Full wwPDB NMR Structure Validation Report (i)

Mar 3, 2022 – 07:36 AM EST

PDB ID	:	2HDC
Title	:	STRUCTURE OF TRANSCRIPTION FACTOR GENESIS/DNA COMPLEX
Authors	:	Jin, C.; Marsden, I.; Chen, X.; Liao, X.
Deposited on	:	1999-05-05

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 (i) symbol.

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

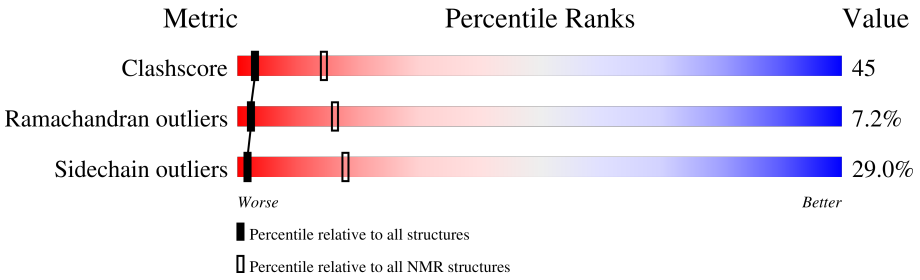
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	B	17	29% 71%
2	C	17	18% 82%
3	A	97	19% 58% 7% 16%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:7-A:87 (81)	0.52	6

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2581 atoms, of which 1080 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	17	493	167	145	67	97	17	0

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	C	17	484	169	135	56	107	17	0

- Molecule 3 is a protein called PROTEIN (TRANSCRIPTION FACTOR).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	A	97	1604	517	800	143	140	4	0

4 Residue-property plots (i)

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

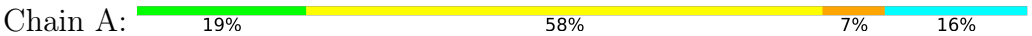
Chain B:

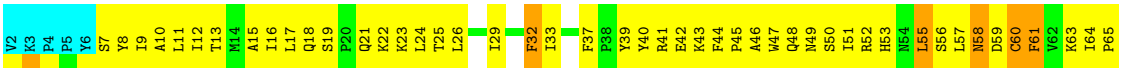
• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*GP*C)-3')

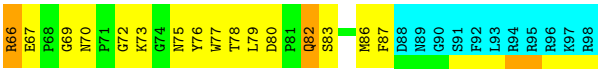
Chain C:

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:







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

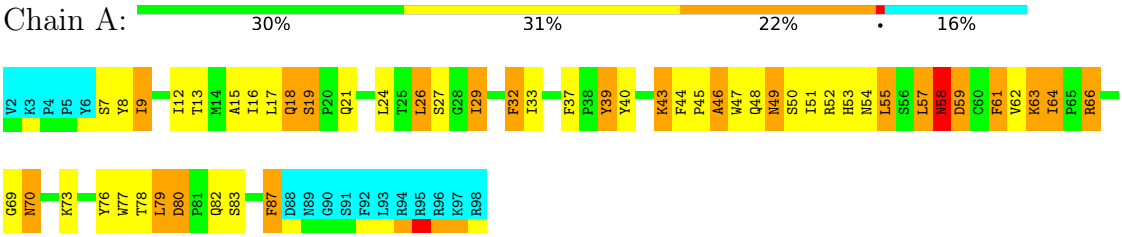
Chain B:

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

Chain C:

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:



4.2.2 Score per residue for model 2

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

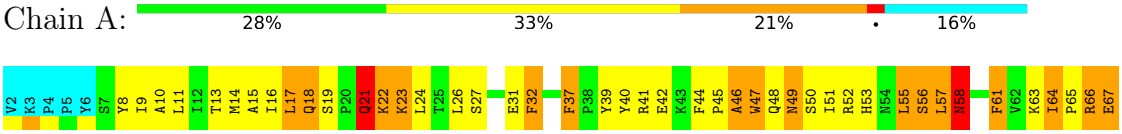
Chain B:

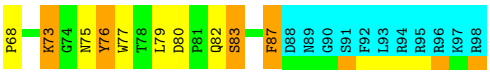
• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*GP*C)-3')

Chain C:

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:





4.2.3 Score per residue for model 3

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

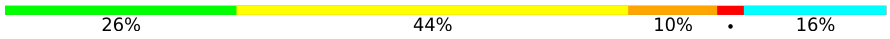
Chain B:

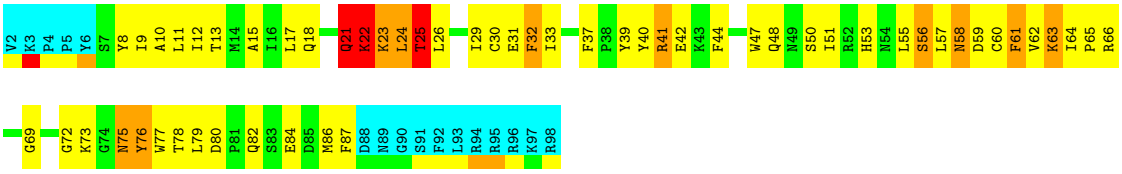
• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*GP*C)-3')

Chain C:

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:





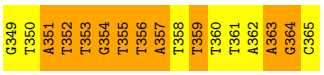
4.2.4 Score per residue for model 4

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

Chain B:

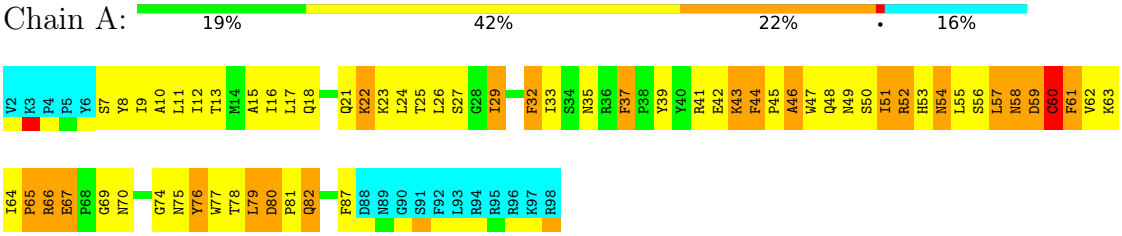
• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*GP*C)-3')

Chain C:



• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:



4.2.5 Score per residue for model 5

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

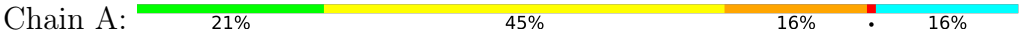
Chain B:

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

Chain C:

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:



4.2.6 Score per residue for model 6 (medoid)

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

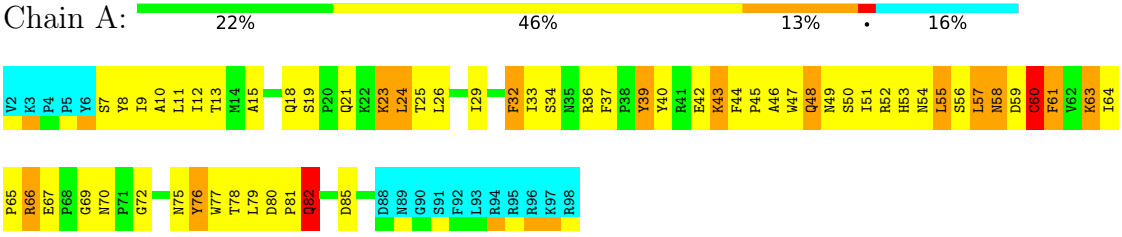
Chain B:

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

Chain C:

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:



4.2.7 Score per residue for model 7

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

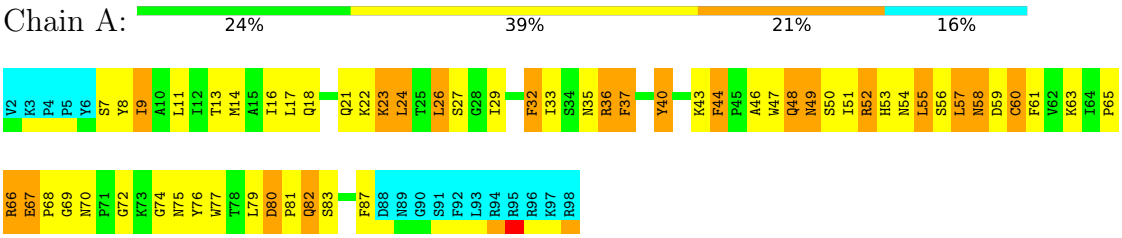
Chain B:

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

Chain C:

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:



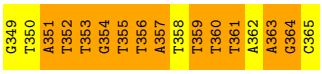
4.2.8 Score per residue for model 8

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

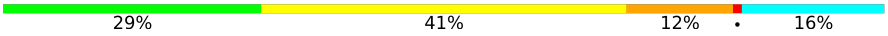
Chain B: 

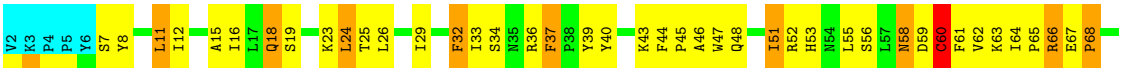
• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*GP*C)-3')

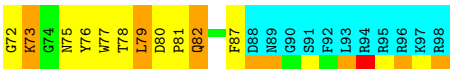
Chain C: 



• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A: 

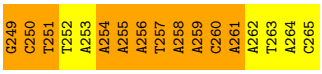




4.2.9 Score per residue for model 9

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

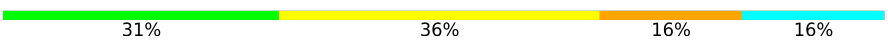
Chain B: 

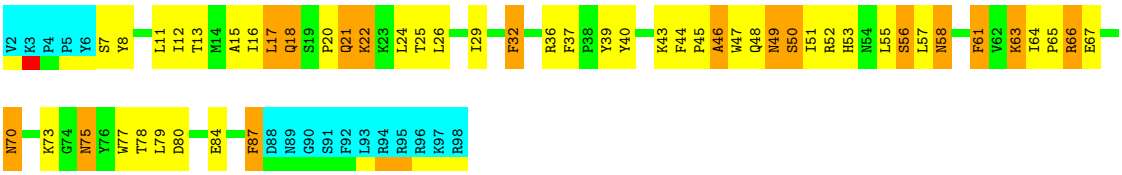


• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*GP*C)-3')

Chain C: 

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A: 



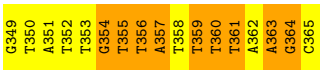
4.2.10 Score per residue for model 10

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

Chain B: 35% 65%

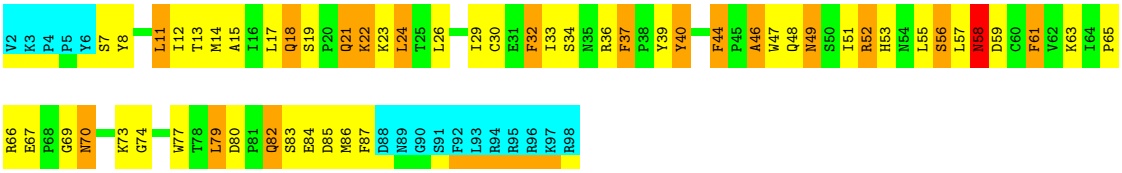
• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*GP*C)-3')

Chain C: 47% 53%



• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A: 27% 38% 18% 16%



4.2.11 Score per residue for model 11

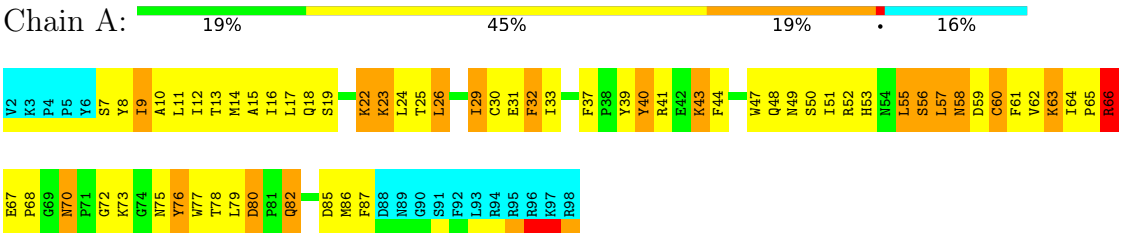
• Molecule 1: DNA (5'-D(P*GP*CP*TP*TP*AP*AP*AP*AP*TP*AP*AP*CP*AP*AP*TP*AP*C)-3')

Chain B: 29% 71%

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

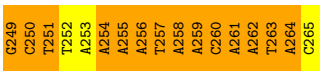
Chain C: 24% 76%

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

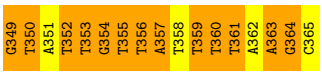


4.2.12 Score per residue for model 12

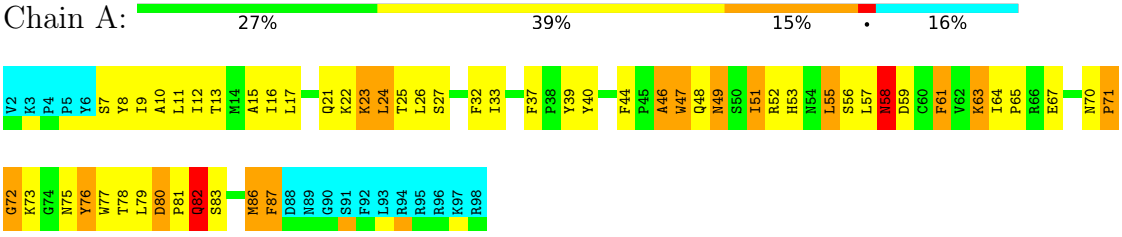
• Molecule 1: DNA (5'-D(P*GP*CP*TP*TP*AP*AP*AP*AP*TP*AP*AP*CP*AP*AP*TP*AP*C)-3')



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



• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

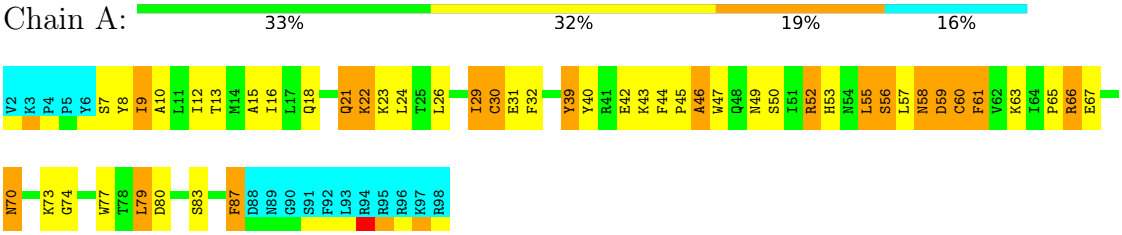


4.2.13 Score per residue for model 13

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

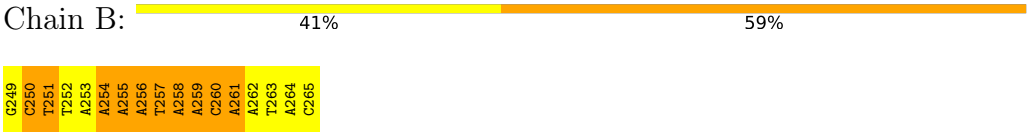
• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*GP*C)-3')

