



Full wwPDB NMR Structure Validation Report ⓘ

Apr 13, 2022 – 12:13 PM JST

PDB ID : 7D3W
Title : Non-specific and specific interactions work cooperatively to promote cytidine deamination catalyzed by APOBEC3A
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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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

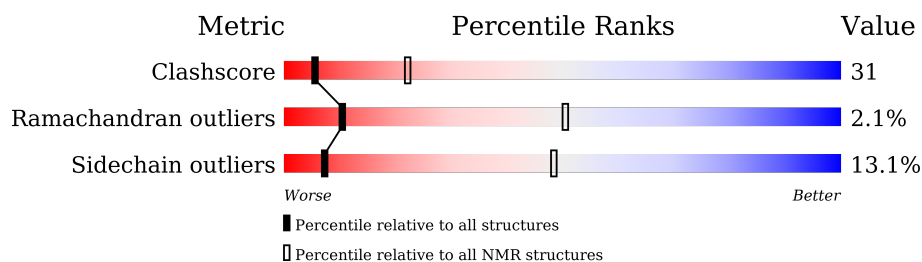
1 Overall quality at a glance

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 ≥ 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	
2	B	10	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:12-A:59, A:70-A:101, A:106-A:197 (172)	0.47	17

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 and 1 single-model cluster was found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3490 atoms, of which 1664 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	

There are 4 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

- 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	B	10	Total	C	H	N	O	P	0
			317	99	118	30	61	9	

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

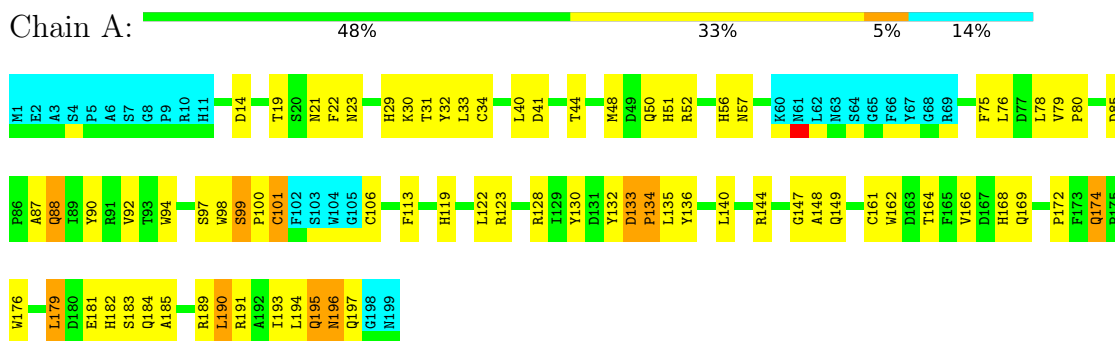
Mol	Chain	Residues	Atoms	
3	A	1	Total	Zn
			1	1

4 Residue-property plots

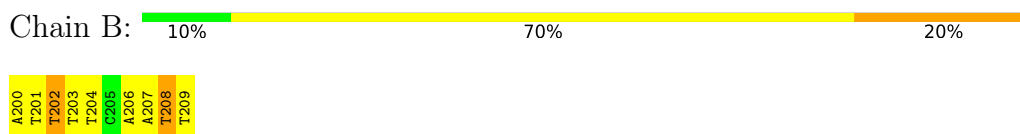
4.1 Average score per residue in the NMR ensemble

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

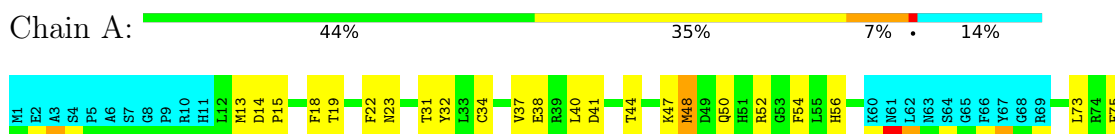


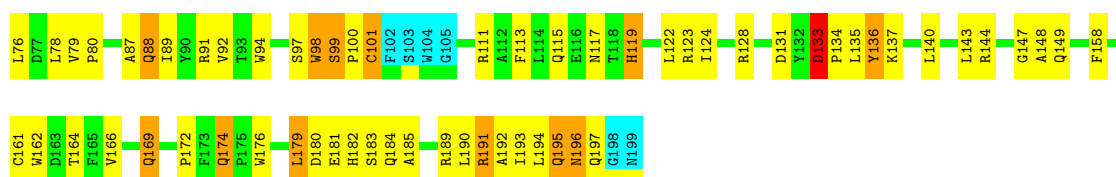
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

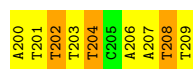
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





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

Chain B: 10% 60% 30%



4.2.2 Score per residue for model 2

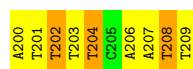
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A: 51% 26% 9% 14%



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

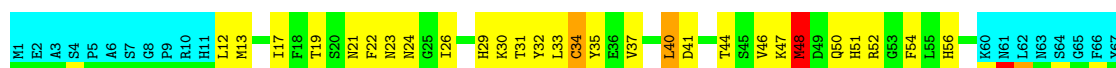
Chain B: 10% 60% 30%



4.2.3 Score per residue for model 3

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

Chain A: 44% 34% 8% 14%





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

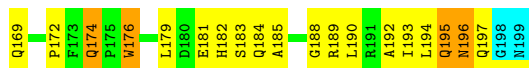
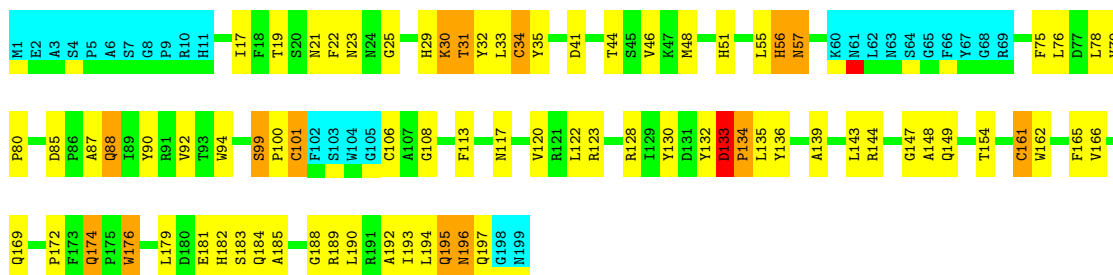
Chain B: 70% 30%



4.2.4 Score per residue for model 4

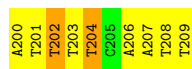
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A: 47% 32% 7% 14%



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

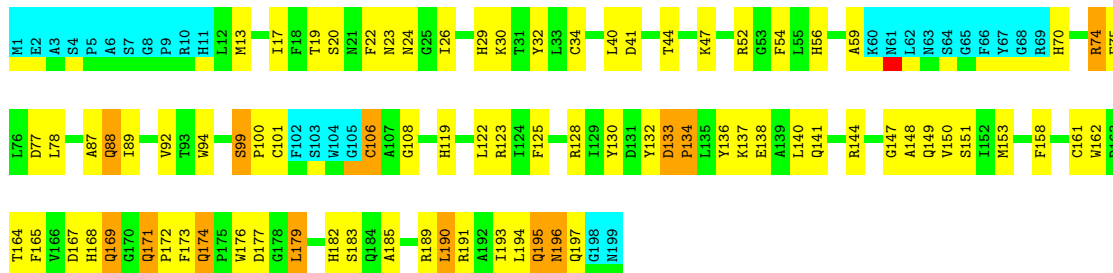
Chain B: 10% 70% 20%



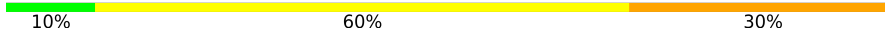
4.2.5 Score per residue for model 5

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

Chain A: 45% 35% 7% 14%



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

Chain B: 

A200
T201
T202
T203
T204
C205
A206
A207
T208
T209

4.2.6 Score per residue for model 6

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

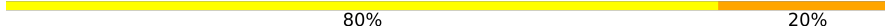
Chain A: 

M1 E2 A3 S4 P5 A6 S7 G8 P9 H11 F18 T19 F22 N23 N24 G25 H29 K30 T31 Y32 L33 C34 D41 T44 H51 R52 Q58 A59 K60 M61 L62 N63 S64 G65 F66 Y67 G68 R69 H70 V79 P80 D85 Q88 I89 Y90 W94 F95 I96

S97 W98 S99 P100 C101 A102 S103 W104 G105 C106 R111 L122 R123 A127 R128 I129 Y132 D133 P134 L135 Y136 L140 Q141 M142 L143 R144 G147 A148 Q149 I152 W162 D163 T164 F165 V166 Q169 Q174 P175 W176 D177 G178 L179 D180 H181 H182 S183 Q184 A185 L186 S187

G188 R189 L190 R191 I192 I193 L194 Q195 N196 Q197 G198 M199

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

Chain B: 

A200
T201
T202
T203
T204
C205
A206
A207
T208
T209

4.2.7 Score per residue for model 7

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

Chain A: 

M1 E2 A3 S4 P5 A6 S7 G8 P9 H11 D14 T19 S20 N21 F22 N23 I26 H29 K30 T31 Y32 V37 L40 M43 H51 H56 N57 Q58 A59 K60 M61 L62 N63 S64 G65 F66 Y67 G68 R69 V79 P80 D85 P86 A87 Q88 I89 Y90 R91

S97 W98 S99 P100 C101 A102 S103 W104 G105 C106 A107 F113 M117 T118 H119 V120 R121 L122 R123 I124 F125 A126 A127 R128 Y130 D133 P134 L135 L140 G147 A148 Q149 V150 S151 I152 M153 E157 H160 C161 W162 D163 T164 F165 V166 H168 Q169 P172 F173 Q174

P175 W176 L179 H182 S183 Q184 A185 R189 L190 I193 L194 Q195 N196 Q197 G198 M199

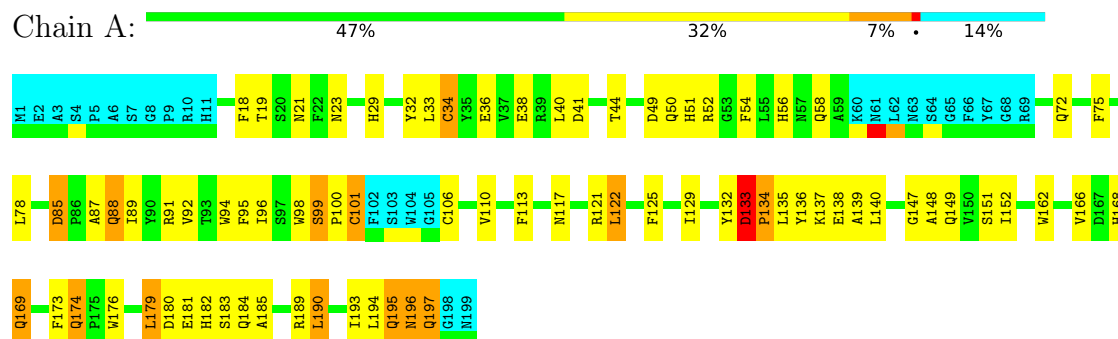
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain B: 

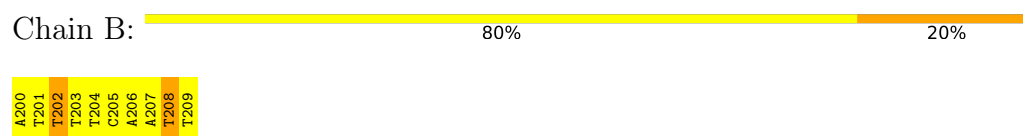
A200
T201
T202
T203
T204
C205
A206
A207
T208
T209

