

# Integrative Structure Validation Report

October 03, 2024 - 12:55 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	9A88
PDB-Dev ID	PDBDEV_00000373
Structure Title	Structure of the pre-incision complex in nucleotide excision repair
Structure Authors	Yu, J.; Yan, C.Y.; Paul, T.; Brewer, L.; Tsutakawa, S.E.; Tsai, C.-L.; Hamdan, S.; Tainer, J.A.; Ivanov, I.

*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)*

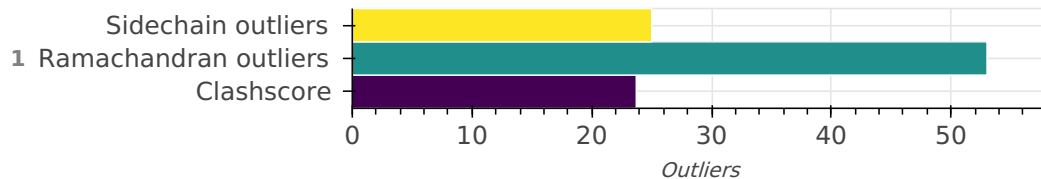
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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.*

Model Quality: MolProbity Analysis



## Ensemble information ?

This entry consists of 0 distinct ensemble(s).

## Summary ?

This entry consists of 1 unique models, with 29 subunits in each model. A total of 25 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 29 flexible or non-rigid units.

## Entry composition ?

There is 1 unique type of models in this entry. This model is titled None/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	General transcription and DNA repair factor IIH helicase subunit XPB	A	A	170
1	2	1	General transcription and DNA repair factor IIH helicase subunit XPB	A	A	473
1	3	2	General transcription and DNA repair factor IIH helicase subunit XPD	B	B	760
1	4	3	General transcription factor IIH subunit 4	C	C	441
1	5	4	General transcription factor IIH subunit 2	D	D	377
1	6	5	General transcription factor IIH subunit 3	E	E	292

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	7	6	General transcription factor IIH subunit 5	F	F	66
1	8	7	DNA repair protein complementing XP-A cells	G	G	273
1	9	8	General transcription factor IIH subunit 1	H	H	154
1	10	9	DNA excision repair protein ERCC-5	I	I	296
1	11	9	DNA excision repair protein ERCC-5	I	I	253
1	12	10	DNA repair endonuclease XPF Gene: ERCC4, ERCC11, XPF	J	J	227
1	13	11	DNA excision repair	K	K	198
1	14	12	Replication protein A 70 kDa DNA-binding subunit, N-terminally processed	L	L	434
1	15	13	Replication protein A 14 kDa subunit	M	M	115
1	16	14	Replication protein A 32 kDa subunit	N	N	225
1	17	15	DNA (66-MER)	O	X	66
1	18	16	DNA (66-MER)	P	Y	66
1	19	17	IRON/SULFUR CLUSTER	Q	B	Not available
1	20	18	ZINC ION	R	D	Not available
1	21	18	ZINC ION	S	D	Not available
1	22	18	ZINC ION	T	D	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	23	18	ZINC ION	U	E	Not available
1	24	18	ZINC ION	V	E	Not available
1	25	18	ZINC ION	W	G	Not available
1	26	18	ZINC ION	Z	L	Not available
1	27	19	MAGNESIUM ION	X	I	Not available
1	28	19	MAGNESIUM ION	Y	J	Not available
1	29	20	water	AA	Y	1

### Datasets used for modeling

*There are 25 unique datasets used to build the models in this entry.*

ID	Dataset type	Database name	Data access code
4	Crosslinking-MS data	File	10.1038/s41467-019-10745-5
1	Experimental model	PDB	6RO4
2	3DEM volume	EMDB	EMD-4970
3	Experimental model	PDB	6TUW
5	De Novo model	Not available	Not available
6	De Novo model	Not available	Not available
7	De Novo model	Not available	Not available
8	Experimental model	PDB	6SXA
9	Experimental model	PDB	6SXB

ID	Dataset type	Database name	Data access code
10	Experimental model	PDB	2BGW
11	De Novo model	Not available	Not available
12	Experimental model	PDB	4GOP
13	Experimental model	PDB	6I52
14	Experimental model	PDB	1JMC
15	Experimental model	PDB	1L1O
16	Experimental model	PDB	2JNW
17	Experimental model	PDB	4MQV
18	De Novo model	Not available	Not available
19	De Novo model	Not available	Not available
20	De Novo model	Not available	Not available
21	De Novo model	Not available	Not available
22	De Novo model	Not available	Not available
23	De Novo model	Not available	Not available
24	De Novo model	Not available	Not available
25	De Novo model	MODEL ARCHIVE	ma-2chon

### Representation

*This entry has only one representation and includes 0 rigid bodies and 29 flexible units.*

Chain ID	Rigid bodies	Non-rigid segments
I	-	1-296, 733-985
B	-	1-760

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
A	-	34-203, 248-720
C	-	1-441
D	-	1-377
E	-	1-292
F	-	1-66
G	-	1-273
H	-	1-154
J	-	1-227
K	-	1-198
L	-	1-434
M	-	1-115
N	-	1-225
O	-	1-66
P	-	1-66
Q	-	None-None
R	-	None-None
S	-	None-None
T	-	None-None
U	-	None-None
V	-	None-None
W	-	None-None
Z	-	None-None
X	-	None-None
Y	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
AA	-	1-1

## 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
				<p>To construct a model of the pre-precision complex (PlnC), we systematically examined the cryo-EM structures and densities of human apo-TFIIH, TFIIH/XPA/DNA, and XPF/ERCC1, the NMR structure of XPA-ERCC1, and the X-ray structures of the XPG catalytic core and RPA-ssDNA (RPA70, RPA32, and RPA14). The TFIIH/XPA/DNA structure (PDB ID: 6RO4 and EMDB accession code: EMD-4970) was the starting point for model building. The PlnC hybrid model has an NER bubble size of 23 nucleotides, matching the 27-nucleotide</p>			

Step number	Protocol ID	Method name	Method type	Method description optimal length of the excision products and the XPF and XPG incision patterns.	Number of computed models	Multi state modeling	Multi scale modeling
				<p>FEN1 shares 30% sequence identity with the XPG catalytic core (PDB ID: 6TUR, 6TUW, and 6VBH). Thus, we modeled DNA-bound XPG based on the human FEN1/DNA X-ray structure (PDB ID: 5UM9). XPG positioning into the hybrid model was based on existing XL-MS data. In addition, positioning of the XPG core required placement of the 3' DNA junction 8 nucleotides away from the expected position of the DNA lesion near XPD's His135 residue. The two XPG gateway helices (GH1, residues 82-126) and (GH2, residues 734-761) were predicted with AlphaFold2 and positioned in the gap between XPD's Arch and Fe-S domains in accordance with the crosslink data. The XPD-anchor domain (residues 157-</p>			



Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	None	<p>296) was predicted by AlphaFold2 and fitted into the TFIIH/XPA/DNA cryo-EM density. The loop connecting GH1 and the XPD-anchor was built with Modeller. To model XPF/ERCC1, we used the cryo-EM structures of XPF/ERCC1 (PDB ID: 6SXA and 6SXB). We first docked the XPF nuclease domain to the 5' junction. The catalytic metal was oriented 3A away from the scissile phosphodiester bond. Mg<sup>2+</sup> ion coordination was based on the Aeropyrum pernix SNF2 structure (PDB ID: 2BGW). A water molecule was placed between Mg<sup>2+</sup> ion and the DNA backbone phosphate group. The ERCC1 (HhH)<sub>2</sub> domain was oriented to interact with the ssDNA through two DNA hairpins based on the 6SXB structure. The long linkers from the ERCC1 central domain to the ERCC1</p>	None	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
				<p>(HhH)2 (residues 214-230) and from the XPF nuclease domain to the XPF (HhH)2 (residues 817-847) were built with Modeller. The SF2 helicase-like N-terminal domain of XPF was omitted from the hybrid PlnC model due to lack of sufficient structural or biochemical restraints. To model RPA, we used following X-ray structures: Ustilago maydis RPA/ssDNA (PDB ID: 4GOP), yeast RPA/ssDNA (PDB ID: 6I52) and human RPA (PDB ID: 1JMC and 1L10). The RPA70AB/ssDNA complex was modeled by superimposing the yeast RPA/ssDNA structure (PDB ID: 1JMC) onto the human apo-RPA 70AB (PDB ID: 6I52). Within PlnC, only RPA70A, 70B, and 70C can engage DNA due to the size of the NER bubble. RPA70AB was placed close to the 3' junction where it interacts with XPG. We reoriented</p>			

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
				<p>RPA70C to bind ssDNA near the 5' junction. The RPA70C/ssDNA was modeled by aligning the <i>Ustilago maydis</i> RPA/ssDNA structure (PDB ID: 4GOP) with the human trimer core structure (PDB ID: 1L10). The orientation of RPA32D and RPA14 follows from the placement of the RPA70C module as they are all connected, forming the trimer core (70C/32D/14). To model XPA, we used the following structures: the cryo-EM TFIIH/XPA/DNA structure (PDB ID: 6RO4), the NMR structure of XPA/ERCC1 (PDB ID: 2JNW), and the human X-ray structure of RPA32C/Smarcal1 N-terminus (PDB ID: 4MQV). The XPA N-terminal extension (residues 1-103), which includes the RPA32C binding helix (residues 22-40), and the C-terminal extension (beta-domain)</p>			

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
				(residues 235-273) lacked known structural homologues and were modeled using AlphaFold2. The beta-domain was fitted into the TFIIH/XPA/DNA density. To position XPA's N-terminal helix (residues 22-40) we used the X-ray structure of RPA32C/Smarcal1 N-terminus. To assemble the complete PInC model, we also modelled loop regions of TFIIH's core subunits (XPB, XPD, p44, p34, and p52) into the TFIIH/XPA/DNA density.			

There are 6 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	<a href="#">AlphaFold2</a>	Not available	model building	<a href="https://alphafold.ebi.ac.uk/">https://alphafold.ebi.ac.uk/</a>
2	<a href="#">Modeller</a>	10.4	model building	<a href="https://salilab.org/modeller/">https://salilab.org/modeller/</a>
3	<a href="#">Clustal Omega</a>	Not available	sequence alignments	<a href="https://www.ebi.ac.uk/jdispatcher/msa/clustalo">https://www.ebi.ac.uk/jdispatcher/msa/clustalo</a>
4	<a href="#">Coot</a>	0.9.8.92	real-space refinement	<a href="https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/">https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/</a>
5	<a href="#">Phenix</a>	1.20.1	real-space refinement	<a href="https://phenix-online.org/">https://phenix-online.org/</a>
6	<a href="#">UCSF Chimera</a>	1.18	model visualization	<a href="https://www.cgl.ucsf.edu/chimera/">https://www.cgl.ucsf.edu/chimera/</a>

## Data quality ?

### 3DEM volume

Validation for this section is under development.

### Crosslinking-MS

Validation for this section is under development.

## Model quality ?

For models with atomic structures, molprobit 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 42 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
CB-CG-CD	106.10	179.97	1
N-CD-CG	103.20	70.21	1
CA-CB-CG	104.50	64.97	1
N-CD-CG	103.20	73.73	1
CA-N-CD	112.00	91.43	1
CA-N-CD	112.00	95.21	1
CA-CB-CG	104.50	83.20	1
CG-SD-CE	100.90	79.13	1
C-N-CA	121.70	139.41	1
CG-CD-NE	112.00	132.75	1
CG-CD-NE	112.00	131.28	1
CA-C-N	116.90	129.87	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	94.97	1
CA-N-CD	112.00	102.25	1
CG-CD-OE1	118.40	103.70	1
O3'-P-OP1	108.00	89.97	1
CG-CD-OE2	118.40	131.42	1
C-N-CA	121.70	131.78	1
C-N-CA	121.70	131.59	1
CA-C-O	120.80	111.48	1
CB-CG-CD	112.60	121.89	1
CA-CB-CG	114.10	103.32	1
C-N-CA	121.70	131.30	1
CG-CD-OE1	118.40	106.28	1
C-N-CA	121.70	131.12	1
C-N-CA	121.70	112.36	1
C-N-CA	121.70	112.87	1
C-N-CA	121.70	130.37	1
C-N-CA	121.70	130.35	1
C-N-CA	121.70	130.16	1
N-CA-C	111.00	124.05	1
C-N-CA	121.70	129.68	1
CA-CB-CG	114.10	122.93	1
CD-NE-CZ	124.40	130.46	1
C-N-CA	121.70	129.38	1
CB-CG-CD	106.10	92.59	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.18	1
CA-CB-CG	114.10	122.41	1
C-N-CA	121.70	114.23	1
C-N-CA	121.70	114.33	1
N-CA-C	111.00	122.44	1
O-C-N	123.00	116.53	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	23.71	1902

All 1902 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:501:GLN:HB2	J:188:MET:HE2	1.141
1	I:273:LEU:HD13	K:48:ASN:HA	1.129
1	H:116:GLU:HG2	H:120:ARG:HD2	1.112
1	G:249:GLU:HB2	G:257:TYR:CE1	1.083
1	B:410:TYR:HB3	B:414:PHE:HD1	1.078
1	G:18:ALA:HB2	M:2:MET:HE2	1.059
1	B:353:SER:HB2	L:273:GLN:HG2	1.049
1	C:140:GLU:OE2	C:144:HIS:HD2	0.999
1	L:252:GLY:O	L:273:GLN:NE2	0.989
1	B:424:ARG:O	I:288:HIS:CE1	0.987
1	C:211:MET:HE2	C:240:SER:HB2	0.976

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:157:GLU:HA	J:160:PRO:HG2	0.966
1	G:237:ARG:HG3	G:239:THR:H	0.951
1	E:143:TYR:CZ	E:147:MET:HE1	0.943
1	H:116:GLU:HG3	H:120:ARG:HH11	0.932
1	G:249:GLU:HB2	G:257:TYR:HE1	0.930
1	B:257:ASP:O	B:260:GLN:HG3	0.928
1	B:410:TYR:HB3	B:414:PHE:CD1	0.927
1	B:543:GLN:H	P:37:DG:H5"	0.924
1	G:167:LYS:HZ1	L:404:ARG:HH22	0.922
1	D:56:ASP:HB3	D:61:MET:HE2	0.916
1	K:149:THR:HG21	K:182:LYS:HD3	0.914
1	H:116:GLU:CG	H:120:ARG:HD2	0.912
1	C:140:GLU:OE2	C:144:HIS:CD2	0.904
1	B:336:LEU:HD21	B:358:LEU:HD12	0.894
1	B:422:ASP:H	B:427:THR:HG22	0.894
1	B:501:GLN:OE1	K:194:PHE:HB3	0.884
1	A:568:LEU:HD11	A:606:PHE:HB3	0.883
1	H:116:GLU:CG	H:120:ARG:HH11	0.881
1	C:132:ASP:O	C:136:GLU:HG2	0.875
1	G:113:MET:HG2	G:114:ASP:H	0.875
1	A:584:THR:HA	K:185:ARG:HD3	0.873
1	H:116:GLU:HG3	H:120:ARG:NH1	0.865
1	A:570:GLU:OE2	K:170:GLU:HG2	0.863



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:273:ILE:HD12	B:276:THR:HB	0.858
1	I:288:HIS:CE1	I:289:TYR:O	0.856
1	K:136:VAL:HG13	K:154:LEU:HD12	0.849
1	J:35:GLY:O	J:150:LEU:HD12	0.846
1	D:246:GLN:HE21	E:251:TYR:HB3	0.843
1	G:167:LYS:NZ	L:404:ARG:HH22	0.843
1	B:657:MET:HE3	B:689:LYS:HB3	0.841
1	N:37:ILE:HB	N:80:GLU:H	0.841
1	G:168:LYS:HB2	G:169:ASN:HA	0.840
1	B:503:ALA:O	J:185:ARG:NH1	0.839
1	B:280:ARG:HH12	B:387:GLU:HG2	0.838
1	J:9:MET:HE3	K:135:ARG:HB3	0.836
1	J:151:ALA:HB1	J:153:THR:H	0.831
1	J:69:MET:HG2	J:76:PRO:HB3	0.825
1	I:273:LEU:HD13	K:48:ASN:CA	0.821
1	D:64:GLN:N	D:64:GLN:OE1	0.820
1	I:271:GLY:HA2	K:51:PRO:HD3	0.819
1	B:288:LEU:HD13	B:324:ARG:HB3	0.816
1	B:360:GLY:H	L:253:VAL:H	0.811
1	N:36:ILE:HG12	N:80:GLU:HG2	0.809
1	B:302:ASP:HB2	B:380:ARG:HE	0.807
1	B:176:ASN:OD1	B:177:LEU:N	0.807
1	O:3:DT:O2	P:65:DG:N2	0.807

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:292:LEU:HD22	B:374:PHE:CD2	0.806
1	B:414:PHE:HE2	B:437:CYS:HB2	0.806
1	A:360:ARG:HH12	A:433:GLN:HB3	0.798
1	B:136:SER:HB3	B:389:THR:HB	0.798
1	B:346:VAL:HG23	L:220:ASN:HD21	0.798
1	G:67:LYS:HB2	K:9:ARG:HD2	0.798
1	I:198:PRO:HB2	I:254:MET:SD	0.797
1	I:169:MET:HA	I:169:MET:HE2	0.796
1	C:81:THR:OG1	C:89:GLN:NE2	0.796
1	B:424:ARG:HE	B:426:PRO:HG2	0.794
1	I:39:LEU:HD12	P:53:DT:H2'	0.793
1	D:263:MET:HE2	D:297:ILE:HG13	0.790
1	G:76:ILE:HG21	K:45:ARG:HB3	0.789
1	B:497:ARG:NH2	B:707:ASN:OD1	0.789
1	D:263:MET:CE	D:297:ILE:HG13	0.787
1	B:543:GLN:HA	B:546:GLU:HB2	0.785
1	J:36:ASP:HB2	J:69:MET:HE1	0.785
1	B:426:PRO:HA	I:290:ILE:HD11	0.783
1	B:138:THR:HB	B:155:CYS:HB3	0.781
1	C:211:MET:HE2	C:240:SER:CB	0.779
1	H:16:GLU:HG3	H:17:MET:HE2	0.779
1	A:569:LYS:HG3	K:184:ARG:HH21	0.776
1	N:109:MET:HA	N:109:MET:HE2	0.775
1	O:39:DG:H2''	O:40:DC:H5''	0.774

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:359:SER:HB2	L:253:VAL:C	0.772
1	B:284:GLU:OE2	B:378:ARG:NH2	0.769
1	A:380:MET:SD	A:381:TRP:CD1	0.764
1	L:253:VAL:HG13	L:278:ASP:HB2	0.764
1	B:416:ILE:HG22	B:435:PHE:HD1	0.762
1	G:32:ARG:HG2	M:83:VAL:HB	0.760
1	G:228:ARG:HE	K:176:PRO:HD2	0.757
1	B:292:LEU:HD22	B:374:PHE:HD2	0.755
1	I:913:LYS:HA	P:66:DT:H2"	0.755
1	A:577:LYS:HD3	A:604:THR:HG21	0.753
1	B:354:PRO:HA	B:415:THR:HA	0.752
1	G:91:VAL:HG11	G:138:LEU:H	0.752
1	J:155:ASP:O	K:148:LYS:NZ	0.752
1	D:340:GLY:HA3	E:146:ARG:HH12	0.751
1	B:386:LEU:HA	I:103:ARG:HE	0.750
1	H:63:ILE:HG23	H:119:ARG:HH21	0.748
1	G:18:ALA:HA	M:2:MET:H	0.747
1	B:424:ARG:HH22	L:228:LYS:H22	0.747
1	E:6:ASP:HB2	E:155:GLN:HB2	0.744
1	I:914:VAL:HG12	I:918:LEU:HG	0.743
1	B:299:ARG:NH2	B:301:THR:O	0.742
1	G:90:VAL:HG22	J:93:ARG:HD3	0.740
1	L:197:LYS:HB2	L:218:ILE:HD11	0.740

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:583:PRO:HD3	P:21:DG:H3'	0.739
1	B:386:LEU:HD12	I:103:ARG:HB3	0.739
1	B:345:ARG:HB3	L:220:ASN:HB3	0.737
1	D:247:HIS:HA	D:279:TYR:HB2	0.736
1	D:315:LEU:HD12	D:316:PHE:CE1	0.736
1	F:31:LYS:NZ	G:269:THR:O	0.736
1	N:106:LEU:HD13	N:111:GLU:HB3	0.735
1	G:130:ARG:NH1	G:130:ARG:O	0.735
1	B:112:ARG:HD2	P:44:DT:H3'	0.734
1	B:209:TYR:HB3	B:213:LEU:HD22	0.734
1	J:41:PRO:HD3	J:146:ALA:HA	0.734
1	J:160:PRO:HA	P:27:DG:H21	0.734
1	M:38:MET:HG3	M:52:GLU:HG2	0.732
1	G:168:LYS:NZ	J:85:SER:OG	0.732
1	B:296:SER:OG	B:307:ASN:ND2	0.729
1	I:32:SER:O	I:36:ASN:ND2	0.729
1	C:423:LEU:C	C:424:MET:HE2	0.728
1	L:396:VAL:HG12	L:406:LYS:H	0.728
1	J:168:GLY:O	J:172:PHE:HB3	0.726
1	B:388:ILE:HD13	I:107:GLU:HB2	0.725
1	A:276:MET:HB2	A:279:GLU:HG2	0.724
1	D:242:MET:HE2	D:303:VAL:HG13	0.724
1	G:34:ARG:HG2	N:224:THR:HB	0.724

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:288:LEU:HB3	B:324:ARG:HD3	0.723
1	G:30:ARG:HD2	G:34:ARG:HH21	0.723
1	I:284:GLU:H	I:288:HIS:HB2	0.723
1	J:45:VAL:HG11	J:79:LEU:HD23	0.723
1	A:360:ARG:NH1	A:433:GLN:HB3	0.722
1	B:240:ASP:O	B:244:ILE:HG12	0.722
1	B:256:LEU:HB3	B:341:LYS:HE2	0.722
1	J:25:ILE:O	J:217:GLN:NE2	0.722
1	A:636:GLU:HG3	A:676:ARG:HD3	0.721
1	B:266:LEU:HD11	B:386:LEU:HD21	0.720
1	A:380:MET:SD	A:381:TRP:NE1	0.719
1	B:347:GLN:O	L:230:ARG:NE	0.719
1	J:13:ARG:HE	J:162:SER:HB3	0.716
1	G:103:VAL:HB	G:113:MET:HA	0.715
1	J:153:THR:O	K:130:GLN:NE2	0.715
1	C:262:ARG:O	C:263:ARG:HD2	0.714
1	A:378:PHE:O	A:382:SER:OG	0.714
1	G:270:TYR:CE2	G:271:GLU:O	0.713
1	L:212:LEU:HB3	L:215:SER:HB3	0.713
1	B:303:ALA:H	B:380:ARG:NH2	0.713
1	B:266:LEU:CD1	B:386:LEU:HD21	0.712
1	B:258:ARG:HH21	I:114:LEU:HD21	0.712
1	L:21:VAL:HG21	L:67:ILE:HD11	0.712
1	G:63:LYS:O	L:323:THR:HB	0.710

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:121:PHE:O	G:185:GLN:NE2	0.710
1	L:111:HIS:O	L:112:HIS:ND1	0.710
1	B:423:ASP:HA	I:288:HIS:HB3	0.709
1	B:343:ARG:HH22	L:250:SER:HB2	0.708
1	L:279:TYR:HB2	L:391:ARG:HH21	0.706
1	A:623:LEU:HB3	A:659:PHE:HB2	0.705
1	B:291:GLY:HA3	B:318:ALA:HA	0.705
1	C:98:ARG:NH1	C:102:ARG:HH12	0.705
1	B:407:VAL:HG13	B:435:PHE:HZ	0.704
1	B:424:ARG:HA	I:251:GLN:HG3	0.704
1	G:167:LYS:HE2	L:404:ARG:HH12	0.704
1	L:229:LEU:O	L:233:PHE:HB2	0.704
1	L:232:TRP:NE1	L:236:GLU:OE1	0.704
1	C:256:GLN:NE2	C:263:ARG:O	0.704
1	B:504:ILE:HA	J:185:ARG:HH12	0.703
1	B:276:THR:HG23	I:758:GLU:HA	0.702
1	B:501:GLN:HB2	J:188:MET:CE	0.700
1	B:387:GLU:OE2	I:100:SER:OG	0.700
1	H:16:GLU:HG3	H:17:MET:CE	0.699
1	I:35:LEU:HD12	I:54:HIS:HB2	0.698
1	I:275:GLU:HB2	K:81:GLN:HE21	0.698
1	B:657:MET:CE	B:689:LYS:HB3	0.697
1	I:244:ASN:ND2	P:37:DG:OP2	0.697
1	L:279:TYR:HB3	L:410:MET:HE1	0.696

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:265:THR:O	B:269:THR:HG23	0.695
1	B:110:SER:OG	B:111:SER:N	0.695
1	E:175:MET:O	E:179:ASN:ND2	0.694
1	B:674:TYR:HB3	B:724:MET:HE2	0.693
1	G:31:LYS:HB3	N:79:PRO:O	0.693
1	L:53:ALA:HB1	L:98:PHE:HE1	0.693
1	B:413:GLY:O	B:438:MET:N	0.693
1	J:162:SER:HB2	P:29:DA:H1'	0.692
1	L:107:CYS:SG	L:108:GLU:N	0.692
1	B:693:LEU:HD22	B:697:ILE:HD11	0.691
1	L:392:VAL:HG22	L:409:VAL:HG22	0.691
1	I:868:THR:OG1	O:6:DG:OP2	0.691
1	J:171:ASP:O	J:175:LYS:HG2	0.690
1	A:565:VAL:O	K:184:ARG:NH2	0.690
1	G:256:MET:HE3	G:257:TYR:H	0.689
1	L:167:MET:HG3	L:232:TRP:HH2	0.688
1	B:223:LYS:HA	B:223:LYS:HE2	0.687
1	I:32:SER:HB2	P:54:DC:H2''	0.687
1	L:8:LEU:HD11	L:17:ILE:HG21	0.687
1	N:165:ALA:HB1	N:194:MET:HE3	0.686
1	G:146:GLN:HE21	J:54:ILE:HB	0.685
1	I:6:LEU:HD23	I:811:SER:HB2	0.684
1	J:26:ASP:HA	J:217:GLN:HG2	0.684
1	J:214:ASN:O	J:218:LEU:HD12	0.683

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:269:THR:HG22	I:106:THR:HB	0.682
1	G:218:LYS:HD2	K:148:LYS:HD2	0.682
1	A:514:MET:SD	A:537:ASN:ND2	0.682
1	K:105:GLU:HG3	K:108:ARG:HH21	0.681
1	G:48:TYR:HD1	G:49:SER:H	0.680
1	I:291:LEU:HD22	I:293:LYS:HE3	0.679
1	L:269:GLU:O	L:270:ASN:HB2	0.678
1	B:309:VAL:HG12	B:409:THR:HB	0.676
1	B:542:TYR:O	B:545:MET:HG2	0.676
1	J:38:ILE:HD12	J:148:THR:HA	0.676
1	H:98:LYS:HB3	H:99:MET:HE2	0.675
1	C:418:ASN:HB3	C:423:LEU:H	0.674
1	D:315:LEU:HD12	D:316:PHE:CD1	0.674
1	C:81:THR:HG23	C:82:GLN:H	0.673
1	C:226:SER:HA	E:102:GLU:HG3	0.673
1	D:47:MET:SD	D:154:SER:OG	0.671
1	B:139:ALA:HB3	B:141:TYR:CZ	0.670
1	B:543:GLN:HB2	P:37:DG:P	0.670
1	M:2:MET:HG2	M:5:LEU:HD12	0.670
1	N:203:VAL:HG13	N:212:ILE:HD11	0.670
1	E:100:LYS:NZ	E:108:ASN:OD1	0.670
1	A:528:LYS:O	A:531:ILE:HG22	0.669
1	I:765:THR:OG1	I:768:MET:HE2	0.668
1	C:103:ILE:HG23	C:108:GLY:HA3	0.667



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:222:LYS:HA	K:152:GLN:HG3	0.667
1	B:542:TYR:HB2	P:37:DG:H4'	0.665
1	K:9:ARG:O	L:317:ARG:NH1	0.665
1	B:515:ALA:HB3	J:185:ARG:HG3	0.664
1	K:8:GLN:HB2	K:14:LEU:HD13	0.664
1	K:44:LEU:HG	K:74:VAL:HA	0.664
1	K:146:VAL:HG13	K:150:ASP:HB2	0.664
1	L:50:GLU:HG3	L:90:VAL:HG13	0.664
1	I:273:LEU:HG	I:274:LYS:N	0.663
1	N:206:LEU:O	N:211:HIS:N	0.663
1	B:236:ALA:HB1	B:239:ILE:HG12	0.662
1	I:295:ILE:HG21	K:81:GLN:HB3	0.662
1	A:327:MET:SD	A:464:LEU:HD13	0.661
1	I:37:GLN:HG2	O:12:DA:C2	0.661
1	B:419:GLU:OE1	B:434:HIS:NE2	0.661
1	B:410:TYR:O	L:270:ASN:ND2	0.661
1	B:416:ILE:HG22	B:435:PHE:CD1	0.660
1	B:668:ILE:C	B:669:ARG:HD2	0.660
1	B:514:ILE:HA	B:517:ILE:CD1	0.659
1	G:167:LYS:NZ	G:168:LYS:O	0.659
1	B:262:ASN:HA	I:110:LEU:HD11	0.658
1	B:414:PHE:CE2	B:437:CYS:HB2	0.658
1	D:272:PRO:HG2	H:71:TYR:CZ	0.658

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:31:LYS:HB2	N:80:GLU:HB2	0.658
1	G:66:PRO:HB3	L:322:ASP:HB2	0.658
1	B:310:LEU:HB2	B:315:LEU:HB3	0.657
1	B:382:LEU:O	B:386:LEU:N	0.657
1	D:312:TYR:O	D:313:HIS:ND1	0.657
1	B:620:MET:HE1	B:624:PRO:HD3	0.656
1	B:368:GLN:N	B:368:GLN:OE1	0.656
1	C:261:SER:O	C:262:ARG:NE	0.656
1	A:673:SER:O	A:677:GLN:HG3	0.655
1	B:569:ILE:HD13	I:237:LEU:HD22	0.654
1	J:34:VAL:HA	K:129:GLU:HB3	0.654
1	B:112:ARG:NH1	P:44:DT:O3'	0.654
1	C:66:GLN:NE2	C:70:THR:OG1	0.654
1	L:190:ARG:NH2	L:252:GLY:H	0.654
1	B:373:ARG:NH2	L:259:ASN:OD1	0.654
1	D:245:PRO:HG3	D:302:LEU:HB3	0.652
1	G:37:MET:HE2	N:211:HIS:HA	0.652
1	I:139:ARG:HH21	I:140:GLU:HB2	0.652
1	J:10:ARG:HG3	J:37:TYR:HB2	0.652
1	C:391:LEU:HB2	F:4:LEU:HB2	0.651
1	E:92:ASN:OD1	E:93:PRO:HD3	0.651
1	J:21:HIS:HA	J:217:GLN:HE22	0.651
1	M:9:ARG:NH1	M:97:TYR:OH	0.651

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:58:LEU:HD23	I:775:LEU:HD23	0.650
1	B:307:ASN:ND2	B:315:LEU:HB2	0.649
1	B:514:ILE:HA	B:517:ILE:HD12	0.649
1	C:16:ARG:HG2	C:214:VAL:HG21	0.649
1	E:63:HIS:HD2	E:118:LEU:HG	0.649
1	G:98:MET:HB3	L:344:ASN:HD21	0.649
1	G:218:LYS:HA	G:221:LYS:HG2	0.649
1	P:33:DA:H2'	P:34:DG:O4'	0.649
1	J:10:ARG:HH12	J:152:ILE:HG23	0.648
1	K:49:LEU:HD22	L:240:LEU:HB2	0.648
1	C:308:ILE:HG12	C:325:VAL:HG21	0.647
1	A:306:ILE:HD13	A:359:LYS:O	0.646
1	C:328:GLN:HG2	C:330:THR:HG23	0.646
1	D:264:ALA:HB3	D:288:TYR:HE1	0.646
1	C:249:ARG:HD3	C:256:GLN:HG3	0.645
1	D:260:SER:O	H:130:HIS:NE2	0.645
1	A:108:CYS:SG	C:295:ASN:ND2	0.644
1	B:71:ILE:HD11	B:225:LEU:HD11	0.643
1	D:139:LEU:HD21	D:159:ILE:HD11	0.642
1	I:33:ILE:HG12	P:55:DT:H4'	0.642
1	B:500:ASP:O	J:188:MET:HE3	0.641
1	L:191:GLN:HB3	L:230:ARG:HH22	0.641
1	M:102:LYS:HD3	N:139:PRO:HG3	0.640
1	K:146:VAL:H	O:41:DG:H5'	0.640

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:133:THR:HB	A:160:THR:HG21	0.639
1	B:257:ASP:O	B:260:GLN:CG	0.638
1	I:273:LEU:CD1	I:295:ILE:O	0.638
1	G:39:ARG:HH21	N:108:ASP:HA	0.638
1	B:311:PRO:HD3	B:409:THR:HG21	0.637
1	A:39:PRO:HA	A:285:ILE:HD13	0.636
1	B:112:ARG:HD2	P:44:DT:C3'	0.636
1	I:267:GLU:HA	I:271:GLY:N	0.636
1	J:166:ASN:HB3	J:167:PRO:HD2	0.636
1	I:969:ASN:ND2	I:971:THR:OG1	0.636
1	L:139:GLY:O	L:194:LEU:N	0.636
1	G:225:GLU:O	K:156:THR:OG1	0.636
1	G:63:LYS:HA	L:325:PHE:HB3	0.635
1	J:138:LYS:HG2	J:141:LYS:HD2	0.635
1	B:252:THR:HB	B:432:ILE:HD13	0.634
1	B:664:VAL:HG13	B:677:MET:HE2	0.634
1	G:86:LYS:HE3	J:96:LEU:HD22	0.634
1	H:78:LEU:HG	H:134:MET:HE3	0.634
1	B:304:HIS:H	B:380:ARG:NH1	0.634
1	B:515:ALA:HB1	J:189:HIS:CD2	0.633
1	G:241:VAL:HG23	G:263:MET:SD	0.633
1	L:86:GLN:NE2	L:132:ASP:O	0.633
1	C:234:VAL:HA	C:263:ARG:HD3	0.632
1	E:67:SER:O	E:139:LYS:NZ	0.632

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:258:HIS:O	I:262:ILE:HG13	0.631
1	J:221:PHE:HE1	K:135:ARG:HD2	0.631
1	N:213:TYR:CZ	N:222:LYS:HB3	0.630
1	I:764:VAL:H	P:54:DC:H5'	0.630
1	L:262:THR:OG1	L:265:GLU:OE1	0.630
1	A:371:VAL:HG21	A:393:THR:HG21	0.629
1	A:455:LEU:HD12	A:483:LEU:HD12	0.629
1	I:102:SER:O	I:106:THR:HG23	0.629
1	J:8:ASP:HA	J:148:THR:HG21	0.629
1	L:115:THR:OG1	L:221:PRO:HB3	0.629
1	G:214:MET:CE	G:217:LYS:HD2	0.628
1	K:146:VAL:HG13	K:150:ASP:CB	0.628
1	G:77:LEU:O	O:30:DC:N4	0.628
1	B:669:ARG:N	B:673:ASP:OD2	0.628
1	C:84:LEU:HG	C:86:GLY:H	0.627
1	I:296:GLN:HB3	K:44:LEU:HB3	0.627
1	B:178:ASP:HA	B:181:LYS:HD2	0.626
1	B:500:ASP:O	B:502:VAL:HG23	0.626
1	G:256:MET:HE3	G:257:TYR:N	0.626
1	B:104:PHE:HE2	B:174:ILE:HD11	0.625
1	B:265:THR:HB	I:110:LEU:HD22	0.625
1	G:31:LYS:CB	N:80:GLU:HB2	0.625
1	B:284:GLU:O	B:288:LEU:HG	0.624
1	B:573:ASP:CG	I:217:THR:HG22	0.624

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:63:LYS:HG3	L:325:PHE:N	0.624
1	A:380:MET:HE1	A:381:TRP:CZ2	0.623
1	C:211:MET:CE	C:240:SER:HB2	0.623
1	C:127:ASP:O	C:131:LEU:HD13	0.622
1	L:168:ASP:OD1	L:170:SER:OG	0.622
1	L:74:TYR:HB2	L:107:CYS:HB2	0.621
1	H:105:ARG:O	H:109:THR:OG1	0.621
1	A:563:ASP:OD1	A:564:ASN:N	0.620
1	B:516:VAL:HA	J:185:ARG:NH2	0.619
1	K:13:VAL:O	K:15:LYS:NZ	0.619
1	B:734:LEU:HA	B:738:LEU:HB2	0.618
1	J:150:LEU:HD21	K:130:GLN:O	0.618
1	N:173:ILE:HG12	N:182:LEU:HD11	0.618
1	B:543:GLN:N	P:37:DG:H5''	0.618
1	C:262:ARG:C	C:263:ARG:HD2	0.617
1	D:288:TYR:OH	D:295:CYS:HB3	0.617
1	B:358:LEU:O	B:362:ALA:N	0.617
1	C:322:PRO:O	C:323:ASN:ND2	0.617
1	B:532:PRO:HB3	D:164:LEU:HD12	0.616
1	I:83:LEU:HD21	I:932:VAL:HG22	0.616
1	L:258:THR:O	L:259:ASN:HB2	0.616
1	G:98:MET:HB3	L:344:ASN:ND2	0.615
1	D:250:ALA:O	E:248:HIS:ND1	0.615
1	N:38:ARG:N	N:50:LYS:O	0.615

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:419:ARG:HD2	A:424:GLU:OE1	0.614
1	B:388:ILE:HG23	B:391:LEU:HD11	0.614
1	G:130:ARG:HG2	L:290:ARG:HH22	0.614
1	C:51:GLN:N	C:89:GLN:O	0.614
1	H:98:LYS:HB3	H:99:MET:CE	0.612
1	B:215:PRO:HD2	B:216:LYS:N	0.611
1	I:295:ILE:HD13	K:81:GLN:HB3	0.611
1	J:11:GLU:HG3	P:30:DA:OP1	0.611
1	B:424:ARG:NH2	L:228:LYS:HZ2	0.611
1	A:538:PRO:O	A:542:ARG:HG3	0.610
1	E:143:TYR:CE2	E:147:MET:HE1	0.610
1	H:33:ALA:O	H:37:ILE:HG13	0.610
1	J:193:ASN:HD21	J:195:ALA:HB3	0.610
1	K:27:VAL:HG12	K:29:PRO:HD2	0.610
1	K:153:THR:HG21	K:183:ALA:HB2	0.609
1	N:206:LEU:HB3	N:211:HIS:HB2	0.609
1	A:373:GLN:NE2	A:616:ASP:HB3	0.608
1	B:109:LEU:HG	B:199:ILE:HD11	0.608
1	B:137:LEU:HD12	B:154:HIS:HA	0.608
1	B:315:LEU:HD12	B:316:GLN:HG3	0.608
1	C:233:SER:C	C:263:ARG:HD3	0.608
1	E:132:LEU:H	E:132:LEU:HD23	0.608
1	G:139:ILE:HD11	G:143:GLU:HB2	0.608
1	J:21:HIS:ND1	J:178:GLY:HA3	0.608

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:211:ARG:HH11	J:61:ARG:NH2	0.608
1	G:237:ARG:HH21	G:240:ILE:HG12	0.607
1	I:95:LYS:HG2	I:761:ALA:HA	0.607
1	J:205:LEU:HD21	J:218:LEU:HD13	0.607
1	E:68:ARG:HE	E:118:LEU:HD13	0.606
1	J:42:GLU:HB2	J:75:ARG:HH21	0.606
1	P:55:DT:H2''	P:56:DT:H5''	0.606
1	M:9:ARG:NH1	M:24:CYS:SG	0.606
1	I:69:ARG:HE	I:983:GLN:HG3	0.605
1	L:216:THR:HG22	L:218:ILE:H	0.605
1	D:279:TYR:OH	D:290:GLU:O	0.605
1	J:45:VAL:HG12	J:46:GLU:H	0.604
1	L:365:LEU:HD11	L:379:VAL:HG11	0.604
1	P:36:DT:H4'	P:37:DG:H5'	0.604
1	B:334:ARG:HH12	L:20:ARG:HH21	0.604
1	K:31:TYR:HB2	K:39:ALA:HB3	0.603
1	L:138:ILE:HG23	L:229:LEU:HD11	0.603
1	G:249:GLU:CB	G:257:TYR:HE1	0.603
1	C:233:SER:O	C:263:ARG:NH1	0.603
1	G:76:ILE:HD13	K:45:ARG:HB3	0.602
1	J:6:VAL:HB	J:146:ALA:H	0.601
1	L:46:ASP:HA	L:113:LEU:HD22	0.601
1	B:411:ALA:HB2	L:270:ASN:N	0.600



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:517:ILE:HG23	B:548:THR:HG23	0.600
1	I:87:THR:HG22	I:91:ARG:HE	0.600
1	M:72:THR:HG1	M:76:THR:HG1	0.600
1	B:305:LEU:HB3	B:376:ALA:HB1	0.599
1	B:516:VAL:HG22	J:185:ARG:NE	0.599
1	H:116:GLU:OE2	H:120:ARG:HD3	0.599
1	B:223:LYS:NZ	B:450:ARG:HD3	0.598
1	L:23:ASN:HD22	L:216:THR:HA	0.598
1	B:303:ALA:HB1	P:43:DA:H1'	0.597
1	B:485:LEU:HD11	B:671:LYS:HG3	0.597
1	K:125:MET:HG2	K:126:GLU:H	0.597
1	M:9:ARG:HH21	N:54:MET:HE3	0.597
1	B:216:LYS:HE2	B:308:PRO:HB3	0.596
1	B:265:THR:O	B:268:LYS:HG2	0.596
1	H:99:MET:HE2	H:99:MET:N	0.596
1	B:546:GLU:OE2	I:240:LYS:HE2	0.596
1	J:157:GLU:HB3	K:147:ASN:OD1	0.596
1	B:273:ILE:HG21	I:103:ARG:HH11	0.595
1	B:336:LEU:O	B:340:VAL:HG23	0.595
1	C:211:MET:HE2	C:240:SER:CA	0.595
1	G:30:ARG:HB2	N:213:TYR:CE1	0.595
1	I:267:GLU:HA	I:271:GLY:H	0.595
1	I:273:LEU:CD1	K:48:ASN:HA	0.595
1	L:167:MET:HG3	L:232:TRP:CH2	0.595

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:149:PRO:O	A:151:GLY:N	0.595
1	B:273:ILE:HG12	I:103:ARG:HD3	0.594
1	H:7:ILE:H	H:7:ILE:HD12	0.594
1	B:215:PRO:HD2	B:216:LYS:H	0.593
1	D:295:CYS:SG	D:298:CYS:HB3	0.593
1	H:63:ILE:HA	H:66:GLU:HG3	0.593
1	B:424:ARG:HE	B:426:PRO:CG	0.593
1	C:94:ASN:OD1	C:97:PHE:N	0.593
1	G:240:ILE:O	G:242:HIS:N	0.593
1	B:112:ARG:CZ	P:44:DT:H5'	0.592
1	K:183:ALA:O	K:186:LEU:HB2	0.592
1	N:36:ILE:HG12	N:80:GLU:CG	0.592
1	J:10:ARG:NH1	K:138:GLU:OE2	0.592
1	G:113:MET:HG2	G:114:ASP:N	0.591
1	I:287:SER:OG	P:36:DT:O4	0.591
1	B:421:PHE:CE1	I:290:ILE:HG13	0.590
1	E:42:MET:HE3	E:108:ASN:HA	0.590
1	J:5:ILE:HB	J:7:VAL:HG23	0.590
1	L:277:PRO:HB3	L:395:LYS:HB2	0.590
1	A:307:ASN:HD22	B:755:GLN:H	0.590
1	C:196:TRP:NE1	C:274:SER:O	0.590
1	B:191:PRO:CD	B:192:TYR:N	0.589
1	I:100:SER:OG	P:48:DG:O6	0.589

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:339:TYR:HD2	B:361:LEU:C	0.588
1	G:86:LYS:O	G:90:VAL:HG23	0.588
1	L:212:LEU:HD23	L:214:SER:H	0.588
1	N:165:ALA:HB1	N:194:MET:CE	0.588
1	P:54:DC:H2''	P:55:DT:H5'	0.587
1	B:27:GLU:OE2	B:30:ARG:NH1	0.587
1	B:345:ARG:HB3	L:220:ASN:CB	0.586
1	B:476:VAL:HG23	B:477:THR:HG23	0.586
1	J:5:ILE:HG22	J:6:VAL:H	0.586
1	G:219:PHE:HD2	J:154:ALA:HB3	0.586
1	K:44:LEU:HD11	K:74:VAL:HG23	0.586
1	O:46:DC:H2'	O:47:DG:C8	0.586
1	B:373:ARG:NE	L:257:ASN:O	0.586
1	G:237:ARG:HG3	G:239:THR:N	0.585
1	B:299:ARG:NH1	P:47:DA:H4'	0.585
1	B:355:PRO:HD2	L:273:GLN:HG3	0.584
1	B:389:THR:HG23	I:104:LYS:HD2	0.584
1	B:439:ASP:HB3	B:639:TYR:HE2	0.584
1	B:81:GLU:OE1	B:176:ASN:ND2	0.584
1	D:59:ARG:NH1	D:132:GLU:OE2	0.584
1	B:211:TYR:HD1	B:221:VAL:HG21	0.583
1	L:55:ALA:HA	L:98:PHE:HB2	0.583
1	B:351:GLN:NE2	L:250:SER:HB3	0.583
1	I:273:LEU:HD11	K:48:ASN:OD1	0.582

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:166:VAL:HG23	A:291:LEU:HG	0.581
1	B:309:VAL:HG13	B:410:TYR:CE2	0.581
1	B:309:VAL:HG21	B:406:LEU:HA	0.581
1	B:657:MET:HE1	B:684:PHE:CD1	0.581
1	G:37:MET:CE	N:211:HIS:HA	0.581
1	G:237:ARG:HD3	G:239:THR:HA	0.581
1	J:122:LEU:H	J:122:LEU:HD23	0.581
1	A:634:ARG:NH1	A:638:GLN:OE1	0.581
1	E:101:TYR:HD1	E:104:LEU:HG	0.580
1	G:165:ILE:O	G:165:ILE:HG13	0.580
1	G:249:GLU:HB2	G:257:TYR:CZ	0.580
1	I:199:GLU:HA	I:254:MET:HE1	0.580
1	M:11:ASN:OD1	M:14:MET:HE3	0.580
1	B:268:LYS:O	B:272:ARG:HG2	0.579
1	B:355:PRO:HA	L:270:ASN:HB3	0.579
1	I:198:PRO:HA	I:201:LYS:HD2	0.579
1	J:164:LYS:HG3	J:175:LYS:HZ3	0.579
1	D:338:CYS:SG	E:146:ARG:NH1	0.579
1	E:173:GLN:N	E:173:GLN:OE1	0.579
1	L:247:ASP:OD1	L:248:LEU:N	0.579
1	L:198:GLY:HA3	L:215:SER:HB2	0.578
1	D:297:ILE:HD12	H:79:ARG:HG2	0.577
1	I:273:LEU:HD12	I:295:ILE:O	0.577
1	K:8:GLN:HB3	K:11:ASN:HB2	0.577

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:125:ARG:NH1	B:125:ARG:O	0.577
1	D:248:THR:HB	D:278:GLY:HA3	0.576
1	D:259:PRO:HD2	H:133:GLU:HG3	0.576
1	B:282:ARG:NH1	P:50:DC:O2	0.576
1	B:348:HIS:HB3	L:249:LYS:HB3	0.575
1	B:407:VAL:HG13	B:435:PHE:CZ	0.575
1	D:263:MET:HE3	D:297:ILE:HG13	0.575
1	G:48:TYR:HD1	G:49:SER:N	0.575
1	J:93:ARG:HH12	J:98:GLN:HE22	0.575
1	B:622:GLY:HA2	B:681:ASP:HB2	0.574
1	G:158:ARG:HH12	G:193:VAL:HG23	0.574
1	A:650:MET:HG2	A:650:MET:O	0.573
1	K:13:VAL:HG23	K:14:LEU:H	0.573
1	M:7:ARG:HH12	N:54:MET:HA	0.573
1	B:112:ARG:HD2	P:44:DT:O3'	0.572
1	B:379:LEU:HD23	B:401:ALA:HB2	0.572
1	C:13:VAL:HG12	C:16:ARG:HH22	0.572
1	E:37:CYS:O	E:41:VAL:HG23	0.572
1	K:131:ASP:CG	K:132:PHE:H	0.572
1	L:347:VAL:HB	L:409:VAL:HG23	0.572
1	B:497:ARG:NH1	B:707:ASN:O	0.572
1	A:650:MET:HE2	A:655:TYR:O	0.571
1	B:369:ARG:H	B:369:ARG:HD3	0.571
1	D:75:LEU:O	D:79:GLU:HG2	0.571

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	O:35:DT:H2"	O:36:DG:N7	0.571
1	A:74:ARG:NH2	D:19:SER:O	0.571
1	J:65:GLN:NE2	K:129:GLU:OE2	0.571
1	A:680:LEU:HD12	A:687:PHE:HZ	0.570
1	H:58:MET:SD	H:59:VAL:HG12	0.570
1	L:52:ARG:HD3	L:88:THR:HG23	0.570
1	B:317:GLU:HB3	B:374:PHE:HZ	0.569
1	B:436:SER:HB2	B:632:ILE:HD11	0.569
1	J:164:LYS:HD2	K:142:THR:HA	0.568
1	C:283:THR:HG22	C:285:HIS:H	0.567
1	C:355:ALA:HB1	C:359:MET:HE3	0.567
1	D:113:ASN:HB2	D:293:VAL:HG23	0.567
1	B:276:THR:O	I:99:SER:HB2	0.567
1	J:80:ILE:HD12	J:123:TRP:CZ3	0.567
1	J:10:ARG:HH22	J:152:ILE:HG22	0.567
1	L:325:PHE:HE1	L:327:ASN:HB3	0.567
1	J:77:VAL:HG12	J:119:LEU:HB2	0.566
1	B:424:ARG:O	I:288:HIS:NE2	0.566
1	A:380:MET:HE1	A:381:TRP:CE2	0.564
1	B:144:ALA:HB2	P:47:DA:N1	0.564
1	B:317:GLU:HB3	B:374:PHE:CZ	0.564
1	B:517:ILE:HG21	B:551:SER:HB3	0.564
1	J:35:GLY:HA2	J:69:MET:SD	0.564

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	K:45:ARG:HH21	L:243:VAL:N	0.564
1	C:49:LEU:HD12	C:50:PRO:O	0.563
1	C:81:THR:HG23	C:82:GLN:N	0.563
1	C:201:GLN:O	C:205:THR:HG23	0.563
1	D:242:MET:CE	D:303:VAL:HG13	0.563
1	D:308:LEU:HD11	E:274:ILE:HD11	0.563
1	G:170:PRO:HB3	L:400:ASN:HB3	0.563
1	L:284:ALA:HA	L:340:ASP:HB3	0.563
1	B:507:LYS:HG2	B:683:ARG:NH1	0.562
1	B:516:VAL:HA	J:185:ARG:HH21	0.562
1	A:388:GLN:HE22	B:755:GLN:HA	0.562
1	C:51:GLN:HB2	C:89:GLN:HB3	0.562
1	I:809:ASP:HA	I:823:ARG:HG3	0.562
1	I:127:ARG:HG2	I:180:PHE:HZ	0.561
1	I:208:MET:HG2	I:243:LEU:HD21	0.561
1	N:124:MET:O	N:130:ASN:ND2	0.561
1	A:106:PRO:HB3	A:109:ARG:HD2	0.560
1	J:9:MET:HE3	K:135:ARG:CB	0.560
1	K:72:VAL:HG11	K:86:LEU:HD13	0.560
1	B:373:ARG:HH21	L:257:ASN:HB2	0.560
1	G:128:ASN:O	G:130:ARG:N	0.560
1	A:34:PRO:HD3	A:280:LEU:HG	0.559
1	A:400:PRO:HB2	A:426:VAL:HG21	0.559
1	A:549:LYS:O	A:553:ARG:HD3	0.559

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:571:TYR:CE2	A:626:ILE:HD12	0.559
1	B:487:ARG:HD2	B:724:MET:HE1	0.559
1	D:263:MET:HE1	D:298:CYS:HB2	0.559
1	G:212:GLU:HA	G:215:LYS:HB2	0.559
1	H:75:GLY:O	H:79:ARG:HG3	0.559
1	J:153:THR:HG23	J:154:ALA:H	0.559
1	K:141:THR:OG1	K:147:ASN:ND2	0.559
1	A:274:GLN:OE1	A:459:GLN:NE2	0.559
1	A:199:LEU:H	A:273:LYS:HZ3	0.558
1	B:508:PHE:CE1	B:509:GLU:HB3	0.557
1	J:157:GLU:HG3	J:160:PRO:HB2	0.557
1	B:35:LYS:HE2	B:452:GLN:HE22	0.556
1	B:349:VAL:HG22	B:350:VAL:H	0.556
1	G:168:LYS:HD3	G:178:MET:HB3	0.556
1	J:35:GLY:C	J:150:LEU:HD12	0.556
1	G:168:LYS:HZ2	J:86:LYS:HG3	0.556
1	L:321:CYS:HB2	L:323:THR:HG22	0.556
1	B:430:ASN:ND2	I:285:ASP:OD2	0.556
1	A:568:LEU:HB3	K:184:ARG:HH22	0.555
1	K:143:VAL:HG21	K:186:LEU:HA	0.555
1	N:83:VAL:HG12	N:105:PRO:HA	0.555
1	B:272:ARG:O	B:276:THR:OG1	0.555
1	D:233:SER:O	E:287:THR:OG1	0.555
1	A:354:ALA:HA	A:437:LEU:CD2	0.554



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:593:LEU:HD11	A:617:LEU:HD13	0.554
1	A:643:VAL:HG21	A:659:PHE:HB3	0.554
1	B:121:VAL:HG23	B:133:LYS:HB3	0.554
1	B:388:ILE:HG23	B:391:LEU:CD1	0.554
1	L:274:GLY:HA2	L:396:VAL:O	0.554
1	A:570:GLU:CA	A:570:GLU:OE2	0.553
1	B:569:ILE:HG12	B:597:LEU:HD11	0.553
1	J:33:GLU:OE2	J:34:VAL:HG22	0.553
1	B:256:LEU:HA	B:259:CYS:SG	0.552
1	I:296:GLN:CB	K:44:LEU:HB3	0.552
1	K:44:LEU:HG	K:73:GLN:O	0.552
1	G:32:ARG:NH1	M:83:VAL:HG21	0.552
1	I:751:LYS:O	I:755:GLN:HG2	0.551
1	L:111:HIS:HB2	L:113:LEU:HD23	0.551
1	B:613:HIS:ND1	B:613:HIS:O	0.551
1	I:284:GLU:OE2	P:38:DA:N6	0.551
1	A:340:LEU:HD23	A:491:ALA:HB2	0.550
1	A:663:VAL:HG13	A:669:GLU:HG2	0.550
1	G:167:LYS:O	G:168:LYS:HD2	0.550
1	A:472:ARG:NH1	O:48:DA:OP1	0.550
1	A:628:SER:HB3	A:639:ARG:HH22	0.548
1	G:35:ALA:HB3	M:86:LYS:HE2	0.548
1	I:193:PHE:HD1	I:196:LEU:HD12	0.548

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:273:LEU:HD23	I:274:LYS:H	0.548
1	K:173:ALA:HA	K:180:PRO:HB3	0.548
1	H:23:LYS:NZ	H:23:LYS:O	0.548
1	D:260:SER:OG	H:133:GLU:OE1	0.548
1	A:368:ALA:N	P:23:DG:OP1	0.548
1	C:42:MET:HE2	C:93:LEU:HG	0.547
1	D:260:SER:HB2	D:285:ARG:O	0.547
1	G:69:ILE:HG22	G:70:ASP:H	0.547
1	G:178:MET:HG3	O:35:DT:H4'	0.547
1	B:351:GLN:HE21	L:250:SER:HB3	0.547
1	L:315:LEU:HG	L:326:PRO:HB3	0.547
1	B:139:ALA:HB3	B:141:TYR:CE1	0.546
1	B:414:PHE:CE2	B:437:CYS:CB	0.546
1	G:237:ARG:CD	G:239:THR:HA	0.546
1	J:11:GLU:O	J:14:SER:N	0.546
1	B:725:ALA:HB1	D:211:VAL:HG21	0.545
1	I:179:PHE:O	I:183:PRO:HG3	0.545
1	B:388:ILE:HD12	B:389:THR:H	0.544
1	C:278:SER:HA	E:2:VAL:HB	0.544
1	D:52:TYR:HE2	D:146:LEU:HD13	0.544
1	F:10:GLU:HB2	F:41:HIS:CD2	0.544
1	I:199:GLU:HG3	I:254:MET:HE1	0.544
1	I:281:VAL:HG23	I:282:VAL:H	0.544
1	K:137:THR:HG23	K:138:GLU:HG2	0.544

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:555:ASN:HD22	D:67:LYS:HA	0.543
1	E:194:CYS:HB3	E:231:PHE:HE2	0.543
1	I:273:LEU:CG	I:274:LYS:N	0.543
1	I:896:TRP:O	I:900:GLN:HG2	0.543
1	J:166:ASN:HB3	J:167:PRO:CD	0.543
1	B:112:ARG:NH1	P:44:DT:H5'	0.543
1	B:601:ARG:NH2	B:624:PRO:O	0.543
1	B:133:LYS:O	B:136:SER:OG	0.543
1	A:38:VAL:HB	A:482:PHE:HB2	0.542
1	B:418:ILE:HA	B:433:LEU:HA	0.542
1	D:293:VAL:O	D:302:LEU:HB2	0.542
1	I:813:ILE:HG12	I:818:ALA:HB2	0.542
1	J:187:LEU:HG	J:205:LEU:HD11	0.542
1	M:53:LEU:HG	M:79:CYS:HB3	0.542
1	G:102:TYR:OH	N:27:GLU:HB3	0.542
1	G:113:MET:CG	G:114:ASP:H	0.542
1	L:52:ARG:NH1	L:88:THR:OG1	0.542
1	A:569:LYS:HG2	K:169:ARG:NH1	0.541
1	G:60:ALA:O	G:61:ASN:HB2	0.541
1	A:599:ASN:ND2	A:602:ILE:H	0.541
1	I:856:TYR:OH	I:929:ASN:O	0.541
1	C:344:ALA:HB1	C:374:ILE:HG22	0.540
1	J:11:GLU:OE1	P:30:DA:OP1	0.540
1	A:39:PRO:HB3	A:284:CYS:O	0.539

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:543:GLN:CA	B:546:GLU:HB2	0.539
1	C:416:PHE:HE2	C:418:ASN:HB2	0.539
1	H:116:GLU:CG	H:120:ARG:NH1	0.539
1	A:570:GLU:OE2	K:170:GLU:CG	0.539
1	A:572:ALA:HB3	K:169:ARG:HH22	0.538
1	C:423:LEU:O	C:424:MET:HE2	0.538
1	G:100:PHE:O	G:113:MET:HB3	0.538
1	G:208:GLN:O	G:212:GLU:HG2	0.538
1	G:168:LYS:NZ	J:86:LYS:HG3	0.538
1	L:167:MET:CG	L:232:TRP:HH2	0.538
1	L:295:MET:HE1	L:330:TYR:HB3	0.538
1	B:345:ARG:O	B:347:GLN:N	0.538
1	B:381:SER:O	B:385:THR:HB	0.537
1	J:213:ALA:O	J:217:GLN:HG3	0.537
1	K:7:ARG:HA	K:9:ARG:HH21	0.537
1	P:60:DG:H5'	P:60:DG:H8	0.537
1	G:106:GLU:N	G:106:GLU:OE1	0.537
1	D:192:SER:OG	D:193:ALA:N	0.537
1	A:536:MET:HE1	A:570:GLU:HG2	0.536
1	B:268:LYS:HG3	I:754:LYS:NZ	0.536
1	G:55:ALA:O	G:56:THR:HG22	0.536
1	L:212:LEU:O	L:215:SER:OG	0.536
1	B:350:VAL:HG23	B:631:ARG:NE	0.535

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:425:THR:O	I:290:ILE:HG12	0.535
1	L:169:THR:HG23	L:229:LEU:HD23	0.535
1	B:256:LEU:HD13	B:341:LYS:CE	0.534
1	D:47:MET:HE2	D:154:SER:N	0.534
1	B:726:GLN:OE1	D:213:LEU:HD13	0.534
1	G:18:ALA:HA	M:2:MET:N	0.534
1	J:172:PHE:HB2	K:142:THR:HG21	0.534
1	M:2:MET:O	M:7:ARG:NE	0.534
1	A:535:THR:HG23	A:627:SER:OG	0.533
1	I:279:ARG:HH11	I:293:LYS:HB2	0.533
1	L:39:LEU:HD12	L:56:PHE:HB3	0.533
1	N:37:ILE:O	N:80:GLU:HG3	0.533
1	B:278:GLU:OE2	P:51:DA:H1'	0.533
1	B:263:LEU:HD21	B:337:LEU:HD22	0.532
1	G:242:HIS:HB2	G:244:HIS:CE1	0.532
1	H:18:GLU:HA	H:18:GLU:OE1	0.532
1	B:509:GLU:OE1	J:180:ASN:ND2	0.532
1	A:599:ASN:HD21	A:601:LYS:HB3	0.531
1	B:344:LEU:HD21	B:433:LEU:HD23	0.531
1	B:368:GLN:HE21	B:371:PRO:HG2	0.531
1	B:424:ARG:HG3	B:426:PRO:HD2	0.531
1	L:190:ARG:O	L:191:GLN:HG2	0.531
1	M:24:CYS:HB2	M:68:VAL:HG13	0.531
1	M:66:GLU:HB3	M:83:VAL:HG23	0.531

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	K:18:ARG:NH1	L:313:ASN:O	0.531
1	A:273:LYS:HB2	A:276:MET:HE3	0.530
1	A:636:GLU:HG3	A:676:ARG:HH11	0.530
1	B:683:ARG:HD2	B:689:LYS:HE2	0.530
1	J:54:ILE:HA	J:57:LEU:HG	0.530
1	B:345:ARG:HH21	L:223:ILE:HD11	0.530
1	C:32:PRO:HD3	C:72:LEU:HD23	0.529
1	G:62:VAL:HG12	G:63:LYS:H	0.529
1	J:158:THR:O	J:160:PRO:HD2	0.529
1	N:37:ILE:HG23	N:49:TYR:HB3	0.529
1	A:395:ASP:OD1	A:396:ALA:N	0.529
1	A:677:GLN:O	A:681:VAL:HG13	0.528
1	J:10:ARG:CD	J:11:GLU:OE1	0.528
1	J:158:THR:C	J:160:PRO:HD2	0.528
1	L:311:GLN:CD	L:315:LEU:HB2	0.528
1	L:394:VAL:HG13	L:407:ALA:HB2	0.528
1	O:27:DG:H2"	O:28:DC:OP2	0.528
1	A:273:LYS:HD3	A:273:LYS:N	0.527
1	B:500:ASP:HA	K:195:LEU:HD11	0.527
1	C:126:ARG:HH21	C:130:SER:HB2	0.527
1	E:13:ILE:HG21	E:41:VAL:HG13	0.527
1	J:133:LEU:HB2	K:84:LYS:HG3	0.527
1	K:4:VAL:HG11	K:15:LYS:HG2	0.527
1	L:190:ARG:HH21	L:276:LYS:H	0.527

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:373:GLN:O	A:377:GLN:HG2	0.526
1	A:514:MET:HG2	A:519:TYR:HD2	0.526
1	B:317:GLU:OE1	B:370:LYS:HE2	0.526
1	J:127:PRO:HA	J:130:THR:HG22	0.526
1	G:200:LEU:O	G:204:LYS:HG3	0.525
1	J:221:PHE:CE1	K:135:ARG:HD2	0.525
1	B:425:THR:N	I:255:ASN:OD1	0.525
1	B:347:GLN:HB2	L:230:ARG:HB2	0.524
1	B:390:ASP:HB2	I:111:LYS:HZ3	0.524
1	B:518:ARG:HD2	J:189:HIS:CE1	0.524
1	J:37:TYR:HE2	J:79:LEU:HD21	0.524
1	L:280:PHE:CE1	L:392:VAL:HB	0.524
1	G:167:LYS:HZ1	L:404:ARG:NH2	0.524
1	A:568:LEU:HD23	K:184:ARG:NH1	0.523
1	A:569:LYS:HD3	K:169:ARG:HG2	0.523
1	C:105:LEU:HA	E:100:LYS:HE3	0.523
1	D:239:LEU:HD11	E:282:CYS:HB2	0.523
1	A:144:SER:O	A:146:THR:N	0.523
1	B:253:ARG:HG3	L:222:ASP:HB2	0.522
1	L:54:THR:HB	L:97:THR:HA	0.522
1	B:263:LEU:CD2	B:337:LEU:HD22	0.521
1	D:261:PHE:HA	H:130:HIS:CE1	0.521
1	D:248:THR:H	D:279:TYR:HB2	0.521

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:762:ALA:HB1	P:53:DT:H3'	0.521
1	L:196:ILE:HB	L:199:ALA:HB2	0.521
1	B:616:ARG:NH1	B:674:TYR:OH	0.521
1	A:61:TYR:O	A:65:MET:HE3	0.520
1	F:38:ASP:C	F:38:ASP:OD2	0.520
1	D:260:SER:HB3	H:134:MET:SD	0.519
1	I:284:GLU:HG3	P:37:DG:O6	0.519
1	N:37:ILE:H	N:80:GLU:HA	0.519
1	N:213:TYR:CE1	N:215:THR:HG22	0.519
1	B:407:VAL:CG1	B:435:PHE:HZ	0.519
1	B:82:LYS:O	B:86:GLU:HG2	0.518
1	L:191:GLN:HG3	L:249:LYS:HG3	0.518
1	L:396:VAL:HG12	L:406:LYS:N	0.518
1	B:498:GLY:N	B:502:VAL:O	0.518
1	D:101:SER:O	D:101:SER:OG	0.518
1	C:215:GLU:HG3	C:241:LEU:HD11	0.517
1	D:110:LEU:HD23	D:149:MET:HE1	0.517
1	F:8:LEU:HG	F:43:PHE:CE1	0.517
1	I:250:VAL:O	I:254:MET:HG2	0.517
1	A:127:VAL:HG11	A:160:THR:HG23	0.516
1	C:391:LEU:HG	F:43:PHE:CE2	0.516
1	I:284:GLU:N	I:288:HIS:HB2	0.516
1	I:837:TYR:HA	I:840:PHE:CE2	0.516
1	J:10:ARG:HD3	J:11:GLU:OE1	0.516



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:514:MET:HE1	A:534:TYR:HA	0.515
1	B:126:PHE:HB2	B:129:ASP:OD1	0.515
1	B:141:TYR:HA	P:47:DA:C2	0.515
1	G:95:GLY:HA2	L:346:TRP:CE2	0.515
1	G:218:LYS:HE3	K:151:SER:OG	0.515
1	J:200:LEU:HD21	J:204:GLU:HB2	0.515
1	K:172:LEU:HD11	K:183:ALA:HB3	0.515
1	L:68:GLU:HB2	L:71:LYS:HG3	0.515
1	L:142:LYS:HD3	L:167:MET:HE1	0.515
1	D:262:SER:H	H:71:TYR:HE2	0.515
1	I:15:ARG:NH1	I:839:ASP:OD2	0.515
1	L:145:GLU:O	L:162:ARG:NH1	0.515
1	D:155:ARG:NH2	D:182:ALA:O	0.515
1	B:349:VAL:HG13	B:351:GLN:H	0.514
1	B:421:PHE:CZ	L:234:ASP:HB3	0.514
1	C:348:ILE:HD13	C:375:ARG:HH21	0.514
1	J:10:ARG:HD3	J:11:GLU:CD	0.514
1	L:190:ARG:CZ	L:252:GLY:H	0.514
1	L:317:ARG:HD3	L:323:THR:O	0.514
1	B:424:ARG:HH22	L:228:LYS:NZ	0.514
1	B:497:ARG:HH12	B:707:ASN:C	0.514
1	B:507:LYS:O	B:511:ARG:NH1	0.514
1	B:135:HIS:HB3	B:389:THR:O	0.513

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:169:ASN:N	G:170:PRO:HD3	0.513
1	J:34:VAL:O	J:73:TYR:OH	0.513
1	E:176:ASN:HA	E:179:ASN:HD22	0.512
1	I:955:LEU:HD22	I:959:ARG:HH21	0.512
1	G:32:ARG:HH11	M:83:VAL:HG11	0.512
1	C:440:ARG:NE	C:440:ARG:O	0.512
1	A:123:LEU:O	A:127:VAL:HG13	0.511
1	B:414:PHE:CD2	B:437:CYS:HA	0.511
1	C:20:HIS:HB2	C:21:PRO:HD3	0.511
1	L:300:PRO:HG2	L:327:ASN:HD21	0.511
1	B:390:ASP:HB2	I:111:LYS:NZ	0.510
1	H:87:VAL:HG22	H:89:THR:HG23	0.510
1	A:179:SER:O	A:267:THR:OG1	0.510
1	B:61:ARG:HH22	B:102:LEU:HD13	0.509
1	I:213:LYS:O	I:217:THR:HG23	0.509
1	G:214:MET:HE3	G:217:LYS:HD2	0.508
1	J:32:LEU:HD22	J:147:ALA:HA	0.508
1	K:46:TYR:O	K:50:HIS:N	0.508
1	I:200:VAL:O	I:204:ILE:HG22	0.507
1	G:31:LYS:NZ	N:38:ARG:O	0.507
1	B:42:MET:SD	B:43:PRO:HD2	0.506
1	B:286:ARG:HD2	P:50:DC:OP1	0.506
1	B:410:TYR:CD2	B:414:PHE:CE1	0.506
1	G:105:CYS:HB2	G:126:CYS:HB3	0.506

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:501:GLN:H	K:195:LEU:HD21	0.506
1	L:88:THR:HG22	L:90:VAL:H	0.506
1	L:249:LYS:O	L:250:SER:HB3	0.506
1	O:60:DT:H2"	O:61:DG:H8	0.506
1	P:34:DG:C8	P:35:DA:C6	0.506
1	B:216:LYS:HZ1	B:308:PRO:HD3	0.505
1	C:119:LEU:H	C:119:LEU:HD23	0.505
1	C:41:ARG:HH12	E:241:LEU:HD22	0.505
1	J:45:VAL:HG12	J:46:GLU:N	0.505
1	G:52:ALA:O	G:54:ALA:N	0.505
1	L:318:CYS:O	L:323:THR:N	0.505
1	B:303:ALA:H	B:380:ARG:CZ	0.504
1	B:627:TYR:HD1	B:630:SER:HB3	0.504
1	E:125:LYS:HG2	E:127:GLN:OE1	0.504
1	I:815:LEU:HD21	I:855:ALA:HB2	0.504
1	B:511:ARG:NH1	P:35:DA:H4'	0.504
1	B:339:TYR:HE2	B:360:GLY:O	0.504
1	A:195:ARG:HH12	A:198:ARG:HE	0.504
1	A:467:THR:OG1	A:468:ALA:N	0.504
1	B:129:ASP:N	B:129:ASP:OD1	0.504
1	C:17:LEU:HA	C:214:VAL:HG23	0.503
1	D:281:CYS:HB2	D:302:LEU:HD11	0.503
1	I:295:ILE:HB	K:82:ALA:HB2	0.503
1	L:142:LYS:HG2	L:244:SER:HB2	0.503

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	L:190:ARG:HD3	L:250:SER:HA	0.503
1	B:424:ARG:NH2	L:228:LYS:HG3	0.503
1	D:339:GLN:N	D:339:GLN:OE1	0.503
1	L:190:ARG:NH2	L:276:LYS:H	0.503
1	A:173:ASN:N	A:434:GLU:OE1	0.503
1	B:657:MET:HE3	B:689:LYS:CB	0.502
1	G:208:GLN:HA	G:211:ARG:HG2	0.502
1	L:320:LYS:HA	O:29:DT:H4'	0.502
1	B:480:THR:O	B:758:GLN:NE2	0.502
1	B:527:MET:O	B:531:VAL:HG12	0.501
1	K:150:ASP:HA	K:153:THR:HB	0.501
1	P:48:DG:H4'	P:49:DG:H5'	0.501
1	G:102:TYR:HD2	N:29:SER:OG	0.501
1	A:697:GLU:CD	A:697:GLU:H	0.501
1	A:40:SER:HB2	A:121:TYR:CE1	0.500
1	B:496:GLY:HA3	B:707:ASN:HD21	0.500
1	I:267:GLU:HB2	I:272:PHE:CD1	0.500
1	I:292:ILE:HB	L:235:ALA:H	0.500
1	P:18:DT:H2''	P:19:DT:O5'	0.500
1	B:280:ARG:HB3	B:385:THR:HG23	0.499
1	B:314:VAL:HG22	L:258:THR:HG23	0.499
1	B:418:ILE:HG22	B:420:PRO:HD3	0.499
1	B:518:ARG:HD2	J:189:HIS:HE1	0.499
1	D:365:VAL:HA	D:369:LEU:HB3	0.499

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:273:LEU:HD11	I:295:ILE:O	0.499
1	I:282:VAL:HG13	P:36:DT:C2	0.499
1	L:286:VAL:HA	L:338:ILE:HG22	0.499
1	B:282:ARG:NH2	P:51:DA:N3	0.499
1	D:64:GLN:CD	D:64:GLN:N	0.499
1	K:181:GLN:NE2	P:20:DC:OP2	0.499
1	B:128:LYS:O	B:131:ASP:HB2	0.498
1	C:180:THR:HG23	C:182:ALA:H	0.498
1	I:169:MET:CE	I:169:MET:HA	0.498
1	I:273:LEU:H	I:273:LEU:HD23	0.498
1	J:6:VAL:O	J:6:VAL:HG12	0.498
1	J:79:LEU:HA	J:123:TRP:HB3	0.498
1	J:157:GLU:HB3	K:147:ASN:CG	0.498
1	A:392:PHE:CD1	A:412:MET:HE3	0.497
1	B:280:ARG:CZ	I:100:SER:HA	0.497
1	B:346:VAL:HG22	L:193:VAL:H	0.497
1	B:733:GLN:HB2	B:738:LEU:HD13	0.497
1	I:756:GLN:O	I:760:ILE:HG12	0.497
1	K:30:ASP:OD1	K:57:ARG:NH2	0.497
1	N:157:MET:O	N:159:ALA:N	0.497
1	A:314:ALA:HB2	A:381:TRP:CD1	0.496
1	A:698:GLU:CD	A:698:GLU:N	0.496
1	B:303:ALA:HB3	P:45:DT:O2	0.496
1	G:56:THR:HG21	L:367:GLU:HB2	0.496

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:157:GLU:CA	J:160:PRO:HG2	0.496
1	L:139:GLY:HA2	L:229:LEU:HD13	0.496
1	A:38:VAL:HG21	A:281:GLN:HG3	0.495
1	B:192:TYR:C	B:192:TYR:CD1	0.495
1	B:304:HIS:CE1	P:45:DT:H3	0.495
1	B:388:ILE:HB	I:107:GLU:OE2	0.495
1	B:426:PRO:O	B:427:THR:HG23	0.495
1	G:22:ALA:HB1	N:216:VAL:HG12	0.495
1	I:127:ARG:HG2	I:180:PHE:CZ	0.495
1	D:113:ASN:OD1	D:116:LYS:N	0.495
1	K:137:THR:OG1	K:147:ASN:OD1	0.495
1	B:264:GLU:CG	L:109:ASP:H	0.494
1	B:627:TYR:HB2	P:36:DT:H72	0.494
1	C:423:LEU:HG	F:37:ILE:HG22	0.494
1	G:98:MET:HE1	G:115:SER:HA	0.494
1	H:95:LYS:O	H:99:MET:HE3	0.494
1	I:273:LEU:CD2	I:273:LEU:H	0.494
1	L:325:PHE:CD2	L:326:PRO:HD2	0.494
1	G:18:ALA:CB	M:2:MET:HE2	0.494
1	O:46:DC:H2'	O:47:DG:N7	0.494
1	P:28:DC:H2''	P:29:DA:C8	0.494
1	A:563:ASP:CG	A:564:ASN:H	0.494
1	J:47:ARG:NH2	J:81:GLU:OE1	0.494
1	L:190:ARG:NH2	L:251:GLY:H	0.494

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:44:CYS:O	J:77:VAL:N	0.494
1	B:299:ARG:HB3	B:302:ASP:OD2	0.493
1	B:439:ASP:HB3	B:639:TYR:CE2	0.493
1	G:48:TYR:CE1	G:51:THR:N	0.493
1	I:33:ILE:O	I:37:GLN:HG3	0.493
1	I:774:GLU:HA	I:777:ARG:HD2	0.493
1	L:315:LEU:HA	L:326:PRO:HA	0.493
1	G:168:LYS:H	G:169:ASN:CG	0.493
1	B:342:TRP:HA	L:220:ASN:HB2	0.492
1	B:358:LEU:HB2	B:372:LEU:HD21	0.492
1	C:23:THR:O	C:27:VAL:HG23	0.492
1	G:33:GLN:HA	G:36:LEU:HB2	0.492
1	G:140:THR:HG22	G:180:LEU:HD23	0.492
1	H:59:VAL:CG2	H:61:ASN:HB2	0.492
1	H:128:VAL:HG22	H:131:ILE:HG12	0.492
1	I:126:LYS:HG2	I:126:LYS:O	0.492
1	I:273:LEU:N	I:273:LEU:HD23	0.492
1	J:173:LEU:HA	J:176:MET:HG3	0.492
1	B:76:THR:OG1	B:77:VAL:N	0.492
1	B:280:ARG:HH22	B:387:GLU:CD	0.492
1	J:159:LEU:O	P:27:DG:N2	0.492
1	B:316:GLN:O	L:430:ARG:NH2	0.492
1	A:273:LYS:HB2	A:276:MET:CE	0.491

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:170:LEU:HD21	B:194:LEU:HD11	0.491
1	B:135:HIS:ND1	B:141:TYR:OH	0.491
1	B:120:GLU:N	B:120:GLU:OE1	0.491
1	A:695:GLY:C	A:698:GLU:OE1	0.490
1	B:662:GLN:O	B:666:ARG:HG2	0.490
1	D:263:MET:HA	D:266:LEU:HD13	0.490
1	D:275:THR:HG22	D:287:LYS:HG3	0.490
1	J:6:VAL:HB	J:146:ALA:N	0.490
1	B:33:ASP:OD1	B:34:ALA:N	0.490
1	B:85:GLU:OE2	B:88:ARG:NH2	0.490
1	G:40:GLN:NE2	M:88:ASP:OD2	0.490
1	A:294:GLU:HB3	A:332:ARG:HD3	0.489
1	B:365:VAL:HG22	L:185:LYS:NZ	0.489
1	B:427:THR:O	B:428:ILE:HG12	0.489
1	J:170:GLN:HB2	K:194:PHE:CE2	0.489
1	L:419:GLU:O	L:422:ARG:HG3	0.489
1	B:372:LEU:HD12	L:255:GLY:HA3	0.488
1	B:223:LYS:HZ1	B:450:ARG:HD3	0.488
1	B:511:ARG:HD2	P:35:DA:H5'	0.488
1	D:266:LEU:HA	D:270:THR:HB	0.488
1	E:143:TYR:OH	E:147:MET:HE1	0.488
1	J:32:LEU:HG	K:131:ASP:OD1	0.488
1	G:137:LYS:O	G:183:LYS:N	0.488
1	B:346:VAL:HG12	B:348:HIS:CD2	0.487



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:326:LEU:HD23	D:327:GLU:N	0.487
1	D:338:CYS:SG	E:146:ARG:HD3	0.487
1	H:108:VAL:HG23	H:111:LEU:HD21	0.487
1	I:273:LEU:CD2	I:274:LYS:H	0.487
1	J:6:VAL:HG13	J:28:GLU:O	0.487
1	L:283:VAL:HG22	L:389:ILE:HG23	0.487
1	N:186:ASP:O	N:190:GLN:HG2	0.487
1	C:15:ASP:N	C:15:ASP:OD1	0.487
1	B:113:LYS:NZ	P:41:DA:OP2	0.487
1	B:379:LEU:O	B:383:LEU:HG	0.486
1	G:28:ILE:HG22	M:83:VAL:HG11	0.486
1	G:130:ARG:CG	L:290:ARG:HH22	0.486
1	M:8:SER:HA	M:113:LEU:HD13	0.486
1	L:166:LEU:O	L:174:VAL:N	0.486
1	B:61:ARG:NH2	B:102:LEU:HD13	0.485
1	B:641:ARG:HB3	B:641:ARG:HH11	0.485
1	D:264:ALA:N	D:266:LEU:HD22	0.485
1	E:101:TYR:CD1	E:104:LEU:HG	0.485
1	J:80:ILE:H	J:123:TRP:CB	0.485
1	L:190:ARG:CZ	L:251:GLY:H	0.485
1	B:573:ASP:OD1	B:574:GLY:N	0.485
1	J:137:LEU:O	J:141:LYS:NZ	0.485
1	B:337:LEU:O	B:341:LYS:HG2	0.484
1	B:410:TYR:CD2	B:414:PHE:HE1	0.484

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:444:ILE:HD12	B:471:LEU:HD13	0.484
1	E:9:ASN:HA	E:158:LYS:O	0.484
1	G:201:GLU:O	G:205:GLU:HG2	0.484
1	G:214:MET:HA	G:217:LYS:HG2	0.484
1	J:9:MET:O	J:10:ARG:HB2	0.484
1	K:17:VAL:HG23	L:312:GLN:HB2	0.484
1	G:244:HIS:ND1	G:262:THR:O	0.484
1	G:194:TRP:O	G:196:SER:N	0.484
1	B:170:LEU:HB3	B:175:TYR:HE2	0.483
1	B:509:GLU:HG3	J:181:ALA:HB3	0.483
1	B:576:GLU:HA	B:579:VAL:CG1	0.483
1	G:249:GLU:HG3	G:257:TYR:OH	0.483
1	L:134:LEU:HB3	L:198:GLY:HA2	0.483
1	B:282:ARG:NH2	I:92:ARG:HH21	0.483
1	I:263:ARG:NH1	I:276:VAL:H	0.483
1	A:375:LYS:HD2	A:391:ARG:HD3	0.482
1	A:380:MET:SD	A:381:TRP:CE2	0.482
1	B:391:LEU:HD22	P:45:DT:C4	0.482
1	C:42:MET:HE1	C:91:LEU:O	0.482
1	C:319:TYR:HB2	C:326:VAL:CG1	0.482
1	D:191:LEU:HG	D:212:ILE:HD12	0.482
1	B:279:GLN:OE1	I:96:ASP:HB3	0.482
1	L:54:THR:HG23	O:20:DT:H72	0.482

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:351:GLN:HE21	L:250:SER:CB	0.482
1	K:146:VAL:N	O:41:DG:H3'	0.482
1	P:30:DA:H2''	P:31:DC:C6	0.482
1	B:215:PRO:CD	B:216:LYS:N	0.482
1	G:123:LEU:HG	G:125:THR:HG23	0.481
1	H:95:LYS:O	H:99:MET:HG2	0.481
1	J:32:LEU:HD21	J:148:THR:O	0.481
1	J:40:THR:HG23	J:42:GLU:HG2	0.481
1	G:32:ARG:NH1	M:83:VAL:HG11	0.481
1	A:99:PHE:O	A:103:ILE:HG12	0.480
1	A:588:GLU:HG2	J:167:PRO:HB2	0.480
1	D:67:LYS:HB3	D:68:PRO:HD3	0.480
1	D:246:GLN:HB3	E:251:TYR:CB	0.480
1	K:154:LEU:O	K:164:LEU:HD21	0.480
1	A:178:GLU:OE2	A:267:THR:OG1	0.480
1	J:171:ASP:OD1	K:142:THR:OG1	0.480
1	G:215:LYS:HA	J:155:ASP:HB3	0.479
1	G:226:LEU:HG	K:152:GLN:OE1	0.479
1	I:39:LEU:HA	I:39:LEU:HD23	0.479
1	I:109:LEU:HD12	I:747:GLN:HG2	0.479
1	I:262:ILE:HG12	L:232:TRP:HD1	0.479
1	L:190:ARG:HA	L:275:ASP:OD2	0.479
1	L:23:ASN:ND2	L:216:THR:HA	0.479
1	K:146:VAL:H	O:41:DG:C5'	0.479

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	O:41:DG:H2''	O:42:DA:N7	0.479
1	H:116:GLU:HG2	H:120:ARG:HH11	0.479
1	E:127:GLN:N	E:127:GLN:OE1	0.479
1	A:39:PRO:HB2	A:288:GLU:HA	0.478
1	A:607:ILE:HG22	A:608:SER:N	0.478
1	B:280:ARG:HB3	B:385:THR:CG2	0.478
1	I:765:THR:HG22	P:52:DG:C8	0.478
1	J:47:ARG:CZ	P:30:DA:H2'	0.478
1	K:73:GLN:HA	K:100:ALA:O	0.478
1	L:398:THR:HA	L:403:SER:HB2	0.478
1	O:55:DT:H2''	O:56:DG:H8	0.478
1	C:433:ASP:N	C:433:ASP:OD1	0.478
1	L:311:GLN:O	L:313:ASN:N	0.478
1	B:158:TYR:CE2	B:162:ASP:HB3	0.477
1	B:211:TYR:CD1	B:221:VAL:HG21	0.477
1	B:332:PHE:HA	B:335:ARG:HE	0.477
1	C:112:TRP:HZ2	E:101:TYR:HA	0.477
1	I:262:ILE:HA	L:232:TRP:HD1	0.477
1	L:12:GLN:HB3	L:80:LEU:HD12	0.477
1	L:233:PHE:HA	L:236:GLU:HB3	0.477
1	N:37:ILE:HG21	N:49:TYR:HD2	0.477
1	O:51:DT:H2'	O:52:DC:C6	0.477
1	O:57:DG:H2''	O:58:DA:H8	0.477
1	J:47:ARG:NH2	P:30:DA:H2'	0.477

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:199:LEU:N	A:273:LYS:HZ3	0.477
1	B:215:PRO:CD	B:216:LYS:H	0.476
1	B:284:GLU:HG3	B:378:ARG:HH12	0.476
1	G:261:CYS:C	G:263:MET:H	0.476
1	D:96:ILE:HD13	D:121:LEU:HD21	0.475
1	D:246:GLN:HG3	E:252:ARG:HA	0.475
1	G:101:ASP:C	G:102:TYR:CG	0.475
1	A:36:GLU:H	A:281:GLN:HE22	0.475
1	K:50:HIS:NE2	K:52:ASP:OD1	0.475
1	L:332:MET:N	L:332:MET:SD	0.475
1	A:398:ASP:N	A:398:ASP:OD1	0.475
1	A:265:THR:HA	A:266:GLN:HA	0.474
1	B:355:PRO:HG2	L:273:GLN:HB2	0.474
1	B:407:VAL:CG1	B:435:PHE:CZ	0.474
1	C:317:MET:HE1	C:325:VAL:CG1	0.474
1	D:135:LEU:HD11	D:159:ILE:HD13	0.474
1	G:173:SER:HB2	P:32:DA:N3	0.474
1	C:98:ARG:HH12	C:102:ARG:HH12	0.474
1	A:551:HIS:HB3	A:556:ASP:HB2	0.473
1	B:508:PHE:CE2	P:33:DA:H2"	0.473
1	I:805:GLY:HA3	I:822:TYR:HE1	0.473
1	B:267:GLN:HE22	L:106:PRO:HB3	0.473
1	L:190:ARG:HB2	L:192:PRO:HD3	0.473

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	M:104:ILE:HG23	M:111:TYR:HB3	0.473
1	E:87:ASN:N	E:109:GLU:OE1	0.473
1	A:126:ALA:O	A:129:VAL:HG22	0.472
1	A:548:ILE:O	A:552:GLU:HG2	0.472
1	B:343:ARG:CZ	L:190:ARG:HD2	0.472
1	B:382:LEU:HD12	B:386:LEU:HB3	0.472
1	B:709:THR:HG23	B:712:GLU:H	0.472
1	C:232:TYR:HB2	C:263:ARG:HG3	0.472
1	L:27:ILE:C	L:28:ARG:HD2	0.472
1	I:768:MET:N	I:768:MET:SD	0.472
1	A:354:ALA:HA	A:437:LEU:HD21	0.471
1	B:170:LEU:HD21	B:194:LEU:HD21	0.471
1	C:203:LEU:HD21	C:217:LEU:HD13	0.471
1	D:47:MET:HB2	D:47:MET:HE3	0.471
1	G:140:THR:HG21	O:35:DT:H5'	0.471
1	G:168:LYS:C	G:170:PRO:HD3	0.471
1	H:101:SER:O	H:105:ARG:HG2	0.471
1	J:179:VAL:HB	J:184:CYS:HB3	0.471
1	N:59:MET:CE	N:98:LEU:HB2	0.471
1	A:120:ALA:O	A:122:SER:N	0.471
1	B:135:HIS:O	B:141:TYR:OH	0.471
1	A:283:ARG:HH21	A:286:HIS:CG	0.470
1	A:437:LEU:HG	A:437:LEU:O	0.470
1	B:302:ASP:O	B:306:ALA:HB2	0.470

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:21:PRO:HB2	C:112:TRP:CZ3	0.470
1	E:224:LEU:HB3	H:28:LEU:HD21	0.470
1	G:219:PHE:CG	K:128:LEU:HD12	0.470
1	I:35:LEU:HD12	I:54:HIS:CB	0.470
1	L:265:GLU:O	L:269:GLU:HB2	0.470
1	B:616:ARG:O	B:676:LEU:N	0.470
1	C:271:ILE:O	E:53:ARG:NH2	0.470
1	G:39:ARG:NH1	M:90:HIS:H	0.470
1	K:45:ARG:HH21	L:243:VAL:H	0.470
1	J:36:ASP:OD1	J:65:GLN:NE2	0.470
1	A:505:VAL:HA	A:657:ALA:O	0.469
1	B:42:MET:HE3	B:48:LYS:HB2	0.469
1	C:237:MET:HE3	C:263:ARG:NH2	0.469
1	C:290:ILE:HD11	C:298:LEU:HD13	0.469
1	G:95:GLY:HA2	L:346:TRP:NE1	0.469
1	J:80:ILE:O	J:80:ILE:HG22	0.469
1	L:187:ASP:OD2	L:189:SER:HB2	0.469
1	K:101:TRP:N	K:105:GLU:OE1	0.469
1	A:695:GLY:O	A:698:GLU:OE1	0.469
1	B:345:ARG:HG2	B:345:ARG:O	0.469
1	B:345:ARG:HB2	L:221:PRO:O	0.468
1	I:50:ILE:O	I:53:PRO:HD3	0.468
1	I:105:THR:HA	I:108:LYS:HD2	0.468
1	K:33:LEU:HD21	K:110:LEU:HD22	0.468

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	K:136:VAL:HG13	K:154:LEU:CD1	0.468
1	K:41:PHE:HZ	K:73:GLN:HE21	0.468
1	K:132:PHE:HE1	K:135:ARG:NE	0.468
1	B:91:LEU:HD22	B:104:PHE:CD2	0.467
1	B:192:TYR:HE1	B:196:ARG:HD3	0.467
1	B:510:THR:CA	B:516:VAL:HG21	0.467
1	J:123:TRP:C	J:123:TRP:CD1	0.467
1	C:126:ARG:NE	C:130:SER:OG	0.467
1	B:386:LEU:HA	I:103:ARG:NE	0.466
1	D:245:PRO:HG3	D:302:LEU:CB	0.466
1	I:139:ARG:HG2	I:177:GLU:HG2	0.466
1	I:253:GLU:HA	I:256:GLN:OE1	0.466
1	J:194:ILE:O	J:197:LEU:HG	0.466
1	L:213:SER:HB2	O:22:DA:C2	0.466
1	L:233:PHE:CE2	L:237:GLY:HA2	0.466
1	N:34:VAL:H	N:115:HIS:CE1	0.466
1	P:26:DC:H2'	P:27:DG:C8	0.466
1	B:8:LEU:HD21	B:59:TYR:HA	0.465
1	B:350:VAL:CG2	B:631:ARG:HG3	0.465
1	C:162:LEU:HD22	C:167:LEU:HD21	0.465
1	I:211:PHE:CZ	I:215:ARG:NE	0.465
1	J:45:VAL:HG22	J:77:VAL:CG2	0.465
1	O:51:DT:H2''	O:52:DC:OP1	0.465



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:273:ILE:HG21	I:103:ARG:NH1	0.464
1	C:198:PHE:HE1	C:251:PHE:CE1	0.464
1	F:7:VAL:HG13	F:44:VAL:HG13	0.464
1	G:206:VAL:O	G:209:GLU:HG3	0.464
1	G:218:LYS:HA	G:221:LYS:CG	0.464
1	G:223:VAL:O	G:227:ARG:HG2	0.464
1	L:72:VAL:HG11	L:109:ASP:HB2	0.464
1	O:56:DG:H2''	O:57:DG:C8	0.464
1	B:45:GLY:H	B:669:ARG:HH21	0.464
1	B:162:ASP:OD1	B:163:ALA:N	0.464
1	B:647:ARG:HH12	O:37:DT:P	0.464
1	A:35:GLN:HB3	A:281:GLN:NE2	0.463
1	G:27:SER:HA	G:30:ARG:HH21	0.463
1	G:221:LYS:HA	G:224:LYS:HB3	0.463
1	I:271:GLY:HA2	K:51:PRO:CD	0.463
1	J:10:ARG:HD2	J:11:GLU:OE2	0.463
1	J:43:MET:HB2	J:43:MET:HE3	0.463
1	B:303:ALA:CB	P:43:DA:H1'	0.462
1	B:486:ALA:HA	B:736:LEU:HD23	0.462
1	G:227:ARG:HD2	G:227:ARG:N	0.462
1	I:296:GLN:HG2	K:48:ASN:HB2	0.462
1	L:259:ASN:C	L:261:LYS:H	0.462
1	P:18:DT:H4'	P:19:DT:OP1	0.462
1	C:256:GLN:O	C:258:LYS:N	0.462

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:308:ILE:HG22	A:355:CYS:HA	0.461
1	A:341:PRO:HG2	A:502:ILE:HD11	0.461
1	G:63:LYS:HE3	L:300:PRO:HD3	0.461
1	G:113:MET:HE1	N:1:GLN:OE1	0.461
1	I:917:LYS:HE3	P:64:DA:H2	0.461
1	J:63:TYR:CZ	K:122:ASP:HB3	0.461
1	A:613:THR:OG1	A:614:SER:N	0.461
1	B:273:ILE:CG1	I:103:ARG:HD3	0.460
1	B:508:PHE:C	B:508:PHE:CD1	0.460
1	I:75:VAL:HG11	I:793:GLN:HB3	0.460
1	O:37:DT:H2"	O:38:DT:C6	0.460
1	B:356:ALA:O	B:359:SER:OG	0.460
1	G:141:LYS:NZ	O:37:DT:OP2	0.460
1	A:505:VAL:HG11	A:640:LEU:HD11	0.459
1	B:547:SER:HA	I:241:ASN:ND2	0.459
1	C:237:MET:HB3	C:241:LEU:HB2	0.459
1	H:120:ARG:CZ	H:128:VAL:CG1	0.459
1	I:54:HIS:HB3	P:53:DT:C2	0.459
1	I:754:LYS:HE2	I:758:GLU:OE2	0.459
1	J:47:ARG:HG3	J:79:LEU:HD11	0.459
1	L:263:LEU:HB3	L:345:GLN:HE21	0.459
1	A:250:ASP:N	A:250:ASP:OD1	0.459
1	A:581:TYR:CE1	K:184:ARG:HG2	0.458
1	G:20:LEU:HG	G:21:PRO:HD3	0.458

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:178:MET:HA	O:36:DG:H5'	0.458
1	H:15:GLN:O	H:18:GLU:HG2	0.458
1	J:10:ARG:CD	J:11:GLU:CD	0.458
1	L:267:LYS:HD3	L:345:GLN:HE22	0.458
1	A:628:SER:OG	A:639:ARG:NH1	0.458
1	B:260:GLN:HA	B:337:LEU:HD21	0.457
1	B:359:SER:HB2	L:253:VAL:O	0.457
1	G:48:TYR:OH	G:51:THR:HG22	0.457
1	J:47:ARG:NH2	J:81:GLU:CD	0.457
1	J:85:SER:HB3	P:32:DA:H61	0.457
1	L:251:GLY:HA3	L:273:GLN:HB3	0.457
1	P:30:DA:H2''	P:31:DC:C5	0.457
1	P:47:DA:C2	P:48:DG:C5	0.457
1	C:387:THR:O	F:8:LEU:N	0.457
1	B:422:ASP:C	B:427:THR:HA	0.456
1	B:502:VAL:CG1	J:185:ARG:HD2	0.456
1	D:56:ASP:O	D:61:MET:HE3	0.456
1	D:150:PRO:HB2	D:152:HIS:ND1	0.456
1	E:133:LEU:HA	E:133:LEU:HD23	0.456
1	D:246:GLN:NE2	E:251:TYR:HB3	0.456
1	H:122:TYR:HB3	H:123:LEU:HD12	0.456
1	I:210:GLU:HB3	I:214:ARG:NH2	0.456
1	J:9:MET:SD	J:149:ALA:C	0.456
1	K:133:VAL:HA	K:155:LEU:HD11	0.456

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	N:5:PRO:HB2	N:119:VAL:HG22	0.456
1	J:156:SER:OG	P:29:DA:OP1	0.456
1	A:76:LEU:HB2	A:143:LEU:O	0.455
1	B:35:LYS:HG2	B:452:GLN:HE21	0.455
1	D:261:PHE:CD2	H:134:MET:HE2	0.455
1	G:168:LYS:CD	G:178:MET:HB3	0.455
1	J:149:ALA:HB3	J:150:LEU:CD2	0.455
1	A:183:ASP:OD1	A:184:VAL:N	0.455
1	D:257:ALA:O	D:285:ARG:NH2	0.455
1	B:55:LEU:O	B:55:LEU:HD12	0.454
1	B:336:LEU:HD12	B:357:PHE:CZ	0.454
1	B:393:ASP:CG	I:111:LYS:HA	0.454
1	D:179:LEU:HD13	D:186:VAL:HG21	0.454
1	F:16:LYS:HE3	F:39:ASP:HA	0.454
1	J:81:GLU:HG2	J:81:GLU:O	0.454
1	J:122:LEU:O	J:123:TRP:CG	0.454
1	J:159:LEU:HG	O:41:DG:N2	0.454
1	K:18:ARG:HB3	L:313:ASN:CG	0.454
1	B:223:LYS:O	B:227:ARG:NH1	0.454
1	C:196:TRP:HE1	C:274:SER:N	0.454
1	J:10:ARG:NE	J:11:GLU:OE1	0.454
1	A:568:LEU:HB3	K:184:ARG:NH2	0.453
1	A:672:TYR:O	A:676:ARG:HG2	0.453
1	B:409:THR:C	L:269:GLU:HG2	0.453

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:519:ASN:HB2	J:185:ARG:HH21	0.453
1	D:272:PRO:HG2	H:71:TYR:CE1	0.453
1	D:315:LEU:CD1	D:316:PHE:CE1	0.453
1	H:59:VAL:HG11	H:63:ILE:HD12	0.453
1	I:262:ILE:HG12	L:232:TRP:CD1	0.453
1	J:21:HIS:HA	J:217:GLN:NE2	0.453
1	G:146:GLN:NE2	J:51:SER:HA	0.453
1	L:234:ASP:N	L:235:ALA:HA	0.453
1	L:318:CYS:HB3	L:323:THR:OG1	0.453
1	O:55:DT:H2''	O:56:DG:C8	0.453
1	B:268:LYS:HG3	I:754:LYS:HZZ	0.452
1	C:232:TYR:C	C:263:ARG:HG2	0.452
1	G:171:HIS:CE1	K:77:LYS:HA	0.452
1	G:205:GLU:O	G:208:GLN:HG2	0.452
1	G:225:GLU:O	G:228:ARG:HB2	0.452
1	B:345:ARG:CB	L:220:ASN:HB3	0.452
1	N:82:TYR:O	N:106:LEU:HG	0.452
1	O:40:DC:H2''	O:41:DG:C8	0.452
1	B:280:ARG:NH2	B:387:GLU:OE2	0.452
1	A:308:ILE:HD13	A:384:ILE:HG13	0.451
1	B:112:ARG:HB2	P:44:DT:H3'	0.451
1	B:135:HIS:CE1	B:141:TYR:OH	0.451
1	B:266:LEU:HA	B:266:LEU:HD13	0.451
1	B:347:GLN:HA	B:420:PRO:HG3	0.451

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	D:108:THR:HG21	D:117:HIS:ND1	0.451
1	D:50:HIS:HE1	D:153:THR:HG21	0.451
1	H:116:GLU:OE2	H:120:ARG:CD	0.451
1	I:53:PRO:HD2	P:53:DT:O4	0.451
1	J:80:ILE:H	J:123:TRP:HB2	0.451
1	L:40:PHE:HE1	L:60:VAL:HA	0.451
1	B:417:ILE:O	B:434:HIS:N	0.451
1	B:709:THR:OG1	B:710:VAL:N	0.451
1	B:121:VAL:HG22	B:130:VAL:HG23	0.450
1	B:260:GLN:HA	B:337:LEU:CD2	0.450
1	G:18:ALA:HB3	M:80:THR:HG21	0.450
1	G:48:TYR:CD1	G:49:SER:N	0.450
1	H:64:GLN:O	H:67:LEU:HG	0.450
1	J:42:GLU:HB2	J:75:ARG:NH2	0.450
1	B:501:GLN:CB	J:188:MET:HE2	0.450
1	K:2:ILE:HA	K:32:VAL:O	0.450
1	P:60:DG:C8	P:60:DG:H5'	0.450
1	C:302:THR:OG1	C:303:GLU:N	0.450
1	G:154:ASP:N	G:154:ASP:OD1	0.450
1	A:140:LEU:HB3	A:148:VAL:HG11	0.449
1	B:264:GLU:HG2	L:109:ASP:HB2	0.449
1	B:416:ILE:HG12	L:273:GLN:OE1	0.449

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:612:HIS:O	B:613:HIS:HB3	0.449
1	E:63:HIS:CD2	E:118:LEU:HG	0.449
1	I:265:GLN:NE2	L:232:TRP:CZ2	0.449
1	B:424:ARG:NE	B:426:PRO:HG2	0.448
1	B:510:THR:HB	B:516:VAL:HG21	0.448
1	C:392:TYR:HB3	F:3:VAL:HG12	0.448
1	G:165:ILE:HD11	G:180:LEU:HD12	0.448
1	H:112:CYS:N	H:113:PRO:HD2	0.448
1	I:112:THR:HG23	I:743:LEU:HD22	0.448
1	K:74:VAL:HG13	K:101:TRP:CD2	0.448
1	L:393:ARG:HH21	L:395:LYS:HB3	0.448
1	M:79:CYS:SG	M:82:TYR:HB3	0.448
1	A:299:ASN:N	A:299:ASN:OD1	0.448
1	A:278:GLU:OE2	A:452:ARG:NH2	0.448
1	A:305:ASP:OD1	A:359:LYS:NZ	0.448
1	J:93:ARG:HG2	J:93:ARG:O	0.448
1	A:194:ILE:HG12	A:280:LEU:HD11	0.447
1	A:310:LEU:HD22	A:352:THR:HG23	0.447
1	B:359:SER:C	B:363:GLN:HG3	0.447
1	B:385:THR:HG22	I:103:ARG:HH21	0.447
1	B:506:SER:HA	B:510:THR:OG1	0.447
1	C:31:LEU:HB3	C:35:ALA:HB3	0.447
1	C:268:ARG:HG2	C:285:HIS:CE1	0.447
1	C:277:VAL:HG22	C:279:GLY:H	0.447

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:168:LYS:HD2	G:178:MET:HE2	0.447
1	G:171:HIS:CD2	J:85:SER:HA	0.447
1	H:145:TRP:O	H:149:ARG:HG2	0.447
1	A:581:TYR:OH	P:21:DG:OP2	0.447
1	A:522:TYR:CE1	A:530:ARG:HB2	0.446
1	B:91:LEU:O	B:91:LEU:HD12	0.446
1	B:410:TYR:CB	B:414:PHE:CD1	0.446
1	C:234:VAL:HA	C:263:ARG:CD	0.446
1	G:167:LYS:HD2	G:168:LYS:C	0.446
1	G:79:GLU:N	G:79:GLU:OE1	0.446
1	L:254:GLY:O	L:256:SER:N	0.446
1	G:239:THR:O	G:240:ILE:C	0.446
1	L:296:TYR:OH	L:331:ARG:NE	0.446
1	A:284:CYS:HA	A:287:LEU:HB2	0.445
1	A:348:LEU:HB2	A:381:TRP:CZ3	0.445
1	C:372:ASP:O	C:376:LEU:HG	0.445
1	G:214:MET:HE2	J:158:THR:HG21	0.445
1	H:109:THR:HG23	H:135:LEU:HD12	0.445
1	I:31:ILE:HG12	I:35:LEU:CD2	0.445
1	I:126:LYS:HG3	I:214:ARG:HD3	0.445
1	J:138:LYS:HE3	J:141:LYS:HB2	0.445
1	J:150:LEU:N	J:150:LEU:HD22	0.445
1	K:145:SER:HB2	K:185:ARG:NH1	0.445
1	M:1:ASP:C	M:3:MET:N	0.445



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:36:GLU:N	A:281:GLN:HE22	0.445
1	C:18:TYR:O	C:100:ASN:ND2	0.445
1	B:272:ARG:HD3	B:272:ARG:N	0.444
1	B:347:GLN:HG3	L:227:TYR:HA	0.444
1	D:285:ARG:HA	D:285:ARG:HD2	0.444
1	I:54:HIS:HB3	P:53:DT:N3	0.444
1	J:12:PHE:HA	J:17:PRO:HG3	0.444
1	J:159:LEU:HD22	P:27:DG:O4'	0.444
1	N:21:PHE:HB2	N:28:ILE:O	0.444
1	L:203:ASP:OD1	L:207:ARG:NH1	0.444
1	L:249:LYS:N	L:275:ASP:OD2	0.444
1	B:293:ARG:NH2	B:316:GLN:O	0.444
1	B:261:GLY:HA3	I:113:PHE:HE2	0.443
1	B:385:THR:HG22	I:103:ARG:NH2	0.443
1	B:726:GLN:OE1	D:213:LEU:HD22	0.443
1	G:98:MET:CE	G:115:SER:HA	0.443
1	G:118:MET:HA	G:122:ASP:HA	0.443
1	I:199:GLU:O	I:203:GLU:HG3	0.443
1	J:10:ARG:HG3	J:36:ASP:O	0.443
1	K:15:LYS:HB2	K:15:LYS:HE2	0.443
1	L:190:ARG:CD	L:250:SER:HA	0.443
1	I:265:GLN:OE1	L:232:TRP:CE2	0.443
1	O:59:DG:C2'	O:60:DT:H71	0.443
1	C:41:ARG:HH21	E:229:TRP:NE1	0.443

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	E:81:PHE:O	E:83:GLY:N	0.443
1	E:236:ASP:N	E:236:ASP:OD1	0.443
1	J:37:TYR:N	J:45:VAL:O	0.443
1	B:37:HIS:O	B:476:VAL:HG22	0.442
1	B:487:ARG:CZ	B:724:MET:HE1	0.442
1	B:526:GLU:HB3	B:714:VAL:HG21	0.442
1	D:242:MET:HE1	D:301:THR:CB	0.442
1	G:219:PHE:CD2	K:128:LEU:HD12	0.442
1	J:50:ILE:HD13	O:35:DT:H5"	0.442
1	J:138:LYS:HB3	J:138:LYS:HE2	0.442
1	G:63:LYS:NZ	L:323:THR:OG1	0.442
1	A:68:LYS:HG3	A:70:ASP:OD1	0.441
1	A:187:HIS:C	A:187:HIS:ND1	0.441
1	F:23:ASP:HB3	F:32:PHE:HB3	0.441
1	I:291:LEU:HA	I:291:LEU:HD23	0.441
1	J:12:PHE:CZ	J:17:PRO:HB3	0.441
1	I:95:LYS:NZ	I:762:ALA:O	0.441
1	J:168:GLY:O	J:172:PHE:CB	0.441
1	A:570:GLU:HA	A:570:GLU:OE2	0.440
1	B:192:TYR:CE1	B:196:ARG:HD3	0.440
1	H:34:SER:HA	H:37:ILE:HD12	0.440
1	H:78:LEU:HA	H:78:LEU:HD13	0.440
1	I:262:ILE:HA	L:232:TRP:CD1	0.440

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:279:ARG:NH1	I:293:LYS:HB2	0.440
1	I:917:LYS:HD3	O:5:DT:H5'	0.440
1	K:155:LEU:HA	K:159:GLY:HA2	0.440
1	I:265:GLN:NE2	L:171:GLY:HA2	0.440
1	P:44:DT:H4'	P:45:DT:C5'	0.440
1	B:33:ASP:C	B:33:ASP:OD1	0.440
1	C:20:HIS:HA	C:100:ASN:OD1	0.439
1	E:92:ASN:H	E:93:PRO:HD3	0.439
1	H:120:ARG:NE	H:128:VAL:HG12	0.439
1	J:169:PRO:HG2	K:194:PHE:CD1	0.439
1	P:34:DG:H2''	P:35:DA:N7	0.439
1	A:196:GLU:N	A:196:GLU:OE1	0.439
1	A:536:MET:HB3	A:536:MET:HE3	0.438
1	H:59:VAL:HG22	H:61:ASN:H	0.438
1	J:43:MET:HE2	J:75:ARG:HD2	0.438
1	J:193:ASN:O	J:196:GLU:HG2	0.438
1	L:221:PRO:HG2	L:223:ILE:HG12	0.438
1	L:272:GLY:HA2	L:394:VAL:O	0.438
1	L:424:LEU:O	L:428:ILE:HG12	0.438
1	M:1:ASP:C	M:3:MET:H	0.438
1	D:56:ASP:OD1	D:57:GLY:N	0.438
1	D:244:PHE:O	D:246:GLN:N	0.438
1	J:171:ASP:OD1	J:172:PHE:N	0.438
1	A:472:ARG:HG2	A:473:GLU:N	0.437

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:351:GLN:O	B:417:ILE:HG12	0.437
1	B:488:VAL:O	B:488:VAL:HG23	0.437
1	D:197:VAL:HA	D:200:VAL:HG12	0.437
1	E:42:MET:HE3	E:108:ASN:CA	0.437
1	G:233:SER:HA	G:236:LYS:HG2	0.437
1	I:7:TRP:CD1	P:57:DG:H5"	0.437
1	I:773:GLN:HG2	I:783:TYR:CE2	0.437
1	K:135:ARG:O	K:139:CYS:HB3	0.437
1	D:340:GLY:CA	E:146:ARG:HH12	0.437
1	B:425:THR:HG23	I:255:ASN:CG	0.436
1	D:109:GLU:CD	D:109:GLU:H	0.436
1	L:190:ARG:CZ	L:276:LYS:HG3	0.436
1	L:263:LEU:HD13	L:345:GLN:HB2	0.436
1	B:355:PRO:CD	L:273:GLN:HG3	0.436
1	L:296:TYR:CD2	L:307:LYS:HG2	0.436
1	O:60:DT:H2"	O:61:DG:C8	0.436
1	A:187:HIS:ND1	A:187:HIS:O	0.436
1	B:563:ARG:HE	D:59:ARG:HH11	0.436
1	C:115:ASP:OD1	C:116:THR:N	0.436
1	K:125:MET:CG	K:126:GLU:H	0.436
1	D:281:CYS:O	D:284:CYS:N	0.436
1	A:45:GLN:HG3	A:46:VAL:N	0.435
1	B:277:ASP:HB2	I:761:ALA:HB1	0.435
1	E:92:ASN:H	E:93:PRO:CD	0.435

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:249:GLU:CG	G:257:TYR:OH	0.435
1	I:263:ARG:NH2	I:275:GLU:HA	0.435
1	I:281:VAL:CG2	I:289:TYR:H	0.435
1	J:205:LEU:CD2	J:218:LEU:HD13	0.435
1	L:134:LEU:HD22	L:198:GLY:HA2	0.435
1	L:377:GLU:O	L:381:GLN:HG2	0.435
1	D:241:ARG:NH2	E:266:TYR:OH	0.435
1	L:340:ASP:N	L:340:ASP:OD2	0.435
1	C:168:MET:SD	C:179:ILE:HG13	0.434
1	C:225:PHE:HB3	E:101:TYR:HE2	0.434
1	G:237:ARG:O	G:240:ILE:HG12	0.434
1	J:191:VAL:HG21	J:197:LEU:HB3	0.434
1	J:162:SER:OG	P:30:DA:H5'	0.434
1	B:269:THR:OG1	B:270:VAL:N	0.434
1	A:502:ILE:HG23	A:644:LEU:HB2	0.433
1	A:533:LEU:HA	A:533:LEU:HD12	0.433
1	C:31:LEU:O	C:36:LYS:HE3	0.433
1	C:220:LEU:HA	C:220:LEU:HD12	0.433
1	C:269:LEU:O	C:269:LEU:HD12	0.433
1	C:405:LEU:HB2	C:409:ARG:HE	0.433
1	J:8:ASP:HB3	J:39:LEU:HA	0.433
1	J:36:ASP:OD2	J:65:GLN:HG2	0.433
1	B:509:GLU:O	J:182:LYS:HB3	0.433

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	L:39:LEU:HB3	O:20:DT:OP1	0.433
1	L:108:GLU:HB3	L:110:ASP:HB3	0.433
1	B:424:ARG:HH22	L:228:LYS:HG3	0.433
1	B:571:THR:OG1	B:572:GLN:N	0.433
1	A:199:LEU:HA	A:273:LYS:NZ	0.432
1	A:527:THR:O	A:529:LYS:HG2	0.432
1	A:587:GLY:O	A:591:GLN:HG2	0.432
1	B:321:GLY:HA2	B:324:ARG:CD	0.432
1	B:425:THR:OG1	B:426:PRO:HD3	0.432
1	E:237:GLN:O	E:241:LEU:HD12	0.432
1	J:34:VAL:HG13	K:129:GLU:HG3	0.432
1	J:129:ALA:O	K:84:LYS:HE2	0.432
1	K:169:ARG:HD3	K:187:PHE:HB3	0.432
1	L:266:VAL:HB	L:345:GLN:NE2	0.432
1	D:263:MET:O	D:265:HIS:N	0.432
1	I:36:ASN:ND2	P:55:DT:O4'	0.432
1	A:472:ARG:NH2	O:48:DA:OP2	0.432
1	A:46:VAL:HG22	A:48:GLU:H	0.431
1	B:304:HIS:C	B:305:LEU:HD22	0.431
1	E:19:PRO:HG3	E:63:HIS:CE1	0.431
1	I:974:ASP:HB3	I:978:PHE:CE2	0.431
1	J:8:ASP:OD2	J:39:LEU:HD23	0.431
1	K:136:VAL:HG12	K:151:SER:HA	0.431
1	L:144:TYR:HB2	L:164:ILE:HG22	0.431

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:122:ASP:O	G:185:GLN:NE2	0.431
1	L:112:HIS:CG	L:112:HIS:O	0.431
1	A:717:LEU:HA	A:717:LEU:HD23	0.430
1	B:216:LYS:HE3	B:304:HIS:O	0.430
1	B:360:GLY:HA3	L:252:GLY:HA2	0.430
1	C:234:VAL:CA	C:263:ARG:HD3	0.430
1	D:281:CYS:HB2	D:302:LEU:HD21	0.430
1	I:282:VAL:HG13	P:36:DT:N3	0.430
1	K:154:LEU:HA	K:164:LEU:HD11	0.430
1	L:212:LEU:HD23	L:214:SER:N	0.430
1	G:63:LYS:CA	L:325:PHE:HB3	0.430
1	N:127:SER:C	N:129:ALA:H	0.430
1	B:192:TYR:OH	P:44:DT:OP1	0.430
1	A:470:LEU:HA	A:470:LEU:HD12	0.429
1	A:551:HIS:HB2	A:558:ILE:HD11	0.429
1	A:569:LYS:HG3	K:184:ARG:NH2	0.429
1	A:640:LEU:O	A:644:LEU:HG	0.429
1	B:329:PHE:HZ	B:379:LEU:HB2	0.429
1	B:462:SER:O	B:464:LEU:HD23	0.429
1	B:18:TYR:HE1	B:737:SER:HB2	0.429
1	D:30:LYS:HD2	D:30:LYS:O	0.429
1	D:242:MET:HE1	D:301:THR:HB	0.429
1	D:355:ASN:HD22	D:374:GLY:HA3	0.429
1	I:54:HIS:HB3	P:53:DT:H3	0.429

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:20:ILE:HG13	J:21:HIS:N	0.429
1	J:162:SER:HA	P:29:DA:N3	0.429
1	L:299:CYS:HB3	L:304:CYS:SG	0.429
1	L:325:PHE:CG	L:326:PRO:HD2	0.429
1	P:40:DC:H1'	P:41:DA:N7	0.429
1	K:7:ARG:NH2	K:26:ASP:OD1	0.429
1	C:402:GLU:N	C:402:GLU:OE1	0.429
1	B:265:THR:HG21	I:110:LEU:HB2	0.428
1	C:73:LEU:HD23	C:79:TRP:CZ2	0.428
1	E:232:LEU:HA	E:232:LEU:HD12	0.428
1	G:218:LYS:HB3	J:154:ALA:HB1	0.428
1	O:2:DC:H6	O:2:DC:H5''	0.428
1	G:258:ARG:NH2	G:260:THR:OG1	0.428
1	A:452:ARG:NH1	A:479:ASP:OD1	0.428
1	B:632:ILE:HA	B:632:ILE:HD12	0.427
1	H:2:THR:HG23	H:4:GLN:HG3	0.427
1	H:12:SER:O	H:15:GLN:HG2	0.427
1	I:296:GLN:HB2	K:76:VAL:HG21	0.427
1	J:7:VAL:HG22	J:25:ILE:HD12	0.427
1	L:256:SER:O	L:269:GLU:HB3	0.427
1	C:237:MET:SD	C:263:ARG:NH2	0.427
1	D:267:ASP:OD1	D:268:GLY:N	0.427
1	I:733:LEU:HB3	I:734:GLU:H	0.427



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:266:LEU:HD21	B:394:PHE:CZ	0.426
1	B:355:PRO:HG3	L:271:LEU:N	0.426
1	F:16:LYS:NZ	F:20:LEU:HD11	0.426
1	J:160:PRO:HG3	P:28:DC:H4'	0.426
1	K:143:VAL:O	K:146:VAL:HB	0.426
1	K:157:THR:HB	K:164:LEU:HD21	0.426
1	L:267:LYS:HA	L:267:LYS:HD2	0.426
1	D:15:ASP:O	D:17:SER:N	0.426
1	D:258:LYS:NZ	H:140:ASN:HD21	0.426
1	I:959:ARG:HH11	I:970:ARG:HH21	0.426
1	A:579:TYR:HB3	A:606:PHE:HB2	0.425
1	B:355:PRO:HA	L:270:ASN:CB	0.425
1	C:51:GLN:HG2	C:91:LEU:HD21	0.425
1	F:50:ASN:O	F:54:GLU:HG2	0.425
1	I:123:PHE:HD1	I:127:ARG:HB2	0.425
1	I:164:GLU:HG3	I:168:ARG:HH21	0.425
1	I:91:ARG:HH22	I:861:ASP:HA	0.425
1	J:37:TYR:HB3	J:46:GLU:HA	0.425
1	K:137:THR:O	K:141:THR:HB	0.425
1	N:81:THR:O	N:83:VAL:HG13	0.425
1	I:763:THR:O	P:53:DT:H4'	0.425
1	B:638:GLU:OE2	B:641:ARG:NH2	0.425
1	A:697:GLU:N	A:697:GLU:OE2	0.425
1	B:162:ASP:C	B:162:ASP:OD1	0.425

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:357:PHE:HD2	B:404:ALA:HA	0.424
1	B:674:TYR:CB	B:724:MET:HE2	0.424
1	D:306:PRO:HA	D:309:ALA:HB3	0.424
1	D:369:LEU:HD11	E:180:VAL:HG12	0.424
1	G:211:ARG:HB2	J:61:ARG:NH2	0.424
1	G:241:VAL:HG23	G:263:MET:CE	0.424
1	J:80:ILE:O	J:81:GLU:CD	0.424
1	L:89:ALA:HB1	L:197:LYS:HG2	0.424
1	L:230:ARG:HD3	L:233:PHE:HB3	0.424
1	B:369:ARG:HH12	L:280:PHE:CB	0.424
1	P:44:DT:H4'	P:45:DT:H5'	0.424
1	I:251:GLN:NE2	I:280:ARG:HH22	0.424
1	K:149:THR:O	K:153:THR:OG1	0.424
1	G:32:ARG:NH2	N:82:TYR:OH	0.424
1	A:580:ILE:HD11	A:589:ARG:HE	0.423
1	B:3:LEU:HA	B:3:LEU:HD12	0.423
1	B:8:LEU:HA	B:8:LEU:HD12	0.423
1	B:358:LEU:HB3	B:372:LEU:HD11	0.423
1	C:217:LEU:HA	C:217:LEU:HD12	0.423
1	C:366:LEU:HA	C:366:LEU:HD13	0.423
1	E:252:ARG:HB3	E:261:LEU:HD22	0.423
1	F:34:ILE:HD11	F:43:PHE:HB3	0.423
1	G:236:LYS:HG3	G:236:LYS:O	0.423
1	I:35:LEU:HB2	P:54:DC:C5	0.423

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:106:THR:HG22	I:754:LYS:HE3	0.423
1	K:160:SER:O	K:164:LEU:HD23	0.423
1	J:37:TYR:O	J:45:VAL:N	0.423
1	A:78:VAL:HG12	A:84:ILE:HG12	0.422
1	A:276:MET:HB2	A:279:GLU:CG	0.422
1	A:562:ALA:HB3	A:568:LEU:HD13	0.422
1	B:304:HIS:HA	P:43:DA:H2	0.422
1	B:591:GLY:N	D:197:VAL:HG21	0.422
1	G:112:PHE:CD1	G:126:CYS:HB2	0.422
1	H:115:GLN:O	H:119:ARG:HG3	0.422
1	I:57:THR:O	I:61:ARG:HG3	0.422
1	I:188:ILE:HD11	I:208:MET:HE1	0.422
1	J:17:PRO:HA	J:20:ILE:HG12	0.422
1	J:42:GLU:O	J:75:ARG:HB2	0.422
1	K:13:VAL:C	K:15:LYS:H	0.422
1	L:265:GLU:HG3	L:269:GLU:OE1	0.422
1	L:299:CYS:SG	L:323:THR:HG21	0.422
1	M:57:LEU:HA	M:57:LEU:HD23	0.422
1	A:704:SER:N	A:708:GLU:OE2	0.422
1	I:147:PRO:O	I:149:LEU:N	0.422
1	A:581:TYR:HD1	K:184:ARG:HH11	0.422
1	A:608:SER:O	A:610:VAL:HG23	0.422
1	B:390:ASP:N	B:390:ASP:OD1	0.422
1	A:347:SER:O	A:351:VAL:HG23	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:517:GLU:HG3	A:713:LEU:HD22	0.421
1	A:607:ILE:HG22	A:608:SER:H	0.421
1	B:749:THR:HA	B:752:ARG:NE	0.421
1	C:169:LYS:O	C:178:CYS:HB3	0.421
1	G:39:ARG:CZ	M:89:SER:HB3	0.421
1	G:98:MET:SD	G:115:SER:HA	0.421
1	B:641:ARG:NH1	G:169:ASN:CG	0.421
1	J:17:PRO:HB2	J:177:PRO:HA	0.421
1	K:17:VAL:HG13	K:19:ASN:H	0.421
1	L:42:LEU:HD13	L:67:ILE:HG12	0.421
1	B:293:ARG:NH1	L:430:ARG:O	0.421
1	K:5:SER:OG	K:27:VAL:O	0.421
1	A:563:ASP:CG	A:564:ASN:N	0.420
1	B:353:SER:HB2	L:273:GLN:CG	0.420
1	B:517:ILE:HG22	B:552:TRP:CD1	0.420
1	G:222:LYS:HA	K:152:GLN:CG	0.420
1	I:205:LEU:HB3	I:247:ILE:HG12	0.420
1	L:28:ARG:HD2	L:28:ARG:N	0.420
1	L:54:THR:HA	O:20:DT:C7	0.420
1	L:279:TYR:CB	L:410:MET:HE1	0.420
1	N:159:ALA:HB1	N:205:PHE:HE1	0.420
1	O:41:DG:H2''	O:42:DA:C8	0.420
1	B:601:ARG:HB2	B:601:ARG:HE	0.420
1	C:274:SER:OG	E:53:ARG:NE	0.420

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:38:VAL:O	A:40:SER:N	0.420
1	A:284:CYS:O	A:287:LEU:N	0.420
1	A:584:THR:HA	K:185:ARG:CD	0.419
1	B:359:SER:O	B:363:GLN:HG3	0.419
1	B:429:ALA:HA	L:227:TYR:CE1	0.419
1	B:445:LYS:O	B:449:GLU:HG3	0.419
1	D:222:LEU:HA	D:222:LEU:HD23	0.419
1	G:66:PRO:O	G:67:LYS:HG3	0.419
1	G:85:GLN:HG2	O:34:DT:O4	0.419
1	G:218:LYS:HZZ	K:137:THR:HG21	0.419
1	B:339:TYR:HD2	B:361:LEU:O	0.419
1	A:387:SER:OG	B:755:GLN:O	0.419
1	B:341:LYS:O	B:344:LEU:N	0.419
1	A:39:PRO:HA	A:285:ILE:HA	0.418
1	A:178:GLU:C	A:178:GLU:CD	0.418
1	A:528:LYS:HD3	A:528:LYS:O	0.418
1	B:135:HIS:CD2	P:45:DT:H2'	0.418
1	B:320:PRO:HG3	B:371:PRO:HG3	0.418
1	B:393:ASP:HB2	I:114:LEU:HB3	0.418
1	B:423:ASP:HB3	I:284:GLU:O	0.418
1	B:629:GLN:HG3	P:35:DA:N1	0.418
1	C:318:LEU:HD12	C:319:TYR:N	0.418
1	H:104:GLU:O	H:108:VAL:HG12	0.418
1	I:88:LEU:HA	I:91:ARG:HD2	0.418

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:64:SER:O	J:67:ILE:HG22	0.418
1	J:80:ILE:HD12	J:123:TRP:CE3	0.418
1	G:219:PHE:CD2	J:154:ALA:HB3	0.418
1	K:8:GLN:O	K:14:LEU:HD22	0.418
1	B:513:ASP:N	B:513:ASP:OD1	0.418
1	J:10:ARG:HH22	J:152:ILE:CG2	0.418
1	E:4:ASP:N	E:4:ASP:OD1	0.418
1	A:112:HIS:HB2	C:293:GLU:OE2	0.417
1	B:423:ASP:HA	I:288:HIS:CB	0.417
1	C:96:ILE:O	C:100:ASN:HB2	0.417
1	C:286:GLN:HG2	C:286:GLN:O	0.417
1	C:317:MET:HE1	C:325:VAL:HG13	0.417
1	E:6:ASP:HB3	E:156:GLU:O	0.417
1	J:10:ARG:CD	J:11:GLU:OE2	0.417
1	J:80:ILE:CD1	J:123:TRP:CZ3	0.417
1	J:125:PRO:CG	K:80:GLN:HA	0.417
1	P:41:DA:H1'	P:42:DC:C5	0.417
1	N:215:THR:OG1	N:216:VAL:N	0.417
1	N:17:VAL:O	N:18:ASP:OD1	0.417
1	B:369:ARG:HD3	B:369:ARG:N	0.416
1	C:78:ILE:HD11	C:97:PHE:CZ	0.416
1	C:134:TYR:HA	C:137:GLU:OE2	0.416
1	C:233:SER:O	C:263:ARG:HD3	0.416
1	G:213:LYS:HA	G:216:GLN:HE21	0.416

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	H:63:ILE:HG23	H:119:ARG:NH2	0.416
1	I:295:ILE:HB	K:82:ALA:N	0.416
1	N:112:PHE:CZ	N:116:ILE:HD11	0.416
1	N:178:ARG:O	N:222:LYS:HD2	0.416
1	F:32:PHE:HZ	F:52:LEU:HD11	0.416
1	G:175:TRP:NE1	P:32:DA:OP2	0.416
1	K:70:LEU:N	K:96:THR:O	0.416
1	A:40:SER:HB2	A:121:TYR:CZ	0.415
1	A:453:ARG:NH1	A:457:ILE:HD11	0.415
1	B:256:LEU:HD22	B:337:LEU:CD1	0.415
1	B:353:SER:HA	B:354:PRO:HD3	0.415
1	F:4:LEU:CD1	G:270:TYR:OH	0.415
1	J:36:ASP:HB3	J:46:GLU:HB2	0.415
1	J:120:ARG:HA	J:120:ARG:HD3	0.415
1	J:154:ALA:HB2	K:130:GLN:CD	0.415
1	A:517:GLU:OE1	A:706:LYS:NZ	0.415
1	A:102:ALA:HA	A:326:LYS:HE2	0.414
1	A:589:ARG:O	A:592:ILE:HG22	0.414
1	B:448:PHE:CD1	B:454:VAL:HG11	0.414
1	B:558:LEU:HD21	I:234:LEU:HD11	0.414
1	C:242:LEU:H	C:242:LEU:HD12	0.414
1	G:56:THR:HG22	L:363:ALA:HB1	0.414
1	H:24:LEU:H	H:24:LEU:HD12	0.414

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:39:LEU:HD12	P:53:DT:C2'	0.414
1	J:150:LEU:HA	J:151:ALA:HA	0.414
1	L:421:GLY:HA3	M:96:LEU:HD21	0.414
1	A:551:HIS:NE2	A:658:PHE:HE2	0.414
1	A:675:LYS:O	A:678:ARG:HG3	0.413
1	B:84:ILE:HA	B:84:ILE:HD13	0.413
1	B:321:GLY:HA2	B:324:ARG:HD2	0.413
1	G:11:ALA:HA	G:15:GLU:HG3	0.413
1	G:118:MET:HE1	G:125:THR:H	0.413
1	L:267:LYS:HG2	L:345:GLN:HE22	0.413
1	G:11:ALA:O	M:5:LEU:HD11	0.413
1	O:56:DG:H2''	O:57:DG:H8	0.413
1	L:141:CYS:N	L:192:PRO:O	0.413
1	A:185:ILE:HG21	A:268:VAL:HG11	0.412
1	B:309:VAL:HG22	B:406:LEU:HD23	0.412
1	E:218:PRO:HG2	E:219:GLN:OE1	0.412
1	K:12:PRO:O	L:317:ARG:HG2	0.412
1	A:195:ARG:NH1	A:198:ARG:HE	0.412
1	L:279:TYR:CB	L:391:ARG:HH21	0.412
1	A:312:PRO:HG2	B:735:GLY:HA3	0.411
1	A:380:MET:C	A:380:MET:SD	0.411
1	A:569:LYS:HG2	K:169:ARG:HH11	0.411
1	B:350:VAL:HG13	B:421:PHE:HD2	0.411
1	B:388:ILE:HA	B:388:ILE:HD12	0.411



Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:154:ALA:HB2	K:130:GLN:OE1	0.411
1	K:161:LEU:HA	K:164:LEU:HB2	0.411
1	L:251:GLY:N	L:275:ASP:HB2	0.411
1	B:422:ASP:HB3	B:423:ASP:H	0.411
1	D:166:THR:O	D:166:THR:OG1	0.411
1	K:45:ARG:NH2	L:238:GLN:OE1	0.411
1	B:409:THR:O	B:409:THR:HG22	0.410
1	B:442:LEU:HA	B:442:LEU:HD13	0.410
1	B:592:ARG:HA	B:592:ARG:HD2	0.410
1	C:34:LEU:HD23	C:38:TRP:HE1	0.410
1	D:340:GLY:HA3	E:146:ARG:NH1	0.410
1	H:45:ALA:C	H:47:MET:H	0.410
1	I:222:MET:HE1	I:232:TYR:HE2	0.410
1	O:57:DG:H2''	O:58:DA:C8	0.410
1	J:181:ALA:O	J:185:ARG:N	0.410
1	A:35:GLN:HG3	A:168:LEU:HD11	0.409
1	A:35:GLN:N	A:291:LEU:HD13	0.409
1	A:320:GLN:HE22	A:345:GLY:HA3	0.409
1	A:368:ALA:O	A:371:VAL:HG22	0.409
1	A:531:ILE:HA	A:534:TYR:CE2	0.409
1	B:236:ALA:HB1	B:239:ILE:CG1	0.409
1	B:466:ILE:HA	B:466:ILE:HD13	0.409
1	D:263:MET:HE1	D:298:CYS:CB	0.409
1	E:68:ARG:HD2	E:118:LEU:HD22	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:47:ARG:HG3	J:79:LEU:CD1	0.409
1	L:12:GLN:HG3	L:15:TRP:CE3	0.409
1	L:261:LYS:HA	L:261:LYS:HD3	0.409
1	N:209:GLU:HB2	N:211:HIS:CE1	0.409
1	O:52:DC:H2"	O:53:DA:H8	0.409
1	N:224:THR:OG1	N:225:ASP:N	0.409
1	A:519:TYR:OH	A:666:ASP:OD1	0.409
1	C:59:LYS:NZ	E:241:LEU:O	0.409
1	I:244:ASN:C	I:244:ASN:OD1	0.409
1	A:480:LEU:HD11	A:484:ILE:HD12	0.408
1	B:170:LEU:HD13	B:175:TYR:CD2	0.408
1	C:14:LEU:HD23	C:17:LEU:HD23	0.408
1	C:106:LEU:HG	E:100:LYS:HD3	0.408
1	E:202:LEU:HA	E:205:GLN:HG3	0.408
1	H:59:VAL:CG2	H:61:ASN:H	0.408
1	J:35:GLY:HA3	J:150:LEU:HG	0.408
1	L:39:LEU:HD21	O:20:DT:H6	0.408
1	L:53:ALA:HB1	L:98:PHE:CE1	0.408
1	N:65:VAL:HG13	N:67:THR:HG23	0.408
1	A:561:PHE:HE1	A:611:GLY:H	0.408
1	I:288:HIS:HE1	I:289:TYR:O	0.408
1	A:199:LEU:CA	A:273:LYS:NZ	0.407
1	B:223:LYS:CA	B:223:LYS:HE2	0.407
1	B:256:LEU:HD13	B:341:LYS:HD3	0.407

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:346:VAL:HG23	L:220:ASN:ND2	0.407
1	C:106:LEU:N	E:100:LYS:HD3	0.407
1	H:116:GLU:CD	H:120:ARG:HD2	0.407
1	I:296:GLN:C	K:44:LEU:HD22	0.407
1	I:856:TYR:OH	I:932:VAL:HB	0.407
1	B:355:PRO:HA	L:270:ASN:CG	0.407
1	G:172:HIS:C	G:174:GLN:H	0.407
1	K:130:GLN:HB3	K:131:ASP:H	0.407
1	B:342:TRP:O	L:220:ASN:ND2	0.407
1	M:95:GLY:H	N:142:ASN:HD21	0.407
1	H:120:ARG:O	H:122:TYR:N	0.407
1	B:541:SER:OG	P:36:DT:OP1	0.407
1	A:34:PRO:O	A:291:LEU:HD22	0.406
1	A:327:MET:CE	A:464:LEU:HD13	0.406
1	A:613:THR:HG21	A:615:PHE:CZ	0.406
1	B:216:LYS:C	B:216:LYS:HD3	0.406
1	B:263:LEU:HD12	B:264:GLU:N	0.406
1	B:411:ALA:HB2	L:270:ASN:CA	0.406
1	B:424:ARG:HA	I:251:GLN:CG	0.406
1	B:480:THR:HG23	B:758:GLN:HE21	0.406
1	C:234:VAL:HB	C:262:ARG:HD3	0.406
1	D:56:ASP:HB3	D:61:MET:CE	0.406
1	G:89:LYS:C	G:91:VAL:H	0.406

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:193:VAL:HG22	G:194:TRP:HD1	0.406
1	B:277:ASP:OD2	I:95:LYS:HB3	0.406
1	J:11:GLU:H	J:16:LEU:HD23	0.406
1	K:137:THR:HB	K:151:SER:CB	0.406
1	N:205:PHE:O	N:209:GLU:HG2	0.406
1	I:222:MET:CE	I:232:TYR:HE2	0.406
1	H:120:ARG:H	H:120:ARG:HG3	0.406
1	L:259:ASN:HB3	L:260:TRP:H	0.406
1	C:272:ASN:N	C:272:ASN:OD1	0.406
1	B:76:THR:HG23	B:78:PRO:HD2	0.405
1	C:283:THR:HG22	C:285:HIS:N	0.405
1	C:317:MET:HB3	C:317:MET:HE3	0.405
1	I:793:GLN:O	I:796:ILE:HG22	0.405
1	J:80:ILE:C	J:81:GLU:CD	0.405
1	J:110:THR:HA	J:113:THR:HG22	0.405
1	J:9:MET:CE	K:135:ARG:CB	0.405
1	B:345:ARG:NE	L:221:PRO:HD2	0.405
1	B:112:ARG:CD	P:44:DT:H3'	0.405
1	A:109:ARG:HH21	A:492:ASN:HB2	0.405
1	D:263:MET:HG2	D:264:ALA:H	0.405
1	G:211:ARG:NH2	P:28:DC:OP1	0.405
1	B:381:SER:O	B:385:THR:CB	0.405
1	I:156:SER:O	I:157:SER:OG	0.405
1	K:144:LYS:HA	O:41:DG:OP2	0.405

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	O:47:DG:H8	O:47:DG:O5'	0.405
1	A:354:ALA:HA	A:437:LEU:HD23	0.404
1	D:291:LEU:HB2	D:292:PRO:HD3	0.404
1	H:98:LYS:C	H:99:MET:HE2	0.404
1	J:116:PHE:HB3	J:117:PRO:HD2	0.404
1	L:265:GLU:HA	L:269:GLU:CD	0.404
1	L:429:ARG:C	L:429:ARG:HD2	0.404
1	B:343:ARG:NE	L:190:ARG:HH11	0.404
1	B:352:GLU:N	B:352:GLU:OE1	0.404
1	B:302:ASP:CB	B:380:ARG:HE	0.404
1	F:38:ASP:OD2	F:40:THR:N	0.404
1	I:139:ARG:O	I:141:ASN:N	0.404
1	B:739:LEU:HG	B:743:GLN:HB2	0.403
1	C:383:ARG:HB3	C:384:LEU:HD12	0.403
1	G:224:LYS:HB2	G:224:LYS:HE2	0.403
1	G:249:GLU:C	G:257:TYR:CE1	0.403
1	H:139:TYR:O	H:142:LEU:HG	0.403
1	J:53:LEU:HD22	J:80:ILE:HD13	0.403
1	L:17:ILE:HD11	L:96:MET:HE1	0.403
1	L:79:THR:HB	L:97:THR:HB	0.403
1	L:321:CYS:HB2	L:323:THR:CG2	0.403
1	B:317:GLU:HG3	L:430:ARG:CZ	0.403
1	M:11:ASN:HA	M:25:PHE:CD1	0.403
1	O:42:DA:C2	O:43:DG:C5	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:508:PHE:CD2	P:33:DA:H2''	0.403
1	B:499:ASN:H	B:519:ASN:HD21	0.403
1	I:273:LEU:CD2	I:273:LEU:N	0.403
1	N:17:VAL:O	N:20:VAL:N	0.403
1	B:128:LYS:HD2	B:392:ALA:HA	0.402
1	B:364:ARG:HA	B:364:ARG:NE	0.402
1	B:514:ILE:HA	B:517:ILE:HD13	0.402
1	G:98:MET:HG2	L:346:TRP:NE1	0.402
1	G:246:TYR:CE2	G:248:PRO:HD3	0.402
1	B:262:ASN:HA	I:110:LEU:HD21	0.402
1	I:222:MET:HA	I:222:MET:HE2	0.402
1	I:279:ARG:HA	I:279:ARG:HD3	0.402
1	K:76:VAL:HG12	K:78:ASP:H	0.402
1	L:190:ARG:HE	L:275:ASP:CB	0.402
1	C:372:ASP:OD1	C:373:GLN:N	0.402
1	N:63:GLN:HA	N:100:ALA:O	0.402
1	A:719:ALA:HA	K:174:LEU:HB2	0.401
1	B:115:LEU:HD12	B:192:TYR:CD2	0.401
1	B:393:ASP:HA	I:114:LEU:HD22	0.401
1	B:487:ARG:NH1	B:724:MET:HE1	0.401
1	C:281:GLY:O	C:360:LEU:HD21	0.401
1	D:48:MET:HB3	D:48:MET:HE3	0.401
1	D:89:ASN:OD1	D:228:PRO:HG3	0.401

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	G:241:VAL:CG2	G:263:MET:HE3	0.401
1	I:102:SER:HA	I:757:GLN:OE1	0.401
1	I:91:ARG:NH2	I:861:ASP:HA	0.401
1	A:493:TRP:HE3	A:685:TYR:HE2	0.401
1	D:261:PHE:CD1	D:261:PHE:N	0.401
1	I:802:GLN:HB3	I:802:GLN:HE21	0.401
1	K:172:LEU:C	K:174:LEU:H	0.401
1	E:52:ASN:HB2	E:55:ASN:OD1	0.401
1	G:31:LYS:O	G:34:ARG:HB2	0.401
1	G:49:SER:O	G:52:ALA:N	0.401
1	G:69:ILE:O	G:71:THR:N	0.401
1	G:123:LEU:O	G:125:THR:N	0.401
1	B:231:VAL:HG21	B:451:PHE:CD1	0.400
1	B:620:MET:HB3	B:620:MET:HE3	0.400
1	B:705:ASN:HA	B:708:LEU:HD13	0.400
1	O:42:DA:H2"	O:43:DG:H8	0.400
1	D:237:CYS:H	E:287:THR:HG21	0.400
1	G:132:ALA:C	G:134:ASP:H	0.400
1	B:393:ASP:O	I:114:LEU:HD13	0.400
1	B:647:ARG:HG3	G:177:ASP:OD2	0.400

### 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
----------	----------	---------	---------	----------

Model ID	Analyzed	Favored	Allowed	Outliers
1	4722	4111	558	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	4194	3175	994	25

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	38	VAL
1	A	65	MET
1	A	187	HIS
1	A	398	ASP
1	B	42	MET
1	B	136	SER
1	B	257	ASP
1	B	266	LEU
1	B	444	ILE
1	B	501	GLN
1	B	546	GLU
1	B	708	LEU
1	C	41	ARG
1	C	359	MET
1	C	424	MET
1	D	295	CYS



Model ID	Chain	Residue ID	Residue type
1	D	315	LEU
1	G	48	TYR
1	G	59	MET
1	G	100	PHE
1	H	30	SER
1	I	247	ILE
1	J	69	MET
1	J	123	TRP
1	L	299	CYS

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

#### 3DEM volume

Validation for this section is under development.

#### Crosslinking-MS

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 lab](#) contributed model validation metrics and software packages.*

*Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB 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.*