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)



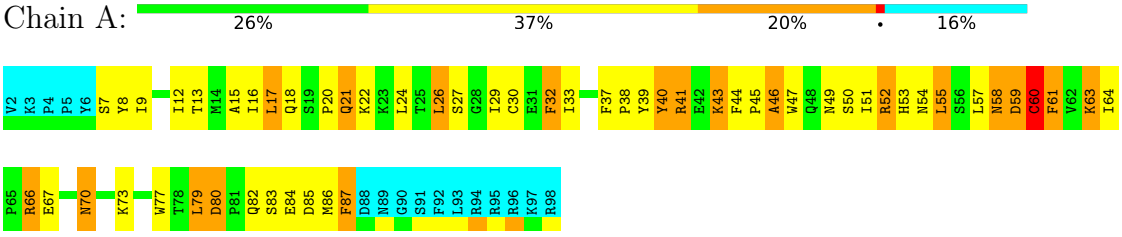
4.2.14 Score per residue for model 14

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



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

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)



4.2.15 Score per residue for model 15

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

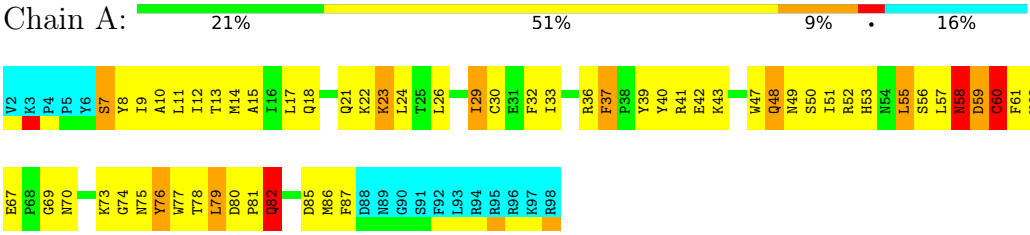
Chain B:

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

Chain C:

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:



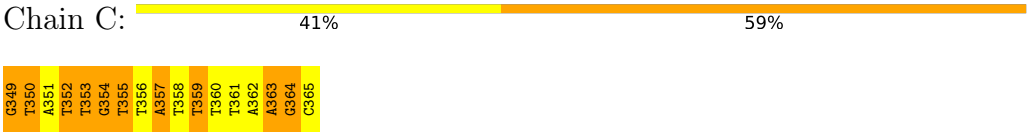
4.2.16 Score per residue for model 16

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

Chain B:

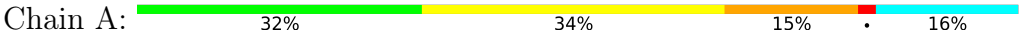
• Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*GP*C)-3')

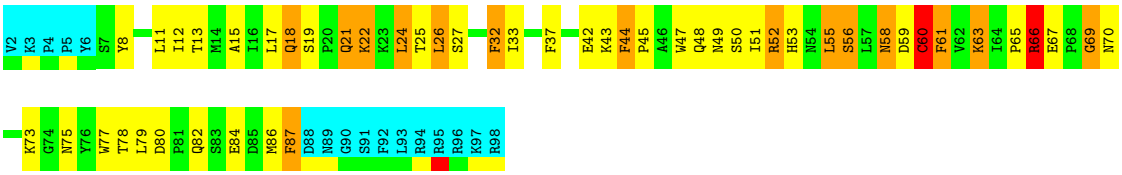
Chain C:



• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:





4.2.17 Score per residue for model 17

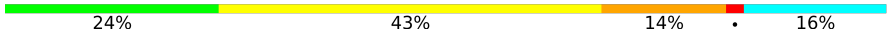
• Molecule 1: DNA (5'-D(P*GP*CP*TP*TP*AP*AP*AP*AP*TP*AP*AP*CP*AP*AP*TP*AP*C)-3')

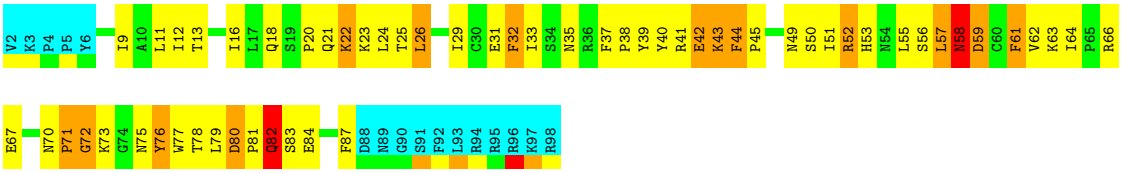
Chain B: 

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

Chain C: 

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

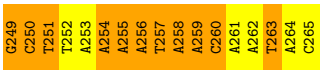
Chain A: 



4.2.18 Score per residue for model 18

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

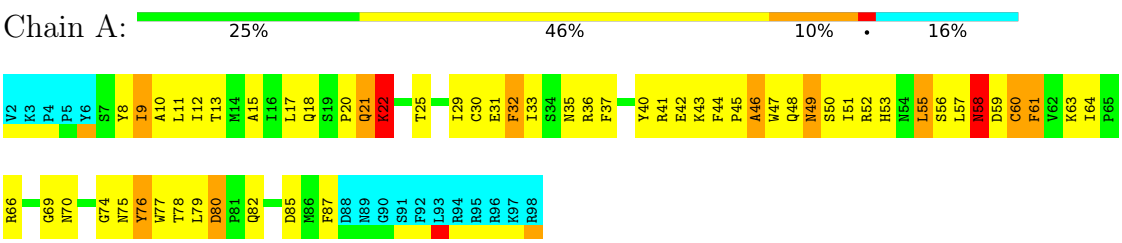
Chain B: 



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

Chain C: 

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

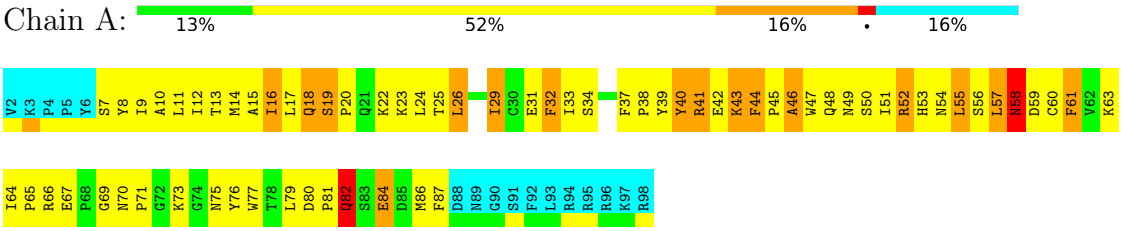


4.2.19 Score per residue for model 19

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

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

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)



4.2.20 Score per residue for model 20

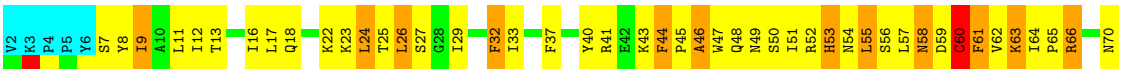
• Molecule 1: DNA (5'-D(P*GP*CP*TP*TP*AP*AP*AP*AP*TP*AP*AP*CP*AP*AP*TP*AP*C)-3')

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

Chain C:

• Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
DYANA	refinement	1.5
DYANA	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	4.98±2.25	13±1/391 (3.4± 0.3%)	5.51±0.64	49±1/600 (8.1± 0.2%)
2	C	3.59±0.38	12±2/389 (3.2± 0.4%)	4.76±0.32	62±2/599 (10.4± 0.3%)
3	A	0.72±0.00	0±0/685 (0.0± 0.0%)	0.92±0.00	0±0/930 (0.0± 0.0%)
All	All	3.42	513/29300 (1.8%)	3.93	2223/42580 (5.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	8.1±1.1	0.0±0.0
2	C	4.2±1.0	0.0±0.0
All	All	246	0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	249	DG	C4'-O4'	277.59	4.22	1.45	20	15
2	C	359	DT	C4'-O4'	60.77	2.05	1.45	18	19
2	C	363	DA	C4'-O4'	44.67	1.89	1.45	9	7
1	B	260	DC	C4'-O4'	42.10	1.87	1.45	3	20
1	B	254	DA	C4'-O4'	-37.77	1.07	1.45	2	20
2	C	360	DT	C4'-O4'	-37.67	1.07	1.45	15	9
1	B	250	DC	C4'-O4'	-37.58	1.07	1.45	7	8
1	B	264	DA	C4'-O4'	-37.00	1.08	1.45	15	7
2	C	358	DT	C4'-O4'	-36.89	1.08	1.45	11	17
1	B	263	DT	C4'-O4'	-36.42	1.08	1.45	15	19
1	B	256	DA	C4'-O4'	36.40	1.81	1.45	6	20
1	B	259	DA	C4'-O4'	-36.35	1.08	1.45	18	19
2	C	352	DT	C4'-O4'	-35.81	1.09	1.45	2	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	261	DA	C4'-O4'	-35.61	1.09	1.45	12	19
2	C	355	DT	C4'-O4'	-35.19	1.09	1.45	10	15
1	B	257	DT	C4'-O4'	-34.80	1.10	1.45	11	16
1	B	255	DA	C4'-O4'	-34.78	1.10	1.45	11	20
2	C	357	DA	C4'-O4'	-34.76	1.10	1.45	6	17
1	B	258	DA	C4'-O4'	-34.08	1.10	1.45	13	8
1	B	253	DA	C4'-O4'	-32.16	1.12	1.45	19	15
2	C	364	DG	C4'-O4'	29.21	1.74	1.45	9	20
1	B	251	DT	C4'-O4'	29.06	1.74	1.45	10	19
2	C	365	DC	C4'-O4'	-28.58	1.16	1.45	6	20
1	B	265	DC	C4'-O4'	-24.70	1.20	1.45	17	17
2	C	354	DG	C4'-O4'	21.69	1.66	1.45	11	19
1	B	262	DA	C4'-O4'	18.69	1.63	1.45	16	17
2	C	361	DT	C4'-O4'	18.45	1.63	1.45	9	15
2	C	353	DT	C4'-O4'	18.07	1.63	1.45	3	19
2	C	362	DA	C4'-O4'	-16.50	1.28	1.45	20	14
2	C	356	DT	C4'-O4'	-15.17	1.29	1.45	10	10
2	C	350	DT	C4'-O4'	14.79	1.59	1.45	16	20
1	B	252	DT	C4'-O4'	14.37	1.59	1.45	2	8
2	C	351	DA	C4'-O4'	9.73	1.54	1.45	2	6
2	C	349	DG	C4'-O4'	-7.22	1.37	1.45	20	10