4.2.8 Score per residue for model 8

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

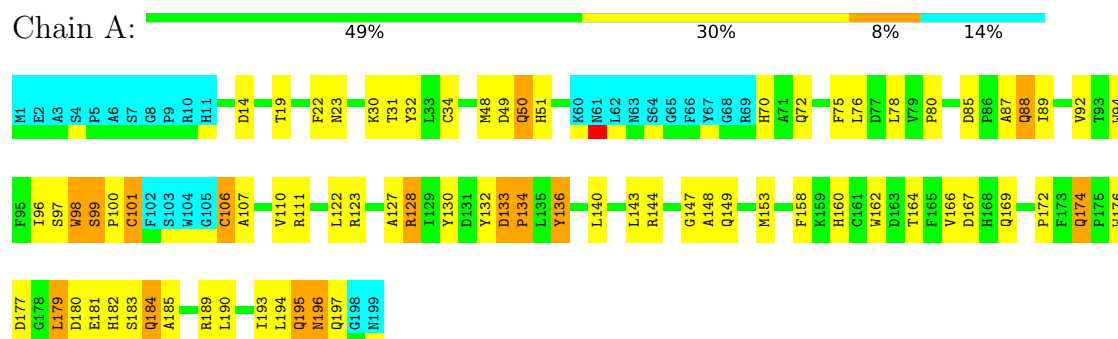


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

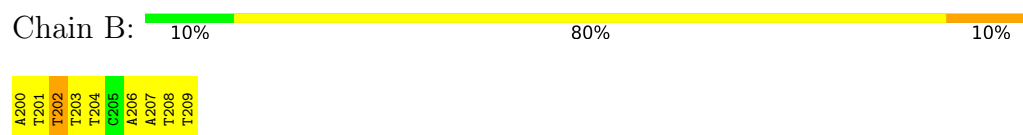


4.2.9 Score per residue for model 9

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

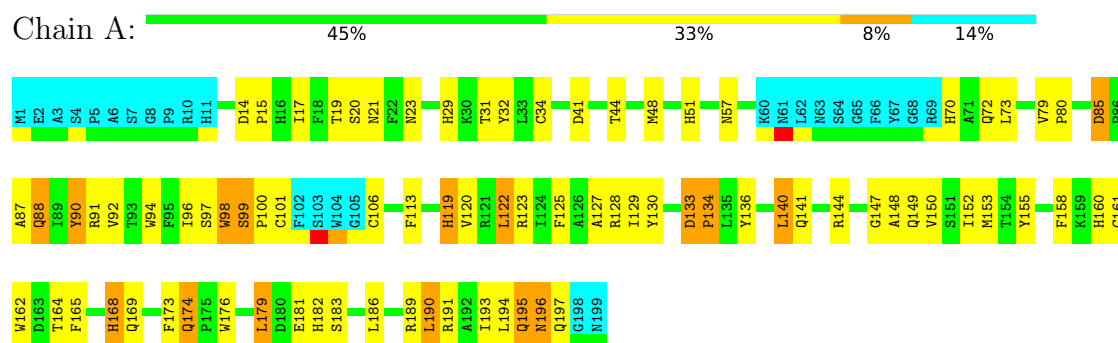


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

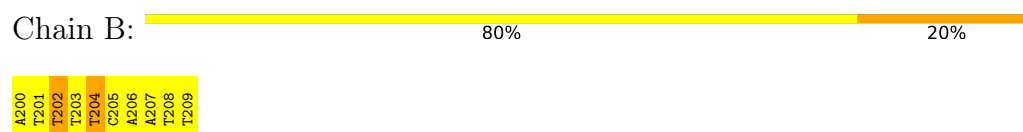


4.2.10 Score per residue for model 10

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

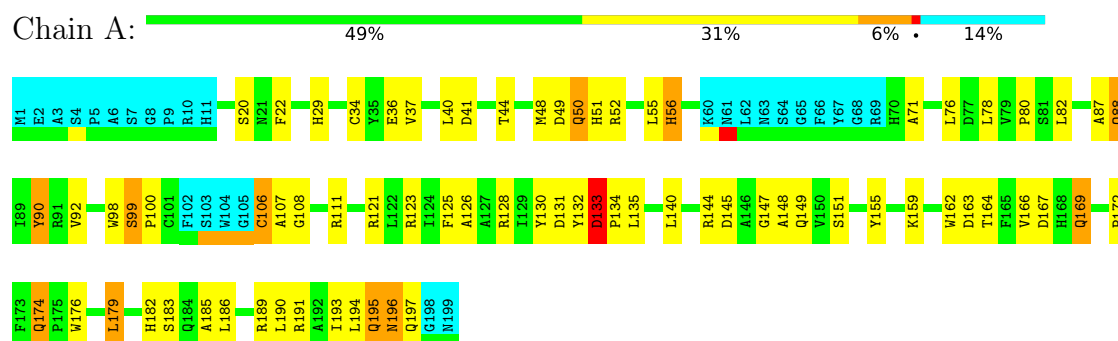


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

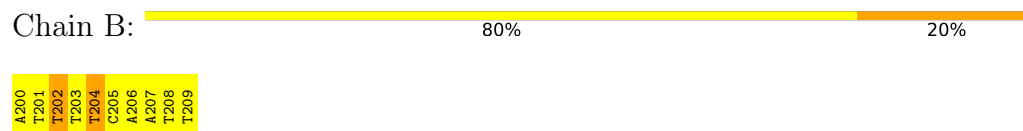


4.2.11 Score per residue for model 11

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

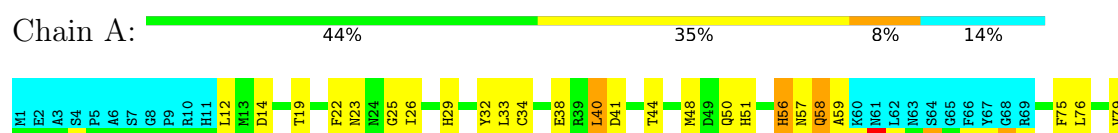


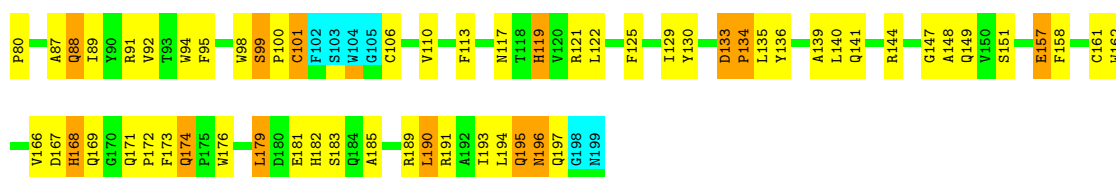
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')



4.2.12 Score per residue for model 12

- 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')

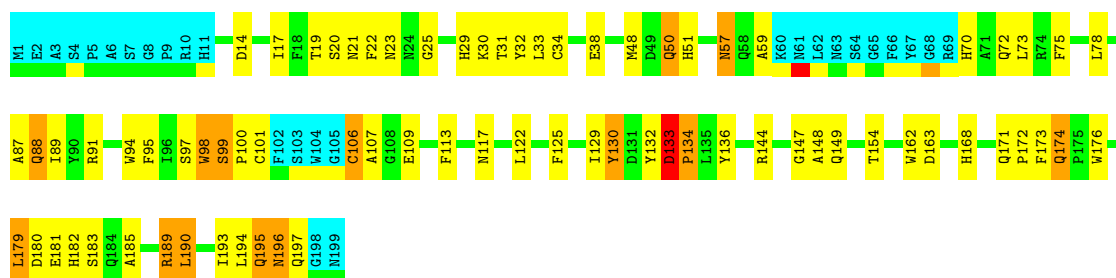
Chain B: 70% 30%



4.2.13 Score per residue for model 13

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

Chain A: 49% 30% 7% 14%



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

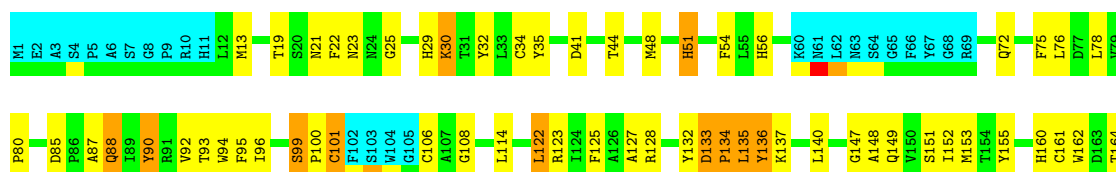
Chain B: 10% 60% 30%



4.2.14 Score per residue for model 14

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

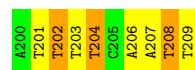
Chain A: 47% 32% 8% 14%





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

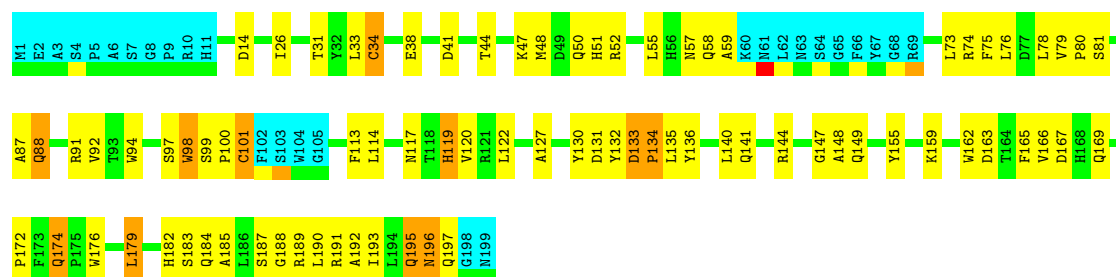
Chain B: 20% 50% 30%



4.2.15 Score per residue for model 15

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

Chain A: 46% 35% 6% 14%



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

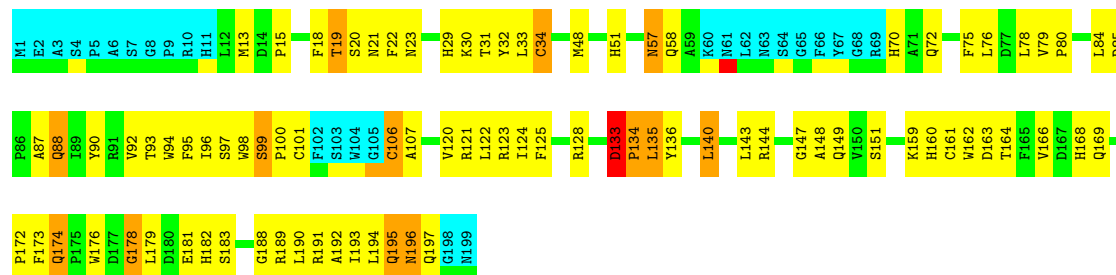
Chain B: 10% 60% 30%



4.2.16 Score per residue for model 16

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

Chain A: 42% 37% 7% 14%



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

Chain B: 

A200
T201
T202
T203
T204
C205
A206
A207
T208
T209

4.2.17 Score per residue for model 17 (medoid)

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


Chain A: 

M1 E2 A3 S4 P5 A6 S7 G8 R10 H11 L12 M13 D14 P15 H16 I17 F18 F19 T19 S20 N21 F22 N23 H29 K30 T31 C34 V37 E38 R39 L40 D41 T44 S45 V46 H51 R52 G53 F54 L55 H56 N57 K60 M61 L62 N63 S64 G65 F66 Y67 G68 R69 F75

L78 V79 P80 D85 P86 A87 Q88 R91 V92 T93 W94 F95 I96 S97 N98 S99 P100 C101 F102 S103 W104 G105 C106 F113 L114 R121 L122 R123 A126 A127 R128 L129 Y130 D131 Y132 D133 P134 L140 L143 R144 D145 A146 G147 A148 Q149 I152 W162 T163 T164 F165

V166 Q169 Q174 P175 W176 L179 D180 H181 H182 S183 Q184 A185 L186 R189 L190 I193 L194 Q195 N196 Q197 G198 M199

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

Chain B: 

A200
T201
T202
T203
T204
C205
A206
A207
T208
T209

4.2.18 Score per residue for model 18

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

Chain A: 

M1 E2 A3 S4 P5 A6 S7 G8 R10 H11 L12 M13 D14 T19 N23 N24 C25 I26 H29 K30 T31 Y32 L33 C34 Y35 D41 M42 G43 T44 K47 H51 R52 G53 F54 L55 H56 N57 Q58 A59 K60 M61 L62 N63 S64 G65 F66 Y67 G68 R69 Q72 W73 L74

F75 L76 D77 L78 V79 P80 A87 Q88 R89 Y90 R91 V92 T93 W94 F95 I96 S97 N98 S99 P100 C101 F102 S103 W104 G105 C106 A107 G108 R111 A112 F113 L114 Q115 E116 M117 L122 R123 D133 P134 L135 Y136 K137 E138 A139 L140 R144 G147 A148 Q149 H160 C161 W162 D163

T164 F165 V166 Q169 Q174 P175 W176 L179 D180 H181 H182 S183 Q184 A185 L186 R189 L190 I193 L194 Q195 N196 Q197 G198 M199

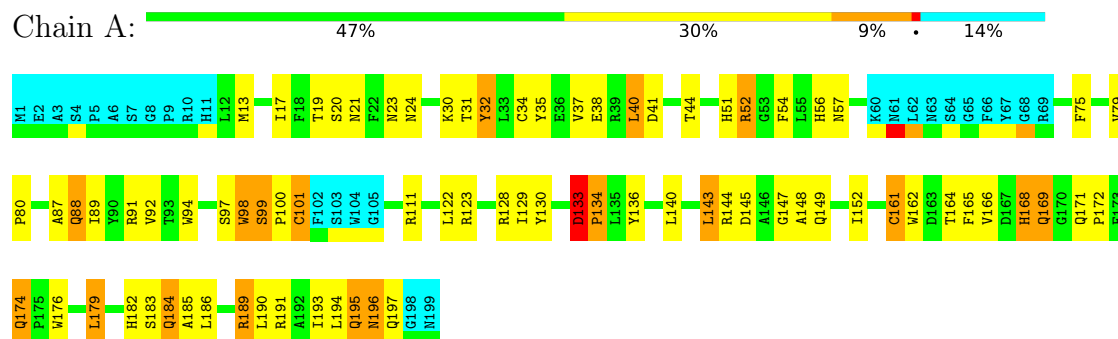
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain B: 

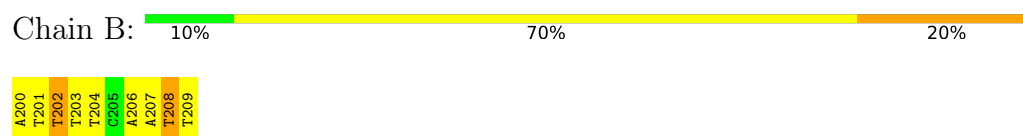
A200
T201
T202
T203
T204
C205
A206
A207
T208
T209

4.2.19 Score per residue for model 19

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

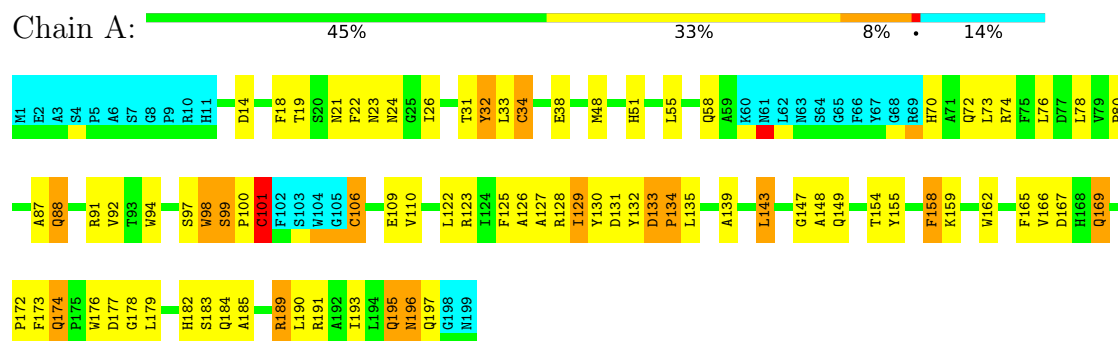


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

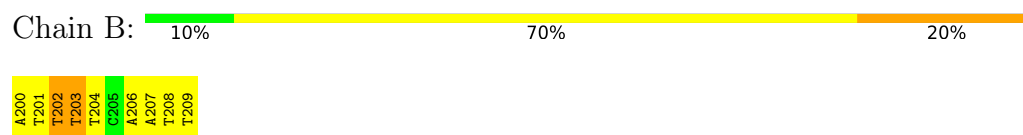


4.2.20 Score per residue for model 20

- 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')



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	2276
Number of shifts mapped to atoms	2276
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

6.1 Standard geometry

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±0/1460 (0.0± 0.0%)	0.91±0.00	0±0/1982 (0.0± 0.0%)
2	B	1.28±0.02	2±1/221 (0.9± 0.3%)	1.70±0.01	10±1/339 (2.8± 0.4%)
All	All	1.04	41/33620 (0.1%)	1.06	192/46420 (0.4%)

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	B	208	DT	C5-C7	5.99	1.53	1.50	5	19
2	B	201	DT	C5-C7	5.51	1.53	1.50	14	13
2	B	204	DT	C5-C7	5.17	1.53	1.50	5	4
2	B	209	DT	C5-C7	5.11	1.53	1.50	11	5

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	B	202	DT	C6-C5-C7	-6.18	119.19	122.90	7	20
2	B	201	DT	C6-C5-C7	-6.11	119.23	122.90	13	19
2	B	208	DT	C6-C5-C7	-6.09	119.25	122.90	5	20
2	B	209	DT	C6-C5-C7	-6.06	119.26	122.90	13	20
2	B	203	DT	C6-C5-C7	-5.87	119.38	122.90	7	20
2	B	204	DT	C6-C5-C7	-5.79	119.43	122.90	18	20
2	B	201	DT	C4-C5-C6	5.48	121.29	118.00	13	2
2	B	202	DT	C4-C5-C6	5.44	121.27	118.00	14	20
2	B	209	DT	C4-C5-C6	5.36	121.22	118.00	13	14
2	B	204	DT	C4-C5-C6	5.18	121.11	118.00	2	14
2	B	203	DT	C4-C5-C6	5.17	121.10	118.00	7	18
2	B	208	DT	C4-C5-C6	5.16	121.09	118.00	13	5

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	1419	1357	1349	88±9
2	B	199	118	118	12±2
All	All	32380	29500	29340	1908

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:TYR:O	1:A:158:PHE:CD1	1.23	1.90	20	1
1:A:158:PHE:CD1	1:A:159:LYS:N	1.02	2.25	20	1
1:A:179:LEU:H	1:A:179:LEU:HD22	0.94	1.21	2	15
1:A:162:TRP:HE1	1:A:168:HIS:CD2	0.92	1.82	12	5
1:A:40:LEU:HD13	1:A:40:LEU:O	0.91	1.64	3	1
1:A:144:ARG:NE	1:A:194:LEU:HD11	0.90	1.80	11	5
1:A:55:LEU:HD22	1:A:74:ARG:HH12	0.90	1.25	20	1
1:A:55:LEU:HD22	1:A:74:ARG:NH1	0.86	1.86	20	1
1:A:136:TYR:OH	1:A:193:ILE:HD11	0.82	1.74	4	5
1:A:33:LEU:HD13	1:A:35:TYR:OH	0.82	1.75	18	1
1:A:155:TYR:O	1:A:158:PHE:CE1	0.80	2.33	20	1
1:A:97:SER:O	1:A:127:ALA:HB3	0.80	1.77	20	6
1:A:78:LEU:O	1:A:78:LEU:HD23	0.79	1.77	1	3
2:B:200:DA:HO5'	2:B:200:DA:H8	0.79	1.13	18	14
1:A:179:LEU:HD22	1:A:179:LEU:N	0.79	1.92	2	15
1:A:40:LEU:C	1:A:40:LEU:HD22	0.76	2.01	3	1
1:A:140:LEU:HD21	1:A:144:ARG:NH1	0.75	1.95	18	1
1:A:40:LEU:HD22	1:A:41:ASP:N	0.75	1.95	3	1
1:A:144:ARG:NH2	1:A:194:LEU:HD22	0.75	1.97	4	1
1:A:162:TRP:CZ2	1:A:168:HIS:CE1	0.75	2.75	7	4
1:A:162:TRP:NE1	1:A:168:HIS:CD2	0.73	2.56	5	5
1:A:21:ASN:ND2	1:A:32:TYR:CD1	0.73	2.57	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:TRP:HE1	1:A:168:HIS:CE1	0.73	2.02	16	5
1:A:31:THR:HG23	1:A:97:SER:OG	0.72	1.85	13	3
1:A:162:TRP:NE1	1:A:168:HIS:CE1	0.72	2.58	16	1
1:A:35:TYR:CD1	1:A:75:PHE:CE1	0.72	2.78	18	1
1:A:99:SER:N	1:A:100:PRO:CD	0.72	2.52	15	18
1:A:174:GLN:H	1:A:174:GLN:NE2	0.71	1.83	17	2
1:A:94:TRP:CH2	1:A:122:LEU:HD11	0.71	2.21	8	5
1:A:113:PHE:CZ	1:A:117:ASN:ND2	0.71	2.59	7	2
1:A:176:TRP:NE1	1:A:179:LEU:HD21	0.71	2.00	4	3
1:A:55:LEU:HD23	1:A:71:ALA:HB1	0.71	1.60	11	1
1:A:24:ASN:ND2	1:A:128:ARG:NH1	0.71	2.39	3	1
1:A:32:TYR:CZ	1:A:54:PHE:CD1	0.70	2.79	2	2
1:A:121:ARG:NH1	1:A:123:ARG:NH1	0.70	2.40	11	2
1:A:184:GLN:N	1:A:184:GLN:OE1	0.70	2.25	2	1
1:A:113:PHE:CE2	1:A:117:ASN:ND2	0.70	2.59	18	1
1:A:168:HIS:CD2	1:A:171:GLN:O	0.70	2.45	12	2
1:A:52:ARG:NH1	1:A:164:THR:HG22	0.70	2.02	3	2
1:A:113:PHE:CE1	1:A:117:ASN:ND2	0.69	2.60	12	3
1:A:179:LEU:H	1:A:179:LEU:CD2	0.69	2.01	18	15
1:A:135:LEU:C	1:A:135:LEU:HD13	0.69	2.08	11	1
1:A:35:TYR:CE1	1:A:75:PHE:CD1	0.69	2.81	18	1
1:A:35:TYR:CE1	1:A:75:PHE:CG	0.69	2.81	18	1
1:A:158:PHE:CG	1:A:159:LYS:N	0.69	2.60	20	1
1:A:133:ASP:H	1:A:134:PRO:CD	0.69	2.00	4	12
1:A:35:TYR:CG	1:A:75:PHE:CE1	0.69	2.81	18	3
1:A:106:CYS:O	1:A:110:VAL:HG23	0.69	1.87	12	2
1:A:23:ASN:ND2	1:A:176:TRP:CE3	0.68	2.61	17	2
1:A:33:LEU:HD11	1:A:72:GLN:NE2	0.68	2.03	18	2
1:A:72:GLN:NE2	1:A:96:ILE:HD11	0.68	2.04	10	1
1:A:140:LEU:HD23	1:A:193:ILE:HG21	0.68	1.65	17	9
1:A:13:MET:SD	1:A:54:PHE:CE1	0.68	2.87	3	3
1:A:174:GLN:NE2	1:A:174:GLN:N	0.68	2.41	17	10
1:A:13:MET:SD	1:A:54:PHE:CZ	0.68	2.87	14	2
1:A:21:ASN:ND2	1:A:32:TYR:CG	0.68	2.61	4	2
1:A:48:MET:SD	1:A:48:MET:N	0.68	2.67	1	2
1:A:33:LEU:C	1:A:33:LEU:HD23	0.67	2.09	2	6
1:A:48:MET:SD	1:A:51:HIS:CE1	0.67	2.88	2	7
1:A:41:ASP:N	1:A:44:THR:O	0.67	2.27	3	15
1:A:91:ARG:HH12	1:A:121:ARG:NH2	0.67	1.87	7	1
1:A:89:ILE:HD11	1:A:121:ARG:HH21	0.67	1.49	12	1
1:A:91:ARG:NH1	1:A:123:ARG:NH2	0.67	2.42	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:TRP:CZ3	1:A:122:LEU:HD11	0.67	2.25	19	11
1:A:135:LEU:HD12	1:A:135:LEU:C	0.67	2.10	6	1
1:A:168:HIS:H	1:A:168:HIS:CD2	0.67	2.07	10	2
1:A:153:MET:SD	1:A:158:PHE:CZ	0.67	2.88	5	1
1:A:92:VAL:CG2	1:A:94:TRP:NE1	0.67	2.58	10	5
1:A:52:ARG:HH22	1:A:164:THR:HG23	0.67	1.50	19	1
1:A:94:TRP:CE2	1:A:122:LEU:HD21	0.66	2.25	15	2
1:A:153:MET:SD	1:A:158:PHE:CE1	0.66	2.88	9	2
1:A:161:CYS:SG	1:A:162:TRP:N	0.66	2.67	14	7
1:A:194:LEU:HD13	1:A:197:GLN:HE21	0.66	1.49	16	2
1:A:89:ILE:HD11	1:A:121:ARG:NH2	0.66	2.06	12	1
1:A:169:GLN:N	1:A:169:GLN:NE2	0.66	2.43	3	5
1:A:33:LEU:HD23	1:A:34:CYS:N	0.66	2.06	18	7
1:A:169:GLN:HE21	1:A:169:GLN:N	0.66	1.89	5	4
1:A:125:PHE:CZ	1:A:153:MET:SD	0.66	2.88	10	1
1:A:182:HIS:CE1	2:B:202:DT:H71	0.66	2.25	8	20
1:A:174:GLN:H	1:A:174:GLN:CD	0.66	1.94	17	2
1:A:133:ASP:O	1:A:135:LEU:N	0.66	2.29	11	3
1:A:136:TYR:CD1	1:A:137:LYS:N	0.66	2.64	14	2
1:A:72:GLN:NE2	1:A:94:TRP:CE3	0.66	2.64	13	3
1:A:29:HIS:CE1	2:B:204:DT:C2	0.66	2.84	4	1
2:B:200:DA:H8	2:B:200:DA:O5'	0.65	1.73	20	14
1:A:88:GLN:HE21	1:A:88:GLN:N	0.65	1.89	16	16
1:A:31:THR:O	1:A:57:ASN:ND2	0.65	2.30	4	2
1:A:98:TRP:CH2	2:B:205:DC:N4	0.65	2.65	11	2
1:A:84:LEU:HD13	1:A:90:TYR:CZ	0.65	2.27	16	1
1:A:72:GLN:NE2	1:A:101:CYS:SG	0.65	2.70	9	1
1:A:185:ALA:HB2	2:B:200:DA:O3'	0.64	1.92	2	14
1:A:13:MET:SD	1:A:54:PHE:CE2	0.64	2.90	19	2
1:A:193:ILE:O	1:A:196:ASN:ND2	0.64	2.30	11	20
1:A:34:CYS:SG	1:A:95:PHE:CD1	0.64	2.89	6	3
1:A:129:ILE:O	1:A:130:TYR:CG	0.64	2.50	12	3
1:A:140:LEU:HD11	1:A:144:ARG:NH2	0.64	2.08	18	1
1:A:174:GLN:O	1:A:174:GLN:NE2	0.64	2.30	6	1
1:A:129:ILE:CG2	1:A:136:TYR:CZ	0.64	2.80	12	1
1:A:168:HIS:O	1:A:168:HIS:ND1	0.64	2.31	12	2
1:A:24:ASN:HD22	1:A:128:ARG:NH1	0.64	1.90	3	1
1:A:122:LEU:HD23	1:A:123:ARG:N	0.64	2.08	7	12
1:A:24:ASN:ND2	1:A:128:ARG:HH11	0.64	1.89	3	1
1:A:140:LEU:C	1:A:140:LEU:HD23	0.64	2.13	7	1
1:A:33:LEU:HD22	1:A:35:TYR:CZ	0.64	2.28	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:PHE:CE2	1:A:153:MET:SD	0.64	2.91	10	1
1:A:37:VAL:HG23	1:A:51:HIS:CD2	0.64	2.28	3	1
1:A:57:ASN:ND2	2:B:206:DA:N3	0.63	2.47	10	2
1:A:196:ASN:ND2	1:A:197:GLN:H	0.63	1.91	11	7
1:A:172:PRO:O	1:A:174:GLN:NE2	0.63	2.32	12	14
1:A:176:TRP:NE1	1:A:179:LEU:HD11	0.63	2.09	6	12
1:A:128:ARG:NH1	1:A:182:HIS:ND1	0.63	2.47	9	1
1:A:155:TYR:CE1	1:A:158:PHE:CZ	0.63	2.86	20	1
1:A:90:TYR:CD1	1:A:90:TYR:N	0.63	2.66	11	5
1:A:144:ARG:CZ	1:A:194:LEU:HD11	0.62	2.23	12	4
1:A:174:GLN:HE21	1:A:174:GLN:N	0.62	1.92	11	6
1:A:106:CYS:SG	1:A:107:ALA:N	0.62	2.71	11	5
1:A:133:ASP:N	1:A:134:PRO:CD	0.62	2.62	15	15
1:A:57:ASN:ND2	1:A:58:GLN:N	0.62	2.47	16	1
1:A:128:ARG:NH1	1:A:182:HIS:CG	0.62	2.68	9	1
1:A:94:TRP:CZ3	1:A:122:LEU:HD21	0.62	2.29	17	1
2:B:200:DA:O5'	2:B:200:DA:C8	0.62	2.53	7	13
1:A:162:TRP:NE1	1:A:168:HIS:NE2	0.62	2.47	19	4
1:A:99:SER:OG	1:A:126:ALA:HB2	0.62	1.95	11	1
1:A:163:ASP:OD1	1:A:164:THR:N	0.61	2.33	16	1
1:A:91:ARG:CZ	1:A:123:ARG:NH2	0.61	2.63	17	1
1:A:88:GLN:NE2	1:A:88:GLN:N	0.61	2.48	18	8
1:A:129:ILE:O	1:A:130:TYR:CD2	0.61	2.54	19	3
1:A:52:ARG:NH1	1:A:164:THR:O	0.61	2.32	17	1
1:A:48:MET:CE	1:A:51:HIS:CE1	0.61	2.83	10	1
1:A:98:TRP:O	1:A:98:TRP:CD1	0.61	2.54	18	2
1:A:179:LEU:O	1:A:183:SER:N	0.61	2.33	9	20
1:A:98:TRP:CD1	1:A:100:PRO:O	0.61	2.53	12	2
2:B:207:DA:H4'	2:B:207:DA:OP1	0.61	1.95	13	20
1:A:99:SER:N	1:A:100:PRO:HD2	0.61	2.11	18	17
1:A:32:TYR:O	1:A:32:TYR:CD1	0.61	2.53	20	1
1:A:22:PHE:CE1	1:A:32:TYR:CZ	0.60	2.89	1	1
1:A:101:CYS:SG	1:A:101:CYS:O	0.60	2.59	15	10
1:A:176:TRP:HE1	1:A:179:LEU:HD21	0.60	1.56	4	3
1:A:121:ARG:HH21	1:A:149:GLN:NE2	0.60	1.94	16	1
1:A:34:CYS:SG	1:A:165:PHE:CE1	0.60	2.93	15	3
1:A:35:TYR:CD1	1:A:75:PHE:CD1	0.60	2.89	18	1
1:A:22:PHE:O	1:A:176:TRP:CZ2	0.60	2.54	20	11
1:A:111:ARG:NH2	1:A:115:GLN:OE1	0.60	2.35	18	2
1:A:37:VAL:CG2	1:A:51:HIS:CD2	0.60	2.85	3	1
1:A:31:THR:HG23	1:A:98:TRP:NE1	0.60	2.12	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:THR:OG1	1:A:98:TRP:CZ2	0.60	2.48	16	1
1:A:32:TYR:OH	1:A:54:PHE:CG	0.60	2.53	18	2
1:A:58:GLN:HE21	2:B:207:DA:P	0.60	2.20	16	2
1:A:87:ALA:C	1:A:88:GLN:NE2	0.59	2.55	12	18
1:A:75:PHE:CE2	1:A:94:TRP:NE1	0.59	2.71	14	10
1:A:119:HIS:O	1:A:119:HIS:ND1	0.59	2.35	12	3
1:A:121:ARG:HH21	1:A:149:GLN:HE22	0.59	1.40	16	1
1:A:92:VAL:CG2	1:A:94:TRP:HE1	0.59	2.09	4	8
1:A:32:TYR:OH	1:A:58:GLN:NE2	0.59	2.35	12	1
1:A:21:ASN:OD1	1:A:32:TYR:CE1	0.59	2.56	16	2
1:A:147:GLY:O	1:A:149:GLN:N	0.59	2.36	4	20
1:A:36:GLU:OE1	1:A:52:ARG:NH1	0.59	2.35	2	1
1:A:19:THR:O	1:A:23:ASN:ND2	0.59	2.35	16	1
1:A:155:TYR:O	1:A:158:PHE:CG	0.59	2.52	20	1
1:A:128:ARG:HH22	1:A:182:HIS:CD2	0.59	2.16	19	2
1:A:33:LEU:HD12	1:A:95:PHE:O	0.59	1.98	12	3
1:A:176:TRP:O	1:A:179:LEU:CD2	0.59	2.51	10	15
1:A:196:ASN:ND2	1:A:197:GLN:N	0.59	2.51	4	18
1:A:155:TYR:CE1	1:A:158:PHE:CE2	0.59	2.91	20	1
1:A:134:PRO:O	1:A:136:TYR:N	0.59	2.36	6	4
1:A:152:ILE:HD12	1:A:186:LEU:HD12	0.59	1.72	6	3
1:A:25:GLY:O	1:A:29:HIS:NE2	0.59	2.36	6	4
1:A:31:THR:CB	1:A:98:TRP:HE1	0.59	2.11	15	1
1:A:97:SER:OG	1:A:98:TRP:CE2	0.58	2.56	1	4
1:A:176:TRP:CD1	1:A:179:LEU:CD1	0.58	2.86	6	2
1:A:98:TRP:CE2	1:A:100:PRO:O	0.58	2.55	13	1
1:A:111:ARG:NH1	1:A:145:ASP:OD2	0.58	2.36	11	2
1:A:54:PHE:CD1	1:A:56:HIS:NE2	0.58	2.71	17	1
1:A:122:LEU:C	1:A:122:LEU:HD23	0.58	2.19	3	9
1:A:30:LYS:NZ	1:A:58:GLN:OE1	0.58	2.36	18	1
1:A:72:GLN:OE1	1:A:94:TRP:CZ3	0.58	2.55	20	1
