Integrative Structure Validation Report

July 22, 2024 - 04:14 PM PDT

The following software was used in the production of this report:

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	9A0R
PDB-Dev ID	PDBDEV_00000063
Structure Title	Integrative structure of transcriptional enhancer factor TEF-1 bound to C-MYC exon
Structure Authors	Filandrova R; Valis K; Cerny J; Chmelik J; Slavata L; Fiala J; Rosulek M; Kavan D; Man P; Chum T; Cebecauer M; Fabris D; Novak P

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

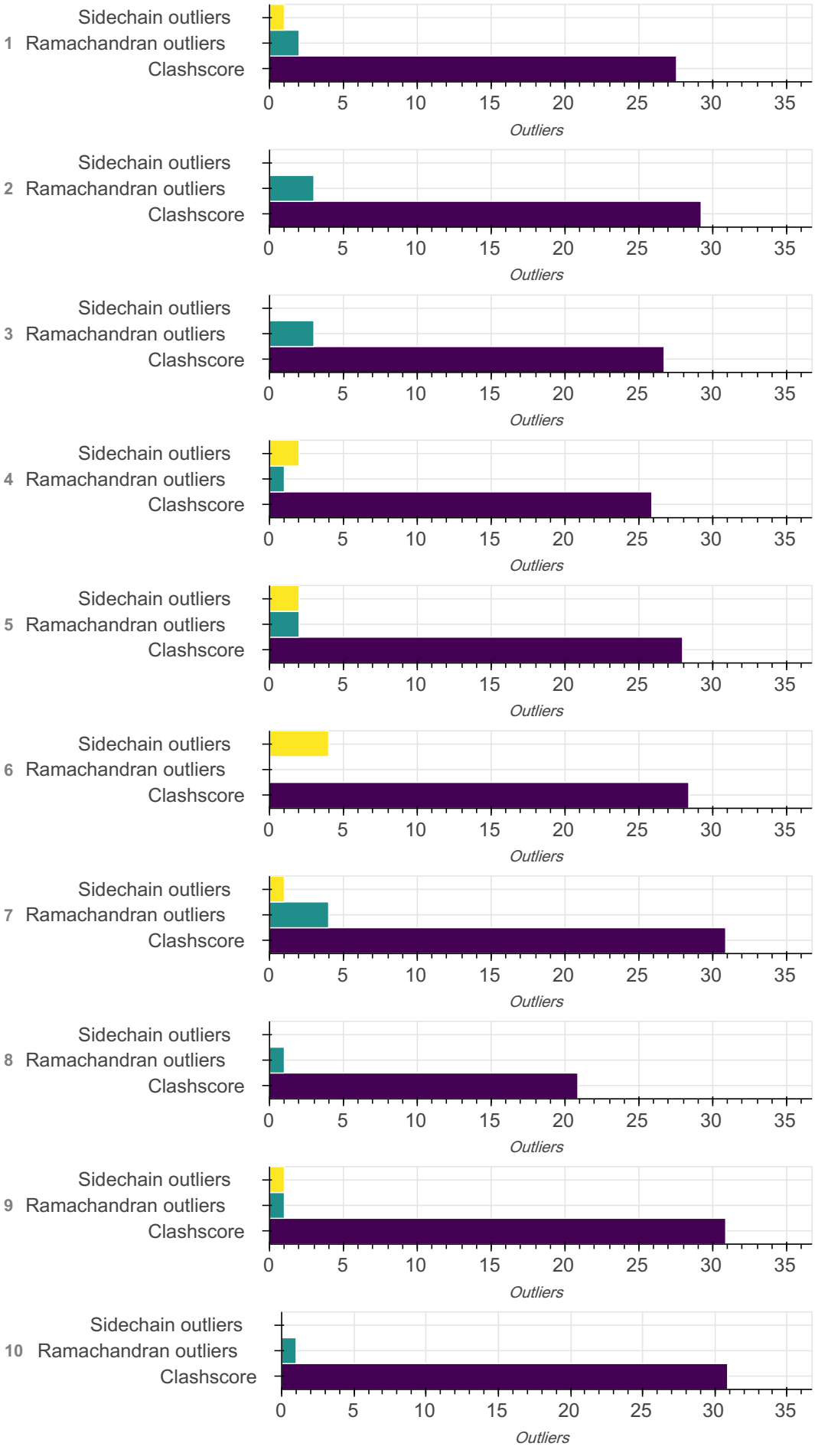
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

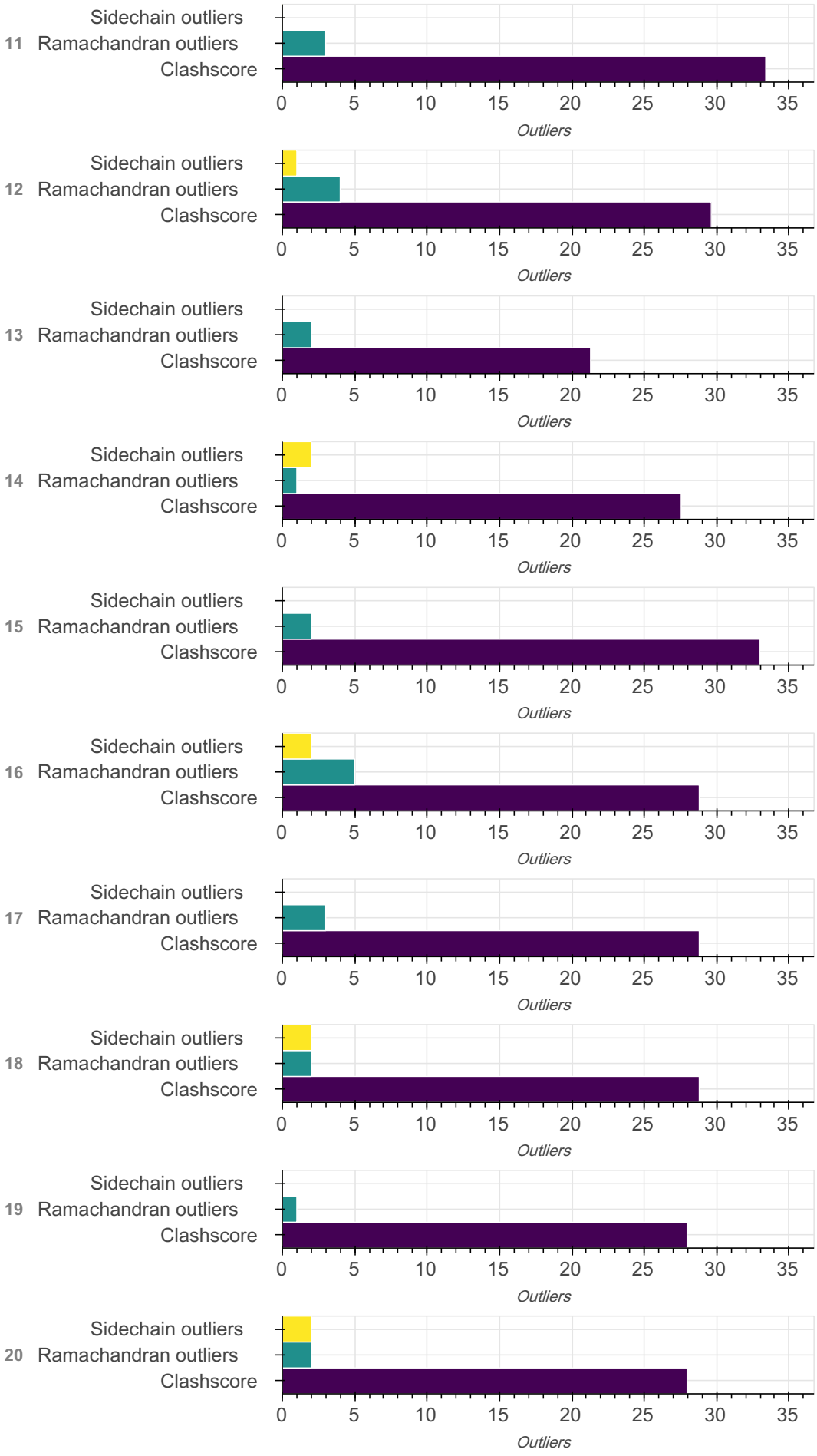
List of references used to build this report is available here.

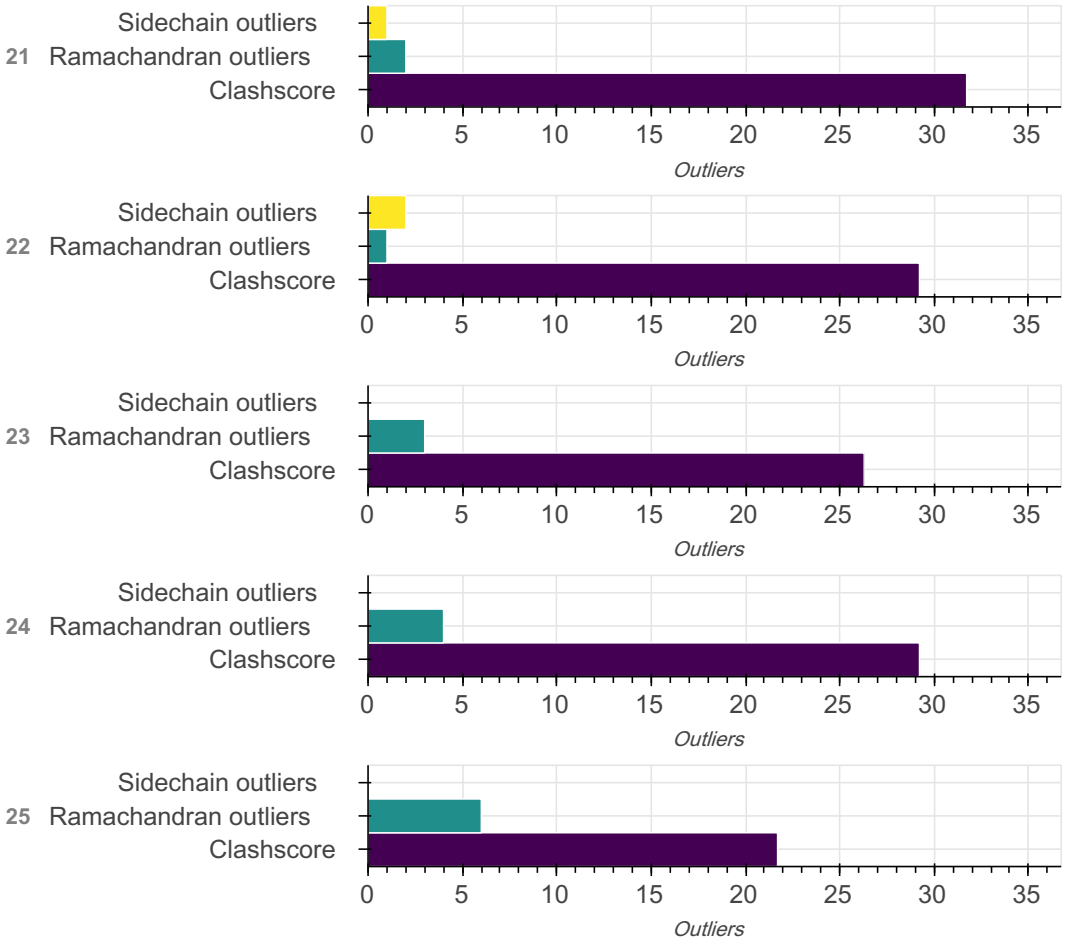
Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis


1
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
2
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
3
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
4
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
5
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
6
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
7
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
8
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
9
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
10
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers


Sidechain outliers
11 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
Sidechain outliers
12 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
Sidechain outliers
13 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
Sidechain outliers
14 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
Sidechain outliers
15 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
Sidechain outliers
16 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
Sidechain outliers
17 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
Sidechain outliers
18 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
Sidechain outliers
19 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers
Sidechain outliers
20 Ramachandran outliers
Clashscore
0 5 10 15 20 25 30 35
Outliers



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 25 unique models, with 2 subunits in each model. A total of 6 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 2 flexible or non-rigid units.

Entry composition

There are 25 unique types of models in this entry.These models are titled Model with the lowest potential energy, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Transcriptional enhancer factor TEF-3	A	A	87
1	2	2	DNA (30-MER)	B	B	30
2	1	1	Transcriptional enhancer factor TEF-3	A	A	87
2	2	2	DNA (30-MER)	B	B	30
3	1	1	Transcriptional enhancer factor TEF-3	A	A	87
3	2	2	DNA (30-MER)	B	B	30
4	1	1	Transcriptional enhancer factor TEF-3	A	A	87
4	2	2	DNA (30-MER)	B	B	30
5	1	1	Transcriptional enhancer factor TEF-3	A	A	87
5	2	2	DNA (30-MER)	B	B	30
6	1	1	Transcriptional enhancer factor TEF-3	A	A	87
6	2	2	DNA (30-MER)	B	B	30
7	1	1	Transcriptional enhancer factor TEF-3	A	A	87
7	2	2	DNA (30-MER)	B	B	30
8	1	1	Transcriptional enhancer factor TEF-3	A	A	87
8	2	2	DNA (30-MER)	B	B	30
9	1	1	Transcriptional enhancer factor TEF-3	A	A	87
9	2	2	DNA (30-MER)	B	B	30

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	1	1	Transcriptional enhancer factor TEF-3	A	A	87
10	2	2	DNA (30-MER)	B	B	30
11	1	1	Transcriptional enhancer factor TEF-3	A	A	87
11	2	2	DNA (30-MER)	B	B	30
12	1	1	Transcriptional enhancer factor TEF-3	A	A	87
12	2	2	DNA (30-MER)	B	B	30
13	1	1	Transcriptional enhancer factor TEF-3	A	A	87
13	2	2	DNA (30-MER)	B	B	30
14	1	1	Transcriptional enhancer factor TEF-3	A	A	87
14	2	2	DNA (30-MER)	B	B	30
15	1	1	Transcriptional enhancer factor TEF-3	A	A	87
15	2	2	DNA (30-MER)	B	B	30
16	1	1	Transcriptional enhancer factor TEF-3	A	A	87
16	2	2	DNA (30-MER)	B	B	30
17	1	1	Transcriptional enhancer factor TEF-3	A	A	87
17	2	2	DNA (30-MER)	B	B	30
18	1	1	Transcriptional enhancer factor TEF-3	A	A	87
18	2	2	DNA (30-MER)	B	B	30

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
19	1	1	Transcriptional enhancer factor TEF-3	A	A	87
19	2	2	DNA (30-MER)	B	B	30
20	1	1	Transcriptional enhancer factor TEF-3	A	A	87
20	2	2	DNA (30-MER)	B	B	30
21	1	1	Transcriptional enhancer factor TEF-3	A	A	87
21	2	2	DNA (30-MER)	B	B	30
22	1	1	Transcriptional enhancer factor TEF-3	A	A	87
22	2	2	DNA (30-MER)	B	B	30
23	1	1	Transcriptional enhancer factor TEF-3	A	A	87
23	2	2	DNA (30-MER)	B	B	30
24	1	1	Transcriptional enhancer factor TEF-3	A	A	87
24	2	2	DNA (30-MER)	B	B	30
25	1	1	Transcriptional enhancer factor TEF-3	A	A	87
25	2	2	DNA (30-MER)	B	B	30

Datasets used for modeling

There are 6 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Mass Spectrometry data	PRIDE	PXD012127

ID	Dataset type	Database name	Data access code
2	Crosslinking-MS data	File	10.17632/27zkz3v729.1
3	Experimental model	PDB	5GZB
4	Comparative model	Not available	Not available
5	Comparative model	Not available	Not available
6	H/D exchange data	File	10.17632/27zkz3v729.1

Representation

This entry has only one representation and includes 0 rigid bodies and 2 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-87
B	-	1-30

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	homology modeling	None	None	25	False	False
2	1	molecular docking	None	None	200	False	False
3	1	molecular dynamics	None	None	300	False	False

There are 5 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location

ID	Software name	Software version	Software classification	Software location
1	MODELLER	9.20	comparative modeling	https://salilab.org/modeller/
2	Make-na	Not available	nucleic acid builder	http://structure.usc.edu/make-na/
3	Modeller	9.24	homology modeling	https://salilab.org/modeller/
4	Haddock	2.2	docking	https://alcazar.science.uu.nl/services/HADDOCK2.2/
5	CNS	1.3	simulated annealing	http://cns-online.org

Data quality

Crosslinking-MS

Validation for this section is under development.