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	249	DG	O4'-C4'-C3'	-121.26	33.25	106.00	20	12
1	B	249	DG	C1'-O4'-C4'	-79.09	31.00	110.10	20	17
2	C	359	DT	O4'-C4'-C3'	-56.61	72.04	106.00	18	14
2	C	363	DA	O4'-C4'-C3'	-48.22	77.07	106.00	9	19
1	B	260	DC	O4'-C4'-C3'	-45.03	78.98	106.00	11	20
1	B	263	DT	O4'-C4'-C3'	-42.83	80.30	106.00	6	17
1	B	255	DA	O4'-C4'-C3'	-42.64	80.42	106.00	18	10
1	B	257	DT	O4'-C4'-C3'	-41.50	81.10	106.00	13	19
1	B	256	DA	O4'-C4'-C3'	-40.44	81.73	106.00	6	16
2	C	364	DG	O4'-C4'-C3'	-39.23	82.46	106.00	9	20
1	B	251	DT	O4'-C4'-C3'	-38.50	82.90	106.00	10	20
1	B	254	DA	O4'-C4'-C3'	-34.83	85.10	106.00	17	1
2	C	358	DT	O4'-C4'-C3'	-32.92	86.25	106.00	13	15
2	C	353	DT	O4'-C4'-C3'	-32.03	86.78	106.00	19	20
1	B	262	DA	O4'-C4'-C3'	-30.30	87.82	106.00	16	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	363	DA	C5'-C4'-O4'	30.25	166.77	109.30	9	1
2	C	354	DG	O4'-C4'-C3'	-30.15	87.91	106.00	11	20
1	B	259	DA	O4'-C4'-C3'	-29.07	88.56	106.00	14	16
1	B	261	DA	O4'-C4'-C3'	-29.05	88.57	106.00	14	19
1	B	253	DA	O4'-C4'-C3'	-28.29	89.02	106.00	3	17
1	B	252	DT	O4'-C4'-C3'	-27.64	89.41	106.00	2	20
2	C	360	DT	O4'-C4'-C3'	-27.48	89.51	106.00	13	19
1	B	263	DT	C5'-C4'-O4'	27.47	161.49	109.30	19	20
1	B	260	DC	C5'-C4'-O4'	26.91	160.43	109.30	6	20
2	C	359	DT	C5'-C4'-O4'	26.88	160.36	109.30	10	18
1	B	256	DA	C5'-C4'-O4'	26.72	160.06	109.30	17	20
1	B	255	DA	C5'-C4'-O4'	26.51	159.67	109.30	19	20
2	C	357	DA	O4'-C4'-C3'	-26.32	90.21	106.00	20	14
2	C	361	DT	O4'-C4'-C3'	-26.02	90.39	106.00	9	20
2	C	351	DA	O4'-C4'-C3'	-25.67	90.60	106.00	2	20
1	B	251	DT	C5'-C4'-O4'	25.45	157.65	109.30	12	20
2	C	358	DT	C5'-C4'-O4'	25.08	156.96	109.30	13	19
2	C	354	DG	C5'-C4'-O4'	25.07	156.93	109.30	9	20
1	B	262	DA	C5'-C4'-O4'	24.98	156.76	109.30	16	20
1	B	257	DT	C5'-C4'-O4'	24.64	156.12	109.30	8	19
1	B	261	DA	C5'-C4'-O4'	24.59	156.01	109.30	11	19
2	C	353	DT	C5'-C4'-O4'	24.55	155.95	109.30	17	20
1	B	265	DC	O4'-C4'-C3'	-24.55	91.27	106.00	8	20
1	B	253	DA	C5'-C4'-O4'	24.45	155.75	109.30	2	19
1	B	259	DA	C5'-C4'-O4'	24.07	155.03	109.30	14	20
1	B	252	DT	C5'-C4'-O4'	23.68	154.30	109.30	2	20
1	B	264	DA	O4'-C4'-C3'	-23.64	91.82	106.00	11	17
2	C	361	DT	C5'-C4'-O4'	23.54	154.03	109.30	9	20
2	C	351	DA	C5'-C4'-O4'	23.30	153.57	109.30	2	20
2	C	355	DT	C5'-C4'-O4'	22.89	152.80	109.30	6	20
2	C	362	DA	O4'-C4'-C3'	-22.86	92.28	106.00	2	16
1	B	264	DA	C5'-C4'-O4'	22.25	151.57	109.30	11	20
2	C	355	DT	O4'-C4'-C3'	-22.24	92.65	106.00	6	17
1	B	258	DA	C5'-C4'-O4'	22.05	151.21	109.30	6	19
1	B	258	DA	O4'-C4'-C3'	-21.93	92.84	106.00	8	17
2	C	362	DA	C5'-C4'-O4'	21.80	150.72	109.30	2	20
1	B	265	DC	C5'-C4'-O4'	21.77	150.66	109.30	13	20
2	C	349	DG	O4'-C4'-C3'	-21.68	92.99	106.00	9	20
2	C	356	DT	C5'-C4'-O4'	21.40	149.97	109.30	20	20
2	C	357	DA	C5'-C4'-O4'	21.12	149.43	109.30	4	20
2	C	350	DT	O4'-C4'-C3'	-20.54	93.67	106.00	9	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	254	DA	C5'-C4'-O4'	20.23	147.74	109.30	17	19
2	C	364	DG	C5'-C4'-O4'	19.42	146.20	109.30	9	6
2	C	356	DT	O4'-C4'-C3'	-19.36	94.38	106.00	11	20
1	B	250	DC	O4'-C4'-C3'	-19.16	94.50	106.00	19	15
2	C	352	DT	C5'-C4'-O4'	15.04	137.88	109.30	7	13
2	C	352	DT	O4'-C4'-C3'	-14.76	97.14	106.00	9	18
2	C	360	DT	C5'-C4'-O4'	-13.60	83.45	109.30	2	18
2	C	360	DT	C1'-O4'-C4'	13.60	123.70	110.10	15	17
1	B	254	DA	C1'-O4'-C4'	13.55	123.65	110.10	2	19
1	B	250	DC	C1'-O4'-C4'	13.47	123.57	110.10	7	19
1	B	263	DT	C1'-O4'-C4'	13.33	123.43	110.10	15	4
2	C	358	DT	C1'-O4'-C4'	13.28	123.38	110.10	11	11
1	B	249	DG	C5'-C4'-O4'	-13.20	84.22	109.30	4	14
1	B	264	DA	C1'-O4'-C4'	13.19	123.29	110.10	15	18
2	C	352	DT	C1'-O4'-C4'	12.90	123.00	110.10	2	11
1	B	259	DA	C1'-O4'-C4'	12.88	122.98	110.10	18	4
1	B	255	DA	C1'-O4'-C4'	12.81	122.91	110.10	17	12
2	C	349	DG	C5'-C4'-O4'	12.63	133.30	109.30	17	15
1	B	256	DA	C1'-O4'-C4'	12.61	122.71	110.10	20	5
2	C	359	DT	C1'-O4'-C4'	12.50	122.60	110.10	13	6
1	B	258	DA	C1'-O4'-C4'	12.39	122.49	110.10	13	16
1	B	261	DA	C1'-O4'-C4'	11.94	122.04	110.10	12	4
2	C	364	DG	C5-C6-N1	11.92	117.46	111.50	11	20
2	C	354	DG	C5-C6-N1	11.91	117.46	111.50	9	20
2	C	349	DG	C5-C6-N1	11.89	117.44	111.50	3	20
1	B	249	DG	C5-C6-N1	11.88	117.44	111.50	3	20
2	C	363	DA	C1'-O4'-C4'	11.74	121.84	110.10	6	14
2	C	355	DT	C1'-O4'-C4'	11.54	121.64	110.10	10	7
2	C	365	DC	C1'-O4'-C4'	11.50	121.60	110.10	6	20
2	C	357	DA	C1'-O4'-C4'	11.23	121.33	110.10	6	9
1	B	257	DT	C1'-O4'-C4'	11.17	121.27	110.10	11	10
2	C	349	DG	C6-N1-C2	-11.08	118.45	125.10	7	20
1	B	249	DG	C6-N1-C2	-11.06	118.46	125.10	2	20
2	C	364	DG	C6-N1-C2	-11.05	118.47	125.10	5	20
2	C	354	DG	C6-N1-C2	-11.04	118.48	125.10	18	20
1	B	253	DA	C1'-O4'-C4'	10.01	120.11	110.10	12	15
1	B	265	DC	C1'-O4'-C4'	9.86	119.96	110.10	17	16
2	C	356	DT	C1'-O4'-C4'	8.95	119.05	110.10	3	16
2	C	365	DC	C5'-C4'-O4'	-8.82	92.55	109.30	20	20
2	C	362	DA	C1'-O4'-C4'	8.80	118.90	110.10	17	20
1	B	262	DA	C1'-O4'-C4'	8.78	118.88	110.10	12	12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	364	DG	N1-C2-N3	8.75	129.15	123.90	4	20
2	C	354	DG	N1-C2-N3	8.73	129.14	123.90	2	20
1	B	249	DG	N1-C2-N3	8.73	129.14	123.90	13	20
2	C	349	DG	N1-C2-N3	8.73	129.14	123.90	11	20
1	B	250	DC	C5'-C4'-O4'	-8.52	93.11	109.30	7	14
1	B	252	DT	C1'-O4'-C4'	8.26	118.36	110.10	10	18
2	C	349	DG	C1'-O4'-C4'	8.24	118.34	110.10	3	20
2	C	351	DA	C1'-O4'-C4'	7.21	117.31	110.10	15	15
2	C	361	DT	C1'-O4'-C4'	7.11	117.20	110.10	15	13
2	C	354	DG	C1'-O4'-C4'	6.99	117.09	110.10	8	6
2	C	350	DT	C5'-C4'-O4'	6.49	121.64	109.30	15	14
2	C	353	DT	C1'-O4'-C4'	6.15	116.25	110.10	18	8
1	B	257	DT	C2-N3-C4	-6.15	123.51	127.20	15	20
2	C	353	DT	C2-N3-C4	-6.14	123.51	127.20	5	20
2	C	359	DT	C2-N3-C4	-6.13	123.52	127.20	3	20
2	C	352	DT	C2-N3-C4	-6.11	123.53	127.20	13	20
2	C	358	DT	C2-N3-C4	-6.10	123.54	127.20	11	20
2	C	356	DT	C2-N3-C4	-6.09	123.55	127.20	9	20
2	C	350	DT	C2-N3-C4	-6.08	123.55	127.20	15	20
1	B	263	DT	C2-N3-C4	-6.08	123.55	127.20	19	20
2	C	361	DT	C2-N3-C4	-6.08	123.55	127.20	6	20
2	C	360	DT	C2-N3-C4	-6.07	123.56	127.20	7	20
1	B	252	DT	C2-N3-C4	-6.07	123.56	127.20	3	20
2	C	355	DT	C2-N3-C4	-6.06	123.56	127.20	14	20
1	B	251	DT	C2-N3-C4	-6.05	123.57	127.20	4	20
1	B	251	DT	C1'-O4'-C4'	5.88	115.98	110.10	9	5
2	C	364	DG	N1-C2-N2	-5.50	111.25	116.20	5	20
1	B	249	DG	N1-C2-N2	-5.49	111.26	116.20	16	20
2	C	349	DG	N1-C2-N2	-5.49	111.26	116.20	10	20
2	C	354	DG	N1-C2-N2	-5.49	111.26	116.20	18	20
2	C	364	DG	C5-C6-O6	-5.47	125.32	128.60	11	20
1	B	249	DG	C5-C6-O6	-5.42	125.35	128.60	1	20
2	C	349	DG	C5-C6-O6	-5.41	125.35	128.60	14	20
2	C	354	DG	C5-C6-O6	-5.41	125.36	128.60	4	20
2	C	350	DT	C1'-O4'-C4'	5.21	115.31	110.10	2	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	255	DA	C4'	20
1	B	260	DC	C4'	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	263	DT	C4'	18
2	C	359	DT	C4'	18
2	C	353	DT	C4'	16
2	C	358	DT	C4'	15
1	B	253	DA	C4'	13
1	B	256	DA	C4'	13
1	B	257	DT	C4'	13
2	C	362	DA	C4'	13
1	B	254	DA	C4'	12
1	B	251	DT	C4'	11
1	B	264	DA	C4'	10
1	B	262	DA	C4'	9
1	B	258	DA	C4'	8
2	C	356	DT	C4'	8
1	B	252	DT	C4'	5
2	C	361	DT	C4'	4
2	C	357	DA	C4'	3
1	B	261	DA	C4'	3
1	B	265	DC	C4'	3
1	B	259	DA	C4'	3
2	C	355	DT	C4'	2
2	C	364	DG	C4'	2
2	C	351	DA	C4'	1
1	B	249	DG	C4'	1
2	C	354	DG	C4'	1
2	C	363	DA	C4'	1

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	348	145	192	26±6
2	C	349	135	197	22±5
3	A	664	652	652	72±13
All	All	27220	18640	20820	2141

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 45.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:261:DA:O4'	1:B:261:DA:C4'	1.39	1.64	13	8
2:C:361:DT:C4'	2:C:361:DT:O4'	1.38	1.63	9	1
1:B:256:DA:O4'	1:B:256:DA:C4'	1.37	1.64	11	12
2:C:364:DG:O4'	2:C:364:DG:C4'	1.36	1.64	15	8
1:B:251:DT:O4'	1:B:251:DT:C4'	1.35	1.65	3	4
1:B:259:DA:C4'	1:B:259:DA:O4'	1.35	1.65	16	4
1:B:255:DA:O4'	1:B:255:DA:C4'	1.34	1.66	15	7
1:B:249:DG:C4'	1:B:249:DG:O4'	1.34	1.64	17	2
2:C:354:DG:C4'	2:C:354:DG:O4'	1.34	1.66	11	3
1:B:262:DA:O4'	1:B:262:DA:C4'	1.33	1.63	16	1
1:B:257:DT:O4'	1:B:257:DT:C4'	1.33	1.65	6	5
1:B:260:DC:O4'	1:B:260:DC:C4'	1.32	1.70	1	17
2:C:359:DT:C4'	2:C:359:DT:O4'	1.31	1.70	1	14
1:B:265:DC:O4'	1:B:265:DC:C4'	1.29	1.64	8	1
1:B:254:DA:C4'	1:B:254:DA:O4'	1.27	1.68	17	1
1:B:263:DT:C4'	1:B:263:DT:O4'	1.27	1.77	2	8
2:C:358:DT:C4'	2:C:358:DT:O4'	1.19	1.68	13	1
2:C:363:DA:C4'	2:C:363:DA:O4'	1.04	1.89	9	1
3:A:16:ILE:HD12	3:A:24:LEU:HD21	0.95	1.35	14	1
3:A:64:ILE:HG22	3:A:76:TYR:O	0.94	1.62	20	10
3:A:9:ILE:O	3:A:13:THR:HG23	0.90	1.65	19	8
3:A:13:THR:HG21	3:A:87:PHE:CE1	0.90	2.00	12	4
3:A:13:THR:O	3:A:17:LEU:HD23	0.89	1.67	11	10
3:A:12:ILE:HD11	3:A:51:ILE:HD11	0.89	1.42	8	1
3:A:23:LYS:O	3:A:24:LEU:HD22	0.87	1.69	3	4
3:A:9:ILE:HG22	3:A:58:ASN:OD1	0.85	1.71	13	2
3:A:47:TRP:O	3:A:51:ILE:HG23	0.85	1.71	6	1
1:B:249:DG:O4'	1:B:249:DG:C5'	0.85	2.24	17	2
3:A:9:ILE:HD11	3:A:58:ASN:OD1	0.84	1.72	17	2
3:A:26:LEU:HD23	3:A:55:LEU:HD23	0.84	1.49	6	2
3:A:16:ILE:HG21	3:A:79:LEU:HD13	0.83	1.50	13	2
3:A:79:LEU:HD23	3:A:80:ASP:O	0.83	1.72	16	14
3:A:16:ILE:HG12	3:A:79:LEU:HD13	0.82	1.50	1	3
1:B:258:DA:C2	2:C:357:DA:C2	0.82	2.68	15	19
3:A:40:TYR:CD2	3:A:47:TRP:CH2	0.82	2.68	7	7
3:A:40:TYR:CD2	3:A:47:TRP:CZ2	0.81	2.69	7	3
2:C:356:DT:H72	3:A:57:LEU:HD11	0.81	1.53	14	1
2:C:355:DT:H72	3:A:52:ARG:NE	0.79	1.92	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:40:TYR:CG	3:A:47:TRP:CH2	0.79	2.71	9	2
3:A:44:PHE:CD1	3:A:47:TRP:CD1	0.79	2.71	16	2
3:A:79:LEU:HD22	3:A:80:ASP:N	0.79	1.92	19	1
3:A:11:LEU:HD22	3:A:37:PHE:CE1	0.78	2.14	2	2
3:A:47:TRP:CE3	3:A:51:ILE:HD11	0.78	2.15	1	2
3:A:26:LEU:HD11	3:A:52:ARG:NH2	0.77	1.94	15	1
3:A:19:SER:OG	3:A:24:LEU:HD23	0.76	1.79	10	1
3:A:8:TYR:HB3	3:A:51:ILE:HD12	0.75	1.57	3	2
3:A:79:LEU:HD13	3:A:80:ASP:O	0.75	1.82	19	1
3:A:53:HIS:CE1	3:A:57:LEU:HD22	0.75	2.16	13	6
3:A:8:TYR:CE2	3:A:12:ILE:HD11	0.75	2.17	6	2
2:C:359:DT:C4'	2:C:360:DT:OP1	0.74	2.34	2	4
3:A:33:ILE:HG21	3:A:47:TRP:CZ3	0.74	2.17	19	7
1:B:255:DA:H1'	1:B:256:DA:H4'	0.74	1.59	11	7
3:A:47:TRP:CZ3	3:A:51:ILE:HD13	0.74	2.18	19	2
3:A:12:ILE:HD11	3:A:51:ILE:CD1	0.74	2.12	8	2
3:A:25:THR:HG23	3:A:75:ASN:O	0.74	1.83	20	4
3:A:79:LEU:HD22	3:A:80:ASP:H	0.74	1.40	19	1
3:A:12:ILE:HD12	3:A:55:LEU:HD13	0.73	1.56	3	3
3:A:19:SER:OG	3:A:24:LEU:HD22	0.73	1.83	16	4
3:A:13:THR:HG21	3:A:87:PHE:CD1	0.73	2.18	14	1
3:A:44:PHE:O	3:A:44:PHE:CG	0.73	2.42	2	2
3:A:12:ILE:HD12	3:A:55:LEU:HG	0.73	1.58	18	6
3:A:32:PHE:CE2	3:A:33:ILE:HD11	0.72	2.19	17	4
3:A:12:ILE:CD1	3:A:51:ILE:HD11	0.72	2.13	8	2
3:A:23:LYS:C	3:A:24:LEU:HD22	0.72	2.04	17	3
3:A:67:GLU:N	3:A:68:PRO:HD3	0.72	1.99	8	1
3:A:11:LEU:HD21	3:A:37:PHE:CZ	0.71	2.19	10	1
3:A:44:PHE:CD1	3:A:47:TRP:NE1	0.71	2.58	16	1
3:A:16:ILE:HD12	3:A:79:LEU:HD13	0.71	1.62	11	3
3:A:16:ILE:CD1	3:A:24:LEU:HD21	0.71	2.14	14	2
3:A:15:ALA:HB2	3:A:32:PHE:CE2	0.71	2.19	1	4
3:A:40:TYR:CG	3:A:47:TRP:CZ2	0.71	2.78	7	4
3:A:61:PHE:HB3	3:A:79:LEU:HD23	0.71	1.62	19	1
3:A:8:TYR:CD1	3:A:47:TRP:CZ3	0.70	2.79	5	1
3:A:25:THR:O	3:A:29:ILE:HD13	0.70	1.87	9	4
2:C:355:DT:H4'	2:C:356:DT:OP1	0.70	1.87	20	3
2:C:364:DG:O4'	2:C:364:DG:C5'	0.70	2.39	10	6
1:B:255:DA:C2	1:B:256:DA:C4	0.70	2.80	9	16
3:A:13:THR:HG21	3:A:87:PHE:CE2	0.69	2.22	13	1
3:A:45:PRO:O	3:A:46:ALA:HB3	0.69	1.86	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:PHE:CE2	3:A:33:ILE:CD1	0.69	2.76	17	4
3:A:44:PHE:CE1	3:A:47:TRP:CB	0.69	2.76	19	1
1:B:257:DT:H73	3:A:53:HIS:ND1	0.69	2.03	6	2
3:A:39:TYR:CE2	3:A:40:TYR:CE1	0.69	2.80	6	2
1:B:255:DA:H2"	1:B:256:DA:OP2	0.68	1.87	19	4
3:A:8:TYR:O	3:A:12:ILE:HD13	0.68	1.87	14	3
1:B:250:DC:H2'	1:B:251:DT:H72	0.68	1.65	6	4
3:A:75:ASN:C	3:A:76:TYR:CD1	0.67	2.66	6	10
3:A:26:LEU:CD2	3:A:55:LEU:HD23	0.67	2.18	6	1
3:A:15:ALA:HB1	3:A:29:ILE:HD11	0.67	1.66	1	2
3:A:11:LEU:HD22	3:A:37:PHE:CZ	0.67	2.23	16	2
3:A:45:PRO:O	3:A:46:ALA:HB2	0.67	1.89	20	8
2:C:354:DG:C8	3:A:52:ARG:NH1	0.67	2.63	19	1
1:B:259:DA:H1'	1:B:260:DC:H4'	0.67	1.67	13	1
3:A:24:LEU:HD23	3:A:29:ILE:HD11	0.67	1.65	15	1
2:C:357:DA:N6	3:A:53:HIS:CD2	0.66	2.63	12	9
3:A:43:LYS:O	3:A:45:PRO:N	0.66	2.28	17	1
2:C:358:DT:C4'	2:C:359:DT:OP1	0.66	2.42	5	2
1:B:257:DT:C2	1:B:258:DA:N7	0.66	2.64	13	9
1:B:257:DT:H72	3:A:50:SER:HA	0.66	1.67	18	3
3:A:24:LEU:HD12	3:A:29:ILE:HG12	0.66	1.66	14	1
3:A:75:ASN:O	3:A:76:TYR:CD1	0.66	2.49	20	8
3:A:46:ALA:HB1	3:A:49:ASN:ND2	0.66	2.05	5	1
1:B:257:DT:H73	3:A:53:HIS:CD2	0.66	2.25	19	4
3:A:53:HIS:CE1	3:A:57:LEU:CD2	0.66	2.79	13	1
3:A:43:LYS:C	3:A:45:PRO:HD3	0.65	2.10	6	2
3:A:8:TYR:CZ	3:A:50:SER:CB	0.65	2.79	18	1
2:C:355:DT:H72	3:A:52:ARG:CZ	0.65	2.21	11	2
3:A:16:ILE:HD12	3:A:79:LEU:CD1	0.65	2.21	11	1
1:B:255:DA:C2'	1:B:256:DA:OP2	0.65	2.45	19	1
1:B:249:DG:O4'	1:B:250:DC:C6	0.65	2.49	20	1
1:B:256:DA:C8	1:B:257:DT:H72	0.65	2.27	2	6
3:A:8:TYR:O	3:A:12:ILE:HD12	0.65	1.92	4	3
2:C:359:DT:H2'	2:C:360:DT:H72	0.65	1.69	17	6
3:A:79:LEU:HD11	3:A:83:SER:CB	0.64	2.22	1	2
1:B:256:DA:N7	3:A:53:HIS:CE1	0.64	2.65	18	3
1:B:257:DT:O4	3:A:53:HIS:CD2	0.64	2.51	18	6
3:A:61:PHE:CD2	3:A:79:LEU:HD12	0.64	2.26	7	8
3:A:11:LEU:CD2	3:A:37:PHE:CE1	0.64	2.81	10	2
3:A:39:TYR:CE2	3:A:40:TYR:CD1	0.64	2.86	14	1
2:C:358:DT:H4'	2:C:359:DT:OP1	0.64	1.92	18	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:67:GLU:N	3:A:68:PRO:CD	0.64	2.60	8	1
3:A:55:LEU:O	3:A:61:PHE:CE2	0.64	2.50	9	6
3:A:8:TYR:CZ	3:A:47:TRP:CZ2	0.64	2.85	19	1
2:C:357:DA:N6	3:A:53:HIS:CE1	0.63	2.66	5	5
1:B:257:DT:H71	3:A:53:HIS:CD2	0.63	2.28	1	2
3:A:61:PHE:HD2	3:A:79:LEU:HD12	0.63	1.51	16	9
3:A:55:LEU:HD22	3:A:61:PHE:CZ	0.63	2.28	14	8
1:B:257:DT:O4	3:A:53:HIS:CG	0.63	2.52	19	17
3:A:37:PHE:CB	3:A:40:TYR:CD2	0.63	2.81	1	5
3:A:16:ILE:HD11	3:A:55:LEU:HD11	0.63	1.70	17	2
3:A:8:TYR:OH	3:A:47:TRP:CZ2	0.63	2.52	19	2
3:A:39:TYR:CD1	3:A:40:TYR:N	0.63	2.67	2	4
3:A:16:ILE:HD12	3:A:24:LEU:HD22	0.62	1.71	1	1
2:C:358:DT:H2'	2:C:359:DT:H72	0.62	1.71	17	4
3:A:13:THR:HG21	3:A:87:PHE:CZ	0.62	2.29	13	2
2:C:363:DA:C4'	2:C:364:DG:OP1	0.62	2.47	10	19
3:A:39:TYR:CD1	3:A:39:TYR:C	0.62	2.73	6	3
2:C:352:DT:H4'	2:C:353:DT:OP1	0.62	1.95	2	1
3:A:51:ILE:HD13	3:A:51:ILE:O	0.62	1.94	8	1
3:A:71:PRO:O	3:A:72:GLY:C	0.62	2.37	20	3
2:C:363:DA:O4'	2:C:364:DG:OP1	0.62	2.17	10	19
3:A:16:ILE:CD1	3:A:79:LEU:HD13	0.62	2.25	7	1
3:A:13:THR:CG2	3:A:87:PHE:CE1	0.62	2.80	12	1
1:B:257:DT:C2	1:B:258:DA:C8	0.62	2.88	10	10
3:A:75:ASN:ND2	3:A:77:TRP:CD1	0.62	2.68	6	2
3:A:15:ALA:O	3:A:24:LEU:HD13	0.61	1.95	14	1
3:A:55:LEU:O	3:A:61:PHE:CZ	0.61	2.53	4	17
1:B:257:DT:O4	3:A:53:HIS:CE1	0.61	2.53	20	3
2:C:352:DT:H2'	2:C:353:DT:H72	0.61	1.72	2	2
3:A:44:PHE:CE1	3:A:46:ALA:O	0.61	2.53	12	2
3:A:44:PHE:CZ	3:A:47:TRP:CE2	0.61	2.88	16	1
3:A:11:LEU:HD22	3:A:37:PHE:CE2	0.61	2.31	3	2
3:A:62:VAL:HG23	3:A:78:THR:HB	0.61	1.73	15	3
3:A:46:ALA:HB1	3:A:49:ASN:HD22	0.61	1.54	5	1
3:A:26:LEU:HD11	3:A:52:ARG:CZ	0.61	2.26	15	1
1:B:254:DA:H2"	1:B:255:DA:OP2	0.60	1.96	17	1
3:A:43:LYS:O	3:A:44:PHE:C	0.60	2.38	14	11
2:C:354:DG:OP2	3:A:77:TRP:CZ2	0.60	2.55	4	8
3:A:59:ASP:O	3:A:60:CYS:CB	0.60	2.49	5	12
3:A:40:TYR:CD1	3:A:47:TRP:CZ2	0.60	2.89	9	2
1:B:261:DA:C2	2:C:354:DG:C2	0.60	2.89	10	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:359:DT:O4'	2:C:359:DT:O3'	0.60	2.10	18	4
3:A:8:TYR:HE2	3:A:12:ILE:HD11	0.60	1.55	6	2
3:A:11:LEU:HD11	3:A:37:PHE:CE2	0.60	2.32	12	2
3:A:45:PRO:O	3:A:46:ALA:CB	0.59	2.49	1	4
3:A:59:ASP:CB	3:A:61:PHE:CD2	0.59	2.84	19	11
3:A:44:PHE:CZ	3:A:46:ALA:O	0.59	2.55	12	2
3:A:8:TYR:CE1	3:A:51:ILE:HG22	0.59	2.32	6	1
1:B:249:DG:C4'	1:B:250:DC:OP1	0.59	2.49	5	3
3:A:64:ILE:HG21	3:A:76:TYR:HD2	0.59	1.58	20	2
2:C:355:DT:C6	2:C:356:DT:H72	0.59	2.33	7	3
2:C:355:DT:H2'	2:C:356:DT:H72	0.59	1.75	10	3
1:B:255:DA:C1'	1:B:256:DA:O5'	0.59	2.51	11	12
2:C:357:DA:H4'	2:C:358:DT:OP1	0.59	1.97	11	5
1:B:256:DA:OP1	3:A:7:SER:HA	0.59	1.97	19	1
3:A:79:LEU:HD11	3:A:83:SER:HB3	0.58	1.75	1	2
1:B:256:DA:OP2	3:A:7:SER:CB	0.58	2.51	8	6
3:A:11:LEU:HD22	3:A:33:ILE:HG23	0.58	1.75	5	1
3:A:49:ASN:OD1	3:A:50:SER:N	0.58	2.36	11	4
2:C:357:DA:C8	2:C:358:DT:H72	0.58	2.33	15	6
2:C:356:DT:C7	3:A:52:ARG:NH2	0.58	2.66	17	2
3:A:44:PHE:CE2	3:A:47:TRP:CB	0.58	2.87	6	3
3:A:79:LEU:HD21	3:A:83:SER:HB3	0.58	1.75	14	2
3:A:59:ASP:HB2	3:A:61:PHE:CE2	0.58	2.33	19	10
3:A:11:LEU:HB3	3:A:33:ILE:HD12	0.58	1.75	5	1
3:A:44:PHE:CZ	3:A:47:TRP:HB2	0.58	2.33	6	4
3:A:40:TYR:CD1	3:A:47:TRP:CH2	0.58	2.90	9	1
3:A:79:LEU:HD23	3:A:80:ASP:N	0.58	2.13	9	3
2:C:357:DA:H2"	2:C:358:DT:OP2	0.58	1.96	15	1
3:A:16:ILE:CD1	3:A:24:LEU:HD22	0.58	2.28	1	1
3:A:16:ILE:HD12	3:A:24:LEU:HG	0.58	1.73	19	1
3:A:55:LEU:HD23	3:A:77:TRP:CZ3	0.58	2.34	17	2
3:A:86:MET:HE1	3:A:87:PHE:CZ	0.58	2.33	11	1
2:C:356:DT:C7	3:A:57:LEU:HD11	0.58	2.27	14	1
2:C:360:DT:C6	2:C:360:DT:H5'	0.58	2.33	15	1
2:C:359:DT:O4'	2:C:360:DT:OP1	0.57	2.22	2	3
3:A:51:ILE:O	3:A:55:LEU:N	0.57	2.36	7	10
3:A:8:TYR:CE1	3:A:50:SER:CB	0.57	2.87	18	2
1:B:257:DT:O2	1:B:258:DA:C8	0.57	2.58	10	3
3:A:44:PHE:CE1	3:A:47:TRP:CE2	0.57	2.91	16	1
1:B:250:DC:H4'	1:B:251:DT:OP1	0.57	1.97	6	3
3:A:44:PHE:CD1	3:A:47:TRP:HB2	0.57	2.34	19	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:355:DT:H72	3:A:52:ARG:CD	0.57	2.30	17	2
1:B:256:DA:H2"	3:A:8:TYR:CE2	0.57	2.34	4	2
3:A:44:PHE:CE2	3:A:47:TRP:HB2	0.57	2.34	6	3
3:A:59:ASP:CB	3:A:61:PHE:CE2	0.57	2.87	12	5
2:C:352:DT:C6	2:C:353:DT:H72	0.57	2.35	7	7
3:A:11:LEU:HD21	3:A:37:PHE:CE1	0.57	2.35	10	2
3:A:44:PHE:CG	3:A:47:TRP:NE1	0.57	2.73	16	1
3:A:52:ARG:NH1	3:A:56:SER:CB	0.56	2.68	4	2
3:A:9:ILE:C	3:A:9:ILE:HD12	0.56	2.20	20	1
3:A:51:ILE:O	3:A:55:LEU:HB2	0.56	2.00	5	9
1:B:257:DT:H2"	1:B:258:DA:OP2	0.56	2.00	13	1
3:A:33:ILE:CG2	3:A:47:TRP:CZ3	0.56	2.87	18	1
3:A:79:LEU:CD2	3:A:80:ASP:O	0.56	2.54	5	11
3:A:56:SER:HA	3:A:61:PHE:CE1	0.56	2.35	16	10
3:A:17:LEU:HD21	3:A:84:GLU:HB2	0.56	1.78	19	1
2:C:363:DA:C1'	2:C:364:DG:OP1	0.56	2.54	6	19
3:A:52:ARG:CZ	3:A:56:SER:OG	0.56	2.53	4	1
3:A:51:ILE:HG13	3:A:52:ARG:N	0.56	2.16	14	3
3:A:75:ASN:C	3:A:76:TYR:CG	0.56	2.79	18	6
3:A:24:LEU:CD1	3:A:29:ILE:HD13	0.56	2.31	13	1
3:A:33:ILE:HG21	3:A:47:TRP:HZ3	0.56	1.60	7	2
3:A:37:PHE:HB2	3:A:40:TYR:CD2	0.56	2.34	1	5
3:A:57:LEU:O	3:A:58:ASN:CB	0.56	2.53	9	11
3:A:63:LYS:HG2	3:A:77:TRP:CE3	0.56	2.35	3	8
3:A:24:LEU:CD2	3:A:29:ILE:HD11	0.56	2.30	4	1
3:A:64:ILE:HG21	3:A:76:TYR:CD2	0.56	2.36	5	4
3:A:9:ILE:HD11	3:A:58:ASN:CG	0.56	2.21	17	1
3:A:47:TRP:CZ3	3:A:51:ILE:HD11	0.56	2.36	1	2
3:A:59:ASP:HB3	3:A:61:PHE:CD2	0.56	2.35	12	4
3:A:76:TYR:CD1	3:A:76:TYR:N	0.56	2.74	6	1
1:B:256:DA:H1'	1:B:257:DT:H4'	0.56	1.78	13	4
3:A:33:ILE:HG23	3:A:37:PHE:CD1	0.55	2.36	14	1
3:A:11:LEU:CD2	3:A:37:PHE:CZ	0.55	2.88	10	2
3:A:25:THR:CG2	3:A:75:ASN:OD1	0.55	2.54	16	2
1:B:256:DA:P	3:A:7:SER:HA	0.55	2.41	13	2
3:A:8:TYR:CE2	3:A:50:SER:HB3	0.55	2.37	18	5
3:A:27:SER:CB	3:A:73:LYS:O	0.55	2.54	2	3
3:A:11:LEU:HD23	3:A:33:ILE:CG2	0.55	2.31	4	1
1:B:254:DA:C2'	1:B:255:DA:O5'	0.55	2.55	20	18
2:C:357:DA:H2'	2:C:358:DT:H72	0.55	1.78	6	5
3:A:53:HIS:O	3:A:57:LEU:CB	0.55	2.55	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:THR:CG2	3:A:75:ASN:O	0.55	2.54	20	3
1:B:250:DC:C6	1:B:251:DT:H72	0.55	2.37	12	17
3:A:26:LEU:HB2	3:A:77:TRP:CE2	0.55	2.37	11	12
2:C:352:DT:O2	3:A:66:ARG:CG	0.55	2.55	4	2
3:A:47:TRP:O	3:A:51:ILE:N	0.55	2.28	5	2
3:A:8:TYR:CD2	3:A:51:ILE:HA	0.55	2.36	6	1
3:A:51:ILE:CG2	3:A:52:ARG:N	0.55	2.70	19	5
3:A:38:PRO:O	3:A:42:GLU:N	0.55	2.40	17	1
1:B:259:DA:N7	3:A:49:ASN:ND2	0.55	2.55	16	11
2:C:359:DT:C1'	2:C:360:DT:OP1	0.55	2.55	6	3
3:A:24:LEU:HD12	3:A:29:ILE:HD11	0.55	1.78	9	1
2:C:354:DG:N7	3:A:52:ARG:NH1	0.54	2.55	14	4
3:A:17:LEU:HD11	3:A:87:PHE:CD2	0.54	2.37	1	1
1:B:262:DA:C8	1:B:263:DT:H72	0.54	2.37	12	9
3:A:65:PRO:O	3:A:67:GLU:N	0.54	2.40	2	7
2:C:351:DA:C2'	2:C:352:DT:H72	0.54	2.31	2	2
2:C:354:DG:OP2	3:A:77:TRP:NE1	0.54	2.40	2	6
3:A:37:PHE:CG	3:A:40:TYR:CE2	0.54	2.95	1	3
3:A:49:ASN:O	3:A:53:HIS:CB	0.54	2.55	9	6
3:A:37:PHE:CD1	3:A:37:PHE:N	0.54	2.76	15	4
3:A:26:LEU:HD22	3:A:26:LEU:O	0.54	2.03	16	1
3:A:44:PHE:O	3:A:47:TRP:CD1	0.54	2.60	12	2
2:C:359:DT:C2'	2:C:360:DT:H71	0.54	2.33	1	1
3:A:12:ILE:HG23	3:A:55:LEU:HD23	0.54	1.79	12	1
3:A:48:GLN:CG	3:A:52:ARG:NH2	0.54	2.71	1	2
3:A:8:TYR:CZ	3:A:50:SER:HB3	0.54	2.37	18	3
1:B:258:DA:N1	2:C:357:DA:C6	0.54	2.75	3	2
3:A:61:PHE:CE1	3:A:77:TRP:CE3	0.54	2.96	7	1
3:A:33:ILE:HG21	3:A:47:TRP:CE3	0.54	2.36	18	1
3:A:65:PRO:O	3:A:66:ARG:C	0.54	2.43	16	7
2:C:354:DG:C4	2:C:355:DT:C5	0.54	2.96	4	5
2:C:359:DT:O4'	2:C:359:DT:C5'	0.54	2.55	18	1
3:A:33:ILE:HG23	3:A:37:PHE:CE1	0.54	2.38	7	2
2:C:354:DG:N7	3:A:52:ARG:NH2	0.54	2.55	6	2
3:A:59:ASP:HB2	3:A:61:PHE:CD2	0.54	2.38	4	5
2:C:351:DA:C8	2:C:352:DT:H72	0.54	2.37	4	5
3:A:64:ILE:CG2	3:A:76:TYR:O	0.54	2.55	18	3
3:A:53:HIS:O	3:A:57:LEU:N	0.53	2.41	7	10
1:B:254:DA:C1'	1:B:255:DA:O5'	0.53	2.56	8	16
2:C:354:DG:OP1	3:A:77:TRP:NE1	0.53	2.41	10	4
3:A:8:TYR:OH	3:A:47:TRP:CE2	0.53	2.61	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:258:DA:N1	2:C:357:DA:N1	0.53	2.56	3	8
1:B:256:DA:OP2	3:A:9:ILE:HG23	0.53	2.03	2	1
1:B:257:DT:C2	1:B:258:DA:C5	0.53	2.96	20	6
3:A:47:TRP:O	3:A:51:ILE:HG22	0.53	2.03	16	3
2:C:359:DT:H4'	2:C:360:DT:OP1	0.53	2.03	6	2
3:A:21:GLN:O	3:A:22:LYS:C	0.53	2.46	9	5
3:A:70:ASN:N	3:A:70:ASN:ND2	0.53	2.57	14	4
1:B:255:DA:H1'	1:B:256:DA:OP2	0.53	2.03	19	1
3:A:15:ALA:HB2	3:A:32:PHE:HE2	0.53	1.57	1	4
3:A:19:SER:OG	3:A:24:LEU:HD13	0.53	2.04	11	2
3:A:24:LEU:O	3:A:77:TRP:N	0.53	2.40	5	9
3:A:15:ALA:O	3:A:18:GLN:CG	0.53	2.56	11	7
3:A:12:ILE:HG13	3:A:55:LEU:HD13	0.53	1.79	17	1
3:A:79:LEU:CD1	3:A:80:ASP:O	0.53	2.55	19	1
3:A:44:PHE:HA	3:A:47:TRP:CD1	0.53	2.39	20	6
1:B:250:DC:C2'	1:B:251:DT:H72	0.53	2.33	19	6
3:A:13:THR:O	3:A:17:LEU:HD12	0.53	2.03	9	1
3:A:8:TYR:CE1	3:A:47:TRP:CZ3	0.53	2.97	13	1
3:A:24:LEU:HD12	3:A:29:ILE:HD13	0.53	1.81	13	1
3:A:44:PHE:CE1	3:A:47:TRP:HB2	0.53	2.38	7	7
3:A:29:ILE:HG22	3:A:30:CYS:N	0.53	2.19	11	5
3:A:36:ARG:HB2	3:A:37:PHE:CE1	0.53	2.38	15	3
3:A:8:TYR:CE1	3:A:50:SER:HB2	0.53	2.39	18	1
3:A:32:PHE:CE2	3:A:33:ILE:HG13	0.53	2.39	4	6
1:B:257:DT:C2'	1:B:258:DA:O5'	0.53	2.57	11	1
3:A:44:PHE:CE2	3:A:47:TRP:CZ2	0.53	2.97	16	1
3:A:15:ALA:HB1	3:A:29:ILE:CD1	0.53	2.34	1	1
3:A:32:PHE:C	3:A:32:PHE:CD1	0.53	2.82	7	2
3:A:63:LYS:HG2	3:A:77:TRP:CZ3	0.53	2.39	14	3
3:A:12:ILE:HG23	3:A:55:LEU:HD13	0.53	1.81	8	1
2:C:355:DT:H72	3:A:52:ARG:NH2	0.53	2.19	11	1
3:A:75:ASN:CG	3:A:76:TYR:N	0.53	2.61	3	1
3:A:8:TYR:CZ	3:A:51:ILE:HG12	0.53	2.39	5	1
3:A:75:ASN:N	3:A:75:ASN:OD1	0.53	2.40	9	3
3:A:16:ILE:HD13	3:A:24:LEU:CD2	0.53	2.34	11	2
3:A:15:ALA:HB1	3:A:29:ILE:CG1	0.53	2.33	18	1
3:A:64:ILE:HG12	3:A:76:TYR:CB	0.52	2.34	1	1
3:A:44:PHE:O	3:A:47:TRP:HD1	0.52	1.87	12	2
3:A:56:SER:HA	3:A:61:PHE:CZ	0.52	2.39	8	6
1:B:259:DA:C1'	1:B:260:DC:O5'	0.52	2.56	13	4
1:B:258:DA:C2	1:B:259:DA:C5	0.52	2.97	14	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:61:PHE:HB2	3:A:78:THR:O	0.52	2.03	9	7
3:A:51:ILE:CG1	3:A:52:ARG:N	0.52	2.72	6	3
3:A:11:LEU:HD13	3:A:33:ILE:HD13	0.52	1.82	8	1
2:C:359:DT:C6	2:C:360:DT:H72	0.52	2.40	20	7
2:C:357:DA:N6	3:A:53:HIS:ND1	0.52	2.57	5	3
3:A:44:PHE:CD2	3:A:47:TRP:NE1	0.52	2.78	3	2
3:A:44:PHE:CZ	3:A:47:TRP:CB	0.52	2.92	6	2
3:A:55:LEU:HG	3:A:77:TRP:CZ3	0.52	2.40	7	5
2:C:354:DG:OP2	3:A:77:TRP:CE2	0.52	2.63	4	4
3:A:8:TYR:CD2	3:A:12:ILE:HG12	0.52	2.40	6	2
3:A:12:ILE:CG2	3:A:55:LEU:HD13	0.52	2.35	8	1
1:B:249:DG:O4'	1:B:249:DG:O5'	0.52	2.28	7	1
3:A:55:LEU:HD13	3:A:77:TRP:CZ3	0.52	2.39	11	3
3:A:8:TYR:CE2	3:A:50:SER:CB	0.52	2.93	16	1
3:A:13:THR:CB	3:A:87:PHE:CZ	0.52	2.93	1	2
1:B:256:DA:C2'	1:B:257:DT:O5'	0.52	2.58	20	4
3:A:57:LEU:O	3:A:58:ASN:CG	0.52	2.49	13	6
2:C:357:DA:N6	3:A:53:HIS:NE2	0.52	2.58	7	3
3:A:44:PHE:CZ	3:A:47:TRP:HB3	0.52	2.40	19	1
3:A:49:ASN:OD1	3:A:49:ASN:C	0.51	2.48	11	1
3:A:13:THR:HB	3:A:87:PHE:CE1	0.51	2.40	20	1
3:A:8:TYR:O	3:A:12:ILE:CD1	0.51	2.58	14	5
3:A:44:PHE:CE1	3:A:47:TRP:CG	0.51	2.98	19	1
2:C:357:DA:C2'	2:C:358:DT:H71	0.51	2.35	20	1
3:A:46:ALA:O	3:A:50:SER:CB	0.51	2.57	14	3
3:A:83:SER:O	3:A:87:PHE:CD2	0.51	2.63	7	2
1:B:250:DC:H5"	1:B:250:DC:C6	0.51	2.41	19	1
3:A:41:ARG:HA	3:A:44:PHE:CD1	0.51	2.40	19	1
3:A:13:THR:O	3:A:16:ILE:HG22	0.51	2.06	19	2
3:A:11:LEU:HD22	3:A:37:PHE:HE2	0.51	1.63	3	1
3:A:8:TYR:O	3:A:11:LEU:N	0.51	2.44	11	7
3:A:7:SER:O	3:A:11:LEU:HD23	0.51	2.06	11	1
3:A:59:ASP:C	3:A:60:CYS:SG	0.51	2.89	11	1
1:B:257:DT:C7	3:A:54:ASN:OD1	0.51	2.58	14	1
3:A:63:LYS:HD3	3:A:77:TRP:CZ3	0.51	2.40	20	1
3:A:26:LEU:C	3:A:26:LEU:HD13	0.51	2.27	6	3
3:A:26:LEU:C	3:A:26:LEU:CD2	0.51	2.78	11	1
3:A:16:ILE:HD12	3:A:24:LEU:CD2	0.51	2.23	14	1
3:A:11:LEU:HD11	3:A:37:PHE:CE1	0.51	2.40	18	2
2:C:355:DT:C2	2:C:356:DT:C5	0.51	2.99	7	5
3:A:12:ILE:HD13	3:A:12:ILE:N	0.51	2.19	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:256:DA:OP2	3:A:7:SER:HA	0.51	2.06	14	1
1:B:255:DA:C1'	1:B:256:DA:OP2	0.51	2.58	19	1
2:C:354:DG:C2'	2:C:355:DT:H71	0.51	2.36	11	12
1:B:259:DA:H4'	1:B:260:DC:OP1	0.51	2.04	4	2
3:A:8:TYR:CE2	3:A:51:ILE:HB	0.51	2.40	6	1
3:A:12:ILE:CG2	3:A:55:LEU:HD23	0.51	2.36	13	1
3:A:63:LYS:HE3	3:A:77:TRP:CH2	0.51	2.40	19	2
1:B:258:DA:C2'	1:B:259:DA:O5'	0.51	2.59	18	1
1:B:257:DT:N3	1:B:258:DA:C5	0.50	2.79	20	4
1:B:264:DA:C2'	1:B:265:DC:O5'	0.50	2.60	15	3
2:C:360:DT:H2'	2:C:361:DT:H72	0.50	1.82	15	1
3:A:44:PHE:CZ	3:A:47:TRP:CZ2	0.50	2.98	16	1
3:A:39:TYR:CD1	3:A:39:TYR:O	0.50	2.64	1	2
3:A:71:PRO:O	3:A:73:LYS:N	0.50	2.45	12	3
3:A:26:LEU:HB2	3:A:77:TRP:CZ2	0.50	2.40	15	2
3:A:56:SER:OG	3:A:57:LEU:HD22	0.50	2.06	3	1
1:B:249:DG:H4'	1:B:250:DC:C5'	0.50	2.35	4	4
1:B:255:DA:H1'	1:B:256:DA:O5'	0.50	2.05	13	4
1:B:259:DA:C2'	1:B:260:DC:O5'	0.50	2.59	13	4
3:A:44:PHE:CD1	3:A:47:TRP:HB3	0.50	2.41	4	1
3:A:32:PHE:O	3:A:32:PHE:CD1	0.50	2.64	5	4
3:A:44:PHE:CD1	3:A:47:TRP:CB	0.50	2.95	19	1
3:A:24:LEU:CD1	3:A:29:ILE:HD11	0.50	2.36	3	1
3:A:79:LEU:HD22	3:A:83:SER:HB2	0.50	1.81	10	1
3:A:24:LEU:HB2	3:A:29:ILE:HD11	0.50	1.82	20	1
3:A:15:ALA:O	3:A:18:GLN:HG3	0.50	2.06	14	8
3:A:61:PHE:C	3:A:61:PHE:CD1	0.50	2.85	2	1
3:A:48:GLN:O	3:A:52:ARG:HB2	0.50	2.07	12	4
3:A:43:LYS:O	3:A:45:PRO:CD	0.50	2.60	17	1
3:A:44:PHE:CE1	3:A:47:TRP:HB3	0.50	2.42	19	1
3:A:10:ALA:O	3:A:13:THR:OG1	0.50	2.25	6	6
2:C:363:DA:O4'	2:C:363:DA:O3'	0.50	2.25	9	1
3:A:63:LYS:HE3	3:A:77:TRP:CZ3	0.50	2.42	19	1
3:A:21:GLN:O	3:A:22:LYS:HB2	0.50	2.07	3	3
1:B:249:DG:H2"	1:B:250:DC:C5'	0.50	2.36	19	1
2:C:359:DT:C2'	2:C:360:DT:H72	0.50	2.37	18	2
3:A:8:TYR:CE2	3:A:12:ILE:CD1	0.50	2.94	6	1
3:A:40:TYR:CE2	3:A:47:TRP:CH2	0.50	2.99	7	2
2:C:354:DG:C2	2:C:355:DT:C4	0.49	3.00	4	1
3:A:67:GLU:HG3	3:A:76:TYR:CE2	0.49	2.41	12	1
3:A:40:TYR:O	3:A:47:TRP:NE1	0.49	2.45	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:354:DG:C8	2:C:355:DT:H72	0.49	2.41	15	2
2:C:353:DT:C2'	3:A:52:ARG:CZ	0.49	2.90	5	1
1:B:255:DA:C2'	1:B:256:DA:O5'	0.49	2.61	3	9
3:A:44:PHE:CG	3:A:47:TRP:HB3	0.49	2.42	4	1
1:B:258:DA:OP2	3:A:46:ALA:HB3	0.49	2.07	10	2
1:B:263:DT:C2'	1:B:264:DA:O5'	0.49	2.60	12	3
3:A:11:LEU:HD13	3:A:33:ILE:HG23	0.49	1.84	12	1
2:C:353:DT:OP1	3:A:74:GLY:N	0.49	2.45	13	1
1:B:250:DC:H2'	1:B:251:DT:C7	0.49	2.38	7	3
1:B:256:DA:C2'	3:A:7:SER:OG	0.49	2.60	6	1
2:C:355:DT:H71	3:A:52:ARG:HD3	0.49	1.83	19	1
3:A:51:ILE:O	3:A:55:LEU:CB	0.49	2.60	6	3
2:C:358:DT:C2'	2:C:359:DT:O5'	0.49	2.61	15	3
3:A:13:THR:HB	3:A:87:PHE:CZ	0.49	2.43	1	2
3:A:11:LEU:HD11	3:A:40:TYR:CE2	0.49	2.42	6	2
3:A:8:TYR:CE2	3:A:50:SER:HB2	0.49	2.43	7	1
1:B:258:DA:OP2	3:A:44:PHE:CE1	0.49	2.66	11	2
3:A:25:THR:HG23	3:A:75:ASN:CG	0.49	2.28	16	1
2:C:356:DT:C2	2:C:357:DA:N7	0.49	2.80	3	1
3:A:33:ILE:CG2	3:A:47:TRP:CH2	0.49	2.96	4	1
1:B:256:DA:OP2	3:A:9:ILE:CG2	0.49	2.61	6	1
1:B:254:DA:H1'	1:B:255:DA:H4'	0.49	1.84	15	3
3:A:12:ILE:HG21	3:A:55:LEU:HA	0.49	1.82	13	1
3:A:8:TYR:CD2	3:A:51:ILE:CG2	0.49	2.96	15	1
3:A:53:HIS:NE2	3:A:57:LEU:HD22	0.49	2.23	7	2
3:A:47:TRP:CE3	3:A:51:ILE:HD13	0.49	2.43	15	2
2:C:360:DT:H4'	2:C:361:DT:OP1	0.49	2.08	15	1
3:A:51:ILE:HG23	3:A:52:ARG:N	0.49	2.22	19	2
1:B:256:DA:P	3:A:7:SER:CB	0.49	3.01	6	1
3:A:11:LEU:HD13	3:A:14:MET:SD	0.49	2.48	11	1
3:A:16:ILE:CD1	3:A:55:LEU:HD11	0.49	2.37	17	1
1:B:257:DT:C7	3:A:53:HIS:CD2	0.49	2.96	1	2
3:A:37:PHE:CD2	3:A:40:TYR:CE2	0.49	3.01	1	3
3:A:19:SER:OG	3:A:24:LEU:CD1	0.49	2.61	19	2
3:A:26:LEU:CD1	3:A:52:ARG:CZ	0.49	2.91	15	1
1:B:263:DT:H2"	1:B:264:DA:OP2	0.49	2.08	17	1
2:C:360:DT:C6	2:C:361:DT:H72	0.48	2.43	10	5
3:A:44:PHE:HB3	3:A:47:TRP:CD1	0.48	2.42	4	1
3:A:13:THR:HA	3:A:87:PHE:CZ	0.48	2.43	10	2
3:A:67:GLU:CB	3:A:68:PRO:HD3	0.48	2.38	2	1
3:A:12:ILE:O	3:A:15:ALA:N	0.48	2.46	11	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:PHE:O	3:A:36:ARG:CG	0.48	2.61	18	1
3:A:29:ILE:HD13	3:A:55:LEU:HD11	0.48	1.82	19	1
3:A:61:PHE:CE1	3:A:77:TRP:CZ3	0.48	3.01	13	4
3:A:36:ARG:HB3	3:A:37:PHE:CD1	0.48	2.43	6	1
3:A:52:ARG:NH2	3:A:56:SER:OG	0.48	2.46	10	1
3:A:11:LEU:HD13	3:A:37:PHE:CE2	0.48	2.43	19	1
3:A:12:ILE:HD13	3:A:54:ASN:HB3	0.48	1.84	4	1
2:C:358:DT:H2'	2:C:359:DT:C7	0.48	2.38	15	4
3:A:24:LEU:HD12	3:A:29:ILE:CD1	0.48	2.38	7	1
3:A:36:ARG:C	3:A:37:PHE:CD1	0.48	2.86	8	1
3:A:39:TYR:CE1	3:A:40:TYR:CD1	0.48	3.01	11	1
3:A:13:THR:HG21	3:A:87:PHE:CG	0.48	2.43	14	1
2:C:352:DT:O5'	3:A:72:GLY:O	0.48	2.32	8	6
1:B:249:DG:C2'	1:B:250:DC:O5'	0.48	2.62	19	1
3:A:37:PHE:CG	3:A:40:TYR:CD2	0.48	3.02	1	3
3:A:45:PRO:HD2	3:A:47:TRP:CD1	0.48	2.44	1	3
2:C:353:DT:O3'	3:A:64:ILE:O	0.48	2.31	8	1
2:C:354:DG:OP1	3:A:64:ILE:N	0.48	2.46	11	1
1:B:253:DA:H2"	1:B:254:DA:OP2	0.48	2.08	10	1
1:B:264:DA:C1'	1:B:265:DC:O5'	0.48	2.62	15	3
2:C:354:DG:N9	2:C:355:DT:H71	0.48	2.23	11	1
3:A:26:LEU:HD23	3:A:26:LEU:O	0.48	2.08	11	1
3:A:9:ILE:HD12	3:A:10:ALA:N	0.48	2.23	12	2
3:A:70:ASN:N	3:A:70:ASN:OD1	0.48	2.46	1	2
1:B:256:DA:N6	3:A:53:HIS:CE1	0.48	2.82	5	3
3:A:24:LEU:O	3:A:25:THR:CG2	0.48	2.62	4	2
3:A:14:MET:O	3:A:18:GLN:CG	0.48	2.62	7	2
3:A:33:ILE:O	3:A:36:ARG:N	0.48	2.42	15	2
3:A:82:GLN:O	3:A:86:MET:CB	0.48	2.62	10	1
3:A:24:LEU:N	3:A:24:LEU:HD23	0.48	2.24	14	2
3:A:63:LYS:CE	3:A:77:TRP:CH2	0.48	2.97	19	1
3:A:63:LYS:HG2	3:A:77:TRP:CD2	0.48	2.44	9	5
3:A:64:ILE:CG1	3:A:76:TYR:O	0.48	2.62	19	2
3:A:65:PRO:O	3:A:67:GLU:OE1	0.48	2.30	4	1
3:A:8:TYR:CE1	3:A:33:ILE:HG13	0.48	2.44	6	1
3:A:11:LEU:HD13	3:A:33:ILE:HD12	0.48	1.86	12	1
1:B:249:DG:C1'	1:B:250:DC:OP1	0.47	2.62	1	3
2:C:349:DG:H2"	2:C:350:DT:OP2	0.47	2.10	12	14
3:A:18:GLN:O	3:A:20:PRO:HD3	0.47	2.09	9	2
3:A:62:VAL:O	3:A:78:THR:O	0.47	2.33	4	6
3:A:8:TYR:OH	3:A:44:PHE:CE2	0.47	2.60	10	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:257:DT:O4	3:A:53:HIS:ND1	0.47	2.47	13	5
3:A:8:TYR:CZ	3:A:51:ILE:HB	0.47	2.43	6	1
3:A:59:ASP:OD1	3:A:79:LEU:CD1	0.47	2.62	12	2
2:C:349:DG:C8	2:C:350:DT:H72	0.47	2.44	12	3
3:A:11:LEU:CD1	3:A:37:PHE:CE2	0.47	2.97	11	1
2:C:359:DT:C2'	2:C:360:DT:O5'	0.47	2.62	17	1
3:A:32:PHE:CE1	3:A:33:ILE:HG13	0.47	2.44	19	1
3:A:48:GLN:OE1	3:A:49:ASN:OD1	0.47	2.32	2	6
3:A:8:TYR:CE2	3:A:51:ILE:HG23	0.47	2.44	5	1
3:A:44:PHE:CD2	3:A:47:TRP:HB2	0.47	2.44	6	1
3:A:13:THR:O	3:A:17:LEU:CD1	0.47	2.62	9	1
3:A:63:LYS:HB3	3:A:77:TRP:CE2	0.47	2.44	14	2
2:C:352:DT:H2'	2:C:353:DT:C7	0.47	2.38	2	2
2:C:359:DT:C2'	2:C:360:DT:C7	0.47	2.93	18	2
3:A:13:THR:HG22	3:A:87:PHE:CE1	0.47	2.44	15	1
3:A:52:ARG:CD	3:A:52:ARG:C	0.47	2.83	17	1
3:A:52:ARG:CD	3:A:52:ARG:O	0.47	2.63	17	1
3:A:8:TYR:O	3:A:12:ILE:HB	0.47	2.09	8	1
1:B:250:DC:H2"	1:B:251:DT:OP2	0.47	2.07	16	2
2:C:358:DT:C6	2:C:359:DT:H72	0.47	2.45	19	1
1:B:258:DA:C2	2:C:357:DA:N1	0.47	2.82	11	3
3:A:15:ALA:CB	3:A:32:PHE:CE2	0.47	2.97	1	1
1:B:258:DA:N6	2:C:357:DA:N6	0.47	2.62	3	1
3:A:13:THR:HG22	3:A:87:PHE:CZ	0.47	2.45	4	2
3:A:24:LEU:HD12	3:A:29:ILE:CG1	0.47	2.39	14	1
2:C:351:DA:C2'	2:C:352:DT:H71	0.47	2.38	8	5
3:A:48:GLN:HG2	3:A:52:ARG:CZ	0.47	2.40	7	4
1:B:256:DA:N6	3:A:53:HIS:NE2	0.47	2.62	4	2
3:A:11:LEU:HG	3:A:37:PHE:CE1	0.47	2.45	4	1
3:A:52:ARG:O	3:A:52:ARG:HD2	0.47	2.09	10	4
3:A:11:LEU:O	3:A:14:MET:CG	0.47	2.62	11	2
1:B:257:DT:C2'	1:B:258:DA:OP2	0.47	2.62	13	1
3:A:8:TYR:CD2	3:A:51:ILE:HG22	0.47	2.44	15	1
3:A:48:GLN:CD	3:A:49:ASN:OD1	0.47	2.53	10	5
3:A:36:ARG:HB3	3:A:37:PHE:CE1	0.47	2.44	6	3
1:B:256:DA:H2"	1:B:257:DT:O5'	0.47	2.10	20	3
3:A:40:TYR:O	3:A:44:PHE:CB	0.47	2.62	10	1
3:A:15:ALA:HB1	3:A:29:ILE:HG13	0.47	1.87	18	1
3:A:15:ALA:HB2	3:A:32:PHE:CE1	0.47	2.45	19	1
2:C:356:DT:H72	3:A:52:ARG:NH2	0.47	2.25	4	1
3:A:75:ASN:ND2	3:A:77:TRP:NE1	0.47	2.63	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:13:THR:HG21	3:A:87:PHE:HE1	0.47	1.62	12	1
3:A:81:PRO:O	3:A:82:GLN:CB	0.47	2.63	6	8
3:A:48:GLN:NE2	3:A:48:GLN:C	0.47	2.68	6	1
3:A:8:TYR:OH	3:A:44:PHE:CZ	0.47	2.66	10	1
3:A:9:ILE:HG13	3:A:10:ALA:N	0.47	2.24	13	2
3:A:67:GLU:CB	3:A:68:PRO:CD	0.46	2.93	7	1
3:A:32:PHE:CE1	3:A:36:ARG:HG3	0.46	2.45	9	2
1:B:256:DA:OP2	3:A:7:SER:HB2	0.46	2.10	11	1
3:A:19:SER:CB	3:A:23:LYS:O	0.46	2.63	11	1
3:A:70:ASN:N	3:A:70:ASN:HD22	0.46	2.08	14	1
1:B:256:DA:C1'	1:B:257:DT:O5'	0.46	2.64	10	4
3:A:12:ILE:HG23	3:A:16:ILE:HD13	0.46	1.86	8	1
3:A:21:GLN:O	3:A:22:LYS:CB	0.46	2.63	17	1
3:A:46:ALA:O	3:A:50:SER:OG	0.46	2.32	20	1
3:A:7:SER:OG	3:A:8:TYR:N	0.46	2.49	12	2
3:A:40:TYR:CE2	3:A:47:TRP:CZ2	0.46	3.03	7	1
3:A:24:LEU:O	3:A:77:TRP:O	0.46	2.33	9	2
1:B:261:DA:C2'	1:B:262:DA:O5'	0.46	2.63	12	1
2:C:359:DT:H1'	2:C:360:DT:C5'	0.46	2.40	15	1
1:B:254:DA:H2"	1:B:255:DA:O5'	0.46	2.11	4	11
3:A:57:LEU:O	3:A:58:ASN:ND2	0.46	2.48	1	6
2:C:352:DT:C2'	2:C:353:DT:O5'	0.46	2.64	8	2
2:C:359:DT:C2	2:C:360:DT:C5	0.46	3.03	2	3
3:A:26:LEU:HD11	3:A:51:ILE:HD11	0.46	1.88	6	1
3:A:11:LEU:HB3	3:A:33:ILE:HD11	0.46	1.87	7	1
1:B:262:DA:H2'	1:B:263:DT:H72	0.46	1.87	12	2
2:C:351:DA:H2"	2:C:352:DT:H71	0.46	1.87	8	5
2:C:358:DT:C2'	2:C:359:DT:C7	0.46	2.94	2	2
3:A:48:GLN:NE2	3:A:49:ASN:OD1	0.46	2.49	4	4
1:B:253:DA:C2'	1:B:254:DA:O5'	0.46	2.62	19	2
3:A:8:TYR:OH	3:A:47:TRP:NE1	0.46	2.48	10	1
3:A:15:ALA:O	3:A:18:GLN:CB	0.46	2.63	11	1
3:A:59:ASP:O	3:A:60:CYS:SG	0.46	2.74	11	1
2:C:359:DT:H2'	2:C:360:DT:C7	0.46	2.39	17	3
3:A:69:GLY:C	3:A:70:ASN:OD1	0.46	2.54	16	1
3:A:11:LEU:CD1	3:A:37:PHE:CE1	0.46	2.99	18	2
3:A:26:LEU:HG	3:A:27:SER:N	0.46	2.26	1	4
2:C:354:DG:C4	2:C:355:DT:C7	0.46	2.99	11	2
2:C:352:DT:O4'	3:A:66:ARG:CD	0.46	2.63	9	1
3:A:16:ILE:HG13	3:A:24:LEU:HD11	0.46	1.86	4	1
1:B:257:DT:H3'	3:A:44:PHE:CZ	0.46	2.46	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:PHE:CE1	3:A:33:ILE:CD1	0.46	2.99	11	1
3:A:64:ILE:HB	3:A:76:TYR:O	0.46	2.11	11	1
1:B:254:DA:C4'	1:B:255:DA:OP1	0.46	2.64	13	2
1:B:254:DA:C2'	1:B:255:DA:OP2	0.46	2.63	17	1
3:A:33:ILE:HG23	3:A:37:PHE:CD2	0.46	2.46	19	1
2:C:352:DT:O3'	3:A:73:LYS:HA	0.45	2.11	2	2
3:A:9:ILE:HD13	3:A:9:ILE:O	0.45	2.11	7	1
3:A:8:TYR:O	3:A:12:ILE:HG12	0.45	2.11	8	2
3:A:8:TYR:HA	3:A:11:LEU:CG	0.45	2.41	8	1
1:B:257:DT:OP2	3:A:8:TYR:CE2	0.45	2.69	11	2
2:C:359:DT:H2'	2:C:360:DT:H71	0.45	1.88	1	1
3:A:39:TYR:CG	3:A:40:TYR:N	0.45	2.84	2	1
3:A:47:TRP:O	3:A:49:ASN:N	0.45	2.50	5	1
2:C:357:DA:H62	3:A:53:HIS:CD2	0.45	2.28	7	5
3:A:52:ARG:HG2	3:A:77:TRP:CH2	0.45	2.45	13	1
1:B:258:DA:N7	3:A:49:ASN:OD1	0.45	2.49	14	2
3:A:32:PHE:CD1	3:A:33:ILE:HG13	0.45	2.46	19	1
3:A:24:LEU:C	3:A:25:THR:HG23	0.45	2.32	17	2
3:A:25:THR:HG23	3:A:75:ASN:OD1	0.45	2.11	6	1
1:B:249:DG:O5'	1:B:249:DG:O3'	0.45	2.34	7	1
3:A:49:ASN:O	3:A:53:HIS:N	0.45	2.49	9	2
1:B:264:DA:H5'	3:A:66:ARG:CZ	0.45	2.41	16	1
1:B:258:DA:OP2	3:A:46:ALA:CB	0.45	2.64	19	1
1:B:249:DG:H4'	1:B:250:DC:OP1	0.45	2.11	5	3
2:C:357:DA:H2'	2:C:358:DT:C7	0.45	2.41	3	3
3:A:8:TYR:C	3:A:10:ALA:N	0.45	2.70	4	2
3:A:16:ILE:HD13	3:A:24:LEU:HD21	0.45	1.88	7	1
3:A:55:LEU:C	3:A:61:PHE:CZ	0.45	2.90	17	4
3:A:63:LYS:HB3	3:A:77:TRP:CD2	0.45	2.46	14	1
3:A:13:THR:HG22	3:A:17:LEU:HD22	0.45	1.88	2	1
3:A:25:THR:HG22	3:A:75:ASN:O	0.45	2.12	12	1
3:A:12:ILE:CG1	3:A:55:LEU:HD13	0.45	2.41	17	1
3:A:41:ARG:O	3:A:41:ARG:NH1	0.45	2.49	3	1
2:C:355:DT:H2'	2:C:356:DT:C7	0.45	2.42	8	2
3:A:11:LEU:HD11	3:A:37:PHE:CZ	0.45	2.47	20	2
1:B:251:DT:C6	1:B:252:DT:H72	0.45	2.47	13	7
2:C:357:DA:C2'	2:C:358:DT:O5'	0.45	2.65	3	1
1:B:257:DT:C7	3:A:50:SER:HA	0.45	2.42	5	1
1:B:258:DA:C2	1:B:259:DA:C6	0.45	3.05	14	1
3:A:26:LEU:CD1	3:A:52:ARG:NH2	0.45	2.75	15	1
3:A:70:ASN:N	3:A:71:PRO:HD3	0.45	2.27	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:65:PRO:HB2	3:A:66:ARG:NH2	0.44	2.27	3	1
3:A:32:PHE:CD1	3:A:32:PHE:O	0.44	2.71	2	1
3:A:70:ASN:CG	3:A:74:GLY:O	0.44	2.56	7	4
3:A:86:MET:HE3	3:A:87:PHE:CD2	0.44	2.47	5	1
3:A:11:LEU:HD21	3:A:37:PHE:CE2	0.44	2.46	12	1
2:C:355:DT:C7	3:A:52:ARG:HD3	0.44	2.43	19	1
3:A:64:ILE:HD12	3:A:65:PRO:O	0.44	2.13	19	1
3:A:55:LEU:O	3:A:55:LEU:HD12	0.44	2.12	2	1
1:B:250:DC:C2'	1:B:251:DT:O5'	0.44	2.65	17	3
2:C:354:DG:OP2	3:A:52:ARG:HD3	0.44	2.12	14	1
3:A:44:PHE:CE1	3:A:47:TRP:NE1	0.44	2.86	16	1
3:A:44:PHE:CE1	3:A:47:TRP:CD1	0.44	3.05	16	1
1:B:256:DA:OP2	3:A:7:SER:CA	0.44	2.65	1	2
1:B:255:DA:C4'	1:B:256:DA:OP1	0.44	2.64	9	2
2:C:354:DG:C5'	3:A:65:PRO:HB3	0.44	2.42	16	2
1:B:256:DA:H2"	1:B:257:DT:OP2	0.44	2.12	14	1
3:A:49:ASN:O	3:A:53:HIS:HB3	0.44	2.12	16	1
3:A:51:ILE:HG23	3:A:52:ARG:H	0.44	1.72	16	1
2:C:358:DT:C2'	2:C:359:DT:H72	0.44	2.43	2	2
2:C:354:DG:OP1	3:A:64:ILE:O	0.44	2.35	8	5
3:A:48:GLN:CG	3:A:52:ARG:CZ	0.44	2.96	6	1
2:C:352:DT:C5'	3:A:72:GLY:O	0.44	2.66	8	1
1:B:249:DG:H4'	1:B:250:DC:H5"	0.44	1.90	12	2
1:B:256:DA:C8	1:B:257:DT:H71	0.44	2.48	10	1
3:A:11:LEU:O	3:A:14:MET:HG2	0.44	2.13	19	1
3:A:24:LEU:HD22	3:A:29:ILE:HD11	0.44	1.89	4	1
2:C:354:DG:OP1	3:A:77:TRP:CE2	0.44	2.70	14	1
2:C:359:DT:C1'	2:C:360:DT:O5'	0.44	2.66	17	1
3:A:61:PHE:C	3:A:61:PHE:HD1	0.44	2.16	2	1
3:A:19:SER:OG	3:A:23:LYS:O	0.44	2.33	11	1
3:A:29:ILE:CG2	3:A:30:CYS:N	0.44	2.80	11	2
3:A:65:PRO:HB2	3:A:66:ARG:CZ	0.43	2.43	5	1
3:A:12:ILE:CD1	3:A:55:LEU:HD22	0.43	2.42	8	1
3:A:37:PHE:HB3	3:A:40:TYR:CG	0.43	2.49	11	1
3:A:61:PHE:CD1	3:A:61:PHE:N	0.43	2.82	16	1
3:A:53:HIS:ND1	3:A:54:ASN:N	0.43	2.66	20	1
3:A:47:TRP:C	3:A:51:ILE:HG23	0.43	2.32	6	1
3:A:37:PHE:HB2	3:A:40:TYR:HB2	0.43	1.89	14	1
3:A:46:ALA:O	3:A:50:SER:HB3	0.43	2.13	14	1
1:B:249:DG:C4	1:B:250:DC:C5	0.43	3.06	18	1
3:A:8:TYR:O	3:A:10:ALA:N	0.43	2.51	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:250:DC:H2"	1:B:251:DT:C7	0.43	2.43	8	2
3:A:13:THR:O	3:A:17:LEU:CD2	0.43	2.59	16	1
3:A:16:ILE:HG12	3:A:79:LEU:CD1	0.43	2.43	17	1
1:B:259:DA:H1'	1:B:260:DC:O5'	0.43	2.13	4	1
3:A:11:LEU:HD11	3:A:37:PHE:HE2	0.43	1.72	12	1
1:B:251:DT:C2'	1:B:252:DT:H72	0.43	2.44	13	1
3:A:12:ILE:CD1	3:A:51:ILE:CD1	0.43	2.95	16	1
3:A:9:ILE:CD1	3:A:58:ASN:OD1	0.43	2.62	18	1
3:A:52:ARG:NE	3:A:52:ARG:O	0.43	2.51	4	1
3:A:8:TYR:HE2	3:A:51:ILE:HG23	0.43	1.73	5	1
3:A:52:ARG:HG3	3:A:77:TRP:CH2	0.43	2.49	6	1
3:A:22:LYS:O	3:A:22:LYS:CG	0.43	2.65	9	1
1:B:262:DA:C2'	1:B:263:DT:H72	0.43	2.43	11	1
3:A:86:MET:CE	3:A:87:PHE:CZ	0.43	3.01	11	1
3:A:38:PRO:O	3:A:41:ARG:CG	0.43	2.67	14	1
3:A:52:ARG:CZ	3:A:56:SER:HB3	0.43	2.43	17	1
3:A:47:TRP:O	3:A:51:ILE:HB	0.43	2.14	18	1
3:A:37:PHE:CD2	3:A:40:TYR:CD2	0.43	3.06	1	1
3:A:64:ILE:HG12	3:A:76:TYR:HB2	0.43	1.89	1	1
3:A:11:LEU:HD23	3:A:33:ILE:HG23	0.43	1.90	4	1
3:A:8:TYR:CG	3:A:51:ILE:HG22	0.43	2.49	15	1
2:C:352:DT:C2'	2:C:353:DT:H72	0.43	2.43	16	1
3:A:13:THR:O	3:A:17:LEU:HD13	0.43	2.14	18	1
2:C:351:DA:C2'	2:C:352:DT:C7	0.43	2.96	2	1
3:A:16:ILE:CG2	3:A:79:LEU:HD13	0.43	2.35	9	1
3:A:13:THR:HG21	3:A:87:PHE:CD2	0.43	2.49	13	1
1:B:263:DT:H4'	1:B:264:DA:OP1	0.43	2.14	11	1
2:C:353:DT:H2"	2:C:354:DG:OP2	0.43	2.13	14	1
3:A:53:HIS:O	3:A:57:LEU:HB2	0.43	2.14	4	2
3:A:16:ILE:HD13	3:A:24:LEU:CD1	0.43	2.43	9	1
3:A:11:LEU:HD13	3:A:37:PHE:CZ	0.43	2.48	19	1
3:A:52:ARG:CG	3:A:53:HIS:N	0.43	2.82	19	1
3:A:70:ASN:ND2	3:A:74:GLY:O	0.43	2.52	5	2
3:A:8:TYR:O	3:A:9:ILE:C	0.43	2.58	18	5
1:B:256:DA:H4'	1:B:257:DT:OP1	0.43	2.14	13	1
3:A:43:LYS:O	3:A:45:PRO:HD3	0.43	2.14	16	1
3:A:18:GLN:C	3:A:20:PRO:HD3	0.43	2.34	17	2
1:B:250:DC:C2'	1:B:251:DT:C7	0.43	2.96	19	1
3:A:34:SER:CB	3:A:41:ARG:HB3	0.43	2.43	19	1
3:A:24:LEU:HD11	3:A:29:ILE:CD1	0.42	2.43	1	1
3:A:79:LEU:C	3:A:79:LEU:HD23	0.42	2.34	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:8:TYR:CD1	3:A:47:TRP:CH2	0.42	3.07	5	1
3:A:16:ILE:CD1	3:A:24:LEU:CD2	0.42	2.97	9	1
2:C:354:DG:H2"	3:A:52:ARG:NH1	0.42	2.28	16	1
2:C:356:DT:H71	3:A:52:ARG:NH2	0.42	2.28	17	1
1:B:249:DG:H1'	1:B:250:DC:C6	0.42	2.49	18	1
3:A:17:LEU:HD11	3:A:84:GLU:HB2	0.42	1.91	19	1
3:A:12:ILE:HG23	3:A:55:LEU:CD1	0.42	2.44	9	1
3:A:13:THR:HB	3:A:87:PHE:CE2	0.42	2.50	9	1
3:A:64:ILE:HD12	3:A:67:GLU:OE1	0.42	2.14	9	1
1:B:257:DT:O2	1:B:258:DA:N9	0.42	2.51	10	1
3:A:8:TYR:CD2	3:A:51:ILE:HD12	0.42	2.49	10	1
3:A:47:TRP:HA	3:A:47:TRP:CE3	0.42	2.49	13	1
2:C:352:DT:O2	3:A:66:ARG:HG3	0.42	2.13	4	1
3:A:55:LEU:HD12	3:A:61:PHE:CZ	0.42	2.49	6	1
3:A:64:ILE:HG21	3:A:76:TYR:HD1	0.42	1.75	6	1
1:B:255:DA:O4'	1:B:256:DA:OP1	0.42	2.37	7	1
3:A:15:ALA:O	3:A:18:GLN:HG2	0.42	2.14	11	2
1:B:257:DT:H1'	1:B:258:DA:C8	0.42	2.49	13	1
2:C:360:DT:C1'	2:C:361:DT:O5'	0.42	2.68	15	1
3:A:12:ILE:N	3:A:12:ILE:HD13	0.42	2.29	16	1
2:C:354:DG:N3	2:C:355:DT:C5	0.42	2.87	4	1
3:A:11:LEU:CD2	3:A:33:ILE:HG23	0.42	2.42	5	1
3:A:11:LEU:N	3:A:11:LEU:HD22	0.42	2.29	7	1
3:A:18:GLN:C	3:A:18:GLN:OE1	0.42	2.58	9	2
3:A:75:ASN:OD1	3:A:75:ASN:C	0.42	2.57	8	1
1:B:257:DT:C1'	1:B:258:DA:O5'	0.42	2.67	11	1
3:A:83:SER:O	3:A:86:MET:CG	0.42	2.68	20	1
1:B:265:DC:OP1	3:A:67:GLU:O	0.42	2.37	2	1
2:C:355:DT:C2'	2:C:356:DT:H71	0.42	2.45	9	1
1:B:263:DT:C1'	1:B:264:DA:O5'	0.42	2.68	11	1
3:A:81:PRO:O	3:A:82:GLN:CG	0.42	2.67	12	1
3:A:8:TYR:HB2	3:A:54:ASN:CG	0.42	2.35	7	2
3:A:8:TYR:CE2	3:A:51:ILE:HG12	0.42	2.50	5	1
3:A:13:THR:OG1	3:A:87:PHE:CZ	0.42	2.72	5	1
3:A:17:LEU:CD2	3:A:87:PHE:CE2	0.42	3.03	10	1
3:A:44:PHE:CG	3:A:47:TRP:HB2	0.42	2.50	19	1
3:A:9:ILE:HD13	3:A:58:ASN:OD1	0.42	2.15	5	1
3:A:47:TRP:O	3:A:48:GLN:C	0.42	2.57	5	1
3:A:8:TYR:CD2	3:A:12:ILE:CG1	0.42	3.02	6	1
2:C:360:DT:C2'	2:C:361:DT:H71	0.42	2.44	8	1
3:A:40:TYR:O	3:A:47:TRP:CD1	0.42	2.72	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:258:DA:C4	1:B:259:DA:N7	0.42	2.88	14	1
3:A:86:MET:HE1	3:A:87:PHE:CE2	0.42	2.50	15	1
2:C:359:DT:H2"	2:C:360:DT:O5'	0.42	2.15	17	1
3:A:57:LEU:O	3:A:58:ASN:HB2	0.42	2.13	17	2
3:A:76:TYR:C	3:A:77:TRP:HD1	0.42	2.18	18	1
3:A:75:ASN:O	3:A:76:TYR:CG	0.42	2.72	19	1
3:A:40:TYR:HB3	3:A:47:TRP:CH2	0.42	2.50	20	1
3:A:44:PHE:CD2	3:A:47:TRP:CD1	0.42	3.07	6	1
1:B:257:DT:O4	3:A:53:HIS:NE2	0.42	2.52	20	1
3:A:44:PHE:CE2	3:A:47:TRP:HB3	0.42	2.50	2	1
1:B:257:DT:H72	3:A:50:SER:O	0.42	2.14	14	2
3:A:11:LEU:CD1	3:A:40:TYR:CE2	0.42	3.03	6	1
3:A:48:GLN:O	3:A:52:ARG:HB3	0.42	2.15	10	1
1:B:258:DA:C4'	1:B:259:DA:OP1	0.42	2.67	13	1
2:C:355:DT:H72	3:A:52:ARG:HD3	0.42	1.92	17	1
3:A:22:LYS:CD	3:A:79:LEU:O	0.42	2.67	19	1
3:A:12:ILE:CD1	3:A:55:LEU:HG	0.42	2.45	5	1
3:A:34:SER:O	3:A:37:PHE:O	0.42	2.37	6	2
2:C:355:DT:C2'	2:C:356:DT:O5'	0.42	2.68	10	1
3:A:19:SER:OG	3:A:24:LEU:HD11	0.41	2.14	19	2
3:A:62:VAL:CG2	3:A:78:THR:HB	0.41	2.45	4	1
3:A:8:TYR:CZ	3:A:33:ILE:HG13	0.41	2.50	6	1
3:A:52:ARG:NH2	3:A:56:SER:HB3	0.41	2.30	16	2
3:A:47:TRP:HZ3	3:A:51:ILE:HD13	0.41	1.69	19	1
3:A:67:GLU:O	3:A:70:ASN:OD1	0.41	2.37	4	2
2:C:353:DT:H2"	3:A:52:ARG:CZ	0.41	2.44	5	1
2:C:353:DT:H2'	3:A:52:ARG:NH2	0.41	2.30	5	1
3:A:52:ARG:O	3:A:52:ARG:CD	0.41	2.69	10	1
2:C:354:DG:OP1	3:A:77:TRP:CZ2	0.41	2.73	14	1
1:B:258:DA:N7	3:A:49:ASN:HB2	0.41	2.30	18	1
1:B:256:DA:C4	1:B:257:DT:C5	0.41	3.09	19	1
3:A:9:ILE:HG22	3:A:54:ASN:CG	0.41	2.35	20	1
2:C:351:DA:C4	2:C:352:DT:C4	0.41	3.08	2	1
2:C:353:DT:O3'	3:A:65:PRO:HA	0.41	2.14	12	2
3:A:25:THR:O	3:A:29:ILE:N	0.41	2.49	4	2
3:A:50:SER:O	3:A:54:ASN:OD1	0.41	2.38	19	3
3:A:12:ILE:HG22	3:A:13:THR:N	0.41	2.31	1	1
1:B:251:DT:H2'	1:B:252:DT:H72	0.41	1.92	6	1
1:B:257:DT:H2"	1:B:258:DA:O5'	0.41	2.14	11	1
3:A:37:PHE:HB3	3:A:39:TYR:CE1	0.41	2.50	14	1
3:A:39:TYR:HE2	3:A:40:TYR:CE1	0.41	2.33	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:256:DA:P	3:A:7:SER:HB2	0.41	2.56	15	1
3:A:33:ILE:HD13	3:A:51:ILE:HD13	0.41	1.92	16	1
1:B:256:DA:OP2	3:A:7:SER:HB3	0.41	2.15	20	2
1:B:256:DA:OP2	3:A:7:SER:OG	0.41	2.30	9	2
3:A:47:TRP:C	3:A:49:ASN:N	0.41	2.72	5	1
3:A:12:ILE:HG23	3:A:55:LEU:CD2	0.41	2.44	12	1
3:A:14:MET:O	3:A:18:GLN:CB	0.41	2.68	15	1
1:B:255:DA:OP2	1:B:255:DA:C4'	0.41	2.69	17	1
3:A:55:LEU:HG	3:A:61:PHE:CZ	0.41	2.51	17	1
2:C:352:DT:C2'	2:C:353:DT:H71	0.41	2.45	3	1
3:A:16:ILE:HD13	3:A:24:LEU:HD11	0.41	1.93	5	1
3:A:67:GLU:CG	3:A:68:PRO:HD2	0.41	2.45	11	1
1:B:261:DA:H4'	1:B:262:DA:OP1	0.41	2.15	12	1
3:A:44:PHE:C	3:A:46:ALA:H	0.41	2.19	8	1
3:A:44:PHE:CG	3:A:47:TRP:CD1	0.41	3.09	10	1
1:B:261:DA:H3'	1:B:261:DA:OP2	0.41	2.16	12	1
3:A:44:PHE:CD1	3:A:47:TRP:CG	0.41	3.08	19	1
3:A:47:TRP:HA	3:A:51:ILE:HD13	0.41	1.92	20	1
3:A:12:ILE:HG23	3:A:55:LEU:HD12	0.41	1.93	10	1
3:A:86:MET:CE	3:A:87:PHE:CE2	0.41	3.03	11	1
3:A:59:ASP:OD1	3:A:79:LEU:HD11	0.41	2.15	12	1
3:A:21:GLN:O	3:A:22:LYS:HG3	0.41	2.16	16	1
3:A:38:PRO:O	3:A:41:ARG:HG3	0.41	2.16	19	1
1:B:249:DG:O4'	1:B:250:DC:H5"	0.41	2.16	20	1
3:A:13:THR:O	3:A:17:LEU:HD22	0.41	2.16	2	1
3:A:33:ILE:HG22	3:A:47:TRP:CH2	0.41	2.50	4	1
3:A:52:ARG:NH1	3:A:56:SER:HB3	0.41	2.30	4	1
2:C:354:DG:OP1	3:A:63:LYS:CB	0.41	2.69	11	1
2:C:355:DT:C7	3:A:52:ARG:CZ	0.41	2.97	11	1
2:C:358:DT:C1'	2:C:359:DT:O5'	0.41	2.69	17	2
1:B:258:DA:C6	2:C:357:DA:N1	0.41	2.88	13	1
3:A:55:LEU:O	3:A:59:ASP:OD1	0.41	2.38	17	1
3:A:49:ASN:HA	3:A:52:ARG:CD	0.41	2.45	19	1
2:C:353:DT:O2	3:A:66:ARG:NH2	0.41	2.54	4	1
2:C:353:DT:H2'	3:A:52:ARG:NH1	0.41	2.31	7	1
3:A:12:ILE:CG1	3:A:51:ILE:HD11	0.41	2.46	8	1
1:B:262:DA:H2"	1:B:263:DT:OP2	0.41	2.15	12	1
2:C:354:DG:C8	2:C:355:DT:C7	0.40	3.04	10	1
3:A:14:MET:HG3	3:A:15:ALA:N	0.40	2.30	10	1
3:A:40:TYR:O	3:A:44:PHE:N	0.40	2.54	10	1
3:A:32:PHE:CD1	3:A:32:PHE:C	0.40	2.91	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:256:DA:OP2	1:B:256:DA:H2'	0.40	2.17	19	1
1:B:249:DG:O4'	1:B:250:DC:C5'	0.40	2.69	20	1
2:C:355:DT:OP2	2:C:355:DT:H3'	0.40	2.16	20	1
3:A:79:LEU:HD21	3:A:83:SER:HB2	0.40	1.93	5	1
3:A:12:ILE:HD11	3:A:51:ILE:HG13	0.40	1.92	9	1
1:B:255:DA:H2"	1:B:256:DA:O5'	0.40	2.16	10	1
3:A:17:LEU:HD21	3:A:87:PHE:CD2	0.40	2.51	10	1
3:A:17:LEU:O	3:A:20:PRO:HD3	0.40	2.16	18	1
3:A:51:ILE:HG22	3:A:55:LEU:HD12	0.40	1.92	18	1
2:C:354:DG:N7	3:A:52:ARG:CZ	0.40	2.85	19	1
1:B:258:DA:OP2	3:A:45:PRO:O	0.40	2.39	1	1
3:A:8:TYR:O	3:A:12:ILE:CB	0.40	2.70	8	1
3:A:82:GLN:O	3:A:82:GLN:CG	0.40	2.69	10	1
3:A:33:ILE:HG13	3:A:51:ILE:CD1	0.40	2.46	11	1
1:B:251:DT:C2'	1:B:252:DT:C7	0.40	2.99	13	1
3:A:8:TYR:CD2	3:A:50:SER:HB3	0.40	2.51	18	1
3:A:29:ILE:O	3:A:32:PHE:N	0.40	2.54	5	1
2:C:357:DA:H62	3:A:53:HIS:CE1	0.40	2.34	9	1
3:A:12:ILE:HD11	3:A:51:ILE:CG1	0.40	2.46	12	1
3:A:82:GLN:O	3:A:86:MET:SD	0.40	2.79	12	1
3:A:17:LEU:HD21	3:A:87:PHE:CG	0.40	2.51	20	1
3:A:70:ASN:OD1	3:A:70:ASN:N	0.40	2.54	20	1
3:A:24:LEU:N	3:A:77:TRP:O	0.40	2.54	2	1
1:B:256:DA:O5'	3:A:7:SER:HB2	0.40	2.17	6	1
3:A:13:THR:OG1	3:A:87:PHE:CE1	0.40	2.59	11	1
3:A:9:ILE:HD12	3:A:9:ILE:C	0.40	2.37	12	1
3:A:8:TYR:CE1	3:A:47:TRP:HB2	0.40	2.52	16	1
3:A:26:LEU:HD23	3:A:75:ASN:ND2	0.40	2.31	19	1
3:A:46:ALA:O	3:A:50:SER:HB2	0.40	2.17	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	81/97 (84%)	62±2 (77±3%)	13±2 (16±2%)	6±1 (7±2%)	2 16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1620/1940 (84%)	1244 (77%)	260 (16%)	116 (7%)	2 16