1:A:31:THR:CG2	1:A:98:TRP:HE1	0.58	2.11	7	5
1:A:27:GLY:N	1:A:29:HIS:NE2	0.58	2.50	2	1
1:A:97:SER:OG	1:A:98:TRP:CD1	0.58	2.55	19	2
1:A:40:LEU:HD13	1:A:41:ASP:N	0.58	2.14	12	2
1:A:195:GLN:CA	1:A:195:GLN:HE21	0.58	2.10	1	20
1:A:92:VAL:O	1:A:92:VAL:HG13	0.58	1.98	20	10
1:A:88:GLN:N	1:A:88:GLN:NE2	0.58	2.51	5	12
1:A:21:ASN:OD1	1:A:32:TYR:CD1	0.58	2.56	16	3
1:A:152:ILE:HG21	1:A:186:LEU:HB3	0.58	1.76	19	5
1:A:30:LYS:O	1:A:32:TYR:CD2	0.58	2.57	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:TYR:CD1	1:A:32:TYR:O	0.58	2.57	19	2
1:A:94:TRP:CZ2	1:A:122:LEU:HD21	0.58	2.34	13	3
1:A:98:TRP:N	1:A:98:TRP:CD1	0.58	2.70	17	1
1:A:162:TRP:O	1:A:166:VAL:N	0.57	2.36	6	13
1:A:140:LEU:HD22	1:A:193:ILE:HG21	0.57	1.76	7	1
1:A:21:ASN:ND2	1:A:30:LYS:O	0.57	2.37	16	2
1:A:91:ARG:HH11	1:A:123:ARG:NH2	0.57	1.96	20	1
1:A:162:TRP:CZ2	1:A:168:HIS:NE2	0.57	2.72	2	4
1:A:122:LEU:HD23	1:A:122:LEU:C	0.57	2.19	7	3
1:A:57:ASN:HD22	1:A:58:GLN:N	0.57	1.96	16	1
1:A:29:HIS:O	2:B:205:DC:C2	0.57	2.57	17	6
1:A:133:ASP:N	1:A:133:ASP:OD1	0.57	2.37	9	3
1:A:181:GLU:O	2:B:200:DA:O5'	0.57	2.22	16	3
1:A:24:ASN:OD1	1:A:128:ARG:NH1	0.57	2.37	20	1
1:A:90:TYR:CZ	1:A:119:HIS:CE1	0.57	2.93	10	1
1:A:122:LEU:HD13	1:A:123:ARG:N	0.57	2.15	14	2
1:A:111:ARG:NH1	1:A:142:MET:O	0.57	2.37	6	1
1:A:114:LEU:HD22	1:A:146:ALA:O	0.57	1.99	17	1
1:A:169:GLN:CD	1:A:169:GLN:N	0.57	2.58	1	5
1:A:38:GLU:N	1:A:38:GLU:OE2	0.57	2.38	12	2
1:A:32:TYR:OH	1:A:54:PHE:CD1	0.57	2.56	2	1
1:A:31:THR:HG23	1:A:98:TRP:HE1	0.57	1.58	7	4
1:A:97:SER:OG	1:A:98:TRP:NE1	0.57	2.38	7	3
1:A:144:ARG:HH21	1:A:194:LEU:CD1	0.57	2.13	3	1
1:A:130:TYR:CE1	2:B:202:DT:OP1	0.57	2.58	15	5
1:A:101:CYS:O	1:A:106:CYS:SG	0.57	2.63	7	1
1:A:38:GLU:OE2	1:A:91:ARG:NH1	0.57	2.38	19	1
2:B:200:DA:C8	2:B:200:DA:O5'	0.57	2.57	9	2
1:A:168:HIS:ND1	1:A:171:GLN:O	0.57	2.37	13	3
1:A:18:PHE:O	1:A:21:ASN:ND2	0.57	2.38	20	1
1:A:17:ILE:N	1:A:17:ILE:CD1	0.57	2.68	3	3
1:A:141:GLN:OE1	1:A:144:ARG:NH1	0.56	2.37	15	2
1:A:52:ARG:CZ	1:A:164:THR:HG22	0.56	2.29	3	1
1:A:91:ARG:NH1	1:A:121:ARG:NH2	0.56	2.52	7	1
1:A:155:TYR:OH	1:A:159:LYS:NZ	0.56	2.36	11	2
1:A:99:SER:H	1:A:100:PRO:CD	0.56	2.14	3	7
1:A:132:TYR:O	1:A:133:ASP:O	0.56	2.22	3	2
1:A:29:HIS:O	1:A:29:HIS:CD2	0.56	2.58	5	1
1:A:72:GLN:OE1	1:A:106:CYS:SG	0.56	2.64	10	2
1:A:144:ARG:CZ	1:A:194:LEU:HD21	0.56	2.30	10	2
1:A:38:GLU:OE2	1:A:91:ARG:CZ	0.56	2.53	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:GLN:N	1:A:169:GLN:CD	0.56	2.58	3	1
1:A:157:GLU:OE1	1:A:161:CYS:SG	0.56	2.63	12	1
1:A:130:TYR:CZ	2:B:202:DT:OP1	0.56	2.59	4	5
1:A:162:TRP:CE2	1:A:168:HIS:NE2	0.56	2.74	7	2
1:A:98:TRP:CE3	1:A:100:PRO:O	0.56	2.58	18	1
1:A:21:ASN:OD1	1:A:22:PHE:CD2	0.56	2.59	20	1
1:A:173:PHE:C	1:A:173:PHE:CD1	0.56	2.79	20	1
1:A:144:ARG:HE	1:A:194:LEU:HD11	0.56	1.57	11	1
1:A:21:ASN:O	1:A:128:ARG:NH1	0.56	2.38	3	1
1:A:184:GLN:NE2	1:A:184:GLN:C	0.56	2.59	19	2
1:A:132:TYR:O	1:A:136:TYR:CD1	0.56	2.59	14	1
1:A:88:GLN:HE21	1:A:88:GLN:CA	0.56	2.14	18	1
1:A:31:THR:OG1	1:A:98:TRP:NE1	0.56	2.39	15	3
1:A:179:LEU:O	1:A:183:SER:CB	0.56	2.54	16	20
1:A:22:PHE:CZ	1:A:32:TYR:OH	0.56	2.56	3	2
1:A:162:TRP:CD1	1:A:168:HIS:CE1	0.56	2.94	16	1
1:A:131:ASP:OD1	1:A:132:TYR:N	0.56	2.39	20	1
1:A:160:HIS:O	1:A:163:ASP:OD1	0.55	2.24	16	1
1:A:40:LEU:HD13	1:A:40:LEU:C	0.55	2.22	3	1
1:A:96:ILE:HD12	1:A:98:TRP:O	0.55	2.01	17	3
1:A:144:ARG:HE	1:A:194:LEU:HD21	0.55	1.62	6	1
1:A:128:ARG:NH1	2:B:204:DT:O4	0.55	2.39	14	1
1:A:174:GLN:NE2	1:A:174:GLN:O	0.55	2.36	17	1
1:A:94:TRP:CD2	1:A:122:LEU:HD21	0.55	2.37	8	1
1:A:90:TYR:CZ	1:A:119:HIS:NE2	0.55	2.73	10	1
1:A:21:ASN:ND2	1:A:32:TYR:CE1	0.55	2.74	19	1
1:A:47:LYS:HZ1	1:A:52:ARG:CZ	0.55	2.14	18	1
1:A:158:PHE:O	1:A:161:CYS:SG	0.55	2.61	10	2
1:A:121:ARG:NH1	1:A:149:GLN:NE2	0.55	2.54	17	1
1:A:128:ARG:NH2	2:B:204:DT:O4	0.55	2.39	10	5
1:A:125:PHE:CZ	1:A:151:SER:OG	0.55	2.57	5	5
1:A:153:MET:SD	1:A:158:PHE:CD1	0.55	3.00	9	1
1:A:36:GLU:OE1	1:A:37:VAL:N	0.54	2.40	11	1
1:A:147:GLY:C	1:A:149:GLN:H	0.54	2.06	4	20
1:A:24:ASN:HD22	1:A:128:ARG:HH11	0.54	1.40	3	1
1:A:99:SER:OG	1:A:128:ARG:O	0.54	2.25	7	3
1:A:36:GLU:OE1	1:A:52:ARG:CZ	0.54	2.55	2	1
1:A:52:ARG:CZ	1:A:164:THR:HG21	0.54	2.32	5	1
1:A:98:TRP:CZ3	2:B:205:DC:N4	0.54	2.75	6	1
1:A:24:ASN:CG	1:A:128:ARG:NH2	0.54	2.61	20	1
1:A:21:ASN:ND2	1:A:29:HIS:CE1	0.54	2.75	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:LEU:O	1:A:183:SER:OG	0.54	2.26	17	14
2:B:206:DA:H4'	2:B:207:DA:OP2	0.54	2.02	2	20
1:A:54:PHE:CE1	1:A:56:HIS:NE2	0.54	2.75	17	1
1:A:47:LYS:NZ	1:A:52:ARG:HH11	0.54	2.01	1	2
2:B:206:DA:H5'	2:B:207:DA:OP2	0.54	2.03	13	20
1:A:27:GLY:O	1:A:29:HIS:CE1	0.54	2.61	2	1
1:A:76:LEU:HD23	1:A:76:LEU:O	0.54	2.03	12	2
1:A:30:LYS:O	1:A:32:TYR:CE2	0.54	2.61	5	1
1:A:29:HIS:O	2:B:205:DC:N3	0.54	2.41	8	1
1:A:19:THR:O	1:A:23:ASN:N	0.54	2.41	5	18
1:A:23:ASN:ND2	1:A:176:TRP:CZ3	0.54	2.76	1	2
1:A:143:LEU:O	1:A:147:GLY:N	0.54	2.38	20	3
1:A:79:VAL:N	1:A:80:PRO:HD2	0.54	2.17	19	10
1:A:194:LEU:N	1:A:194:LEU:HD22	0.54	2.17	9	8
1:A:179:LEU:N	1:A:179:LEU:HD12	0.54	2.18	16	2
1:A:162:TRP:NE1	1:A:168:HIS:ND1	0.54	2.56	16	1
1:A:168:HIS:CD2	1:A:168:HIS:H	0.54	2.21	5	3
1:A:168:HIS:ND1	1:A:168:HIS:N	0.53	2.54	2	3
1:A:129:ILE:HG21	1:A:136:TYR:OH	0.53	2.03	12	4
1:A:21:ASN:OD1	1:A:98:TRP:CZ2	0.53	2.62	10	1
1:A:144:ARG:NH2	1:A:194:LEU:HD21	0.53	2.18	17	2
1:A:140:LEU:O	1:A:140:LEU:HD13	0.53	2.04	16	2
1:A:168:HIS:CD2	1:A:168:HIS:N	0.53	2.75	10	1
1:A:40:LEU:C	1:A:40:LEU:CD2	0.53	2.72	3	1
1:A:144:ARG:HH22	1:A:197:GLN:HE22	0.53	1.46	4	1
1:A:184:GLN:HE21	1:A:185:ALA:CA	0.53	2.16	7	1
1:A:36:GLU:CD	1:A:52:ARG:NH2	0.53	2.62	8	1
2:B:206:DA:C4'	2:B:207:DA:OP2	0.53	2.57	2	20
1:A:135:LEU:HD12	1:A:136:TYR:N	0.53	2.18	6	1
1:A:135:LEU:O	1:A:135:LEU:HD13	0.53	2.03	16	2
1:A:26:ILE:HD13	2:B:203:DT:OP1	0.53	2.03	18	5
1:A:26:ILE:CD1	2:B:203:DT:OP1	0.53	2.57	7	2
1:A:141:GLN:OE1	1:A:144:ARG:CZ	0.53	2.57	3	1
1:A:169:GLN:CD	1:A:169:GLN:H	0.53	2.06	20	1
1:A:56:HIS:ND1	1:A:57:ASN:N	0.53	2.57	4	1
1:A:125:PHE:CE2	1:A:151:SER:OG	0.53	2.55	7	5
1:A:144:ARG:NE	1:A:194:LEU:HD22	0.52	2.18	1	1
1:A:50:GLN:O	1:A:51:HIS:ND1	0.52	2.42	8	1
1:A:143:LEU:HD13	1:A:143:LEU:O	0.52	2.05	19	1
1:A:31:THR:OG1	1:A:57:ASN:ND2	0.52	2.41	2	1
1:A:160:HIS:CE1	1:A:164:THR:HG1	0.52	2.22	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:THR:CG2	1:A:97:SER:OG	0.52	2.55	13	2
1:A:132:TYR:O	1:A:136:TYR:CB	0.52	2.57	5	5
1:A:140:LEU:HD23	1:A:140:LEU:O	0.52	2.04	7	1
1:A:162:TRP:CE2	1:A:168:HIS:CE1	0.52	2.97	8	2
1:A:24:ASN:CG	1:A:128:ARG:NH1	0.52	2.62	5	1
1:A:88:GLN:N	1:A:88:GLN:CD	0.52	2.62	18	1
1:A:40:LEU:HB2	1:A:89:ILE:HG23	0.52	1.81	5	3
1:A:195:GLN:CA	1:A:195:GLN:NE2	0.52	2.73	6	20
1:A:173:PHE:C	1:A:174:GLN:NE2	0.52	2.63	5	5
1:A:121:ARG:NH1	1:A:123:ARG:HH11	0.52	2.01	7	2
1:A:32:TYR:OH	1:A:165:PHE:CZ	0.52	2.62	10	1
1:A:194:LEU:N	1:A:194:LEU:CD2	0.52	2.73	19	8
1:A:29:HIS:ND1	2:B:204:DT:O2	0.52	2.43	4	1
1:A:160:HIS:CE1	1:A:164:THR:OG1	0.52	2.62	10	3
1:A:31:THR:HG1	1:A:98:TRP:HE1	0.52	1.48	15	1
1:A:174:GLN:O	1:A:174:GLN:CD	0.52	2.48	6	1
1:A:30:LYS:CE	1:A:58:GLN:OE1	0.52	2.57	18	1
1:A:18:PHE:CE1	1:A:22:PHE:CE1	0.52	2.97	16	2
1:A:24:ASN:CG	1:A:128:ARG:HH11	0.52	2.08	5	2
1:A:141:GLN:OE1	1:A:197:GLN:NE2	0.52	2.43	5	2
1:A:160:HIS:O	1:A:164:THR:OG1	0.52	2.27	16	4
2:B:200:DA:H8	2:B:200:DA:HO5'	0.52	1.33	4	1
1:A:184:GLN:NE2	1:A:184:GLN:O	0.52	2.43	19	2
1:A:35:TYR:CD2	1:A:75:PHE:CE1	0.51	2.99	3	1
1:A:138:GLU:CG	1:A:139:ALA:N	0.51	2.72	18	1
1:A:180:ASP:OD1	1:A:181:GLU:N	0.51	2.43	17	6
1:A:133:ASP:O	1:A:134:PRO:O	0.51	2.29	15	2
1:A:134:PRO:C	1:A:136:TYR:N	0.51	2.63	6	2
1:A:174:GLN:N	1:A:174:GLN:CD	0.51	2.62	17	1
1:A:72:GLN:CD	1:A:94:TRP:CZ3	0.51	2.84	20	1
1:A:158:PHE:CD1	1:A:158:PHE:N	0.51	2.78	20	1
1:A:31:THR:OG1	1:A:98:TRP:CZ3	0.51	2.56	2	1
1:A:31:THR:OG1	1:A:57:ASN:CG	0.51	2.49	19	3
1:A:25:GLY:O	1:A:29:HIS:CE1	0.51	2.63	13	2
1:A:125:PHE:CD1	1:A:151:SER:O	0.51	2.64	14	1
1:A:119:HIS:CD2	1:A:120:VAL:HG23	0.51	2.40	15	1
1:A:29:HIS:O	1:A:30:LYS:O	0.51	2.27	4	2
1:A:136:TYR:CE1	1:A:140:LEU:HD23	0.51	2.41	16	1
1:A:113:PHE:CE1	1:A:117:ASN:OD1	0.51	2.64	15	2
1:A:160:HIS:NE2	1:A:164:THR:OG1	0.51	2.42	10	2
1:A:30:LYS:O	1:A:32:TYR:CD1	0.51	2.64	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ASN:CG	1:A:128:ARG:CZ	0.51	2.79	20	1
1:A:130:TYR:OH	1:A:189:ARG:NH1	0.51	2.44	13	3
1:A:49:ASP:OD1	1:A:50:GLN:N	0.50	2.44	11	3
1:A:144:ARG:NH1	1:A:190:LEU:HD11	0.50	2.21	2	1
1:A:184:GLN:HE21	1:A:185:ALA:N	0.50	2.05	7	1
1:A:176:TRP:O	1:A:178:GLY:N	0.50	2.44	16	1
1:A:162:TRP:O	1:A:166:VAL:O	0.50	2.30	3	6
1:A:17:ILE:N	1:A:17:ILE:HD12	0.50	2.21	3	3
1:A:140:LEU:HD13	1:A:193:ILE:HG21	0.50	1.84	7	1
1:A:160:HIS:CD2	1:A:164:THR:OG1	0.50	2.65	10	2
1:A:88:GLN:N	1:A:88:GLN:HE21	0.50	2.04	15	3
1:A:144:ARG:CZ	1:A:197:GLN:NE2	0.50	2.75	15	1
1:A:20:SER:O	1:A:29:HIS:CD2	0.50	2.64	11	1
1:A:176:TRP:NE1	1:A:179:LEU:CD1	0.50	2.74	16	1
1:A:91:ARG:HH11	1:A:123:ARG:CZ	0.50	2.20	20	1
1:A:136:TYR:CZ	1:A:193:ILE:HD11	0.50	2.42	9	2
1:A:106:CYS:O	1:A:110:VAL:HG13	0.50	2.06	9	1
1:A:121:ARG:NH2	1:A:149:GLN:NE2	0.50	2.59	16	1
1:A:174:GLN:N	1:A:174:GLN:NE2	0.50	2.59	11	2
1:A:95:PHE:CE1	1:A:153:MET:SD	0.50	3.04	14	1
1:A:194:LEU:N	1:A:194:LEU:HD12	0.50	2.22	8	3
1:A:173:PHE:CD1	1:A:174:GLN:N	0.50	2.80	8	2
1:A:163:ASP:O	1:A:167:ASP:OD1	0.50	2.29	11	2
1:A:159:LYS:O	1:A:163:ASP:OD1	0.50	2.29	16	1
1:A:133:ASP:CB	1:A:134:PRO:CD	0.50	2.90	7	2
1:A:117:ASN:OD1	1:A:117:ASN:O	0.50	2.30	18	2
1:A:57:ASN:OD1	1:A:58:GLN:N	0.50	2.45	2	1
2:B:206:DA:C5'	2:B:207:DA:OP2	0.49	2.60	7	20
1:A:24:ASN:OD1	1:A:176:TRP:NE1	0.49	2.45	5	1
1:A:133:ASP:H	1:A:134:PRO:HD2	0.49	1.67	6	8
1:A:24:ASN:CA	1:A:128:ARG:HH11	0.49	2.19	6	1
1:A:140:LEU:HD23	1:A:193:ILE:HD13	0.49	1.82	11	1
1:A:24:ASN:ND2	1:A:128:ARG:NH2	0.49	2.60	20	1
1:A:52:ARG:NH2	1:A:164:THR:HG23	0.49	2.21	19	2
1:A:29:HIS:CE1	2:B:204:DT:O2	0.49	2.64	4	1
1:A:191:ARG:O	1:A:195:GLN:NE2	0.49	2.45	6	1
1:A:121:ARG:HH11	1:A:149:GLN:NE2	0.49	2.05	8	1
1:A:33:LEU:C	1:A:33:LEU:CD2	0.49	2.81	16	6
1:A:18:PHE:CE1	1:A:22:PHE:CE2	0.49	3.00	6	2
1:A:24:ASN:CB	1:A:128:ARG:HH11	0.49	2.20	5	1
1:A:74:ARG:HH11	1:A:77:ASP:CB	0.49	2.20	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:PHE:O	1:A:117:ASN:OD1	0.49	2.30	7	2
1:A:56:HIS:CD2	1:A:56:HIS:H	0.49	2.25	14	1
1:A:190:LEU:O	1:A:190:LEU:HD13	0.49	2.08	3	9
1:A:51:HIS:CD2	1:A:82:LEU:HD22	0.49	2.43	11	1
1:A:173:PHE:CE1	1:A:174:GLN:O	0.49	2.66	16	1
1:A:19:THR:O	1:A:23:ASN:CG	0.49	2.51	2	5
1:A:136:TYR:CE2	1:A:140:LEU:HD11	0.49	2.42	1	1
1:A:132:TYR:O	1:A:136:TYR:CG	0.49	2.66	15	2
1:A:110:VAL:HG23	1:A:111:ARG:N	0.49	2.22	9	1
1:A:130:TYR:O	1:A:131:ASP:OD1	0.49	2.30	11	2
1:A:38:GLU:OE2	1:A:91:ARG:O	0.49	2.30	20	2
1:A:32:TYR:CZ	1:A:58:GLN:NE2	0.49	2.81	12	1
1:A:110:VAL:HG11	1:A:143:LEU:HD21	0.49	1.85	20	1
1:A:48:MET:CB	1:A:51:HIS:ND1	0.48	2.76	12	3
1:A:179:LEU:N	1:A:179:LEU:CD1	0.48	2.76	16	1
1:A:91:ARG:NH1	1:A:123:ARG:HH11	0.48	2.06	10	1
1:A:135:LEU:HD13	1:A:135:LEU:O	0.48	2.08	11	1
1:A:47:LYS:NZ	1:A:52:ARG:CZ	0.48	2.76	18	1
1:A:141:GLN:OE1	1:A:196:ASN:OD1	0.48	2.32	10	1
1:A:135:LEU:C	1:A:135:LEU:CD1	0.48	2.80	11	2
1:A:98:TRP:CD1	1:A:131:ASP:OD1	0.48	2.67	11	1
1:A:89:ILE:CD1	1:A:121:ARG:NH2	0.48	2.77	12	1
1:A:85:ASP:O	1:A:90:TYR:OH	0.48	2.30	10	2
1:A:150:VAL:HG11	1:A:190:LEU:HD21	0.48	1.84	5	1
1:A:174:GLN:NE2	1:A:174:GLN:CA	0.48	2.76	11	4
1:A:48:MET:SD	1:A:51:HIS:ND1	0.48	2.87	14	1
1:A:158:PHE:CD2	1:A:173:PHE:CE1	0.48	3.01	20	1
1:A:99:SER:H	1:A:100:PRO:HD2	0.48	1.66	18	3
1:A:17:ILE:O	1:A:20:SER:OG	0.48	2.30	13	4
1:A:98:TRP:CD1	1:A:98:TRP:O	0.48	2.66	8	2
1:A:98:TRP:CD2	1:A:100:PRO:O	0.48	2.67	13	1
1:A:114:LEU:HD21	1:A:122:LEU:HB2	0.48	1.86	15	2
1:A:168:HIS:C	1:A:169:GLN:NE2	0.48	2.67	5	2
1:A:129:ILE:CG2	1:A:136:TYR:OH	0.48	2.61	13	3
1:A:56:HIS:ND1	1:A:56:HIS:O	0.48	2.46	12	2
1:A:56:HIS:CD2	1:A:56:HIS:N	0.48	2.82	14	1
1:A:47:LYS:NZ	1:A:52:ARG:NH1	0.48	2.61	18	1
1:A:181:GLU:OE2	2:B:202:DT:O4	0.48	2.32	8	8
1:A:30:LYS:NZ	1:A:58:GLN:NE2	0.48	2.62	6	1
1:A:121:ARG:HH11	1:A:149:GLN:HE22	0.48	1.50	8	1
1:A:144:ARG:HH12	1:A:190:LEU:HD11	0.48	1.69	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:PRO:C	1:A:136:TYR:H	0.48	2.12	15	2
1:A:49:ASP:OD1	1:A:49:ASP:N	0.48	2.47	8	3
1:A:152:ILE:HD11	1:A:190:LEU:HD23	0.48	1.86	8	1
1:A:184:GLN:O	1:A:184:GLN:NE2	0.48	2.47	8	2
1:A:59:ALA:O	2:B:208:DT:OP1	0.48	2.31	15	1
1:A:33:LEU:HD23	1:A:33:LEU:C	0.48	2.29	18	1
1:A:176:TRP:HE1	1:A:179:LEU:HD11	0.47	1.69	2	5
1:A:72:GLN:OE1	1:A:94:TRP:CE3	0.47	2.67	2	1
1:A:167:ASP:O	1:A:169:GLN:NE2	0.47	2.46	3	3
1:A:36:GLU:CD	1:A:52:ARG:HH22	0.47	2.12	8	1
1:A:36:GLU:OE1	1:A:52:ARG:NH2	0.47	2.47	8	1
1:A:55:LEU:HD13	1:A:74:ARG:HD2	0.47	1.84	15	1
1:A:91:ARG:HH12	1:A:121:ARG:HH22	0.47	1.50	7	1
1:A:98:TRP:CD1	1:A:98:TRP:C	0.47	2.87	8	4
1:A:20:SER:O	1:A:29:HIS:ND1	0.47	2.47	16	1
1:A:98:TRP:NE1	1:A:128:ARG:NH1	0.47	2.62	16	1
1:A:140:LEU:HD11	1:A:144:ARG:CZ	0.47	2.38	18	1
1:A:15:PRO:O	1:A:19:THR:OG1	0.47	2.31	1	4
1:A:75:PHE:CE1	1:A:78:LEU:HD23	0.47	2.45	18	1
1:A:32:TYR:O	1:A:32:TYR:CG	0.47	2.67	20	1
1:A:88:GLN:NE2	1:A:88:GLN:CA	0.47	2.76	18	5
1:A:31:THR:O	1:A:57:ASN:OD1	0.47	2.33	4	2
1:A:19:THR:O	1:A:23:ASN:OD1	0.47	2.33	9	1
1:A:52:ARG:NH2	1:A:164:THR:CG2	0.47	2.77	19	2
1:A:98:TRP:CD1	1:A:98:TRP:N	0.47	2.82	7	1
1:A:196:ASN:CG	1:A:197:GLN:N	0.47	2.67	11	7
1:A:52:ARG:HH21	1:A:164:THR:CG2	0.47	2.22	6	1
1:A:72:GLN:HE21	1:A:96:ILE:CD1	0.47	2.23	14	2
1:A:119:HIS:C	1:A:119:HIS:ND1	0.47	2.64	10	1
1:A:36:GLU:CD	1:A:37:VAL:N	0.47	2.68	11	1
1:A:39:ARG:N	1:A:46:VAL:O	0.47	2.47	17	1
1:A:58:GLN:NE2	2:B:207:DA:OP1	0.47	2.48	20	1
1:A:48:MET:CE	1:A:51:HIS:CG	0.47	2.97	14	6
1:A:119:HIS:O	1:A:119:HIS:CG	0.47	2.68	15	3
1:A:37:VAL:HG23	1:A:51:HIS:NE2	0.47	2.25	3	1
1:A:37:VAL:HG22	1:A:51:HIS:ND1	0.47	2.25	17	2
1:A:188:GLY:O	1:A:192:ALA:HB2	0.47	2.10	6	5
1:A:34:CYS:SG	1:A:165:PHE:CZ	0.47	3.01	15	1
1:A:79:VAL:HG21	1:A:113:PHE:CZ	0.47	2.45	15	3
1:A:167:ASP:O	1:A:167:ASP:OD1	0.47	2.33	20	2
1:A:194:LEU:HD13	1:A:197:GLN:NE2	0.47	2.22	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LYS:NZ	1:A:56:HIS:NE2	0.47	2.63	19	1
1:A:92:VAL:O	1:A:92:VAL:CG1	0.46	2.63	1	5
1:A:179:LEU:N	1:A:179:LEU:CD2	0.46	2.66	2	4
1:A:176:TRP:CD1	1:A:179:LEU:HD11	0.46	2.45	6	1
1:A:174:GLN:N	1:A:174:GLN:HE21	0.46	2.09	7	2
1:A:150:VAL:HG11	1:A:190:LEU:HD11	0.46	1.87	10	1
1:A:174:GLN:CD	1:A:174:GLN:N	0.46	2.68	18	1
1:A:158:PHE:N	1:A:158:PHE:HD1	0.46	2.07	20	1
1:A:51:HIS:ND1	1:A:51:HIS:O	0.46	2.49	9	2
1:A:56:HIS:ND1	1:A:56:HIS:N	0.46	2.62	11	2
1:A:98:TRP:CZ2	1:A:100:PRO:O	0.46	2.68	13	1
1:A:136:TYR:CE1	1:A:140:LEU:HD11	0.46	2.45	19	1
1:A:162:TRP:CD1	1:A:162:TRP:C	0.46	2.88	6	8
1:A:135:LEU:O	1:A:139:ALA:CB	0.46	2.64	8	3
1:A:177:ASP:O	1:A:177:ASP:OD1	0.46	2.33	20	3
1:A:152:ILE:HG22	1:A:186:LEU:HD12	0.46	1.87	17	2
1:A:32:TYR:CD1	1:A:32:TYR:C	0.46	2.89	7	1
1:A:166:VAL:CG1	1:A:168:HIS:CE1	0.46	2.98	7	1
1:A:121:ARG:CZ	1:A:123:ARG:HH11	0.46	2.23	11	1
1:A:47:LYS:HZ3	1:A:52:ARG:NH1	0.46	2.08	18	1
1:A:57:ASN:OD1	1:A:57:ASN:N	0.46	2.49	18	1
1:A:72:GLN:CD	1:A:94:TRP:CE3	0.46	2.89	16	1
1:A:73:LEU:N	1:A:109:GLU:OE1	0.46	2.48	20	1
1:A:24:ASN:CB	1:A:128:ARG:NH1	0.46	2.79	5	1
1:A:122:LEU:O	1:A:149:GLN:OE1	0.46	2.34	14	1
1:A:136:TYR:CG	1:A:137:LYS:N	0.46	2.81	14	1
1:A:121:ARG:NH1	1:A:149:GLN:CD	0.46	2.68	17	1
1:A:12:LEU:HD12	1:A:12:LEU:N	0.46	2.25	18	1
1:A:181:GLU:OE1	2:B:202:DT:O4	0.46	2.33	4	1
1:A:128:ARG:NH2	1:A:182:HIS:CD2	0.46	2.84	5	1
1:A:85:ASP:N	1:A:85:ASP:OD1	0.46	2.47	8	1
1:A:47:LYS:HZ1	1:A:52:ARG:HH11	0.46	1.53	1	1
1:A:132:TYR:O	1:A:136:TYR:CD2	0.46	2.69	6	1
1:A:31:THR:CG2	1:A:98:TRP:NE1	0.46	2.78	9	1
1:A:91:ARG:CZ	1:A:123:ARG:HH21	0.46	2.24	17	1
1:A:99:SER:OG	1:A:126:ALA:HB1	0.46	2.10	20	1
1:A:162:TRP:CE3	1:A:166:VAL:HG21	0.45	2.46	17	2
1:A:133:ASP:N	1:A:134:PRO:HD2	0.45	2.25	15	4
1:A:113:PHE:CZ	1:A:117:ASN:OD1	0.45	2.69	13	1
1:A:95:PHE:CZ	1:A:127:ALA:HB2	0.45	2.46	14	1
1:A:35:TYR:CB	1:A:75:PHE:CE1	0.45	3.00	4	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	0.45	2.79	5	2
1:A:144:ARG:HE	1:A:194:LEU:CD2	0.45	2.23	6	1
1:A:162:TRP:HE1	1:A:168:HIS:HE2	0.45	1.52	8	1
1:A:168:HIS:CG	1:A:171:GLN:O	0.45	2.69	12	2
1:A:133:ASP:OD1	1:A:133:ASP:C	0.45	2.55	16	1
1:A:35:TYR:CD1	1:A:75:PHE:CZ	0.45	3.05	18	1
1:A:40:LEU:HD13	1:A:41:ASP:H	0.45	1.70	19	1
1:A:117:ASN:O	1:A:117:ASN:CG	0.45	2.54	7	1
1:A:160:HIS:CD2	1:A:164:THR:HG1	0.45	2.29	7	2
1:A:133:ASP:C	1:A:135:LEU:N	0.45	2.70	11	2
1:A:73:LEU:HD12	1:A:76:LEU:HD12	0.45	1.86	15	2
1:A:94:TRP:CE3	1:A:122:LEU:HD21	0.45	2.46	17	1
1:A:180:ASP:O	1:A:184:GLN:CD	0.45	2.55	2	1
1:A:58:GLN:CG	1:A:58:GLN:O	0.45	2.65	8	1
1:A:95:PHE:CE2	1:A:125:PHE:CG	0.45	3.04	16	1
1:A:128:ARG:HH22	1:A:182:HIS:CE1	0.45	2.29	5	1
1:A:20:SER:OG	1:A:29:HIS:CE1	0.45	2.69	7	1
1:A:132:TYR:O	1:A:133:ASP:C	0.45	2.55	3	2
1:A:73:LEU:HD13	1:A:109:GLU:OE1	0.45	2.12	13	1
1:A:129:ILE:HG23	1:A:136:TYR:CZ	0.45	2.47	10	1
1:A:35:TYR:C	1:A:35:TYR:CD1	0.45	2.90	14	1
1:A:21:ASN:ND2	1:A:22:PHE:CD2	0.45	2.85	20	1
1:A:40:LEU:CB	1:A:89:ILE:HG23	0.45	2.41	7	2
1:A:98:TRP:HE1	1:A:128:ARG:NH1	0.45	2.10	16	1
1:A:140:LEU:C	1:A:140:LEU:CD2	0.44	2.85	7	1
1:A:88:GLN:O	1:A:119:HIS:CE1	0.44	2.69	12	2
1:A:180:ASP:O	1:A:183:SER:OG	0.44	2.35	8	1
1:A:184:GLN:HG3	1:A:185:ALA:N	0.44	2.28	19	1
1:A:48:MET:CE	1:A:51:HIS:CD2	0.44	3.00	7	1
1:A:38:GLU:OE1	1:A:91:ARG:O	0.44	2.35	8	1
1:A:140:LEU:HD11	1:A:144:ARG:HH22	0.44	1.69	18	1
1:A:124:ILE:CD1	1:A:143:LEU:HD21	0.44	2.43	16	2
1:A:32:TYR:CE1	1:A:56:HIS:CD2	0.44	3.06	4	1
1:A:144:ARG:NH1	1:A:197:GLN:HE21	0.44	2.11	15	1
1:A:91:ARG:HH11	1:A:123:ARG:CD	0.44	2.25	1	1
1:A:122:LEU:C	1:A:122:LEU:CD2	0.44	2.86	6	6
1:A:140:LEU:O	1:A:144:ARG:CB	0.44	2.65	19	1
1:A:135:LEU:O	1:A:139:ALA:N	0.44	2.44	20	2
1:A:162:TRP:CD1	1:A:163:ASP:N	0.44	2.86	13	1
1:A:162:TRP:HE1	1:A:168:HIS:CG	0.44	2.31	16	1
1:A:13:MET:SD	1:A:54:PHE:CD1	0.44	3.11	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:ASP:H	1:A:134:PRO:HD3	0.44	1.70	4	2
1:A:140:LEU:HD22	1:A:193:ILE:CG2	0.44	2.43	7	1
1:A:121:ARG:HE	1:A:149:GLN:HE22	0.44	1.55	11	1
1:A:131:ASP:OD1	1:A:132:TYR:CD2	0.44	2.71	15	1
1:A:52:ARG:HH22	1:A:164:THR:CG2	0.44	2.22	19	1
1:A:147:GLY:C	1:A:149:GLN:N	0.44	2.72	16	20
1:A:76:LEU:O	1:A:80:PRO:CD	0.44	2.66	3	7
1:A:79:VAL:N	1:A:80:PRO:CD	0.44	2.81	18	3
1:A:182:HIS:CE1	2:B:202:DT:C7	0.44	2.99	8	5
1:A:169:GLN:NE2	1:A:169:GLN:CA	0.44	2.81	5	1
1:A:22:PHE:O	1:A:176:TRP:CH2	0.44	2.71	9	1
1:A:128:ARG:CZ	2:B:204:DT:O4	0.44	2.66	11	1
1:A:144:ARG:NH1	1:A:197:GLN:NE2	0.44	2.65	15	1
1:A:101:CYS:O	1:A:101:CYS:SG	0.44	2.76	18	1
1:A:35:TYR:CG	1:A:75:PHE:CZ	0.43	3.06	3	1
1:A:179:LEU:CD1	1:A:179:LEU:N	0.43	2.81	6	1
1:A:21:ASN:OD1	1:A:21:ASN:C	0.43	2.56	20	1
1:A:135:LEU:C	1:A:137:LYS:N	0.43	2.71	1	1
1:A:153:MET:SD	1:A:157:GLU:OE2	0.43	2.77	7	1
1:A:160:HIS:O	1:A:164:THR:CB	0.43	2.66	7	2
1:A:163:ASP:O	1:A:166:VAL:O	0.43	2.36	7	1
1:A:88:GLN:O	1:A:90:TYR:CE1	0.43	2.71	14	2
1:A:133:ASP:C	1:A:135:LEU:H	0.43	2.17	18	2
1:A:129:ILE:HG21	1:A:136:TYR:CZ	0.43	2.48	12	1
1:A:99:SER:H	1:A:100:PRO:HD3	0.43	1.73	15	1
1:A:194:LEU:N	1:A:194:LEU:CD1	0.43	2.81	17	1
1:A:12:LEU:N	1:A:12:LEU:CD1	0.43	2.81	18	1
1:A:22:PHE:CE1	1:A:32:TYR:CE1	0.43	3.07	1	1
1:A:110:VAL:CG2	1:A:111:ARG:N	0.43	2.80	9	1
1:A:129:ILE:HG23	1:A:136:TYR:CE1	0.43	2.48	12	1
1:A:184:GLN:O	1:A:187:SER:OG	0.43	2.31	15	1
1:A:30:LYS:NZ	1:A:56:HIS:CE1	0.43	2.85	17	1
1:A:35:TYR:CZ	1:A:75:PHE:CD1	0.43	3.06	18	1
1:A:51:HIS:O	1:A:52:ARG:C	0.43	2.57	3	1
1:A:157:GLU:O	1:A:161:CYS:SG	0.43	2.75	3	1
1:A:166:VAL:HG12	1:A:168:HIS:ND1	0.43	2.29	8	1
1:A:72:GLN:OE1	1:A:94:TRP:CH2	0.43	2.71	20	1
1:A:13:MET:CE	1:A:32:TYR:OH	0.43	2.67	2	1
1:A:135:LEU:O	1:A:139:ALA:HB2	0.43	2.13	4	1
1:A:14:ASP:HB2	1:A:17:ILE:HD12	0.43	1.88	17	1
1:A:94:TRP:CZ3	1:A:122:LEU:CD2	0.43	3.01	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:CYS:HG	1:A:165:PHE:HZ	0.43	1.57	20	1
1:A:37:VAL:O	1:A:38:GLU:CD	0.43	2.57	1	1
1:A:31:THR:C	1:A:57:ASN:HD21	0.43	2.17	4	1
1:A:30:LYS:NZ	1:A:58:GLN:HE22	0.43	2.12	6	1
1:A:94:TRP:CH2	1:A:122:LEU:HD21	0.43	2.48	17	1
1:A:152:ILE:CG2	1:A:186:LEU:HD12	0.43	2.44	17	1
1:A:21:ASN:CG	1:A:22:PHE:N	0.43	2.72	20	1
1:A:184:GLN:O	1:A:184:GLN:OE1	0.43	2.36	4	1
1:A:136:TYR:OH	1:A:193:ILE:CG1	0.43	2.67	14	1
1:A:38:GLU:OE1	1:A:91:ARG:NH1	0.43	2.52	15	1
1:A:113:PHE:CD1	1:A:117:ASN:OD1	0.43	2.72	15	1
1:A:40:LEU:HD22	1:A:41:ASP:CA	0.43	2.44	3	1
1:A:90:TYR:CZ	1:A:120:VAL:HG22	0.43	2.49	4	2
1:A:72:GLN:NE2	1:A:96:ILE:CD1	0.43	2.82	8	2
1:A:173:PHE:CD1	1:A:173:PHE:C	0.43	2.90	16	1
1:A:91:ARG:NH1	1:A:123:ARG:CZ	0.43	2.82	17	1
1:A:167:ASP:O	1:A:167:ASP:CG	0.43	2.55	20	1
1:A:52:ARG:CZ	1:A:164:THR:CG2	0.43	2.96	5	2
1:A:162:TRP:CH2	1:A:166:VAL:HG11	0.43	2.49	17	1
1:A:90:TYR:CE2	1:A:119:HIS:CE1	0.42	3.07	10	1
1:A:157:GLU:CD	1:A:157:GLU:C	0.42	2.78	12	1
1:A:40:LEU:O	1:A:40:LEU:CD1	0.42	2.54	3	1
1:A:99:SER:OG	1:A:140:LEU:HD21	0.42	2.13	5	2
1:A:119:HIS:NE2	1:A:120:VAL:HG23	0.42	2.29	10	1
1:A:57:ASN:ND2	1:A:57:ASN:C	0.42	2.70	16	1
1:A:31:THR:HG21	1:A:57:ASN:ND2	0.42	2.30	17	1
1:A:95:PHE:CE1	1:A:125:PHE:CG	0.42	3.08	13	1
1:A:47:LYS:CD	1:A:52:ARG:HH12	0.42	2.28	15	1
1:A:84:LEU:HD13	1:A:90:TYR:CE1	0.42	2.48	16	1
1:A:92:VAL:HG22	1:A:94:TRP:NE1	0.42	2.28	20	1
1:A:137:LYS:HG3	1:A:193:ILE:HG23	0.42	1.92	3	1
1:A:180:ASP:CG	1:A:181:GLU:N	0.42	2.73	8	2
1:A:167:ASP:OD1	1:A:169:GLN:NE2	0.42	2.53	3	3
1:A:37:VAL:O	1:A:37:VAL:HG23	0.42	2.14	17	1
1:A:39:ARG:O	1:A:46:VAL:N	0.42	2.49	17	1
1:A:29:HIS:O	1:A:29:HIS:CG	0.42	2.72	5	1
1:A:129:ILE:HG23	1:A:136:TYR:OH	0.42	2.14	6	2
1:A:89:ILE:HG23	1:A:89:ILE:O	0.42	2.15	9	2
1:A:144:ARG:NH1	1:A:194:LEU:HD21	0.42	2.29	10	1
1:A:168:HIS:CG	1:A:168:HIS:O	0.42	2.73	16	1
1:A:190:LEU:C	1:A:190:LEU:CD1	0.42	2.89	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ARG:HH11	1:A:182:HIS:CE1	0.42	2.32	9	1
1:A:12:LEU:N	1:A:12:LEU:CD2	0.42	2.83	12	1
1:A:21:ASN:OD1	1:A:22:PHE:N	0.42	2.52	20	1
1:A:135:LEU:O	1:A:137:LYS:N	0.41	2.53	1	1
1:A:27:GLY:H	1:A:29:HIS:CE1	0.41	2.32	2	1
1:A:94:TRP:CE3	1:A:122:LEU:HD11	0.41	2.50	18	1
1:A:48:MET:HE1	1:A:51:HIS:CD2	0.41	2.50	7	1
1:A:93:THR:CG2	1:A:95:PHE:CE1	0.41	3.04	16	1
1:A:129:ILE:C	1:A:130:TYR:CG	0.41	2.93	20	1
1:A:41:ASP:CB	1:A:44:THR:O	0.41	2.67	3	1
1:A:188:GLY:O	1:A:192:ALA:CB	0.41	2.68	4	1
1:A:22:PHE:CE1	1:A:32:TYR:OH	0.41	2.60	6	1
1:A:190:LEU:HD13	1:A:190:LEU:C	0.41	2.36	6	1
1:A:113:PHE:O	1:A:117:ASN:N	0.41	2.49	15	1
1:A:31:THR:OG1	1:A:57:ASN:OD1	0.41	2.36	17	1
1:A:144:ARG:CZ	1:A:197:GLN:HE22	0.41	2.28	19	1
1:A:184:GLN:CG	1:A:185:ALA:N	0.41	2.83	19	1
1:A:180:ASP:OD1	1:A:180:ASP:N	0.41	2.53	1	4
1:A:121:ARG:HH11	1:A:123:ARG:HH11	0.41	1.58	7	1
1:A:32:TYR:OH	1:A:54:PHE:CE1	0.41	2.67	8	1
1:A:57:ASN:O	1:A:59:ALA:N	0.41	2.52	12	1
1:A:89:ILE:O	1:A:89:ILE:HG23	0.41	2.15	19	2
1:A:91:ARG:HH22	1:A:121:ARG:NH2	0.41	2.13	7	1
1:A:166:VAL:CG1	1:A:168:HIS:ND1	0.41	2.83	8	1
1:A:31:THR:OG1	1:A:97:SER:OG	0.41	2.37	13	1
1:A:187:SER:O	1:A:191:ARG:CG	0.41	2.68	2	1
1:A:56:HIS:H	1:A:56:HIS:HD1	0.41	1.56	11	1
1:A:148:ALA:O	1:A:149:GLN:OE1	0.41	2.39	3	1
1:A:40:LEU:HD12	1:A:40:LEU:N	0.41	2.30	11	1
1:A:157:GLU:HG3	1:A:158:PHE:N	0.41	2.31	12	1
1:A:98:TRP:CZ3	1:A:128:ARG:NH1	0.41	2.89	7	1
1:A:162:TRP:CD2	1:A:173:PHE:CB	0.41	3.04	14	1
1:A:196:ASN:ND2	1:A:196:ASN:C	0.41	2.73	1	1
1:A:168:HIS:O	1:A:169:GLN:OE1	0.41	2.39	7	1
1:A:93:THR:OG1	1:A:123:ARG:NE	0.41	2.54	14	1
1:A:162:TRP:CE2	1:A:168:HIS:CD2	0.41	3.09	19	1
1:A:144:ARG:HH21	1:A:194:LEU:CD2	0.41	2.28	5	1
1:A:153:MET:SD	1:A:158:PHE:CE2	0.41	3.14	5	1
1:A:21:ASN:OD1	1:A:32:TYR:CG	0.41	2.74	14	1
1:A:162:TRP:O	1:A:166:VAL:HB	0.41	2.16	16	1
1:A:21:ASN:OD1	1:A:22:PHE:CG	0.41	2.74	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:ARG:CD	1:A:192:ALA:N	0.40	2.84	1	1
1:A:47:LYS:O	1:A:48:MET:O	0.40	2.38	3	1
1:A:33:LEU:O	1:A:55:LEU:N	0.40	2.53	4	1
1:A:144:ARG:NH2	1:A:194:LEU:CD2	0.40	2.78	4	1
1:A:37:VAL:HG22	1:A:51:HIS:CE1	0.40	2.51	19	2
1:A:75:PHE:CE1	1:A:94:TRP:NE1	0.40	2.89	15	1
1:A:129:ILE:C	1:A:130:TYR:CD2	0.40	2.95	20	1
1:A:154:THR:O	1:A:155:TYR:C	0.40	2.58	20	1
1:A:23:ASN:OD1	1:A:176:TRP:CZ3	0.40	2.74	2	1
1:A:31:THR:O	1:A:57:ASN:CG	0.40	2.60	4	1
1:A:92:VAL:HG13	1:A:122:LEU:HD22	0.40	1.92	10	1
1:A:122:LEU:C	1:A:122:LEU:CD1	0.40	2.89	10	1
1:A:181:GLU:HG3	1:A:182:HIS:N	0.40	2.31	14	1
1:A:31:THR:CG2	1:A:57:ASN:ND2	0.40	2.85	17	1
1:A:99:SER:OG	1:A:126:ALA:CB	0.40	2.69	17	1
1:A:134:PRO:O	1:A:135:LEU:C	0.40	2.59	3	1
1:A:185:ALA:HB2	2:B:200:DA:C3'	0.40	2.46	8	1
1:A:184:GLN:C	1:A:184:GLN:CD	0.40	2.79	9	1
1:A:96:ILE:CD1	1:A:98:TRP:O	0.40	2.69	16	1
1:A:134:PRO:O	1:A:137:LYS:N	0.40	2.47	18	1
1:A:184:GLN:CD	1:A:184:GLN:O	0.40	2.60	1	1
1:A:40:LEU:C	1:A:40:LEU:CD1	0.40	2.87	3	1
1:A:181:GLU:O	2:B:200:DA:C5'	0.40	2.70	6	2
1:A:137:LYS:HG3	1:A:138:GLU:N	0.40	2.32	8	1
1:A:141:GLN:CD	1:A:196:ASN:OD1	0.40	2.60	10	1
1:A:94:TRP:CE2	1:A:122:LEU:CD2	0.40	3.03	15	1
1:A:79:VAL:CB	1:A:80:PRO:CD	0.40	2.99	2	1
1:A:133:ASP:O	1:A:134:PRO:C	0.40	2.58	7	1
1:A:75:PHE:CD1	1:A:94:TRP:CZ2	0.40	3.09	15	1
1:A:113:PHE:CD1	1:A:113:PHE:C	0.40	2.95	17	1
1:A:130:TYR:OH	1:A:189:ARG:NE	0.40	2.54	20	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	172/199 (86%)	157±1 (91±1%)	11±1 (6±1%)	4±1 (2±1%)	10	50
All	All	3440/3980 (86%)	3146 (91%)	221 (6%)	73 (2%)	10	50

All 11 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	148	ALA	20
1	A	134	PRO	19
1	A	133	ASP	9
1	A	50	GLN	8
1	A	101	CYS	4
1	A	178	GLY	4
1	A	48	MET	3
1	A	30	LYS	2
1	A	135	LEU	2
1	A	51	HIS	1
1	A	58	GLN	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	151/171 (88%)	131±2 (87±1%)	20±2 (13±1%)	7	48
All	All	3020/3420 (88%)	2625 (87%)	395 (13%)	7	48

All 69 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	174	GLN	20
1	A	189	ARG	20
1	A	190	LEU	20
1	A	195	GLN	20
1	A	196	ASN	20
1	A	99	SER	19

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Mol	Chain	Res	Type	Models (Total)
1	A	133	ASP	19
1	A	34	CYS	18
1	A	101	CYS	18
1	A	169	GLN	16
1	A	179	LEU	15
1	A	98	TRP	11
1	A	14	ASP	10
1	A	191	ARG	10
1	A	78	LEU	10
1	A	85	ASP	10
1	A	56	HIS	9
1	A	106	CYS	9
1	A	119	HIS	7
1	A	90	TYR	6
1	A	168	HIS	5
1	A	184	GLN	5
1	A	165	PHE	4
1	A	40	LEU	4
1	A	57	ASN	4
1	A	136	TYR	3
1	A	140	LEU	3
1	A	143	LEU	3
1	A	176	TRP	3
1	A	51	HIS	3
1	A	122	LEU	3
1	A	48	MET	2
1	A	73	LEU	2
1	A	13	MET	2
1	A	46	VAL	2
1	A	171	GLN	2
1	A	154	THR	2
1	A	161	CYS	2
1	A	155	TYR	2
1	A	130	TYR	2
1	A	135	LEU	2
1	A	32	TYR	2
1	A	76	LEU	1
1	A	131	ASP	1
1	A	29	HIS	1
1	A	12	LEU	1
1	A	30	LYS	1
1	A	153	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	31	THR	1
1	A	74	ARG	1
1	A	18	PHE	1
1	A	197	GLN	1
1	A	128	ARG	1
1	A	186	LEU	1
1	A	157	GLU	1
1	A	50	GLN	1
1	A	173	PHE	1
1	A	58	GLN	1
1	A	81	SER	1
1	A	19	THR	1
1	A	41	ASP	1
1	A	114	LEU	1
1	A	42	ASN	1
1	A	96	ILE	1
1	A	52	ARG	1
1	A	125	PHE	1
1	A	129	ILE	1
1	A	158	PHE	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 1 ligands modelled in this entry, 1 is 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-nospecific_20200915.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	2276
Number of shifts mapped to atoms	2276
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	192	0.06 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	176	0.64 ± 0.15	Should be applied
$^{13}\text{C}'$	173	-0.02 ± 0.11	None needed (< 0.5 ppm)
^{15}N	181	-0.34 ± 0.31	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. 1815 atoms were assigned a chemical shift out of a possible 2412. 23 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	814/846 (96%)	328/337 (97%)	325/344 (94%)	161/165 (98%)
Sidechain	800/1113 (72%)	521/656 (79%)	273/396 (69%)	6/61 (10%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	118/265 (45%)	102/138 (74%)	14/106 (13%)	2/21 (10%)
Overall	1815/2412 (75%)	1034/1239 (83%)	612/916 (67%)	169/257 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 2039 atoms were assigned a chemical shift out of a possible 2732. 24 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	919/977 (94%)	373/389 (96%)	365/398 (92%)	181/190 (95%)
Sidechain	896/1256 (71%)	586/744 (79%)	304/441 (69%)	6/71 (8%)
Aromatic	141/311 (45%)	117/162 (72%)	21/125 (17%)	3/24 (12%)
Overall	2039/2732 (75%)	1159/1403 (83%)	690/1034 (67%)	190/295 (64%)

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	A	70	HIS	CE1	118.42	149.70 – 125.30	-7.8
1	A	66	PHE	CD2	124.86	137.34 – 125.84	-5.9
1	A	66	PHE	CD1	124.86	137.63 – 125.43	-5.5
1	A	72	GLN	CB	38.88	38.36 – 19.96	5.3
1	A	131	ASP	CB	32.21	49.06 – 32.66	-5.3
1	A	172	PRO	CG	32.94	32.66 – 21.76	5.3
1	A	179	LEU	HG	-0.22	3.16 – -0.14	-5.2
1	A	97	SER	HB3	2.44	5.25 – 2.45	-5.0

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *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:

