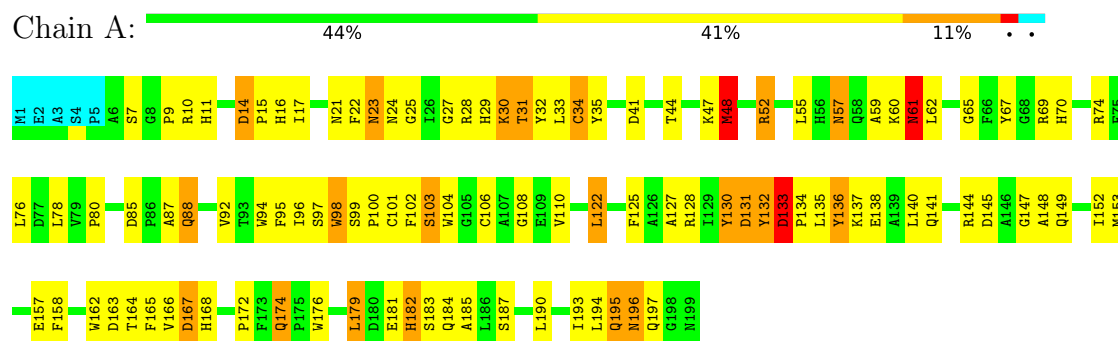


## 4.2 Scores per residue for each member of the ensemble

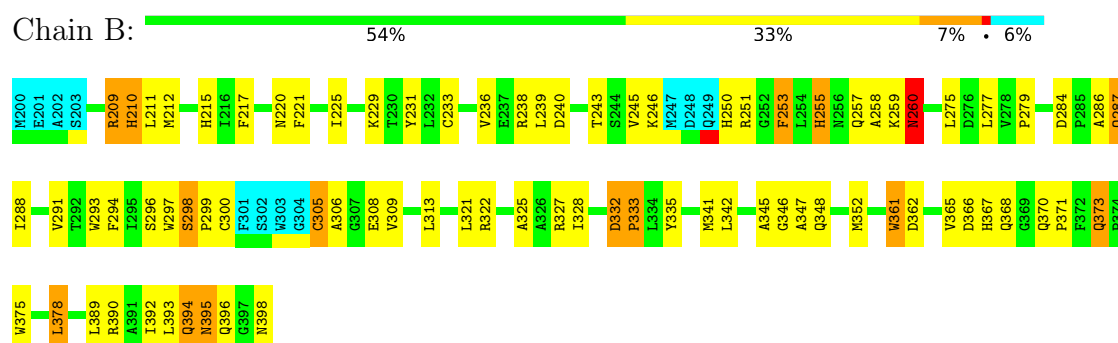
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

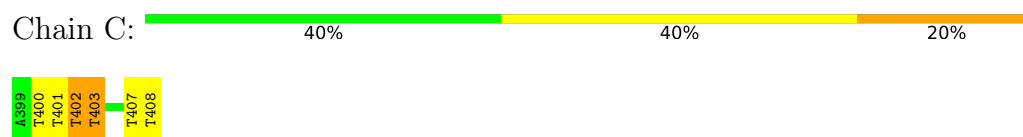
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

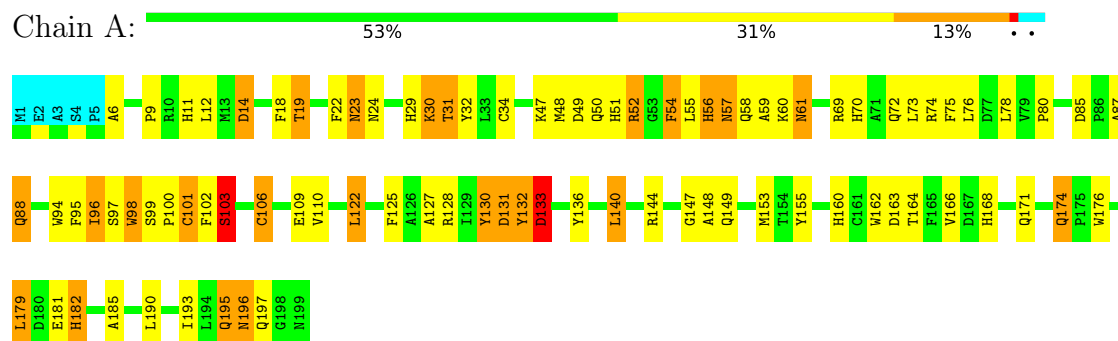


- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



### 4.2.2 Score per residue for model 2

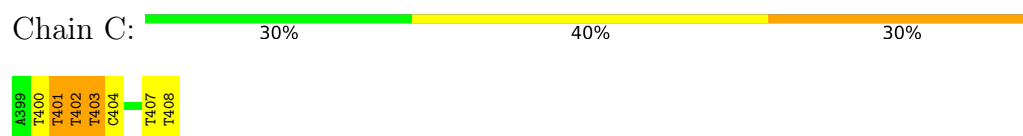
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



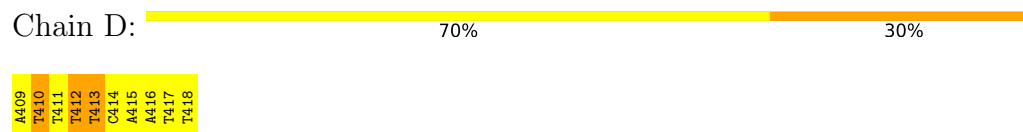
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

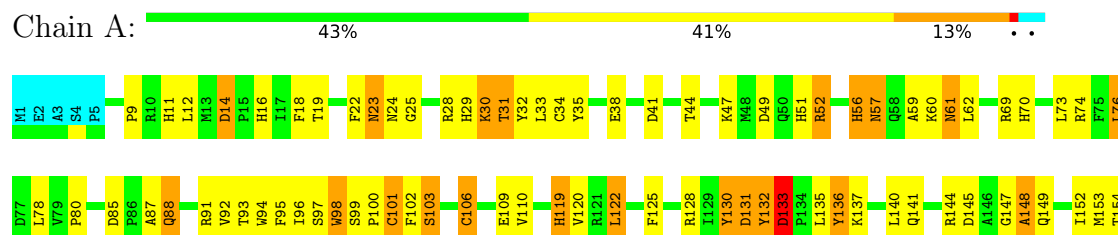


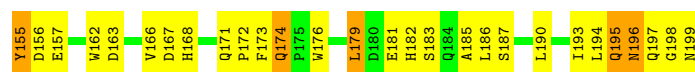
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



### 4.2.3 Score per residue for model 3

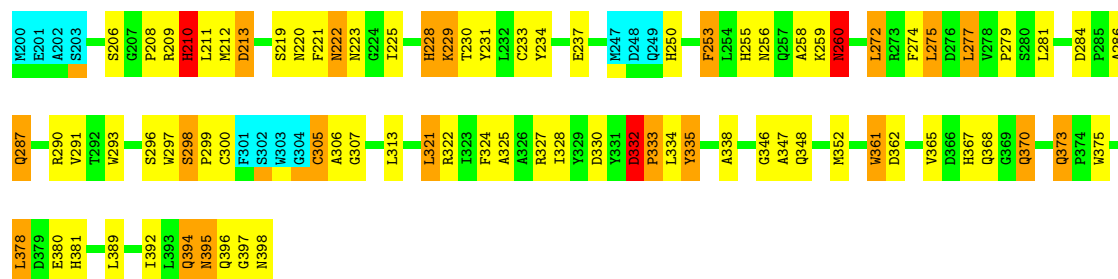
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B:



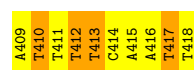
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain C:



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

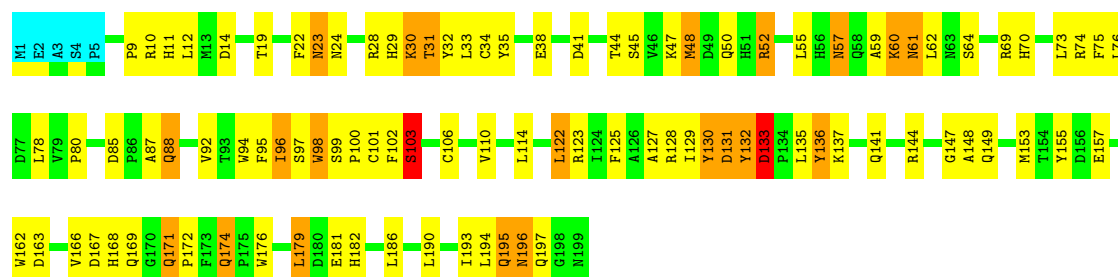
Chain D:



#### 4.2.4 Score per residue for model 4

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

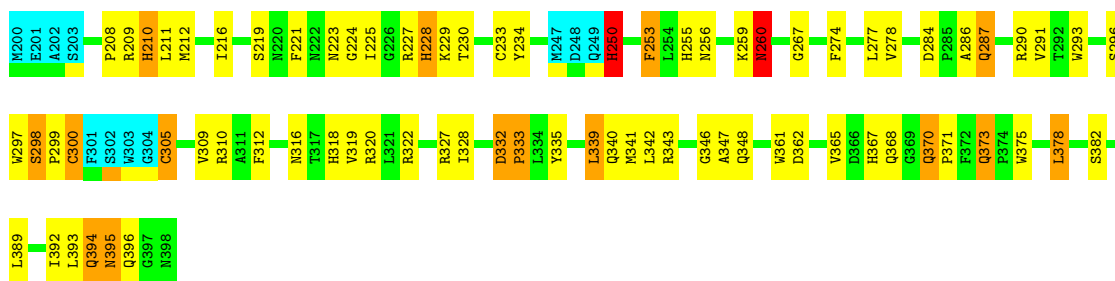
Chain A:



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B:





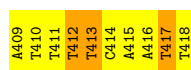
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain C: 40% 40% 20%



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

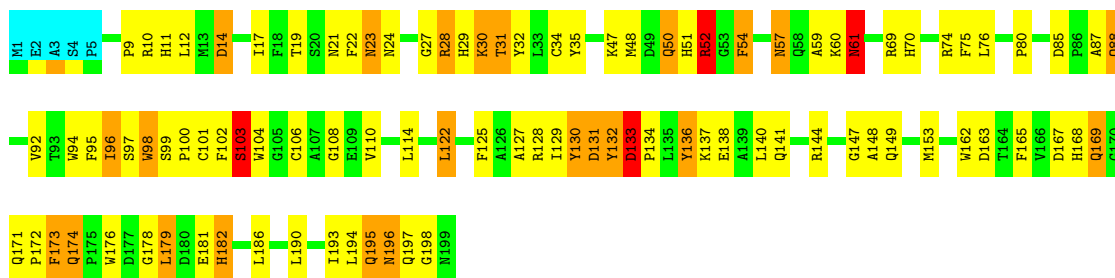
Chain D: 70% 30%



#### 4.2.5 Score per residue for model 5 (medoid)

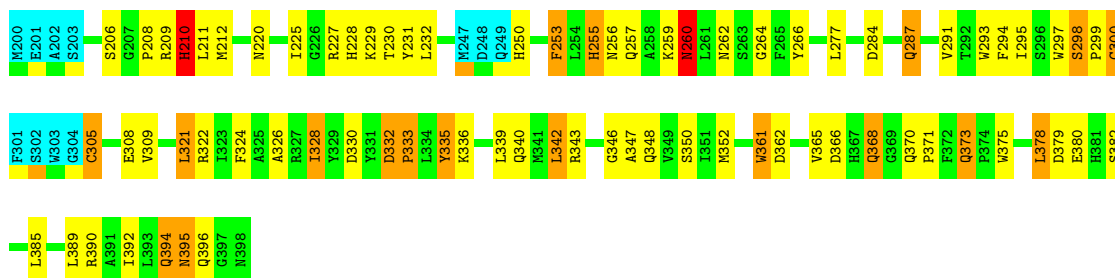
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A: 49% 35% 12% ..

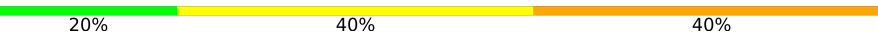


- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 56% 29% 9% 6%

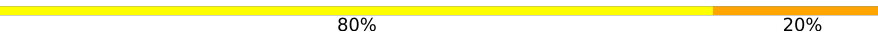


- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain C: 



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

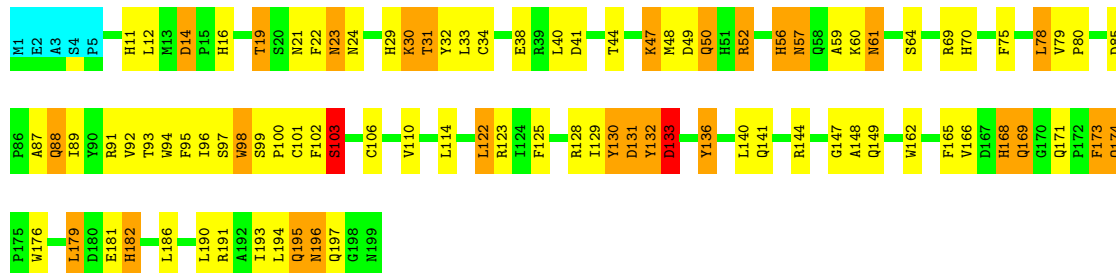
Chain D: 



#### 4.2.6 Score per residue for model 6

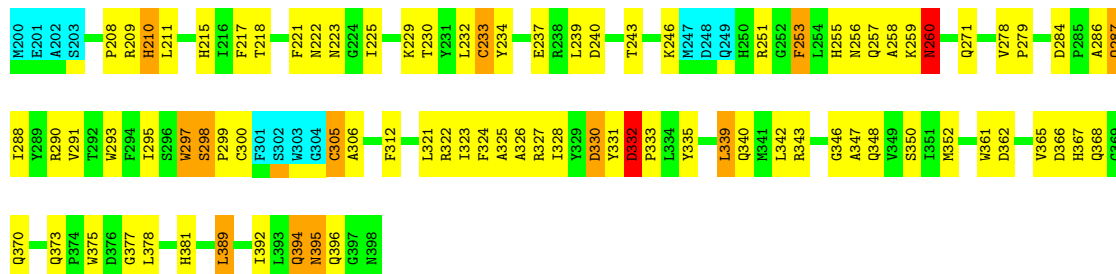
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A: 



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain C: 



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain D:  60% 40%

A409  
T410  
T411  
T412  
T413  
C414  
A415  
A416  
T417  
T418

#### 4.2.7 Score per residue for model 7

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A:  44% 39% 15%

M1 E2 A3 S4 P5 H11 L12 M13 D14 P15 H16 I17 F18 T19 S20 N21 F22 N23 N24 G25 R28 H29 K30 T31 Y32 L33 C34 Y35 E38 R39 L40 D41 N42 G43 T44 S45 V46 K47 M48 D49 Q50 H51 R52 G53 F54 L55 H56 N57 Q58 A59 K60 N61 L62 R69 H70

R74 V79 P80 D85 P86 A87 Q88 R91 W94 S97 S99 P100 C101 F102 S103 W104 G105 C106 A107 V110 H119 L122 R123 T124 F125 A126 R128 I129 Y130 D131 Y132 D133 P134 L135 Y136 K137 E138 A139 L140 Q141 G147 A148 Q149 M153 T154 Y155 W162

D163 T164 F166 V166 D167 H168 P172 F173 Q174 L179 D180 E181 S182 S183 L186 L190 I193 L194 Q195 M196 Q197 G198 N199

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B:  56% 30% 8% 6%

W200 E201 S202 S203 P208 R209 H210 L211 M212 D213 F217 N220 N222 N223 G224 I225 H228 K229 T230 Y231 L232 C233 Y234 E235 K246 M247 D248 Q249 H250 R251 G252 F253 L254 H255 N256 Q257 A258 K259 W260 F274 L277 V278 P279 A286 Q287 W293 F294 Y295 S296 W297

S298 P299 C300 F301 S302 W303 C305 A306 F312 K316 F317 H318 L321 R322 R327 L328 Y329 D332 P333 L334 Y335 L339 G346 A347 Q346 M352 K361 D362 Y365 D366 H367 Q368 C369 Q370 P371 F372 Q373 P374 K375 L378 D379 S382 R388 L389 R390 A391

I392 L393 Q394 N395 Q396 G397 N398

- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain C:  40% 40% 20%

A399  
T400  
T401  
T402  
T403  
T407  
T408

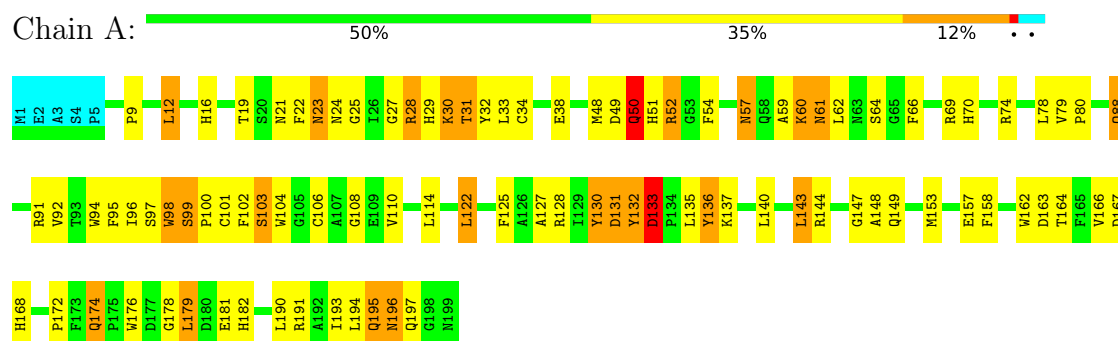
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain D:  60% 40%

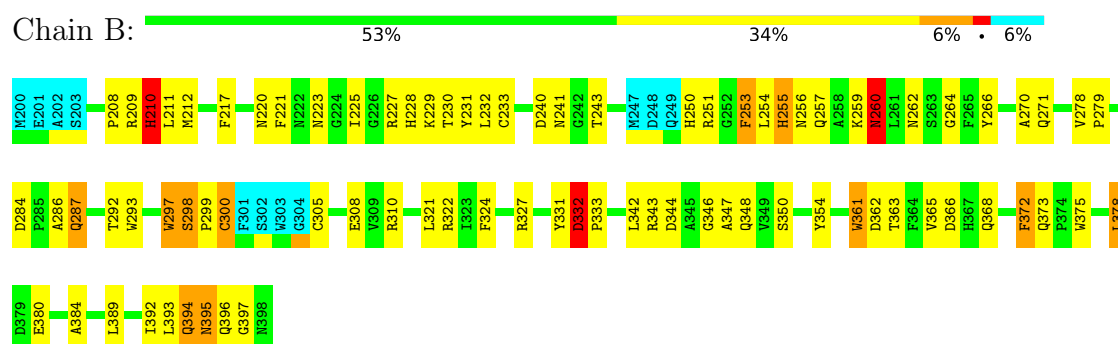
A409  
T410  
T411  
T412  
T413  
C414  
A415  
A416  
T417  
T418

### 4.2.8 Score per residue for model 8

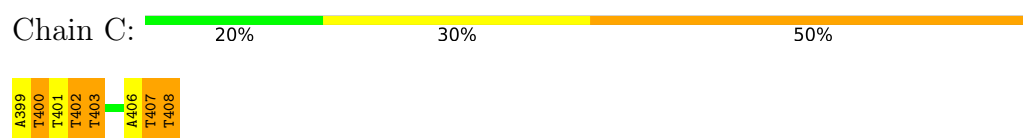
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



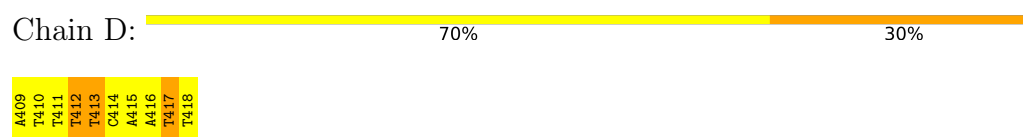
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



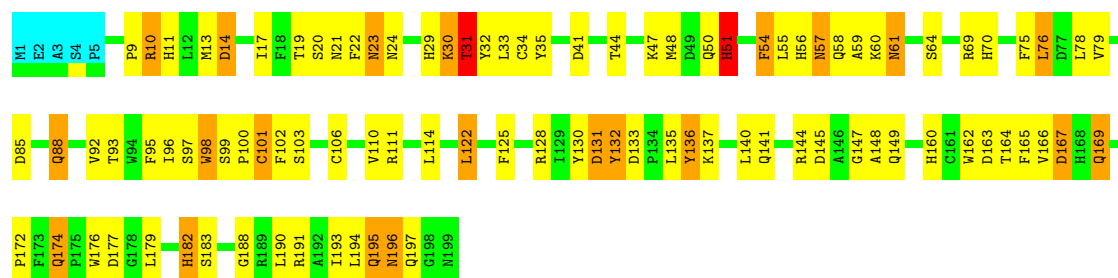
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



### 4.2.9 Score per residue for model 9

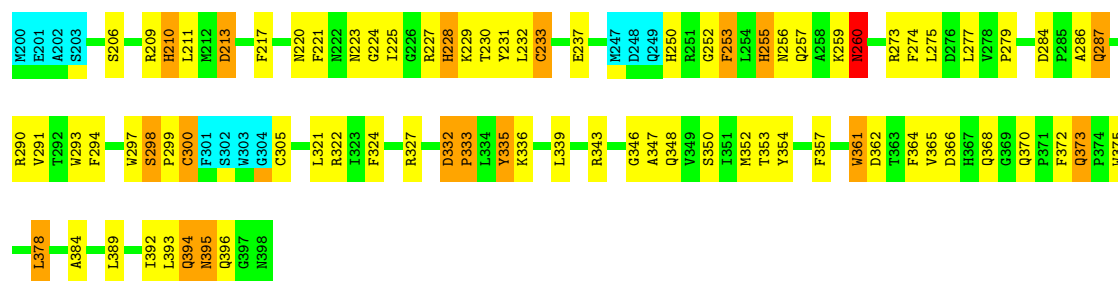
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 54% 31% 9% 6%



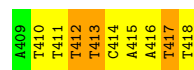
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain C: 30% 40% 30%



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

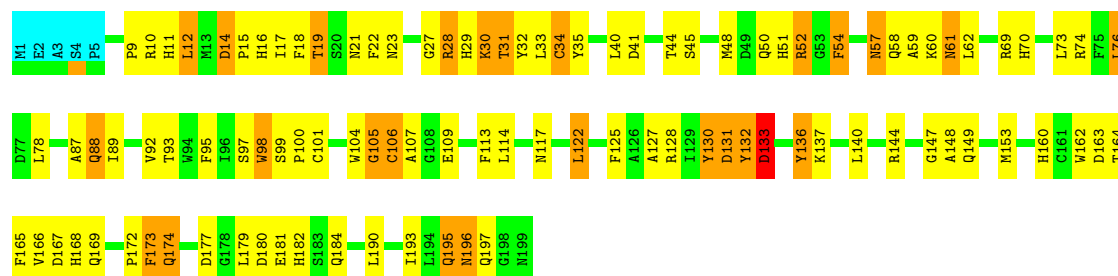
Chain D: 10% 60% 30%



#### 4.2.10 Score per residue for model 10

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

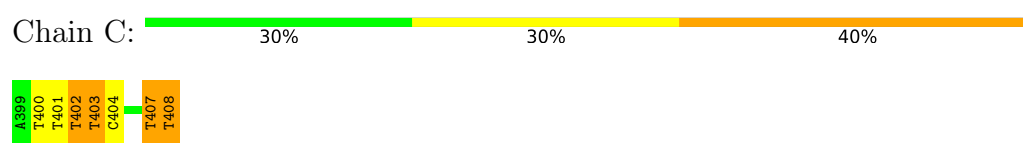
Chain A: 47% 38% 13%



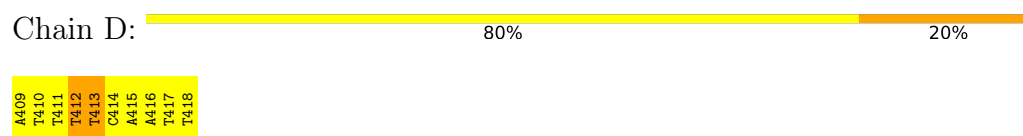
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

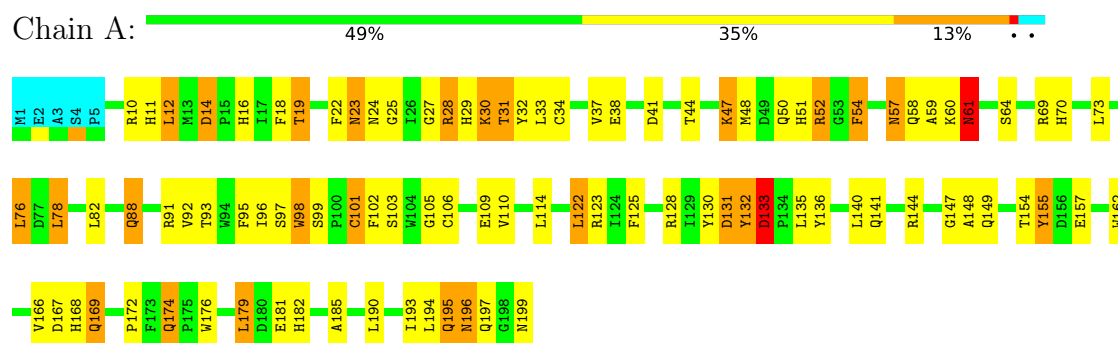


- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

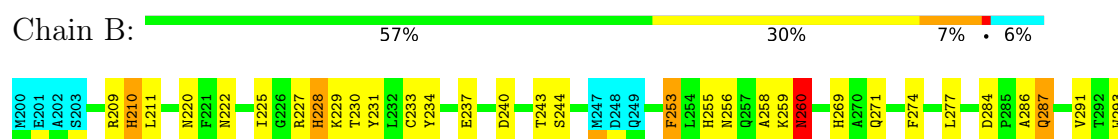


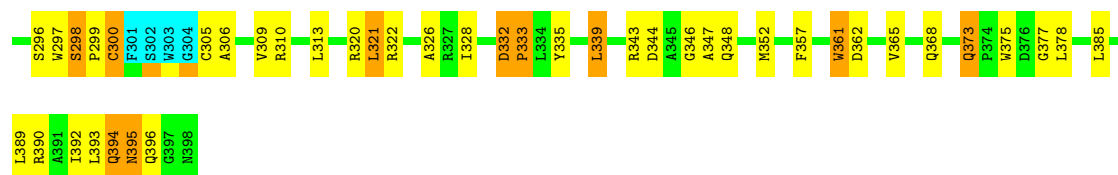
#### 4.2.11 Score per residue for model 11

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





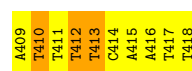
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain C: 40% 40% 20%



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

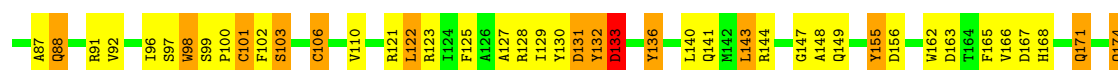
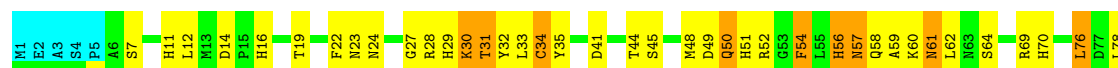
Chain D: 70% 30%



#### 4.2.12 Score per residue for model 12

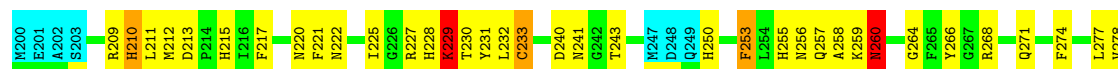
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A: 52% 33% 13% • •

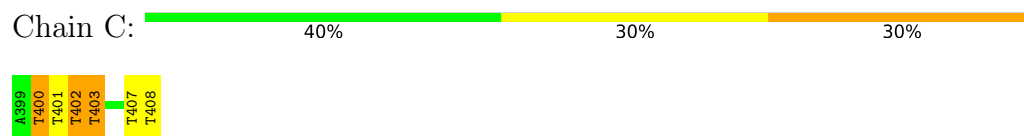


- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

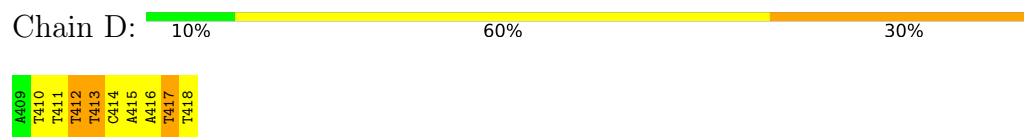
Chain B: 50% 35% 8% • 6%



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

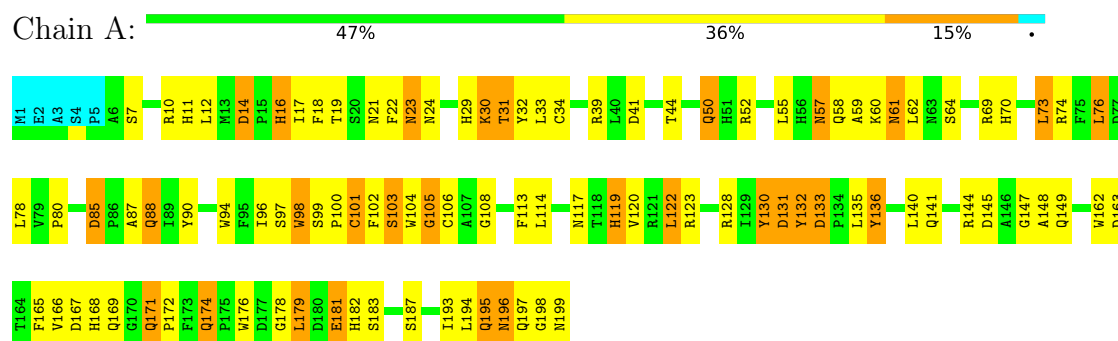


- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

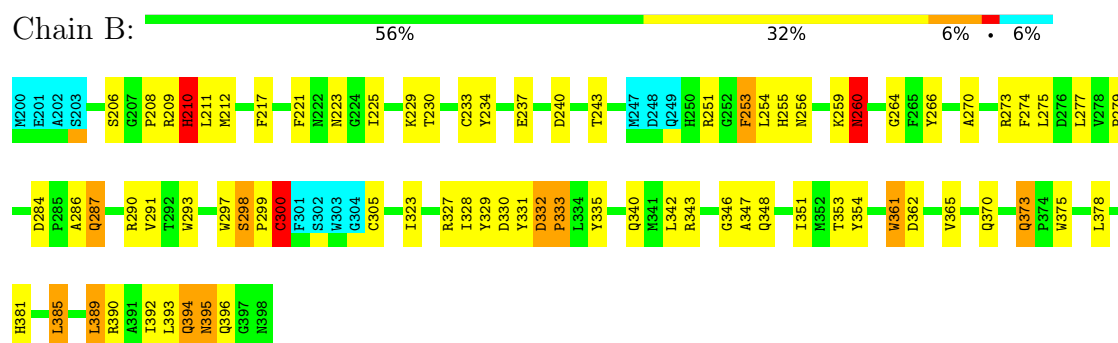


#### 4.2.13 Score per residue for model 13

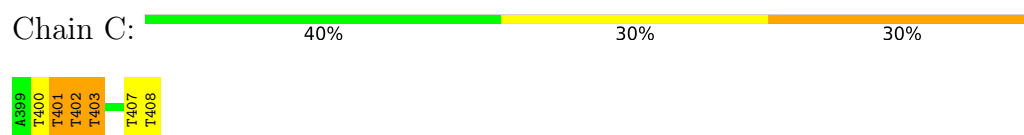
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



Chain D:  70% 30%

A409  
T410  
T411  
T412  
T413  
C414  
A415  
A416  
T417  
T418

#### 4.2.14 Score per residue for model 14

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A:  45% 37% 14% • •

M1 E2 A3 S4 P5 A6 S7 G8 P9 R10 H11 H12 M13 M14 D14 P15 H16 T19 S20 N21 F22 N23 N24 G25 T26 G27 R28 R29 K30 T31 Y32 L33 C34 E38 S45 W46 K47 M48 D49 Q50 H51 H52 G53 P54 L55 H56 N57 Q58 A59 R60 N61 R69 H70 L76 D77 L78

D85 P86 A87 Q88 R91 W94 F95 I96 S97 Q98 S99 P100 C101 F102 W104 G105 A107 G108 L114 H119 V120 R121 R122 T31 R123 L124 F125 R128 I129 Y130 D131 Y132 D133 P134 L135 Y136 K137 Q141 R144 G147 A148 Q149 V150 S151 E157 W162 D163 T164

F165 V166 D167 H168 Q169 P172 F173 Q174 P175 W176 D180 E181 H182 S183 Q184 A185 L186 S187 R191 A192 I193 L194 Q195 N196 G198 N199

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B:  52% 35% 7% • 6%

W200 E201 A202 S203 G207 P208 R209 H210 L211 M212 D213 F217 N220 F221 L225 H228 K229 T230 Y231 L232 C233 D240 N241 G242 T243 M247 D248 Q249 H250 R251 G252 F253 L254 H255 A258 K259 W260 L261 N262 S263 G264 F265 Y266 G267 R268 L272 L281 D284 P285

A286 Q287 V291 W293 W297 S298 P299 C300 F301 S302 V303 G304 A306 V309 R310 K320 L321 R322 A325 A326 D332 P333 L334 Y335 K336 L339 Q340 R343 D344 A345 G346 A347 Q348 K352 W361 D362 T363 F364 V365 D366 H367 Q368 G369 Q370 Q373 P374 W375

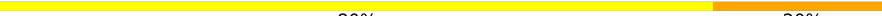
D376 G377 L378 D379 H380 E381 S382 L389 R390 A391 I392 L393 Q394 N395 Q396 G397 N398

- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain C:  40% 30% 30%

A399  
T400  
T401  
T402  
T403  
T407  
T408

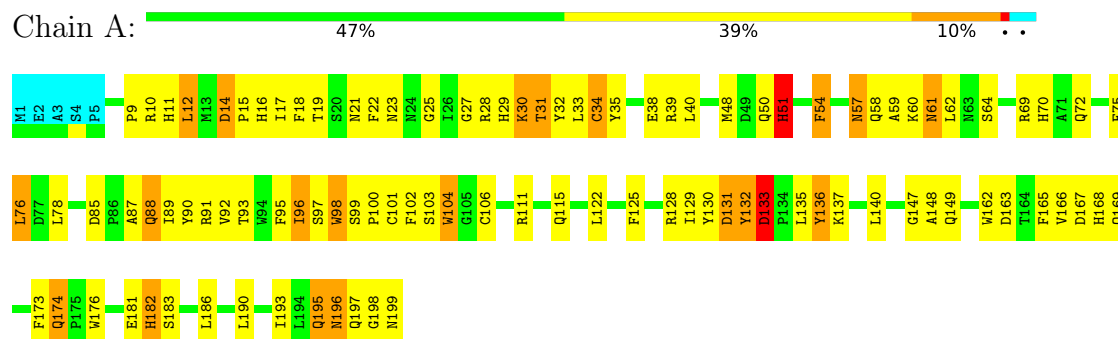
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain D:  80% 20%

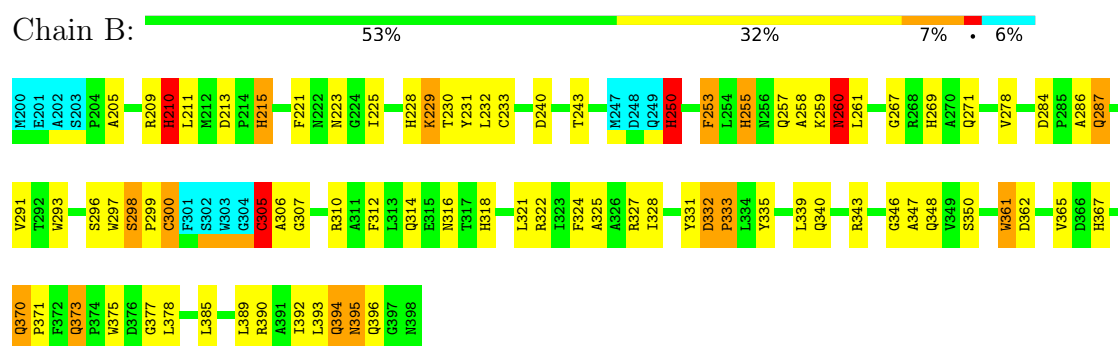
A409  
T410  
T411  
T412  
T413  
C414  
A415  
A416  
T417  
T418

### 4.2.15 Score per residue for model 15

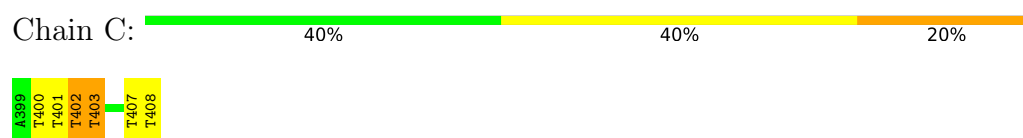
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



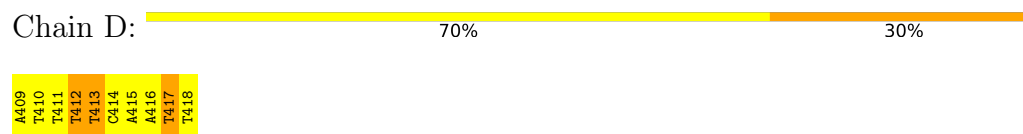
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



### 4.2.16 Score per residue for model 16

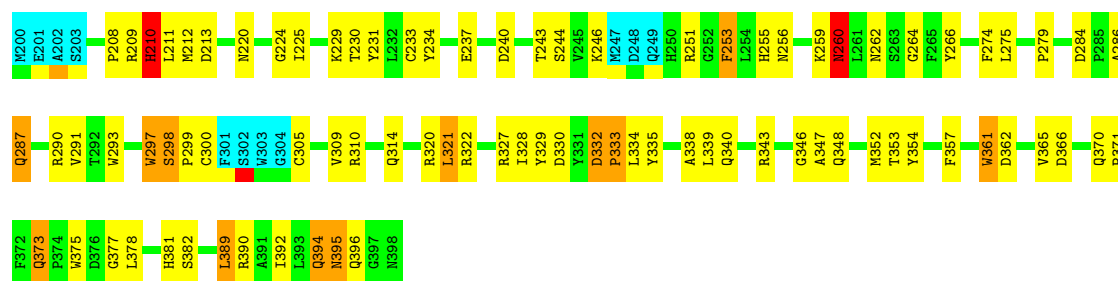
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





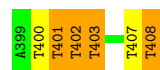
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 52% 36% 6% • 6%



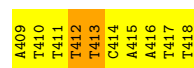
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

Chain C: 40% 20% 40%



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

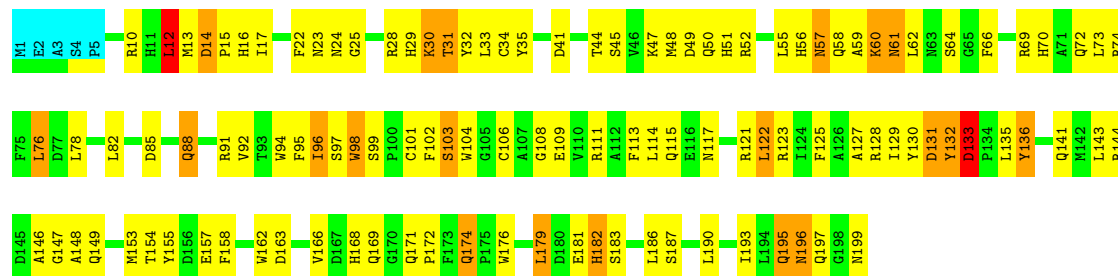
Chain D: 80% 20%



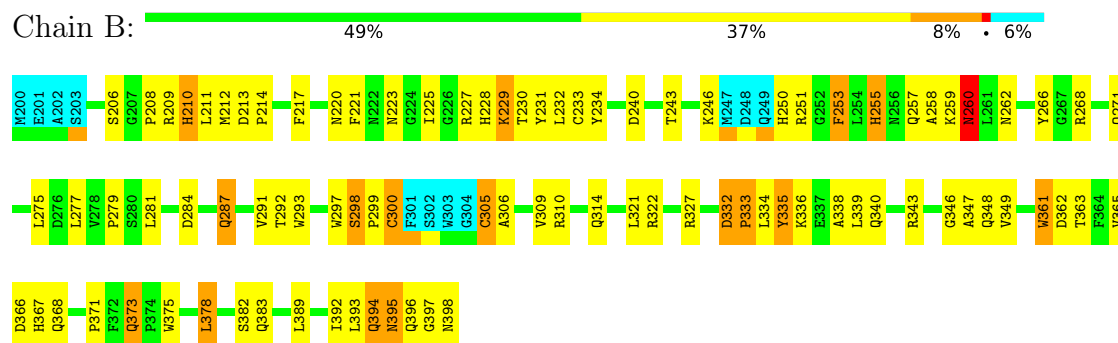
#### 4.2.17 Score per residue for model 17

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

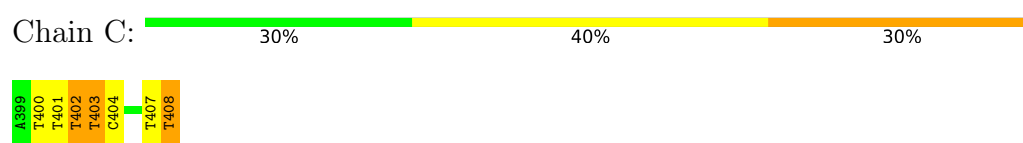
Chain A: 40% 46% 10% • •



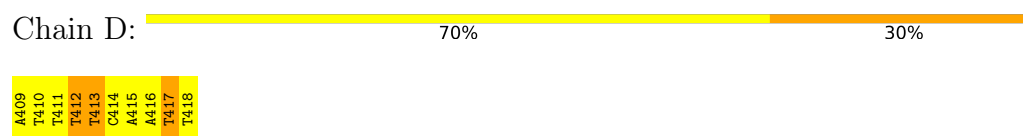
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

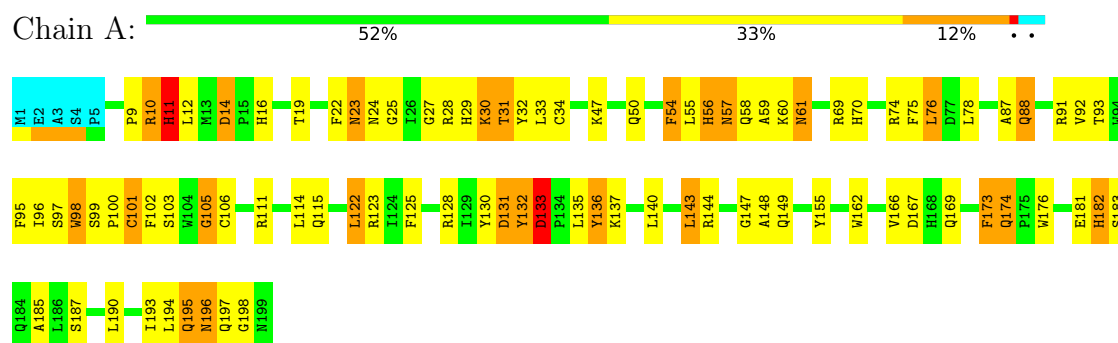


- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

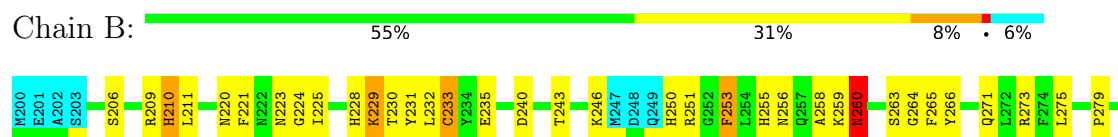


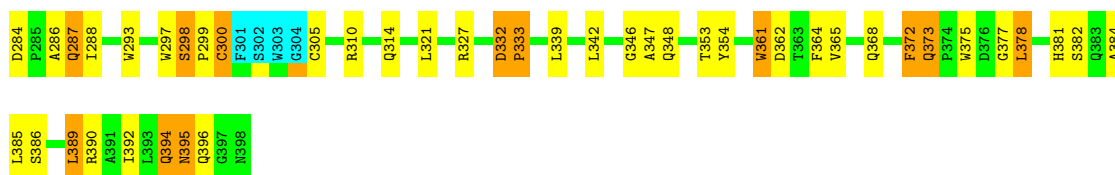
#### 4.2.18 Score per residue for model 18

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

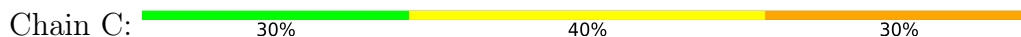


- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

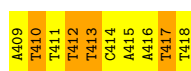




- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

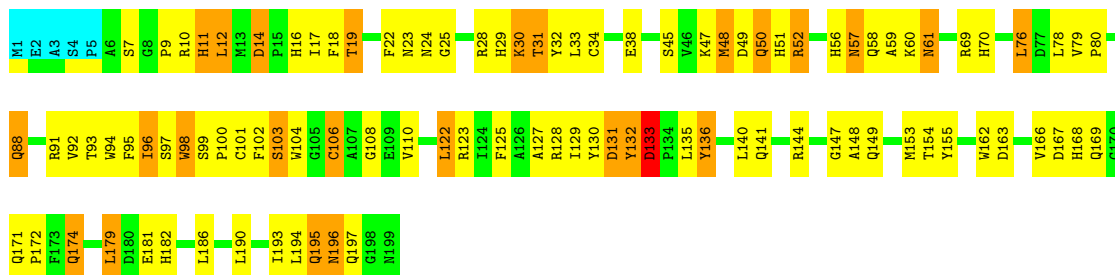


- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

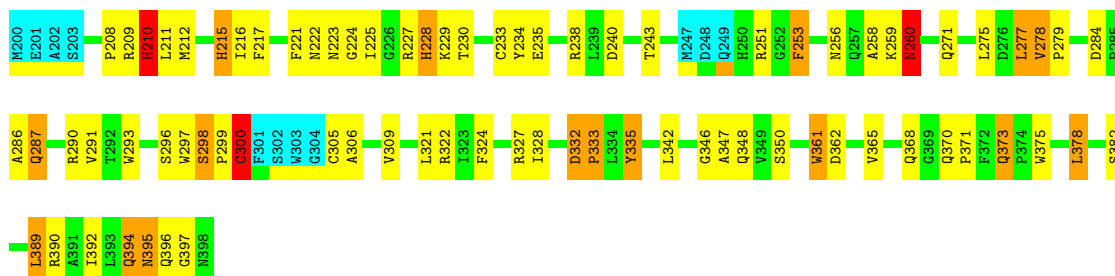


#### 4.2.19 Score per residue for model 19

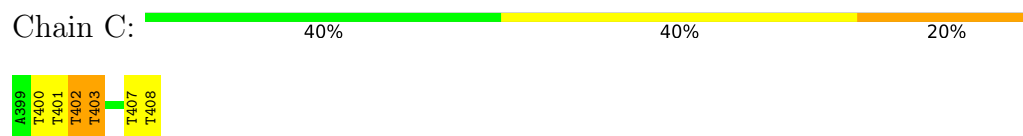
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



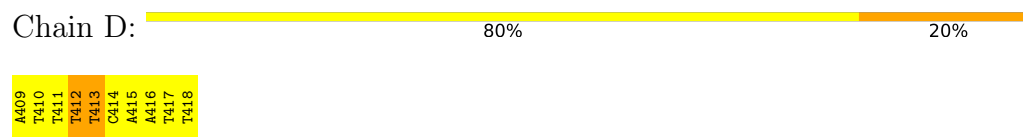
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

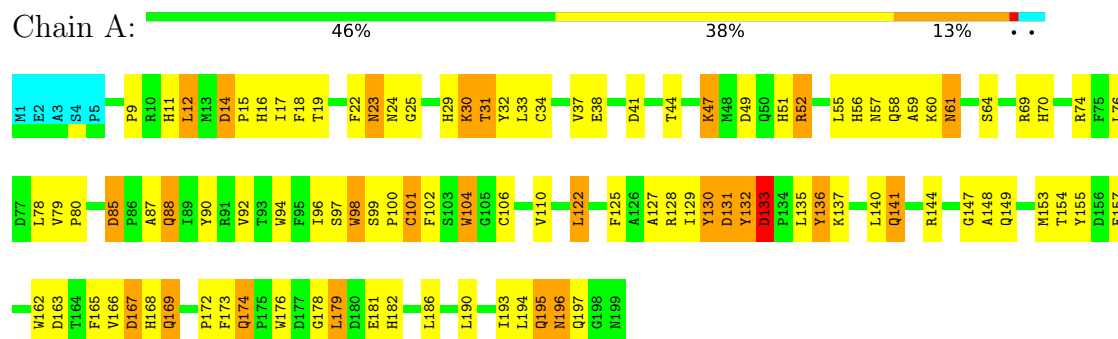


- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')

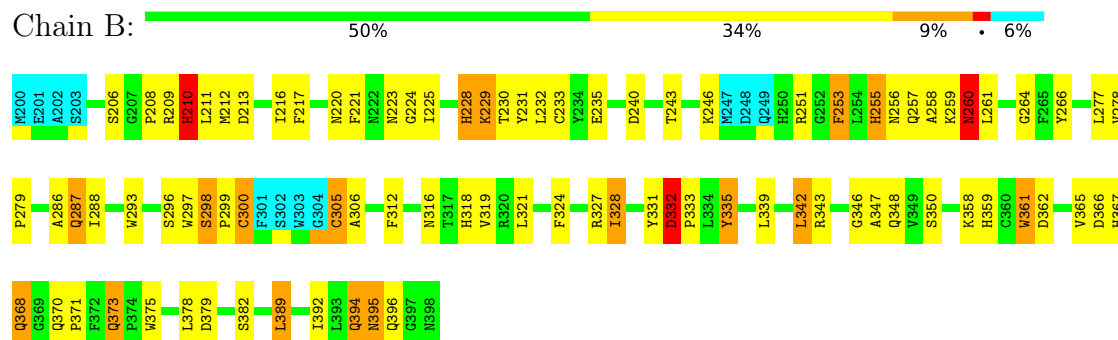


#### 4.2.20 Score per residue for model 20

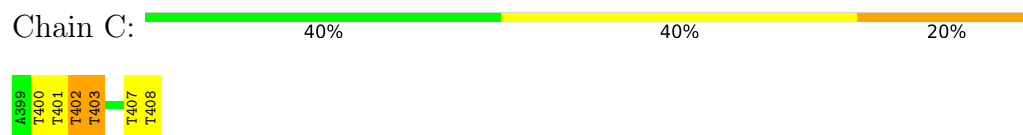
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



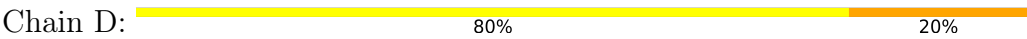
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*TP\*TP\*CP\*AP\*AP\*TP\*T)-3')



A409	T410	T411	T412	T413	C414	A415	A416	T417	T418
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## 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
X-PLOR NIH	structure calculation	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	4564
Number of shifts mapped to atoms	4564
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%



## 6 Model quality (i)

### 6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.00±0.00	0±0/1638 ( 0.0± 0.0%)	0.92±0.00	1±0/2218 ( 0.0± 0.0%)
1	B	1.00±0.00	0±0/1583 ( 0.0± 0.0%)	0.90±0.00	0±0/2144 ( 0.0± 0.0%)
2	C	1.38±0.04	1±1/221 ( 0.5± 0.6%)	1.74±0.01	11±1/339 ( 3.3± 0.4%)
2	D	1.28±0.01	1±1/221 ( 0.4± 0.3%)	1.71±0.01	12±1/339 ( 3.4± 0.2%)
All	All	1.05	37/73260 ( 0.1%)	1.06	464/100800 ( 0.5%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	402	DT	C5-C7	6.17	1.53	1.50	8	3
2	C	401	DT	C5-C7	5.70	1.53	1.50	8	8
2	C	407	DT	C5-C7	5.25	1.53	1.50	8	1
2	D	412	DT	C5-C7	5.23	1.53	1.50	11	4
2	D	418	DT	C5-C7	5.16	1.53	1.50	20	4
2	C	408	DT	C5-C7	5.16	1.53	1.50	6	6
2	D	411	DT	C5-C7	5.11	1.53	1.50	12	5
2	D	410	DT	C5-C7	5.10	1.53	1.50	11	3
2	C	402	DT	C4'-O4'	-5.04	1.40	1.45	20	1
2	C	400	DT	C5-C7	5.03	1.53	1.50	3	1
2	C	401	DT	C4'-O4'	-5.01	1.40	1.45	8	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	402	DT	C6-C5-C7	-7.81	118.22	122.90	17	19
2	C	401	DT	C6-C5-C7	-6.89	118.77	122.90	16	19
2	C	403	DT	C6-C5-C7	-6.88	118.77	122.90	16	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	D	417	DT	C6-C5-C7	-6.88	118.77	122.90	20	20
2	D	410	DT	C6-C5-C7	-6.51	119.00	122.90	4	20
2	C	407	DT	C6-C5-C7	-6.43	119.04	122.90	15	20
2	C	400	DT	C6-C5-C7	-6.32	119.11	122.90	8	20
2	D	413	DT	C6-C5-C7	-6.29	119.13	122.90	9	20
1	A	130	TYR	CB-CG-CD1	-6.18	117.29	121.00	1	13
2	D	412	DT	C6-C5-C7	-6.06	119.26	122.90	13	20
2	C	408	DT	C6-C5-C7	-6.04	119.28	122.90	14	20
2	C	403	DT	C4-C5-C6	6.00	121.60	118.00	11	20
2	D	411	DT	C6-C5-C7	-5.99	119.31	122.90	9	20
2	D	418	DT	C6-C5-C7	-5.98	119.31	122.90	14	20
2	C	401	DT	O4'-C1'-N1	-5.81	103.93	108.00	8	4
2	C	402	DT	O4'-C1'-N1	-5.78	103.96	108.00	8	8
2	D	413	DT	C4-C5-C6	5.70	121.42	118.00	10	20
2	C	400	DT	C4-C5-C6	5.45	121.27	118.00	8	20
2	D	417	DT	C4-C5-C6	5.39	121.23	118.00	8	18
2	C	401	DT	C4-C5-C6	5.38	121.22	118.00	5	11
2	C	402	DT	C4-C5-C6	5.36	121.22	118.00	17	9
2	D	411	DT	C4-C5-C6	5.36	121.22	118.00	9	20
2	D	412	DT	C4-C5-C6	5.33	121.20	118.00	13	20
2	D	410	DT	C4-C5-C6	5.30	121.18	118.00	5	15
2	C	407	DT	C4-C5-C6	5.27	121.16	118.00	16	15
2	C	408	DT	C4-C5-C6	5.23	121.14	118.00	15	16
2	D	418	DT	C4-C5-C6	5.23	121.14	118.00	15	17

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	A	1591	1512	1503	135±10
1	B	1538	1471	1462	100±11
2	C	199	117	118	5±2
2	D	199	117	118	22±3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	70580	64340	64020	4584

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:378:LEU:H	1:B:378:LEU:HD22	0.94	1.23	10	12
1:A:179:LEU:HD22	1:A:179:LEU:H	0.93	1.22	3	15
1:B:250:HIS:NE2	1:B:281:LEU:HD21	0.90	1.81	10	1
1:B:361:TRP:CE3	1:B:365:VAL:HG21	0.88	2.03	9	17
1:B:343:ARG:HH11	1:B:393:LEU:HD11	0.88	1.28	17	1
1:A:144:ARG:HE	1:A:194:LEU:HD11	0.88	1.29	16	3
1:A:119:HIS:CD2	1:A:120:VAL:HG23	0.87	2.05	14	3
1:B:205:ALA:HB1	1:B:209:ARG:HH22	0.86	1.28	15	1
1:B:298:SER:OG	1:B:339:LEU:HD21	0.85	1.70	12	2
1:A:144:ARG:NE	1:A:194:LEU:HD11	0.85	1.86	16	3
1:B:225:ILE:HD12	2:C:402:DT:OP2	0.85	1.72	1	19
1:A:16:HIS:CG	1:B:258:ALA:HB3	0.85	2.06	20	11
1:A:78:LEU:HD11	1:B:209:ARG:NE	0.85	1.87	3	2
1:B:335:TYR:OH	1:B:392:ILE:HD11	0.85	1.71	3	5
1:B:335:TYR:CE1	1:B:339:LEU:HD11	0.84	2.07	15	1
1:A:140:LEU:HD23	1:A:193:ILE:HG21	0.83	1.47	6	1
1:A:62:LEU:HD11	2:D:417:DT:OP1	0.83	1.74	12	6
1:A:16:HIS:ND1	1:B:258:ALA:HB3	0.82	1.88	11	6
1:B:205:ALA:HB1	1:B:209:ARG:NH2	0.82	1.90	15	1
1:A:31:THR:HG22	1:A:98:TRP:CZ2	0.79	2.12	14	20
1:A:140:LEU:HD13	1:A:193:ILE:HD13	0.79	1.54	7	11
1:B:343:ARG:NH1	1:B:393:LEU:HD11	0.79	1.92	17	1
1:A:62:LEU:HD21	2:D:417:DT:OP1	0.79	1.78	1	2
1:B:361:TRP:CD1	1:B:362:ASP:N	0.78	2.51	12	20
1:A:14:ASP:CG	1:A:17:ILE:HD12	0.78	1.98	19	7
1:B:293:TRP:CH2	1:B:321:LEU:HD11	0.78	2.14	1	4
1:A:162:TRP:HE1	1:A:168:HIS:CD2	0.78	1.96	16	4
1:A:12:LEU:HD23	1:A:167:ASP:CG	0.78	1.99	3	1
1:B:339:LEU:HD23	1:B:392:ILE:HG21	0.78	1.56	16	4
1:A:31:THR:HG23	1:A:32:TYR:N	0.78	1.94	14	20
1:A:102:PHE:CE2	1:A:135:LEU:HD13	0.77	2.13	14	4
1:B:246:LYS:HZ3	1:B:251:ARG:HE	0.77	1.16	16	1
1:A:179:LEU:HD22	1:A:179:LEU:N	0.77	1.95	9	15
1:B:378:LEU:HD22	1:B:378:LEU:N	0.76	1.96	7	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:ASP:OD1	1:A:17:ILE:HD12	0.76	1.80	15	3
1:A:94:TRP:CH2	1:A:122:LEU:HD11	0.76	2.16	20	10
1:B:230:THR:HG23	1:B:256:ASN:OD1	0.75	1.81	13	4
1:A:94:TRP:CE2	1:A:122:LEU:HD21	0.75	2.17	2	10
1:A:78:LEU:HD23	1:A:78:LEU:O	0.75	1.82	4	5
1:A:14:ASP:OD2	1:A:17:ILE:HD12	0.74	1.83	1	4
1:A:144:ARG:HH11	1:A:194:LEU:HD11	0.74	1.41	3	1
1:A:96:ILE:HD12	1:A:96:ILE:H	0.74	1.43	5	1
1:A:57:ASN:H	1:A:57:ASN:ND2	0.73	1.81	17	10
1:A:33:LEU:O	1:A:33:LEU:HD23	0.73	1.84	10	8
1:B:335:TYR:CD1	1:B:336:LYS:N	0.73	2.57	5	3
1:A:140:LEU:HD13	1:A:193:ILE:HG21	0.72	1.61	19	3
1:B:305:CYS:O	1:B:309:VAL:HG23	0.72	1.85	10	9
1:A:129:ILE:HD11	1:A:186:LEU:CD1	0.72	2.14	16	9
1:B:293:TRP:CZ2	1:B:321:LEU:HD21	0.71	2.20	5	5
1:B:220:ASN:ND2	1:B:231:TYR:CZ	0.71	2.59	5	5
1:A:102:PHE:CD1	1:A:135:LEU:HD13	0.71	2.21	9	2
1:A:57:ASN:N	1:A:57:ASN:ND2	0.71	2.39	3	9
1:A:102:PHE:CE1	1:A:135:LEU:HD13	0.71	2.20	15	3
1:A:162:TRP:NE1	1:A:168:HIS:CD2	0.71	2.59	6	4
1:B:220:ASN:ND2	1:B:231:TYR:CE2	0.70	2.59	8	2
1:A:16:HIS:CD2	1:B:258:ALA:HB3	0.70	2.21	20	1
1:A:182:HIS:ND1	1:A:183:SER:N	0.70	2.38	14	4
1:B:335:TYR:CD2	1:B:336:LYS:N	0.70	2.60	12	3
1:A:91:ARG:NE	1:A:121:ARG:NH1	0.70	2.40	16	1
1:A:144:ARG:NH1	1:A:194:LEU:HD11	0.70	2.02	3	1
1:A:22:PHE:CE2	1:A:32:TYR:CZ	0.70	2.80	10	1
1:A:179:LEU:H	1:A:179:LEU:CD2	0.70	1.99	12	15
1:B:230:THR:HG22	1:B:256:ASN:OD1	0.70	1.87	3	1
1:A:31:THR:HG22	1:A:98:TRP:CH2	0.70	2.22	9	20
1:B:361:TRP:CZ2	1:B:367:HIS:CD2	0.70	2.80	12	4
1:B:220:ASN:ND2	1:B:231:TYR:CG	0.70	2.59	11	2
1:B:220:ASN:ND2	1:B:231:TYR:CE1	0.70	2.60	17	5
1:B:225:ILE:N	2:C:403:DT:H72	0.69	2.02	11	14
1:A:95:PHE:CE1	1:A:125:PHE:CD1	0.69	2.80	11	5
1:A:95:PHE:CE1	1:A:125:PHE:CD2	0.69	2.80	1	3
1:B:246:LYS:NZ	1:B:251:ARG:NH1	0.69	2.41	7	6
1:B:232:LEU:C	1:B:232:LEU:HD23	0.69	2.08	8	10
1:A:10:ARG:NH2	1:B:277:LEU:HD11	0.69	2.02	5	1
1:B:231:TYR:CE2	1:B:255:HIS:CD2	0.69	2.81	7	3
1:A:91:ARG:NH1	1:A:123:ARG:NH2	0.69	2.40	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:312:PHE:CZ	1:B:316:ASN:ND2	0.69	2.61	4	5
1:B:253:PHE:O	1:B:254:LEU:HD12	0.69	1.88	13	1
1:A:162:TRP:CE3	1:A:166:VAL:HG21	0.69	2.22	18	1
1:B:217:PHE:CE1	1:B:221:PHE:CE1	0.69	2.81	1	3
1:A:95:PHE:CE2	1:A:125:PHE:CD2	0.69	2.81	18	5
1:A:48:MET:SD	1:A:48:MET:N	0.69	2.65	1	3
1:A:56:HIS:ND1	1:A:56:HIS:N	0.69	2.40	2	2
1:A:57:ASN:ND2	1:A:57:ASN:N	0.69	2.41	10	10
1:B:320:ARG:NH2	1:B:322:ARG:HE	0.69	1.86	4	1
1:B:343:ARG:NH1	1:B:396:GLN:NE2	0.69	2.41	6	4
1:A:135:LEU:C	1:A:135:LEU:HD12	0.69	2.08	17	1
1:B:231:TYR:CZ	1:B:255:HIS:NE2	0.69	2.60	3	2
1:B:294:PHE:CE1	1:B:324:PHE:CD1	0.69	2.81	9	1
1:A:106:CYS:O	1:A:110:VAL:HG23	0.69	1.88	2	14
1:A:162:TRP:NE1	1:A:168:HIS:NE2	0.68	2.41	2	2
1:B:305:CYS:SG	1:B:306:ALA:N	0.68	2.66	7	7
1:A:136:TYR:CG	1:A:137:LYS:N	0.68	2.61	10	13
1:B:361:TRP:NE1	1:B:367:HIS:CD2	0.68	2.61	6	5
1:B:361:TRP:CZ2	1:B:365:VAL:HG11	0.68	2.24	9	2
1:B:231:TYR:CE2	1:B:255:HIS:CG	0.68	2.81	18	1
1:B:255:HIS:ND1	1:B:255:HIS:N	0.68	2.40	1	7
1:B:231:TYR:CE1	1:B:255:HIS:CE1	0.68	2.81	12	1
1:B:246:LYS:HZ3	1:B:251:ARG:HH12	0.68	1.30	7	1
1:B:253:PHE:CE2	1:B:364:PHE:CE1	0.68	2.81	10	1
1:B:231:TYR:CD1	1:B:255:HIS:ND1	0.68	2.62	12	1
1:B:378:LEU:H	1:B:378:LEU:CD2	0.68	2.01	10	12
1:A:54:PHE:CZ	1:A:56:HIS:CE1	0.68	2.81	14	2
1:A:131:ASP:O	1:A:132:TYR:CB	0.68	2.42	8	20
1:A:95:PHE:CE2	1:A:125:PHE:CD1	0.68	2.82	6	3
1:B:217:PHE:CE2	1:B:221:PHE:CE2	0.68	2.82	12	5
1:B:361:TRP:NE1	1:B:367:HIS:NE2	0.68	2.41	12	6
1:B:212:MET:SD	1:B:253:PHE:CE2	0.68	2.87	2	1
1:A:96:ILE:HD12	1:A:96:ILE:N	0.68	2.03	5	1
1:B:312:PHE:CE2	1:B:316:ASN:ND2	0.67	2.61	2	3
1:B:367:HIS:ND1	1:B:370:GLN:NE2	0.67	2.42	7	1
1:A:11:HIS:CG	1:A:11:HIS:O	0.67	2.47	5	8
1:B:367:HIS:CE1	1:B:370:GLN:NE2	0.67	2.62	7	1
1:A:144:ARG:HE	1:A:194:LEU:HD21	0.67	1.49	6	2
1:B:294:PHE:CE1	1:B:352:MET:SD	0.67	2.88	7	1
1:B:217:PHE:CZ	1:B:221:PHE:CZ	0.67	2.83	1	2
1:A:144:ARG:NH2	1:A:197:GLN:NE2	0.67	2.42	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:TRP:CZ2	1:A:168:HIS:CD2	0.67	2.83	11	2
1:B:255:HIS:CD2	1:B:257:GLN:H	0.67	2.08	12	2
1:B:250:HIS:CD2	1:B:281:LEU:HD21	0.67	2.24	10	1
1:A:140:LEU:HD22	1:A:193:ILE:HG21	0.67	1.66	11	1
1:A:97:SER:O	1:A:128:ARG:N	0.67	2.28	6	20
1:A:119:HIS:NE2	1:A:120:VAL:HG23	0.67	2.05	13	3
1:B:217:PHE:CE2	1:B:221:PHE:CE1	0.67	2.83	19	2
1:B:255:HIS:CE1	1:B:257:GLN:NE2	0.67	2.63	15	4
1:B:255:HIS:CE1	1:B:257:GLN:H	0.66	2.07	7	1
1:A:140:LEU:HD23	1:A:140:LEU:C	0.66	2.10	11	3
1:B:255:HIS:H	1:B:255:HIS:CD2	0.66	2.06	2	1
1:A:98:TRP:CZ3	2:D:414:DC:C2	0.66	2.83	12	20
1:B:294:PHE:CD2	1:B:352:MET:SD	0.66	2.88	1	3
1:A:11:HIS:ND1	1:B:210:HIS:O	0.66	2.29	3	6
1:B:220:ASN:ND2	1:B:231:TYR:CD2	0.66	2.63	2	2
1:B:326:ALA:HB2	1:B:352:MET:CE	0.66	2.21	6	3
1:A:182:HIS:CE1	2:D:409:DA:C6	0.66	2.84	3	13
1:B:320:ARG:NH1	1:B:322:ARG:NH1	0.66	2.43	11	1
1:B:361:TRP:O	1:B:365:VAL:HG23	0.66	1.90	11	20
1:B:233:CYS:SG	1:B:364:PHE:CZ	0.66	2.88	9	1
1:B:294:PHE:CE2	1:B:352:MET:SD	0.66	2.89	12	3
1:A:102:PHE:CZ	1:A:135:LEU:HD13	0.66	2.25	14	2
1:A:28:ARG:HH11	1:A:31:THR:N	0.66	1.89	3	1
1:A:94:TRP:CZ2	1:A:122:LEU:HD21	0.66	2.26	13	4
1:A:129:ILE:HD11	1:A:186:LEU:HD13	0.66	1.67	7	9
1:A:127:ALA:HB2	1:A:153:MET:CE	0.66	2.21	5	2
1:B:340:GLN:NE2	1:B:392:ILE:HG22	0.66	2.06	5	2
1:A:34:CYS:SG	1:A:165:PHE:CZ	0.66	2.88	13	9
1:B:290:ARG:NE	1:B:322:ARG:NH2	0.66	2.44	10	1
1:A:10:ARG:HH12	1:B:273:ARG:NH1	0.66	1.89	18	2
1:B:378:LEU:HD12	1:B:378:LEU:N	0.66	2.06	2	8
1:B:312:PHE:CE1	1:B:316:ASN:ND2	0.65	2.64	15	2
1:B:255:HIS:CD2	1:B:256:ASN:N	0.65	2.64	7	1
1:B:361:TRP:HE1	1:B:367:HIS:CD2	0.65	2.08	6	2
1:A:125:PHE:CD1	1:A:153:MET:SD	0.65	2.89	7	1
1:B:294:PHE:CD1	1:B:352:MET:SD	0.65	2.89	7	1
1:A:135:LEU:HD12	1:A:136:TYR:N	0.65	2.05	9	3
1:B:290:ARG:NH1	1:B:322:ARG:HH21	0.65	1.89	19	1
1:A:182:HIS:NE2	2:D:409:DA:N6	0.65	2.44	19	2
1:A:125:PHE:CD2	1:A:153:MET:SD	0.65	2.89	3	1
1:B:343:ARG:HH12	1:B:396:GLN:NE2	0.65	1.88	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:335:TYR:CZ	1:B:339:LEU:HD11	0.65	2.26	15	1
1:B:287:GLN:HE21	1:B:287:GLN:N	0.65	1.89	14	19
1:A:182:HIS:CE1	2:D:409:DA:N6	0.65	2.65	11	4
1:A:144:ARG:NH2	1:A:197:GLN:HE22	0.65	1.90	19	3
1:B:340:GLN:HE22	1:B:343:ARG:NH2	0.65	1.90	13	1
1:B:373:GLN:H	1:B:373:GLN:NE2	0.65	1.90	11	4
1:A:11:HIS:CD2	1:B:212:MET:SD	0.65	2.90	12	2
1:B:298:SER:N	1:B:299:PRO:CD	0.65	2.60	5	20
1:A:182:HIS:NE2	2:D:409:DA:C6	0.65	2.64	8	3
1:B:320:ARG:CZ	1:B:348:GLN:NE2	0.65	2.60	14	1
1:B:373:GLN:HE21	1:B:373:GLN:N	0.65	1.90	2	6
1:A:102:PHE:CD2	1:A:135:LEU:HD13	0.65	2.27	17	1
1:B:332:ASP:H	1:B:333:PRO:CD	0.64	2.04	12	14
1:A:54:PHE:CE1	1:A:56:HIS:NE2	0.64	2.65	14	1
1:A:193:ILE:O	1:A:196:ASN:ND2	0.64	2.31	16	20
1:A:50:GLN:NE2	1:A:52:ARG:NH1	0.64	2.46	7	2
1:B:228:HIS:ND1	1:B:228:HIS:N	0.64	2.43	11	1
1:A:45:SER:CB	1:A:91:ARG:NH1	0.64	2.61	17	1
1:A:58:GLN:HE21	1:A:60:LYS:N	0.64	1.90	19	1
1:A:88:GLN:HE21	1:A:88:GLN:N	0.64	1.90	8	17
1:B:255:HIS:CD2	1:B:256:ASN:H	0.64	2.10	7	1
1:B:228:HIS:NE2	1:B:259:LYS:NZ	0.64	2.45	20	1
1:A:144:ARG:NH1	1:A:197:GLN:NE2	0.64	2.46	10	1
1:A:29:HIS:NE2	2:D:415:DA:N7	0.64	2.46	12	18
1:A:144:ARG:CZ	1:A:197:GLN:NE2	0.64	2.60	2	4
1:B:255:HIS:N	1:B:255:HIS:CD2	0.64	2.66	10	2
1:B:300:CYS:SG	1:B:300:CYS:O	0.64	2.56	15	10
1:B:271:GLN:NE2	1:B:293:TRP:CE3	0.64	2.66	12	1
1:A:28:ARG:NH1	1:A:128:ARG:HE	0.64	1.90	19	1
1:B:392:ILE:O	1:B:395:ASN:ND2	0.64	2.31	1	20
1:B:246:LYS:HZ3	1:B:251:ARG:NE	0.64	1.90	16	1
1:A:174:GLN:NE2	1:A:174:GLN:N	0.63	2.46	18	8
1:B:361:TRP:HE1	1:B:367:HIS:CE1	0.63	2.10	6	1
1:B:255:HIS:CE1	1:B:257:GLN:CG	0.63	2.81	8	3
1:A:11:HIS:CE1	1:B:212:MET:SD	0.63	2.91	20	1
1:A:174:GLN:H	1:A:174:GLN:NE2	0.63	1.90	2	2
1:B:231:TYR:CZ	1:B:255:HIS:CD2	0.63	2.86	18	2
1:B:343:ARG:HH11	1:B:396:GLN:NE2	0.63	1.90	6	2
1:B:297:TRP:HE1	1:B:327:ARG:NH1	0.63	1.92	8	1
1:B:343:ARG:CZ	1:B:396:GLN:NE2	0.63	2.61	5	2
1:B:310:ARG:NH1	1:B:341:MET:SD	0.63	2.71	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:GLN:HE22	1:A:193:ILE:HG22	0.63	1.53	14	1
1:A:144:ARG:CZ	1:A:197:GLN:HE21	0.63	2.07	10	4
1:A:140:LEU:HD23	1:A:140:LEU:O	0.63	1.93	12	3
1:B:222:ASN:ND2	2:C:403:DT:C2	0.63	2.67	19	3
1:B:251:ARG:NH2	1:B:363:THR:HG23	0.63	2.07	8	2
1:A:54:PHE:O	1:A:54:PHE:CD1	0.63	2.51	12	4
1:A:58:GLN:NE2	1:A:60:LYS:H	0.63	1.91	19	1
1:A:11:HIS:ND1	1:B:253:PHE:CE2	0.63	2.67	1	1
1:A:54:PHE:CZ	1:A:56:HIS:NE2	0.63	2.66	14	2
1:B:253:PHE:CZ	1:B:255:HIS:ND1	0.63	2.67	16	2
1:A:29:HIS:CE1	2:D:414:DC:OP1	0.63	2.52	17	11
1:B:253:PHE:C	1:B:253:PHE:CD2	0.63	2.70	9	7
1:B:253:PHE:CD1	1:B:253:PHE:C	0.63	2.71	12	5
1:A:57:ASN:HD22	1:A:58:GLN:N	0.63	1.91	18	7
1:A:50:GLN:NE2	1:A:52:ARG:CZ	0.62	2.62	4	1
1:A:48:MET:SD	1:A:51:HIS:CE1	0.62	2.91	10	3
1:B:290:ARG:CZ	1:B:322:ARG:NH1	0.62	2.62	4	1
1:A:33:LEU:C	1:A:33:LEU:HD23	0.62	2.14	7	3
1:A:48:MET:CE	1:A:51:HIS:CE1	0.62	2.82	5	5
1:B:220:ASN:ND2	1:B:231:TYR:CD1	0.62	2.67	16	2
1:A:52:ARG:O	1:B:209:ARG:N	0.62	2.32	19	7
1:A:69:ARG:NH1	1:A:104:TRP:HE1	0.62	1.92	20	2
1:A:29:HIS:O	2:D:415:DA:OP2	0.62	2.18	18	20
1:A:34:CYS:SG	1:A:165:PHE:CE1	0.62	2.89	7	5
1:B:290:ARG:HE	1:B:322:ARG:NH2	0.62	1.92	10	1
1:B:367:HIS:CG	1:B:367:HIS:O	0.62	2.53	1	4
1:A:168:HIS:ND1	1:A:168:HIS:O	0.62	2.32	6	2
1:B:361:TRP:CE2	1:B:367:HIS:CD2	0.62	2.88	12	4
1:A:162:TRP:HE1	1:A:168:HIS:CE1	0.62	2.12	5	2
1:A:54:PHE:O	1:A:54:PHE:CD2	0.62	2.52	10	4
1:B:231:TYR:CE1	1:B:255:HIS:ND1	0.62	2.68	12	1
1:B:297:TRP:N	1:B:297:TRP:CD1	0.62	2.67	16	1
1:A:162:TRP:O	1:A:166:VAL:N	0.62	2.33	6	19
1:A:92:VAL:HG13	1:A:92:VAL:O	0.62	1.95	12	16
2:D:418:DT:H73	2:D:418:DT:OP2	0.62	1.95	6	1
1:A:144:ARG:NH1	1:A:197:GLN:HE21	0.62	1.93	10	1
1:A:11:HIS:CD2	1:B:212:MET:CG	0.62	2.83	19	1
1:A:127:ALA:HB2	1:A:153:MET:SD	0.61	2.35	2	6
1:A:60:LYS:NZ	2:D:416:DA:N7	0.61	2.46	10	2
1:A:174:GLN:N	1:A:174:GLN:HE21	0.61	1.91	3	7
1:B:321:LEU:HD23	1:B:322:ARG:N	0.61	2.09	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:367:HIS:O	1:B:367:HIS:ND1	0.61	2.33	12	5
1:B:343:ARG:CZ	1:B:396:GLN:HE21	0.61	2.08	5	1
1:A:172:PRO:O	1:A:174:GLN:NE2	0.61	2.34	3	15
1:A:9:PRO:O	1:B:210:HIS:CE1	0.61	2.53	5	8
1:B:246:LYS:NZ	1:B:251:ARG:HH12	0.61	1.93	6	2
1:A:31:THR:N	1:A:57:ASN:OD1	0.61	2.33	20	19
1:B:367:HIS:CE1	1:B:370:GLN:O	0.61	2.54	12	5
1:A:91:ARG:HH11	1:A:123:ARG:NH2	0.61	1.94	6	2
1:A:19:THR:O	1:A:23:ASN:N	0.61	2.34	3	17
1:A:10:ARG:HH11	1:B:273:ARG:NH1	0.61	1.93	9	1
1:B:259:LYS:O	1:B:260:ASN:ND2	0.61	2.34	8	20
1:B:371:PRO:O	1:B:373:GLN:NE2	0.61	2.34	15	10
1:A:14:ASP:N	1:A:14:ASP:OD2	0.61	2.33	20	5
1:A:58:GLN:HE21	1:A:60:LYS:H	0.61	1.38	19	1
1:B:230:THR:HG22	1:B:256:ASN:CG	0.61	2.16	9	1
1:B:318:HIS:CD2	1:B:319:VAL:HG23	0.61	2.31	20	4
1:A:10:ARG:NE	1:B:234:TYR:OH	0.61	2.34	19	2
1:A:57:ASN:HD22	1:A:58:GLN:H	0.60	1.38	12	7
1:B:212:MET:SD	1:B:253:PHE:CE1	0.60	2.94	10	1
1:A:181:GLU:OE2	1:A:182:HIS:CE1	0.60	2.54	13	1
1:A:38:GLU:N	1:A:38:GLU:OE1	0.60	2.35	3	1
1:B:223:ASN:O	1:B:327:ARG:NE	0.60	2.34	7	1
1:A:140:LEU:HD22	1:A:144:ARG:HH22	0.60	1.55	20	2
1:A:14:ASP:OD1	1:A:14:ASP:N	0.60	2.33	13	13
1:A:55:LEU:HD22	1:A:74:ARG:HH21	0.60	1.56	4	4
1:B:253:PHE:CD2	1:B:253:PHE:C	0.60	2.73	4	5
1:B:342:LEU:O	1:B:346:GLY:N	0.60	2.33	8	7
1:B:367:HIS:ND1	1:B:370:GLN:O	0.60	2.34	6	6
1:A:144:ARG:CZ	1:A:197:GLN:HE22	0.60	2.09	4	1
1:B:237:GLU:OE2	1:B:290:ARG:NH1	0.60	2.35	16	2
1:B:367:HIS:O	1:B:367:HIS:CG	0.60	2.54	12	2
1:A:155:TYR:CE2	1:A:156:ASP:OD1	0.60	2.54	12	2
1:B:210:HIS:CD2	1:B:210:HIS:O	0.60	2.53	7	1
1:A:56:HIS:O	1:A:56:HIS:CD2	0.60	2.54	18	2
1:A:56:HIS:H	1:A:74:ARG:HH11	0.60	1.39	3	1
1:B:220:ASN:OD1	1:B:231:TYR:CE2	0.60	2.54	20	4
1:B:246:LYS:HZ3	1:B:251:ARG:HH11	0.60	1.39	20	1
1:A:100:PRO:O	1:A:130:TYR:CD2	0.60	2.54	8	18
1:B:324:PHE:CE2	1:B:350:SER:OG	0.60	2.55	6	4
1:A:60:LYS:O	1:B:215:HIS:NE2	0.60	2.34	1	3
1:A:60:LYS:O	1:A:61:ASN:CB	0.60	2.48	12	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:GLN:N	1:A:88:GLN:NE2	0.60	2.49	7	15
1:A:141:GLN:OE1	1:A:197:GLN:NE2	0.60	2.35	1	4
1:B:229:LYS:O	1:B:231:TYR:CE2	0.60	2.55	2	5
1:B:230:THR:N	1:B:256:ASN:OD1	0.60	2.34	19	6
1:A:125:PHE:CE2	1:A:157:GLU:OE1	0.60	2.55	14	3
1:A:18:PHE:CE1	1:A:32:TYR:OH	0.60	2.55	10	1
1:A:18:PHE:CD1	1:A:32:TYR:OH	0.60	2.55	10	2
1:B:229:LYS:O	1:B:231:TYR:CD1	0.60	2.55	17	4
1:A:25:GLY:O	1:A:128:ARG:NH2	0.60	2.35	15	5
1:B:296:SER:OG	1:B:297:TRP:CD1	0.60	2.55	3	5
1:A:56:HIS:CG	1:B:213:ASP:OD1	0.60	2.55	16	3
1:A:61:ASN:ND2	1:A:64:SER:H	0.60	1.95	11	1
1:A:11:HIS:O	1:A:11:HIS:CD2	0.60	2.55	3	3
1:B:340:GLN:OE1	1:B:343:ARG:NH1	0.60	2.35	13	3
1:B:250:HIS:O	1:B:250:HIS:ND1	0.60	2.35	10	1
1:A:111:ARG:NH2	1:A:115:GLN:OE1	0.60	2.35	18	3
1:B:230:THR:O	1:B:256:ASN:ND2	0.59	2.35	2	1
1:A:21:ASN:O	1:A:28:ARG:NH2	0.59	2.35	10	2
1:A:61:ASN:ND2	1:A:64:SER:OG	0.59	2.34	15	3
1:B:223:ASN:O	1:B:327:ARG:NH2	0.59	2.35	17	3
1:A:49:ASP:OD2	1:A:51:HIS:NE2	0.59	2.35	7	1
1:A:121:ARG:NE	1:A:123:ARG:HE	0.59	1.95	16	1
1:B:290:ARG:NH1	1:B:322:ARG:NH2	0.59	2.50	19	1
1:A:11:HIS:CE1	1:B:253:PHE:CE1	0.59	2.89	20	1
1:A:74:ARG:NH1	1:B:366:ASP:OD2	0.59	2.35	5	6
1:A:97:SER:OG	1:A:98:TRP:CE2	0.59	2.55	12	8
1:B:253:PHE:CD2	1:B:253:PHE:O	0.59	2.56	17	9
1:B:373:GLN:NE2	1:B:373:GLN:N	0.59	2.49	7	12
1:B:362:ASP:OD2	1:B:367:HIS:NE2	0.59	2.35	6	1
1:A:60:LYS:O	1:B:215:HIS:CE1	0.59	2.55	12	1
1:A:12:LEU:HD13	1:A:167:ASP:CG	0.59	2.17	18	2
1:A:58:GLN:NE2	2:D:416:DA:N6	0.59	2.50	20	1
1:A:69:ARG:O	1:A:70:HIS:CD2	0.59	2.56	7	20
1:B:321:LEU:C	1:B:321:LEU:HD23	0.59	2.18	19	10
1:B:361:TRP:NE1	1:B:362:ASP:OD1	0.59	2.35	3	5
1:B:253:PHE:O	1:B:253:PHE:CD1	0.59	2.55	19	2
1:A:180:ASP:OD1	1:A:184:GLN:NE2	0.59	2.35	14	2
1:B:378:LEU:N	1:B:378:LEU:CD1	0.59	2.65	2	8
1:A:56:HIS:O	1:A:56:HIS:ND1	0.59	2.35	12	3
1:B:232:LEU:HD23	1:B:233:CYS:N	0.59	2.13	12	4
1:A:49:ASP:OD2	1:A:51:HIS:CE1	0.59	2.56	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:MET:CG	1:A:49:ASP:H	0.59	2.11	14	1
1:A:9:PRO:O	1:B:210:HIS:NE2	0.59	2.36	8	6
1:B:229:LYS:O	1:B:231:TYR:CD2	0.59	2.55	8	5
1:B:297:TRP:CZ2	1:B:330:ASP:OD1	0.59	2.55	2	1
1:A:101:CYS:O	1:A:101:CYS:SG	0.59	2.60	7	9
1:B:228:HIS:O	1:B:230:THR:N	0.59	2.35	12	6
1:B:320:ARG:NH2	1:B:322:ARG:NE	0.59	2.50	4	1
1:B:361:TRP:CD2	1:B:365:VAL:HG21	0.59	2.32	9	2
1:A:50:GLN:O	1:A:51:HIS:ND1	0.59	2.36	15	2
1:B:310:ARG:NH2	1:B:314:GLN:OE1	0.59	2.35	15	4
1:B:220:ASN:OD1	1:B:231:TYR:CD1	0.59	2.56	1	3
1:B:246:LYS:NZ	1:B:251:ARG:HH11	0.59	1.93	20	4
1:A:168:HIS:ND1	1:A:171:GLN:O	0.59	2.36	2	2
1:B:229:LYS:NZ	2:C:403:DT:O4	0.59	2.33	19	2
1:A:14:ASP:OD1	1:B:255:HIS:CE1	0.59	2.56	5	1
1:A:21:ASN:ND2	1:A:31:THR:OG1	0.59	2.35	13	4
1:B:229:LYS:O	1:B:255:HIS:CE1	0.59	2.55	13	2
1:A:121:ARG:NH2	1:A:123:ARG:HH11	0.59	1.96	17	2
1:B:343:ARG:CZ	1:B:396:GLN:HE22	0.59	2.11	20	1
1:A:11:HIS:O	1:A:11:HIS:CG	0.59	2.55	3	3
1:A:24:ASN:OD1	1:A:176:TRP:CD1	0.59	2.55	8	4
1:A:102:PHE:CE1	1:A:135:LEU:HD21	0.59	2.33	19	2
1:B:271:GLN:OE1	1:B:293:TRP:CZ3	0.59	2.56	15	2
1:B:297:TRP:CD1	1:B:330:ASP:OD1	0.59	2.56	12	1
1:A:181:GLU:OE2	1:A:182:HIS:NE2	0.59	2.36	13	1
1:B:361:TRP:O	1:B:365:VAL:CG2	0.59	2.51	2	19
1:A:33:LEU:HD23	1:A:33:LEU:C	0.59	2.18	19	8
1:B:297:TRP:CD1	1:B:299:PRO:O	0.59	2.56	5	1
1:B:220:ASN:OD1	1:B:231:TYR:CZ	0.59	2.55	7	2
1:A:51:HIS:N	1:B:206:SER:O	0.59	2.35	9	1
1:A:141:GLN:OE1	1:A:144:ARG:NH1	0.59	2.35	17	1
1:A:33:LEU:HD13	1:A:96:ILE:HG23	0.59	1.75	8	6
1:A:125:PHE:CZ	1:A:157:GLU:OE1	0.59	2.56	8	4
1:B:223:ASN:O	1:B:327:ARG:NH1	0.59	2.34	7	3
1:A:135:LEU:HD12	1:A:135:LEU:C	0.59	2.18	18	2
1:A:25:GLY:O	1:A:128:ARG:NH1	0.59	2.36	11	7
1:A:56:HIS:H	1:A:74:ARG:NH1	0.59	1.96	3	1
1:A:167:ASP:OD2	1:A:169:GLN:NE2	0.59	2.36	11	2
1:B:229:LYS:O	1:B:231:TYR:CZ	0.59	2.56	9	1
1:A:11:HIS:CD2	1:B:253:PHE:CE2	0.59	2.90	11	1
1:B:237:GLU:OE1	1:B:290:ARG:NH1	0.58	2.35	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:297:TRP:CD2	1:B:330:ASP:OD1	0.58	2.56	6	1
1:B:230:THR:OG1	1:B:256:ASN:ND2	0.58	2.36	13	1
1:A:18:PHE:CE2	1:A:22:PHE:CE2	0.58	2.91	2	1
1:B:220:ASN:OD1	1:B:231:TYR:CE1	0.58	2.56	18	2
1:A:50:GLN:O	1:A:51:HIS:CG	0.58	2.56	15	2
1:B:230:THR:O	1:B:255:HIS:ND1	0.58	2.36	13	2
1:B:235:GLU:OE2	1:B:251:ARG:NH2	0.58	2.36	18	1
1:B:324:PHE:CE1	1:B:350:SER:OG	0.58	2.55	19	1
1:B:225:ILE:HD11	1:B:327:ARG:HH12	0.58	1.58	2	1
1:B:291:VAL:CG2	1:B:293:TRP:NE1	0.58	2.66	3	12
1:B:293:TRP:CZ2	1:B:321:LEU:HD11	0.58	2.33	18	4
1:A:10:ARG:O	1:A:12:LEU:HD23	0.58	1.98	14	3
1:A:166:VAL:HG12	1:A:168:HIS:CD2	0.58	2.33	11	1
1:A:39:ARG:NH2	1:A:90:TYR:OH	0.58	2.36	15	2
1:B:255:HIS:CD2	1:B:255:HIS:N	0.58	2.69	2	1
1:B:320:ARG:NH1	1:B:348:GLN:OE1	0.58	2.36	4	1
1:A:60:LYS:NZ	2:D:416:DA:C5	0.58	2.70	5	1
1:A:49:ASP:O	1:A:50:GLN:CB	0.58	2.51	16	2
1:A:22:PHE:O	1:A:24:ASN:ND2	0.58	2.37	9	10
1:A:102:PHE:O	1:A:103:SER:CB	0.58	2.51	12	11
1:B:332:ASP:N	1:B:333:PRO:CD	0.58	2.66	12	17
1:B:362:ASP:N	1:B:362:ASP:OD1	0.58	2.36	20	1
1:A:21:ASN:OD1	1:A:28:ARG:NH2	0.58	2.36	1	5
1:A:35:TYR:OH	1:B:209:ARG:NE	0.58	2.37	10	2
1:B:326:ALA:HB2	1:B:352:MET:SD	0.58	2.38	11	1
1:A:24:ASN:OD1	1:A:176:TRP:NE1	0.58	2.36	1	9
1:A:88:GLN:O	1:A:119:HIS:ND1	0.58	2.36	7	4
1:B:253:PHE:CD1	1:B:253:PHE:O	0.58	2.57	15	3
1:B:297:TRP:CG	1:B:330:ASP:OD1	0.58	2.56	12	2
1:B:310:ARG:NH1	1:B:344:ASP:OD2	0.58	2.37	8	2
1:A:78:LEU:HD12	1:B:209:ARG:NH2	0.58	2.13	9	1
1:B:296:SER:OG	1:B:297:TRP:CE2	0.58	2.55	10	1
1:B:361:TRP:NE1	1:B:362:ASP:OD2	0.58	2.37	18	3
1:A:181:GLU:OE1	1:A:182:HIS:N	0.58	2.36	13	1
1:A:94:TRP:CD2	1:A:122:LEU:HD21	0.58	2.34	5	9
1:A:195:GLN:CA	1:A:195:GLN:HE21	0.58	2.12	5	20
1:B:225:ILE:HD11	1:B:327:ARG:NH1	0.58	2.12	2	1
1:A:168:HIS:CD2	1:A:171:GLN:O	0.58	2.57	6	2
1:A:125:PHE:CZ	1:A:127:ALA:HB2	0.58	2.34	12	1
1:A:31:THR:CG2	1:A:32:TYR:N	0.58	2.66	8	17
1:B:227:ARG:O	1:B:228:HIS:CB	0.58	2.51	19	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ALA:C	1:A:88:GLN:NE2	0.58	2.58	13	15
1:A:54:PHE:CD1	1:A:54:PHE:C	0.58	2.76	18	5
1:A:103:SER:OG	1:A:106:CYS:N	0.58	2.36	11	3
1:A:56:HIS:CD2	1:B:213:ASP:OD1	0.58	2.56	12	1
1:B:298:SER:OG	1:B:325:ALA:HB2	0.57	1.99	15	5
1:B:346:GLY:O	1:B:348:GLN:N	0.57	2.37	2	20
1:A:144:ARG:NE	1:A:194:LEU:HD22	0.57	2.13	19	3
1:A:11:HIS:ND1	1:A:11:HIS:O	0.57	2.37	14	3
1:B:209:ARG:HH12	1:B:368:GLN:HE22	0.57	1.41	14	1
1:A:72:GLN:HE21	1:A:96:ILE:CD1	0.57	2.12	2	2
1:B:362:ASP:N	1:B:362:ASP:OD2	0.57	2.35	2	1
1:B:297:TRP:CH2	1:B:327:ARG:NH2	0.57	2.72	3	1
1:B:297:TRP:NE1	1:B:299:PRO:O	0.57	2.37	5	1
1:B:232:LEU:HD11	1:B:271:GLN:NE2	0.57	2.13	15	2
1:A:12:LEU:HD23	1:A:12:LEU:H	0.57	1.58	14	2
1:A:40:LEU:HD21	1:A:43:GLY:H	0.57	1.60	7	1
1:A:130:TYR:O	1:A:130:TYR:CD2	0.57	2.57	12	7
1:A:69:ARG:NE	1:A:103:SER:OG	0.57	2.38	1	2
1:B:220:ASN:O	1:B:327:ARG:NH1	0.57	2.38	3	1
1:B:361:TRP:HE1	1:B:367:HIS:HE2	0.57	1.39	20	3
1:B:225:ILE:CD1	1:B:327:ARG:HH12	0.57	2.12	2	1
1:A:21:ASN:OD1	1:A:28:ARG:NH1	0.57	2.37	8	1
1:B:340:GLN:OE1	1:B:396:GLN:NE2	0.57	2.38	10	2
1:B:394:GLN:HE21	1:B:394:GLN:CA	0.57	2.12	4	20
1:A:25:GLY:N	1:A:128:ARG:HH12	0.57	1.97	11	1
1:A:56:HIS:CE1	1:B:213:ASP:OD2	0.57	2.58	3	1
1:A:96:ILE:N	1:A:96:ILE:CD1	0.57	2.67	5	1
1:A:162:TRP:HE1	1:A:168:HIS:CG	0.57	2.16	6	2
1:B:229:LYS:NZ	2:C:404:DC:O2	0.57	2.38	6	1
1:A:51:HIS:NE2	1:A:82:LEU:HD22	0.57	2.15	17	1
1:A:144:ARG:NH2	1:A:197:GLN:OE1	0.57	2.38	19	1
1:A:12:LEU:N	1:A:12:LEU:HD22	0.57	2.14	2	1
1:A:12:LEU:CD1	1:A:12:LEU:N	0.57	2.68	3	1
1:A:141:GLN:NE2	1:A:196:ASN:HD21	0.57	1.98	7	1
1:B:229:LYS:N	1:B:256:ASN:OD1	0.57	2.38	18	3
1:A:136:TYR:CD2	1:A:136:TYR:C	0.57	2.79	20	3
1:B:362:ASP:OD1	1:B:367:HIS:CE1	0.57	2.58	12	1
1:A:174:GLN:NE2	1:A:174:GLN:H	0.57	1.98	18	1
1:A:91:ARG:NH1	1:A:123:ARG:HH21	0.57	1.98	18	2
1:B:320:ARG:NH1	1:B:322:ARG:HH11	0.57	1.98	11	1
1:B:217:PHE:CE1	1:B:221:PHE:CE2	0.57	2.93	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:209:ARG:C	1:B:211:LEU:H	0.56	2.04	12	20
1:B:209:ARG:O	1:B:211:LEU:N	0.56	2.36	7	17
1:A:174:GLN:H	1:A:174:GLN:CD	0.56	2.03	12	3
1:A:52:ARG:O	1:B:208:PRO:CB	0.56	2.53	5	7
1:A:182:HIS:ND1	2:D:409:DA:N6	0.56	2.52	16	4
1:A:34:CYS:SG	1:A:165:PHE:CE2	0.56	2.96	6	2
1:A:111:ARG:NH1	1:A:145:ASP:OD2	0.56	2.37	9	1
1:B:253:PHE:O	1:B:253:PHE:CD2	0.56	2.58	13	1
1:A:167:ASP:OD1	1:A:169:GLN:NE2	0.56	2.38	20	3
1:A:59:ALA:O	2:D:416:DA:P	0.56	2.64	20	12
1:A:131:ASP:OD1	2:D:413:DT:N3	0.56	2.37	11	15
1:A:132:TYR:CG	1:A:133:ASP:N	0.56	2.73	2	20
1:B:286:ALA:C	1:B:287:GLN:NE2	0.56	2.59	9	17
1:A:196:ASN:ND2	1:A:197:GLN:H	0.56	1.98	3	5
1:B:231:TYR:OH	1:B:255:HIS:CE1	0.56	2.58	3	1
1:A:125:PHE:CE1	1:A:157:GLU:OE1	0.56	2.59	4	2
1:A:40:LEU:CD2	1:A:43:GLY:H	0.56	2.14	7	1
1:A:54:PHE:CD2	1:A:54:PHE:C	0.56	2.77	11	3
1:B:223:ASN:C	1:B:327:ARG:NH2	0.56	2.59	9	3
1:A:121:ARG:CG	1:A:149:GLN:HE22	0.56	2.14	12	1
1:A:114:LEU:CD1	1:A:146:ALA:HB1	0.56	2.29	17	1
1:A:27:GLY:O	1:A:28:ARG:NE	0.56	2.38	18	7
1:A:35:TYR:CD1	1:A:35:TYR:C	0.56	2.79	10	2
1:A:130:TYR:CD2	1:A:130:TYR:O	0.56	2.58	7	12
1:B:298:SER:H	1:B:299:PRO:CD	0.56	2.14	16	9
1:B:353:THR:HG22	1:B:354:TYR:N	0.56	2.16	2	5
1:A:60:LYS:O	1:A:61:ASN:ND2	0.56	2.39	3	1
1:B:231:TYR:CZ	1:B:255:HIS:CE1	0.56	2.94	12	2
1:A:95:PHE:CE2	1:A:125:PHE:CG	0.56	2.94	18	5
1:A:140:LEU:CD2	1:A:193:ILE:HD13	0.56	2.31	6	1
1:B:220:ASN:CG	1:B:231:TYR:CE2	0.56	2.79	12	4
1:B:268:ARG:HE	1:B:272:LEU:HD22	0.56	1.60	14	1
1:A:136:TYR:CD1	1:A:136:TYR:C	0.56	2.78	12	11
1:B:287:GLN:N	1:B:287:GLN:NE2	0.56	2.53	6	19
1:A:24:ASN:OD1	1:A:176:TRP:CE2	0.56	2.58	3	3
1:B:275:LEU:O	1:B:278:VAL:HG13	0.56	2.01	19	1
1:A:125:PHE:CE2	1:A:157:GLU:OE2	0.56	2.59	3	1
1:B:292:THR:OG1	1:B:322:ARG:NH1	0.56	2.39	8	2
1:B:321:LEU:HD23	1:B:321:LEU:C	0.56	2.21	9	1
1:A:165:PHE:CE1	1:B:210:HIS:NE2	0.56	2.73	12	1
1:A:69:ARG:CZ	1:A:104:TRP:HE1	0.56	2.14	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:HIS:CE1	1:A:58:GLN:O	0.56	2.59	18	1
1:B:223:ASN:O	1:B:327:ARG:CZ	0.56	2.54	17	2
1:A:168:HIS:NE2	1:A:171:GLN:OE1	0.56	2.39	3	1
1:B:224:GLY:O	1:B:327:ARG:NH2	0.56	2.39	16	6
1:B:264:GLY:O	1:B:266:TYR:CD1	0.56	2.59	2	5
1:B:255:HIS:CE1	1:B:257:GLN:CD	0.56	2.79	9	3
1:A:10:ARG:CZ	1:A:12:LEU:HD12	0.56	2.31	18	1
1:B:235:GLU:OE1	1:B:251:ARG:NH1	0.56	2.39	18	1
1:A:30:LYS:C	1:A:57:ASN:HD21	0.55	2.04	19	12
1:A:144:ARG:NE	1:A:194:LEU:HD21	0.55	2.16	6	3
1:B:361:TRP:CH2	1:B:365:VAL:HG11	0.55	2.35	9	4
1:A:41:ASP:N	1:A:44:THR:O	0.55	2.39	13	12
1:A:181:GLU:OE1	2:D:409:DA:C6	0.55	2.59	8	6
1:B:343:ARG:NH1	1:B:396:GLN:HE21	0.55	1.98	6	1
1:A:91:ARG:NE	1:A:121:ARG:HH11	0.55	1.99	16	1
1:A:21:ASN:OD1	1:A:28:ARG:CZ	0.55	2.54	8	3
1:B:339:LEU:HD13	1:B:339:LEU:O	0.55	2.01	11	4
1:A:181:GLU:OE2	2:D:409:DA:N6	0.55	2.39	13	7
1:B:262:ASN:ND2	2:C:408:DT:OP1	0.55	2.39	16	3
1:A:78:LEU:HD11	1:B:209:ARG:CD	0.55	2.31	12	1
1:A:144:ARG:HH21	1:A:197:GLN:HE22	0.55	1.42	14	1
1:A:143:LEU:O	1:A:147:GLY:N	0.55	2.36	17	1
1:A:153:MET:SD	1:A:157:GLU:OE2	0.55	2.64	20	1
1:A:16:HIS:NE2	1:B:260:ASN:ND2	0.55	2.54	13	2
1:A:113:PHE:CE2	1:A:117:ASN:OD1	0.55	2.59	10	2
1:B:343:ARG:NE	1:B:393:LEU:HD11	0.55	2.16	14	1
1:A:88:GLN:HE21	1:A:88:GLN:CA	0.55	2.14	7	1
1:A:143:LEU:HD13	1:A:143:LEU:O	0.55	2.02	18	3
1:A:140:LEU:HD22	1:A:144:ARG:NH2	0.55	2.16	20	2
1:A:95:PHE:CE1	1:A:125:PHE:CG	0.55	2.95	11	3
1:A:61:ASN:HD21	1:A:64:SER:H	0.55	1.44	11	1
1:B:271:GLN:OE1	1:B:293:TRP:CH2	0.55	2.59	12	1
1:A:38:GLU:OE2	1:A:91:ARG:NH1	0.55	2.40	15	1
1:A:98:TRP:CZ2	2:D:414:DC:O4'	0.55	2.59	8	18
1:A:182:HIS:CE1	2:D:409:DA:C5	0.55	2.95	1	9
1:B:250:HIS:CE1	1:B:281:LEU:HD22	0.55	2.37	3	1
1:A:52:ARG:CZ	1:A:164:THR:HG23	0.55	2.32	8	1
1:A:141:GLN:OE1	1:A:196:ASN:ND2	0.55	2.40	19	3
1:A:181:GLU:OE1	2:D:409:DA:N6	0.55	2.40	8	8
1:B:271:GLN:OE1	1:B:305:CYS:SG	0.55	2.64	10	5
1:A:45:SER:CB	1:A:91:ARG:HH21	0.55	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:320:ARG:CZ	1:B:348:GLN:HE22	0.55	2.14	14	1
1:A:60:LYS:O	1:A:61:ASN:CG	0.55	2.45	3	12
1:A:167:ASP:O	1:A:167:ASP:OD2	0.55	2.25	4	7
1:A:56:HIS:N	1:A:74:ARG:HH11	0.55	2.00	3	1
1:A:174:GLN:N	1:A:174:GLN:NE2	0.55	2.54	3	2
1:A:54:PHE:C	1:A:54:PHE:CD2	0.55	2.80	7	2
1:B:335:TYR:CE1	1:B:392:ILE:HD11	0.55	2.36	11	1
1:B:250:HIS:CD2	1:B:281:LEU:CD2	0.55	2.89	17	1
1:A:31:THR:O	1:A:57:ASN:ND2	0.55	2.39	15	14
1:A:98:TRP:CD2	2:D:414:DC:C6	0.55	2.94	19	20
1:B:220:ASN:CG	1:B:231:TYR:CG	0.55	2.80	16	2
1:B:293:TRP:CZ3	1:B:321:LEU:HD11	0.55	2.37	9	3
1:B:305:CYS:O	1:B:309:VAL:CG2	0.55	2.55	1	3
1:B:229:LYS:O	1:B:231:TYR:CE1	0.55	2.60	16	5
1:B:368:GLN:N	1:B:368:GLN:CD	0.55	2.60	5	2
1:B:230:THR:O	1:B:255:HIS:CE1	0.55	2.60	13	2
1:A:111:ARG:CZ	1:A:115:GLN:OE1	0.55	2.55	15	3
1:A:162:TRP:CD1	1:A:163:ASP:N	0.55	2.74	5	15
1:B:296:SER:OG	1:B:297:TRP:NE1	0.55	2.40	4	3
1:A:50:GLN:CD	1:A:52:ARG:NH1	0.55	2.61	4	2
1:B:373:GLN:H	1:B:373:GLN:CD	0.55	2.05	14	3
1:A:38:GLU:CD	1:A:91:ARG:NH1	0.55	2.60	15	1
1:A:56:HIS:N	1:A:56:HIS:CD2	0.55	2.75	17	1
1:A:144:ARG:NH2	1:A:193:ILE:HG21	0.55	2.16	20	1
1:B:246:LYS:HZ3	1:B:251:ARG:NH1	0.54	2.00	1	4
1:B:291:VAL:CG2	1:B:293:TRP:HE1	0.54	2.14	14	13
1:A:106:CYS:O	1:A:110:VAL:CG2	0.54	2.56	7	6
1:A:136:TYR:C	1:A:136:TYR:CD2	0.54	2.79	13	4
1:A:122:LEU:HD13	1:A:123:ARG:N	0.54	2.17	11	5
1:A:38:GLU:OE1	1:A:91:ARG:NH1	0.54	2.39	7	2
1:A:125:PHE:CE1	1:A:153:MET:SD	0.54	3.00	7	1
1:A:104:TRP:CD1	1:A:104:TRP:N	0.54	2.73	15	1
1:B:235:GLU:OE1	1:B:251:ARG:CZ	0.54	2.55	18	1
1:A:132:TYR:O	1:A:133:ASP:O	0.54	2.24	1	20
1:B:395:ASN:ND2	1:B:396:GLN:N	0.54	2.55	19	20
1:B:278:VAL:HG21	1:B:312:PHE:CZ	0.54	2.38	7	7
1:A:10:ARG:HH12	1:B:273:ARG:CZ	0.54	2.15	13	1
1:A:35:TYR:OH	1:B:209:ARG:CB	0.54	2.56	4	4
1:A:155:TYR:C	1:A:155:TYR:CD1	0.54	2.79	12	2
1:A:78:LEU:O	1:A:78:LEU:HD13	0.54	2.02	6	1
1:B:227:ARG:C	1:B:228:HIS:CG	0.54	2.80	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:GLY:O	1:A:28:ARG:NH1	0.54	2.39	19	1
1:A:16:HIS:CB	1:B:258:ALA:HB3	0.54	2.32	1	8
1:A:57:ASN:N	1:A:57:ASN:HD22	0.54	2.00	3	13
1:B:321:LEU:HD13	1:B:322:ARG:N	0.54	2.17	5	5
1:A:173:PHE:CE2	1:A:174:GLN:O	0.54	2.61	10	3
1:A:59:ALA:O	2:D:416:DA:OP2	0.54	2.25	9	18
1:A:62:LEU:HD11	2:D:417:DT:P	0.54	2.42	1	2
1:B:220:ASN:ND2	1:B:220:ASN:O	0.54	2.40	2	1
1:B:278:VAL:N	1:B:279:PRO:HD2	0.54	2.16	19	5
1:B:271:GLN:NE2	1:B:300:CYS:SG	0.54	2.80	10	1
1:A:10:ARG:O	1:A:12:LEU:N	0.54	2.39	18	3
1:A:176:TRP:O	1:A:179:LEU:CD2	0.54	2.56	12	14
1:B:275:LEU:O	1:B:279:PRO:CD	0.54	2.56	19	9
1:B:381:HIS:NE2	2:C:401:DT:O4	0.54	2.41	2	3
1:A:56:HIS:N	1:A:56:HIS:ND1	0.54	2.56	3	1
1:A:103:SER:OG	1:A:106:CYS:CB	0.54	2.56	11	3
1:B:221:PHE:O	1:B:223:ASN:ND2	0.54	2.40	4	3
1:B:229:LYS:CA	1:B:256:ASN:OD1	0.54	2.55	7	2
1:A:121:ARG:HH21	1:A:123:ARG:HH11	0.54	1.46	17	1
1:B:306:ALA:HB1	1:B:341:MET:SD	0.54	2.43	1	1
1:A:114:LEU:HD21	1:A:122:LEU:HB2	0.54	1.80	11	10
1:A:27:GLY:O	1:A:28:ARG:CZ	0.54	2.56	10	3
1:B:342:LEU:HD13	1:B:342:LEU:O	0.54	2.02	10	3
1:A:169:GLN:CD	1:A:169:GLN:N	0.54	2.61	10	2
1:A:106:CYS:SG	1:A:107:ALA:N	0.54	2.81	10	1
1:B:343:ARG:NH2	1:B:396:GLN:HE22	0.54	2.00	9	1
1:B:212:MET:SD	1:B:253:PHE:CD1	0.54	3.01	10	1
1:B:215:HIS:C	1:B:215:HIS:ND1	0.54	2.60	15	1
1:A:154:THR:HG22	1:A:155:TYR:N	0.53	2.18	19	7
1:B:343:ARG:NH2	1:B:396:GLN:NE2	0.53	2.56	9	3
1:A:181:GLU:OE2	1:A:182:HIS:CD2	0.53	2.61	13	1
1:A:52:ARG:NH2	1:A:164:THR:HG23	0.53	2.18	1	2
1:A:76:LEU:HD13	1:A:76:LEU:O	0.53	2.02	15	11
1:A:57:ASN:ND2	1:A:57:ASN:H	0.53	2.01	14	9
1:B:217:PHE:CE1	1:B:221:PHE:CZ	0.53	2.96	1	1
1:A:140:LEU:HG	1:A:193:ILE:HG21	0.53	1.80	2	1
1:B:230:THR:CG2	1:B:256:ASN:OD1	0.53	2.56	5	1
1:A:181:GLU:OE1	2:D:409:DA:C5	0.53	2.62	8	1
1:A:162:TRP:CD1	1:A:162:TRP:C	0.53	2.82	16	18
1:A:50:GLN:OE1	1:A:52:ARG:NH1	0.53	2.41	7	2
1:B:343:ARG:HE	1:B:393:LEU:HD11	0.53	1.62	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ARG:HH11	1:B:273:ARG:HH11	0.53	1.44	9	1
1:B:320:ARG:NH1	1:B:348:GLN:NE2	0.53	2.56	14	1
1:A:102:PHE:CD1	1:A:135:LEU:HD23	0.53	2.39	1	1
1:A:195:GLN:CA	1:A:195:GLN:NE2	0.53	2.72	12	19
1:B:297:TRP:CE2	1:B:330:ASP:OD2	0.53	2.61	2	1
1:A:35:TYR:C	1:A:35:TYR:CD2	0.53	2.82	5	3
1:B:236:VAL:HG21	1:B:250:HIS:CE1	0.53	2.38	10	1
1:A:181:GLU:OE2	2:D:409:DA:C5	0.53	2.62	13	1
1:A:61:ASN:ND2	1:A:61:ASN:C	0.53	2.61	11	1
1:A:104:TRP:O	1:A:108:GLY:N	0.53	2.40	16	7
1:A:173:PHE:C	1:A:174:GLN:NE2	0.53	2.61	3	1
1:A:33:LEU:HD23	1:A:33:LEU:O	0.53	2.03	16	2
1:B:395:ASN:ND2	1:B:396:GLN:H	0.53	2.00	19	2
1:B:228:HIS:CE1	1:B:259:LYS:NZ	0.53	2.77	20	1
1:B:343:ARG:NE	1:B:396:GLN:HE22	0.53	2.00	20	1
1:A:196:ASN:ND2	1:A:197:GLN:N	0.53	2.57	3	19
1:B:293:TRP:CH2	1:B:321:LEU:HD21	0.53	2.38	5	1
1:B:293:TRP:CE2	1:B:321:LEU:HD11	0.53	2.39	8	4
1:B:328:ILE:CG2	1:B:335:TYR:CE1	0.53	2.92	1	2
1:B:375:TRP:O	1:B:378:LEU:CD2	0.53	2.57	8	12
1:A:162:TRP:O	1:A:166:VAL:O	0.53	2.27	6	2
1:A:12:LEU:H	1:A:12:LEU:HD23	0.53	1.63	11	2
1:B:271:GLN:OE1	1:B:309:VAL:HG21	0.53	2.04	19	1
1:A:17:ILE:CD1	1:A:17:ILE:N	0.53	2.72	20	1
1:A:147:GLY:O	1:A:149:GLN:N	0.53	2.40	6	20
1:B:373:GLN:N	1:B:373:GLN:NE2	0.53	2.56	2	4
1:A:181:GLU:OE2	2:D:409:DA:N7	0.53	2.42	20	3
1:B:322:ARG:HH11	1:B:350:SER:CB	0.53	2.16	9	2
1:B:335:TYR:CE2	1:B:339:LEU:HD12	0.53	2.39	9	3
1:A:22:PHE:C	1:A:24:ASN:H	0.52	2.08	13	18
1:B:346:GLY:C	1:B:348:GLN:H	0.52	2.08	8	20
1:A:60:LYS:CE	2:D:417:DT:O4	0.52	2.56	9	5
1:A:144:ARG:NE	1:A:194:LEU:CD2	0.52	2.72	6	3
1:A:140:LEU:HD22	1:A:193:ILE:CG2	0.52	2.34	11	1
1:B:291:VAL:HG13	1:B:291:VAL:O	0.52	2.04	1	3
1:B:375:TRP:NE1	1:B:378:LEU:HD11	0.52	2.20	14	4
1:B:287:GLN:NE2	1:B:287:GLN:N	0.52	2.57	12	1
1:B:220:ASN:ND2	1:B:231:TYR:CB	0.52	2.72	11	2
1:B:394:GLN:CA	1:B:394:GLN:NE2	0.52	2.73	1	20
1:B:361:TRP:CG	1:B:362:ASP:N	0.52	2.77	12	4
1:B:367:HIS:CE1	1:B:370:GLN:HE22	0.52	2.20	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:PRO:CG	1:A:168:HIS:NE2	0.52	2.73	20	4
1:A:140:LEU:CD1	1:A:193:ILE:HD13	0.52	2.35	1	6
1:B:225:ILE:O	2:C:403:DT:C7	0.52	2.57	7	10
1:B:339:LEU:HD13	1:B:392:ILE:CD1	0.52	2.35	15	3
1:A:18:PHE:CD2	1:A:32:TYR:OH	0.52	2.62	13	1
1:A:33:LEU:HD12	1:A:34:CYS:N	0.52	2.19	13	1
1:B:228:HIS:CE1	1:B:259:LYS:HZ2	0.52	2.20	20	1
1:A:131:ASP:OD1	2:D:413:DT:C2	0.52	2.62	14	13
1:B:328:ILE:CG2	1:B:335:TYR:OH	0.52	2.58	3	3
1:B:212:MET:O	1:B:366:ASP:N	0.52	2.42	12	1
1:A:38:GLU:OE2	1:A:91:ARG:CZ	0.52	2.58	15	1
1:A:31:THR:O	1:A:57:ASN:OD1	0.52	2.28	6	6
1:B:274:PHE:CE1	1:B:277:LEU:HD23	0.52	2.39	4	2
1:B:339:LEU:HD13	1:B:392:ILE:HD13	0.52	1.82	17	4
1:A:181:GLU:CD	2:D:409:DA:N7	0.52	2.63	3	17
1:B:331:TYR:O	1:B:332:ASP:O	0.52	2.28	8	3
1:A:55:LEU:HD21	1:B:209:ARG:NH2	0.52	2.19	9	1
1:A:27:GLY:H	1:A:128:ARG:HH12	0.52	1.46	10	1
1:B:240:ASP:N	1:B:243:THR:O	0.52	2.41	17	11
1:B:268:ARG:O	1:B:269:HIS:O	0.52	2.27	2	1
1:B:228:HIS:C	1:B:230:THR:N	0.52	2.62	12	6
1:A:49:ASP:O	1:A:50:GLN:O	0.52	2.28	7	3
1:A:88:GLN:N	1:A:88:GLN:CD	0.52	2.63	7	1
1:B:220:ASN:CG	1:B:231:TYR:CZ	0.52	2.83	12	3
1:B:373:GLN:CD	1:B:373:GLN:H	0.52	2.07	18	2
1:B:232:LEU:HD11	1:B:271:GLN:HE21	0.52	1.65	8	1
1:A:58:GLN:O	1:A:58:GLN:CG	0.52	2.58	17	3
1:A:141:GLN:CD	1:A:197:GLN:NE2	0.52	2.63	11	1
1:A:61:ASN:OD1	1:A:61:ASN:O	0.52	2.27	12	1
1:A:50:GLN:O	1:B:206:SER:O	0.52	2.28	2	4
1:A:168:HIS:CD2	1:A:168:HIS:H	0.52	2.24	5	2
1:A:195:GLN:NE2	1:A:195:GLN:CA	0.52	2.73	2	1
1:B:220:ASN:CG	1:B:231:TYR:CD2	0.52	2.84	2	2
1:A:64:SER:O	1:A:66:PHE:CD2	0.52	2.63	8	2
1:A:121:ARG:HH21	1:A:149:GLN:NE2	0.52	2.01	12	1
1:B:271:GLN:CD	1:B:293:TRP:CZ3	0.52	2.84	12	1
1:A:55:LEU:HD22	1:A:74:ARG:CD	0.52	2.35	13	2
1:A:52:ARG:NH1	1:A:164:THR:O	0.52	2.43	14	1
1:A:88:GLN:NE2	1:A:88:GLN:N	0.51	2.57	4	5
1:A:96:ILE:HD12	1:A:98:TRP:O	0.51	2.05	19	7
1:A:18:PHE:CZ	1:A:22:PHE:CD1	0.51	2.98	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:343:ARG:NH1	1:B:396:GLN:CD	0.51	2.63	13	1
1:B:332:ASP:N	1:B:332:ASP:OD2	0.51	2.43	18	1
1:A:28:ARG:NH1	1:A:128:ARG:NE	0.51	2.58	19	1
1:B:359:HIS:O	1:B:362:ASP:OD1	0.51	2.28	20	1
1:A:140:LEU:HD13	1:A:140:LEU:O	0.51	2.06	2	1
1:B:277:LEU:HD13	1:B:277:LEU:O	0.51	2.05	19	2
1:B:227:ARG:O	1:B:228:HIS:C	0.51	2.48	12	1
1:B:255:HIS:CE1	1:B:257:GLN:HE21	0.51	2.23	1	2
1:B:393:LEU:HD22	1:B:393:LEU:N	0.51	2.20	11	8
1:A:73:LEU:CD1	1:A:109:GLU:OE1	0.51	2.58	10	2
1:A:134:PRO:O	1:A:138:GLU:OE1	0.51	2.28	7	1
1:B:274:PHE:CE2	1:B:277:LEU:HD23	0.51	2.40	11	2
1:A:62:LEU:CD1	2:D:417:DT:OP1	0.51	2.58	8	2
1:A:57:ASN:HD22	1:A:57:ASN:N	0.51	2.04	18	2
1:A:12:LEU:N	1:A:12:LEU:CD2	0.51	2.73	2	1
1:B:329:TYR:O	1:B:330:ASP:OD1	0.51	2.28	16	2
1:B:375:TRP:CD1	1:B:378:LEU:CD1	0.51	2.94	14	4
1:B:388:ARG:O	1:B:392:ILE:HD12	0.51	2.05	7	1
1:B:362:ASP:OD1	1:B:367:HIS:NE2	0.51	2.43	12	1
1:B:255:HIS:CE1	1:B:257:GLN:N	0.51	2.78	7	1
1:B:340:GLN:NE2	1:B:343:ARG:NH2	0.51	2.59	13	1
1:A:59:ALA:O	2:D:416:DA:OP1	0.51	2.29	8	8
1:B:328:ILE:HG21	1:B:335:TYR:OH	0.51	2.06	19	4
1:A:25:GLY:O	1:A:128:ARG:CZ	0.51	2.58	11	2
1:A:56:HIS:HD1	1:B:213:ASP:CG	0.51	2.09	9	1
1:B:232:LEU:HD23	1:B:232:LEU:O	0.51	2.05	14	1
1:B:320:ARG:NH1	1:B:348:GLN:HE21	0.51	2.04	14	1
1:B:235:GLU:CD	1:B:251:ARG:HH22	0.51	2.09	7	3
1:A:28:ARG:HH22	1:A:128:ARG:HH11	0.51	1.49	11	1
1:B:367:HIS:ND1	1:B:367:HIS:C	0.51	2.64	12	2
1:A:12:LEU:HD22	1:A:167:ASP:OD1	0.51	2.06	14	1
1:B:320:ARG:NE	1:B:348:GLN:HE22	0.51	2.03	14	1
1:A:88:GLN:N	1:A:88:GLN:HE21	0.51	2.04	20	2
1:A:194:LEU:HD13	1:A:197:GLN:NE2	0.51	2.21	9	1
1:A:155:TYR:CD2	1:A:155:TYR:C	0.51	2.81	16	1
1:A:22:PHE:O	1:A:176:TRP:CZ2	0.51	2.64	20	2
1:A:30:LYS:O	1:A:31:THR:O	0.51	2.29	20	19
1:B:212:MET:SD	1:B:253:PHE:CZ	0.51	3.04	2	1
1:B:335:TYR:OH	1:B:392:ILE:CD1	0.51	2.55	2	1
1:A:78:LEU:CD1	1:B:209:ARG:NH2	0.51	2.74	9	1
1:A:24:ASN:OD1	1:A:176:TRP:CG	0.51	2.63	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:358:LYS:O	1:B:362:ASP:OD1	0.51	2.29	20	1
1:B:217:PHE:CZ	1:B:221:PHE:CE1	0.50	2.99	2	2
1:A:51:HIS:O	1:A:52:ARG:C	0.50	2.50	14	6
1:B:297:TRP:CH2	1:B:327:ARG:NH1	0.50	2.78	4	1
1:A:194:LEU:N	1:A:194:LEU:CD2	0.50	2.75	4	7
1:B:274:PHE:CE1	1:B:293:TRP:NE1	0.50	2.79	7	2
1:B:228:HIS:C	1:B:230:THR:H	0.50	2.09	12	3
1:A:194:LEU:CD1	1:A:197:GLN:NE2	0.50	2.74	9	1
1:A:58:GLN:NE2	2:D:416:DA:H62	0.50	2.04	20	1
1:A:147:GLY:C	1:A:149:GLN:H	0.50	2.09	6	20
1:B:361:TRP:CD1	1:B:362:ASP:OD1	0.50	2.64	4	4
1:B:332:ASP:OD1	1:B:332:ASP:N	0.50	2.44	6	1
1:B:343:ARG:HH22	1:B:396:GLN:HE22	0.50	1.49	9	1
1:A:11:HIS:NE2	1:B:212:MET:SD	0.50	2.85	12	1
1:B:234:TYR:CD1	1:B:274:PHE:CE2	0.50	2.99	16	1
1:B:250:HIS:CD2	1:B:281:LEU:HD22	0.50	2.41	17	1
1:A:88:GLN:O	1:A:119:HIS:CE1	0.50	2.65	3	1
1:B:373:GLN:N	1:B:373:GLN:CD	0.50	2.64	7	2
1:A:61:ASN:HD21	1:A:64:SER:N	0.50	2.04	11	1
1:B:331:TYR:O	1:B:335:TYR:CB	0.50	2.60	13	3
1:B:320:ARG:NH2	1:B:322:ARG:HH11	0.50	2.04	16	1
2:D:412:DT:H3'	2:D:412:DT:O2	0.50	2.07	8	14
2:D:412:DT:O2	2:D:412:DT:C3'	0.50	2.59	8	20
1:B:367:HIS:ND1	1:B:370:GLN:CD	0.50	2.64	7	2
1:A:173:PHE:CD1	1:A:173:PHE:C	0.50	2.85	5	2
1:B:232:LEU:C	1:B:232:LEU:CD2	0.50	2.80	20	10
1:B:393:LEU:N	1:B:393:LEU:CD2	0.50	2.75	11	9
1:B:228:HIS:CD2	1:B:259:LYS:CE	0.50	2.95	2	1
1:B:359:HIS:O	1:B:362:ASP:OD2	0.50	2.30	2	1
1:A:38:GLU:OE1	1:A:91:ARG:O	0.50	2.30	3	1
1:A:49:ASP:O	1:B:206:SER:O	0.50	2.30	20	3
1:A:173:PHE:CD2	1:A:174:GLN:N	0.50	2.80	14	4
1:A:182:HIS:CD2	2:D:409:DA:N6	0.50	2.80	8	1
1:A:103:SER:OG	1:A:104:TRP:N	0.50	2.42	13	1
1:A:185:ALA:HB1	2:D:410:DT:O4	0.50	2.06	18	5
1:A:165:PHE:CD1	1:B:210:HIS:CE1	0.50	3.00	12	1
1:A:73:LEU:HD13	1:A:73:LEU:O	0.50	2.07	13	1
1:B:232:LEU:CD1	1:B:271:GLN:NE2	0.50	2.75	15	1
1:B:343:ARG:NE	1:B:393:LEU:HD22	0.50	2.22	9	1
1:B:209:ARG:NH1	1:B:368:GLN:HE22	0.50	2.04	14	1
1:A:45:SER:CB	1:A:91:ARG:HH11	0.50	2.19	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:HIS:CD2	2:D:414:DC:C2	0.50	3.00	9	20
1:A:55:LEU:HD21	1:B:209:ARG:NE	0.50	2.22	2	1
1:B:255:HIS:CG	1:B:256:ASN:N	0.50	2.80	7	2
1:B:384:ALA:CB	2:C:400:DT:P	0.50	3.00	18	4
1:B:329:TYR:O	1:B:330:ASP:OD2	0.50	2.29	12	2
1:A:61:ASN:OD1	1:A:66:PHE:O	0.50	2.30	16	1
1:B:272:LEU:HD13	1:B:272:LEU:O	0.49	2.07	3	1
1:A:91:ARG:CZ	1:A:123:ARG:NH2	0.49	2.75	14	1
1:B:335:TYR:CZ	1:B:339:LEU:HD22	0.49	2.42	16	1
1:A:98:TRP:CE3	2:D:414:DC:C2	0.49	3.01	14	18
1:A:19:THR:O	1:A:23:ASN:CG	0.49	2.51	15	5
1:B:275:LEU:HD13	1:B:275:LEU:O	0.49	2.07	3	1
1:A:61:ASN:CG	1:A:61:ASN:O	0.49	2.50	13	5
1:A:127:ALA:HB2	1:A:153:MET:HE1	0.49	1.84	5	1
1:A:61:ASN:HD21	1:A:64:SER:CB	0.49	2.20	9	2
1:A:49:ASP:OD2	1:A:49:ASP:N	0.49	2.45	12	1
1:B:335:TYR:CG	1:B:336:LYS:N	0.49	2.79	17	3
1:A:177:ASP:O	1:A:177:ASP:OD2	0.49	2.30	10	1
1:A:61:ASN:OD1	1:A:61:ASN:N	0.49	2.43	16	1
1:A:121:ARG:CZ	1:A:123:ARG:HH11	0.49	2.20	16	1
1:A:153:MET:SD	1:A:158:PHE:CZ	0.49	3.06	17	1
1:A:9:PRO:O	1:A:11:HIS:N	0.49	2.43	9	6
1:A:132:TYR:O	1:A:133:ASP:C	0.49	2.49	7	18
1:B:343:ARG:HH22	1:B:395:ASN:HD21	0.49	1.50	4	1
1:A:13:MET:SD	1:B:210:HIS:CD2	0.49	3.05	9	1
1:A:11:HIS:CD2	1:B:253:PHE:CZ	0.49	3.01	15	1
1:A:18:PHE:CZ	1:A:22:PHE:CE1	0.49	3.00	15	1
1:B:378:LEU:N	1:B:378:LEU:CD2	0.49	2.70	18	5
1:A:50:GLN:O	1:A:51:HIS:CB	0.49	2.60	15	2
1:A:125:PHE:CE1	1:A:157:GLU:OE2	0.49	2.65	1	1
1:B:234:TYR:CD1	1:B:274:PHE:CE1	0.49	3.00	3	1
1:B:237:GLU:CD	1:B:237:GLU:N	0.49	2.65	3	1
1:A:178:GLY:O	1:A:182:HIS:ND1	0.49	2.45	13	1
1:A:48:MET:CG	1:A:49:ASP:N	0.49	2.75	14	1
1:B:264:GLY:O	1:B:266:TYR:CD2	0.49	2.66	16	2
2:D:412:DT:O2	2:D:412:DT:H3'	0.49	2.08	13	6
1:B:335:TYR:CE1	1:B:339:LEU:HD12	0.49	2.42	12	2
1:A:196:ASN:O	1:A:199:ASN:OD1	0.49	2.30	15	1
1:B:232:LEU:HD12	1:B:233:CYS:N	0.49	2.23	18	1
1:A:122:LEU:O	1:A:149:GLN:OE1	0.49	2.30	12	3
1:B:210:HIS:O	1:B:210:HIS:CG	0.49	2.65	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:CD1	1:A:109:GLU:OE2	0.49	2.61	17	2
1:A:23:ASN:OD1	1:A:23:ASN:O	0.49	2.31	14	2
1:B:267:GLY:O	1:B:268:ARG:C	0.49	2.51	14	1
1:B:290:ARG:HH11	1:B:322:ARG:HH21	0.49	1.47	19	1
1:A:125:PHE:CE2	1:A:127:ALA:HB2	0.49	2.43	20	1
1:A:88:GLN:NE2	1:A:88:GLN:CA	0.49	2.76	7	9
1:A:24:ASN:C	1:A:128:ARG:NH1	0.49	2.66	2	1
1:A:38:GLU:OE2	1:A:91:ARG:O	0.49	2.31	8	1
1:A:141:GLN:OE1	1:A:196:ASN:OD1	0.49	2.31	19	4
1:A:173:PHE:O	1:A:173:PHE:CG	0.49	2.64	18	1
1:A:22:PHE:O	1:A:24:ASN:N	0.49	2.46	6	14
1:A:21:ASN:ND2	1:A:32:TYR:CE1	0.49	2.81	13	1
1:A:24:ASN:OD1	1:A:176:TRP:CZ2	0.48	2.66	3	1
1:A:52:ARG:O	1:B:208:PRO:CA	0.48	2.61	7	10
1:A:29:HIS:CD2	2:D:415:DA:OP2	0.48	2.66	12	2
1:B:340:GLN:OE1	1:B:396:GLN:OE1	0.48	2.31	6	1
1:A:100:PRO:HB3	1:A:140:LEU:HD21	0.48	1.85	20	2
1:A:7:SER:OG	1:B:207:GLY:CA	0.48	2.61	14	1
1:A:194:LEU:N	1:A:194:LEU:HD22	0.48	2.24	4	6
1:A:30:LYS:C	1:A:57:ASN:ND2	0.48	2.66	17	8
1:A:12:LEU:HD23	1:A:167:ASP:OD2	0.48	2.08	3	1
1:A:19:THR:O	1:A:23:ASN:OD1	0.48	2.31	19	4
1:B:235:GLU:CD	1:B:251:ARG:NH2	0.48	2.66	18	4
1:A:49:ASP:O	1:A:50:GLN:OE1	0.48	2.32	8	1
1:B:326:ALA:HB2	1:B:352:MET:HE1	0.48	1.84	14	1
1:A:173:PHE:O	1:A:173:PHE:CD2	0.48	2.67	18	1
1:B:275:LEU:HD13	1:B:308:GLU:HG2	0.48	1.86	1	1
1:B:220:ASN:CG	1:B:231:TYR:CE1	0.48	2.87	3	1
1:B:250:HIS:O	1:B:250:HIS:CG	0.48	2.66	10	1
1:B:328:ILE:HG23	1:B:335:TYR:CZ	0.48	2.43	16	1
1:A:60:LYS:O	1:B:215:HIS:CD2	0.48	2.67	1	1
1:A:100:PRO:HG2	1:A:130:TYR:O	0.48	2.08	1	13
1:B:361:TRP:O	1:B:365:VAL:CB	0.48	2.62	20	13
1:A:93:THR:CG2	1:A:95:PHE:CE2	0.48	2.97	11	4
1:B:225:ILE:N	2:C:403:DT:C7	0.48	2.76	11	9
1:B:340:GLN:OE1	1:B:395:ASN:ND2	0.48	2.47	5	1
1:A:179:LEU:N	1:A:179:LEU:HD12	0.48	2.23	7	1
1:A:181:GLU:OE1	1:A:181:GLU:C	0.48	2.51	13	1
2:D:415:DA:C8	2:D:415:DA:O5'	0.48	2.67	8	13
1:B:264:GLY:O	1:B:266:TYR:CE1	0.48	2.67	13	4
1:B:321:LEU:O	1:B:348:GLN:OE1	0.48	2.31	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:N	1:A:12:LEU:HD12	0.48	2.23	3	1
1:A:60:LYS:O	1:A:61:ASN:HB2	0.48	2.08	6	2
1:A:167:ASP:CG	1:A:167:ASP:O	0.48	2.52	3	1
1:A:119:HIS:ND1	1:A:119:HIS:O	0.48	2.47	7	1
1:A:153:MET:CE	1:A:158:PHE:CE1	0.48	2.96	8	1
1:B:211:LEU:N	1:B:211:LEU:HD22	0.48	2.22	9	1
1:B:237:GLU:OE1	1:B:290:ARG:NE	0.48	2.46	9	1
1:A:180:ASP:CG	1:A:184:GLN:HE21	0.48	2.11	14	2
1:A:140:LEU:C	1:A:140:LEU:CD2	0.48	2.82	11	1
1:B:372:PHE:CE2	1:B:373:GLN:O	0.48	2.67	12	1
1:A:9:PRO:C	1:A:11:HIS:H	0.48	2.12	14	7
1:B:373:GLN:NE2	1:B:373:GLN:CA	0.48	2.76	17	5
1:B:375:TRP:O	1:B:377:GLY:N	0.48	2.46	2	4
1:A:141:GLN:O	1:A:145:ASP:OD1	0.48	2.31	3	2
1:B:221:PHE:C	1:B:223:ASN:H	0.48	2.11	3	2
1:A:181:GLU:OE2	2:D:409:DA:C6	0.48	2.66	13	3
1:B:366:ASP:OD1	1:B:366:ASP:O	0.48	2.31	6	3
1:B:397:GLY:O	1:B:398:ASN:OD1	0.48	2.31	17	2
1:B:254:LEU:HD23	1:B:270:ALA:HB1	0.48	1.83	13	1
1:B:228:HIS:CD2	1:B:259:LYS:NZ	0.48	2.82	14	1
1:B:334:LEU:O	1:B:338:ALA:CB	0.48	2.62	3	4
1:B:367:HIS:ND1	1:B:370:GLN:CB	0.48	2.77	10	2
1:A:197:GLN:CG	1:A:198:GLY:N	0.48	2.77	5	3
1:B:217:PHE:CE1	1:B:221:PHE:CD1	0.48	3.01	9	1
1:A:55:LEU:HD22	1:A:74:ARG:HD3	0.48	1.86	13	1
1:A:64:SER:O	1:A:66:PHE:CD1	0.48	2.67	16	1
1:A:72:GLN:HE21	1:A:96:ILE:HD12	0.48	1.68	2	1
1:B:339:LEU:HG	1:B:392:ILE:HD13	0.48	1.84	4	3
1:A:198:GLY:O	1:A:199:ASN:OXT	0.48	2.31	13	2
1:B:234:TYR:C	1:B:234:TYR:CD2	0.48	2.87	6	1
1:B:240:ASP:O	1:B:243:THR:N	0.48	2.46	14	3
1:B:237:GLU:OE1	1:B:290:ARG:O	0.48	2.32	13	2
1:A:114:LEU:HD12	1:A:146:ALA:HB1	0.48	1.85	17	1
1:B:278:VAL:HG13	1:B:279:PRO:HD3	0.48	1.86	19	1
1:A:31:THR:HG21	1:A:97:SER:OG	0.48	2.08	17	5
1:A:173:PHE:CD1	1:A:174:GLN:N	0.48	2.82	5	2
1:B:217:PHE:CE2	1:B:221:PHE:CZ	0.48	3.02	6	2
1:B:228:HIS:O	1:B:229:LYS:C	0.48	2.52	17	5
1:A:174:GLN:CD	1:A:174:GLN:N	0.48	2.66	12	1
1:B:253:PHE:CZ	1:B:255:HIS:CE1	0.48	3.02	16	2
1:B:395:ASN:O	1:B:398:ASN:O	0.48	2.31	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:389:LEU:O	1:B:389:LEU:HD13	0.48	2.09	2	7
1:B:290:ARG:NH2	1:B:322:ARG:NH1	0.48	2.62	4	1
1:A:10:ARG:NH2	1:B:277:LEU:CD1	0.48	2.76	5	1
1:A:60:LYS:NZ	2:D:417:DT:O4	0.48	2.47	9	2
1:A:60:LYS:NZ	2:D:416:DA:N6	0.48	2.62	16	1
1:A:144:ARG:CZ	1:A:194:LEU:HD21	0.47	2.39	1	2
1:A:183:SER:O	1:A:187:SER:CB	0.47	2.63	3	5
1:A:49:ASP:OD1	1:A:49:ASP:N	0.47	2.47	7	1
1:B:372:PHE:O	1:B:372:PHE:CG	0.47	2.67	18	2
1:A:35:TYR:OH	1:B:209:ARG:CD	0.47	2.62	10	1
1:B:343:ARG:NH2	1:B:349:VAL:CG2	0.47	2.77	17	1
1:B:263:SER:OG	1:B:265:PHE:CD1	0.47	2.57	18	1
1:A:144:ARG:HH12	1:A:197:GLN:NE2	0.47	2.07	13	1
1:A:168:HIS:ND1	1:A:168:HIS:N	0.47	2.62	16	1
1:A:12:LEU:HD13	1:A:167:ASP:OD2	0.47	2.10	18	1
1:A:33:LEU:HD23	1:A:55:LEU:HD12	0.47	1.86	20	1
1:B:295:ILE:HD12	1:B:297:TRP:O	0.47	2.08	7	1
1:A:177:ASP:OD1	1:A:177:ASP:O	0.47	2.31	9	1
1:A:94:TRP:CZ2	1:A:122:LEU:HD11	0.47	2.44	1	4
1:B:396:GLN:CG	1:B:397:GLY:N	0.47	2.77	2	4
1:B:223:ASN:O	2:C:402:DT:O4	0.47	2.32	9	5
1:B:229:LYS:O	1:B:230:THR:C	0.47	2.51	19	2
1:B:340:GLN:HE21	1:B:392:ILE:HG22	0.47	1.69	5	1
1:B:297:TRP:CE3	1:B:330:ASP:OD1	0.47	2.67	6	1
1:B:372:PHE:O	1:B:372:PHE:CD1	0.47	2.66	18	2
1:B:335:TYR:CD1	1:B:335:TYR:C	0.47	2.85	20	2
1:B:318:HIS:NE2	1:B:319:VAL:HG23	0.47	2.24	20	1
1:A:105:GLY:O	1:A:106:CYS:C	0.47	2.51	13	3
1:A:144:ARG:HH22	1:A:197:GLN:HE22	0.47	1.50	8	1
1:B:343:ARG:HE	1:B:393:LEU:CD1	0.47	2.22	8	1
1:B:228:HIS:C	1:B:256:ASN:OD1	0.47	2.53	2	1
1:B:377:GLY:O	1:B:381:HIS:CG	0.47	2.68	2	4
1:A:22:PHE:CE2	1:A:32:TYR:OH	0.47	2.67	10	1
1:A:38:GLU:OE1	1:A:47:LYS:CG	0.47	2.62	11	2
1:B:323:ILE:CD1	1:B:342:LEU:HD21	0.47	2.39	13	1
1:A:62:LEU:CD2	2:D:417:DT:OP1	0.47	2.61	13	3
1:A:183:SER:O	1:A:187:SER:OG	0.47	2.31	17	4
1:A:102:PHE:CD1	1:A:135:LEU:CD1	0.47	2.98	4	1
2:D:418:DT:O5'	2:D:418:DT:H6	0.47	1.93	6	1
1:B:210:HIS:C	1:B:210:HIS:CD2	0.47	2.88	8	1
1:B:361:TRP:CD1	1:B:362:ASP:OD2	0.47	2.67	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ARG:NH1	1:B:234:TYR:OH	0.47	2.46	10	1
1:A:11:HIS:O	1:A:11:HIS:ND1	0.47	2.48	10	1
1:B:237:GLU:OE1	1:B:237:GLU:N	0.47	2.47	10	2
1:B:215:HIS:ND1	1:B:215:HIS:O	0.47	2.47	15	1
1:B:220:ASN:CG	1:B:231:TYR:CD1	0.47	2.88	3	2
1:B:225:ILE:N	2:C:403:DT:H73	0.47	2.25	4	1
1:A:69:ARG:CZ	1:A:103:SER:OG	0.47	2.63	6	1
1:B:218:THR:O	1:B:222:ASN:OD1	0.47	2.32	6	1
1:A:105:GLY:O	1:A:109:GLU:CB	0.47	2.62	11	1
1:A:102:PHE:CE2	1:A:135:LEU:HD23	0.47	2.45	13	1
1:B:232:LEU:HD22	1:B:254:LEU:HD12	0.47	1.86	14	1
1:A:152:ILE:CD1	1:A:187:SER:OG	0.47	2.63	3	2
1:B:225:ILE:HD13	2:C:402:DT:OP2	0.47	2.10	2	1
1:B:262:ASN:OD1	2:C:408:DT:OP1	0.47	2.33	14	5
1:A:12:LEU:CB	1:A:167:ASP:OD1	0.47	2.63	15	2
1:B:393:LEU:N	1:B:393:LEU:HD22	0.47	2.23	8	1
1:B:211:LEU:N	1:B:211:LEU:CD2	0.47	2.77	9	1
1:A:7:SER:OG	1:A:50:GLN:OE1	0.47	2.30	19	1
1:A:58:GLN:OE1	1:B:215:HIS:CD2	0.47	2.67	19	1
1:A:22:PHE:C	1:A:24:ASN:N	0.47	2.67	6	17
1:A:153:MET:CE	1:A:158:PHE:CE2	0.47	2.97	1	1
1:B:225:ILE:CD1	1:B:327:ARG:NH1	0.47	2.77	2	1
1:B:250:HIS:ND1	1:B:250:HIS:N	0.47	2.63	9	1
1:B:357:PHE:O	1:B:361:TRP:N	0.47	2.46	9	2
1:A:27:GLY:O	1:A:28:ARG:NH1	0.47	2.48	11	1
1:B:224:GLY:O	1:B:327:ARG:CZ	0.47	2.63	16	1
1:B:214:PRO:CG	1:B:367:HIS:NE2	0.47	2.78	17	1
1:A:162:TRP:O	1:A:166:VAL:HG23	0.47	2.10	18	1
1:B:229:LYS:CB	2:C:404:DC:N3	0.47	2.78	18	1
1:B:298:SER:N	1:B:299:PRO:HD2	0.46	2.25	7	9
1:B:313:LEU:HD21	1:B:321:LEU:HB2	0.46	1.86	11	2
1:B:218:THR:O	1:B:222:ASN:CG	0.46	2.54	6	1
1:A:105:GLY:O	1:A:108:GLY:N	0.46	2.48	13	1
1:A:33:LEU:HD12	1:A:96:ILE:CG2	0.46	2.39	16	1
1:A:134:PRO:C	1:A:136:TYR:N	0.46	2.68	1	1
1:A:49:ASP:CG	1:A:52:ARG:HH11	0.46	2.13	2	1
1:B:379:ASP:O	1:B:382:SER:OG	0.46	2.32	20	4
1:A:132:TYR:CD2	1:A:133:ASP:N	0.46	2.83	19	4
1:A:181:GLU:CD	1:A:182:HIS:N	0.46	2.69	13	1
1:A:102:PHE:O	1:A:103:SER:OG	0.46	2.31	12	7
1:A:179:LEU:N	1:A:179:LEU:CD2	0.46	2.70	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:266:TYR:O	1:B:268:ARG:N	0.46	2.48	17	3
1:A:49:ASP:O	1:A:50:GLN:CD	0.46	2.54	8	1
1:A:62:LEU:N	1:A:62:LEU:CD2	0.46	2.78	10	1
1:B:313:LEU:HD13	1:B:345:ALA:HB1	0.46	1.87	12	1
1:A:141:GLN:O	1:A:145:ASP:OD2	0.46	2.34	1	1
1:B:353:THR:HG22	1:B:354:TYR:H	0.46	1.70	13	2
1:A:174:GLN:NE2	1:A:174:GLN:CA	0.46	2.78	8	3
1:B:221:PHE:C	1:B:223:ASN:N	0.46	2.69	3	6
1:B:361:TRP:O	1:B:365:VAL:N	0.46	2.44	17	2
1:A:60:LYS:CE	2:D:416:DA:C5	0.46	2.99	11	7
1:B:291:VAL:HG22	1:B:293:TRP:NE1	0.46	2.26	14	2
1:B:381:HIS:CE1	2:C:401:DT:O4	0.46	2.69	2	2
1:B:230:THR:OG1	1:B:256:ASN:OD1	0.46	2.33	5	3
1:A:15:PRO:O	1:A:19:THR:OG1	0.46	2.30	15	2
1:B:264:GLY:O	1:B:266:TYR:CE2	0.46	2.69	16	2
1:A:24:ASN:C	1:A:128:ARG:HH12	0.46	2.14	2	1
1:A:162:TRP:O	1:A:166:VAL:CB	0.46	2.63	2	3
1:A:59:ALA:C	2:D:416:DA:OP2	0.46	2.54	4	11
1:B:237:GLU:OE2	1:B:290:ARG:O	0.46	2.33	3	1
1:B:229:LYS:CB	2:C:404:DC:O2	0.46	2.64	9	4
1:A:41:ASP:O	1:A:44:THR:N	0.46	2.46	7	1
1:B:239:LEU:HB2	1:B:288:ILE:HG23	0.46	1.87	1	2
1:B:313:LEU:CD1	1:B:345:ALA:HB1	0.46	2.41	1	1
1:A:74:ARG:HH12	1:B:366:ASP:CG	0.46	2.12	5	3
1:B:340:GLN:OE1	1:B:395:ASN:OD1	0.46	2.34	5	4
1:B:294:PHE:CE2	1:B:324:PHE:CD2	0.46	3.03	5	1
1:B:297:TRP:CZ3	1:B:327:ARG:NH2	0.46	2.84	16	1
1:A:144:ARG:HH22	1:A:196:ASN:HD21	0.46	1.54	17	1
1:B:328:ILE:CG2	1:B:335:TYR:CE2	0.46	2.98	19	1
1:A:30:LYS:C	1:A:57:ASN:OD1	0.46	2.55	11	13
1:A:38:GLU:OE2	1:A:45:SER:C	0.46	2.54	14	2
1:B:320:ARG:HH22	1:B:322:ARG:NE	0.46	2.09	4	1
1:A:168:HIS:ND1	1:A:171:GLN:NE2	0.46	2.64	13	1
1:B:343:ARG:HH21	1:B:393:LEU:HD23	0.46	1.70	13	1
1:A:48:MET:HE3	1:A:51:HIS:CE1	0.46	2.45	19	1
1:B:209:ARG:C	1:B:211:LEU:N	0.46	2.69	12	16
1:B:324:PHE:CD1	1:B:350:SER:O	0.46	2.69	5	1
1:A:173:PHE:C	1:A:173:PHE:CD2	0.46	2.84	7	1
1:A:180:ASP:CG	1:A:184:GLN:NE2	0.46	2.70	14	2
1:B:237:GLU:OE1	1:B:244:SER:C	0.46	2.54	11	2
1:B:328:ILE:HD12	1:B:385:LEU:HD13	0.46	1.88	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:328:ILE:CG2	1:B:335:TYR:CZ	0.46	2.98	4	3
1:A:61:ASN:O	1:A:61:ASN:OD1	0.46	2.33	4	1
1:A:38:GLU:OE2	1:A:45:SER:OG	0.46	2.29	7	1
1:B:297:TRP:HE1	1:B:327:ARG:HH11	0.46	1.52	8	1
1:A:7:SER:CB	1:A:50:GLN:HE22	0.46	2.24	12	1
1:A:61:ASN:OD1	1:A:64:SER:CB	0.46	2.64	12	1
1:A:78:LEU:CD1	1:B:209:ARG:NE	0.46	2.79	18	1
1:A:56:HIS:NE2	1:B:216:ILE:CD1	0.46	2.79	20	1
1:A:11:HIS:CD2	1:A:11:HIS:C	0.45	2.87	3	2
1:B:328:ILE:HD11	1:B:385:LEU:HD13	0.45	1.88	5	1
1:B:366:ASP:O	1:B:366:ASP:CG	0.45	2.55	6	4
1:A:10:ARG:H	1:B:252:GLY:CA	0.45	2.24	9	1
1:A:38:GLU:OE1	1:A:45:SER:C	0.45	2.55	16	2
1:A:61:ASN:C	1:A:61:ASN:OD1	0.45	2.52	6	2
1:B:246:LYS:HZ1	1:B:251:ARG:NH1	0.45	2.09	20	2
1:B:229:LYS:C	1:B:256:ASN:OD1	0.45	2.54	12	2
1:B:227:ARG:CB	1:B:228:HIS:CE1	0.45	3.00	11	1
1:B:237:GLU:OE1	1:B:244:SER:O	0.45	2.34	11	1
1:B:293:TRP:CE2	1:B:321:LEU:HD21	0.45	2.47	2	1
1:A:59:ALA:N	2:D:416:DA:OP2	0.45	2.49	3	2
1:B:334:LEU:O	1:B:338:ALA:N	0.45	2.43	3	1
1:A:33:LEU:C	1:A:33:LEU:CD2	0.45	2.85	12	5
1:A:38:GLU:N	1:A:38:GLU:CD	0.45	2.70	8	1
1:B:234:TYR:CG	1:B:274:PHE:CE2	0.45	3.05	11	1
1:B:261:LEU:N	1:B:261:LEU:HD12	0.45	2.27	20	2
1:A:196:ASN:O	1:A:199:ASN:O	0.45	2.34	16	2
1:B:343:ARG:HH21	1:B:349:VAL:HG21	0.45	1.71	17	1
1:A:23:ASN:CG	1:A:23:ASN:O	0.45	2.55	1	1
1:A:98:TRP:CE3	2:D:414:DC:C4	0.45	3.04	11	14
1:B:366:ASP:CG	1:B:366:ASP:O	0.45	2.54	10	1
1:A:92:VAL:O	1:A:92:VAL:CG1	0.45	2.63	12	2
1:B:287:GLN:N	1:B:287:GLN:HE21	0.45	2.08	12	1
1:B:378:LEU:O	1:B:382:SER:OG	0.45	2.31	19	2
1:B:332:ASP:H	1:B:333:PRO:HD2	0.45	1.71	13	12
1:A:125:PHE:CG	1:A:153:MET:SD	0.45	3.10	3	1
1:B:234:TYR:CD1	1:B:234:TYR:C	0.45	2.89	4	2
1:B:259:LYS:C	2:C:407:DT:OP1	0.45	2.55	10	3
1:A:79:VAL:N	1:A:80:PRO:HD2	0.45	2.26	8	5
1:A:173:PHE:CD2	1:A:173:PHE:C	0.45	2.87	10	3
1:B:224:GLY:O	1:B:327:ARG:NH1	0.45	2.50	16	1
1:A:167:ASP:O	1:A:167:ASP:CG	0.45	2.55	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:PHE:CE1	1:A:94:TRP:NE1	0.45	2.85	2	1
1:A:31:THR:O	1:A:57:ASN:CG	0.45	2.55	3	2
1:B:255:HIS:CD2	1:B:255:HIS:H	0.45	2.28	5	2
1:A:194:LEU:HD12	1:A:194:LEU:N	0.45	2.27	6	1
1:A:47:LYS:O	1:A:48:MET:O	0.45	2.34	16	1
1:B:222:ASN:OD1	1:B:222:ASN:C	0.45	2.55	19	1
1:A:144:ARG:HD3	1:A:194:LEU:HD11	0.45	1.88	1	1
1:B:291:VAL:HG22	1:B:293:TRP:HE1	0.45	1.70	1	1
1:B:376:ASP:O	1:B:376:ASP:OD2	0.45	2.35	2	2
1:A:144:ARG:NE	1:A:194:LEU:CD1	0.45	2.78	5	2
1:A:78:LEU:CD1	1:B:209:ARG:HH21	0.45	2.25	9	1
1:A:182:HIS:ND1	1:A:182:HIS:C	0.45	2.70	14	1
1:A:141:GLN:CG	1:A:196:ASN:OD1	0.45	2.64	20	1
1:B:361:TRP:O	1:B:365:VAL:HB	0.45	2.12	20	4
1:A:168:HIS:CD2	1:A:171:GLN:OE1	0.45	2.70	3	1
1:A:93:THR:CG2	1:A:95:PHE:CE1	0.45	3.00	18	5
1:A:105:GLY:O	1:A:107:ALA:N	0.45	2.50	7	1
1:B:283:LEU:HD22	1:B:289:TYR:CG	0.45	2.46	10	1
1:A:136:TYR:OH	1:A:193:ILE:HD11	0.45	2.12	14	1
1:B:261:LEU:N	1:B:261:LEU:CD1	0.45	2.80	15	2
1:B:343:ARG:CD	1:B:396:GLN:NE2	0.45	2.80	20	1
1:B:221:PHE:O	1:B:223:ASN:N	0.45	2.50	3	1
1:A:61:ASN:OD1	1:A:64:SER:OG	0.45	2.31	4	2
1:A:134:PRO:O	1:A:138:GLU:OE2	0.45	2.34	5	1
1:A:69:ARG:NH1	1:A:103:SER:OG	0.45	2.49	6	1
1:B:327:ARG:NH1	1:B:381:HIS:NE2	0.45	2.65	6	1
1:A:199:ASN:OXT	1:A:199:ASN:OD1	0.45	2.35	11	1
1:B:375:TRP:NE1	1:B:378:LEU:CD1	0.45	2.80	14	2
1:A:10:ARG:NH1	1:B:273:ARG:NH1	0.45	2.61	18	1
1:A:102:PHE:CE1	1:A:135:LEU:HD22	0.45	2.47	18	1
1:A:17:ILE:N	1:A:17:ILE:HD12	0.45	2.26	20	1
1:B:297:TRP:CD1	1:B:297:TRP:N	0.45	2.85	4	1
1:A:40:LEU:HD23	1:A:40:LEU:C	0.45	2.32	7	1
1:A:125:PHE:CE1	1:A:127:ALA:HB2	0.45	2.47	12	2
1:B:359:HIS:O	1:B:363:THR:OG1	0.45	2.29	10	1
1:B:320:ARG:HH21	1:B:322:ARG:HH11	0.45	1.54	16	1
1:A:134:PRO:O	1:A:136:TYR:N	0.44	2.49	1	1
1:B:397:GLY:O	1:B:398:ASN:OXT	0.44	2.34	3	1
1:A:160:HIS:O	1:A:164:THR:OG1	0.44	2.30	10	3
1:B:397:GLY:O	1:B:398:ASN:C	0.44	2.56	3	2
1:A:50:GLN:CD	1:A:52:ARG:CZ	0.44	2.85	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:HIS:ND1	1:A:171:GLN:CB	0.44	2.80	19	3
1:B:253:PHE:CE2	1:B:364:PHE:CD1	0.44	3.05	10	1
1:A:85:ASP:OD1	1:A:90:TYR:OH	0.44	2.35	20	1
1:A:62:LEU:CD1	1:A:62:LEU:N	0.44	2.80	4	1
1:A:62:LEU:N	1:A:62:LEU:HD12	0.44	2.27	4	1
1:B:378:LEU:O	1:B:382:SER:N	0.44	2.43	17	3
1:A:173:PHE:CE1	1:A:174:GLN:O	0.44	2.70	6	1
1:B:362:ASP:OD1	1:B:367:HIS:O	0.44	2.36	7	1
1:A:56:HIS:ND1	1:B:213:ASP:CG	0.44	2.71	9	1
1:B:335:TYR:CZ	1:B:339:LEU:CD1	0.44	2.99	15	1
1:B:343:ARG:NH1	1:B:393:LEU:HD21	0.44	2.26	17	1
1:A:58:GLN:CD	1:A:58:GLN:O	0.44	2.56	19	1
1:B:366:ASP:OD1	1:B:366:ASP:N	0.44	2.51	1	2
1:B:219:SER:O	1:B:222:ASN:CG	0.44	2.56	3	1
1:B:323:ILE:HD13	1:B:342:LEU:HD21	0.44	1.88	13	2
1:B:240:ASP:O	1:B:241:ASN:C	0.44	2.56	14	3
1:A:10:ARG:NH1	1:B:250:HIS:O	0.44	2.51	10	1
1:B:343:ARG:NH2	1:B:396:GLN:HE21	0.44	2.10	15	1
1:A:131:ASP:O	1:A:132:TYR:HB3	0.44	2.13	2	17
1:A:141:GLN:CD	1:A:196:ASN:OD1	0.44	2.56	1	8
1:A:35:TYR:CG	1:A:75:PHE:CE1	0.44	3.05	5	1
1:A:194:LEU:N	1:A:194:LEU:CD1	0.44	2.81	6	1
1:B:230:THR:CB	1:B:256:ASN:OD1	0.44	2.64	8	1
1:A:22:PHE:CZ	1:A:32:TYR:CE1	0.44	3.06	10	1
1:B:253:PHE:CE1	1:B:364:PHE:CD1	0.44	3.05	14	1
1:A:34:CYS:CB	1:A:165:PHE:CZ	0.44	3.00	15	1
1:B:297:TRP:CZ2	1:B:327:ARG:NH2	0.44	2.86	2	1
1:A:75:PHE:CD2	1:A:75:PHE:C	0.44	2.90	4	1
1:B:219:SER:C	1:B:229:LYS:NZ	0.44	2.71	4	1
1:A:154:THR:HG22	1:A:155:TYR:H	0.44	1.72	7	2
1:A:168:HIS:CG	1:A:171:GLN:HE21	0.44	2.30	12	1
1:B:398:ASN:OXT	1:B:398:ASN:OD1	0.44	2.36	14	2
1:A:51:HIS:O	1:A:52:ARG:O	0.44	2.35	14	2
1:B:255:HIS:NE2	1:B:257:GLN:CG	0.44	2.81	15	1
1:B:310:ARG:CZ	1:B:314:GLN:OE1	0.44	2.66	17	1
1:B:384:ALA:HB1	2:C:400:DT:OP1	0.44	2.13	18	1
1:B:366:ASP:OD1	1:B:368:GLN:NE2	0.44	2.51	20	1
1:B:297:TRP:CD2	1:B:330:ASP:OD2	0.44	2.71	2	1
1:A:30:LYS:O	1:A:30:LYS:CG	0.44	2.64	3	1
1:A:144:ARG:O	1:A:148:ALA:HB2	0.44	2.11	3	1
1:B:210:HIS:CD2	1:B:210:HIS:C	0.44	2.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LYS:C	1:A:61:ASN:CG	0.44	2.76	16	3
1:A:95:PHE:CZ	1:A:125:PHE:CD1	0.44	3.05	11	1
1:A:144:ARG:NH2	1:A:197:GLN:CG	0.44	2.80	17	1
1:B:380:GLU:CG	1:B:381:HIS:N	0.44	2.81	12	2
1:A:75:PHE:CZ	1:A:92:VAL:HG21	0.44	2.48	6	3
1:B:361:TRP:CD1	1:B:367:HIS:NE2	0.44	2.86	6	1
1:A:20:SER:O	1:A:23:ASN:CG	0.44	2.56	7	1
1:A:102:PHE:CE1	1:A:135:LEU:CD2	0.44	3.00	19	2
1:B:222:ASN:O	2:C:402:DT:O4	0.44	2.36	11	2
1:B:268:ARG:HE	1:B:272:LEU:CD2	0.44	2.24	14	1
1:A:76:LEU:O	1:A:80:PRO:CD	0.43	2.66	16	8
1:B:367:HIS:ND1	1:B:370:GLN:OE1	0.43	2.50	3	1
1:A:91:ARG:HH11	1:A:123:ARG:HH21	0.43	1.56	12	3
1:A:61:ASN:OD1	1:A:61:ASN:C	0.43	2.55	13	2
1:B:267:GLY:O	1:B:268:ARG:O	0.43	2.36	14	1
1:B:321:LEU:C	1:B:321:LEU:CD2	0.43	2.87	19	1
1:A:69:ARG:CZ	1:A:104:TRP:NE1	0.43	2.81	20	1
1:B:328:ILE:HG23	1:B:335:TYR:CE1	0.43	2.48	1	1
1:A:140:LEU:HD23	1:A:193:ILE:HD13	0.43	1.88	6	1
1:B:259:LYS:O	2:C:407:DT:OP1	0.43	2.36	8	1
1:B:343:ARG:NE	1:B:393:LEU:CD2	0.43	2.81	9	1
1:B:352:MET:CE	1:B:357:PHE:CE2	0.43	3.01	9	1
1:B:278:VAL:N	1:B:279:PRO:CD	0.43	2.81	19	1
1:A:11:HIS:CE1	1:B:253:PHE:CE2	0.43	3.07	1	1
1:A:162:TRP:O	1:A:166:VAL:HB	0.43	2.13	2	2
1:B:324:PHE:CD2	1:B:324:PHE:C	0.43	2.90	3	1
1:B:255:HIS:CD2	1:B:257:GLN:CG	0.43	3.01	15	3
1:A:50:GLN:C	1:B:206:SER:O	0.43	2.56	9	2
1:B:233:CYS:SG	1:B:253:PHE:CE2	0.43	3.11	10	1
1:A:28:ARG:NH2	1:A:128:ARG:HH11	0.43	2.11	11	1
1:A:56:HIS:NE2	1:A:74:ARG:NH1	0.43	2.65	18	1
1:B:238:ARG:O	1:B:245:VAL:N	0.43	2.49	1	1
1:B:228:HIS:O	1:B:256:ASN:CB	0.43	2.66	2	1
1:B:295:ILE:CG2	1:B:297:TRP:O	0.43	2.67	5	2
1:A:11:HIS:CD2	1:A:11:HIS:H	0.43	2.32	7	1
1:A:23:ASN:O	1:A:23:ASN:CG	0.43	2.57	14	2
1:B:343:ARG:NH1	1:B:396:GLN:CG	0.43	2.81	13	1
1:A:132:TYR:CD1	1:A:133:ASP:N	0.43	2.85	2	2
1:A:130:TYR:CE1	2:D:413:DT:H2''	0.43	2.48	7	8
1:B:380:GLU:O	2:C:399:DA:O5'	0.43	2.30	5	2
2:D:418:DT:OP2	2:D:418:DT:C7	0.43	2.65	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:HIS:CD2	1:A:58:GLN:O	0.43	2.71	12	2
1:A:198:GLY:O	1:A:199:ASN:O	0.43	2.36	15	1
1:A:50:GLN:CA	1:B:206:SER:O	0.43	2.66	18	1
1:B:361:TRP:CD2	1:B:372:PHE:CB	0.43	3.01	18	1
1:A:183:SER:O	1:A:187:SER:N	0.43	2.48	1	2
1:B:297:TRP:CE2	1:B:330:ASP:OD1	0.43	2.72	2	1
1:A:198:GLY:O	1:A:199:ASN:C	0.43	2.56	3	1
1:A:75:PHE:CE2	1:A:94:TRP:NE1	0.43	2.87	5	1
1:B:340:GLN:HE21	1:B:392:ILE:CG2	0.43	2.27	5	1
1:A:16:HIS:NE2	1:B:260:ASN:CG	0.43	2.72	13	1
1:B:253:PHE:CE2	1:B:255:HIS:CE1	0.43	3.06	16	1
1:B:343:ARG:CZ	1:B:393:LEU:HD21	0.43	2.44	17	1
1:A:134:PRO:C	1:A:136:TYR:H	0.43	2.17	1	1
1:B:296:SER:O	1:B:327:ARG:N	0.43	2.51	1	2
1:B:346:GLY:C	1:B:348:GLN:N	0.43	2.72	2	19
1:A:40:LEU:HB2	1:A:89:ILE:HG23	0.43	1.89	15	3
1:A:12:LEU:HD13	1:A:167:ASP:OD1	0.43	2.13	14	1
1:A:75:PHE:CE1	1:A:78:LEU:HD22	0.43	2.48	18	2
1:B:212:MET:SD	1:B:253:PHE:CD2	0.43	3.12	2	1
1:A:93:THR:HG22	1:A:95:PHE:CE2	0.43	2.49	10	2
1:A:61:ASN:CG	1:A:64:SER:OG	0.43	2.57	6	1
1:A:138:GLU:OE1	1:A:138:GLU:N	0.43	2.47	7	1
1:B:318:HIS:O	1:B:318:HIS:CG	0.43	2.70	7	1
1:B:210:HIS:CD2	1:B:210:HIS:N	0.43	2.86	11	3
1:B:395:ASN:HD21	1:B:396:GLN:HE21	0.43	1.56	10	1
1:A:10:ARG:CZ	1:B:234:TYR:OH	0.43	2.67	16	1
1:A:153:MET:SD	1:A:158:PHE:CE1	0.43	3.12	17	1
1:B:384:ALA:CB	2:C:400:DT:OP1	0.43	2.66	18	1
1:A:168:HIS:CD2	1:A:168:HIS:N	0.43	2.86	2	1
1:A:129:ILE:CD1	1:A:186:LEU:CD1	0.43	2.95	4	3
1:A:16:HIS:NE2	2:C:406:DA:OP1	0.43	2.52	8	1
1:A:60:LYS:O	1:A:61:ASN:OD1	0.43	2.37	8	1
1:B:220:ASN:ND2	1:B:231:TYR:OH	0.43	2.52	9	1
1:A:48:MET:CE	1:A:51:HIS:CG	0.43	3.01	12	1
1:A:14:ASP:OD2	1:A:17:ILE:CD1	0.43	2.67	5	1
1:A:40:LEU:HD23	1:A:41:ASP:N	0.43	2.29	7	1
1:B:250:HIS:NE2	1:B:281:LEU:HD22	0.43	2.29	14	1
1:A:11:HIS:CD2	1:B:253:PHE:CE1	0.43	3.07	15	1
1:A:12:LEU:CD2	1:A:12:LEU:H	0.42	2.27	2	1
1:A:55:LEU:HD21	1:B:209:ARG:HE	0.42	1.73	2	1
1:B:237:GLU:CD	1:B:290:ARG:O	0.42	2.58	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:332:ASP:OD2	1:B:332:ASP:C	0.42	2.56	9	1
1:A:62:LEU:N	1:A:62:LEU:HD22	0.42	2.29	10	1
1:A:37:VAL:O	1:A:38:GLU:CD	0.42	2.57	20	2
1:A:113:PHE:CE2	1:A:117:ASN:ND2	0.42	2.87	13	1
1:A:198:GLY:O	1:A:199:ASN:OD1	0.42	2.37	14	1
1:A:65:GLY:O	1:A:67:TYR:CE2	0.42	2.72	1	1
1:B:246:LYS:HZ1	1:B:251:ARG:HH12	0.42	1.56	6	1
1:A:22:PHE:CZ	1:A:32:TYR:CZ	0.42	3.07	10	1
1:A:22:PHE:CD2	1:A:32:TYR:OH	0.42	2.70	10	1
1:B:351:ILE:HD12	1:B:385:LEU:HD12	0.42	1.90	13	1
1:A:182:HIS:CG	1:A:183:SER:N	0.42	2.85	15	1
1:B:290:ARG:HH11	1:B:322:ARG:NH2	0.42	2.12	19	1
1:A:141:GLN:O	1:A:145:ASP:CG	0.42	2.58	1	1
1:B:352:MET:CE	1:B:357:PHE:CE1	0.42	3.02	16	2
1:A:98:TRP:CD2	2:D:414:DC:C5	0.42	3.08	19	1
1:B:230:THR:OG1	1:B:256:ASN:CG	0.42	2.58	5	2
1:A:57:ASN:C	1:A:57:ASN:HD22	0.42	2.16	7	1
1:B:254:LEU:CD1	1:B:270:ALA:HB1	0.42	2.45	8	1
1:B:274:PHE:CE2	1:B:293:TRP:NE1	0.42	2.87	9	1
1:B:230:THR:HG23	1:B:297:TRP:CD1	0.42	2.49	10	1
1:A:144:ARG:HD2	1:A:194:LEU:HD11	0.42	1.90	13	1
1:A:181:GLU:CG	1:A:182:HIS:N	0.42	2.82	13	1
1:A:129:ILE:CG1	1:A:186:LEU:HD22	0.42	2.44	17	2
1:B:230:THR:HG23	1:B:297:TRP:NE1	0.42	2.30	10	1
1:A:78:LEU:HD13	1:B:209:ARG:NH2	0.42	2.28	11	1
1:A:168:HIS:CE1	1:A:171:GLN:HE21	0.42	2.31	12	1
1:A:60:LYS:CE	2:D:416:DA:C6	0.42	3.03	15	5
1:A:196:ASN:CG	1:A:197:GLN:N	0.42	2.73	16	4
1:A:50:GLN:CB	1:B:206:SER:O	0.42	2.67	5	1
1:B:329:TYR:O	1:B:329:TYR:CD1	0.42	2.73	16	1
1:B:395:ASN:CG	1:B:396:GLN:N	0.42	2.73	19	2
1:A:11:HIS:N	1:A:11:HIS:CD2	0.42	2.88	18	1
1:A:144:ARG:CD	1:A:194:LEU:CD2	0.42	2.97	18	1
1:B:382:SER:O	1:B:386:SER:CB	0.42	2.68	18	1
1:B:384:ALA:HB2	2:C:400:DT:P	0.42	2.55	18	1
1:B:287:GLN:NE2	1:B:287:GLN:CA	0.42	2.83	1	11
1:A:186:LEU:N	1:A:186:LEU:CD1	0.42	2.83	3	1
1:B:340:GLN:CD	1:B:395:ASN:OD1	0.42	2.58	4	1
1:A:27:GLY:H	1:A:128:ARG:HH22	0.42	1.57	5	1
1:B:335:TYR:CE2	1:B:339:LEU:CD1	0.42	3.02	5	1
1:A:119:HIS:O	1:A:119:HIS:CG	0.42	2.69	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:HIS:CG	1:A:82:LEU:HD22	0.42	2.50	11	1
1:A:102:PHE:CZ	1:A:135:LEU:CD2	0.42	3.03	11	1
1:A:167:ASP:O	1:A:169:GLN:NE2	0.42	2.53	14	1
1:A:95:PHE:CZ	1:A:125:PHE:CD2	0.42	3.07	18	1
1:B:229:LYS:CG	2:C:404:DC:H42	0.42	2.28	2	1
2:D:415:DA:O5'	2:D:415:DA:C8	0.42	2.73	14	5
1:A:50:GLN:HE22	1:A:52:ARG:NH1	0.42	2.12	7	1
1:B:372:PHE:CD1	1:B:373:GLN:N	0.42	2.87	7	1
1:B:217:PHE:CE2	1:B:221:PHE:CD2	0.42	3.08	10	2
1:B:343:ARG:HH21	1:B:393:LEU:CD2	0.42	2.27	13	1
1:B:385:LEU:CD1	1:B:385:LEU:N	0.42	2.83	18	1
1:A:18:PHE:CE2	1:A:22:PHE:CE1	0.42	3.08	3	2
1:A:73:LEU:HD13	1:A:109:GLU:OE2	0.42	2.15	3	1
1:A:45:SER:O	1:A:45:SER:OG	0.42	2.36	10	1
1:B:361:TRP:CE2	1:B:372:PHE:HB2	0.42	2.50	12	1
1:B:236:VAL:HG23	1:B:236:VAL:O	0.42	2.15	1	1
1:A:28:ARG:NH1	1:A:31:THR:N	0.42	2.64	3	1
1:A:186:LEU:N	1:A:186:LEU:HD12	0.42	2.29	3	1
1:A:97:SER:OG	1:A:98:TRP:CD1	0.42	2.73	6	1
1:B:220:ASN:OD1	1:B:231:TYR:OH	0.42	2.30	7	1
1:A:31:THR:CG2	1:A:98:TRP:CZ2	0.42	2.97	13	1
1:B:321:LEU:C	1:B:321:LEU:CD1	0.41	2.89	3	2
1:B:385:LEU:N	1:B:385:LEU:CD2	0.41	2.82	2	1
1:A:31:THR:HG23	1:A:32:TYR:H	0.41	1.73	4	1
1:A:178:GLY:H	1:A:179:LEU:HD22	0.41	1.75	8	3
1:A:50:GLN:CD	1:A:52:ARG:HH11	0.41	2.15	7	1
1:A:199:ASN:OD1	1:A:199:ASN:C	0.41	2.58	11	1
1:A:100:PRO:O	1:A:130:TYR:CG	0.41	2.73	8	5
1:B:324:PHE:CD2	1:B:325:ALA:N	0.41	2.88	3	1
1:B:335:TYR:CZ	1:B:392:ILE:HD11	0.41	2.49	3	1
1:A:191:ARG:O	1:A:195:GLN:N	0.41	2.49	6	1
1:A:41:ASP:O	1:A:42:ASN:C	0.41	2.59	7	1
1:B:229:LYS:NZ	1:B:255:HIS:CE1	0.41	2.88	7	1
1:B:229:LYS:HZ3	1:B:255:HIS:CE1	0.41	2.33	7	1
1:B:324:PHE:CZ	1:B:350:SER:OG	0.41	2.70	8	1
1:B:343:ARG:NE	1:B:393:LEU:CD1	0.41	2.82	8	1
1:A:16:HIS:HE2	1:B:260:ASN:ND2	0.41	2.12	13	1
1:A:140:LEU:O	1:A:144:ARG:CB	0.41	2.69	13	1
1:A:18:PHE:CE1	1:A:22:PHE:CE1	0.41	3.08	15	1
1:A:147:GLY:C	1:A:149:GLN:N	0.41	2.73	6	5
1:B:353:THR:CG2	1:B:354:TYR:N	0.41	2.83	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:TYR:CD2	1:A:35:TYR:C	0.41	2.93	3	2
1:A:122:LEU:C	1:A:122:LEU:CD1	0.41	2.88	11	3
1:A:75:PHE:CE1	1:A:79:VAL:HG23	0.41	2.51	9	1
1:B:321:LEU:CD1	1:B:321:LEU:C	0.41	2.89	11	1
1:A:131:ASP:C	2:D:413:DT:O2	0.41	2.58	14	2
1:A:155:TYR:CD1	1:A:155:TYR:O	0.41	2.74	12	1
1:A:10:ARG:NH2	1:B:254:LEU:HD11	0.41	2.31	13	1
1:A:11:HIS:C	1:B:210:HIS:CE1	0.41	2.94	16	1
1:B:288:ILE:HG23	1:B:288:ILE:O	0.41	2.15	20	2
1:A:7:SER:HG	1:A:50:GLN:CD	0.41	2.19	19	1
1:B:291:VAL:O	1:B:291:VAL:CG1	0.41	2.68	1	1
1:A:97:SER:OG	1:A:98:TRP:CD2	0.41	2.74	12	3
1:A:102:PHE:C	1:A:103:SER:OG	0.41	2.58	2	3
1:A:125:PHE:CD2	1:A:151:SER:O	0.41	2.74	14	1
1:B:223:ASN:H	1:B:327:ARG:HH11	0.41	1.58	3	1
1:A:93:THR:HG22	1:A:95:PHE:CE1	0.41	2.50	6	2
1:A:16:HIS:NE2	1:B:265:PHE:CE1	0.41	2.89	10	1
1:A:60:LYS:NZ	2:D:416:DA:C6	0.41	2.89	16	1
1:A:155:TYR:CE2	1:A:175:PRO:CG	0.41	3.02	16	1
1:B:330:ASP:O	1:B:330:ASP:OD1	0.41	2.39	5	1
1:B:218:THR:O	1:B:222:ASN:N	0.41	2.54	6	1
1:B:332:ASP:CB	1:B:333:PRO:CD	0.41	2.98	6	3
1:A:56:HIS:CE1	1:A:74:ARG:NH2	0.41	2.88	7	1
1:B:229:LYS:CA	1:B:255:HIS:NE2	0.41	2.83	11	1
1:A:144:ARG:HH12	1:A:197:GLN:HE21	0.41	1.56	13	1
1:B:310:ARG:HH11	1:B:344:ASP:CB	0.41	2.28	14	1
1:B:328:ILE:HG22	1:B:335:TYR:OH	0.41	2.15	20	1
1:B:246:LYS:CD	1:B:251:ARG:NH1	0.41	2.84	2	1
1:A:73:LEU:HD12	1:A:76:LEU:HD12	0.41	1.93	4	1
1:B:310:ARG:NH2	1:B:341:MET:O	0.41	2.53	4	1
1:A:104:TRP:CG	1:A:105:GLY:N	0.41	2.88	10	1
1:A:187:SER:O	1:A:191:ARG:CG	0.41	2.68	14	1
1:A:62:LEU:HD13	2:D:417:DT:OP1	0.41	2.16	15	1
1:A:10:ARG:O	1:A:12:LEU:CD2	0.41	2.69	17	1
1:A:72:GLN:NE2	1:A:96:ILE:CD1	0.41	2.83	17	1
1:B:234:TYR:CD2	1:B:234:TYR:C	0.41	2.94	19	2
1:A:56:HIS:CE1	1:B:216:ILE:HD11	0.41	2.51	19	1
1:B:320:ARG:HH21	1:B:322:ARG:HE	0.41	1.55	4	1
1:B:340:GLN:NE2	1:B:392:ILE:CG2	0.41	2.82	5	1
1:A:141:GLN:OE1	1:A:196:ASN:CG	0.41	2.59	16	2
1:A:12:LEU:H	1:A:12:LEU:CD2	0.41	2.26	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:LYS:CG	1:A:138:GLU:N	0.41	2.84	1	1
1:A:137:LYS:HG3	1:A:138:GLU:N	0.41	2.31	1	1
1:B:250:HIS:CE1	1:B:281:LEU:HD13	0.41	2.51	3	1
1:B:221:PHE:CE2	1:B:294:PHE:CE2	0.41	3.09	7	1
1:A:99:SER:N	1:A:100:PRO:HD2	0.41	2.31	8	1
1:B:232:LEU:CD1	1:B:271:GLN:HE21	0.41	2.28	8	1
1:A:188:GLY:O	1:A:191:ARG:CG	0.41	2.69	9	1
1:A:177:ASP:OD2	1:A:177:ASP:C	0.41	2.59	10	1
1:A:166:VAL:CG1	1:A:168:HIS:CD2	0.41	3.03	11	1
1:A:119:HIS:NE2	1:A:120:VAL:CG2	0.41	2.80	14	1
1:A:70:HIS:CE1	1:A:101:CYS:SG	0.41	3.13	2	1
1:A:167:ASP:OD2	1:A:167:ASP:C	0.41	2.59	4	1
1:A:138:GLU:OE2	1:A:138:GLU:N	0.41	2.47	5	1
1:A:17:ILE:O	1:A:20:SER:OG	0.41	2.31	9	1
1:A:195:GLN:HE21	1:A:195:GLN:N	0.41	2.14	12	1
1:B:271:GLN:NE2	1:B:293:TRP:CZ3	0.41	2.88	12	1
1:A:122:LEU:CD1	1:A:122:LEU:C	0.41	2.89	14	1
1:A:155:TYR:CD2	1:A:155:TYR:O	0.41	2.74	16	1
1:B:246:LYS:HZ2	1:B:251:ARG:NH1	0.40	2.12	1	1
1:B:216:ILE:O	1:B:219:SER:OG	0.40	2.33	4	1
1:A:62:LEU:HD23	2:D:418:DT:H73	0.40	1.91	7	1
1:B:329:TYR:O	1:B:329:TYR:CD2	0.40	2.74	7	1
1:A:61:ASN:ND2	1:A:61:ASN:O	0.40	2.54	11	1
1:A:78:LEU:HD23	1:A:78:LEU:C	0.40	2.34	12	1
1:A:7:SER:OG	1:A:50:GLN:NE2	0.40	2.53	13	1
1:A:85:ASP:O	1:A:119:HIS:CE1	0.40	2.74	13	1
1:A:45:SER:OG	1:A:91:ARG:NH1	0.40	2.53	17	1
1:A:92:VAL:CG2	1:A:94:TRP:HE1	0.40	2.29	20	1
1:A:92:VAL:HG22	1:A:94:TRP:HE1	0.40	1.75	20	1
1:B:330:ASP:OD2	1:B:330:ASP:O	0.40	2.39	3	1
1:A:62:LEU:HD23	2:D:418:DT:C7	0.40	2.46	7	1
1:B:318:HIS:O	1:B:318:HIS:ND1	0.40	2.54	7	1
1:B:393:LEU:CD1	1:B:396:GLN:NE2	0.40	2.85	7	1
1:B:223:ASN:O	2:C:402:DT:C4	0.40	2.74	9	1
1:B:224:GLY:C	1:B:327:ARG:HH22	0.40	2.19	9	1
1:A:16:HIS:CG	1:B:258:ALA:CB	0.40	3.04	12	1
1:B:351:ILE:HD13	1:B:385:LEU:HB3	0.40	1.93	2	1
1:B:361:TRP:CD1	1:B:361:TRP:C	0.40	2.91	8	1
1:A:28:ARG:NH2	1:A:128:ARG:NH1	0.40	2.69	11	1
1:B:234:TYR:CD2	1:B:274:PHE:CE1	0.40	3.09	13	1
1:B:343:ARG:HH12	1:B:396:GLN:HE21	0.40	1.56	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:220:ASN:ND2	1:B:220:ASN:C	0.40	2.73	2	1
1:B:395:ASN:ND2	1:B:395:ASN:C	0.40	2.75	2	1
1:A:38:GLU:OE2	1:A:47:LYS:CG	0.40	2.69	6	1
1:A:102:PHE:CZ	1:A:135:LEU:HD21	0.40	2.52	11	1
1:A:132:TYR:N	2:D:413:DT:O2	0.40	2.54	11	1
1:B:310:ARG:NH1	1:B:341:MET:CG	0.40	2.85	12	1
1:B:220:ASN:OD1	1:B:231:TYR:CB	0.40	2.69	16	1
1:A:15:PRO:HG2	1:A:168:HIS:NE2	0.40	2.32	17	1
1:A:40:LEU:HD21	1:A:43:GLY:N	0.40	2.29	7	1
1:B:216:ILE:HG22	1:B:220:ASN:OD1	0.40	2.17	10	1
1:B:342:LEU:O	1:B:342:LEU:CD1	0.40	2.70	10	1
1:A:16:HIS:CE1	1:B:258:ALA:HB3	0.40	2.50	11	1
1:B:234:TYR:CD1	1:B:234:TYR:O	0.40	2.75	11	1
1:B:297:TRP:CZ3	1:B:300:CYS:SG	0.40	3.14	13	1
1:A:121:ARG:CZ	1:A:123:ARG:HE	0.40	2.30	16	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	193/199 (97%)	172±2 (89±1%)	12±2 (6±1%)	9±1 (5±1%)	4	27
1	B	187/199 (94%)	168±2 (90±1%)	14±2 (7±1%)	5±1 (3±1%)	8	42
All	All	7600/7960 (95%)	6804 (90%)	514 (7%)	282 (4%)	6	34

All 30 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	30	LYS	20
1	A	31	THR	20
1	A	61	ASN	20
1	A	132	TYR	20
1	A	148	ALA	20
1	B	210	HIS	20

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Mol	Chain	Res	Type	Models (Total)
1	B	260	ASN	20
1	B	347	ALA	20
1	A	133	ASP	18
1	B	333	PRO	17
1	A	103	SER	12
1	A	50	GLN	12
1	A	23	ASN	11
1	A	10	ARG	6
1	B	332	ASP	6
1	B	229	LYS	6
1	B	228	HIS	5
1	A	48	MET	4
1	A	52	ARG	4
1	A	105	GLY	4
1	B	300	CYS	4
1	B	250	HIS	2
1	A	51	HIS	2
1	A	12	LEU	2
1	A	11	HIS	2
1	B	267	GLY	1
1	B	269	HIS	1
1	B	222	ASN	1
1	B	268	ARG	1
1	B	305	CYS	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/171 (98%)	140±3 (84±2%)	27±3 (16±2%)	5	42
1	B	162/171 (95%)	141±2 (87±1%)	21±2 (13±1%)	7	48
All	All	6580/6840 (96%)	5615 (85%)	965 (15%)	6	45

All 108 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	88	GLN	20
1	A	98	TRP	20
1	A	99	SER	20
1	A	101	CYS	20
1	A	122	LEU	20
1	A	131	ASP	20
1	A	136	TYR	20
1	A	174	GLN	20
1	A	195	GLN	20
1	A	196	ASN	20
1	B	260	ASN	20
1	B	287	GLN	20
1	B	298	SER	20
1	B	332	ASP	20
1	B	373	GLN	20
1	B	389	LEU	20
1	B	394	GLN	20
1	B	395	ASN	20
1	A	57	ASN	19
1	B	233	CYS	19
1	A	14	ASP	18
1	A	133	ASP	18
1	A	190	LEU	18
1	B	253	PHE	18
1	B	300	CYS	18
1	B	361	TRP	18
1	B	284	ASP	17
1	B	368	GLN	16
1	A	34	CYS	15
1	A	47	LYS	15
1	A	179	LEU	15
1	B	210	HIS	15
1	A	85	ASP	14
1	A	12	LEU	14
1	B	305	CYS	13
1	A	52	ARG	12
1	A	182	HIS	12
1	B	297	TRP	12
1	B	378	LEU	12
1	A	169	GLN	12
1	B	255	HIS	11
1	B	390	ARG	11
1	A	96	ILE	11

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Mol	Chain	Res	Type	Models (Total)
1	B	335	TYR	11
1	A	76	LEU	11
1	A	78	LEU	10
1	A	54	PHE	10
1	B	370	GLN	9
1	B	212	MET	8
1	B	277	LEU	8
1	A	103	SER	8
1	A	106	CYS	8
1	B	213	ASP	8
1	A	28	ARG	8
1	A	48	MET	7
1	A	19	THR	7
1	A	56	HIS	7
1	A	155	TYR	7
1	A	168	HIS	6
1	B	321	LEU	5
1	A	173	PHE	5
1	A	61	ASN	4
1	B	339	LEU	4
1	A	119	HIS	4
1	A	60	LYS	4
1	A	171	GLN	4
1	B	328	ILE	4
1	B	342	LEU	4
1	A	167	ASP	3
1	A	143	LEU	3
1	B	372	PHE	3
1	B	228	HIS	3
1	A	141	GLN	3
1	B	250	HIS	2
1	A	11	HIS	2
1	B	318	HIS	2
1	A	191	ARG	2
1	A	51	HIS	2
1	A	23	ASN	2
1	A	16	HIS	2
1	A	13	MET	2
1	A	104	TRP	2
1	B	215	HIS	2
1	A	64	SER	2
1	A	184	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	B	209	ARG	1
1	A	140	LEU	1
1	B	220	ASN	1
1	B	272	LEU	1
1	B	275	LEU	1
1	B	352	MET	1
1	B	330	ASP	1
1	B	230	THR	1
1	B	232	LEU	1
1	A	50	GLN	1
1	B	354	TYR	1
1	A	31	THR	1
1	B	367	HIS	1
1	B	229	LYS	1
1	A	73	LEU	1
1	A	181	GLU	1
1	B	385	LEU	1
1	A	176	TRP	1
1	A	7	SER	1
1	A	111	ARG	1
1	B	383	GLN	1
1	B	364	PHE	1
1	B	278	VAL	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 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

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 75% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *A3A\_shifts-2plus2\_20200918.txt*

#### 7.1.1 Bookkeeping

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

Total number of shifts	4564
Number of shifts mapped to atoms	4564
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	17

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	384	$0.04 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	350	$0.68 \pm 0.09$	Should be applied
$^{13}\text{C}'$	345	$-0.02 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	362	$-0.31 \pm 0.23$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 3978 atoms were assigned a chemical shift out of a possible 5285. 47 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	1786/1876 (95%)	724/747 (97%)	709/764 (93%)	353/365 (97%)
Sidechain	1751/2432 (72%)	1151/1439 (80%)	580/852 (68%)	20/141 (14%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	275/601 (46%)	232/313 (74%)	38/241 (16%)	5/47 (11%)
Overall	3978/5285 (75%)	2273/2715 (84%)	1327/1997 (66%)	378/573 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 4090 atoms were assigned a chemical shift out of a possible 5464. 47 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	1837/1954 (94%)	746/778 (96%)	729/796 (92%)	362/380 (95%)
Sidechain	1801/2512 (72%)	1183/1488 (80%)	598/882 (68%)	20/142 (14%)
Aromatic	286/622 (46%)	238/324 (73%)	42/250 (17%)	6/48 (12%)
Overall	4090/5464 (75%)	2333/2806 (83%)	1369/2068 (66%)	388/590 (66%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

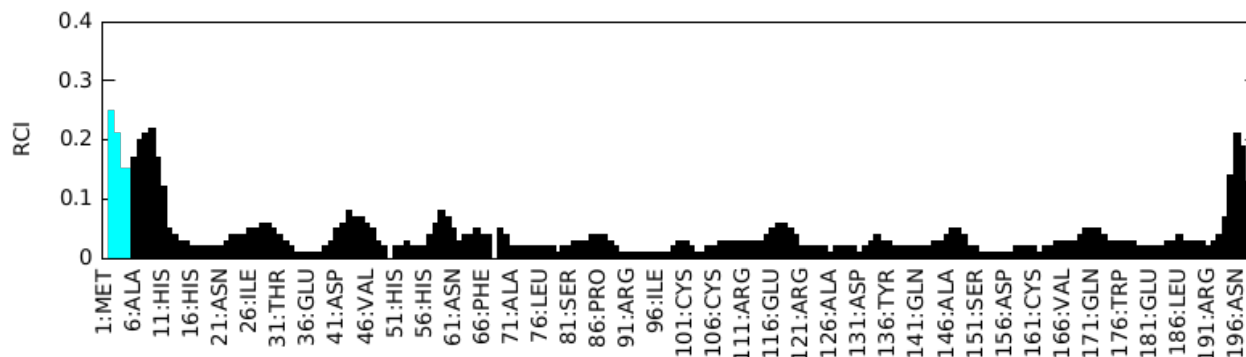
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	94	TRP	HE1	5.58	12.85 – 7.35	-8.2
1	B	293	TRP	HE1	5.58	12.85 – 7.35	-8.2
1	A	70	HIS	CE1	118.42	149.70 – 125.30	-7.8
1	B	269	HIS	CE1	118.42	149.70 – 125.30	-7.8
1	A	66	PHE	CD2	124.86	137.34 – 125.84	-5.9
1	B	265	PHE	CD2	124.86	137.34 – 125.84	-5.9
1	A	66	PHE	CD1	124.86	137.63 – 125.43	-5.5
1	B	265	PHE	CD1	124.86	137.63 – 125.43	-5.5
1	A	72	GLN	CB	38.88	38.36 – 19.96	5.3
1	B	271	GLN	CB	38.88	38.36 – 19.96	5.3
1	A	131	ASP	CB	32.21	49.06 – 32.66	-5.3
1	B	330	ASP	CB	32.21	49.06 – 32.66	-5.3
1	B	371	PRO	CG	32.94	32.66 – 21.76	5.3
1	B	378	LEU	HG	-0.22	3.16 – -0.14	-5.2
1	A	179	LEU	HG	-0.21	3.16 – -0.14	-5.2
1	A	97	SER	HB3	2.44	5.25 – 2.45	-5.0
1	B	296	SER	HB3	2.44	5.25 – 2.45	-5.0

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

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