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	58	ASN	20
3	A	82	GLN	17
3	A	46	ALA	14
3	A	66	ARG	14
3	A	60	CYS	13
3	A	69	GLY	11
3	A	22	LYS	6
3	A	23	LYS	6
3	A	21	GLN	4
3	A	71	PRO	3
3	A	72	GLY	3
3	A	25	THR	1
3	A	65	PRO	1
3	A	48	GLN	1
3	A	68	PRO	1
3	A	44	PHE	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	74/89 (83%)	53±4 (71±5%)	21±4 (29±5%)	2 18
All	All	1480/1780 (83%)	1051 (71%)	429 (29%)	2 18

All 61 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	32	PHE	19
3	A	63	LYS	18
3	A	61	PHE	16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
3	A	55	LEU	14
3	A	21	GLN	13
3	A	58	ASN	13
3	A	73	LYS	13
3	A	80	ASP	13
3	A	22	LYS	13
3	A	66	ARG	12
3	A	23	LYS	12
3	A	18	GLN	11
3	A	41	ARG	11
3	A	76	TYR	11
3	A	26	LEU	10
3	A	70	ASN	10
3	A	42	GLU	10
3	A	56	SER	10
3	A	29	ILE	9
3	A	57	LEU	9
3	A	87	PHE	9
3	A	24	LEU	9
3	A	52	ARG	9
3	A	43	LYS	8
3	A	49	ASN	8
3	A	79	LEU	8
3	A	67	GLU	8
3	A	40	TYR	8
3	A	60	CYS	8
3	A	82	GLN	7
3	A	31	GLU	7
3	A	48	GLN	7
3	A	84	GLU	7
3	A	9	ILE	6
3	A	59	ASP	6
3	A	37	PHE	6
3	A	44	PHE	6
3	A	86	MET	5
3	A	50	SER	4
3	A	35	ASN	4
3	A	85	ASP	4
3	A	39	TYR	3
3	A	64	ILE	3
3	A	17	LEU	3
3	A	27	SER	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
3	A	51	ILE	3
3	A	30	CYS	3
3	A	19	SER	2
3	A	47	TRP	2
3	A	83	SER	2
3	A	75	ASN	2
3	A	36	ARG	2
3	A	11	LEU	2
3	A	14	MET	1
3	A	25	THR	1
3	A	54	ASN	1
3	A	34	SER	1
3	A	7	SER	1
3	A	12	ILE	1
3	A	16	ILE	1
3	A	53	HIS	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided