

# Integrative Structure Validation Report ?

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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	9A1V
PDB-Dev ID	PDBDEV_00000124
Structure Title	Integrative model of Nucleotide excision repair complex of XPA and RPA on 5' junction substrate
Structure Authors	DSouza, A.; Topolska-Wos, A.M.; Chazin, W.J.

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

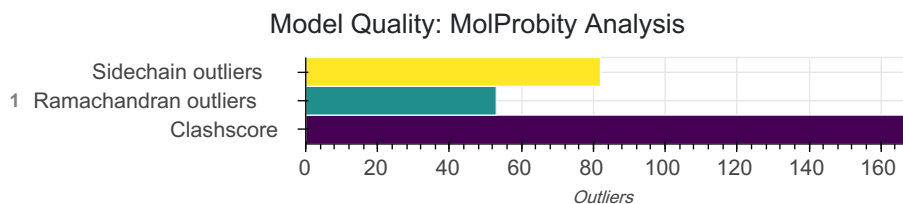
*We welcome your comments at [pdb-dev@mail.wwpdb.org](mailto:pdb-dev@mail.wwpdb.org)*

*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](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.*



## Ensemble information ?

*This entry consists of 0 distinct ensemble(s).*



## Representation ?

This entry has only one representation and includes 0 rigid bodies and 14 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-238, 239-253, 254-434
B	-	1-128, 129-226
C	-	1-115
D	-	1-28, 29-48, 49-97, 98-239
E	-	1-18
F	-	1-40
G	-	None-None
H	-	None-None

## 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	None	None	None	1	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	<a href="https://salilab.org/modeller/">Modeller</a>	9v4	model building	<a href="https://salilab.org/modeller/">https://salilab.org/modeller/</a>
2	<a href="https://modbase.compbio.ucsf.edu/foxsdock/">FoXSDock</a>	main.c2a7893	model building	<a href="https://modbase.compbio.ucsf.edu/foxsdock/">https://modbase.compbio.ucsf.edu/foxsdock/</a>

## Data quality ?

### SAS:Scattering profile

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

## Model quality ?

For models with atomic structures, molprobtity 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 ?

There are 505 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
P-O5'-C5'	120.00	65.50	1
C3'-O3'-P	120.20	171.11	1
C3'-O3'-P	120.20	69.52	1
P-O5'-C5'	120.00	164.88	1
O3'-P-O5'	104.00	146.56	1
P-O5'-C5'	120.00	157.46	1
O3'-P-O5'	104.00	141.20	1
P-O5'-C5'	120.00	156.68	1
C3'-O3'-P	120.20	152.55	1
OP1-P-O5'	109.00	46.86	1
C4'-C3'-O3'	110.00	140.12	1
C2'-C1'-N1	113.50	140.67	1
N-CA-C	112.10	156.99	1
P-O5'-C5'	120.00	146.80	1
C4'-C3'-O3'	110.00	135.88	1
C3'-O3'-P	120.20	146.08	1
C3'-O3'-P	120.20	145.89	1
O5'-C5'-C4'	110.80	135.59	1
C5'-C4'-O4'	109.40	84.64	1
CA-C-N	116.20	148.91	1
P-O5'-C5'	120.00	144.15	1
CA-C-N	116.90	139.43	1
C4'-C3'-C2'	102.40	79.89	1
C-N-CA	121.70	148.28	1
O3'-P-OP1	108.00	64.52	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	147.56	1
C4'-C3'-O3'	110.00	131.44	1
C2-N1-C6	120.60	99.24	1
O4'-C1'-N1	108.40	129.74	1
O3'-P-O5'	104.00	125.31	1
O3'-P-OP2	108.00	65.67	1
C4'-C3'-O3'	110.00	131.11	1
C-CA-CB	109.10	140.02	1
C5'-C4'-C3'	114.90	135.54	1
O4'-C1'-N1	108.40	128.86	1
C2'-C1'-N1	113.50	133.84	1
C3'-C2'-C1'	101.60	121.71	1
C2'-C1'-N1	113.50	133.45	1
O3'-C3'-C2'	111.50	131.43	1
O3'-P-O5'	104.00	123.68	1
C-N-CA	121.70	145.29	1
C-N-CA	121.70	145.26	1
CA-C-N	116.20	142.12	1
C-N-CA	121.70	144.83	1
O3'-P-O5'	104.00	123.10	1
C-N-CA	121.70	144.38	1
C4'-C3'-O3'	110.00	128.77	1
C-N-CA	121.70	144.17	1
C4'-C3'-O3'	110.00	128.63	1
O5'-C5'-C4'	110.80	128.80	1
C5'-C4'-C3'	114.90	132.75	1
C2-N1-C6	120.60	102.88	1
O3'-C3'-C2'	111.50	128.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C1'-N1	113.50	130.93	1
CA-C-O	120.80	101.23	1
C4'-C3'-O3'	110.00	127.07	1
C4-C5-C6	117.60	100.74	1
O5'-C5'-C4'	110.80	94.22	1
C-N-CA	121.70	141.57	1
N-CA-C	111.00	141.86	1
C3'-O3'-P	120.20	136.61	1
C-N-CA	121.70	141.34	1
C1'-N1-C2	119.70	135.79	1
OP2-P-O5'	108.00	76.06	1
CA-C-N	116.20	137.32	1
O4'-C1'-N1	108.40	124.23	1
C5'-C4'-C3'	114.90	130.69	1
O3'-C3'-C2'	111.50	95.78	1
C-N-CA	121.70	140.54	1
C4'-C3'-C2'	102.40	86.92	1
C-N-CA	121.70	140.24	1
C3'-O3'-P	120.20	135.41	1
OP1-P-OP2	120.00	89.59	1
N-CA-C	112.10	137.08	1
N-CA-C	112.10	137.07	1
O5'-C5'-C4'	110.80	125.73	1
CA-CB-CG	113.80	103.90	1
CA-CB-CG	113.80	103.97	1
O-C-N	123.00	107.32	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5'-C4'-O4'	109.40	95.29	1
N-CA-CB	110.50	94.65	1
C2-N3-C4	120.00	106.12	1
C-N-CA	121.70	138.35	1
O3'-P-O5'	104.00	90.21	1
N-CA-C	111.00	136.43	1
CA-CB-CG	112.60	121.53	1
CA-CB-CG	112.60	103.72	1
O-C-N	123.00	108.92	1
C4'-C3'-O3'	110.00	96.97	1
N3-C4-C5	121.80	108.77	1
C-CA-CB	110.50	97.62	1
O4'-C1'-C2'	106.40	93.56	1
C2-N1-C6	120.60	107.76	1
CA-CB-CG	112.60	104.08	1
C2-N1-C6	120.60	107.88	1
P-O5'-C5'	120.00	132.68	1
O4'-C1'-N1	108.40	95.76	1
O5'-C5'-C4'	110.80	123.43	1
P-O5'-C5'	120.00	107.44	1
CA-C-N	116.20	132.82	1
CA-CB-CG	113.80	105.52	1
C2'-C1'-N1	113.50	125.86	1
N-CA-C	111.00	133.99	1
C3'-C2'-C1'	101.60	113.91	1
N-CA-C	112.10	132.59	1
C5'-C4'-O4'	109.40	97.12	1
C-CA-CB	109.10	91.13	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5'-C4'-C3'	114.90	127.09	1
C-N-CA	121.70	136.33	1
O3'-P-O5'	104.00	91.86	1
N-CA-C	111.00	133.55	1
C3'-C2'-C1'	101.60	89.52	1
CA-C-N	116.90	128.96	1
C2'-C1'-N1	113.50	125.56	1
O-C-N	123.00	110.27	1
O4'-C1'-C2'	106.40	94.50	1
O2-C2-N3	121.90	110.04	1
O4'-C1'-N1	108.40	120.23	1
CA-CB-CG	113.80	106.05	1
O3'-P-O5'	104.00	115.61	1
CA-CB-CG	113.80	106.11	1
CB-CG-ND2	116.40	104.88	1
N-CA-C	111.00	132.40	1
C1'-N1-C2	119.70	131.03	1
O4'-C1'-N1	108.40	119.68	1
C-N-CA	121.70	135.22	1
CA-CB-CG	113.80	106.33	1
C-N-CA	121.70	135.12	1
O-C-N	123.00	111.19	1
C-N-CA	121.70	134.97	1
N-CA-CB	111.50	99.08	1
C-CA-CB	110.10	96.31	1
CA-CB-CG	113.80	106.55	1



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	123.81	1
C-N-CA	121.70	134.50	1
P-O5'-C5'	120.00	109.46	1
CA-C-O	121.00	99.93	1
C5'-C4'-C3'	114.90	125.30	1
CA-CB-CG	113.90	101.46	1
C-N-CA	121.70	109.28	1
C-N-CA	121.70	134.05	1
CA-C-N	116.20	129.88	1
O4'-C4'-C3'	105.40	95.15	1
C5'-C4'-C3'	114.90	104.67	1
CA-CB-CG	113.80	107.00	1
C4'-O4'-C1'	109.70	119.86	1
CA-C-N	116.90	127.04	1
N-CA-C	111.00	129.89	1
CA-C-O	120.80	109.37	1
N1-C2-N3	118.90	108.83	1
O4'-C1'-C2'	106.40	96.36	1
O4'-C4'-C3'	105.40	115.43	1
CA-CB-CG	113.80	107.16	1
N3-C4-C5	121.80	111.84	1
C-N-CA	121.70	133.61	1
C3'-C2'-C1'	101.60	111.51	1
O3'-P-OP1	108.00	88.18	1
CA-CB-CG	113.80	107.20	1
O3'-P-O5'	104.00	113.89	1
C-N-CA	121.70	133.55	1
C-CA-CB	110.10	97.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	107.26	1
C4'-O4'-C1'	109.70	99.91	1
C4'-C3'-O3'	110.00	119.73	1
N-CA-C	111.00	129.09	1
CA-CB-CG	113.80	107.34	1
OP2-P-O5'	108.00	127.33	1
C-N-CA	121.70	110.13	1
P-O5'-C5'	120.00	110.36	1
O5'-C5'-C4'	110.80	120.42	1
C-CA-CB	110.10	97.92	1
CA-CB-CG	113.80	107.45	1
C-N-CA	121.70	133.12	1
C-N-CA	121.70	133.10	1
C-N-CA	121.70	133.08	1
CA-CB-CG	113.80	107.48	1
C5'-C4'-C3'	114.90	124.33	1
C4'-O4'-C1'	109.70	100.31	1
C-N-CA	121.70	132.95	1
N-CA-CB	110.50	121.11	1
CA-CB-CG	113.80	107.58	1
CA-CB-CG	113.80	107.59	1
C-N-CA	121.70	132.83	1
CA-CB-CG	113.80	107.63	1
CA-CB-CG	113.80	107.64	2
O5'-C5'-C4'	110.80	120.01	1
C-N-CA	121.70	132.75	1
O5'-C5'-C4'	110.80	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5'-C4'-C3'	114.90	105.71	1
O3'-P-O5'	104.00	113.13	1
CA-CB-CG	113.80	107.72	1
OP2-P-O5'	108.00	89.76	1
C-CA-CB	110.10	98.56	1
C-N-CA	121.70	132.63	1
C-N-CA	121.70	132.58	1
N3-C4-N4	117.90	126.91	1
C-N-CA	121.70	132.51	1
C1'-N1-C6	119.70	128.69	1
C-CA-CB	110.10	98.71	1
C-N-CA	121.70	132.44	1
O3'-C3'-C2'	111.50	102.59	1
C1'-N1-C2	119.70	110.79	1
O3'-P-O5'	104.00	112.90	1
CA-C-N	116.20	128.06	1
C-N-CA	121.70	132.35	1
N-CA-CB	110.50	120.55	1
N3-C4-N4	117.90	109.05	1
N-CA-C	111.00	127.42	1
CA-C-N	116.20	127.91	1
C-CA-CB	110.10	98.99	1
C-CA-CB	110.10	99.01	1
CA-C-N	116.20	127.86	1
O4'-C1'-C2'	106.40	97.68	1
C-N-CA	121.70	132.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5'-C4'-O4'	109.40	118.10	1
OD1-CG-ND2	122.60	128.39	1
C-N-CA	121.70	132.11	1
CA-CB-CG	113.80	108.03	1
CA-CB-CG	112.60	106.83	1
CA-CB-CG	114.10	125.63	1
O4'-C1'-C2'	106.40	97.78	1
CA-C-O	120.80	111.06	1
N-CA-C	111.00	127.03	1
CA-CB-CG	113.80	108.11	1
CA-C-O	119.00	101.94	1
C-N-CA	122.60	150.95	1
C2-N3-C4	120.00	128.50	1
C4'-C3'-O3'	110.00	118.35	1
O4'-C1'-N1	108.40	116.73	1
CA-C-N	116.90	125.23	1
C-CA-CB	110.10	99.59	1
CA-CB-CG	113.90	103.97	1
C-N-CA	121.70	131.63	1
CG1-CB-CG2	110.80	122.89	1
CA-CB-CG	112.60	107.11	1
CA-C-N	116.20	127.16	1
N-CA-CB	110.50	101.19	1
CA-CB-CG	113.80	108.33	1
CA-CB-CG	112.60	107.13	1
CA-CB-CG	112.60	118.07	1
N3-C4-C5	121.80	113.60	1
CA-CB-CG	112.60	107.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	125.06	1
C-CA-CB	110.10	120.40	1
C-N-CA	121.70	131.43	1
C3'-C2'-C1'	101.60	109.70	1
C-CA-CB	110.10	99.85	1
C4'-O4'-C1'	109.70	117.76	1
N3-C4-N4	117.90	125.94	1
C-N-CA	121.70	131.33	1
C-N-CD	125.00	103.14	1
N-CA-C	111.00	125.91	1
C-CA-CB	110.10	99.99	1
O5'-C5'-C4'	110.80	118.77	1
OG1-CB-CG2	109.30	119.86	1
C-CA-CB	110.10	100.10	1
P-O5'-C5'	120.00	127.89	1
CA-CB-CG	113.80	108.55	1
CB-CG-CD	112.60	103.67	1
O4'-C4'-C3'	105.40	97.53	1
N-CA-C	111.00	125.67	1
N-CA-CB	110.50	119.37	1
N-CA-C	112.10	99.06	1
C2'-C1'-N1	113.50	105.69	1
N-CA-CB	110.50	119.35	1
C-N-CA	121.70	131.07	1
N-CA-CB	111.50	120.30	1
O-C-N	123.00	114.74	1
CA-CB-CG	113.80	118.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	126.51	1
N-CA-C	111.00	125.43	1
CA-CB-CG	112.60	107.45	1
O-C-N	123.00	114.77	1
C-CA-CB	110.50	102.79	1
CA-C-N	116.20	126.47	1
N-CA-C	111.00	125.37	1
P-O5'-C5'	120.00	112.35	1
C-N-CA	121.70	130.87	1
C4'-C3'-O3'	110.00	117.63	1
CA-CB-CG	113.80	108.72	1
N-CA-C	111.00	96.78	1
CA-C-N	116.20	126.35	1
N-CA-C	111.00	125.18	1
C-N-CA	121.70	112.59	1
CA-CB-CG	113.80	108.74	1
CA-C-N	116.20	126.30	1
C5'-C4'-C3'	114.90	107.34	1
C-CA-CB	110.10	100.52	1
O3'-P-O5'	104.00	111.56	1
C4'-O4'-C1'	109.70	117.24	1
N-CA-CB	110.50	119.04	1
CA-CB-CG1	110.40	101.88	1
CA-CB-CG	112.60	107.59	1
O4'-C1'-N1	108.40	115.90	1
C-N-CA	121.70	130.69	1
CA-C-N	116.20	126.19	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	126.14	2
N-CA-C	111.00	124.90	1
CA-C-O	120.80	112.38	1
CA-CB-CG	113.90	105.00	1
N-CA-CB	103.00	108.40	1
CB-CG-CD	112.60	104.27	1
C-N-CA	121.70	112.88	1
CA-CB-CG	112.60	107.70	1
O4'-C1'-C2'	106.40	99.05	1
CA-C-N	116.20	125.99	1
CA-CB-CG	112.60	107.71	1
N-CA-C	111.00	124.63	1
N-CA-C	111.00	124.62	1
ND1-CE1-NE2	108.40	113.26	1
O3'-P-OP2	108.00	93.44	1
C-CA-CB	110.50	103.23	1
CA-N-CD	112.00	105.24	1
CA-CB-CG	112.60	107.78	1
CA-CB-CG	113.80	108.99	1
N-CA-CB	110.50	102.33	1
N-CA-C	111.00	124.45	1
CA-CB-CG	112.60	107.81	1
N1-C2-O2	119.20	126.35	1
O2-C2-N3	121.90	114.75	1
CA-C-N	116.20	125.73	1
N-CA-C	111.00	124.33	1
N-CA-CB	110.50	118.59	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.25	1
C-CA-CB	110.10	101.08	1
C3'-C2'-C1'	101.60	108.72	1
N-CA-C	112.10	123.96	1
C5'-C4'-C3'	114.90	107.79	1
N-CA-C	112.10	123.94	1
CA-C-N	116.20	125.67	1
CD2-NE2-CE1	109.00	104.27	1
N-CA-CB	110.50	118.54	1
C4'-C3'-C2'	102.40	95.32	1
N-CA-CB	110.50	118.53	1
CD2-NE2-CE1	109.00	104.28	1
N-CA-CB	110.50	118.51	1
C3'-C2'-C1'	101.60	108.66	1
N-CA-C	111.00	124.18	1
CA-C-N	116.20	125.62	1
C5'-C4'-C3'	114.90	107.85	1
N-CA-C	111.00	124.17	1
C-CA-CB	110.10	119.02	1
CA-C-N	116.90	123.94	2
CA-CB-CG	112.60	107.91	1
CA-CB-CG	112.60	107.92	1
CA-C-N	116.90	123.88	1
C-CA-CB	110.10	101.27	1
CA-CB-CG	112.60	107.95	1
C-CA-CB	110.50	103.54	1



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N3-C4-N4	117.90	124.85	1
CA-CB-CG	112.60	107.97	2
C-N-CA	121.70	130.01	1
CA-C-N	116.20	125.43	1
CA-CB-CG	112.60	107.99	2
C5'-C4'-C3'	114.90	107.99	1
CA-CB-CG	112.60	108.00	1
C-CA-CB	110.10	101.36	1
CA-CB-CG2	110.50	118.31	1
CA-C-N	116.90	123.78	1
N-CA-CB	110.50	118.29	1
CA-CB-CG	112.60	108.02	1
O3'-C3'-C2'	111.50	104.64	1
C-N-CA	121.70	113.47	1
O4'-C1'-C2'	106.40	99.55	1
CA-CB-CG	112.60	108.03	2
O-C-N	123.00	115.70	1
CA-C-N	116.20	125.32	1
CA-CB-CG	112.60	108.05	1
C-N-CA	121.70	129.89	1
N1-C2-N3	118.90	112.08	1
CD2-NE2-CE1	109.00	104.45	1
N-CA-C	113.30	126.46	1
C-CA-CB	110.10	101.48	1
CD2-NE2-CE1	109.00	104.47	1
N-CA-CB	110.50	118.20	1
C-CA-CB	110.10	101.50	1
CA-CB-CG	112.60	108.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	118.18	1
N3-C4-N4	117.90	124.67	1
N-CA-C	113.30	126.38	1
CD2-NE2-CE1	109.00	104.49	2
CA-C-N	116.20	125.21	1
CA-CB-CG	112.60	108.10	1
C-N-CA	121.70	129.80	1
CA-C-N	116.90	123.65	1
C-N-CA	121.70	113.61	1
N-CA-CB	103.00	107.94	1
CA-C-N	116.20	125.18	1
N-CA-CB	103.00	107.93	1
CD2-NE2-CE1	109.00	104.51	1
C-CA-CB	110.10	101.58	1
O-C-N	123.00	115.86	1
CD2-NE2-CE1	109.00	104.53	1
CD2-NE2-CE1	109.00	104.54	1
CA-CB-CG	112.60	108.14	1
N-CA-CB	103.00	107.90	1
O3'-P-OP1	108.00	94.64	1
CD2-NE2-CE1	109.00	104.55	1
N-CA-C	113.30	126.19	1
CA-CB-CG	112.60	108.16	2
CD2-NE2-CE1	109.00	104.56	2
CA-CB-CG	112.60	108.17	2
CD2-NE2-CE1	109.00	104.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CE1	109.00	104.58	1
N-CA-CB	110.50	118.01	1
C-N-CA	121.70	129.64	1
CD2-NE2-CE1	109.00	104.59	1
N-CA-C	112.10	123.12	1
CD2-NE2-CE1	109.00	104.60	2
CB-CG-CD	112.60	105.12	1
CA-CB-CG	112.60	108.20	1
CD2-NE2-CE1	109.00	104.61	1
O3'-P-OP2	108.00	121.16	1
C-CA-CB	110.10	101.77	1
CA-CB-CG	113.90	106.01	1
CA-CB-CG	112.60	108.23	1
C-CA-CB	110.10	101.79	1
O-C-N	123.00	116.01	1
C-N-CA	121.70	129.56	1
CA-CB-CG	113.80	109.43	1
C5'-C4'-C3'	114.90	108.35	1
C-CA-CB	110.10	101.82	1
N-CA-CB	110.40	116.93	1
N-CA-CB	103.00	107.78	1
CA-CB-CG	112.60	108.26	1
C-CA-CB	111.60	102.93	1
C5'-C4'-C3'	114.90	108.40	1
C-CA-CB	111.40	103.18	1
CA-CB-CG	112.60	108.28	1
ND1-CE1-NE2	108.40	112.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2'-C1'-N1	113.50	119.98	1
C-N-CA	121.70	113.93	1
O3'-C3'-C2'	111.50	105.04	1
CA-CB-CG	113.80	109.49	1
C-N-CA	121.70	113.95	1
C5'-C4'-O4'	109.40	115.85	1
CA-CB-CG	112.60	108.30	2
CD-NE-CZ	124.40	118.39	1
N-CA-CB	110.50	117.79	1
C-CA-CB	111.60	103.03	1
CA-CB-CG	112.60	108.32	1
C-N-CD	125.00	107.45	1
CA-CB-CG	112.60	108.33	1
N-CA-CB	110.50	117.75	1
C-N-CA	121.70	114.03	1
N-CA-CB	110.50	117.73	1
C-N-CA	121.70	129.36	1
CA-CB-CG	114.10	105.62	1
CA-CB-CG	113.80	109.57	1
CA-CB-CG	112.60	108.37	1
C-CA-CB	111.40	103.36	1
C-N-CA	121.70	129.32	1
N-CA-C	113.30	101.04	1
O4'-C1'-N1	108.40	114.73	1
O4'-C1'-C2'	106.40	100.09	1
CA-C-N	116.20	124.61	1
N-CA-C	111.00	122.76	1
O-C-N	123.00	116.29	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.23	1
CA-CB-CG	112.60	108.42	1
CD-NE-CZ	124.40	118.57	1
C-N-CA	121.70	114.21	1
C-N-CA	121.70	114.22	1
CA-CB-CG	112.60	108.45	1
CA-CB-CG	112.60	108.46	1
C1'-N1-C2	119.70	125.90	1
CA-CB-CG	113.80	109.67	1
N-CA-C	111.00	99.45	1
C1'-N1-C2	119.70	113.53	1
C-CA-CB	110.10	102.29	1
N-CA-CB	110.50	117.49	1
N-CA-C	113.30	125.21	1
CA-CB-CG	112.60	108.50	1
O-C-N	123.00	116.45	1
N-CA-CB	103.00	107.50	1
C2'-C1'-N1	113.50	107.37	1
C-CA-CB	110.50	104.37	1
C4'-O4'-C1'	109.70	115.82	1
C-CA-CB	110.10	102.36	1
CA-C-O	120.80	113.88	1
N-CA-C	111.00	99.64	1
N-CA-C	113.30	101.55	1
C-N-CA	121.70	114.42	1
N-CA-CB	110.50	117.37	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
P-O5'-C5'	120.00	126.04	1
CB-CG-CD	112.60	105.75	1
CA-CB-CG	112.60	108.57	2
CA-N-CD	112.00	106.37	1
CA-CB-CG	113.80	109.78	1
CA-CB-CG	112.60	108.58	1
CA-CB-CG	112.60	108.59	1
N-CA-CB	110.50	117.30	1

### 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
1	166.70	1843

All 1843 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	D:181:TYR:CZ	E:13:DT:H5'	1.712
1	D:181:TYR:CE1	E:13:DT:H5'	1.625
1	C:105:HIS:CE1	D:53:ALA:CB	1.622
1	D:135:LYS:HD3	E:16:DT:C4	1.594
1	D:130:ARG:HB3	E:15:DT:C3'	1.564
1	D:177:ASP:CB	F:33:DC:H5'	1.542
1	B:155:PHE:CA	B:155:PHE:N	1.521
1	D:177:ASP:HB2	F:33:DC:C5'	1.480
1	C:105:HIS:CE1	D:53:ALA:HB3	1.479
1	D:130:ARG:HB3	E:15:DT:C2'	1.479
1	B:157:PRO:C	B:158:ALA:N	1.471
1	D:181:TYR:CE1	E:13:DT:C5'	1.459
1	B:156:MET:CA	B:156:MET:N	1.443

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:1:ASP:N	D:46:ARG:HH21	1.437
1	B:156:MET:C	B:157:PRO:N	1.409
1	D:172:HIS:CE1	E:10:DC:O2	1.400
1	D:130:ARG:CG	E:16:DT:P	1.398
1	B:156:MET:C	B:156:MET:CA	1.390
1	D:130:ARG:HG2	E:16:DT:P	1.388
1	D:137:LYS:CG	E:16:DT:H5'	1.387
1	B:157:PRO:CA	B:157:PRO:N	1.384
1	D:130:ARG:NH2	E:16:DT:C6	1.381
1	B:157:PRO:C	B:157:PRO:CA	1.364
1	D:130:ARG:CB	E:15:DT:H2"	1.364
1	B:148:GLY:HA3	D:46:ARG:CZ	1.361
1	B:148:GLY:HA3	D:46:ARG:NH2	1.352
1	D:175:TRP:CH2	E:10:DC:H4'	1.346
1	D:130:ARG:HB2	E:16:DT:OP1	1.340
1	D:135:LYS:NZ	E:16:DT:O4	1.321
1	D:130:ARG:CB	E:15:DT:C2'	1.316
1	D:135:LYS:CD	E:16:DT:C4	1.312
1	B:148:GLY:C	D:46:ARG:HH12	1.305
1	D:127:ASP:O	E:15:DT:C1'	1.295
1	D:126:CYS:HA	E:16:DT:OP2	1.280
1	D:130:ARG:HG2	E:16:DT:O5'	1.279
1	A:133:SER:OG	D:113:MET:SD	1.275
1	D:174:GLN:C	E:11:DT:H2"	1.263
1	B:155:PHE:C	B:155:PHE:CA	1.259
1	D:64:ALA:HB3	E:15:DT:O5'	1.258
1	D:64:ALA:CB	E:15:DT:O5'	1.248

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:105:HIS:ND1	D:54:ALA:N	1.248
1	A:85:LYS:HD2	E:14:DT:C2	1.247
1	D:137:LYS:NZ	E:16:DT:H2"	1.242
1	D:137:LYS:CG	E:16:DT:C5'	1.235
1	A:248:LEU:O	F:7:DC:H2'	1.235
1	D:168:LYS:CE	E:13:DT:O2	1.220
1	D:175:TRP:CH2	E:10:DC:C4'	1.220
1	D:175:TRP:N	E:11:DT:H2"	1.219
1	A:250:SER:OG	F:7:DC:OP1	1.219
1	D:177:ASP:CB	F:33:DC:C5'	1.210
1	D:130:ARG:HB3	E:15:DT:O3'	1.208
1	D:130:ARG:CG	E:16:DT:O5'	1.202
1	D:139:ILE:HD13	E:14:DT:C5'	1.201
1	B:224:ASP:HB2	D:39:ARG:NH2	1.200
1	C:4:ASP:OD2	D:48:TYR:CA	1.200
1	C:1:ASP:CA	D:46:ARG:HH21	1.195
1	D:126:CYS:CA	E:16:DT:OP2	1.194
1	D:130:ARG:CB	E:16:DT:OP1	1.188
1	D:181:TYR:CZ	E:13:DT:C5'	1.188
1	D:130:ARG:CB	E:16:DT:P	1.185
1	D:173:SER:C	E:11:DT:H3'	1.182
1	C:1:ASP:N	D:46:ARG:NH2	1.182
1	B:129:ASN:HB2	F:28:DC:OP2	1.181
1	D:67:LYS:HB2	D:166:VAL:HB	1.181
1	B:148:GLY:CA	D:46:ARG:HH22	1.180
1	D:141:LYS:HB3	F:32:DC:OP2	1.180
1	D:168:LYS:NZ	E:13:DT:O2	1.176
1	D:106:GLU:CD	H:1:ZN2:ZN2	1.170



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:5:ILE:HD11	A:49:GLY:HA3	1.169
1	D:181:TYR:CG	E:14:DT:OP1	1.169
1	D:130:ARG:CD	E:16:DT:O5'	1.163
1	D:179:LYS:HD2	E:12:DT:C4'	1.161
1	A:11:TYR:OH	E:12:DT:C3'	1.159
1	D:172:HIS:CE1	E:10:DC:C2	1.157
1	D:108:CYS:SG	E:16:DT:H4'	1.157
1	D:149:LEU:HD13	D:187:VAL:HG12	1.156
1	D:137:LYS:HG2	E:16:DT:C5'	1.154
1	D:125:THR:O	E:16:DT:OP2	1.154
1	A:38:LYS:HD3	A:58:GLU:HB2	1.143
1	D:135:LYS:HD3	E:16:DT:C5	1.139
1	D:172:HIS:NE2	E:10:DC:C2	1.137
1	D:134:ASP:H	E:15:DT:H73	1.133
1	D:169:ASN:O	E:13:DT:OP1	1.132
1	A:201:VAL:HG13	A:211:VAL:HG13	1.131
1	B:191:LYS:HE2	B:194:SER:HB3	1.130
1	A:91:LYS:HE2	A:93:ASP:HB3	1.128
1	D:168:LYS:HE3	E:13:DT:O2	1.128
1	D:181:TYR:CZ	E:13:DT:H3'	1.126
1	A:131:LYS:HD2	A:134:LEU:HB2	1.123
1	B:155:PHE:CB	B:226:GLU:HB3	1.123
1	D:126:CYS:HA	E:16:DT:P	1.122
1	A:138:ILE:HD12	A:200:ARG:HD2	1.120
1	A:86:GLN:OE1	D:117:LEU:CG	1.120
1	A:248:LEU:O	F:7:DC:C2'	1.119

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:32:ILE:HG13	C:41:LEU:HD23	1.118
1	D:131:ASP:O	E:15:DT:C7	1.115
1	D:177:ASP:HB3	F:33:DC:H5'	1.115
1	D:181:TYR:HH	E:13:DT:C5'	1.110
1	D:127:ASP:H	E:15:DT:H2'	1.110
1	B:148:GLY:CA	D:46:ARG:NH2	1.108
1	B:148:GLY:HA3	D:46:ARG:NH1	1.106
1	D:139:ILE:HD13	E:14:DT:H5'	1.106
1	D:230:VAL:HB	D:236:LYS:HD3	1.105
1	B:224:ASP:CB	D:39:ARG:NH2	1.102
1	D:150:LEU:HD12	D:204:LYS:HG2	1.100
1	A:140:ILE:HG13	A:167:MET:HB3	1.099
1	D:127:ASP:N	E:15:DT:H2'	1.099
1	D:179:LYS:HA	F:32:DC:H5'	1.097
1	D:127:ASP:O	E:15:DT:C2'	1.095
1	D:138:LEU:HD23	D:184:LEU:HD11	1.094
1	D:62:VAL:HA	D:135:LYS:H	1.089
1	D:162:LEU:HD21	D:190:SER:HB3	1.086
1	D:65:ALA:HB3	D:139:ILE:HD13	1.084
1	D:139:ILE:CD1	E:14:DT:H5'	1.084
1	D:127:ASP:H	E:15:DT:C2'	1.084
1	D:145:LYS:HD3	D:182:LEU:HG	1.081
1	D:175:TRP:HH2	E:10:DC:C4'	1.081
1	A:178:LEU:CD1	F:7:DC:H42	1.081
1	D:173:SER:N	E:12:DT:OP1	1.080
1	D:135:LYS:CE	E:16:DT:C4	1.079
1	D:175:TRP:N	E:11:DT:C2'	1.078

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:130:ARG:CB	E:15:DT:O3'	1.077
1	D:168:LYS:HG3	E:13:DT:C4'	1.077
1	D:168:LYS:HG3	E:13:DT:H4'	1.077
1	B:224:ASP:OD2	D:39:ARG:NH1	1.077
1	C:105:HIS:CG	D:54:ALA:HA	1.076
1	A:90:VAL:HG21	A:199:ALA:HB2	1.074
1	B:214:THR:O	D:43:LEU:HD23	1.074
1	B:155:PHE:HB3	B:226:GLU:HB3	1.069
1	D:131:ASP:O	E:15:DT:H72	1.065
1	D:135:LYS:HE2	E:16:DT:N3	1.063
1	B:168:VAL:HG13	B:169:LEU:HD23	1.061
1	D:130:ARG:HG2	E:15:DT:O3'	1.061
1	A:178:LEU:HD13	F:7:DC:H42	1.058
1	D:67:LYS:HE2	E:14:DT:O5'	1.053
1	D:62:VAL:HG22	D:136:HIS:H	1.053
1	B:148:GLY:C	D:46:ARG:NH1	1.051
1	D:168:LYS:CG	E:13:DT:H4'	1.050
1	D:130:ARG:HB2	E:15:DT:H2"	1.042
1	D:181:TYR:OH	E:13:DT:H5'	1.041
1	A:28:ARG:HE	A:39:LEU:HD13	1.039
1	B:181:LEU:HD13	B:222:SER:HA	1.039
1	A:249:LYS:HG3	F:7:DC:H5"	1.037
1	C:105:HIS:CE1	D:53:ALA:HB1	1.037
1	A:119:ASP:HB3	A:137:ILE:HG12	1.036
1	B:148:GLY:CA	D:46:ARG:HH12	1.034
1	D:63:LYS:CA	D:138:LEU:HA	1.034
1	B:184:GLN:HG3	B:199:LYS:H22	1.032
1	D:181:TYR:CE2	E:13:DT:H3'	1.027

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:149:ASN:N	D:46:ARG:HH12	1.027
1	C:2:MET:CE	D:48:TYR:H	1.026
1	D:62:VAL:HA	D:135:LYS:N	1.025
1	A:133:SER:CB	D:113:MET:SD	1.022
1	A:85:LYS:HA	E:14:DT:N3	1.021
1	D:63:LYS:HB3	D:138:LEU:HD13	1.018
1	B:187:LYS:HB3	B:199:LYS:HE3	1.017
1	D:173:SER:C	E:11:DT:C3'	1.015
1	D:139:ILE:CD1	E:14:DT:C5'	1.014
1	B:148:GLY:CA	D:46:ARG:NH1	1.012
1	D:181:TYR:OH	E:13:DT:C5'	1.011
1	D:130:ARG:HD3	E:16:DT:O5'	1.010
1	D:215:LYS:HA	D:218:LYS:HE3	1.009
1	D:137:LYS:HZ3	E:16:DT:H2"	1.009
1	D:130:ARG:CG	E:15:DT:O3'	1.005
1	A:52:ARG:HH22	A:81:LYS:HD3	1.004
1	A:86:GLN:OE1	D:117:LEU:CD1	1.004
1	D:135:LYS:CE	E:16:DT:N3	1.004
1	A:178:LEU:HD13	F:7:DC:N4	0.997
1	A:161:LYS:H	A:161:LYS:HD2	0.994
1	A:23:ASN:HD21	A:44:LEU:HD23	0.988
1	B:171:LEU:HD22	B:172:ILE:HD12	0.987
1	A:70:ASN:HD22	A:71:LYS:HD2	0.984
1	D:62:VAL:HG11	D:137:LYS:HB2	0.983
1	A:86:GLN:OE1	D:117:LEU:HG	0.983
1	A:142:LYS:HG3	A:165:TYR:CZ	0.982

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:2:MET:HE1	D:48:TYR:O	0.982
1	A:194:LEU:HD21	A:230:ARG:HD2	0.980
1	A:179:TRP:CH2	A:218:ILE:HD12	0.979
1	B:224:ASP:CB	D:39:ARG:HH22	0.973
1	C:10:ILE:HG13	C:102:LYS:HD3	0.971
1	A:86:GLN:OE1	D:117:LEU:HD11	0.970
1	D:177:ASP:HB3	F:33:DC:P	0.970
1	D:185:GLN:NE2	E:17:DT:OP2	0.968
1	D:154:ASP:HA	D:157:LYS:HE2	0.967
1	A:85:LYS:NZ	D:128:ASN:HA	0.965
1	B:154:SER:CB	B:225:ALA:HA	0.963
1	D:127:ASP:O	E:15:DT:H1'	0.962
1	A:19:ALA:HB1	A:73:TYR:CE2	0.957
1	D:149:LEU:HD11	D:191:LEU:HB2	0.957
1	B:155:PHE:C	B:155:PHE:HA	0.956
1	D:64:ALA:HA	D:139:ILE:HB	0.956
1	D:126:CYS:C	E:15:DT:H3'	0.953
1	D:107:GLU:H	D:125:THR:HG21	0.952
1	C:8:SER:OG	D:51:THR:HG22	0.951
1	D:142:THR:HG23	D:145:LYS:HE3	0.951
1	A:234:ASP:HA	A:238:GLN:HB3	0.950
1	A:203:ASP:HB3	A:209:LEU:HB3	0.947
1	C:1:ASP:CA	D:46:ARG:NH2	0.943
1	D:137:LYS:HG3	E:16:DT:C5'	0.939
1	D:137:LYS:HZ1	D:185:GLN:HB2	0.939
1	A:116:VAL:HG12	A:117:GLN:H	0.938
1	D:137:LYS:HE3	D:183:LYS:HD2	0.937

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:94:LEU:HD11	C:96:LEU:HG	0.936
1	A:11:TYR:OH	E:12:DT:C2'	0.936
1	C:1:ASP:H1	D:46:ARG:HH21	0.936
1	D:179:LYS:HD2	E:12:DT:H4'	0.934
1	A:75:PHE:HB2	A:106:PRO:HG2	0.933
1	D:40:GLN:HA	D:43:LEU:HG	0.933
1	D:191:LEU:HD12	D:201:GLU:HG2	0.932
1	B:154:SER:HA	B:223:THR:HG23	0.931
1	D:62:VAL:HG12	E:15:DT:C5	0.931
1	D:174:GLN:C	E:11:DT:C2'	0.931
1	A:51:ILE:HG23	A:91:LYS:HG2	0.930
1	A:201:VAL:CG1	A:211:VAL:HG13	0.927
1	A:1:LYS:HG2	A:17:ILE:HG23	0.925
1	D:172:HIS:ND1	E:11:DT:H5"	0.925
1	A:98:PHE:CE1	F:1:DC:O2	0.924
1	A:119:ASP:HB3	A:137:ILE:CG1	0.923
1	D:127:ASP:O	E:15:DT:H2'	0.923
1	D:137:LYS:HZ3	E:16:DT:C2'	0.920
1	A:234:ASP:HA	A:238:GLN:CB	0.919
1	B:149:ASN:N	D:46:ARG:NH1	0.918
1	C:105:HIS:ND1	D:53:ALA:CB	0.917
1	D:67:LYS:CB	D:166:VAL:HB	0.917
1	A:153:ARG:HD3	A:156:ASN:HD22	0.916
1	A:98:PHE:CE1	F:1:DC:C2	0.915
1	A:180:GLY:H	A:212:LEU:HD11	0.915
1	D:181:TYR:CD2	E:14:DT:OP1	0.915
1	D:212:GLU:HG2	D:213:LYS:HD2	0.913
1	A:5:ILE:CD1	A:49:GLY:HA3	0.910

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:165:ILE:HG12	D:182:LEU:HD11	0.910
1	D:139:ILE:HD11	D:181:TYR:HB3	0.909
1	A:3:VAL:HG22	A:17:ILE:HD11	0.908
1	A:73:TYR:HD2	A:108:GLU:HB3	0.908
1	B:155:PHE:HB3	B:226:GLU:CB	0.908
1	D:65:ALA:CB	D:139:ILE:HD13	0.908
1	B:155:PHE:CA	B:226:GLU:HB2	0.907
1	B:155:PHE:HB2	B:223:THR:OG1	0.907
1	B:214:THR:O	D:43:LEU:CD2	0.906
1	D:149:LEU:CD1	D:187:VAL:HG12	0.906
1	D:181:TYR:HE1	E:13:DT:H5"	0.904
1	B:169:LEU:HD12	B:202:VAL:HG11	0.903
1	D:163:LYS:CG	D:186:ILE:HD12	0.903
1	B:157:PRO:N	B:161:LEU:HD11	0.902
1	A:30:TRP:HA	A:39:LEU:HD23	0.900
1	A:196:ILE:CG1	A:219:ALA:HB3	0.900
1	D:163:LYS:HG2	D:186:ILE:HG23	0.900
1	A:56:PHE:HD2	A:60:VAL:HG12	0.897
1	B:171:LEU:CD2	B:172:ILE:HD12	0.897
1	D:233:SER:HB2	D:235:TRP:CD1	0.897
1	C:4:ASP:OD2	D:48:TYR:HA	0.896
1	D:149:LEU:CD1	D:191:LEU:HB2	0.896
1	B:154:SER:H	B:223:THR:HG23	0.895
1	D:40:GLN:HA	D:43:LEU:CG	0.895
1	A:194:LEU:HB3	A:227:TYR:CD2	0.891
1	D:62:VAL:HG21	D:130:ARG:CZ	0.891

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:134:ASP:N	E:15:DT:H73	0.891
1	A:56:PHE:HA	A:99:ASN:CG	0.889
1	A:54:THR:HA	A:97:THR:HG23	0.888
1	A:140:ILE:CG1	A:167:MET:HB3	0.888
1	B:181:LEU:HD13	B:222:SER:CA	0.888
1	D:62:VAL:C	D:134:ASP:H	0.888
1	B:148:GLY:CA	D:46:ARG:CZ	0.886
1	D:137:LYS:HA	D:137:LYS:HE3	0.885
1	D:181:TYR:HE1	E:13:DT:C5'	0.885
1	D:177:ASP:HB3	F:32:DC:O3'	0.884
1	B:191:LYS:CE	B:194:SER:HB3	0.882
1	D:166:VAL:CG2	D:181:TYR:HB2	0.882
1	D:172:HIS:NE2	E:10:DC:O2	0.882
1	A:60:VAL:HB	A:99:ASN:OD1	0.880
1	D:28:ILE:CG2	D:30:ARG:HG2	0.879
1	D:63:LYS:HB2	D:134:ASP:HA	0.879
1	D:155:LEU:HB3	D:162:LEU:HG	0.878
1	D:163:LYS:HG2	D:186:ILE:HD12	0.878
1	D:230:VAL:CB	D:236:LYS:HD3	0.878
1	A:5:ILE:HD11	A:49:GLY:CA	0.877
1	B:154:SER:N	B:223:THR:HG23	0.877
1	B:154:SER:CA	B:223:THR:HG23	0.876
1	B:155:PHE:N	B:225:ALA:C	0.876
1	D:62:VAL:HG22	D:136:HIS:N	0.876
1	D:149:LEU:HD21	D:191:LEU:HD23	0.875
1	A:85:LYS:HB2	A:88:THR:HG22	0.874
1	B:195:VAL:HG23	B:196:SER:H	0.872
1	B:155:PHE:CB	B:226:GLU:CB	0.871



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:63:LYS:HB3	D:138:LEU:CD1	0.871
1	D:149:LEU:CG	D:191:LEU:HB2	0.871
1	D:62:VAL:CA	D:135:LYS:H	0.870
1	A:5:ILE:HD13	A:6:ALA:N	0.869
1	A:24:LYS:HB3	A:217:ILE:CG1	0.869
1	D:63:LYS:HA	D:131:ASP:O	0.867
1	D:129:CYS:O	E:15:DT:C2	0.867
1	C:1:ASP:HA	D:46:ARG:HH21	0.867
1	A:164:ILE:HG12	A:178:LEU:CD2	0.865
1	D:134:ASP:H	E:15:DT:C7	0.865
1	D:181:TYR:CB	E:14:DT:OP1	0.862
1	A:131:LYS:CD	A:134:LEU:HB2	0.860
1	D:175:TRP:CE3	E:11:DT:C5	0.860
1	D:106:GLU:OE2	E:16:DT:OP1	0.860
1	A:20:ARG:HG2	A:45:VAL:HG12	0.859
1	A:42:LEU:HD21	A:96:MET:HE1	0.859
1	A:176:ALA:HB3	A:209:LEU:CD2	0.859
1	D:106:GLU:OE1	H:1:ZN2:ZN2	0.859
1	D:127:ASP:C	E:15:DT:H2'	0.858
1	D:138:LEU:HD12	D:139:ILE:N	0.855
1	B:181:LEU:CD1	B:222:SER:HA	0.854
1	C:45:GLU:HG2	C:99:GLU:CD	0.854
1	D:130:ARG:NH2	E:16:DT:H6	0.850
1	A:23:ASN:ND2	A:44:LEU:HD23	0.849
1	D:135:LYS:NZ	E:16:DT:C4	0.848
1	D:89:LYS:HG2	D:90:VAL:HG23	0.847
1	D:127:ASP:O	E:15:DT:O4'	0.847

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:77:LYS:HB2	A:104:VAL:HG22	0.845
1	A:82:ILE:C	E:13:DT:C7	0.845
1	D:137:LYS:HG2	E:16:DT:H5'	0.845
1	B:169:LEU:HD21	B:191:LYS:HE3	0.844
1	C:105:HIS:HE1	D:53:ALA:CB	0.844
1	C:108:PRO:HD2	D:55:ALA:O	0.843
1	D:32:ARG:HH12	D:34:ARG:HA	0.843
1	D:137:LYS:HA	D:183:LYS:HD2	0.843
1	A:42:LEU:HD13	A:43:GLU:N	0.842
1	D:62:VAL:N	D:135:LYS:HB3	0.842
1	B:129:ASN:CB	F:28:DC:OP2	0.841
1	D:37:MET:O	D:40:GLN:HG3	0.841
1	A:138:ILE:CD1	A:200:ARG:HD2	0.840
1	D:64:ALA:CA	D:131:ASP:HB2	0.840
1	D:199:ALA:HA	D:202:GLU:OE2	0.839
1	D:62:VAL:N	D:135:LYS:H	0.839
1	A:196:ILE:HG12	A:219:ALA:HB3	0.838
1	D:135:LYS:HD3	E:16:DT:O4	0.838
1	D:127:ASP:N	E:15:DT:H3'	0.837
1	A:123:ILE:HB	A:126:LEU:HG	0.836
1	B:224:ASP:HB3	D:39:ARG:HH22	0.836
1	B:155:PHE:H	B:225:ALA:N	0.836
1	D:173:SER:CA	E:11:DT:H3'	0.835
1	A:38:LYS:HD3	A:58:GLU:CB	0.834
1	A:2:VAL:O	A:17:ILE:HG12	0.833
1	A:20:ARG:CG	A:45:VAL:HG12	0.833

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:69:ILE:HD13	D:70:ASP:N	0.833
1	A:209:LEU:HD13	A:210:SER:N	0.832
1	A:5:ILE:HA	A:47:GLU:OE2	0.831
1	D:67:LYS:HD2	D:168:LYS:CG	0.831
1	D:131:ASP:HB3	E:15:DT:O5'	0.831
1	A:50:GLU:HG2	A:51:ILE:H	0.830
1	C:23:VAL:HG12	C:71:VAL:HG22	0.830
1	C:105:HIS:ND1	D:53:ALA:HB1	0.830
1	D:138:LEU:HD23	D:184:LEU:CD1	0.830
1	D:201:GLU:O	D:204:LYS:HD3	0.830
1	D:165:ILE:HG12	D:182:LEU:CD1	0.829
1	D:65:ALA:HB2	D:139:ILE:HG21	0.827
1	D:76:ILE:HG13	D:78:GLU:HG3	0.827
1	B:148:GLY:HA3	D:46:ARG:HH22	0.826
1	D:181:TYR:CZ	E:13:DT:C3'	0.825
1	A:28:ARG:NE	A:39:LEU:HD13	0.823
1	A:150:ILE:HG12	A:159:VAL:HG12	0.823
1	B:145:SER:HB3	C:23:VAL:HG22	0.823
1	B:187:LYS:HE2	B:191:LYS:NZ	0.822
1	D:230:VAL:HA	D:235:TRP:HE1	0.822
1	D:227:ARG:O	D:230:VAL:HG22	0.822
1	D:168:LYS:HD3	D:169:ASN:H	0.821
1	D:133:ASP:N	E:15:DT:C5	0.821
1	B:154:SER:HA	B:223:THR:CG2	0.820
1	C:2:MET:HE1	D:48:TYR:C	0.820
1	A:85:LYS:H22	D:128:ASN:HA	0.820
1	B:174:ALA:HB2	B:223:THR:HG21	0.819
1	D:137:LYS:NZ	E:16:DT:C2'	0.819

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:131:LYS:HD2	A:134:LEU:CB	0.818
1	C:1:ASP:HA	D:46:ARG:NH2	0.818
1	D:28:ILE:HG21	D:30:ARG:HG2	0.817
1	D:137:LYS:HG3	E:16:DT:P	0.817
1	D:165:ILE:HG21	D:180:LEU:HB3	0.816
1	C:108:PRO:CD	D:56:THR:HA	0.815
1	D:181:TYR:OH	E:13:DT:O5'	0.815
1	D:137:LYS:HG3	E:15:DT:O3'	0.814
1	A:150:ILE:HG12	A:159:VAL:CG1	0.813
1	B:155:PHE:CA	B:226:GLU:CB	0.813
1	D:40:GLN:HB2	D:43:LEU:HD12	0.813
1	D:150:LEU:HD12	D:204:LYS:CG	0.813
1	A:133:SER:HB2	D:113:MET:SD	0.811
1	C:1:ASP:H1	D:46:ARG:NH2	0.811
1	A:44:LEU:HD11	A:91:LYS:HG3	0.810
1	A:43:GLU:OE1	A:68:GLU:HG2	0.810
1	D:62:VAL:HG23	D:135:LYS:HB3	0.810
1	A:1:LYS:HE3	A:15:TRP:CH2	0.809
1	A:83:ALA:N	E:13:DT:H71	0.809
1	B:155:PHE:N	B:223:THR:OG1	0.809
1	C:1:ASP:H2	D:46:ARG:NH2	0.809
1	D:25:ARG:CZ	D:25:ARG:HA	0.808
1	D:28:ILE:HD13	D:30:ARG:HE	0.808
1	A:73:TYR:CD2	A:108:GLU:HB3	0.807
1	A:178:LEU:CD1	F:7:DC:N4	0.807
1	A:220:ASN:HB2	A:221:PRO:HD3	0.807

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:168:VAL:HA	B:171:LEU:CD1	0.806
1	B:183:PHE:HB3	B:219:HIS:NE2	0.806
1	D:125:THR:C	E:16:DT:OP2	0.806
1	A:249:LYS:HG3	F:7:DC:C5'	0.805
1	B:168:VAL:HG22	B:172:ILE:HD13	0.805
1	D:145:LYS:CD	D:182:LEU:HG	0.805
1	A:51:ILE:CG2	A:91:LYS:HG2	0.803
1	B:165:GLN:O	B:168:VAL:HG12	0.803
1	D:233:SER:HB2	D:235:TRP:HD1	0.803
1	A:142:LYS:HD2	A:167:MET:SD	0.802
1	D:142:THR:HA	D:145:LYS:CE	0.802
1	A:91:LYS:CE	A:93:ASP:HB3	0.801
1	A:138:ILE:H	A:138:ILE:HD13	0.801
1	B:145:SER:CB	C:23:VAL:HG22	0.801
1	D:64:ALA:HA	D:139:ILE:CB	0.800
1	D:137:LYS:HD2	E:16:DT:H5"	0.800
1	A:42:LEU:HD22	A:54:THR:O	0.799
1	A:53:ALA:HB3	A:96:MET:SD	0.799
1	B:156:MET:C	B:157:PRO:CD	0.799
1	B:162:THR:HB	B:167:GLN:OE1	0.799
1	A:201:VAL:HG13	A:211:VAL:CG1	0.798
1	A:117:GLN:OE1	A:217:ILE:HB	0.798
1	D:149:LEU:HD13	D:187:VAL:CG1	0.798
1	A:11:TYR:OH	E:12:DT:O3'	0.797
1	A:70:ASN:ND2	A:71:LYS:HD2	0.796
1	A:140:ILE:CG2	A:169:THR:HA	0.796
1	D:142:THR:HA	D:145:LYS:HE3	0.796
1	D:158:ARG:HD2	D:161:PRO:HG2	0.796

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:169:LEU:HD13	B:187:LYS:NZ	0.795
1	B:181:LEU:HD23	B:182:ASN:N	0.795
1	D:62:VAL:CG1	D:137:LYS:HB2	0.795
1	B:154:SER:HB2	B:225:ALA:HA	0.794
1	D:230:VAL:HB	D:236:LYS:CD	0.794
1	A:179:TRP:HA	A:212:LEU:HD13	0.793
1	B:202:VAL:HA	B:205:LEU:HD21	0.793
1	A:1:LYS:HE3	A:15:TRP:CZ2	0.791
1	D:215:LYS:HA	D:218:LYS:CE	0.791
1	D:175:TRP:HE3	E:11:DT:C5	0.791
1	A:18:CYS:SG	A:76:SER:HB3	0.790
1	A:200:ARG:NH2	A:210:SER:HB2	0.790
1	B:131:GLN:CD	B:132:PRO:HD2	0.790
1	C:28:ARG:HB3	C:43:ASP:OD1	0.790
1	D:62:VAL:CA	E:15:DT:C4	0.790
1	D:222:LYS:O	D:225:GLU:HG2	0.790
1	D:63:LYS:CB	D:138:LEU:HD13	0.788
1	D:175:TRP:CE3	E:11:DT:C7	0.788
1	D:40:GLN:HA	D:43:LEU:CD1	0.787
1	A:140:ILE:HG21	A:169:THR:HG22	0.786
1	A:225:GLU:O	A:228:LYS:HG3	0.786
1	D:130:ARG:CD	E:16:DT:P	0.786
1	A:82:ILE:C	E:13:DT:H71	0.785
1	C:105:HIS:CG	D:54:ALA:CA	0.784
1	A:11:TYR:OH	E:12:DT:H3'	0.783
1	D:126:CYS:CA	E:15:DT:H3'	0.783

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:96:MET:HE2	F:2:DC:H42	0.782
1	A:178:LEU:O	A:212:LEU:HD22	0.781
1	D:131:ASP:HB3	E:15:DT:C4'	0.781
1	D:64:ALA:CA	D:139:ILE:HB	0.780
1	D:171:HIS:CG	E:12:DT:O2	0.780
1	A:44:LEU:HD12	A:52:ARG:O	0.776
1	C:33:HIS:CG	C:34:PRO:HD2	0.776
1	D:62:VAL:HG21	D:130:ARG:NE	0.776
1	D:67:LYS:HE3	E:14:DT:OP1	0.776
1	D:138:LEU:CD2	D:184:LEU:HD11	0.776
1	C:34:PRO:HD3	C:40:ILE:HG22	0.775
1	D:62:VAL:HG13	D:137:LYS:N	0.775
1	D:175:TRP:CD2	E:11:DT:C7	0.775
1	B:155:PHE:C	B:226:GLU:HB2	0.774
1	C:10:ILE:HG23	C:102:LYS:NZ	0.773
1	A:5:ILE:CD1	A:7:SER:H	0.772
1	A:38:LYS:HG2	A:39:LEU:H	0.772
1	A:124:ASP:OD2	A:173:VAL:HB	0.772
1	B:155:PHE:CB	B:155:PHE:N	0.772
1	D:40:GLN:CB	D:43:LEU:HD12	0.772
1	D:127:ASP:N	E:15:DT:C2'	0.772
1	D:130:ARG:N	E:15:DT:C2'	0.772
1	B:173:LYS:HG3	B:181:LEU:CD2	0.771
1	D:220:ASP:O	D:223:VAL:HG22	0.771
1	D:171:HIS:N	E:12:DT:O2	0.771
1	D:205:GLU:O	D:208:GLN:HG3	0.770
1	B:157:PRO:HA	B:157:PRO:N	0.770
1	A:17:ILE:HB	A:77:LYS:HD2	0.769

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:138:ILE:HG13	A:200:ARG:NH1	0.769
1	B:167:GLN:HA	B:170:ASN:ND2	0.769
1	D:177:ASP:HB2	F:33:DC:H5"	0.769
1	B:173:LYS:HG3	B:181:LEU:HD21	0.768
1	D:132:ALA:C	E:15:DT:H72	0.768
1	D:149:LEU:CD2	D:191:LEU:HD23	0.768
1	B:215:VAL:HG22	D:42:ARG:HH21	0.767
1	D:168:LYS:HD3	D:169:ASN:N	0.767
1	D:191:LEU:HD12	D:201:GLU:CG	0.767
1	C:10:ILE:CG1	C:102:LYS:HD3	0.766
1	D:135:LYS:CE	E:16:DT:O4	0.766
1	A:3:VAL:HG22	A:17:ILE:CD1	0.765
1	A:138:ILE:HD12	A:200:ARG:CD	0.765
1	C:66:GLU:OE2	C:83:VAL:HG21	0.765
1	C:90:HIS:CG	C:91:PRO:HD3	0.765
1	C:112:PRO:HD3	D:55:ALA:HB3	0.765
1	D:181:TYR:CE1	E:13:DT:H5"	0.762
1	D:201:GLU:OE1	D:204:LYS:HE3	0.762
1	A:81:LYS:HA	A:81:LYS:HZ3	0.761
1	D:64:ALA:N	D:131:ASP:HB2	0.761
1	A:51:ILE:HG23	A:91:LYS:CG	0.760
1	A:82:ILE:C	E:13:DT:H73	0.760
1	A:86:GLN:OE1	D:117:LEU:CD2	0.760
1	A:228:LYS:HD3	A:229:LEU:N	0.759
1	A:153:ARG:CD	A:156:ASN:HB2	0.758
1	B:195:VAL:HG23	B:198:ILE:H	0.758
1	A:1:LYS:HE3	A:15:TRP:CE2	0.757



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:85:LYS:HA	E:14:DT:C2	0.757
1	C:32:ILE:CG1	C:41:LEU:HD23	0.757
1	D:62:VAL:N	D:133:ASP:HB2	0.757
1	F:6:DC:H5'	F:7:DC:C5	0.757
1	A:3:VAL:CG2	A:17:ILE:HD11	0.756
1	A:200:ARG:CZ	A:210:SER:HB2	0.756
1	B:202:VAL:HA	B:205:LEU:CD2	0.756
1	D:127:ASP:N	E:15:DT:C3'	0.756
1	A:53:ALA:O	A:97:THR:HG22	0.755
1	D:62:VAL:HG12	E:15:DT:C6	0.754
1	D:149:LEU:HD21	D:191:LEU:HB2	0.754
1	D:172:HIS:HB3	E:12:DT:H5'	0.754
1	A:52:ARG:NH2	A:81:LYS:HD3	0.753
1	D:139:ILE:HD11	D:181:TYR:CB	0.752
1	D:146:GLN:HG2	D:156:GLU:OE2	0.752
1	D:179:LYS:CD	E:12:DT:H4'	0.752
1	D:60:ALA:N	F:28:DC:OP1	0.752
1	B:129:ASN:HD21	D:61:ASN:HB3	0.751
1	B:163:VAL:HG13	B:166:ASN:H	0.749
1	C:105:HIS:ND1	D:54:ALA:CA	0.749
1	A:142:LYS:O	A:192:PRO:HB3	0.748
1	A:4:PRO:HB3	A:8:LEU:HD23	0.747
1	A:30:TRP:HB2	A:39:LEU:HD21	0.746
1	A:115:THR:HB	A:118:PHE:CE1	0.745
1	A:190:ARG:HG2	A:191:GLN:CD	0.744
1	D:57:GLY:HA2	F:27:DC:OP1	0.744
1	D:139:ILE:CD1	D:181:TYR:HB3	0.744

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:172:HIS:ND1	E:10:DC:O2	0.744
1	C:54:MET:HE2	C:58:ASP:OD2	0.743
1	B:163:VAL:O	B:167:GLN:HG2	0.741
1	B:184:GLN:HB3	B:219:HIS:CE1	0.741
1	C:105:HIS:NE2	D:53:ALA:HB3	0.741
1	D:130:ARG:NH2	E:16:DT:N1	0.741
1	B:141:ASN:HB3	B:142:PRO:HD2	0.740
1	D:139:ILE:HD13	E:14:DT:P	0.739
1	A:140:ILE:HG21	A:169:THR:CG2	0.738
1	D:127:ASP:CA	E:15:DT:H2'	0.738
1	D:212:GLU:O	D:215:LYS:HG2	0.737
1	D:131:ASP:O	E:15:DT:H71	0.737
1	A:20:ARG:HD2	A:45:VAL:HB	0.736
1	D:191:LEU:O	D:191:LEU:HD13	0.736
1	B:207:ASN:HB2	B:212:TYR:CE1	0.735
1	B:215:VAL:HG22	D:42:ARG:NH2	0.735
1	D:97:VAL:HG23	D:98:MET:H	0.735
1	D:99:GLU:HG2	D:100:PHE:H	0.735
1	D:138:LEU:HG	D:140:THR:HG23	0.735
1	D:142:THR:CG2	D:145:LYS:HE3	0.735
1	D:126:CYS:CB	E:16:DT:OP2	0.735
1	A:17:ILE:CB	A:77:LYS:HD2	0.734
1	C:33:HIS:HE1	C:37:LYS:HD2	0.734
1	D:64:ALA:HB3	E:15:DT:C5'	0.734
1	D:141:LYS:CB	F:31:DG:H3'	0.734
1	A:21:VAL:HG22	A:73:TYR:HD1	0.733
1	D:209:GLU:HA	D:212:GLU:CD	0.733

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:47:GLU:HG2	A:48:SER:H	0.731
1	D:97:VAL:O	D:98:MET:HG3	0.731
1	A:139:GLY:O	A:140:ILE:HG23	0.730
1	A:231:GLY:HA2	A:234:ASP:OD2	0.730
1	D:139:ILE:CD1	E:14:DT:H5"	0.730
1	B:149:ASN:H	D:46:ARG:NH1	0.729
1	A:1:LYS:HE3	A:15:TRP:CZ3	0.728
1	D:203:ALA:O	D:206:VAL:HG12	0.728
1	B:155:PHE:HE2	B:206:SER:HG	0.728
1	A:140:ILE:CG2	A:169:THR:HG22	0.727
1	D:64:ALA:CB	E:15:DT:P	0.727
1	D:123:LEU:O	D:123:LEU:HD13	0.727
1	D:163:LYS:CG	D:186:ILE:HG23	0.727
1	F:31:DG:H2"	F:32:DC:C6	0.727
1	A:179:TRP:CZ2	A:197:LYS:HD3	0.726
1	D:130:ARG:HG2	D:137:LYS:HG3	0.726
1	D:130:ARG:H	E:15:DT:C2'	0.726
1	A:77:LYS:HG3	A:104:VAL:HG23	0.725
1	B:157:PRO:C	B:157:PRO:HA	0.725
1	D:145:LYS:HE2	D:182:LEU:CD2	0.725
1	D:64:ALA:HB1	E:15:DT:O5'	0.725
1	D:145:LYS:HE2	D:182:LEU:HD23	0.724
1	A:115:THR:HG22	A:116:VAL:H	0.723
1	D:62:VAL:HG13	D:137:LYS:H	0.723
1	D:65:ALA:CB	D:139:ILE:HG21	0.723
1	A:85:LYS:NZ	D:128:ASN:CA	0.723

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:158:ARG:CD	D:161:PRO:HG2	0.723
1	D:179:LYS:HB2	D:181:TYR:HE1	0.723
1	D:173:SER:H	E:12:DT:P	0.723
1	B:185:ASP:HA	B:188:ASN:HD21	0.722
1	B:187:LYS:HE2	B:191:LYS:HZ1	0.722
1	B:183:PHE:HD2	B:219:HIS:HD2	0.722
1	A:194:LEU:HB3	A:227:TYR:CE2	0.721
1	A:30:TRP:CA	A:39:LEU:HD23	0.720
1	A:82:ILE:CG2	A:96:MET:HB3	0.720
1	B:156:MET:C	B:156:MET:CB	0.720
1	D:112:PHE:CZ	D:129:CYS:HB3	0.720
1	D:178:MET:HE1	D:180:LEU:HD11	0.720
1	D:149:LEU:HD11	D:191:LEU:CB	0.719
1	A:90:VAL:HG21	A:199:ALA:CB	0.718
1	A:115:THR:HG21	A:118:PHE:CZ	0.718
1	B:181:LEU:HD22	B:221:LYS:O	0.718
1	D:149:LEU:O	D:149:LEU:HD23	0.717
1	E:10:DC:H2"	E:11:DT:OP2	0.717
1	A:20:ARG:HG3	A:47:GLU:HB2	0.716
1	B:172:ILE:HG22	B:182:ASN:ND2	0.716
1	D:87:ILE:O	D:87:ILE:HD12	0.716
1	D:163:LYS:HG2	D:186:ILE:CG2	0.716
1	D:230:VAL:HA	D:235:TRP:NE1	0.716
1	A:1:LYS:HD3	A:17:ILE:CG2	0.715
1	A:145:GLU:HB2	A:165:TYR:HE2	0.715
1	D:212:GLU:HG2	D:213:LYS:N	0.715
1	A:45:VAL:O	A:51:ILE:HG13	0.714
1	D:141:LYS:NZ	F:31:DG:O3'	0.714

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:54:THR:HA	A:97:THR:CG2	0.712
1	A:72:VAL:HG13	A:74:TYR:CE2	0.712
1	A:140:ILE:C	A:194:LEU:HD22	0.711
1	B:187:LYS:HB3	B:199:LYS:CE	0.711
1	D:62:VAL:CB	E:15:DT:C4	0.711
1	D:69:ILE:HG21	D:96:PRO:HG3	0.710
1	D:121:PHE:CE1	D:164:PHE:HB3	0.710
1	D:149:LEU:CD2	D:191:LEU:HB2	0.710
1	A:142:LYS:HG3	A:165:TYR:CE1	0.709
1	D:135:LYS:CD	E:16:DT:N3	0.709
1	D:159:GLU:HG2	D:160:PRO:CD	0.709
1	D:137:LYS:CD	E:16:DT:C5'	0.708
1	D:171:HIS:HB2	E:12:DT:O3'	0.707
1	A:85:LYS:HD2	E:14:DT:N1	0.706
1	D:33:GLN:HB3	D:36:LEU:HB3	0.706
1	D:165:ILE:HG23	D:182:LEU:HD22	0.706
1	D:199:ALA:O	D:202:GLU:HG2	0.706
1	A:56:PHE:CD2	A:60:VAL:HG12	0.705
1	A:140:ILE:HG22	A:169:THR:HA	0.705
1	D:67:LYS:HD2	D:168:LYS:HG2	0.705
1	D:77:LEU:HD23	D:78:GLU:N	0.705
1	B:157:PRO:N	B:161:LEU:CD1	0.704
1	B:171:LEU:HD22	B:172:ILE:N	0.704
1	D:121:PHE:CD1	D:164:PHE:HB3	0.704
1	D:170:PRO:HG3	D:177:ASP:O	0.704
1	D:28:ILE:HG23	D:30:ARG:HG2	0.702
1	B:206:SER:OG	B:211:ILE:HB	0.701

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:215:VAL:HB	B:220:PHE:CE1	0.701
1	D:64:ALA:HB3	D:131:ASP:HB3	0.701
1	D:209:GLU:HA	D:212:GLU:OE1	0.701
1	B:156:MET:HA	B:156:MET:N	0.701
1	A:24:LYS:CB	A:217:ILE:HD11	0.700
1	A:194:LEU:CD2	A:230:ARG:HD2	0.700
1	B:155:PHE:C	B:225:ALA:O	0.700
1	B:169:LEU:HD13	B:187:LYS:HZ3	0.699
1	A:52:ARG:NH2	A:95:GLU:HB3	0.698
1	A:167:MET:HE1	A:195:ALA:HB3	0.698
1	D:32:ARG:HH22	D:34:ARG:HD3	0.698
1	B:168:VAL:HG22	B:172:ILE:CD1	0.697
1	D:116:TYR:HA	D:119:ASN:HD21	0.697
1	D:141:LYS:HG2	F:31:DG:O3'	0.696
1	D:158:ARG:CG	D:161:PRO:HG2	0.696
1	A:115:THR:HB	A:118:PHE:HE1	0.695
1	A:249:LYS:HD2	F:8:DC:OP2	0.695
1	D:19:GLU:C	D:20:LEU:HD12	0.695
1	D:178:MET:HE1	D:180:LEU:CD1	0.695
1	D:137:LYS:NZ	D:185:GLN:HB2	0.695
1	A:212:LEU:O	A:212:LEU:HD23	0.694
1	D:149:LEU:HD21	D:191:LEU:CD2	0.694
1	A:145:GLU:HB2	A:165:TYR:CE2	0.693
1	A:82:ILE:HG23	A:96:MET:HB3	0.691
1	B:209:GLY:HA3	B:211:ILE:CD1	0.691
1	A:1:LYS:HG3	A:15:TRP:NE1	0.690
1	D:122:ASP:C	D:124:PRO:HD2	0.690

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:170:PRO:HA	D:179:LYS:HD2	0.690
1	A:77:LYS:HB2	A:104:VAL:CG2	0.689
1	B:168:VAL:CG1	B:169:LEU:HD23	0.689
1	D:137:LYS:HE3	D:183:LYS:CD	0.689
1	A:1:LYS:HE3	A:15:TRP:CD2	0.688
1	A:162:ARG:NH2	A:164:ILE:HD11	0.688
1	D:62:VAL:HG11	D:130:ARG:HG3	0.688
1	D:215:LYS:HE3	D:219:PHE:HE2	0.688
1	A:120:PHE:O	A:137:ILE:HG13	0.687
1	B:155:PHE:CE2	B:206:SER:OG	0.687
1	F:5:DC:H2"	F:6:DC:C5	0.686
1	D:175:TRP:HH2	E:10:DC:C5'	0.686
1	B:185:ASP:HA	B:188:ASN:ND2	0.685
1	D:141:LYS:HB3	F:32:DC:P	0.684
1	A:17:ILE:CG2	A:77:LYS:HD2	0.683
1	A:20:ARG:HB3	A:45:VAL:CG1	0.683
1	D:40:GLN:O	D:43:LEU:HB2	0.683
1	D:135:LYS:HG3	D:136:HIS:N	0.683
1	D:149:LEU:HD21	D:191:LEU:CB	0.683
1	D:163:LYS:CB	D:186:ILE:HG23	0.683
1	B:157:PRO:C	B:157:PRO:CB	0.682
1	D:130:ARG:HD3	E:16:DT:P	0.682
1	D:168:LYS:CB	E:13:DT:H4'	0.682
1	D:191:LEU:CD1	D:201:GLU:HG2	0.682
1	B:173:LYS:CG	B:181:LEU:HD21	0.681
1	B:183:PHE:HB3	B:219:HIS:CD2	0.681
1	D:65:ALA:N	D:139:ILE:HB	0.681

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:167:MET:CE	A:195:ALA:HB3	0.680
1	A:194:LEU:HD21	A:230:ARG:CD	0.680
1	B:167:GLN:HA	B:170:ASN:HD21	0.680
1	B:169:LEU:HD21	B:191:LYS:CE	0.680
1	A:23:ASN:OD1	A:44:LEU:HB3	0.679
1	A:38:LYS:CD	A:58:GLU:HB2	0.679
1	A:85:LYS:HE3	D:66:PRO:HG3	0.679
1	A:137:ILE:O	A:137:ILE:HD12	0.679
1	C:94:LEU:CD1	C:96:LEU:HG	0.679
1	A:85:LYS:CD	E:14:DT:C2	0.679
1	F:6:DC:H5'	F:7:DC:H5	0.679
1	A:24:LYS:HG3	A:24:LYS:O	0.678
1	A:220:ASN:CB	A:221:PRO:HD3	0.678
1	C:90:HIS:CD2	C:91:PRO:HD3	0.678
1	D:131:ASP:HB3	E:15:DT:C5'	0.678
1	D:175:TRP:CE3	E:11:DT:H72	0.678
1	D:230:VAL:CG2	D:236:LYS:HG2	0.678
1	A:21:VAL:CG2	A:73:TYR:HD1	0.677
1	A:30:TRP:HE3	A:39:LEU:HD21	0.677
1	A:64:PHE:O	A:67:ILE:HG22	0.677
1	D:181:TYR:CE1	E:13:DT:C4'	0.677
1	B:155:PHE:N	B:225:ALA:N	0.677
1	D:171:HIS:CA	E:12:DT:O2	0.677
1	A:86:GLN:OE1	D:117:LEU:HD21	0.675
1	E:14:DT:H2'	E:15:DT:OP1	0.675
1	B:155:PHE:HE2	B:206:SER:OG	0.675
1	B:183:PHE:CD2	B:219:HIS:HD2	0.674



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:149:ASN:H	D:46:ARG:HH12	0.674
1	A:5:ILE:HD13	A:7:SER:H	0.673
1	A:153:ARG:HG2	A:158:GLU:O	0.673
1	A:228:LYS:CD	A:229:LEU:HD23	0.673
1	D:137:LYS:HD3	D:183:LYS:HZ2	0.672
1	A:140:ILE:HD12	A:167:MET:C	0.671
1	A:1:LYS:HD3	A:17:ILE:HG22	0.670
1	A:171:GLY:O	A:172:LYS:HG2	0.670
1	B:155:PHE:C	B:226:GLU:OE1	0.670
1	D:155:LEU:HD22	D:158:ARG:HH21	0.670
1	A:42:LEU:CD2	A:96:MET:HE1	0.669
1	A:213:SER:O	A:216:THR:HG22	0.669
1	C:105:HIS:ND1	D:53:ALA:C	0.669
1	A:177:THR:HA	A:210:SER:HB3	0.668
1	A:179:TRP:CE3	A:212:LEU:HD13	0.668
1	A:180:GLY:H	A:212:LEU:CD1	0.668
1	B:168:VAL:HA	B:171:LEU:HD11	0.668
1	D:62:VAL:CA	D:133:ASP:HB2	0.668
1	D:130:ARG:HH22	E:16:DT:N1	0.667
1	A:20:ARG:HB3	A:45:VAL:HG11	0.666
1	A:77:LYS:CG	A:104:VAL:HG23	0.666
1	B:154:SER:H	B:223:THR:CG2	0.666
1	E:12:DT:H1'	E:12:DT:OP1	0.666
1	C:4:ASP:OD2	D:48:TYR:CB	0.665
1	D:68:ILE:H	D:68:ILE:HD13	0.665
1	D:108:CYS:SG	D:130:ARG:HD3	0.664
1	A:8:LEU:O	A:10:PRO:HD3	0.663

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:29:THR:HG21	A:40:PHE:CZ	0.663
1	D:28:ILE:HD13	D:30:ARG:NE	0.663
1	D:235:TRP:CE3	D:236:LYS:HE2	0.663
1	A:153:ARG:HH11	A:156:ASN:ND2	0.663
1	A:79:THR:CG2	A:81:LYS:HE2	0.662
1	B:168:VAL:O	B:171:LEU:HD13	0.662
1	D:90:VAL:O	D:91:VAL:HG13	0.662
1	A:4:PRO:HB3	A:8:LEU:CD2	0.661
1	A:75:PHE:O	A:106:PRO:HD2	0.661
1	A:140:ILE:HG21	A:169:THR:HA	0.661
1	A:153:ARG:HD3	A:156:ASN:ND2	0.661
1	D:172:HIS:CG	F:31:DG:N2	0.660
1	D:127:ASP:H	E:15:DT:C3'	0.660
1	A:140:ILE:HB	A:168:ASP:O	0.659
1	A:145:GLU:HG3	A:165:TYR:HD2	0.659
1	B:215:VAL:HB	B:220:PHE:CD1	0.659
1	D:62:VAL:HG11	D:137:LYS:CB	0.659
1	D:63:LYS:C	D:139:ILE:H	0.659
1	D:159:GLU:HG2	D:160:PRO:HD2	0.659
1	E:1:DG:H2"	E:2:DG:C8	0.659
1	D:137:LYS:CD	E:16:DT:H5'	0.658
1	D:183:LYS:O	D:187:VAL:HG23	0.657
1	D:40:GLN:HA	D:43:LEU:HD12	0.656
1	D:117:LEU:H	D:117:LEU:HD22	0.656
1	D:126:CYS:CA	E:16:DT:P	0.656
1	A:131:LYS:C	A:131:LYS:HD3	0.655

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:120:PHE:N	A:137:ILE:HG12	0.653
1	D:66:PRO:O	D:67:LYS:HD3	0.653
1	C:10:ILE:HG23	C:102:LYS:CD	0.652
1	A:161:LYS:HD2	A:161:LYS:N	0.651
1	D:63:LYS:C	D:138:LEU:HA	0.651
1	D:137:LYS:CD	E:16:DT:H5"	0.650
1	D:149:LEU:C	D:149:LEU:HD23	0.650
1	D:195:GLY:O	D:200:LEU:HD12	0.650
1	A:85:LYS:HB2	A:88:THR:CG2	0.649
1	A:190:ARG:HG2	A:191:GLN:OE1	0.649
1	A:228:LYS:C	A:228:LYS:HD3	0.649
1	B:209:GLY:C	B:211:ILE:HD12	0.649
1	D:62:VAL:CA	E:15:DT:O4	0.649
1	A:1:LYS:HG2	A:17:ILE:CG2	0.648
1	D:62:VAL:HB	E:15:DT:C4	0.648
1	D:168:LYS:HB3	E:13:DT:H5"	0.648
1	D:165:ILE:CG1	D:182:LEU:HD11	0.648
1	D:108:CYS:SG	E:16:DT:C4'	0.647
1	A:85:LYS:O	A:88:THR:HG22	0.646
1	A:115:THR:HG22	A:116:VAL:N	0.646
1	D:62:VAL:N	D:133:ASP:CB	0.645
1	B:155:PHE:CB	B:223:THR:OG1	0.644
1	D:142:THR:HA	D:145:LYS:HG3	0.643
1	D:212:GLU:CG	D:213:LYS:HD2	0.643
1	A:153:ARG:HG3	A:156:ASN:HB2	0.642
1	D:231:ARG:HG3	D:232:SER:N	0.642
1	D:67:LYS:NZ	E:13:DT:C1'	0.642
1	D:67:LYS:CE	E:14:DT:O5'	0.642

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:189:ARG:HD3	E:17:DT:O2	0.641
1	B:167:GLN:NE2	B:170:ASN:HD21	0.641
1	A:1:LYS:HE3	A:15:TRP:CE3	0.640
1	D:62:VAL:C	D:134:ASP:N	0.640
1	A:35:GLY:O	A:36:GLU:HG3	0.638
1	A:44:LEU:HD11	A:91:LYS:CG	0.638
1	A:61:ASP:OD1	A:65:PRO:HG2	0.638
1	D:157:LYS:HG3	D:158:ARG:N	0.638
1	D:137:LYS:CE	D:183:LYS:HD2	0.638
1	A:30:TRP:HE3	A:39:LEU:CD2	0.637
1	A:44:LEU:HG	A:51:ILE:HD11	0.637
1	A:138:ILE:HG13	A:200:ARG:HH11	0.637
1	A:222:ASP:CG	A:224:PRO:HD2	0.637
1	D:209:GLU:O	D:213:LYS:HD3	0.637
1	D:227:ARG:HH11	D:238:GLU:HB3	0.637
1	A:24:LYS:HZ2	A:215:SER:HB2	0.636
1	B:156:MET:HB3	B:161:LEU:HD13	0.636
1	B:211:ILE:H	B:211:ILE:HD12	0.635
1	C:39:PHE:HD1	C:53:LEU:CD1	0.635
1	C:108:PRO:HD2	D:56:THR:HA	0.635
1	A:28:ARG:NH2	A:62:LYS:HE2	0.634
1	D:64:ALA:HB1	D:118:MET:SD	0.634
1	D:142:THR:CA	D:145:LYS:HE3	0.634
1	D:168:LYS:HE3	E:13:DT:C2	0.634
1	C:105:HIS:CG	D:54:ALA:N	0.634
1	C:1:ASP:C	D:47:PRO:HD2	0.633
1	D:7:ALA:O	D:9:PRO:HD3	0.633

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:4:PRO:CB	A:8:LEU:HD23	0.632
1	A:196:ILE:O	A:196:ILE:HG13	0.632
1	D:63:LYS:HG3	D:63:LYS:O	0.632
1	B:166:ASN:ND2	B:202:VAL:HG22	0.631
1	D:137:LYS:CG	E:16:DT:H5"	0.631
1	A:1:LYS:H3	A:17:ILE:HG21	0.630
1	B:202:VAL:O	B:205:LEU:HD23	0.629
1	D:64:ALA:HB3	D:131:ASP:CB	0.629
1	D:138:LEU:HB3	D:184:LEU:HG	0.629
1	A:19:ALA:HB1	A:73:TYR:HE2	0.628
1	A:30:TRP:HB2	A:39:LEU:CD2	0.628
1	B:187:LYS:HD2	B:199:LYS:HD2	0.628
1	D:67:LYS:HG3	D:166:VAL:CG2	0.628
1	D:146:GLN:HG2	D:156:GLU:CD	0.628
1	D:168:LYS:HB3	D:179:LYS:NZ	0.628
1	A:96:MET:HE2	F:2:DC:N4	0.627
1	C:34:PRO:CD	C:40:ILE:HG22	0.627
1	A:82:ILE:O	E:13:DT:H73	0.627
1	A:116:VAL:HG12	A:117:GLN:N	0.626
1	A:176:ALA:O	A:209:LEU:HD22	0.626
1	B:215:VAL:CG2	D:42:ARG:NH2	0.626
1	D:62:VAL:CG2	D:135:LYS:HB3	0.626
1	D:164:PHE:C	D:165:ILE:HG13	0.626
1	A:6:ALA:HB2	A:20:ARG:HE	0.625
1	A:179:TRP:HE3	A:212:LEU:HD13	0.625
1	A:234:ASP:HB3	A:238:GLN:OE1	0.625
1	B:155:PHE:CA	B:225:ALA:O	0.625

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:177:ASP:HB2	F:33:DC:H5'	0.625
1	D:212:GLU:OE2	D:213:LYS:HE3	0.624
1	D:214:MET:C	D:218:LYS:HE2	0.624
1	A:11:TYR:H	A:11:TYR:HD1	0.624
1	B:195:VAL:HG23	B:196:SER:N	0.623
1	C:39:PHE:HD1	C:53:LEU:HD13	0.623
1	D:196:SER:O	D:197:GLN:HB2	0.623
1	A:132:ASP:CG	A:204:PHE:HD2	0.622
1	D:130:ARG:CG	E:16:DT:OP1	0.622
1	D:151:LYS:HB3	D:151:LYS:NZ	0.622
1	D:158:ARG:HD2	D:161:PRO:CG	0.622
1	C:105:HIS:HE1	D:53:ALA:HB1	0.621
1	A:85:LYS:CE	D:66:PRO:HG3	0.620
1	B:211:ILE:HG13	B:226:GLU:OE1	0.620
1	D:18:ALA:O	D:19:GLU:HB2	0.620
1	D:32:ARG:NH1	D:34:ARG:HA	0.620
1	A:56:PHE:HA	A:99:ASN:ND2	0.619
1	B:172:ILE:O	B:176:PRO:HD3	0.619
1	D:162:LEU:HD13	D:163:LYS:HB2	0.619
1	A:234:ASP:HA	A:238:GLN:HB2	0.618
1	D:176:GLY:CA	E:11:DT:O2	0.618
1	D:222:LYS:HA	D:225:GLU:CD	0.618
1	B:181:LEU:HB3	B:221:LYS:O	0.617
1	D:14:LEU:N	D:14:LEU:HD12	0.617
1	D:172:HIS:NE2	E:10:DC:N3	0.617
1	A:42:LEU:HD23	A:55:ALA:HB2	0.616
1	D:90:VAL:O	D:91:VAL:HG22	0.616

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:11:TYR:HA	A:81:LYS:HG3	0.615
1	B:184:GLN:HG3	B:199:LYS:NZ	0.615
1	C:40:ILE:HG13	C:52:GLU:CG	0.615
1	D:135:LYS:CD	E:16:DT:O4	0.615
1	A:200:ARG:HG3	A:210:SER:OG	0.614
1	B:166:ASN:HD21	B:202:VAL:HG22	0.614
1	D:68:ILE:CG2	D:117:LEU:HD12	0.614
1	D:175:TRP:CD2	E:11:DT:H71	0.614
1	A:140:ILE:CD1	A:167:MET:HB3	0.613
1	D:137:LYS:HD2	E:16:DT:C5'	0.613
1	C:108:PRO:CD	D:55:ALA:O	0.612
1	D:130:ARG:CD	E:16:DT:OP1	0.612
1	A:30:TRP:CE3	A:39:LEU:HG	0.611
1	A:44:LEU:HD11	A:51:ILE:HG12	0.610
1	C:94:LEU:HD11	C:96:LEU:CG	0.609
1	D:166:VAL:HG23	D:181:TYR:HB2	0.609
1	D:172:HIS:CB	E:12:DT:H5'	0.609
1	A:17:ILE:HG21	A:77:LYS:HE3	0.608
1	B:157:PRO:C	B:158:ALA:CA	0.608
1	D:28:ILE:HG12	D:29:GLU:N	0.608
1	D:63:LYS:N	D:138:LEU:HA	0.608
1	D:137:LYS:CE	D:137:LYS:HA	0.607
1	A:247:ASP:O	A:248:LEU:HD23	0.606
1	B:169:LEU:HD12	B:202:VAL:CG1	0.606
1	C:2:MET:CE	D:48:TYR:N	0.606
1	A:17:ILE:HG21	A:77:LYS:CE	0.605

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:24:LYS:HB3	A:217:ILE:HG12	0.605
1	A:140:ILE:HG13	A:167:MET:HE3	0.605
1	A:176:ALA:HB3	A:209:LEU:HD21	0.605
1	B:157:PRO:CA	B:161:LEU:HD11	0.605
1	B:129:ASN:HD21	D:61:ASN:CB	0.605
1	D:181:TYR:C	D:182:LEU:HD22	0.605
1	A:81:LYS:CA	A:81:LYS:HZ3	0.604
1	B:195:VAL:CG2	B:198:ILE:HG22	0.604
1	B:211:ILE:N	B:211:ILE:HD12	0.604
1	C:33:HIS:CE1	C:37:LYS:HD2	0.604
1	D:64:ALA:C	D:139:ILE:HB	0.604
1	D:172:HIS:N	E:12:DT:H5'	0.604
1	A:47:GLU:HG2	A:48:SER:N	0.603
1	D:25:ARG:HA	D:25:ARG:NH1	0.603
1	D:117:LEU:N	D:117:LEU:HD22	0.603
1	D:177:ASP:CG	F:33:DC:C5'	0.603
1	A:2:VAL:C	A:4:PRO:HD3	0.602
1	A:2:VAL:O	A:4:PRO:HD3	0.602
1	A:120:PHE:C	A:137:ILE:HD11	0.602
1	D:131:ASP:HB3	E:15:DT:P	0.602
1	A:69:VAL:O	A:72:VAL:HG12	0.601
1	A:140:ILE:HD12	A:168:ASP:N	0.601
1	A:180:GLY:N	A:212:LEU:HD21	0.601
1	B:206:SER:HA	B:211:ILE:HD13	0.601
1	B:183:PHE:HD2	B:219:HIS:CD2	0.601
1	D:173:SER:O	E:11:DT:C2'	0.601
1	D:141:LYS:CG	F:31:DG:O3'	0.601
1	D:67:LYS:CG	D:166:VAL:HB	0.600



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:71:THR:HG22	D:72:GLY:N	0.599
1	D:136:HIS:HB3	D:137:LYS:NZ	0.599
1	D:154:ASP:O	D:157:LYS:HG2	0.599
1	A:19:ALA:HB1	A:73:TYR:CZ	0.598
1	A:137:ILE:C	A:137:ILE:HD12	0.598
1	B:162:THR:CG2	B:166:ASN:HB2	0.598
1	D:163:LYS:HE2	D:189:ARG:NE	0.598
1	D:179:LYS:HB2	D:181:TYR:CE1	0.598
1	D:215:LYS:HE3	D:219:PHE:CE2	0.598
1	A:150:ILE:CG1	A:159:VAL:HG12	0.597
1	A:162:ARG:C	A:162:ARG:HD3	0.597
1	D:143:GLU:OE2	D:147:GLU:HG3	0.597
1	D:226:LEU:O	D:230:VAL:HG13	0.597
1	B:168:VAL:O	B:172:ILE:HD13	0.596
1	D:231:ARG:NH2	D:239:THR:HA	0.596
1	A:91:LYS:HB3	A:91:LYS:NZ	0.595
1	A:98:PHE:CZ	F:1:DC:C2	0.595
1	A:179:TRP:CH2	A:197:LYS:HD3	0.595
1	B:131:GLN:HG3	B:132:PRO:N	0.595
1	A:69:VAL:HG12	A:70:ASN:N	0.594
1	D:162:LEU:C	D:162:LEU:HD13	0.594
1	D:175:TRP:HH2	E:10:DC:H4'	0.594
1	A:234:ASP:CA	A:238:GLN:HB3	0.593
1	D:214:MET:O	D:218:LYS:HD3	0.593
1	A:166:LEU:N	A:166:LEU:HD22	0.592
1	B:162:THR:HG22	B:166:ASN:HB2	0.592

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:137:LYS:CA	D:183:LYS:HD2	0.592
1	A:73:TYR:HD2	A:108:GLU:CB	0.592
1	D:25:ARG:NH1	D:26:ALA:H	0.592
1	A:24:LYS:HB3	A:217:ILE:HG13	0.591
1	A:153:ARG:CG	A:156:ASN:HB2	0.591
1	A:194:LEU:CD1	A:196:ILE:HG23	0.591
1	B:162:THR:HG22	B:163:VAL:N	0.591
1	B:173:LYS:O	B:181:LEU:HD21	0.591
1	D:172:HIS:CG	F:31:DG:H22	0.591
1	D:224:LYS:NZ	D:228:ARG:HH11	0.591
1	A:54:THR:CA	A:97:THR:HG23	0.590
1	C:39:PHE:CE2	C:41:LEU:HD21	0.590
1	D:138:LEU:HB3	D:184:LEU:CD1	0.590
1	D:168:LYS:CG	E:13:DT:C4'	0.590
1	B:190:LEU:C	B:190:LEU:HD13	0.589
1	D:162:LEU:CD2	D:190:SER:HB3	0.589
1	D:168:LYS:NZ	E:12:DT:H3	0.589
1	A:57:ASN:CG	A:98:PHE:HZ	0.588
1	A:201:VAL:HG12	A:211:VAL:O	0.588
1	C:39:PHE:HE2	C:41:LEU:HD21	0.588
1	A:87:PHE:HE1	A:131:LYS:HZ1	0.588
1	B:131:GLN:CG	B:132:PRO:HD2	0.587
1	B:154:SER:HB3	B:225:ALA:HA	0.587
1	D:64:ALA:HB3	E:15:DT:P	0.587
1	D:99:GLU:HG2	D:100:PHE:N	0.587
1	D:112:PHE:CE1	D:127:ASP:HB3	0.587
1	D:192:GLU:O	D:196:SER:HA	0.587
1	D:222:LYS:CE	D:226:LEU:HD11	0.587

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:20:ARG:CB	A:45:VAL:HG12	0.586
1	A:134:LEU:HG	A:135:VAL:N	0.586
1	A:140:ILE:HG21	A:169:THR:CA	0.586
1	D:64:ALA:HB1	E:15:DT:P	0.586
1	D:76:ILE:O	D:76:ILE:HG13	0.586
1	D:235:TRP:CZ3	D:236:LYS:HE2	0.586
1	F:34:DG:H2'	F:35:DC:C6	0.586
1	A:193:VAL:HG12	A:194:LEU:N	0.585
1	A:142:LYS:HG3	A:165:TYR:CE2	0.584
1	A:162:ARG:HH22	A:164:ILE:HD11	0.584
1	B:155:PHE:CA	B:226:GLU:HB3	0.584
1	D:116:TYR:HA	D:119:ASN:ND2	0.584
1	A:121:THR:N	A:137:ILE:HD11	0.583
1	B:215:VAL:HG12	B:216:ASP:N	0.583
1	A:74:TYR:CD1	A:107:CYS:HA	0.582
1	A:78:GLY:O	A:79:THR:HB	0.581
1	B:186:LEU:C	B:186:LEU:HD13	0.581
1	A:1:LYS:HB3	A:15:TRP:CZ2	0.580
1	B:187:LYS:HZ2	B:199:LYS:HG3	0.580
1	D:149:LEU:HD22	D:151:LYS:NZ	0.580
1	D:154:ASP:HA	D:157:LYS:CE	0.580
1	D:159:GLU:HG2	D:160:PRO:HD3	0.580
1	D:172:HIS:CD2	E:10:DC:O2	0.580
1	D:209:GLU:HA	D:212:GLU:OE2	0.580
1	A:223:ILE:O	A:223:ILE:HG23	0.579
1	D:64:ALA:HB2	D:137:LYS:O	0.579
1	D:149:LEU:HD13	D:151:LYS:NZ	0.579

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:149:LEU:O	D:204:LYS:HE2	0.579
1	D:67:LYS:NZ	E:13:DT:H1'	0.579
1	A:29:THR:HG22	A:40:PHE:O	0.578
1	D:64:ALA:O	E:14:DT:C2'	0.578
1	D:16:GLN:N	D:17:PRO:HD3	0.577
1	A:194:LEU:C	A:194:LEU:HD13	0.576
1	D:8:LEU:H	D:8:LEU:HD12	0.576
1	D:8:LEU:N	D:8:LEU:HD12	0.576
1	D:128:ASN:HA	D:131:ASP:OD1	0.576
1	A:26:GLN:HG2	A:27:ILE:N	0.574
1	A:43:GLU:CD	A:68:GLU:HG2	0.574
1	A:44:LEU:HD21	A:51:ILE:CD1	0.574
1	A:18:CYS:HG	A:76:SER:HB3	0.574
1	A:248:LEU:C	F:7:DC:H2'	0.574
1	A:172:LYS:HG3	A:172:LYS:O	0.573
1	A:209:LEU:HD13	A:210:SER:H	0.573
1	D:68:ILE:HD12	D:117:LEU:HD12	0.573
1	A:162:ARG:CZ	A:164:ILE:HD11	0.572
1	D:139:ILE:CG1	D:181:TYR:HB3	0.572
1	D:221:LYS:O	D:224:LYS:HG2	0.572
1	B:156:MET:CB	B:156:MET:N	0.572
1	A:120:PHE:H	A:137:ILE:HG12	0.571
1	D:28:ILE:HG12	D:30:ARG:H	0.571
1	D:62:VAL:HG13	D:137:LYS:CA	0.571
1	A:21:VAL:HG12	A:22:THR:N	0.570
1	A:21:VAL:HG22	A:73:TYR:CD1	0.570
1	A:145:GLU:CB	A:165:TYR:CE2	0.570

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:154:SER:CA	B:224:ASP:O	0.570
1	D:30:ARG:HG3	D:30:ARG:O	0.570
1	D:68:ILE:N	D:68:ILE:HD13	0.570
1	D:130:ARG:HG2	E:16:DT:C5'	0.570
1	D:234:VAL:O	D:234:VAL:HG12	0.570
1	D:165:ILE:HG22	D:166:VAL:N	0.569
1	D:199:ALA:HA	D:202:GLU:CD	0.569
1	D:86:LYS:HG2	D:87:ILE:H	0.568
1	A:177:THR:HG22	A:178:LEU:N	0.565
1	D:162:LEU:HD11	D:190:SER:OG	0.565
1	D:222:LYS:HA	D:225:GLU:OE1	0.565
1	A:42:LEU:HD22	A:54:THR:C	0.564
1	A:123:ILE:HB	A:126:LEU:CG	0.564
1	A:151:THR:HG22	A:160:ALA:O	0.564
1	B:145:SER:HB2	C:23:VAL:HG22	0.564
1	D:33:GLN:O	D:37:MET:HG2	0.564
1	D:189:ARG:O	D:192:GLU:HG2	0.564
1	A:5:ILE:HD12	A:7:SER:H	0.563
1	B:215:VAL:CG2	D:42:ARG:HH21	0.563
1	D:137:LYS:HG3	E:16:DT:O5'	0.563
1	A:245:ILE:HG22	A:246:SER:N	0.562
1	D:20:LEU:N	D:20:LEU:HD12	0.562
1	D:126:CYS:N	E:16:DT:OP2	0.562
1	A:44:LEU:CD2	A:51:ILE:HD11	0.561
1	A:66:LEU:N	A:66:LEU:HD12	0.561
1	A:77:LYS:HG3	A:104:VAL:CG2	0.561
1	D:1:MET:HE3	D:1:MET:N	0.561

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:139:ILE:CD1	E:14:DT:OP1	0.561
1	D:230:VAL:HG21	D:236:LYS:HG2	0.561
1	A:179:TRP:HE3	A:212:LEU:CD1	0.560
1	A:56:PHE:HD2	A:60:VAL:CG1	0.560
1	D:106:GLU:OE2	H:1:ZN2:ZN2	0.560
1	A:123:ILE:HG22	A:125:ASP:H	0.559
1	A:148:THR:O	A:148:THR:HG23	0.559
1	B:154:SER:C	B:223:THR:CG2	0.559
1	D:32:ARG:HH22	D:34:ARG:CD	0.559
1	D:64:ALA:HA	D:139:ILE:N	0.559
1	A:145:GLU:HG3	A:165:TYR:CD2	0.558
1	A:175:THR:CG2	A:200:ARG:HH22	0.557
1	D:40:GLN:CA	D:43:LEU:HD12	0.557
1	D:138:LEU:HD11	D:140:THR:HG22	0.557
1	D:207:ARG:NH1	D:211:ARG:HH21	0.557
1	A:85:LYS:CA	E:14:DT:N3	0.557
1	D:61:ASN:N	D:61:ASN:HD22	0.556
1	A:119:ASP:CB	A:137:ILE:HG12	0.555
1	A:228:LYS:HD2	A:229:LEU:HD23	0.555
1	B:198:ILE:HG23	B:199:LYS:N	0.555
1	A:38:LYS:CG	A:39:LEU:H	0.554
1	A:218:ILE:O	A:218:ILE:HG23	0.554
1	D:231:ARG:HH21	D:239:THR:HA	0.554
1	A:44:LEU:HD21	A:51:ILE:HD13	0.553
1	B:186:LEU:O	B:186:LEU:HD13	0.553
1	A:26:GLN:HG2	A:27:ILE:H	0.552

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:73:TYR:HE2	A:108:GLU:CD	0.552
1	A:164:ILE:HG12	A:178:LEU:HD23	0.552
1	B:163:VAL:HG22	B:164:ALA:N	0.552
1	B:195:VAL:HG23	B:198:ILE:HG22	0.552
1	A:82:ILE:HG12	A:83:ALA:N	0.551
1	A:142:LYS:HA	A:165:TYR:CE1	0.551
1	A:196:ILE:HG21	A:222:ASP:OD2	0.551
1	D:62:VAL:HG23	D:135:LYS:CB	0.551
1	D:230:VAL:HG23	D:236:LYS:HG2	0.551
1	A:137:ILE:HG22	A:198:GLY:HA2	0.550
1	D:89:LYS:HG2	D:90:VAL:CG2	0.550
1	D:136:HIS:O	D:184:LEU:HB2	0.550
1	D:133:ASP:N	E:15:DT:C7	0.550
1	A:52:ARG:CZ	A:95:GLU:HB3	0.549
1	C:10:ILE:HG22	D:52:ALA:HB1	0.549
1	D:68:ILE:HG21	D:117:LEU:CD1	0.549
1	D:132:ALA:C	E:15:DT:C7	0.549
1	D:142:THR:CB	D:145:LYS:HE3	0.549
1	D:186:ILE:HG22	D:187:VAL:N	0.549
1	D:207:ARG:HD2	D:211:ARG:NH2	0.549
1	F:37:DG:H2'	F:38:DG:C8	0.549
1	D:63:LYS:HB2	D:134:ASP:CA	0.548
1	D:64:ALA:C	D:131:ASP:HB2	0.548
1	A:153:ARG:HH11	A:156:ASN:HD22	0.548
1	A:17:ILE:HB	A:77:LYS:CD	0.547
1	D:126:CYS:HB2	E:16:DT:OP2	0.547
1	D:130:ARG:HG2	D:137:LYS:CG	0.547
1	A:1:LYS:HG3	A:15:TRP:CE2	0.546

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:42:LEU:C	A:42:LEU:HD13	0.546
1	A:175:THR:HG21	A:200:ARG:HH22	0.546
1	D:67:LYS:HD2	D:168:LYS:CB	0.546
1	D:91:VAL:O	D:92:HIS:HB2	0.546
1	D:222:LYS:C	D:222:LYS:HD3	0.546
1	D:224:LYS:O	D:228:ARG:HG2	0.546
1	D:129:CYS:O	E:15:DT:N3	0.546
1	B:224:ASP:OD2	D:39:ARG:CZ	0.546
1	A:28:ARG:HH21	A:39:LEU:HD12	0.545
1	A:72:VAL:HG13	A:74:TYR:HE2	0.545
1	B:215:VAL:H	B:220:PHE:HD1	0.545
1	A:121:THR:HA	A:137:ILE:HD11	0.544
1	B:154:SER:HB2	B:224:ASP:O	0.544
1	D:127:ASP:CG	D:128:ASN:H	0.544
1	D:191:LEU:C	D:191:LEU:HD13	0.544
1	A:121:THR:HA	A:137:ILE:CD1	0.543
1	A:175:THR:HG21	A:200:ARG:NH2	0.543
1	B:154:SER:C	B:226:GLU:N	0.543
1	D:141:LYS:NZ	D:179:LYS:HG2	0.543
1	D:180:LEU:N	D:180:LEU:HD22	0.543
1	A:249:LYS:CG	F:7:DC:H5"	0.543
1	A:72:VAL:HG22	A:73:TYR:N	0.542
1	D:122:ASP:HB3	D:124:PRO:HD2	0.542
1	C:101:VAL:HG12	D:54:ALA:CB	0.541
1	C:112:PRO:CD	D:55:ALA:HB3	0.541
1	D:163:LYS:HG2	D:186:ILE:CD1	0.541



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:168:LYS:HD2	D:179:LYS:NZ	0.541
1	D:172:HIS:CB	F:31:DG:N2	0.541
1	A:5:ILE:HD13	A:6:ALA:H	0.540
1	A:63:PHE:CE2	A:64:PHE:CZ	0.540
1	A:86:GLN:CD	D:117:LEU:HD21	0.540
1	B:173:LYS:HE3	B:221:LYS:HB2	0.540
1	D:60:ALA:C	D:61:ASN:HD22	0.540
1	D:63:LYS:N	D:134:ASP:HA	0.540
1	A:17:ILE:HD12	A:75:PHE:CD1	0.539
1	B:203:ASP:OD2	B:221:LYS:HE2	0.539
1	D:80:GLU:HA	D:80:GLU:OE1	0.539
1	D:80:GLU:O	D:81:GLU:HB2	0.539
1	B:129:ASN:ND2	F:28:DC:OP2	0.539
1	A:67:ILE:HG23	A:68:GLU:N	0.538
1	A:140:ILE:O	A:194:LEU:HD22	0.538
1	B:139:ILE:C	B:139:ILE:HD12	0.538
1	B:214:THR:HB	B:217:ASP:O	0.538
1	D:62:VAL:HB	E:15:DT:N3	0.538
1	D:158:ARG:HG3	D:161:PRO:HG2	0.538
1	A:63:PHE:HD2	A:64:PHE:CD2	0.537
1	B:154:SER:C	B:223:THR:OG1	0.537
1	B:171:LEU:C	B:171:LEU:HD22	0.537
1	B:209:GLY:O	B:210:HIS:HB3	0.537
1	D:145:LYS:CE	D:182:LEU:HG	0.537
1	D:181:TYR:CZ	E:13:DT:C4'	0.537
1	D:62:VAL:N	E:15:DT:O4	0.537
1	A:30:TRP:HE3	A:39:LEU:CG	0.536
1	D:63:LYS:HB3	D:138:LEU:CB	0.536

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:66:PRO:HD3	E:15:DT:P	0.536
1	D:149:LEU:HD22	D:151:LYS:HZ2	0.536
1	A:63:PHE:CD2	A:64:PHE:CE2	0.535
1	D:139:ILE:HD12	E:14:DT:C5'	0.535
1	D:227:ARG:NH1	D:239:THR:HG22	0.535
1	A:37:GLY:O	A:38:LYS:HB2	0.534
1	C:25:PHE:CZ	C:67:VAL:HG11	0.534
1	C:7:ARG:NE	C:115:ILE:HG22	0.534
1	D:150:LEU:CD1	D:204:LYS:HG2	0.534
1	A:248:LEU:O	F:7:DC:C3'	0.533
1	D:61:ASN:C	D:135:LYS:N	0.532
1	D:67:LYS:NZ	D:168:LYS:HG3	0.532
1	A:90:VAL:CG2	A:199:ALA:HB2	0.531
1	D:63:LYS:CG	D:138:LEU:HD13	0.531
1	D:139:ILE:HD12	E:14:DT:H5'	0.531
1	A:24:LYS:HB3	A:217:ILE:CD1	0.529
1	D:91:VAL:O	D:91:VAL:HG23	0.529
1	D:97:VAL:HG23	D:98:MET:N	0.529
1	D:62:VAL:H	D:133:ASP:HB2	0.529
1	D:197:GLN:HA	D:197:GLN:OE1	0.529
1	D:239:THR:OXT	D:239:THR:HG23	0.529
1	A:74:TYR:HD1	A:107:CYS:HA	0.528
1	D:62:VAL:CG1	D:137:LYS:H	0.528
1	D:151:LYS:HE3	D:155:LEU:HD12	0.528
1	D:236:LYS:HD2	D:236:LYS:N	0.528
1	D:177:ASP:HB3	F:33:DC:C5'	0.527
1	D:151:LYS:NZ	D:187:VAL:HG13	0.527

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:224:LYS:NZ	D:228:ARG:HD3	0.527
1	E:10:DC:H1'	E:11:DT:O5'	0.527
1	F:3:DC:H4'	F:4:DC:H5	0.527
1	A:75:PHE:CB	A:106:PRO:HG2	0.526
1	D:62:VAL:CG1	D:137:LYS:CB	0.526
1	D:106:GLU:HG2	D:108:CYS:H	0.526
1	D:114:ASP:OD2	D:125:THR:HG23	0.526
1	D:141:LYS:NZ	F:31:DG:C3'	0.526
1	A:209:LEU:HD13	A:210:SER:O	0.525
1	D:149:LEU:HG	D:191:LEU:HB2	0.525
1	D:223:VAL:HG23	D:224:LYS:N	0.524
1	D:232:SER:O	D:234:VAL:HG23	0.524
1	A:190:ARG:NE	A:191:GLN:HE22	0.524
1	A:240:LEU:HG	A:241:ASP:N	0.523
1	D:106:GLU:HG3	D:125:THR:HG22	0.523
1	D:138:LEU:HB3	D:184:LEU:HD12	0.523
1	A:222:ASP:C	A:224:PRO:HD2	0.522
1	B:157:PRO:CA	B:157:PRO:O	0.522
1	B:176:PRO:HG3	B:182:ASN:OD1	0.522
1	A:179:TRP:CZ2	A:218:ILE:HD12	0.521
1	B:168:VAL:HG13	B:169:LEU:CD2	0.521
1	B:169:LEU:N	B:169:LEU:HD23	0.521
1	B:187:LYS:NZ	B:199:LYS:HG3	0.521
1	B:209:GLY:HA3	B:211:ILE:HD11	0.521
1	D:117:LEU:CD2	D:117:LEU:H	0.521
1	D:138:LEU:CG	D:140:THR:HG23	0.521

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:135:VAL:O	A:135:VAL:HG23	0.520
1	B:154:SER:C	B:225:ALA:C	0.520
1	C:10:ILE:HG23	C:102:LYS:HZ2	0.520
1	D:181:TYR:CD2	E:14:DT:P	0.520
1	A:248:LEU:C	F:7:DC:C2'	0.520
1	A:52:ARG:NH2	A:81:LYS:HZ2	0.520
1	A:51:ILE:HG23	A:91:LYS:CD	0.519
1	A:81:LYS:HA	A:81:LYS:NZ	0.519
1	A:228:LYS:HD2	A:229:LEU:CD2	0.519
1	B:156:MET:C	B:156:MET:HB3	0.519
1	B:171:LEU:HD21	B:172:ILE:HD12	0.519
1	B:180:GLY:HA2	B:220:PHE:CE2	0.519
1	C:2:MET:CE	D:48:TYR:CA	0.519
1	C:32:ILE:HG13	C:41:LEU:CD2	0.519
1	C:94:LEU:HD13	C:96:LEU:HD23	0.519
1	D:138:LEU:HB3	D:184:LEU:CG	0.518
1	D:151:LYS:HD2	D:187:VAL:HG13	0.518
1	A:30:TRP:CE3	A:39:LEU:HD21	0.517
1	A:179:TRP:HA	A:212:LEU:CD1	0.517
1	B:156:MET:C	B:161:LEU:CD1	0.517
1	D:63:LYS:HD3	D:134:ASP:CG	0.517
1	D:173:SER:C	E:11:DT:C2'	0.517
1	A:1:LYS:CD	A:1:LYS:H3	0.516
1	D:67:LYS:HD2	D:168:LYS:HB2	0.516
1	A:142:LYS:CA	A:165:TYR:CE1	0.515
1	B:205:LEU:H	B:205:LEU:HD23	0.515
1	D:158:ARG:HE	D:162:LEU:HB2	0.515
1	A:138:ILE:N	A:138:ILE:HD13	0.514

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:154:SER:C	B:223:THR:HG23	0.514
1	D:103:VAL:HG23	D:113:MET:HE3	0.514
1	D:139:ILE:HD13	E:14:DT:OP1	0.514
1	A:64:PHE:HD1	A:67:ILE:HG21	0.513
1	A:52:ARG:HE	A:96:MET:C	0.513
1	B:155:PHE:N	B:225:ALA:CA	0.513
1	A:99:ASN:N	A:99:ASN:HD22	0.513
1	B:214:THR:HA	B:220:PHE:O	0.512
1	D:132:ALA:C	E:15:DT:C5	0.512
1	D:215:LYS:HG3	D:216:GLN:N	0.512
1	B:154:SER:C	B:225:ALA:CA	0.511
1	C:39:PHE:CD1	C:53:LEU:HD13	0.511
1	D:61:ASN:C	D:135:LYS:H	0.511
1	A:3:VAL:HG22	A:17:ILE:CG1	0.510
1	A:38:LYS:HD2	A:57:ASN:HD22	0.510
1	D:191:LEU:HD12	D:201:GLU:CD	0.510
1	A:44:LEU:CD1	A:91:LYS:HG3	0.509
1	D:136:HIS:HB3	D:137:LYS:HZ1	0.509
1	D:163:LYS:HG3	D:186:ILE:HD12	0.509
1	A:72:VAL:CG1	A:74:TYR:CE2	0.508
1	A:164:ILE:HG12	A:178:LEU:HD22	0.508
1	A:99:ASN:H	A:99:ASN:HD22	0.508
1	C:10:ILE:HG22	D:53:ALA:H	0.507
1	D:137:LYS:HZ2	E:16:DT:H1'	0.507
1	C:4:ASP:OD1	D:49:SER:O	0.507
1	A:27:ILE:HG12	A:28:ARG:N	0.506

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:66:LEU:H	A:66:LEU:HD12	0.506
1	C:33:HIS:HE1	C:37:LYS:CD	0.506
1	A:2:VAL:C	A:17:ILE:HG12	0.505
1	A:58:GLU:HG2	A:59:GLN:N	0.505
1	A:153:ARG:HD3	A:156:ASN:HB2	0.505
1	B:180:GLY:CA	B:220:PHE:CE2	0.505
1	C:103:ILE:CD1	C:107:PHE:CE2	0.505
1	D:155:LEU:HD22	D:158:ARG:NH2	0.505
1	D:235:TRP:CD2	D:236:LYS:HE2	0.505
1	E:8:DG:H2''	E:9:DG:H5'	0.505
1	D:130:ARG:CB	E:15:DT:C3'	0.505
1	A:91:LYS:HD3	A:93:ASP:HB2	0.504
1	B:155:PHE:CA	B:155:PHE:H	0.504
1	D:135:LYS:HG3	E:16:DT:C2	0.504
1	B:148:GLY:N	D:46:ARG:NH2	0.504
1	A:162:ARG:NH1	A:164:ILE:HD11	0.503
1	A:165:TYR:CD1	A:166:LEU:N	0.503
1	D:112:PHE:CE1	D:127:ASP:CB	0.503
1	D:222:LYS:HE2	D:226:LEU:HD11	0.503
1	B:215:VAL:CG2	B:220:PHE:CE1	0.502
1	C:10:ILE:HG23	C:102:LYS:HD2	0.502
1	D:142:THR:OG1	D:180:LEU:HB2	0.502
1	A:17:ILE:O	A:17:ILE:HG13	0.501
1	A:167:MET:HE2	A:197:LYS:NZ	0.501
1	A:216:THR:O	A:216:THR:HG23	0.501
1	D:62:VAL:HG21	D:130:ARG:NH2	0.501
1	A:64:PHE:CG	A:105:MET:CE	0.500
1	A:121:THR:O	A:121:THR:HG23	0.500

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:238:GLN:HG2	A:238:GLN:O	0.499
1	B:167:GLN:HA	B:167:GLN:NE2	0.499
1	C:25:PHE:CZ	C:67:VAL:CG1	0.499
1	C:101:VAL:HG12	D:54:ALA:HB1	0.499
1	D:142:THR:HG23	D:156:GLU:HG2	0.499
1	D:230:VAL:HG21	D:236:LYS:CG	0.499
1	D:62:VAL:CG1	E:15:DT:C5	0.499
1	A:47:GLU:CG	A:48:SER:H	0.499
1	A:24:LYS:HD2	A:215:SER:O	0.498
1	A:131:LYS:HD3	A:132:ASP:O	0.498
1	C:10:ILE:HG23	C:102:LYS:HZ3	0.498
1	D:155:LEU:N	D:155:LEU:HD23	0.498
1	A:190:ARG:HG2	A:191:GLN:NE2	0.497
1	C:25:PHE:CE1	C:67:VAL:HG11	0.497
1	D:138:LEU:HD11	D:140:THR:CG2	0.497
1	A:87:PHE:HE1	A:131:LYS:NZ	0.497
1	A:12:GLN:HG2	A:12:GLN:O	0.496
1	A:29:THR:CG2	A:40:PHE:CZ	0.496
1	A:79:THR:HG23	A:81:LYS:HE2	0.496
1	A:115:THR:CB	A:118:PHE:CE1	0.496
1	A:163:ASN:CB	A:184:ASP:HB2	0.496
1	D:34:ARG:HG2	D:34:ARG:HH11	0.496
1	E:3:DC:H2"	E:4:DC:C6	0.496
1	A:88:THR:OG1	F:3:DC:C2	0.496
1	D:65:ALA:H	D:139:ILE:HD12	0.495
1	D:230:VAL:CG2	D:236:LYS:HD3	0.495
1	A:117:GLN:HE22	A:217:ILE:HG22	0.494

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:195:VAL:HG22	B:198:ILE:CG2	0.494
1	D:102:TYR:CG	D:103:VAL:N	0.494
1	D:63:LYS:H	D:138:LEU:CA	0.494
1	A:249:LYS:HG2	A:250:SER:N	0.493
1	D:69:ILE:C	D:69:ILE:HD13	0.493
1	D:63:LYS:H	D:138:LEU:N	0.493
1	D:185:GLN:HE22	E:17:DT:P	0.493
1	A:17:ILE:HG22	A:77:LYS:HD2	0.492
1	A:24:LYS:HA	A:70:ASN:OD1	0.492
1	A:179:TRP:CE3	A:212:LEU:CD1	0.492
1	B:168:VAL:HG13	B:169:LEU:N	0.492
1	D:172:HIS:CE1	E:11:DT:H5"	0.492
1	A:64:PHE:CD1	A:105:MET:HE3	0.491
1	A:85:LYS:HE3	E:14:DT:H1'	0.491
1	C:25:PHE:CE1	C:67:VAL:CG1	0.491
1	D:189:ARG:HA	D:192:GLU:HG2	0.491
1	A:98:PHE:HE1	F:1:DC:O2	0.491
1	A:22:THR:OG1	A:70:ASN:HA	0.490
1	A:158:GLU:HG2	A:159:VAL:N	0.490
1	B:141:ASN:HB3	B:142:PRO:CD	0.490
1	C:2:MET:HE1	D:48:TYR:CA	0.490
1	D:154:ASP:HA	D:157:LYS:HG2	0.490
1	D:179:LYS:HB2	E:13:DT:H5"	0.490
1	E:6:DG:H2"	E:7:DC:C6	0.490
1	D:171:HIS:CB	E:12:DT:O3'	0.490
1	A:52:ARG:HA	A:91:LYS:HE3	0.489



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:61:ASN:C	D:135:LYS:CB	0.489
1	D:197:GLN:CD	D:198:GLU:H	0.489
1	A:24:LYS:HB3	A:217:ILE:HD11	0.488
1	A:145:GLU:HG2	A:146:ASP:O	0.488
1	B:173:LYS:HA	B:182:ASN:ND2	0.488
1	D:162:LEU:O	D:163:LYS:HD3	0.488
1	D:165:ILE:HG23	D:182:LEU:CD2	0.488
1	D:179:LYS:CB	D:181:TYR:CE1	0.488
1	A:44:LEU:CG	A:51:ILE:HD11	0.487
1	A:64:PHE:H	A:65:PRO:HD2	0.487
1	B:198:ILE:O	B:202:VAL:HG23	0.487
1	D:101:ASP:O	D:102:TYR:HB2	0.487
1	D:166:VAL:HG22	D:181:TYR:O	0.487
1	A:1:LYS:CE	A:15:TRP:CE2	0.486
1	D:172:HIS:CE1	E:10:DC:H1'	0.486
1	B:154:SER:N	B:223:THR:O	0.486
1	B:176:PRO:HG3	B:182:ASN:CG	0.485
1	D:64:ALA:HA	D:139:ILE:CA	0.485
1	D:227:ARG:NH1	D:238:GLU:HB3	0.485
1	D:99:GLU:O	D:100:PHE:HD1	0.485
1	A:21:VAL:CG2	A:73:TYR:CD1	0.484
1	B:187:LYS:HD3	B:187:LYS:O	0.484
1	C:33:HIS:CE1	C:37:LYS:HG3	0.484
1	A:2:VAL:HG12	A:3:VAL:N	0.483
1	A:30:TRP:CE3	A:39:LEU:CD2	0.483
1	A:85:LYS:HG3	D:128:ASN:CG	0.483
1	A:163:ASN:HB2	A:184:ASP:HB2	0.483
1	B:215:VAL:HG22	D:42:ARG:CZ	0.483

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:39:PHE:CD1	C:53:LEU:CD1	0.483
1	D:151:LYS:HB3	D:151:LYS:HZ1	0.483
1	D:68:ILE:HG23	D:117:LEU:HD12	0.482
1	D:153:CYS:HA	D:156:GLU:OE1	0.482
1	E:7:DC:H2"	E:8:DG:C5'	0.482
1	A:91:LYS:C	A:91:LYS:HD2	0.481
1	B:206:SER:O	B:211:ILE:HD13	0.481
1	D:8:LEU:CD1	D:8:LEU:H	0.481
1	D:62:VAL:HG23	D:135:LYS:CG	0.481
1	D:68:ILE:HG21	D:117:LEU:HD12	0.481
1	D:85:GLN:HA	D:85:GLN:HE21	0.481
1	D:89:LYS:O	D:90:VAL:HB	0.481
1	D:122:ASP:O	D:123:LEU:HB3	0.481
1	A:70:ASN:HD22	A:71:LYS:N	0.481
1	A:75:PHE:O	A:105:MET:HA	0.480
1	A:140:ILE:O	A:167:MET:HE1	0.480
1	B:173:LYS:HG3	B:181:LEU:HD22	0.480
1	A:85:LYS:CD	E:14:DT:N1	0.480
1	A:1:LYS:CE	A:15:TRP:CD2	0.479
1	A:44:LEU:HD12	A:52:ARG:C	0.479
1	A:91:LYS:HD2	A:93:ASP:N	0.479
1	D:106:GLU:HG2	D:108:CYS:N	0.479
1	D:99:GLU:CG	D:100:PHE:H	0.479
1	A:21:VAL:HG21	A:114:PRO:HG2	0.478
1	A:38:LYS:HG2	A:39:LEU:N	0.478
1	B:131:GLN:HG3	B:132:PRO:CD	0.478

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:145:SER:HB2	C:23:VAL:HG13	0.478
1	B:173:LYS:HE3	B:221:LYS:CB	0.478
1	B:129:ASN:OD1	D:61:ASN:CG	0.478
1	A:3:VAL:HA	A:17:ILE:O	0.477
1	D:34:ARG:HG2	D:34:ARG:NH1	0.477
1	D:163:LYS:HE2	D:189:ARG:HE	0.477
1	D:210:ASN:O	D:214:MET:HG2	0.477
1	F:3:DC:H4'	F:4:DC:C5	0.477
1	F:5:DC:H4'	F:6:DC:O4'	0.477
1	D:139:ILE:O	D:139:ILE:HG23	0.477
1	B:179:GLU:CD	B:179:GLU:H	0.476
1	D:62:VAL:CG1	D:130:ARG:HG3	0.476
1	D:98:MET:O	D:99:GLU:HB3	0.475
1	D:224:LYS:HZ1	D:228:ARG:HH11	0.475
1	B:215:VAL:CG2	B:220:PHE:HE1	0.474
1	A:20:ARG:HD2	A:45:VAL:CB	0.473
1	A:56:PHE:CD2	A:99:ASN:HB3	0.473
1	B:131:GLN:HG3	B:132:PRO:HD2	0.473
1	D:85:GLN:HA	D:85:GLN:NE2	0.473
1	A:24:LYS:HZ1	A:215:SER:HA	0.472
1	A:249:LYS:HG3	F:7:DC:C4'	0.472
1	B:145:SER:HB2	C:23:VAL:CG2	0.472
1	B:165:GLN:HA	B:165:GLN:NE2	0.472
1	D:198:GLU:O	D:201:GLU:HB2	0.472
1	D:230:VAL:CA	D:235:TRP:NE1	0.472
1	A:115:THR:CG2	A:118:PHE:CZ	0.470
1	B:168:VAL:C	B:171:LEU:HD13	0.470
1	B:168:VAL:HA	B:171:LEU:HD13	0.470

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:211:ILE:CD1	B:211:ILE:H	0.470
1	A:56:PHE:CZ	A:105:MET:CE	0.469
1	A:142:LYS:C	A:165:TYR:HE1	0.469
1	D:151:LYS:HG3	D:156:GLU:OE2	0.469
1	D:116:TYR:CE2	D:120:HIS:CE1	0.468
1	D:178:MET:HB2	D:178:MET:HE2	0.468
1	F:3:DC:H5"	F:4:DC:OP2	0.467
1	A:142:LYS:HE3	A:165:TYR:CD2	0.466
1	B:154:SER:CA	B:225:ALA:HA	0.466
1	D:172:HIS:HB3	E:12:DT:C5'	0.466
1	A:91:LYS:CD	A:93:ASP:CB	0.465
1	D:149:LEU:HD13	D:151:LYS:HZ2	0.465
1	D:149:LEU:HD21	D:191:LEU:CG	0.465
1	A:57:ASN:CG	A:98:PHE:CZ	0.463
1	A:212:LEU:C	A:212:LEU:HD23	0.463
1	D:62:VAL:CG2	D:135:LYS:CB	0.463
1	A:85:LYS:HZ3	D:128:ASN:CA	0.463
1	D:61:ASN:C	D:135:LYS:HB3	0.463
1	D:149:LEU:HD22	D:151:LYS:HB3	0.463
1	D:28:ILE:CD1	D:30:ARG:HE	0.463
1	D:64:ALA:N	D:137:LYS:O	0.463
1	A:51:ILE:HG23	A:91:LYS:HD3	0.462
1	B:162:THR:HB	B:167:GLN:CD	0.462
1	B:187:LYS:HG3	B:199:LYS:HE2	0.462
1	D:46:ARG:HB2	D:47:PRO:CD	0.462
1	D:166:VAL:O	D:166:VAL:HG23	0.462

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:164:PHE:O	D:182:LEU:HD13	0.462
1	D:224:LYS:HG3	D:225:GLU:N	0.462
1	A:29:THR:HG21	A:40:PHE:CE1	0.461
1	A:94:TYR:HB2	A:95:GLU:OE1	0.461
1	B:181:LEU:HD23	B:182:ASN:H	0.461
1	A:75:PHE:CZ	A:108:GLU:CD	0.460
1	A:121:THR:CA	A:137:ILE:HD11	0.460
1	A:145:GLU:HA	A:165:TYR:CD2	0.460
1	B:207:ASN:CB	B:212:TYR:CE1	0.460
1	D:62:VAL:CG2	D:135:LYS:CG	0.460
1	D:76:ILE:HD11	D:78:GLU:OE2	0.460
1	D:137:LYS:HB3	D:183:LYS:HZ2	0.460
1	A:115:THR:CG2	A:116:VAL:H	0.460
1	A:116:VAL:CG1	A:117:GLN:H	0.460
1	A:228:LYS:HD3	A:229:LEU:HD23	0.459
1	B:180:GLY:CA	B:220:PHE:HE2	0.459
1	D:121:PHE:C	D:121:PHE:CD1	0.459
1	D:67:LYS:CG	D:166:VAL:CG2	0.459
1	D:67:LYS:HZ3	D:168:LYS:HG3	0.459
1	D:151:LYS:HB2	D:155:LEU:HD12	0.458
1	B:129:ASN:OD1	D:61:ASN:ND2	0.458
1	D:141:LYS:HZ2	F:31:DG:C3'	0.458
1	A:1:LYS:CB	A:15:TRP:NE1	0.457
1	A:50:GLU:HG2	A:51:ILE:N	0.457
1	D:222:LYS:HE3	D:226:LEU:HD11	0.457
1	A:4:PRO:HD2	A:17:ILE:O	0.456
1	A:142:LYS:HE3	A:165:TYR:CG	0.456

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:98:MET:HE3	D:98:MET:N	0.456
1	D:138:LEU:CB	D:184:LEU:HG	0.456
1	D:118:MET:SD	E:15:DT:C5'	0.456
1	A:140:ILE:CD1	A:167:MET:CB	0.455
1	D:97:VAL:C	D:98:MET:HG3	0.455
1	D:165:ILE:HG12	D:182:LEU:CD2	0.455
1	A:29:THR:O	A:29:THR:HG23	0.455
1	D:172:HIS:CG	E:10:DC:O2	0.455
1	B:155:PHE:HA	B:155:PHE:O	0.454
1	C:10:ILE:CG2	C:102:LYS:CD	0.454
1	D:179:LYS:HE3	E:12:DT:O2	0.454
1	D:201:GLU:HA	D:204:LYS:CD	0.454
1	B:203:ASP:O	B:212:TYR:HE1	0.454
1	A:204:PHE:C	A:204:PHE:CD1	0.453
1	B:191:LYS:NZ	B:194:SER:HB3	0.453
1	A:151:THR:O	A:151:THR:HG23	0.453
1	A:8:LEU:HG	A:8:LEU:O	0.452
1	A:1:LYS:CD	A:17:ILE:CG2	0.452
1	A:140:ILE:HA	A:230:ARG:HD3	0.452
1	A:6:ALA:HB2	A:20:ARG:NE	0.451
1	A:20:ARG:HD3	A:45:VAL:O	0.451
1	A:196:ILE:CD1	A:219:ALA:HB3	0.451
1	D:162:LEU:HD21	D:190:SER:CB	0.451
1	C:1:ASP:H2	D:46:ARG:CZ	0.451
1	A:30:TRP:CB	A:39:LEU:CD2	0.450
1	A:60:VAL:O	A:60:VAL:HG12	0.450
1	A:80:LEU:HB2	A:98:PHE:HB3	0.450
1	C:94:LEU:CD1	C:96:LEU:CD2	0.450

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:17:ILE:CG2	A:77:LYS:CE	0.449
1	A:68:GLU:CD	A:74:TYR:CD2	0.449
1	A:81:LYS:NZ	A:97:THR:HA	0.449
1	D:71:THR:HG22	D:72:GLY:H	0.449
1	D:237:ARG:HG3	D:237:ARG:O	0.449
1	A:40:PHE:C	A:40:PHE:CD1	0.448
1	A:52:ARG:CZ	A:95:GLU:CB	0.448
1	B:166:ASN:OD1	B:205:LEU:HD11	0.448
1	B:129:ASN:HD21	D:61:ASN:CG	0.448
1	D:158:ARG:NE	D:162:LEU:HB2	0.448
1	B:156:MET:HB3	B:161:LEU:CD1	0.447
1	B:225:ALA:O	B:226:GLU:HB2	0.447
1	C:10:ILE:CG2	C:102:LYS:HD2	0.447
1	C:103:ILE:CD1	C:107:PHE:CD2	0.447
1	A:144:TYR:C	A:165:TYR:CZ	0.446
1	A:199:ALA:HB3	A:216:THR:CB	0.446
1	B:150:PHE:CD1	B:150:PHE:N	0.446
1	B:180:GLY:C	B:220:PHE:CE2	0.446
1	D:142:THR:CA	D:145:LYS:HG3	0.446
1	D:172:HIS:HE1	E:10:DC:H1'	0.446
1	D:135:LYS:CD	E:16:DT:C5	0.446
1	B:181:LEU:CD2	B:182:ASN:N	0.446
1	D:40:GLN:HB2	D:40:GLN:HE21	0.446
1	D:69:ILE:O	D:69:ILE:HG23	0.446
1	A:194:LEU:CD1	A:196:ILE:CG2	0.445
1	B:220:PHE:C	B:220:PHE:CD1	0.445

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:149:LEU:O	D:150:LEU:HB2	0.445
1	D:206:VAL:HG13	D:207:ARG:N	0.445
1	A:146:ASP:CG	A:147:ALA:H	0.444
1	A:249:LYS:HA	F:7:DC:H3'	0.444
1	B:181:LEU:HD23	B:182:ASN:HB2	0.444
1	B:215:VAL:HG22	D:42:ARG:NE	0.444
1	D:99:GLU:O	D:100:PHE:HB2	0.444
1	D:228:ARG:O	D:231:ARG:HG2	0.444
1	D:62:VAL:N	D:135:LYS:CB	0.444
1	D:107:GLU:H	D:125:THR:CG2	0.444
1	A:77:LYS:CB	A:104:VAL:CG2	0.443
1	B:183:PHE:CB	B:219:HIS:CD2	0.443
1	C:39:PHE:CE2	C:41:LEU:CD2	0.443
1	D:30:ARG:O	D:31:LYS:HB3	0.443
1	D:62:VAL:CB	D:133:ASP:HB2	0.443
1	A:1:LYS:CG	A:15:TRP:NE1	0.443
1	A:83:ALA:N	E:13:DT:C7	0.443
1	A:1:LYS:CG	A:17:ILE:CG2	0.442
1	B:173:LYS:HB2	B:173:LYS:NZ	0.442
1	B:215:VAL:CB	B:220:PHE:CE1	0.442
1	D:84:GLU:OE2	D:86:LYS:HD3	0.442
1	D:144:ALA:HB1	D:148:TYR:CE2	0.442
1	D:144:ALA:HB1	D:148:TYR:HE2	0.442
1	D:163:LYS:HA	D:163:LYS:HD3	0.442
1	A:1:LYS:CG	A:15:TRP:CE2	0.441
1	A:20:ARG:CG	A:46:ASP:C	0.441
1	D:119:ASN:O	D:123:LEU:HA	0.441
1	D:121:PHE:HE1	D:164:PHE:HB3	0.441



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:230:VAL:CB	D:235:TRP:NE1	0.441
1	A:56:PHE:CD2	A:99:ASN:CB	0.440
1	A:199:ALA:HB3	A:216:THR:HB	0.440
1	B:168:VAL:CA	B:171:LEU:HD13	0.440
1	D:155:LEU:CB	D:162:LEU:HG	0.440
1	A:193:VAL:CG1	A:194:LEU:N	0.440
1	D:180:LEU:N	F:32:DC:OP1	0.440
1	A:227:TYR:C	A:227:TYR:CD1	0.439
1	D:64:ALA:H	D:131:ASP:HA	0.439
1	D:136:HIS:C	D:138:LEU:H	0.439
1	D:142:THR:HG23	D:145:LYS:CE	0.439
1	A:1:LYS:HG3	A:15:TRP:CD1	0.438
1	B:172:ILE:HG22	B:182:ASN:HD22	0.438
1	B:207:ASN:CA	B:212:TYR:CE1	0.438
1	D:68:ILE:CG2	D:117:LEU:CD1	0.438
1	D:77:LEU:C	D:77:LEU:HD23	0.438
1	D:116:TYR:C	D:116:TYR:CD1	0.438
1	A:75:PHE:HB2	A:106:PRO:CG	0.437
1	B:203:ASP:CG	B:221:LYS:HZ3	0.437
1	B:209:GLY:CA	B:211:ILE:CD1	0.437
1	F:33:DC:H2'	F:34:DG:O4'	0.437
1	A:91:LYS:HB3	A:91:LYS:HZ3	0.436
1	B:187:LYS:CB	B:199:LYS:CE	0.436
1	D:106:GLU:CD	D:112:PHE:CE1	0.436
1	D:183:LYS:O	D:186:ILE:HB	0.436
1	D:61:ASN:O	D:135:LYS:N	0.436
1	D:62:VAL:HG12	D:130:ARG:O	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:64:ALA:O	D:131:ASP:HB2	0.435
1	D:130:ARG:NH1	D:137:LYS:HG2	0.435
1	D:171:HIS:CD2	E:12:DT:O2	0.435
1	A:54:THR:HG23	A:97:THR:HG23	0.434
1	A:123:ILE:O	A:126:LEU:HB2	0.434
1	B:141:ASN:CB	B:142:PRO:HD2	0.434
1	D:82:GLU:HG3	D:82:GLU:O	0.434
1	A:142:LYS:C	A:165:TYR:CE1	0.433
1	A:144:TYR:O	A:165:TYR:CE1	0.433
1	D:222:LYS:HE2	D:226:LEU:CD1	0.433
1	A:79:THR:CG2	A:81:LYS:CE	0.432
1	A:82:ILE:HG12	A:83:ALA:H	0.432
1	A:200:ARG:CZ	A:210:SER:CB	0.432
1	B:207:ASN:HB2	B:212:TYR:CZ	0.432
1	C:103:ILE:HD12	C:107:PHE:CD2	0.432
1	D:159:GLU:CD	D:159:GLU:H	0.432
1	D:177:ASP:CB	F:33:DC:P	0.432
1	D:166:VAL:HG21	D:181:TYR:HB2	0.432
1	B:129:ASN:ND2	D:60:ALA:O	0.432
1	A:150:ILE:O	A:150:ILE:HG23	0.432
1	A:54:THR:CA	A:97:THR:CG2	0.431
1	A:140:ILE:HG22	A:230:ARG:NH1	0.431
1	B:157:PRO:C	B:158:ALA:O	0.431
1	C:103:ILE:HD11	C:107:PHE:CE2	0.431
1	D:126:CYS:CA	E:15:DT:C3'	0.431
1	D:139:ILE:HG21	E:14:DT:OP2	0.431
1	D:165:ILE:CG2	D:180:LEU:HB3	0.431

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:145:LYS:CE	D:182:LEU:CD2	0.431
1	D:90:VAL:CG1	D:91:VAL:N	0.431
1	B:147:ALA:C	C:1:ASP:H1	0.430
1	D:139:ILE:HG12	D:181:TYR:HB3	0.430
1	A:96:MET:CE	F:2:DC:H42	0.430
1	A:56:PHE:CD2	A:60:VAL:CG1	0.429
1	A:52:ARG:HE	A:96:MET:CA	0.429
1	A:108:GLU:CG	A:109:ASP:N	0.429
1	A:178:LEU:HG	A:209:LEU:HD11	0.429
1	D:1:MET:C	D:1:MET:HE3	0.429
1	D:34:ARG:O	D:37:MET:HB2	0.429
1	D:65:ALA:H	D:139:ILE:HB	0.429
1	A:24:LYS:H22	A:215:SER:CB	0.429
1	A:138:ILE:HD12	A:200:ARG:HB2	0.428
1	B:187:LYS:CB	B:199:LYS:HE3	0.428
1	D:62:VAL:CG1	D:137:LYS:CA	0.428
1	D:137:LYS:HD3	D:183:LYS:NZ	0.428
1	A:84:ASN:ND2	A:85:LYS:H	0.428
1	B:162:THR:CG2	B:163:VAL:N	0.428
1	B:224:ASP:HB3	D:39:ARG:NH2	0.428
1	D:71:THR:CG2	D:72:GLY:N	0.428
1	D:224:LYS:HB2	D:224:LYS:NZ	0.428
1	B:183:PHE:CD2	B:219:HIS:CD2	0.427
1	D:54:ALA:O	D:55:ALA:HB2	0.427
1	D:230:VAL:CG2	D:236:LYS:CG	0.427
1	A:47:GLU:CG	A:48:SER:N	0.427
1	A:245:ILE:CG2	A:246:SER:N	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:148:GLY:HA2	D:46:ARG:HH22	0.427
1	D:90:VAL:HG12	D:91:VAL:N	0.427
1	A:1:LYS:HB2	A:15:TRP:HE1	0.426
1	A:1:LYS:N	A:17:ILE:HG21	0.426
1	A:138:ILE:CG1	A:200:ARG:HD2	0.426
1	B:202:VAL:CA	B:205:LEU:CD2	0.426
1	D:62:VAL:CA	D:134:ASP:N	0.426
1	D:63:LYS:HB3	D:138:LEU:CG	0.426
1	D:230:VAL:HB	D:235:TRP:NE1	0.426
1	D:233:SER:O	D:234:VAL:HB	0.426
1	B:198:ILE:CG2	B:199:LYS:N	0.426
1	A:30:TRP:CE3	A:39:LEU:CG	0.425
1	B:191:LYS:HZ3	B:194:SER:CB	0.425
1	D:106:GLU:CD	D:112:PHE:HE1	0.425
1	A:138:ILE:CD1	A:138:ILE:N	0.425
1	A:85:LYS:HE3	D:66:PRO:CG	0.424
1	A:111:HIS:O	A:113:LEU:HD23	0.424
1	B:137:ALA:HA	B:138:PRO:HD3	0.424
1	B:180:GLY:HA2	B:220:PHE:CD2	0.424
1	F:2:DC:H2'	F:3:DC:C6	0.424
1	A:26:GLN:CG	A:27:ILE:N	0.424
1	A:69:VAL:HG12	A:70:ASN:H	0.423
1	B:224:ASP:HB2	D:39:ARG:CZ	0.423
1	B:168:VAL:CG1	B:169:LEU:N	0.423
1	D:223:VAL:CG2	D:224:LYS:N	0.423
1	D:176:GLY:C	E:11:DT:O2	0.423
1	B:191:LYS:HB3	B:191:LYS:NZ	0.422

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:109:GLY:O	D:110:LYS:HB2	0.422
1	D:130:ARG:HH21	D:135:LYS:HG2	0.422
1	D:165:ILE:HG12	D:182:LEU:HD21	0.422
1	D:137:LYS:HZ2	E:16:DT:C2'	0.422
1	D:62:VAL:N	D:135:LYS:N	0.422
1	D:230:VAL:CG2	D:231:ARG:N	0.422
1	B:173:LYS:O	B:181:LEU:CD2	0.422
1	B:129:ASN:CG	F:28:DC:OP2	0.422
1	A:17:ILE:CG2	A:77:LYS:CD	0.421
1	A:19:ALA:CB	A:108:GLU:CD	0.421
1	A:27:ILE:HG12	A:28:ARG:H	0.421
1	A:98:PHE:CD1	F:1:DC:N3	0.421
1	A:128:ASN:ND2	A:207:ARG:HD2	0.421
1	B:173:LYS:HD3	B:212:TYR:HB2	0.421
1	D:62:VAL:CG1	D:130:ARG:O	0.421
1	D:131:ASP:CG	E:15:DT:OP1	0.421
1	D:138:LEU:HD12	D:139:ILE:C	0.421
1	D:179:LYS:HB3	F:32:DC:OP1	0.421
1	D:182:LEU:CD2	D:182:LEU:N	0.421
1	E:8:DG:H2'	E:9:DG:C8	0.421
1	A:58:GLU:CG	A:59:GLN:H	0.420
1	B:173:LYS:C	B:181:LEU:HD21	0.420
1	B:207:ASN:HB2	B:212:TYR:HE1	0.420
1	D:104:ILE:HG22	D:114:ASP:HB2	0.420
1	D:151:LYS:CE	D:187:VAL:HG13	0.420
1	D:182:LEU:N	D:182:LEU:HD22	0.420
1	D:207:ARG:HD2	D:211:ARG:CZ	0.420

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:144:TYR:CG	A:145:GLU:N	0.420
1	D:68:ILE:HG21	D:117:LEU:HD13	0.419
1	D:217:LYS:O	D:221:LYS:HG2	0.419
1	D:236:LYS:HB3	D:236:LYS:NZ	0.419
1	C:108:PRO:HD2	D:55:ALA:C	0.418
1	D:201:GLU:HA	D:204:LYS:HD2	0.418
1	D:64:ALA:N	D:131:ASP:CB	0.418
1	A:90:VAL:O	A:90:VAL:HG12	0.418
1	A:137:ILE:HG22	A:199:ALA:H	0.417
1	A:179:TRP:CA	A:212:LEU:HD13	0.417
1	D:64:ALA:C	D:139:ILE:CG2	0.417
1	D:67:LYS:HG3	D:166:VAL:HG23	0.417
1	B:184:GLN:HA	B:199:LYS:HZ1	0.417
1	D:65:ALA:N	D:139:ILE:CB	0.417
1	A:56:PHE:CG	A:99:ASN:HB3	0.416
1	A:131:LYS:HD3	A:131:LYS:O	0.416
1	D:131:ASP:CB	E:15:DT:P	0.416
1	D:172:HIS:CD2	E:10:DC:C2	0.416
1	A:72:VAL:CG2	A:73:TYR:N	0.416
1	B:154:SER:CB	B:224:ASP:O	0.416
1	A:154:SER:OG	F:9:DC:OP2	0.416
1	D:57:GLY:CA	F:27:DC:OP1	0.416
1	A:85:LYS:CB	A:88:THR:HG22	0.415
1	B:145:SER:HB2	C:23:VAL:CG1	0.415
1	B:172:ILE:HG22	B:182:ASN:HD21	0.415
1	D:138:LEU:HD12	D:139:ILE:H	0.415
1	B:202:VAL:C	B:205:LEU:HD23	0.414

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:33:GLN:HB3	D:36:LEU:CB	0.414
1	D:63:LYS:HD3	D:134:ASP:OD2	0.414
1	D:138:LEU:HD12	D:139:ILE:O	0.414
1	A:138:ILE:CG1	A:200:ARG:HH11	0.414
1	D:206:VAL:CG1	D:207:ARG:N	0.414
1	A:38:LYS:CG	A:39:LEU:N	0.413
1	A:154:SER:CB	F:9:DC:OP2	0.413
1	D:63:LYS:CB	D:134:ASP:HA	0.413
1	D:136:HIS:HB2	E:16:DT:H1'	0.413
1	D:222:LYS:C	D:222:LYS:CD	0.413
1	E:2:DG:H2''	E:3:DC:O4'	0.413
1	A:66:LEU:CD1	A:66:LEU:H	0.413
1	A:69:VAL:CG1	A:70:ASN:N	0.413
1	A:166:LEU:CD2	A:166:LEU:N	0.413
1	A:177:THR:CG2	A:178:LEU:N	0.413
1	B:153:ASN:C	B:223:THR:O	0.412
1	B:191:LYS:HG2	B:194:SER:H	0.412
1	B:195:VAL:CG2	B:198:ILE:CG2	0.412
1	D:99:GLU:O	D:100:PHE:CD1	0.412
1	D:138:LEU:C	D:138:LEU:HD12	0.412
1	A:67:ILE:CG2	A:68:GLU:N	0.412
1	B:155:PHE:H	B:225:ALA:H	0.412
1	A:85:LYS:HG3	D:128:ASN:ND2	0.411
1	A:137:ILE:CG2	A:198:GLY:HA2	0.411
1	A:24:LYS:NZ	A:215:SER:HA	0.411
1	B:169:LEU:HD13	B:187:LYS:HZ1	0.411
1	B:195:VAL:N	B:198:ILE:CG2	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:10:ILE:HG13	C:102:LYS:CD	0.411
1	D:77:LEU:C	D:77:LEU:CD2	0.411
1	D:121:PHE:CE1	D:165:ILE:O	0.411
1	D:163:LYS:CB	D:186:ILE:CG2	0.411
1	A:21:VAL:CG1	A:22:THR:N	0.411
1	A:26:GLN:CG	A:27:ILE:H	0.411
1	D:165:ILE:CG2	D:166:VAL:N	0.411
1	A:3:VAL:HA	A:17:ILE:CG1	0.410
1	A:20:ARG:HD3	A:45:VAL:C	0.410
1	D:141:LYS:CG	F:32:DC:P	0.410
1	E:4:DC:H2'	E:5:DC:C6	0.410
1	A:34:ARG:H	A:34:ARG:HG2	0.410
1	A:249:LYS:CG	A:250:SER:N	0.410
1	D:68:ILE:CD1	D:68:ILE:N	0.410
1	D:98:MET:SD	D:99:GLU:N	0.410
1	A:123:ILE:HB	A:126:LEU:CD1	0.409
1	A:145:GLU:CA	A:165:TYR:CE2	0.409
1	B:147:ALA:C	C:1:ASP:N	0.409
1	B:177:ARG:HB2	B:178:PRO:HD3	0.409
1	D:53:ALA:O	D:54:ALA:HB2	0.409
1	D:168:LYS:HG3	E:13:DT:O4'	0.409
1	D:227:ARG:HH12	D:239:THR:HG22	0.409
1	A:138:ILE:CD1	A:200:ARG:HH11	0.409
1	A:19:ALA:HB1	A:108:GLU:CD	0.408
1	B:187:LYS:C	B:187:LYS:HD3	0.408
1	B:190:LEU:C	B:190:LEU:CD1	0.408
1	D:63:LYS:C	D:131:ASP:O	0.408



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:175:TRP:CD2	E:11:DT:O4'	0.408
1	A:161:LYS:CD	A:161:LYS:H	0.408
1	B:154:SER:HB3	B:226:GLU:H	0.408
1	A:63:PHE:CD2	A:64:PHE:CZ	0.407
1	A:158:GLU:CG	A:159:VAL:N	0.407
1	A:162:ARG:HD3	A:162:ARG:O	0.407
1	D:106:GLU:OE1	D:112:PHE:CZ	0.407
1	D:230:VAL:HG23	D:231:ARG:N	0.407
1	A:180:GLY:N	A:212:LEU:CD2	0.406
1	B:155:PHE:HA	B:211:ILE:HA	0.406
1	B:179:GLU:C	B:181:LEU:H	0.406
1	C:18:PHE:HD2	C:19:ILE:HG13	0.406
1	C:33:HIS:CE1	C:37:LYS:CG	0.406
1	A:222:ASP:OD1	A:227:TYR:CD2	0.406
1	D:191:LEU:C	D:191:LEU:CD1	0.405
1	D:152:ASP:OD2	D:194:TRP:CZ2	0.405
1	B:203:ASP:OD1	B:212:TYR:CZ	0.405
1	B:214:THR:O	D:43:LEU:HD22	0.405
1	D:63:LYS:O	D:139:ILE:HG22	0.405
1	A:20:ARG:HG2	A:46:ASP:O	0.404
1	A:223:ILE:C	A:223:ILE:HD13	0.404
1	C:47:LYS:HB3	C:47:LYS:NZ	0.404
1	D:63:LYS:HB3	D:138:LEU:HB2	0.404
1	D:215:LYS:O	D:219:PHE:CD2	0.404
1	A:27:ILE:CG1	A:28:ARG:N	0.404
1	D:28:ILE:CG1	D:29:GLU:N	0.404
1	A:1:LYS:CE	A:15:TRP:CE3	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:144:TYR:CE2	A:145:GLU:O	0.403
1	B:155:PHE:CA	B:225:ALA:C	0.403
1	B:181:LEU:HD23	B:182:ASN:CB	0.403
1	D:171:HIS:ND1	E:13:DT:O5'	0.403
1	A:30:TRP:CA	A:39:LEU:CD2	0.402
1	A:75:PHE:CD1	A:108:GLU:OE1	0.402
1	A:145:GLU:CG	A:165:TYR:CD2	0.402
1	A:124:ASP:CG	A:169:THR:CG2	0.402
1	A:24:LYS:HB2	A:217:ILE:HD11	0.402
1	B:171:LEU:C	B:171:LEU:CD2	0.402
1	B:186:LEU:C	B:186:LEU:CD1	0.402
1	D:62:VAL:HB	D:130:ARG:O	0.402
1	D:64:ALA:CB	D:131:ASP:HB2	0.402
1	A:29:THR:O	A:39:LEU:HA	0.401
1	A:110:ASP:OD1	A:114:PRO:HD2	0.401
1	B:224:ASP:HB2	D:39:ARG:HH21	0.401
1	C:1:ASP:CA	D:46:ARG:CZ	0.401
1	C:7:ARG:HE	C:115:ILE:HG22	0.401
1	D:112:PHE:CZ	D:129:CYS:CB	0.401
1	D:201:GLU:O	D:205:GLU:HG3	0.401

#### 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	Analysed	Favored	Allowed	Outliers
1	1003	897	53	53

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	882	709	91	82

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	1	LYS
1	A	5	ILE
1	A	65	PRO
1	A	70	ASN
1	A	81	LYS
1	A	91	LYS
1	A	99	ASN
1	A	131	LYS
1	A	138	ILE
1	A	155	ASN
1	A	161	LYS
1	A	162	ARG
1	A	166	LEU
1	A	211	VAL
1	A	223	ILE
1	A	228	LYS
1	A	286	VAL
1	A	291	LYS
1	A	295	MET
1	A	302	GLN
1	A	351	GLN
1	A	357	ILE
1	A	384	ASN
1	A	395	LYS
1	A	413	LYS

Model ID	Chain	Residue ID	Residue type
1	A	418	ARG
1	A	422	ARG
1	A	428	ILE
1	B	23	ILE
1	B	28	ILE
1	B	38	ARG
1	B	59	MET
1	B	84	LYS
1	B	99	VAL
1	B	102	LYS
1	B	116	ILE
1	B	128	LYS
1	B	171	LEU
1	B	173	LYS
1	B	187	LYS
1	B	191	LYS
1	B	211	ILE
1	C	7	ARG
1	C	19	ILE
1	C	41	LEU
1	C	47	LYS
1	C	77	ILE
1	C	96	LEU
1	C	103	ILE
1	D	1	MET
1	D	19	GLU
1	D	25	ARG

Model ID	Chain	Residue ID	Residue type
1	D	40	GLN
1	D	51	THR
1	D	61	ASN
1	D	68	ILE
1	D	69	ILE
1	D	83	GLU
1	D	89	LYS
1	D	93	GLN
1	D	98	MET
1	D	117	LEU
1	D	119	ASN
1	D	135	LYS
1	D	137	LYS
1	D	151	LYS
1	D	157	LYS
1	D	159	GLU
1	D	163	LYS
1	D	167	LYS
1	D	178	MET
1	D	179	LYS
1	D	197	GLN
1	D	198	GLU
1	D	204	LYS
1	D	212	GLU
1	D	215	LYS
1	D	218	LYS
1	D	222	LYS
1	D	224	LYS

Model ID	Chain	Residue ID	Residue type
1	D	235	TRP
1	D	236	LYS

### Fit of model to data used for modeling ?

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

### Fit of model to data used for validation ?

Validation for this section is under development.

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