H/D exchange

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

Model quality

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers

Bond angle outliers do not exist or can not be evaluated for this model

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes

Model ID	Clash score	Number of clashes
1	27.55	66
2	29.22	70
3	26.71	64
4	25.88	62
5	27.96	67
6	28.38	68
7	30.88	74
8	20.87	50
9	30.88	74
10	30.88	74
11	33.39	80
12	29.63	71
13	21.29	51
14	27.55	66
15	32.97	79
16	28.80	69
17	28.80	69
18	28.80	69
19	27.96	67
20	27.96	67
21	31.72	76
22	29.22	70
23	26.29	63

Model ID	Clash score	Number of clashes
24	29.22	70
25	21.70	52

All 1688 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:19:DT:H2'	B:20:DG:C8	0.806
1	B:12:DA:H1'	B:20:DG:N2	0.803
1	B:8:DT:H2'	B:9:DT:C6	0.790
1	B:27:DC:H2'	B:28:DT:H6	0.789
1	A:18:PRO:HA	A:35:ARG:HE	0.783
1	B:18:DC:H2'	B:19:DT:C6	0.768
1	A:23:LYS:HZ2	A:35:ARG:HB3	0.718
1	B:18:DC:H3'	B:19:DT:H71	0.701
1	B:26:DA:H2'	B:27:DC:C6	0.700
1	B:27:DC:H2'	B:28:DT:C6	0.696
1	B:21:DG:C2	B:22:DA:H1'	0.669
1	B:14:DC:H2'	B:15:DG:H8	0.661
1	B:18:DC:H2'	B:19:DT:H6	0.653
1	B:11:DC:H2'	B:12:DA:O4'	0.645
1	B:3:DA:H2'	B:4:DG:O4'	0.643
1	B:8:DT:H2'	B:9:DT:H6	0.641
1	B:5:DT:H2'	B:6:DA:C8	0.636
1	B:23:DA:H2'	B:24:DT:O4'	0.635
1	B:24:DT:H2'	B:25:DT:C6	0.608

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:9:DT:H73	B:9:DT:OP2	0.604
1	B:28:DT:H2'	B:29:DA:C8	0.602
1	A:58:SER:HB3	B:7:DA:H61	0.594
1	B:12:DA:H1'	B:20:DG:H22	0.592
1	B:25:DT:H2'	B:26:DA:O4'	0.578
1	B:6:DA:H2'	B:7:DA:C8	0.569
1	B:4:DG:N2	B:28:DT:H1'	0.568
1	B:22:DA:O2'	B:23:DA:H5'	0.561
1	A:61:GLN:OE1	B:22:DA:H5'	0.542
1	B:11:DC:O2'	B:12:DA:H5'	0.539
1	B:7:DA:H2'	B:8:DT:C6	0.537
1	B:14:DC:H2'	B:15:DG:C8	0.536
1	B:24:DT:H2'	B:25:DT:H6	0.535
1	B:1:DG:O2'	B:2:DT:H5'	0.534
1	B:9:DT:H2'	B:10:DC:H6	0.533
1	B:9:DT:H2'	B:10:DC:O4'	0.533
1	A:15:ILE:H	A:15:ILE:HD12	0.508
1	B:13:DG:H2'	B:14:DC:C6	0.498
1	B:13:DG:H2'	B:14:DC:H6	0.495
1	B:10:DC:H2'	B:11:DC:C6	0.494
1	B:28:DT:H2'	B:29:DA:H8	0.491
1	A:52:THR:O	A:55:GLN:HG2	0.484
1	B:25:DT:O2'	B:26:DA:H5'	0.478

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:15:ILE:N	A:15:ILE:HD12	0.475
1	B:6:DA:H8	B:6:DA:O5'	0.473
1	A:25:ILE:O	A:32:MET:HA	0.471
1	A:43:ILE:N	A:43:ILE:HD12	0.466
1	A:53:ARG:H	A:53:ARG:HD3	0.461
1	B:13:DG:O2'	B:14:DC:H5'	0.457
1	B:26:DA:H2'	B:27:DC:H6	0.455
1	B:9:DT:H2'	B:10:DC:C6	0.453
1	B:27:DC:H3'	B:28:DT:H71	0.449
1	B:27:DC:O2'	B:28:DT:H5'	0.440
1	A:13:LEU:HD23	A:39:ILE:HD13	0.432
1	B:2:DT:N3	B:29:DA:C2	0.430
1	A:53:ARG:HD3	A:53:ARG:N	0.427
1	A:5:ILE:N	A:5:ILE:HD12	0.423
1	B:12:DA:H1'	B:20:DG:H21	0.423
1	B:21:DG:N2	B:22:DA:H1'	0.419
1	B:7:DA:H2'	B:8:DT:H6	0.417
1	B:5:DT:O2	B:26:DA:H2	0.417
1	B:6:DA:H2'	B:7:DA:O4'	0.414
1	B:22:DA:H2'	B:23:DA:O4'	0.408
1	A:19:CYS:H	A:35:ARG:HD2	0.406
1	A:52:THR:O	A:56:VAL:HG23	0.404
1	A:17:PRO:HA	A:18:PRO:HD3	0.401

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:9:DT:H2'	B:10:DC:O4'	0.921
2	A:18:PRO:HA	A:35:ARG:HE	0.824
2	B:19:DT:H2'	B:20:DG:C8	0.823
2	B:24:DT:H2'	B:25:DT:C6	0.822
2	B:10:DC:H2'	B:11:DC:C6	0.782
2	B:4:DG:N2	B:28:DT:H1'	0.777
2	B:7:DA:H2'	B:8:DT:C6	0.758
2	B:18:DC:H2'	B:19:DT:C6	0.756
2	B:27:DC:H2'	B:28:DT:H6	0.709
2	A:55:GLN:HB3	B:8:DT:H73	0.704
2	A:23:LYS:HE3	A:35:ARG:HB3	0.686
2	B:19:DT:H2'	B:20:DG:H8	0.683
2	B:6:DA:H2'	B:7:DA:C8	0.680
2	B:12:DA:H1'	B:20:DG:N2	0.668
2	B:13:DG:H1	B:17:DG:H1	0.657
2	B:27:DC:H2'	B:28:DT:C6	0.638
2	B:23:DA:H2'	B:24:DT:O4'	0.632
2	B:26:DA:H2'	B:27:DC:C6	0.632
2	B:24:DT:H2'	B:25:DT:H6	0.619
2	B:25:DT:H73	B:25:DT:OP1	0.604
2	A:61:GLN:OE1	B:22:DA:H5'	0.588
2	B:4:DG:H22	B:28:DT:H1'	0.585
2	A:55:GLN:HB3	B:8:DT:C7	0.582

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:3:DA:H2'	B:4:DG:O4'	0.579
2	B:8:DT:O2'	B:9:DT:H5'	0.573
2	B:25:DT:H2'	B:26:DA:O4'	0.566
2	B:22:DA:H2'	B:23:DA:O4'	0.562
2	B:25:DT:O2'	B:26:DA:H5'	0.557
2	B:7:DA:H2'	B:8:DT:H6	0.554
2	B:23:DA:H3'	B:24:DT:H71	0.545
2	A:63:LEU:HD23	A:66:ARG:HH21	0.540
2	A:18:PRO:HA	A:35:ARG:NE	0.535
2	B:11:DC:H2'	B:12:DA:H8	0.533
2	B:11:DC:H2'	B:12:DA:O4'	0.532
2	B:10:DC:H2'	B:11:DC:H6	0.515
2	A:53:ARG:H	A:53:ARG:HD3	0.508
2	B:28:DT:H2'	B:29:DA:C8	0.501
2	B:21:DG:C2	B:22:DA:H1'	0.492
2	B:13:DG:O2'	B:14:DC:H5'	0.491
2	A:52:THR:O	A:56:VAL:HG23	0.489
2	A:15:ILE:H	A:15:ILE:HD12	0.480
2	A:15:ILE:N	A:15:ILE:HD12	0.480
2	B:1:DG:O2'	B:2:DT:H5'	0.480
2	B:11:DC:O2'	B:12:DA:H5'	0.473
2	B:26:DA:H2'	B:27:DC:H6	0.473
2	A:36:ASN:ND2	A:60:ILE:HD11	0.464

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:13:DG:H2'	B:14:DC:H6	0.460
2	B:27:DC:O2'	B:28:DT:H5'	0.458
2	B:23:DA:O2'	B:24:DT:H5'	0.455
2	B:22:DA:O2'	B:23:DA:H5'	0.450
2	A:64:ALA:HA	A:67:LYS:HE2	0.448
2	A:19:CYS:H	A:35:ARG:HD2	0.447
2	B:12:DA:H1'	B:20:DG:H21	0.446
2	A:43:ILE:N	A:43:ILE:HD12	0.443
2	B:23:DA:H2'	B:24:DT:C6	0.441
2	B:23:DA:H2'	B:24:DT:H6	0.441
2	B:28:DT:H2'	B:29:DA:O4'	0.436
2	B:5:DT:H2'	B:6:DA:O4'	0.433
2	B:14:DC:H2'	B:15:DG:O4'	0.431
2	B:11:DC:H2'	B:12:DA:C8	0.429
2	B:8:DT:H2'	B:9:DT:C6	0.424
2	B:28:DT:O2'	B:29:DA:H5'	0.423
2	A:18:PRO:HG3	A:35:ARG:HH21	0.420
2	A:23:LYS:HB3	A:23:LYS:HE2	0.419
2	B:4:DG:H21	B:28:DT:H1'	0.418
2	B:23:DA:C2	B:24:DT:C2	0.411
2	A:32:MET:HB3	B:19:DT:H4'	0.406
2	B:5:DT:O2	B:26:DA:H2	0.406
2	B:13:DG:H2'	B:14:DC:C6	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:14:DC:O2'	B:15:DG:H5'	0.401
3	B:9:DT:H2'	B:10:DC:O4'	0.934
3	B:24:DT:H2'	B:25:DT:C6	0.837
3	B:10:DC:H2'	B:11:DC:C6	0.804
3	A:18:PRO:HA	A:35:ARG:HE	0.802
3	B:19:DT:H2'	B:20:DG:C8	0.782
3	B:4:DG:N2	B:28:DT:H1'	0.762
3	B:19:DT:H2'	B:20:DG:H8	0.729
3	B:18:DC:H2'	B:19:DT:C6	0.712
3	B:10:DC:H2'	B:11:DC:H6	0.711
3	A:55:GLN:HB3	B:8:DT:H73	0.708
3	B:27:DC:H2'	B:28:DT:H6	0.690
3	B:7:DA:H2'	B:8:DT:C6	0.689
3	B:6:DA:H2'	B:7:DA:C8	0.677
3	A:55:GLN:HB3	B:8:DT:C7	0.666
3	B:24:DT:H2'	B:25:DT:H6	0.641
3	B:25:DT:H73	B:25:DT:OP1	0.633
3	B:23:DA:H2'	B:24:DT:O4'	0.629
3	B:3:DA:H2'	B:4:DG:O4'	0.619
3	B:27:DC:H2'	B:28:DT:C6	0.615
3	B:26:DA:H2'	B:27:DC:C6	0.609
3	B:25:DT:H2'	B:26:DA:O4'	0.606
3	B:22:DA:H2'	B:23:DA:C8	0.585

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:53:ARG:H	A:53:ARG:HD3	0.582
3	B:25:DT:O2'	B:26:DA:H5'	0.581
3	A:32:MET:HB3	B:19:DT:H4'	0.576
3	B:4:DG:H22	B:28:DT:H1'	0.558
3	A:15:ILE:H	A:15:ILE:HD12	0.557
3	B:8:DT:O2'	B:9:DT:H5'	0.555
3	B:23:DA:H3'	B:24:DT:H71	0.550
3	B:28:DT:H2'	B:29:DA:C8	0.546
3	B:11:DC:H2'	B:12:DA:H8	0.531
3	B:23:DA:H2'	B:24:DT:C6	0.525
3	B:23:DA:H2'	B:24:DT:H6	0.523
3	A:23:LYS:HE3	A:35:ARG:H	0.504
3	B:12:DA:H1'	B:20:DG:N2	0.499
3	B:11:DC:H2'	B:12:DA:C8	0.497
3	B:7:DA:H2'	B:8:DT:H6	0.494
3	B:23:DA:O2'	B:24:DT:H5'	0.489
3	B:1:DG:O2'	B:2:DT:H5'	0.487
3	A:63:LEU:O	A:67:LYS:HG3	0.485
3	B:11:DC:H2'	B:12:DA:O4'	0.469
3	B:17:DG:H2'	B:18:DC:O4'	0.465
3	A:15:ILE:N	A:15:ILE:HD12	0.464
3	B:13:DG:O2'	B:14:DC:H5'	0.463
3	A:5:ILE:HG21	A:51:ARG:HH11	0.456

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	B:7:DA:H8	B:7:DA:O5'	0.448
3	A:52:THR:O	A:56:VAL:HG23	0.447
3	B:18:DC:H2'	B:19:DT:H6	0.447
3	B:28:DT:O2'	B:29:DA:H5'	0.447
3	B:28:DT:H2'	B:29:DA:O4'	0.443
3	B:27:DC:O2'	B:28:DT:H5'	0.440
3	B:5:DT:H2'	B:6:DA:C8	0.437
3	A:55:GLN:NE2	B:7:DA:H3'	0.432
3	B:13:DG:H2'	B:14:DC:H6	0.432
3	B:26:DA:H2'	B:27:DC:H6	0.432
3	A:63:LEU:HD23	A:66:ARG:HH21	0.429
3	B:5:DT:O2	B:26:DA:H2	0.424
3	A:19:CYS:H	A:35:ARG:HD2	0.422
3	A:5:ILE:N	A:5:ILE:HD12	0.418
3	B:2:DT:H2'	B:3:DA:C8	0.411
3	B:9:DT:H71	B:9:DT:OP2	0.404
3	A:58:SER:HB3	B:7:DA:N6	0.403
3	B:8:DT:H2'	B:9:DT:C6	0.401
3	B:9:DT:H2'	B:10:DC:C5'	0.401
4	B:4:DG:H2'	B:5:DT:O4'	0.879
4	B:6:DA:H2'	B:7:DA:C8	0.810
4	B:5:DT:H2'	B:6:DA:C8	0.777
4	B:8:DT:H2'	B:9:DT:C6	0.774

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:23:LYS:HZ2	A:35:ARG:HB3	0.748
4	B:26:DA:H2'	B:27:DC:C6	0.738
4	B:12:DA:H1'	B:20:DG:N2	0.732
4	B:8:DT:H2'	B:9:DT:H6	0.678
4	B:23:DA:H2'	B:24:DT:H6	0.675
4	B:23:DA:H2'	B:24:DT:C6	0.658
4	B:9:DT:H2'	B:10:DC:C6	0.647
4	B:24:DT:H2'	B:25:DT:C6	0.623
4	B:24:DT:H2'	B:25:DT:H6	0.617
4	B:12:DA:H1'	B:20:DG:H22	0.606
4	B:18:DC:O2'	B:19:DT:H5'	0.599
4	B:27:DC:O2'	B:28:DT:H5'	0.577
4	B:3:DA:H2'	B:4:DG:O4'	0.572
4	A:41:ARG:HA	A:44:LYS:HD2	0.561
4	B:7:DA:O2'	B:8:DT:H5'	0.557
4	B:11:DC:H1'	B:21:DG:H21	0.556
4	B:21:DG:H2'	B:22:DA:C8	0.549
4	B:20:DG:H2'	B:21:DG:O4'	0.547
4	A:23:LYS:NZ	A:35:ARG:HB3	0.543
4	B:25:DT:H2'	B:26:DA:C8	0.537
4	B:21:DG:H2'	B:22:DA:H8	0.535
4	B:26:DA:H2'	B:27:DC:O4'	0.530
4	B:13:DG:O2'	B:14:DC:H5'	0.529

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	B:6:DA:H2'	B:7:DA:H8	0.526
4	B:28:DT:H2'	B:29:DA:O4'	0.524
4	B:1:DG:H3'	B:2:DT:H71	0.522
4	B:10:DC:H2'	B:11:DC:H6	0.519
4	B:11:DC:H1'	B:21:DG:N2	0.517
4	B:10:DC:O2'	B:11:DC:H5'	0.514
4	B:5:DT:H2'	B:6:DA:H8	0.501
4	B:17:DG:H2'	B:18:DC:C6	0.500
4	B:17:DG:H2'	B:18:DC:O4'	0.500
4	A:31:LYS:HB3	A:31:LYS:NZ	0.495
4	B:27:DC:H2'	B:28:DT:H6	0.494
4	B:9:DT:H2'	B:10:DC:O4'	0.484
4	B:28:DT:H2'	B:29:DA:C8	0.483
4	B:28:DT:O2'	B:29:DA:H5'	0.477
4	B:11:DC:H2'	B:12:DA:C8	0.473
4	B:10:DC:H6	B:10:DC:O5'	0.472
4	B:11:DC:H2'	B:12:DA:O4'	0.469
4	A:52:THR:HG22	A:54:LYS:H	0.456
4	B:4:DG:H8	B:4:DG:O5'	0.456
4	B:19:DT:H2'	B:20:DG:C8	0.446
4	B:27:DC:H2'	B:28:DT:C6	0.440
4	B:10:DC:H2'	B:11:DC:C6	0.439
4	B:14:DC:H2'	B:15:DG:H8	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	B:5:DT:H71	B:5:DT:OP1	0.433
4	A:38:LEU:O	A:41:ARG:HG3	0.421
4	B:24:DT:O2'	B:25:DT:H5'	0.420
4	B:1:DG:H2'	B:2:DT:C6	0.419
4	B:26:DA:H2'	B:27:DC:H6	0.419
4	B:19:DT:H6	B:19:DT:O5'	0.417
4	B:13:DG:N2	B:19:DT:H1'	0.416
4	B:26:DA:H8	B:26:DA:O5'	0.416
4	B:19:DT:H73	B:19:DT:OP2	0.415
4	A:18:PRO:HA	A:35:ARG:NE	0.412
5	B:5:DT:H2'	B:6:DA:C8	0.850
5	B:4:DG:H2'	B:5:DT:O4'	0.849
5	B:6:DA:H2'	B:7:DA:C8	0.817
5	B:5:DT:H71	B:5:DT:OP1	0.792
5	B:8:DT:H2'	B:9:DT:C6	0.780
5	B:12:DA:H1'	B:20:DG:N2	0.777
5	B:9:DT:H2'	B:10:DC:C6	0.736
5	B:26:DA:H2'	B:27:DC:C6	0.710
5	A:31:LYS:HB3	A:31:LYS:HZ2	0.700
5	A:23:LYS:HZ2	A:35:ARG:HB3	0.700
5	B:10:DC:H2'	B:11:DC:H6	0.692
5	B:27:DC:O2'	B:28:DT:H5'	0.677
5	B:8:DT:H2'	B:9:DT:H6	0.655

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	B:21:DG:H2'	B:22:DA:H8	0.647
5	B:6:DA:H2'	B:7:DA:H8	0.640
5	B:21:DG:H2'	B:22:DA:C8	0.612
5	B:12:DA:H1'	B:20:DG:H22	0.604
5	B:23:DA:H2'	B:24:DT:O4'	0.604
5	B:10:DC:H2'	B:11:DC:C6	0.598
5	A:41:ARG:HA	A:44:LYS:HD2	0.590
5	A:23:LYS:NZ	A:35:ARG:HB3	0.580
5	B:25:DT:H2'	B:26:DA:C8	0.558
5	B:1:DG:H3'	B:2:DT:H71	0.557
5	B:26:DA:H2'	B:27:DC:O4'	0.557
5	B:20:DG:H2'	B:21:DG:O4'	0.552
5	B:7:DA:H2'	B:8:DT:H6	0.532
5	B:7:DA:H2'	B:8:DT:C6	0.527
5	B:19:DT:H2'	B:20:DG:C8	0.523
5	B:28:DT:H2'	B:29:DA:C8	0.520
5	B:3:DA:H2'	B:4:DG:O4'	0.514
5	B:10:DC:O2'	B:11:DC:H5'	0.512
5	A:40:ALA:HB2	A:56:VAL:HG21	0.505
5	B:4:DG:C2'	B:5:DT:H5'	0.505
5	B:23:DA:O2'	B:24:DT:H5'	0.504
5	B:24:DT:H2'	B:25:DT:H6	0.499
5	B:11:DC:H1'	B:21:DG:H21	0.496

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	B:13:DG:O2'	B:14:DC:H5'	0.492
5	B:11:DC:H2'	B:12:DA:C8	0.490
5	B:24:DT:H2'	B:25:DT:C6	0.485
5	B:23:DA:H2'	B:24:DT:H6	0.483
5	B:9:DT:H2'	B:10:DC:H6	0.482
5	B:11:DC:H1'	B:21:DG:N2	0.480
5	A:31:LYS:HB3	A:31:LYS:NZ	0.479
5	A:55:GLN:HG2	B:8:DT:C7	0.479
5	B:1:DG:H2'	B:2:DT:C6	0.478
5	B:4:DG:H8	B:4:DG:O5'	0.475
5	B:7:DA:O2'	B:8:DT:H5'	0.474
5	B:28:DT:H2'	B:29:DA:O4'	0.473
5	A:38:LEU:O	A:41:ARG:HG3	0.470
5	B:4:DG:H2'	B:5:DT:C4'	0.469
5	B:24:DT:O2'	B:25:DT:H5'	0.468
5	A:52:THR:HG22	A:54:LYS:H	0.465
5	B:28:DT:H2'	B:29:DA:H8	0.457
5	B:17:DG:H2'	B:18:DC:O4'	0.454
5	B:4:DG:H2'	B:5:DT:C5'	0.453
5	B:19:DT:H6	B:19:DT:O5'	0.451
5	B:17:DG:H2'	B:18:DC:C6	0.449
5	A:13:LEU:HD23	A:39:ILE:HD13	0.437
5	B:26:DA:H2'	B:27:DC:H6	0.433

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:52:THR:HG22	A:53:ARG:N	0.425
5	B:23:DA:H2'	B:24:DT:C6	0.424
5	B:28:DT:O2'	B:29:DA:H5'	0.423
5	B:4:DG:H2'	B:5:DT:H5'	0.415
5	B:22:DA:O2'	B:23:DA:H5'	0.411
5	B:9:DT:H2'	B:10:DC:O4'	0.410
5	B:11:DC:H2'	B:12:DA:O4'	0.408
6	B:21:DG:H2'	B:22:DA:O4'	0.866
6	B:2:DT:H2'	B:3:DA:C8	0.805
6	B:2:DT:H2'	B:3:DA:H8	0.759
6	B:20:DG:H2'	B:21:DG:O4'	0.756
6	B:23:DA:H2'	B:24:DT:C6	0.738
6	B:6:DA:H2'	B:7:DA:C8	0.729
6	B:23:DA:H2'	B:24:DT:H6	0.720
6	B:27:DC:H2'	B:28:DT:H6	0.720
6	B:5:DT:H2'	B:6:DA:O4'	0.709
6	A:34:GLY:H	A:37:GLU:HG3	0.704
6	B:6:DA:H2'	B:7:DA:H8	0.703
6	A:53:ARG:H	A:53:ARG:HD2	0.701
6	B:23:DA:H3'	B:24:DT:H71	0.701
6	B:7:DA:H3'	B:8:DT:H71	0.679
6	B:26:DA:H2'	B:27:DC:C6	0.677
6	B:27:DC:H2'	B:28:DT:C6	0.677

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	B:17:DG:O2'	B:18:DC:H5'	0.663
6	B:21:DG:C2	B:22:DA:H1'	0.661
6	B:9:DT:H2'	B:10:DC:C6	0.659
6	B:18:DC:H2'	B:19:DT:O4'	0.635
6	B:28:DT:H2'	B:29:DA:O4'	0.622
6	A:53:ARG:HG2	A:54:LYS:HD2	0.621
6	B:1:DG:H2'	B:2:DT:O4'	0.621
6	B:7:DA:H2'	B:8:DT:O4'	0.617
6	B:7:DA:O2'	B:8:DT:H5'	0.604
6	B:24:DT:H2'	B:25:DT:C6	0.586
6	B:8:DT:O2'	B:9:DT:H5'	0.584
6	B:22:DA:H2'	B:23:DA:C8	0.570
6	B:16:DC:H2'	B:17:DG:C8	0.559
6	B:24:DT:H2'	B:25:DT:H6	0.550
6	B:28:DT:O2'	B:29:DA:H5'	0.541
6	B:12:DA:H8	B:12:DA:O5'	0.532
6	A:23:LYS:HZ2	A:36:ASN:H	0.525
6	B:9:DT:H2'	B:10:DC:H6	0.522
6	B:1:DG:O2'	B:2:DT:H5'	0.513
6	B:11:DC:H2'	B:12:DA:O4'	0.512
6	B:22:DA:O2'	B:23:DA:H5'	0.508
6	B:23:DA:H2'	B:24:DT:O4'	0.499
6	A:39:ILE:O	A:43:ILE:HG12	0.497

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	B:22:DA:H2'	B:23:DA:H8	0.493
6	B:21:DG:O2'	B:22:DA:H5'	0.487
6	B:1:DG:H3'	B:2:DT:H71	0.482
6	A:63:LEU:O	A:67:LYS:HG3	0.472
6	B:7:DA:H2'	B:8:DT:H6	0.470
6	A:32:MET:N	A:32:MET:SD	0.470
6	B:7:DA:C2	B:8:DT:H1'	0.466
6	B:18:DC:C2'	B:19:DT:H5'	0.464
6	A:17:PRO:HA	A:18:PRO:HD3	0.458
6	A:31:LYS:HB3	A:31:LYS:NZ	0.456
6	A:52:THR:HG22	A:54:LYS:H	0.454
6	A:23:LYS:NZ	A:36:ASN:H	0.454
6	B:27:DC:O2'	B:28:DT:H5'	0.453
6	B:3:DA:H2'	B:4:DG:C8	0.451
6	B:12:DA:H2'	B:13:DG:O4'	0.450
6	B:22:DA:H2'	B:23:DA:O4'	0.444
6	B:12:DA:O2'	B:13:DG:H5'	0.441
6	A:49:LYS:HB3	A:49:LYS:NZ	0.439
6	A:62:VAL:CG1	B:6:DA:H62	0.437
6	B:1:DG:H2'	B:2:DT:C6	0.436
6	B:26:DA:C2	B:27:DC:C2	0.436
6	B:18:DC:H6	B:18:DC:O5'	0.430
6	B:18:DC:H2'	B:19:DT:C5'	0.424

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:62:VAL:HG12	B:6:DA:H62	0.416
6	B:12:DA:H61	B:18:DC:N4	0.416
6	B:5:DT:H3	B:26:DA:H2	0.414
6	B:21:DG:N3	B:22:DA:H1'	0.409
6	B:18:DC:O2'	B:19:DT:H5'	0.406
7	B:19:DT:H2'	B:20:DG:C8	0.792
7	B:8:DT:H2'	B:9:DT:C6	0.751
7	A:18:PRO:HA	A:35:ARG:HE	0.748
7	B:19:DT:H2'	B:20:DG:H8	0.733
7	B:4:DG:N2	B:28:DT:H1'	0.727
7	B:9:DT:H2'	B:10:DC:O4'	0.718
7	B:18:DC:H2'	B:19:DT:C6	0.703
7	A:55:GLN:HB3	B:8:DT:H73	0.697
7	B:24:DT:H2'	B:25:DT:C6	0.682
7	B:6:DA:H2'	B:7:DA:C8	0.664
7	B:8:DT:H2'	B:9:DT:H6	0.656
7	B:10:DC:H2'	B:11:DC:C6	0.656
7	B:27:DC:H2'	B:28:DT:H6	0.649
7	B:27:DC:H2'	B:28:DT:C6	0.638
7	B:23:DA:H2'	B:24:DT:C6	0.605
7	B:25:DT:H73	B:25:DT:OP1	0.600
7	B:24:DT:H2'	B:25:DT:H6	0.590
7	B:22:DA:H2'	B:23:DA:O4'	0.584

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	B:26:DA:H2'	B:27:DC:C6	0.583
7	B:25:DT:H2'	B:26:DA:O4'	0.573
7	A:13:LEU:HD23	A:39:ILE:HD13	0.560
7	B:23:DA:H2'	B:24:DT:H6	0.553
7	B:18:DC:H2'	B:19:DT:H6	0.552
7	B:24:DT:H2'	B:25:DT:O4'	0.547
7	B:28:DT:H2'	B:29:DA:C8	0.544
7	B:25:DT:O2'	B:26:DA:H5'	0.536
7	B:22:DA:H2'	B:23:DA:C8	0.528
7	B:5:DT:H3	B:26:DA:H2	0.526
7	B:5:DT:H2'	B:6:DA:C8	0.525
7	A:9:PHE:HA	A:43:ILE:HD11	0.523
7	A:23:LYS:HE3	A:35:ARG:H	0.522
7	A:18:PRO:HA	A:35:ARG:NE	0.515
7	B:10:DC:H2'	B:11:DC:H6	0.515
7	B:4:DG:H22	B:28:DT:H1'	0.505
7	B:13:DG:O2'	B:14:DC:H5'	0.502
7	B:11:DC:H2'	B:12:DA:O4'	0.501
7	B:23:DA:O2'	B:24:DT:H5'	0.495
7	A:63:LEU:O	A:67:LYS:HG3	0.490
7	B:13:DG:H2'	B:14:DC:H6	0.489
7	A:19:CYS:H	A:35:ARG:HD2	0.488
7	B:11:DC:H2'	B:12:DA:H8	0.487

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	B:1:DG:H2'	B:2:DT:H6	0.484
7	A:15:ILE:H	A:15:ILE:HD12	0.482
7	A:52:THR:O	A:56:VAL:HG23	0.482
7	B:2:DT:H2'	B:3:DA:C8	0.482
7	B:1:DG:H2'	B:2:DT:C6	0.479
7	A:15:ILE:N	A:15:ILE:HD12	0.477
7	B:7:DA:H2'	B:8:DT:C6	0.471
7	B:11:DC:O2'	B:12:DA:H5'	0.470
7	B:14:DC:H2'	B:15:DG:H8	0.466
7	B:23:DA:C2	B:24:DT:C2	0.465
7	B:3:DA:H2'	B:4:DG:O4'	0.462
7	B:9:DT:H2'	B:10:DC:C6	0.458
7	B:9:DT:H2'	B:10:DC:H6	0.457
7	A:55:GLN:HB3	B:8:DT:C7	0.454
7	A:43:ILE:N	A:43:ILE:HD12	0.451
7	A:5:ILE:HG21	A:51:ARG:HH11	0.440
7	B:14:DC:H2'	B:15:DG:C8	0.436
7	B:21:DG:C2	B:22:DA:H1'	0.435
7	A:63:LEU:HD23	A:66:ARG:HH21	0.432
7	B:23:DA:H3'	B:24:DT:H71	0.430
7	B:12:DA:H1'	B:20:DG:N2	0.428
7	B:14:DC:O2'	B:15:DG:H5'	0.428
7	A:53:ARG:H	A:53:ARG:HD3	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	B:18:DC:H3'	B:19:DT:H71	0.424
7	B:23:DA:H2'	B:24:DT:O4'	0.423
7	B:27:DC:O2'	B:28:DT:H5'	0.421
7	B:13:DG:H2'	B:14:DC:C6	0.419
7	A:25:ILE:O	A:32:MET:HA	0.418
7	B:7:DA:H2'	B:8:DT:H6	0.413
7	B:17:DG:H2'	B:18:DC:O4'	0.411
7	B:28:DT:O2'	B:29:DA:H5'	0.411
7	B:11:DC:H2'	B:12:DA:C8	0.406
7	B:22:DA:H2'	B:23:DA:H8	0.406
8	B:4:DG:N2	B:28:DT:H1'	0.865
8	B:4:DG:H2'	B:5:DT:O4'	0.768
8	B:24:DT:H2'	B:25:DT:O4'	0.715
8	B:4:DG:H22	B:28:DT:H1'	0.656
8	A:19:CYS:H	A:35:ARG:HD2	0.642
8	B:21:DG:H2'	B:22:DA:H8	0.638
8	B:5:DT:H2'	B:6:DA:O4'	0.629
8	B:22:DA:H2'	B:23:DA:C8	0.617
8	B:21:DG:H2'	B:22:DA:C8	0.596
8	B:19:DT:H2'	B:20:DG:O4'	0.594
8	B:6:DA:H2'	B:7:DA:C8	0.579
8	B:6:DA:H2'	B:7:DA:H8	0.551
8	B:28:DT:O2'	B:29:DA:H5'	0.551

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	B:13:DG:H2'	B:14:DC:O4'	0.548
8	B:27:DC:O2'	B:28:DT:H5'	0.541
8	A:36:ASN:HD21	A:57:SER:HB3	0.535
8	A:31:LYS:HB3	A:31:LYS:NZ	0.528
8	B:18:DC:H2'	B:19:DT:H6	0.528
8	B:25:DT:H73	B:25:DT:OP1	0.527
8	A:40:ALA:O	A:44:LYS:HG2	0.524
8	B:18:DC:H2'	B:19:DT:C6	0.518
8	B:27:DC:H2'	B:28:DT:H6	0.513
8	B:19:DT:O2'	B:20:DG:H5'	0.511
8	B:1:DG:H2'	B:2:DT:C6	0.506
8	B:9:DT:H2'	B:10:DC:O4'	0.502
8	B:4:DG:H21	B:28:DT:H1'	0.500
8	B:20:DG:H2'	B:21:DG:O4'	0.485
8	B:5:DT:H71	B:5:DT:OP1	0.479
8	A:24:ILE:H	A:24:ILE:HD12	0.477
8	A:55:GLN:O	A:59:HIS:HB2	0.474
8	B:2:DT:O2'	B:3:DA:H5'	0.471
8	B:27:DC:H2'	B:28:DT:C6	0.466
8	B:4:DG:C2	B:5:DT:H1'	0.458
8	A:26:LEU:H	A:26:LEU:HD12	0.457
8	A:24:ILE:N	A:24:ILE:HD12	0.450
8	B:1:DG:H3'	B:2:DT:H71	0.448

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	B:26:DA:H2'	B:27:DC:C6	0.447
8	B:24:DT:O2'	B:25:DT:H5'	0.446
8	B:23:DA:C2	B:24:DT:C2	0.444
8	B:23:DA:H8	B:23:DA:O5'	0.415
8	B:17:DG:H2'	B:18:DC:O4'	0.411
8	A:13:LEU:HD23	A:39:ILE:HD13	0.410
8	A:53:ARG:HD3	A:53:ARG:N	0.410
8	B:13:DG:C2'	B:14:DC:H5'	0.407
8	B:20:DG:H2'	B:21:DG:C8	0.407
8	A:2:SER:HA	A:3:PRO:HD3	0.405
8	B:2:DT:H2'	B:3:DA:O4'	0.404
8	B:10:DC:H6	B:10:DC:O5'	0.404
8	B:26:DA:H2'	B:27:DC:O4'	0.400
9	A:18:PRO:HA	A:35:ARG:HE	0.845
9	B:4:DG:N2	B:28:DT:H1'	0.795
9	B:24:DT:H3'	B:25:DT:H71	0.794
9	B:6:DA:H2'	B:7:DA:C8	0.767
9	B:24:DT:H2'	B:25:DT:C6	0.739
9	B:5:DT:H2'	B:6:DA:C8	0.737
9	A:2:SER:H	A:3:PRO:HD2	0.717
9	A:55:GLN:HB3	B:8:DT:H73	0.712
9	B:9:DT:H2'	B:10:DC:O4'	0.697
9	B:27:DC:H2'	B:28:DT:H6	0.690

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	B:23:DA:H2'	B:24:DT:O4'	0.687
9	B:19:DT:H2'	B:20:DG:C8	0.683
9	B:23:DA:H3'	B:24:DT:H71	0.662
9	B:18:DC:H2'	B:19:DT:C6	0.640
9	B:10:DC:H2'	B:11:DC:C6	0.638
9	B:3:DA:H2'	B:4:DG:O4'	0.630
9	B:8:DT:H2'	B:9:DT:C6	0.613
9	B:12:DA:H1'	B:20:DG:N2	0.609
9	A:55:GLN:HB3	B:8:DT:C7	0.591
9	A:61:GLN:OE1	B:22:DA:H5'	0.589
9	B:5:DT:H2'	B:6:DA:H8	0.584
9	B:27:DC:H2'	B:28:DT:C6	0.584
9	B:24:DT:H2'	B:25:DT:H6	0.583
9	B:11:DC:H2'	B:12:DA:O4'	0.580
9	B:26:DA:H2'	B:27:DC:C6	0.575
9	B:7:DA:H2'	B:8:DT:C6	0.570
9	A:15:ILE:H	A:15:ILE:HD12	0.562
9	A:53:ARG:H	A:53:ARG:HD3	0.555
9	B:25:DT:O2'	B:26:DA:H5'	0.541
9	B:23:DA:O2'	B:24:DT:H5'	0.539
9	B:25:DT:H2'	B:26:DA:O4'	0.538
9	A:32:MET:CB	B:19:DT:H4'	0.534
9	B:8:DT:H2'	B:9:DT:H6	0.528

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	B:7:DA:H2'	B:8:DT:H6	0.524
9	A:32:MET:HB2	B:19:DT:H4'	0.523
9	B:4:DG:H22	B:28:DT:H1'	0.521
9	A:63:LEU:O	A:67:LYS:HG3	0.516
9	B:18:DC:H2'	B:19:DT:H6	0.504
9	B:19:DT:H2'	B:20:DG:H8	0.495
9	B:11:DC:O2'	B:12:DA:H5'	0.494
9	B:21:DG:C2	B:22:DA:H1'	0.493
9	A:15:ILE:N	A:15:ILE:HD12	0.485
9	B:14:DC:H2'	B:15:DG:H8	0.482
9	A:52:THR:O	A:56:VAL:HG23	0.477
9	B:17:DG:H2'	B:18:DC:O4'	0.469
9	B:10:DC:H2'	B:11:DC:H6	0.462
9	B:27:DC:O2'	B:28:DT:H5'	0.455
9	B:28:DT:O2'	B:29:DA:H5'	0.451
9	B:11:DC:H2'	B:12:DA:H8	0.450
9	B:22:DA:O2'	B:23:DA:H5'	0.450
9	A:43:ILE:N	A:43:ILE:HD12	0.449
9	B:4:DG:H21	B:28:DT:H1'	0.446
9	A:53:ARG:HD3	A:53:ARG:N	0.445
9	B:13:DG:O2'	B:14:DC:H5'	0.441
9	B:1:DG:H2'	B:2:DT:H6	0.440
9	A:18:PRO:HA	A:35:ARG:NE	0.437

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	B:1:DG:O2'	B:2:DT:H5'	0.434
9	B:5:DT:O2	B:26:DA:H2	0.434
9	B:22:DA:C2	B:23:DA:C4	0.428
9	A:18:PRO:HG3	A:35:ARG:HH21	0.427
9	B:14:DC:H2'	B:15:DG:C8	0.426
9	A:36:ASN:HD21	A:56:VAL:HG12	0.425
9	B:1:DG:H2'	B:2:DT:C6	0.422
9	B:8:DT:O2'	B:9:DT:H5'	0.421
9	A:23:LYS:HE3	A:35:ARG:H	0.418
9	B:13:DG:H2'	B:14:DC:H6	0.418
9	B:25:DT:H2'	B:26:DA:C8	0.414
9	A:32:MET:HB3	B:19:DT:H4'	0.413
9	B:8:DT:H3	B:23:DA:N6	0.411
9	A:19:CYS:H	A:35:ARG:HD2	0.410
9	B:24:DT:H2'	B:25:DT:O4'	0.408
9	B:2:DT:O2'	B:3:DA:H5'	0.406
9	B:8:DT:N3	B:23:DA:N6	0.404
9	B:27:DC:H6	B:27:DC:O5'	0.403
10	B:19:DT:H2'	B:20:DG:H8	0.900
10	B:10:DC:H2'	B:11:DC:C6	0.890
10	A:18:PRO:HA	A:35:ARG:HE	0.888
10	B:24:DT:H2'	B:25:DT:C6	0.847
10	B:8:DT:H2'	B:9:DT:C6	0.836

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	B:19:DT:H2'	B:20:DG:C8	0.832
10	B:18:DC:H2'	B:19:DT:C6	0.798
10	B:26:DA:H2'	B:27:DC:C6	0.766
10	B:8:DT:H2'	B:9:DT:H6	0.749
10	B:9:DT:H2'	B:10:DC:O4'	0.748
10	B:27:DC:H2'	B:28:DT:H6	0.743
10	B:23:DA:H3'	B:24:DT:H71	0.731
10	B:10:DC:H2'	B:11:DC:H6	0.725
10	B:24:DT:H2'	B:25:DT:H6	0.719
10	B:23:DA:H2'	B:24:DT:O4'	0.699
10	B:13:DG:H1	B:17:DG:H1	0.685
10	B:27:DC:H2'	B:28:DT:C6	0.676
10	B:13:DG:H2'	B:14:DC:H6	0.666
10	B:28:DT:H2'	B:29:DA:H8	0.663
10	B:22:DA:H2'	B:23:DA:O4'	0.661
10	B:3:DA:H2'	B:4:DG:O4'	0.648
10	B:7:DA:H2'	B:8:DT:C6	0.633
10	B:28:DT:H2'	B:29:DA:C8	0.623
10	B:9:DT:O2'	B:10:DC:H5'	0.613
10	B:4:DG:N2	B:28:DT:H1'	0.606
10	B:1:DG:O2'	B:2:DT:H5'	0.589
10	A:53:ARG:H	A:53:ARG:HD3	0.584
10	B:21:DG:C2	B:22:DA:H1'	0.578

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	B:13:DG:H2'	B:14:DC:C6	0.575
10	B:19:DT:H73	B:19:DT:OP2	0.571
10	A:23:LYS:HE3	A:35:ARG:HB3	0.567
10	B:7:DA:H2'	B:8:DT:H71	0.556
10	B:6:DA:H2'	B:7:DA:C8	0.554
10	B:11:DC:H2'	B:12:DA:H8	0.549
10	A:55:GLN:HB3	B:8:DT:H73	0.548
10	A:61:GLN:OE1	B:22:DA:H5'	0.548
10	B:24:DT:H3'	B:25:DT:H71	0.534
10	B:11:DC:H2'	B:12:DA:C8	0.531
10	B:25:DT:O2'	B:26:DA:H5'	0.529
10	A:63:LEU:O	A:67:LYS:HG3	0.526
10	B:5:DT:H2'	B:6:DA:O4'	0.525
10	B:26:DA:H2'	B:27:DC:H6	0.507
10	A:52:THR:O	A:56:VAL:HG23	0.502
10	B:11:DC:H2'	B:12:DA:O4'	0.499
10	A:18:PRO:HG3	A:35:ARG:HH21	0.497
10	B:28:DT:H2'	B:29:DA:O4'	0.492
10	A:23:LYS:HE3	A:35:ARG:H	0.483
10	B:25:DT:H2'	B:26:DA:O4'	0.479
10	B:11:DC:H6	B:11:DC:O5'	0.470
10	A:15:ILE:N	A:15:ILE:HD12	0.467
10	B:22:DA:O2'	B:23:DA:H5'	0.466

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	B:23:DA:H2'	B:24:DT:C6	0.466
10	B:28:DT:O2'	B:29:DA:H5'	0.465
10	B:27:DC:O2'	B:28:DT:H5'	0.464
10	A:13:LEU:HD23	A:39:ILE:HD13	0.463
10	A:43:ILE:N	A:43:ILE:HD12	0.462
10	A:40:ALA:O	A:44:LYS:HG2	0.456
10	A:15:ILE:H	A:15:ILE:HD12	0.454
10	B:23:DA:H2'	B:24:DT:H6	0.447
10	B:13:DG:O2'	B:14:DC:H5'	0.445
10	B:2:DT:H2'	B:3:DA:O4'	0.436
10	A:18:PRO:HA	A:35:ARG:NE	0.434
10	B:27:DC:H3'	B:28:DT:H71	0.432
10	A:19:CYS:H	A:35:ARG:HD2	0.429
10	B:4:DG:H22	B:28:DT:H1'	0.426
10	A:55:GLN:HB3	B:8:DT:C7	0.420
10	B:28:DT:C2	B:29:DA:C8	0.417
10	A:63:LEU:HD23	A:66:ARG:HH21	0.416
10	A:65:ARG:O	A:69:ARG:HB2	0.414
10	B:7:DA:H2'	B:8:DT:H6	0.412
10	A:2:SER:HA	A:3:PRO:HD3	0.409
10	B:23:DA:C2	B:24:DT:H1'	0.401
10	B:11:DC:O2'	B:12:DA:H5'	0.400
11	B:8:DT:H2'	B:9:DT:H6	0.862

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	B:8:DT:H2'	B:9:DT:C6	0.861
11	B:24:DT:H2'	B:25:DT:C6	0.846
11	A:18:PRO:HA	A:35:ARG:HE	0.841
11	B:19:DT:H2'	B:20:DG:C8	0.827
11	B:18:DC:H2'	B:19:DT:C6	0.802
11	B:27:DC:H2'	B:28:DT:H6	0.769
11	B:22:DA:H2'	B:23:DA:O4'	0.695
11	B:26:DA:H2'	B:27:DC:C6	0.695
11	B:9:DT:H2'	B:10:DC:C6	0.673
11	B:27:DC:H2'	B:28:DT:C6	0.672
11	B:6:DA:H2'	B:7:DA:C8	0.669
11	B:24:DT:H2'	B:25:DT:H6	0.664
11	B:23:DA:H2'	B:24:DT:O4'	0.658
11	B:18:DC:H2'	B:19:DT:H6	0.657
11	B:7:DA:H2'	B:8:DT:C6	0.635
11	B:4:DG:N2	B:28:DT:H1'	0.634
11	B:8:DT:H3'	B:9:DT:H71	0.618
11	B:9:DT:H2'	B:10:DC:H6	0.610
11	B:13:DG:H2'	B:14:DC:H6	0.606
11	B:19:DT:H2'	B:20:DG:H8	0.599
11	B:3:DA:H2'	B:4:DG:O4'	0.594
11	B:18:DC:H3'	B:19:DT:H71	0.593
11	B:9:DT:H2'	B:10:DC:O4'	0.590

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	B:12:DA:H1'	B:20:DG:N2	0.574
11	B:28:DT:H2'	B:29:DA:C8	0.562
11	B:24:DT:H3'	B:25:DT:H71	0.561
11	B:21:DG:N2	B:22:DA:H1'	0.560
11	A:18:PRO:HA	A:35:ARG:NE	0.552
11	B:10:DC:H2'	B:11:DC:C6	0.552
11	A:63:LEU:O	A:67:LYS:HG3	0.545
11	B:24:DT:H73	B:24:DT:OP1	0.544
11	B:1:DG:O2'	B:2:DT:H5'	0.534
11	B:13:DG:H2'	B:14:DC:C6	0.532
11	B:28:DT:H2'	B:29:DA:H8	0.532
11	A:32:MET:HB3	B:19:DT:H4'	0.528
11	B:7:DA:H2'	B:8:DT:H71	0.523
11	B:25:DT:O2'	B:26:DA:H5'	0.511
11	B:25:DT:H2'	B:26:DA:O4'	0.509
11	A:19:CYS:H	A:35:ARG:HD2	0.507
11	B:22:DA:O2'	B:23:DA:H5'	0.504
11	A:23:LYS:HE3	A:35:ARG:H	0.501
11	A:58:SER:HB3	B:7:DA:H61	0.491
11	A:15:ILE:N	A:15:ILE:HD12	0.481
11	A:15:ILE:H	A:15:ILE:HD12	0.479
11	B:28:DT:H2'	B:29:DA:O4'	0.479
11	A:52:THR:O	A:56:VAL:HG23	0.476

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	B:13:DG:O2'	B:14:DC:H5'	0.475
11	B:27:DC:O2'	B:28:DT:H5'	0.469
11	A:32:MET:CB	B:19:DT:H4'	0.467
11	A:55:GLN:HB3	B:8:DT:H73	0.464
11	B:21:DG:C2	B:22:DA:H1'	0.464
11	B:17:DG:H2'	B:18:DC:O4'	0.463
11	A:53:ARG:H	A:53:ARG:HD3	0.462
11	B:28:DT:O2'	B:29:DA:H5'	0.462
11	A:61:GLN:OE1	B:22:DA:H5'	0.460
11	A:5:ILE:N	A:5:ILE:HD12	0.459
11	B:23:DA:H2'	B:24:DT:C6	0.459
11	B:7:DA:H2'	B:8:DT:H6	0.458
11	A:27:SER:OG	A:31:LYS:HE3	0.451
11	B:13:DG:H22	B:17:DG:H1	0.450
11	A:52:THR:O	A:55:GLN:HG2	0.447
11	B:26:DA:H2'	B:27:DC:H6	0.441
11	B:23:DA:H2'	B:24:DT:H6	0.438
11	B:11:DC:H2'	B:12:DA:O4'	0.436
11	A:36:ASN:HD21	A:56:VAL:HG12	0.435
11	A:53:ARG:HD3	A:53:ARG:N	0.434
11	B:23:DA:O2'	B:24:DT:H5'	0.434
11	A:63:LEU:HD23	A:66:ARG:HH21	0.431
11	A:18:PRO:HG3	A:35:ARG:HH21	0.424

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	B:4:DG:H22	B:28:DT:H1'	0.423
11	B:10:DC:O2'	B:11:DC:H5'	0.422
11	A:40:ALA:O	A:44:LYS:HG2	0.417
11	B:11:DC:H6	B:11:DC:O5'	0.412
11	B:2:DT:H2'	B:3:DA:O4'	0.409
11	A:55:GLN:HB3	B:8:DT:C7	0.408
11	A:52:THR:HG22	A:54:LYS:H	0.402
11	B:18:DC:O2'	B:19:DT:H5'	0.401
12	B:5:DT:H2'	B:6:DA:C8	0.863
12	B:4:DG:H2'	B:5:DT:O4'	0.846
12	B:8:DT:H2'	B:9:DT:C6	0.799
12	B:6:DA:H2'	B:7:DA:C8	0.789
12	B:12:DA:H1'	B:20:DG:N2	0.789
12	B:26:DA:H2'	B:27:DC:C6	0.737
12	B:8:DT:H2'	B:9:DT:H6	0.713
12	B:21:DG:H2'	B:22:DA:H8	0.700
12	B:9:DT:H2'	B:10:DC:C6	0.687
12	B:10:DC:H2'	B:11:DC:H6	0.669
12	B:21:DG:H2'	B:22:DA:C8	0.669
12	B:12:DA:H1'	B:20:DG:H22	0.638
12	B:10:DC:H2'	B:11:DC:C6	0.611
12	A:41:ARG:HA	A:44:LYS:HD2	0.605
12	B:23:DA:H3'	B:24:DT:H71	0.602

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	B:23:DA:H2'	B:24:DT:H6	0.600
12	B:23:DA:H2'	B:24:DT:C6	0.593
12	B:6:DA:H2'	B:7:DA:H8	0.590
12	A:23:LYS:HZ2	A:35:ARG:HB3	0.574
12	B:17:DG:H2'	B:18:DC:O4'	0.572
12	B:28:DT:H2'	B:29:DA:O4'	0.572
12	B:3:DA:H2'	B:4:DG:O4'	0.567
12	B:11:DC:H2'	B:12:DA:C8	0.559
12	A:5:ILE:HG23	A:43:ILE:HG21	0.558
12	B:11:DC:H1'	B:21:DG:N2	0.552
12	B:9:DT:H2'	B:10:DC:H6	0.548
12	A:23:LYS:NZ	A:35:ARG:HB3	0.544
12	B:20:DG:H2'	B:21:DG:O4'	0.542
12	B:28:DT:O2'	B:29:DA:H5'	0.535
12	A:23:LYS:HZ2	A:36:ASN:H	0.517
12	B:27:DC:H2'	B:28:DT:H6	0.515
12	B:24:DT:O2'	B:25:DT:H5'	0.512
12	B:5:DT:H71	B:5:DT:OP1	0.510
12	B:11:DC:H1'	B:21:DG:H21	0.509
12	B:26:DA:H2'	B:27:DC:O4'	0.508
12	B:1:DG:H3'	B:2:DT:H71	0.507
12	A:64:ALA:HA	A:67:LYS:HE3	0.503
12	B:25:DT:H2'	B:26:DA:C8	0.503

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	B:27:DC:O2'	B:28:DT:H5'	0.501
12	A:52:THR:HG22	A:53:ARG:N	0.498
12	A:47:THR:HG23	A:49:LYS:H	0.495
12	B:23:DA:H2'	B:24:DT:O4'	0.495
12	B:19:DT:H2'	B:20:DG:C8	0.493
12	B:18:DC:O2'	B:19:DT:H5'	0.483
12	B:27:DC:H2'	B:28:DT:C6	0.479
12	B:14:DC:H2'	B:15:DG:H8	0.474
12	B:7:DA:O2'	B:8:DT:H5'	0.473
12	B:1:DG:H2'	B:2:DT:O4'	0.469
12	B:10:DC:O2'	B:11:DC:H5'	0.468
12	B:24:DT:H2'	B:25:DT:H6	0.463
12	B:11:DC:H2'	B:12:DA:O4'	0.457
12	B:13:DG:O2'	B:14:DC:H5'	0.455
12	A:52:THR:HG22	A:53:ARG:H	0.449
12	A:38:LEU:O	A:41:ARG:HG3	0.444
12	B:19:DT:H6	B:19:DT:O5'	0.443
12	A:31:LYS:HB3	A:31:LYS:NZ	0.432
12	B:24:DT:H2'	B:25:DT:C6	0.432
12	B:26:DA:H8	B:26:DA:O5'	0.429
12	B:17:DG:O2'	B:18:DC:H5'	0.427
12	B:28:DT:H2'	B:29:DA:C8	0.427
12	B:4:DG:H8	B:4:DG:O5'	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
12	A:55:GLN:HG2	B:8:DT:C7	0.421
12	B:23:DA:O2'	B:24:DT:H5'	0.419
12	B:8:DT:H3'	B:9:DT:H71	0.418
12	A:5:ILE:HD11	A:49:LYS:HG2	0.415
12	B:22:DA:O2'	B:23:DA:H5'	0.408
12	A:23:LYS:NZ	A:36:ASN:H	0.404
12	B:27:DC:H6	B:27:DC:O5'	0.403
12	B:5:DT:H2'	B:6:DA:H8	0.402
12	B:1:DG:O2'	B:2:DT:H5'	0.401
13	B:4:DG:N2	B:28:DT:H1'	0.817
13	B:4:DG:H2'	B:5:DT:O4'	0.730
13	B:24:DT:H2'	B:25:DT:O4'	0.724
13	B:22:DA:H2'	B:23:DA:C8	0.662
13	B:5:DT:H2'	B:6:DA:O4'	0.651
13	B:4:DG:H22	B:28:DT:H1'	0.639
13	B:13:DG:H2'	B:14:DC:O4'	0.611
13	A:41:ARG:HA	A:44:LYS:HE2	0.605
13	B:27:DC:O2'	B:28:DT:H5'	0.591
13	B:28:DT:O2'	B:29:DA:H5'	0.588
13	B:18:DC:H2'	B:19:DT:H6	0.585
13	B:1:DG:H3'	B:2:DT:H71	0.582
13	B:19:DT:H2'	B:20:DG:O4'	0.579
13	B:6:DA:H2'	B:7:DA:C8	0.574

Model ID	Atom-1	Atom-2	Clash overlap (Å)
13	B:18:DC:H2'	B:19:DT:C6	0.574
13	A:23:LYS:NZ	A:35:ARG:H	0.560
13	A:31:LYS:HB3	A:31:LYS:NZ	0.541
13	B:19:DT:O2'	B:20:DG:H5'	0.541
13	B:21:DG:H2'	B:22:DA:H8	0.539
13	B:21:DG:H2'	B:22:DA:C8	0.537
13	B:25:DT:H73	B:25:DT:OP1	0.536
13	B:9:DT:H2'	B:10:DC:O4'	0.515
13	B:20:DG:H2'	B:21:DG:C8	0.515
13	B:6:DA:H2'	B:7:DA:H8	0.507
13	A:24:ILE:H	A:24:ILE:HD12	0.506
13	A:23:LYS:HZ1	A:35:ARG:H	0.501
13	A:55:GLN:O	A:59:HIS:HB2	0.493
13	A:5:ILE:HG12	A:47:THR:HG21	0.492
13	B:1:DG:H2'	B:2:DT:O4'	0.477
13	A:33:TYR:HD2	A:37:GLU:HB3	0.476
13	A:64:ALA:HA	A:67:LYS:HE2	0.470
13	B:4:DG:C2	B:5:DT:H1'	0.470
13	B:26:DA:H2'	B:27:DC:C6	0.468
13	B:26:DA:H2'	B:27:DC:H6	0.467
13	B:20:DG:H2'	B:21:DG:O4'	0.465
13	B:5:DT:H71	B:5:DT:OP1	0.461
13	B:28:DT:H2'	B:29:DA:O4'	0.449

Model ID	Atom-1	Atom-2	Clash overlap (Å)
13	B:2:DT:H2'	B:3:DA:C8	0.448
13	A:24:ILE:N	A:24:ILE:HD12	0.447
13	B:24:DT:O2'	B:25:DT:H5'	0.440
13	B:10:DC:H6	B:10:DC:O5'	0.436
13	B:23:DA:H8	B:23:DA:O5'	0.434
13	B:27:DC:H2'	B:28:DT:O4'	0.419
13	B:13:DG:C2'	B:14:DC:H5'	0.417
13	B:9:DT:O2'	B:10:DC:H5'	0.415
13	B:16:DC:H6	B:16:DC:O5'	0.415
13	B:17:DG:H2'	B:18:DC:O4'	0.415
13	A:49:LYS:HE3	A:51:ARG:HH22	0.404
13	B:2:DT:O2'	B:3:DA:H5'	0.402
13	B:2:DT:H2'	B:3:DA:O4'	0.401
14	B:4:DG:H2'	B:5:DT:O4'	0.842
14	B:5:DT:H2'	B:6:DA:C8	0.809
14	B:6:DA:H2'	B:7:DA:C8	0.780
14	B:26:DA:H2'	B:27:DC:C6	0.761
14	B:8:DT:H2'	B:9:DT:C6	0.724
14	B:12:DA:H1'	B:20:DG:N2	0.694
14	B:9:DT:H2'	B:10:DC:C6	0.665
14	B:19:DT:H2'	B:20:DG:C8	0.641
14	B:21:DG:H2'	B:22:DA:C8	0.630
14	B:6:DA:H2'	B:7:DA:H8	0.626

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	B:21:DG:H2'	B:22:DA:H8	0.624
14	A:41:ARG:HA	A:44:LYS:HD2	0.615
14	B:8:DT:H2'	B:9:DT:H6	0.608
14	B:13:DG:O2'	B:14:DC:H5'	0.589
14	B:12:DA:H1'	B:20:DG:H22	0.584
14	B:3:DA:H2'	B:4:DG:O4'	0.582
14	B:23:DA:H2'	B:24:DT:O4'	0.582
14	B:17:DG:H2'	B:18:DC:C6	0.576
14	B:24:DT:H2'	B:25:DT:H6	0.567
14	B:11:DC:H1'	B:21:DG:H21	0.552
14	B:24:DT:H2'	B:25:DT:C6	0.545
14	B:10:DC:H2'	B:11:DC:H6	0.544
14	B:27:DC:O2'	B:28:DT:H5'	0.536
14	B:23:DA:H2'	B:24:DT:C6	0.532
14	B:23:DA:H2'	B:24:DT:H6	0.524
14	A:23:LYS:NZ	A:35:ARG:HB3	0.515
14	B:5:DT:H73	B:5:DT:OP1	0.513
14	B:7:DA:H2'	B:8:DT:C6	0.510
14	B:10:DC:O2'	B:11:DC:H5'	0.510
14	B:4:DG:H8	B:4:DG:O5'	0.510
14	B:27:DC:H2'	B:28:DT:H6	0.507
14	B:11:DC:H2'	B:12:DA:O4'	0.503
14	B:7:DA:H2'	B:8:DT:H6	0.502

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	A:23:LYS:HZ2	A:36:ASN:H	0.501
14	B:26:DA:H2'	B:27:DC:O4'	0.497
14	A:23:LYS:HZ3	A:35:ARG:HB3	0.495
14	A:52:THR:HG22	A:53:ARG:N	0.492
14	B:28:DT:H2'	B:29:DA:O4'	0.490
14	B:9:DT:H2'	B:10:DC:O4'	0.486
14	B:24:DT:O2'	B:25:DT:H5'	0.484
14	A:63:LEU:HD23	A:66:ARG:HH11	0.482
14	B:28:DT:O2'	B:29:DA:H5'	0.481
14	B:25:DT:H2'	B:26:DA:C8	0.473
14	B:10:DC:H2'	B:11:DC:C6	0.471
14	A:31:LYS:HB3	A:31:LYS:NZ	0.467
14	B:1:DG:H3'	B:2:DT:H71	0.465
14	B:18:DC:H6	B:18:DC:O5'	0.463
14	B:22:DA:C2	B:23:DA:C4	0.454
14	A:64:ALA:HA	A:67:LYS:HG3	0.453
14	B:27:DC:H2'	B:28:DT:C6	0.451
14	B:11:DC:H1'	B:21:DG:N2	0.450
14	B:1:DG:H2'	B:2:DT:O4'	0.444
14	B:23:DA:O2'	B:24:DT:H5'	0.444
14	B:19:DT:H6	B:19:DT:O5'	0.444
14	B:23:DA:H3'	B:24:DT:H71	0.443
14	B:10:DC:H6	B:10:DC:O5'	0.440

Model ID	Atom-1	Atom-2	Clash overlap (Å)
14	A:55:GLN:HG2	B:8:DT:C7	0.437
14	A:38:LEU:O	A:41:ARG:HG3	0.429
14	A:18:PRO:HA	A:35:ARG:NE	0.415
14	B:28:DT:H2'	B:29:DA:C8	0.410
14	B:27:DC:H6	B:27:DC:O5'	0.410
14	B:14:DC:H2'	B:15:DG:H8	0.409
14	B:7:DA:O2'	B:8:DT:H5'	0.408
14	B:11:DC:H2'	B:12:DA:C8	0.401
15	B:19:DT:H2'	B:20:DG:C8	0.935
15	B:9:DT:H2'	B:10:DC:O4'	0.901
15	A:18:PRO:HA	A:35:ARG:HE	0.833
15	B:24:DT:H2'	B:25:DT:C6	0.814
15	B:19:DT:H2'	B:20:DG:H8	0.787
15	B:18:DC:H2'	B:19:DT:C6	0.785
15	B:27:DC:H2'	B:28:DT:H6	0.769
15	B:10:DC:H2'	B:11:DC:C6	0.762
15	B:6:DA:H2'	B:7:DA:C8	0.755
15	B:4:DG:N2	B:28:DT:H1'	0.755
15	B:23:DA:H2'	B:24:DT:O4'	0.741
15	A:55:GLN:HB3	B:8:DT:H73	0.707
15	A:64:ALA:HA	A:67:LYS:HE2	0.687
15	B:10:DC:H2'	B:11:DC:H6	0.684
15	B:26:DA:H2'	B:27:DC:C6	0.683

Model ID	Atom-1	Atom-2	Clash overlap (Å)
15	B:3:DA:H2'	B:4:DG:O4'	0.668
15	B:27:DC:H2'	B:28:DT:C6	0.664
15	A:55:GLN:HE22	B:7:DA:H3'	0.663
15	B:7:DA:H2'	B:8:DT:C6	0.663
15	A:32:MET:HB3	B:19:DT:H4'	0.623
15	B:23:DA:H3'	B:24:DT:H71	0.617
15	B:24:DT:H2'	B:25:DT:H6	0.604
15	A:36:ASN:HD21	A:56:VAL:HG12	0.598
15	A:32:MET:CB	B:19:DT:H4'	0.572
15	A:55:GLN:NE2	B:7:DA:H3'	0.572
15	B:28:DT:H2'	B:29:DA:C8	0.566
15	B:18:DC:H2'	B:19:DT:H6	0.565
15	B:11:DC:H2'	B:12:DA:H8	0.562
15	B:1:DG:O2'	B:2:DT:H5'	0.560
15	B:25:DT:O2'	B:26:DA:H5'	0.553
15	B:28:DT:H2'	B:29:DA:H8	0.550
15	B:25:DT:H2'	B:26:DA:O4'	0.548
15	B:19:DT:H73	B:19:DT:OP2	0.539
15	B:13:DG:H2'	B:14:DC:H6	0.536
15	A:23:LYS:HE3	A:35:ARG:H	0.524
15	B:11:DC:H2'	B:12:DA:O4'	0.523
15	B:13:DG:H2'	B:14:DC:C6	0.519
15	A:15:ILE:H	A:15:ILE:HD12	0.517

Model ID	Atom-1	Atom-2	Clash overlap (Å)
15	B:11:DC:H2'	B:12:DA:C8	0.517
15	B:8:DT:O2'	B:9:DT:H5'	0.510
15	B:14:DC:H2'	B:15:DG:H8	0.500
15	B:4:DG:H22	B:28:DT:H1'	0.496
15	A:15:ILE:N	A:15:ILE:HD12	0.477
15	A:52:THR:O	A:56:VAL:HG23	0.477
15	B:2:DT:H2'	B:3:DA:O4'	0.471
15	B:28:DT:O2'	B:29:DA:H5'	0.471
15	B:26:DA:H2'	B:27:DC:H6	0.467
15	B:27:DC:O2'	B:28:DT:H5'	0.466
15	B:6:DA:H2'	B:7:DA:H8	0.464
15	B:9:DT:H71	B:9:DT:OP2	0.462
15	B:19:DT:C2'	B:20:DG:H8	0.461
15	B:14:DC:H2'	B:15:DG:C8	0.460
15	A:55:GLN:HB3	B:8:DT:C7	0.458
15	A:19:CYS:H	A:35:ARG:HD2	0.456
15	B:13:DG:O2'	B:14:DC:H5'	0.456
15	B:27:DC:H3'	B:28:DT:H71	0.455
15	A:53:ARG:H	A:53:ARG:HD3	0.452
15	B:7:DA:H2'	B:8:DT:H6	0.448
15	A:3:PRO:HG2	A:4:ASP:H	0.447
15	B:17:DG:H2'	B:18:DC:O4'	0.446
15	A:53:ARG:HD3	A:53:ARG:N	0.437

Model ID	Atom-1	Atom-2	Clash overlap (Å)
15	B:24:DT:H3'	B:25:DT:H71	0.433
15	B:21:DG:C2	B:22:DA:H1'	0.431
15	B:23:DA:H2'	B:24:DT:C6	0.430
15	A:27:SER:OG	A:31:LYS:HE3	0.425
15	A:61:GLN:OE1	B:22:DA:H5'	0.424
15	B:9:DT:H2'	B:10:DC:C4'	0.423
15	B:28:DT:H2'	B:29:DA:O4'	0.422
15	B:9:DT:H2'	B:10:DC:C5'	0.420
15	A:2:SER:HA	A:3:PRO:HD2	0.416
15	A:43:ILE:N	A:43:ILE:HD12	0.416
15	B:22:DA:O2'	B:23:DA:H5'	0.416
15	B:9:DT:C2'	B:10:DC:H5'	0.414
15	B:8:DT:H2'	B:9:DT:C6	0.413
15	B:23:DA:H2'	B:24:DT:H6	0.413
15	B:22:DA:H2'	B:23:DA:O4'	0.408
15	B:11:DC:O2'	B:12:DA:H5'	0.407
15	B:24:DT:C2	B:25:DT:C5	0.406
16	B:26:DA:H2'	B:27:DC:C6	0.909
16	B:12:DA:H2'	B:13:DG:H8	0.815
16	B:12:DA:H2'	B:13:DG:C8	0.790
16	A:23:LYS:HZ3	A:35:ARG:HB3	0.763
16	B:5:DT:H2'	B:6:DA:C8	0.752
16	B:17:DG:H2'	B:18:DC:C6	0.737

Model ID	Atom-1	Atom-2	Clash overlap (Å)
16	B:24:DT:H2'	B:25:DT:C6	0.728
16	B:4:DG:H2'	B:5:DT:H5'	0.706
16	B:27:DC:H2'	B:28:DT:C6	0.698
16	B:2:DT:H2'	B:3:DA:C8	0.697
16	B:24:DT:H2'	B:25:DT:H6	0.689
16	A:66:ARG:HH22	B:5:DT:H3'	0.680
16	B:7:DA:H2'	B:8:DT:C6	0.678
16	B:8:DT:H2'	B:9:DT:H6	0.673
16	B:26:DA:H2'	B:27:DC:H6	0.672
16	B:22:DA:H2'	B:23:DA:H8	0.668
16	B:4:DG:C2'	B:5:DT:H5'	0.654
16	B:7:DA:H3'	B:8:DT:H71	0.640
16	B:8:DT:O2'	B:9:DT:H5'	0.626
16	A:64:ALA:HA	A:67:LYS:HE2	0.620
16	B:4:DG:H2'	B:5:DT:C5'	0.620
16	B:27:DC:H2'	B:28:DT:H6	0.620
16	B:12:DA:H1'	B:20:DG:N2	0.612
16	A:54:LYS:HA	A:54:LYS:HE2	0.609
16	B:23:DA:O2'	B:24:DT:H5'	0.605
16	B:28:DT:H2'	B:29:DA:O4'	0.603
16	B:10:DC:H2'	B:11:DC:C6	0.595
16	A:40:ALA:O	A:44:LYS:HG2	0.593
16	B:28:DT:H73	B:28:DT:OP1	0.590

Model ID	Atom-1	Atom-2	Clash overlap (Å)
16	B:13:DG:O2'	B:14:DC:H5'	0.589
16	B:10:DC:H2'	B:11:DC:H6	0.587
16	B:23:DA:H2'	B:24:DT:O4'	0.581
16	B:7:DA:H2'	B:8:DT:H6	0.579
16	B:22:DA:H2'	B:23:DA:C8	0.578
16	B:13:DG:N2	B:19:DT:H1'	0.576
16	B:4:DG:H2'	B:5:DT:O4'	0.573
16	A:31:LYS:HB3	A:31:LYS:NZ	0.563
16	B:28:DT:H2'	B:29:DA:C8	0.562
16	B:8:DT:H2'	B:9:DT:C6	0.540
16	B:21:DG:H2'	B:22:DA:O4'	0.534
16	B:18:DC:H2'	B:19:DT:H6	0.531
16	B:13:DG:H2'	B:14:DC:O4'	0.529
16	B:18:DC:H3'	B:19:DT:H71	0.524
16	B:7:DA:H2'	B:8:DT:O4'	0.512
16	B:12:DA:H2	B:19:DT:H3	0.509
16	B:24:DT:O2'	B:25:DT:H5'	0.500
16	B:18:DC:H2'	B:19:DT:C6	0.484
16	B:24:DT:H3'	B:25:DT:H71	0.483
16	B:29:DA:H2'	B:30:DC:C6	0.479
16	B:6:DA:H2'	B:7:DA:C8	0.478
16	B:18:DC:H6	B:18:DC:O5'	0.474
16	B:16:DC:H2'	B:17:DG:C8	0.473

Model ID	Atom-1	Atom-2	Clash overlap (Å)
16	B:28:DT:H2'	B:29:DA:H8	0.470
16	B:4:DG:H2'	B:5:DT:C4'	0.467
16	A:60:ILE:O	A:60:ILE:HD13	0.459
16	B:27:DC:O2'	B:28:DT:H5'	0.459
16	B:1:DG:H2'	B:2:DT:C6	0.445
16	B:25:DT:H2'	B:26:DA:O4'	0.440
16	A:32:MET:CE	B:19:DT:H5"	0.437
16	B:4:DG:N2	B:28:DT:H1'	0.435
16	B:11:DC:H1'	B:21:DG:N2	0.428
16	B:6:DA:O2'	B:7:DA:H5'	0.414
16	B:4:DG:H22	B:28:DT:H1'	0.407
16	B:11:DC:H2'	B:12:DA:O4'	0.405
16	B:29:DA:H2'	B:30:DC:H6	0.405
16	B:6:DA:H2'	B:7:DA:O4'	0.405
16	B:2:DT:H2'	B:3:DA:H8	0.403
17	B:8:DT:H3'	B:9:DT:H71	0.952
17	B:18:DC:H2'	B:19:DT:C6	0.900
17	B:17:DG:H2'	B:18:DC:O4'	0.852
17	B:5:DT:H2'	B:6:DA:O4'	0.805
17	B:4:DG:H3'	B:5:DT:H71	0.794
17	B:10:DC:H2'	B:11:DC:C6	0.767
17	B:10:DC:H2'	B:11:DC:H6	0.756
17	B:4:DG:N2	B:28:DT:H1'	0.733

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	B:25:DT:H2'	B:26:DA:O4'	0.724
17	B:13:DG:O2'	B:14:DC:H5'	0.720
17	A:32:MET:HE1	B:18:DC:H4'	0.693
17	B:19:DT:H2'	B:20:DG:C8	0.691
17	B:26:DA:H2'	B:27:DC:C6	0.685
17	B:12:DA:H2'	B:13:DG:H8	0.659
17	A:23:LYS:HZ2	A:35:ARG:HB3	0.647
17	B:12:DA:H1'	B:20:DG:N2	0.624
17	B:18:DC:H2'	B:19:DT:H6	0.617
17	B:19:DT:H2'	B:20:DG:H8	0.594
17	A:61:GLN:NE2	B:22:DA:H3'	0.593
17	A:40:ALA:HB2	A:56:VAL:HG21	0.588
17	B:28:DT:O2'	B:29:DA:H5'	0.587
17	B:12:DA:H2'	B:13:DG:C8	0.586
17	B:27:DC:H2'	B:28:DT:H6	0.568
17	B:26:DA:H2'	B:27:DC:H6	0.561
17	A:23:LYS:CE	B:20:DG:H5''	0.559
17	A:31:LYS:HB3	A:31:LYS:NZ	0.558
17	B:8:DT:H2'	B:9:DT:C6	0.554
17	B:4:DG:H2'	B:5:DT:C6	0.552
17	A:23:LYS:HZ1	A:36:ASN:H	0.550
17	A:23:LYS:HE3	B:20:DG:H5''	0.525
17	B:21:DG:H2'	B:22:DA:O4'	0.521

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	A:47:THR:HG23	A:49:LYS:H	0.510
17	A:41:ARG:HA	A:44:LYS:HD2	0.508
17	B:28:DT:H2'	B:29:DA:O4'	0.507
17	B:5:DT:C2'	B:6:DA:H5'	0.502
17	A:23:LYS:NZ	A:35:ARG:HB3	0.501
17	B:5:DT:H2'	B:6:DA:C5'	0.501
17	B:4:DG:H22	B:28:DT:H1'	0.498
17	B:11:DC:H2'	B:12:DA:O4'	0.493
17	B:5:DT:H2'	B:6:DA:H5'	0.490
17	A:52:THR:HB	A:55:GLN:HG3	0.481
17	A:61:GLN:HE21	B:22:DA:H3'	0.475
17	B:27:DC:H2'	B:28:DT:C6	0.468
17	B:10:DC:H6	B:10:DC:O5'	0.467
17	B:22:DA:H8	B:22:DA:O5'	0.459
17	B:22:DA:O2'	B:23:DA:H5'	0.454
17	B:9:DT:H2'	B:10:DC:O4'	0.452
17	B:12:DA:O2'	B:13:DG:H5'	0.450
17	B:1:DG:H2'	B:2:DT:H6	0.447
17	B:19:DT:O2'	B:20:DG:H5'	0.447
17	B:5:DT:H2'	B:6:DA:C4'	0.445
17	B:2:DT:H2'	B:3:DA:O4'	0.436
17	B:21:DG:H2'	B:22:DA:C8	0.435
17	B:4:DG:H21	B:28:DT:H1'	0.433

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	A:65:ARG:HA	A:65:ARG:HE	0.430
17	B:12:DA:H1'	B:20:DG:H22	0.428
17	B:8:DT:H2'	B:9:DT:H6	0.427
17	B:22:DA:H2'	B:23:DA:O4'	0.427
17	A:15:ILE:N	A:15:ILE:HD12	0.426
17	B:4:DG:C3'	B:5:DT:H71	0.425
17	B:27:DC:H6	B:27:DC:O5'	0.425
17	B:1:DG:H2'	B:2:DT:C6	0.424
17	A:55:GLN:HE21	B:8:DT:P	0.422
17	A:52:THR:HG22	A:53:ARG:N	0.420
17	B:12:DA:H61	B:18:DC:H42	0.419
17	B:20:DG:H2'	B:21:DG:C8	0.410
17	B:23:DA:H8	B:23:DA:O5'	0.403
17	B:7:DA:N1	B:25:DT:N3	0.403
17	B:27:DC:H3'	B:28:DT:H71	0.401
18	B:4:DG:H2'	B:5:DT:O4'	0.820
18	B:6:DA:H2'	B:7:DA:C8	0.750
18	B:26:DA:H2'	B:27:DC:C6	0.744
18	B:8:DT:H2'	B:9:DT:C6	0.731
18	B:5:DT:H2'	B:6:DA:C8	0.716
18	B:9:DT:H2'	B:10:DC:C6	0.657
18	A:41:ARG:HA	A:44:LYS:HD2	0.646
18	B:12:DA:H1'	B:20:DG:N2	0.642

Model ID	Atom-1	Atom-2	Clash overlap (Å)
18	B:8:DT:H2'	B:9:DT:H6	0.618
18	B:27:DC:O2'	B:28:DT:H5'	0.612
18	B:24:DT:H2'	B:25:DT:H6	0.596
18	B:24:DT:H2'	B:25:DT:C6	0.591
18	B:19:DT:H2'	B:20:DG:C8	0.584
18	B:25:DT:H2'	B:26:DA:C8	0.558
18	B:18:DC:O2'	B:19:DT:H5'	0.553
18	A:18:PRO:HA	A:35:ARG:NE	0.549
18	B:11:DC:H1'	B:21:DG:H21	0.546
18	B:12:DA:H1'	B:20:DG:H22	0.546
18	B:23:DA:H2'	B:24:DT:H6	0.540
18	B:10:DC:H2'	B:11:DC:H6	0.538
18	B:17:DG:H2'	B:18:DC:C6	0.538
18	B:3:DA:H2'	B:4:DG:O4'	0.535
18	B:6:DA:H2'	B:7:DA:H8	0.535
18	B:23:DA:O2'	B:24:DT:H5'	0.527
18	B:13:DG:O2'	B:14:DC:H5'	0.525
18	A:23:LYS:NZ	A:35:ARG:HB3	0.523
18	B:4:DG:H8	B:4:DG:O5'	0.523
18	B:1:DG:H3'	B:2:DT:H71	0.521
18	B:26:DA:H2'	B:27:DC:O4'	0.519
18	A:52:THR:HG22	A:53:ARG:N	0.516
18	B:21:DG:H2'	B:22:DA:C8	0.515

Model ID	Atom-1	Atom-2	Clash overlap (Å)
18	B:21:DG:H2'	B:22:DA:H8	0.509
18	B:28:DT:H2'	B:29:DA:O4'	0.509
18	A:23:LYS:HZ2	A:35:ARG:HB3	0.506
18	B:7:DA:H2'	B:8:DT:C6	0.506
18	B:28:DT:H2'	B:29:DA:C8	0.506
18	B:27:DC:H2'	B:28:DT:H6	0.497
18	B:11:DC:H1'	B:21:DG:N2	0.495
18	B:20:DG:H2'	B:21:DG:O4'	0.491
18	A:52:THR:HG22	A:53:ARG:H	0.488
18	B:10:DC:O2'	B:11:DC:H5'	0.488
18	B:9:DT:H2'	B:10:DC:O4'	0.486
18	B:23:DA:H2'	B:24:DT:O4'	0.485
18	A:18:PRO:HA	A:35:ARG:HE	0.484
18	A:31:LYS:HB3	A:31:LYS:NZ	0.468
18	B:22:DA:C2	B:23:DA:C4	0.465
18	B:28:DT:H2'	B:29:DA:H8	0.465
18	B:23:DA:H2'	B:24:DT:C6	0.464
18	B:7:DA:H2'	B:8:DT:H6	0.463
18	B:10:DC:H2'	B:11:DC:C6	0.461
18	B:28:DT:O2'	B:29:DA:H5'	0.461
18	A:6:GLU:O	A:10:GLN:HG2	0.452
18	B:19:DT:H6	B:19:DT:O5'	0.443
18	B:18:DC:H2'	B:19:DT:O4'	0.442

Model ID	Atom-1	Atom-2	Clash overlap (Å)
18	B:1:DG:H2'	B:2:DT:O4'	0.441
18	B:11:DC:H2'	B:12:DA:O4'	0.439
18	A:38:LEU:O	A:41:ARG:HG3	0.438
18	B:23:DA:H3'	B:24:DT:H71	0.438
18	B:26:DA:H2'	B:27:DC:H6	0.438
18	B:11:DC:H2'	B:12:DA:C8	0.433
18	B:22:DA:H2'	B:23:DA:C8	0.433
18	B:26:DA:H8	B:26:DA:O5'	0.426
18	B:10:DC:H6	B:10:DC:O5'	0.425
18	B:1:DG:H2'	B:2:DT:C6	0.418
18	B:6:DA:H2'	B:7:DA:O4'	0.416
18	A:55:GLN:HG2	B:8:DT:C7	0.415
18	B:7:DA:O2'	B:8:DT:H5'	0.401
18	B:24:DT:O2'	B:25:DT:H5'	0.400
19	B:9:DT:H2'	B:10:DC:O4'	0.913
19	A:55:GLN:HB3	B:8:DT:H73	0.886
19	A:18:PRO:HA	A:35:ARG:HE	0.878
19	B:24:DT:H2'	B:25:DT:C6	0.827
19	B:19:DT:H2'	B:20:DG:C8	0.794
19	B:18:DC:H2'	B:19:DT:C6	0.772
19	B:4:DG:N2	B:28:DT:H1'	0.756
19	B:10:DC:H2'	B:11:DC:C6	0.740
19	B:12:DA:H1'	B:20:DG:N2	0.727

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	B:26:DA:H2'	B:27:DC:C6	0.701
19	B:22:DA:H2'	B:23:DA:O4'	0.676
19	B:13:DG:H1	B:17:DG:H1	0.666
19	A:55:GLN:HB3	B:8:DT:C7	0.665
19	B:7:DA:H2'	B:8:DT:C6	0.659
19	A:18:PRO:HA	A:35:ARG:NE	0.626
19	B:23:DA:H3'	B:24:DT:H71	0.621
19	B:24:DT:H2'	B:25:DT:H6	0.613
19	B:8:DT:O2'	B:9:DT:H5'	0.605
19	B:6:DA:H2'	B:7:DA:C8	0.600
19	B:3:DA:H2'	B:4:DG:O4'	0.593
19	B:27:DC:H2'	B:28:DT:H6	0.586
19	B:28:DT:O2'	B:29:DA:H5'	0.584
19	B:11:DC:H2'	B:12:DA:O4'	0.583
19	B:25:DT:H73	B:25:DT:OP1	0.582
19	A:63:LEU:O	A:67:LYS:HG3	0.572
19	B:23:DA:H2'	B:24:DT:O4'	0.569
19	B:1:DG:H2'	B:2:DT:C6	0.568
19	B:7:DA:H2'	B:8:DT:H71	0.568
19	B:27:DC:O2'	B:28:DT:H5'	0.548
19	A:61:GLN:OE1	B:22:DA:H5'	0.543
19	A:19:CYS:H	A:35:ARG:HD2	0.542
19	B:13:DG:H2'	B:14:DC:H6	0.530

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:15:ILE:H	A:15:ILE:HD12	0.524
19	B:4:DG:H22	B:28:DT:H1'	0.523
19	B:13:DG:O2'	B:14:DC:H5'	0.521
19	B:10:DC:H2'	B:11:DC:C5	0.515
19	B:2:DT:O2'	B:3:DA:H5'	0.513
19	B:26:DA:H2'	B:27:DC:H6	0.512
19	B:19:DT:H2'	B:20:DG:H8	0.509
19	B:1:DG:H2'	B:2:DT:H6	0.504
19	A:52:THR:O	A:56:VAL:HG23	0.503
19	B:23:DA:H2'	B:24:DT:H6	0.503
19	A:47:THR:HG23	A:49:LYS:H	0.502
19	B:11:DC:O2'	B:12:DA:H5'	0.501
19	B:12:DA:H1'	B:20:DG:H21	0.500
19	A:23:LYS:HE3	A:35:ARG:HB3	0.496
19	B:23:DA:H2'	B:24:DT:C6	0.495
19	B:25:DT:H2'	B:26:DA:O4'	0.493
19	B:5:DT:H2'	B:6:DA:O4'	0.492
19	B:25:DT:O2'	B:26:DA:H5'	0.491
19	B:22:DA:O2'	B:23:DA:H5'	0.477
19	B:27:DC:H2'	B:28:DT:C6	0.473
19	A:53:ARG:H	A:53:ARG:HD3	0.469
19	A:5:ILE:N	A:5:ILE:HD12	0.468
19	A:5:ILE:H	A:5:ILE:HD12	0.463

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	A:55:GLN:HE21	B:8:DT:C7	0.460
19	B:23:DA:O2'	B:24:DT:H5'	0.460
19	B:28:DT:H2'	B:29:DA:O4'	0.458
19	A:15:ILE:N	A:15:ILE:HD12	0.456
19	B:12:DA:H1'	B:20:DG:H22	0.430
19	B:13:DG:H2'	B:14:DC:C6	0.428
19	B:9:DT:H2'	B:10:DC:C4'	0.421
19	A:27:SER:OG	A:31:LYS:HE3	0.418
19	A:19:CYS:SG	A:35:ARG:HB2	0.406
19	B:9:DT:H2'	B:10:DC:C5'	0.404
19	B:25:DT:H2'	B:26:DA:C8	0.404
20	B:4:DG:H2'	B:5:DT:O4'	0.860
20	B:8:DT:H2'	B:9:DT:C6	0.825
20	B:5:DT:H2'	B:6:DA:C8	0.787
20	B:9:DT:H2'	B:10:DC:C6	0.742
20	B:6:DA:H2'	B:7:DA:C8	0.740
20	B:8:DT:H2'	B:9:DT:H6	0.710
20	B:27:DC:O2'	B:28:DT:H5'	0.687
20	B:24:DT:H2'	B:25:DT:C6	0.679
20	B:6:DA:H2'	B:7:DA:H8	0.655
20	B:26:DA:H2'	B:27:DC:O4'	0.648
20	B:24:DT:H2'	B:25:DT:H6	0.644
20	B:26:DA:H2'	B:27:DC:C6	0.638

Model ID	Atom-1	Atom-2	Clash overlap (Å)
20	A:23:LYS:HZ2	A:35:ARG:HB3	0.616
20	B:25:DT:H2'	B:26:DA:C8	0.609
20	B:12:DA:H1'	B:20:DG:N2	0.588
20	A:41:ARG:HA	A:44:LYS:HD2	0.565
20	A:23:LYS:NZ	A:35:ARG:HB3	0.564
20	B:13:DG:O2'	B:14:DC:H5'	0.563
20	B:1:DG:H3'	B:2:DT:H71	0.559
20	A:66:ARG:NH2	B:4:DG:H5''	0.556
20	B:3:DA:H2'	B:4:DG:O4'	0.555
20	B:21:DG:H2'	B:22:DA:H8	0.554
20	B:23:DA:H2'	B:24:DT:H6	0.544
20	B:28:DT:H2'	B:29:DA:C8	0.543
20	B:11:DC:H2'	B:12:DA:C8	0.542
20	A:66:ARG:HH22	B:4:DG:H5''	0.539
20	B:21:DG:H2'	B:22:DA:C8	0.537
20	B:19:DT:H2'	B:20:DG:C8	0.534
20	B:4:DG:C2'	B:5:DT:H5'	0.516
20	B:4:DG:H2'	B:5:DT:C4'	0.511
20	B:23:DA:H2'	B:24:DT:C6	0.509
20	B:1:DG:H2'	B:2:DT:C6	0.504
20	B:10:DC:O2'	B:11:DC:H5'	0.496
20	B:12:DA:H1'	B:20:DG:H22	0.496
20	B:23:DA:H2'	B:24:DT:O4'	0.496

Model ID	Atom-1	Atom-2	Clash overlap (Å)
20	B:11:DC:H1'	B:21:DG:H21	0.490
20	B:7:DA:O2'	B:8:DT:H5'	0.489
20	B:10:DC:H6	B:10:DC:O5'	0.485
20	B:26:DA:H2'	B:27:DC:H6	0.484
20	B:4:DG:H2'	B:5:DT:C5'	0.479
20	B:17:DG:O2'	B:18:DC:H5'	0.479
20	A:24:ILE:HD11	A:32:MET:SD	0.465
20	B:4:DG:H8	B:4:DG:O5'	0.460
20	B:27:DC:H2'	B:28:DT:H6	0.459
20	B:11:DC:H2'	B:12:DA:O4'	0.454
20	B:8:DT:H3'	B:9:DT:H71	0.453
20	B:23:DA:O2'	B:24:DT:H5'	0.450
20	B:10:DC:H2'	B:11:DC:H6	0.447
20	B:6:DA:H2'	B:7:DA:O4'	0.446
20	B:4:DG:H2'	B:5:DT:H5'	0.442
20	B:25:DT:H2'	B:26:DA:O4'	0.441
20	B:17:DG:H2'	B:18:DC:O4'	0.439
20	A:13:LEU:HD23	A:39:ILE:HD13	0.435
20	B:28:DT:H2'	B:29:DA:H8	0.435
20	A:52:THR:HG22	A:54:LYS:H	0.434
20	B:22:DA:C2	B:23:DA:C4	0.432
20	B:11:DC:H1'	B:21:DG:N2	0.430
20	B:28:DT:H2'	B:29:DA:O4'	0.422

Model ID	Atom-1	Atom-2	Clash overlap (Å)
20	B:13:DG:N2	B:19:DT:H1'	0.419
20	B:19:DT:H6	B:19:DT:O5'	0.415
20	B:19:DT:H73	B:19:DT:OP2	0.411
20	B:9:DT:H2'	B:10:DC:O4'	0.407
20	A:31:LYS:HB3	A:31:LYS:NZ	0.406
20	B:13:DG:H2'	B:14:DC:O4'	0.405
20	A:12:ALA:HB1	A:39:ILE:HG23	0.401
21	B:19:DT:H2'	B:20:DG:C8	0.894
21	B:8:DT:H2'	B:9:DT:C6	0.828
21	B:24:DT:H2'	B:25:DT:C6	0.823
21	B:4:DG:N2	B:28:DT:H1'	0.817
21	B:18:DC:H2'	B:19:DT:C6	0.786
21	B:23:DA:H3'	B:24:DT:H71	0.774
21	B:6:DA:H2'	B:7:DA:C8	0.773
21	B:8:DT:H2'	B:9:DT:H6	0.729
21	B:22:DA:H2'	B:23:DA:O4'	0.710
21	B:27:DC:H2'	B:28:DT:H6	0.708
21	B:23:DA:H2'	B:24:DT:O4'	0.692
21	B:19:DT:H2'	B:20:DG:H8	0.689
21	B:24:DT:H2'	B:25:DT:H6	0.670
21	B:9:DT:H2'	B:10:DC:O4'	0.665
21	B:5:DT:H2'	B:6:DA:C8	0.664
21	B:12:DA:H1'	B:20:DG:N2	0.662

Model ID	Atom-1	Atom-2	Clash overlap (Å)
21	B:14:DC:H2'	B:15:DG:C8	0.628
21	B:18:DC:H2'	B:19:DT:H6	0.621
21	B:11:DC:H2'	B:12:DA:H8	0.613
21	B:25:DT:H2'	B:26:DA:O4'	0.611
21	B:27:DC:H2'	B:28:DT:C6	0.602
21	B:25:DT:O2'	B:26:DA:H5'	0.591
21	B:3:DA:H2'	B:4:DG:O4'	0.579
21	B:11:DC:H2'	B:12:DA:C8	0.574
21	B:8:DT:H3'	B:9:DT:H71	0.546
21	B:26:DA:H2'	B:27:DC:C6	0.546
21	B:21:DG:C2	B:22:DA:H1'	0.545
21	A:55:GLN:HB3	B:8:DT:H73	0.537
21	B:4:DG:H22	B:28:DT:H1'	0.535
21	B:1:DG:O2'	B:2:DT:H5'	0.529
21	B:6:DA:H2'	B:7:DA:H8	0.529
21	B:10:DC:H2'	B:11:DC:C6	0.528
21	B:28:DT:H2'	B:29:DA:C8	0.527
21	A:5:ILE:H	A:5:ILE:HD12	0.523
21	B:18:DC:H3'	B:19:DT:H71	0.514
21	B:5:DT:H2'	B:6:DA:H8	0.512
21	B:11:DC:H2'	B:12:DA:O4'	0.512
21	A:44:LYS:HB3	A:50:THR:HA	0.504
21	B:13:DG:O2'	B:14:DC:H5'	0.501

Model ID	Atom-1	Atom-2	Clash overlap (Å)
21	B:14:DC:H2'	B:15:DG:H8	0.499
21	A:52:THR:O	A:56:VAL:HG23	0.497
21	A:53:ARG:H	A:53:ARG:HD3	0.496
21	B:28:DT:O2'	B:29:DA:H5'	0.495
21	B:23:DA:H2'	B:24:DT:C6	0.489
21	B:4:DG:H21	B:28:DT:H1'	0.484
21	B:22:DA:O2'	B:23:DA:H5'	0.474
21	B:17:DG:H2'	B:18:DC:O4'	0.471
21	A:32:MET:HB3	B:19:DT:H4'	0.470
21	B:28:DT:H2'	B:29:DA:H8	0.469
21	A:15:ILE:H	A:15:ILE:HD12	0.468
21	A:36:ASN:HD21	A:56:VAL:HG12	0.461
21	B:23:DA:H2'	B:24:DT:H6	0.459
21	B:13:DG:H2'	B:14:DC:C6	0.457
21	A:15:ILE:N	A:15:ILE:HD12	0.456
21	B:13:DG:H2'	B:14:DC:H6	0.454
21	A:61:GLN:OE1	B:22:DA:H5'	0.452
21	A:64:ALA:HA	A:67:LYS:HE3	0.448
21	B:9:DT:H2'	B:10:DC:H6	0.442
21	B:27:DC:H6	B:27:DC:O5'	0.442
21	B:27:DC:O2'	B:28:DT:H5'	0.438
21	A:55:GLN:HB3	B:8:DT:C7	0.436
21	A:23:LYS:NZ	A:35:ARG:HB3	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
21	A:27:SER:OG	A:31:LYS:HE3	0.428
21	B:10:DC:O2'	B:11:DC:H5'	0.423
21	A:23:LYS:HZ3	A:35:ARG:HB3	0.422
21	B:24:DT:H3'	B:25:DT:H71	0.422
21	A:5:ILE:HG21	A:51:ARG:HH11	0.421
21	A:53:ARG:HD3	A:53:ARG:N	0.421
21	B:11:DC:O2'	B:12:DA:H5'	0.419
21	B:21:DG:N2	B:22:DA:H1'	0.418
21	A:5:ILE:N	A:5:ILE:HD12	0.416
21	A:32:MET:CB	B:19:DT:H4'	0.415
21	A:43:ILE:N	A:43:ILE:HD12	0.415
21	B:23:DA:C2	B:24:DT:H1'	0.414
21	B:7:DA:H2'	B:8:DT:C6	0.413
21	B:28:DT:H2'	B:29:DA:O4'	0.412
22	B:26:DA:H2'	B:27:DC:C6	0.913
22	B:5:DT:H2'	B:6:DA:C8	0.810
22	B:12:DA:H2'	B:13:DG:H8	0.802
22	B:12:DA:H2'	B:13:DG:C8	0.790
22	A:41:ARG:HA	A:44:LYS:HE2	0.763
22	B:24:DT:H2'	B:25:DT:C6	0.757
22	A:32:MET:HE1	B:19:DT:H5"	0.755
22	B:17:DG:H2'	B:18:DC:C6	0.737
22	B:24:DT:H2'	B:25:DT:H6	0.725

Model ID	Atom-1	Atom-2	Clash overlap (Å)
22	B:28:DT:H2'	B:29:DA:C8	0.721
22	B:27:DC:H3'	B:28:DT:H71	0.720
22	B:22:DA:H2'	B:23:DA:H8	0.707
22	B:27:DC:H2'	B:28:DT:C6	0.692
22	B:7:DA:H2'	B:8:DT:C6	0.689
22	B:28:DT:H2'	B:29:DA:H8	0.681
22	B:2:DT:H2'	B:3:DA:C8	0.675
22	B:4:DG:N2	B:28:DT:H1'	0.665
22	B:22:DA:H2'	B:23:DA:C8	0.663
22	B:8:DT:H2'	B:9:DT:H6	0.661
22	B:27:DC:H2'	B:28:DT:H6	0.652
22	B:4:DG:H2'	B:5:DT:O4'	0.640
22	B:8:DT:O2'	B:9:DT:H5'	0.636
22	B:8:DT:H73	B:8:DT:OP1	0.635
22	A:54:LYS:HA	A:54:LYS:HE2	0.618
22	B:23:DA:H2'	B:24:DT:O4'	0.615
22	B:25:DT:H73	B:25:DT:OP2	0.610
22	B:23:DA:O2'	B:24:DT:H5'	0.606
22	B:7:DA:H2'	B:8:DT:H6	0.599
22	B:10:DC:H2'	B:11:DC:C6	0.598
22	B:10:DC:H2'	B:11:DC:H6	0.597
22	B:12:DA:H1'	B:20:DG:N2	0.587
22	B:13:DG:O2'	B:14:DC:H5'	0.577

Model ID	Atom-1	Atom-2	Clash overlap (Å)
22	B:8:DT:H2'	B:9:DT:C6	0.572
22	B:13:DG:N2	B:19:DT:H1'	0.543
22	B:21:DG:H2'	B:22:DA:O4'	0.541
22	B:6:DA:H2'	B:7:DA:C8	0.529
22	A:64:ALA:HA	A:67:LYS:HE2	0.528
22	B:13:DG:H2'	B:14:DC:O4'	0.522
22	B:18:DC:H3'	B:19:DT:H71	0.511
22	B:26:DA:H2'	B:27:DC:H6	0.510
22	B:29:DA:H2'	B:30:DC:C6	0.498
22	B:18:DC:H2'	B:19:DT:H6	0.496
22	B:12:DA:H2	B:19:DT:H3	0.490
22	B:4:DG:C2	B:5:DT:H1'	0.486
22	B:18:DC:H6	B:18:DC:O5'	0.484
22	A:23:LYS:NZ	A:35:ARG:H	0.480
22	A:60:ILE:O	A:60:ILE:HD13	0.473
22	A:66:ARG:HH22	B:5:DT:H3'	0.470
22	B:4:DG:C2'	B:5:DT:H5'	0.467
22	B:16:DC:H2'	B:17:DG:C8	0.466
22	B:24:DT:O2'	B:25:DT:H5'	0.465
22	B:18:DC:H2'	B:19:DT:C6	0.461
22	B:4:DG:H2'	B:5:DT:H5'	0.453
22	B:7:DA:H2'	B:8:DT:O4'	0.453
22	B:4:DG:H22	B:28:DT:H1'	0.452

Model ID	Atom-1	Atom-2	Clash overlap (Å)
22	B:11:DC:H1'	B:21:DG:N2	0.448
22	B:5:DT:H73	B:5:DT:OP2	0.441
22	B:6:DA:C2	B:7:DA:C4	0.441
22	B:1:DG:O2'	B:2:DT:H5'	0.437
22	B:4:DG:H2'	B:5:DT:C5'	0.434
22	B:6:DA:C2	B:26:DA:N3	0.434
22	B:5:DT:H2'	B:6:DA:H8	0.429
22	A:40:ALA:O	A:44:LYS:HG2	0.424
22	B:27:DC:O2'	B:28:DT:H5'	0.423
22	B:21:DG:H2'	B:22:DA:C8	0.415
22	B:6:DA:H2'	B:7:DA:O4'	0.414
22	A:23:LYS:HZ3	A:36:ASN:H	0.412
22	A:12:ALA:HB1	A:39:ILE:HG23	0.408
22	B:1:DG:H2'	B:2:DT:C6	0.404
22	B:11:DC:H2'	B:12:DA:O4'	0.404
23	B:18:DC:H2'	B:19:DT:C6	0.865
23	B:10:DC:H2'	B:11:DC:C6	0.857
23	B:19:DT:H2'	B:20:DG:H8	0.802
23	B:24:DT:H2'	B:25:DT:C6	0.760
23	B:10:DC:H2'	B:11:DC:H6	0.759
23	B:22:DA:H2'	B:23:DA:O4'	0.715
23	B:4:DG:N2	B:28:DT:H1'	0.710
23	B:27:DC:H2'	B:28:DT:H6	0.692

Model ID	Atom-1	Atom-2	Clash overlap (Å)
23	B:9:DT:H2'	B:10:DC:O4'	0.679
23	B:19:DT:H2'	B:20:DG:C8	0.668
23	B:9:DT:H3	B:22:DA:H61	0.666
23	B:7:DA:H2'	B:8:DT:C6	0.663
23	B:6:DA:H2'	B:7:DA:C8	0.662
23	B:27:DC:H2'	B:28:DT:C6	0.652
23	B:8:DT:H2'	B:9:DT:C6	0.649
23	A:2:SER:H	A:3:PRO:HD2	0.629
23	B:13:DG:H2'	B:14:DC:H6	0.598
23	B:23:DA:H2'	B:24:DT:O4'	0.593
23	B:26:DA:H2'	B:27:DC:C6	0.584
23	B:24:DT:H2'	B:25:DT:H6	0.582
23	B:18:DC:H2'	B:19:DT:H6	0.579
23	A:53:ARG:H	A:53:ARG:HD3	0.560
23	A:61:GLN:OE1	B:22:DA:H5'	0.558
23	B:25:DT:H2'	B:26:DA:O4'	0.557
23	A:23:LYS:HE3	A:35:ARG:H	0.546
23	B:9:DT:O2'	B:10:DC:H5'	0.543
23	B:26:DA:H2'	B:27:DC:H6	0.543
23	B:25:DT:O2'	B:26:DA:H5'	0.537
23	B:1:DG:H2'	B:2:DT:H6	0.531
23	B:13:DG:H2'	B:14:DC:C6	0.519
23	B:7:DA:H2'	B:8:DT:H71	0.518

Model ID	Atom-1	Atom-2	Clash overlap (Å)
23	B:1:DG:H2'	B:2:DT:C6	0.515
23	B:13:DG:O2'	B:14:DC:H5'	0.513
23	A:52:THR:O	A:56:VAL:HG23	0.511
23	B:19:DT:H73	B:19:DT:OP2	0.501
23	B:28:DT:H2'	B:29:DA:C8	0.488
23	B:3:DA:H2'	B:4:DG:O4'	0.487
23	B:21:DG:C2	B:22:DA:H1'	0.486
23	B:22:DA:O2'	B:23:DA:H5'	0.485
23	B:24:DT:H73	B:24:DT:OP1	0.481
23	B:11:DC:H2'	B:12:DA:O4'	0.473
23	B:7:DA:H2'	B:8:DT:H6	0.462
23	B:4:DG:H22	B:28:DT:H1'	0.462
23	A:15:ILE:N	A:15:ILE:HD12	0.459
23	B:9:DT:H73	B:9:DT:OP2	0.451
23	A:43:ILE:N	A:43:ILE:HD12	0.448
23	A:58:SER:HB3	B:7:DA:H61	0.447
23	B:11:DC:O2'	B:12:DA:H5'	0.444
23	B:28:DT:O2'	B:29:DA:H5'	0.439
23	A:44:LYS:HB3	A:50:THR:HA	0.434
23	A:15:ILE:H	A:15:ILE:HD12	0.431
23	B:24:DT:H3'	B:25:DT:H71	0.431
23	B:2:DT:O2'	B:3:DA:H5'	0.429
23	A:2:SER:N	A:3:PRO:HD2	0.426

Model ID	Atom-1	Atom-2	Clash overlap (Å)
23	A:5:ILE:N	A:5:ILE:HD12	0.416
23	B:27:DC:O2'	B:28:DT:H5'	0.415
23	B:9:DT:C2'	B:10:DC:H5'	0.414
23	B:23:DA:C2	B:24:DT:H1'	0.411
23	B:28:DT:H2'	B:29:DA:O4'	0.411
23	A:55:GLN:HB3	B:8:DT:C7	0.409
23	B:23:DA:O2'	B:24:DT:H5'	0.409
23	A:55:GLN:NE2	B:7:DA:H3'	0.401
24	B:8:DT:H3'	B:9:DT:H71	0.873
24	B:10:DC:H2'	B:11:DC:C6	0.873
24	A:23:LYS:HE3	B:20:DG:H5"	0.826
24	B:5:DT:H2'	B:6:DA:O4'	0.823
24	B:17:DG:H2'	B:18:DC:O4'	0.822
24	B:13:DG:O2'	B:14:DC:H5'	0.742
24	A:23:LYS:CE	B:20:DG:H5"	0.722
24	B:20:DG:H2'	B:21:DG:C8	0.707
24	A:23:LYS:HZ1	A:36:ASN:H	0.699
24	A:53:ARG:HH22	B:19:DT:H5"	0.696
24	B:12:DA:H1'	B:20:DG:H22	0.694
24	B:25:DT:H2'	B:26:DA:O4'	0.691
24	B:21:DG:H2'	B:22:DA:O4'	0.668
24	B:19:DT:H2'	B:20:DG:C8	0.664
24	B:19:DT:H2'	B:20:DG:H8	0.658

Model ID	Atom-1	Atom-2	Clash overlap (Å)
24	B:4:DG:N2	B:28:DT:H1'	0.657
24	B:7:DA:H2	B:25:DT:H3	0.655
24	B:11:DC:H2'	B:12:DA:O4'	0.653
24	B:20:DG:H2'	B:21:DG:H8	0.623
24	B:9:DT:H2'	B:10:DC:O4'	0.620
24	B:18:DC:H2'	B:19:DT:C6	0.614
24	B:27:DC:H2'	B:28:DT:H6	0.608
24	B:27:DC:H6	B:27:DC:O5'	0.595
24	B:21:DG:N2	B:22:DA:H1'	0.588
24	A:23:LYS:NZ	A:36:ASN:H	0.588
24	A:65:ARG:HA	A:65:ARG:HE	0.587
24	A:52:THR:HB	A:55:GLN:HG3	0.583
24	A:31:LYS:HB3	A:31:LYS:NZ	0.556
24	B:21:DG:O2'	B:22:DA:H5'	0.555
24	A:23:LYS:HZ2	A:35:ARG:H	0.549
24	B:4:DG:H3'	B:5:DT:H71	0.543
24	B:4:DG:H21	B:28:DT:H1'	0.522
24	B:11:DC:H6	B:11:DC:O5'	0.520
24	B:4:DG:H2'	B:5:DT:C6	0.509
24	B:12:DA:H1'	B:20:DG:N2	0.505
24	B:12:DA:H2'	B:13:DG:H8	0.491
24	A:44:LYS:HG2	A:51:ARG:H	0.483
24	A:23:LYS:HZ2	A:35:ARG:N	0.480

Model ID	Atom-1	Atom-2	Clash overlap (Å)
24	B:13:DG:C2'	B:14:DC:H5'	0.479
24	B:27:DC:H2'	B:28:DT:C6	0.479
24	B:10:DC:H2'	B:11:DC:H6	0.469
24	B:3:DA:H2'	B:4:DG:C8	0.468
24	B:4:DG:H2'	B:5:DT:H6	0.468
24	B:28:DT:O2'	B:29:DA:H5'	0.468
24	B:27:DC:O2'	B:28:DT:H5'	0.466
24	A:31:LYS:HB3	A:31:LYS:HZ2	0.456
24	A:63:LEU:O	A:67:LYS:HG3	0.456
24	B:21:DG:C2	B:22:DA:H1'	0.454
24	B:26:DA:H2'	B:27:DC:O4'	0.454
24	B:2:DT:H2'	B:3:DA:O4'	0.448
24	B:22:DA:H8	B:22:DA:O5'	0.446
24	B:12:DA:O2'	B:13:DG:H5'	0.442
24	A:47:THR:HG23	A:48:GLY:N	0.440
24	B:21:DG:H21	B:22:DA:H1'	0.440
24	B:11:DC:H2'	B:12:DA:H8	0.436
24	B:20:DG:C2	B:21:DG:C4	0.436
24	A:23:LYS:HZ2	A:35:ARG:HB3	0.435
24	B:19:DT:H71	B:19:DT:OP2	0.435
24	A:52:THR:HG22	A:54:LYS:H	0.428
24	B:26:DA:O2'	B:27:DC:H5'	0.427
24	B:5:DT:C2'	B:6:DA:H5'	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
24	B:20:DG:H2'	B:21:DG:O4'	0.423
24	B:28:DT:H2'	B:29:DA:O4'	0.421
24	A:15:ILE:N	A:15:ILE:HD12	0.420
24	B:23:DA:H8	B:23:DA:O5'	0.417
24	B:8:DT:H2'	B:9:DT:C6	0.403
24	B:9:DT:O2'	B:10:DC:H5'	0.403
24	B:11:DC:H2'	B:12:DA:C8	0.403
24	B:12:DA:H2'	B:13:DG:C8	0.401
24	B:10:DC:H6	B:10:DC:O5'	0.400
25	B:24:DT:H2'	B:25:DT:O4'	0.767
25	B:5:DT:H2'	B:6:DA:O4'	0.692
25	B:4:DG:N2	B:28:DT:H1'	0.684
25	B:22:DA:H2'	B:23:DA:C8	0.675
25	B:27:DC:H2'	B:28:DT:H6	0.664
25	A:19:CYS:H	A:35:ARG:HD2	0.648
25	B:28:DT:O2'	B:29:DA:H5'	0.639
25	B:13:DG:H2'	B:14:DC:O4'	0.622
25	B:4:DG:H3'	B:5:DT:H71	0.597
25	A:23:LYS:HZ1	A:35:ARG:H	0.592
25	B:9:DT:H2'	B:10:DC:O4'	0.588
25	B:25:DT:H73	B:25:DT:OP1	0.579
25	B:27:DC:H2'	B:28:DT:C6	0.579
25	B:19:DT:H2'	B:20:DG:O4'	0.568

Model ID	Atom-1	Atom-2	Clash overlap (Å)
25	A:40:ALA:O	A:44:LYS:HG2	0.566
25	B:7:DA:N6	B:23:DA:H61	0.557
25	B:3:DA:H2'	B:4:DG:O4'	0.549
25	B:2:DT:O2'	B:3:DA:H5'	0.548
25	B:7:DA:H61	B:23:DA:H61	0.543
25	B:6:DA:H2'	B:7:DA:C8	0.533
25	B:1:DG:H3'	B:2:DT:H71	0.528
25	A:64:ALA:HA	A:67:LYS:HE2	0.526
25	B:1:DG:H2'	B:2:DT:C6	0.523
25	A:31:LYS:HB3	A:31:LYS:NZ	0.520
25	B:21:DG:H2'	B:22:DA:O4'	0.520
25	B:23:DA:H8	B:23:DA:O5'	0.506
25	A:2:SER:N	A:3:PRO:HD3	0.499
25	B:27:DC:O2'	B:28:DT:H5'	0.492
25	B:26:DA:H2'	B:27:DC:O4'	0.487
25	B:24:DT:O2'	B:25:DT:H5'	0.483
25	B:20:DG:H2'	B:21:DG:O4'	0.476
25	B:19:DT:O2'	B:20:DG:H5'	0.475
25	B:7:DA:H61	B:23:DA:N6	0.474
25	B:10:DC:H2'	B:11:DC:H6	0.471
25	B:6:DA:H8	B:6:DA:O5'	0.465
25	A:24:ILE:H	A:24:ILE:HD12	0.454
25	B:10:DC:H2'	B:11:DC:C6	0.453

Model ID	Atom-1	Atom-2	Clash overlap (Å)
25	B:16:DC:H6	B:16:DC:O5'	0.451
25	A:24:ILE:N	A:24:ILE:HD12	0.449
25	B:23:DA:C2	B:24:DT:C2	0.448
25	B:17:DG:H2'	B:18:DC:C6	0.441
25	B:26:DA:H2'	B:27:DC:C6	0.438
25	A:23:LYS:NZ	A:35:ARG:H	0.435
25	B:4:DG:H2'	B:5:DT:C6	0.431
25	B:4:DG:H2'	B:5:DT:O4'	0.426
25	A:4:ASP:C	A:6:GLU:H	0.419
25	B:25:DT:H2'	B:26:DA:O4'	0.415
25	A:13:LEU:HD23	A:39:ILE:HD13	0.412
25	B:17:DG:H2'	B:18:DC:O4'	0.411
25	B:4:DG:H22	B:28:DT:H1'	0.411
25	A:33:TYR:HD2	A:37:GLU:HB3	0.410

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	85	71	12	2
2	85	70	12	3
3	85	70	12	3
4	85	72	12	1
5	85	71	12	2
6	85	72	13	0

Model ID	Analyzed	Favored	Allowed	Outliers
7	85	67	14	4
8	85	76	8	1
9	85	73	11	1
10	85	75	9	1
11	85	67	15	3
12	85	74	7	4
13	85	75	8	2
14	85	72	12	1
15	85	71	12	2
16	85	71	9	5
17	85	72	10	3
18	85	68	15	2
19	85	74	10	1
20	85	70	13	2
21	85	72	11	2
22	85	75	9	1
23	85	71	11	3
24	85	65	16	4
25	85	66	13	6

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	75	68	6	1

Model ID	Analyzed	Favored	Allowed	Outliers
2	75	69	6	0
3	75	66	9	0
4	75	71	2	2
5	75	72	1	2
6	75	67	4	4
7	75	68	6	1
8	75	69	6	0
9	75	69	5	1
10	75	71	4	0
11	75	68	7	0
12	75	70	4	1
13	75	69	6	0
14	75	71	2	2
15	75	67	8	0
16	75	66	7	2
17	75	72	3	0
18	75	70	3	2
19	75	69	6	0
20	75	72	1	2
21	75	68	6	1
22	75	69	4	2
23	75	68	7	0
24	75	70	5	0

Model ID	Analyzed	Favored	Allowed	Outliers
25	75	70	5	0

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	31	LYS
4	A	31	LYS
5	A	31	LYS
5	A	38	LEU
6	A	31	LYS
6	A	49	LYS
6	A	53	ARG
7	A	31	LYS
9	A	31	LYS
12	A	31	LYS
14	A	31	LYS
14	A	38	LEU
16	A	60	ILE
18	A	31	LYS
20	A	31	LYS
20	A	38	LEU
21	A	53	ARG
22	A	31	LYS
22	A	60	ILE

Fit of model to data used for modeling

Crosslinking-MS

Validation for this section is under development.

H/D exchange

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The PDB-Dev team and members of Sali labcontributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded byRCSB PDB (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from RCSB PDB, Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the SASBDB repository are acknowledged for their advice and support in implementing SAS validation methods.

Members of the wwPDB Integrative/Hybrid Methods Task Force provided recommendations and community support for the project.