Full wwPDB EM Validation Report (i)

Mar 3, 2024 – 08:56 AM EST

PDB ID	:	6BZO
EMDB ID	:	EMD-7319
Title	:	Mtb RNAP Holo/RbpA/Fidaxomicin/upstream fork DNA
Authors	:	Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.
Deposited on	:	2017-12-25
Resolution	:	3.38 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

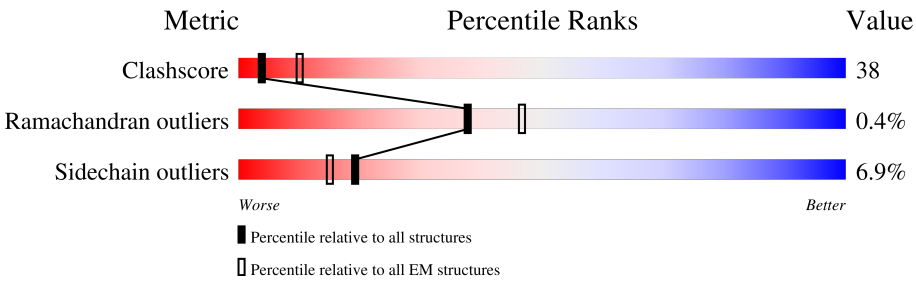
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	35% 28% • 35%
1	B	347	28% 38% • 32%
2	C	1181	43% 46% • 6%
3	D	1324	• 45% 46% • 5%
4	E	110	27% 45% • 25%
5	F	531	28% 29% • 39%
6	J	111	48% 38% 11% •
7	O	31	26% 74%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	P	26	38% 62%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 27336 atoms, of which 74 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	226	1724	1085	297	339	3	0	0
1	B	237	1775	1120	304	348	3	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1111	8556	5361	1504	1652	39	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879
C	1186	GLY	-	expression tag	UNP V9Z879
C	1187	ALA	-	expression tag	UNP V9Z879

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1263	9857	6175	1791	1850	41	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A0A045J9E2
D	1318	HIS	-	expression tag	UNP A0A045J9E2
D	1319	HIS	-	expression tag	UNP A0A045J9E2
D	1320	HIS	-	expression tag	UNP A0A045J9E2
D	1321	HIS	-	expression tag	UNP A0A045J9E2
D	1322	HIS	-	expression tag	UNP A0A045J9E2
D	1323	HIS	-	expression tag	UNP A0A045J9E2
D	1324	HIS	-	expression tag	UNP A0A045J9E2

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	83	649	414	108	127	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	326	2588	1617	467	495	9	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP A0A045HD00
F	-1	PRO	-	expression tag	UNP A0A045HD00
F	0	HIS	-	expression tag	UNP A0A045HD00

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	107	872	539	162	168	3	0	0

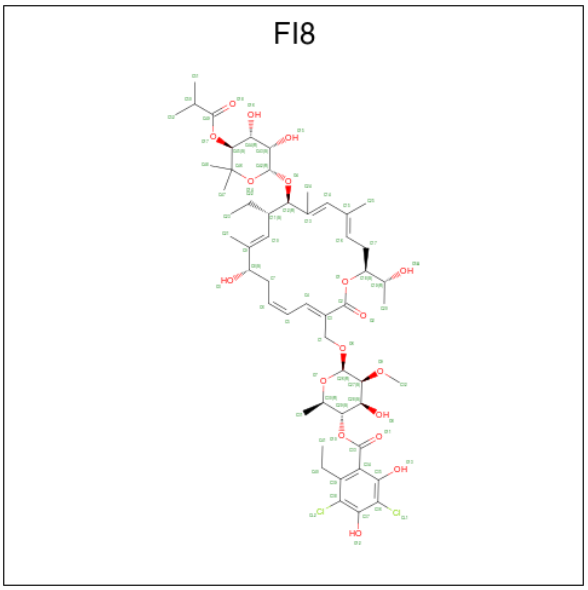
- Molecule 7 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	O	31	634	305	114	185	30	0	0

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	P	26	526	254	94	153	25	0	0

- Molecule 9 is Fidaxomicin (three-letter code: FI8) (formula: $C_{52}H_{74}Cl_2O_{18}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	H	O	
9	C	1	146	52	2	74	18	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	D	2	2	2	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	D	1	1	1	0

- Molecule 12 is water.

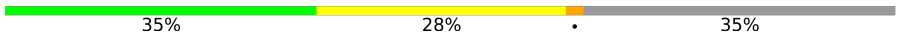
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
12	C	2	2	2	0
			Total	O	
12	D	4	4	4	0

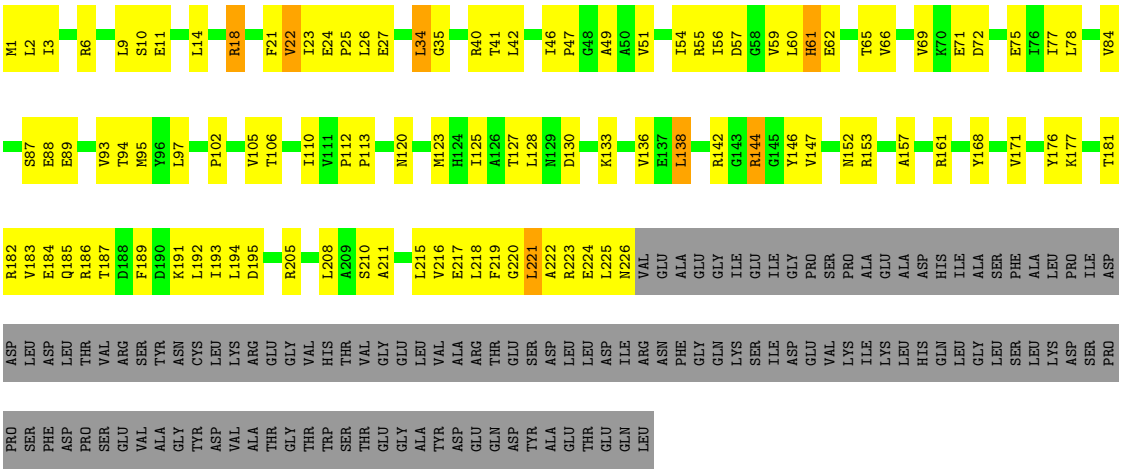
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase subunit alpha

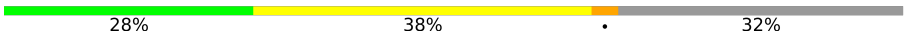
Chain A:

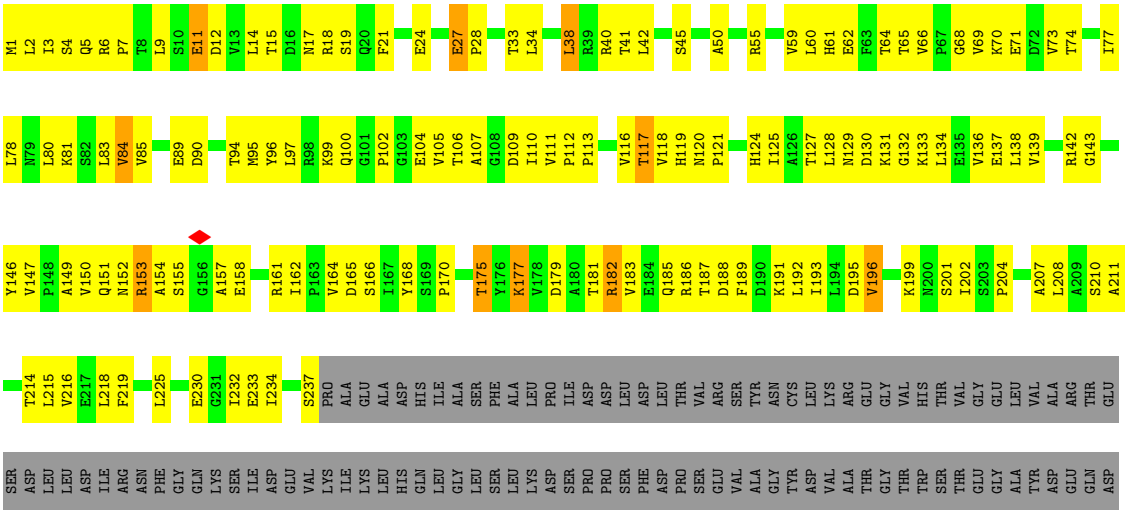


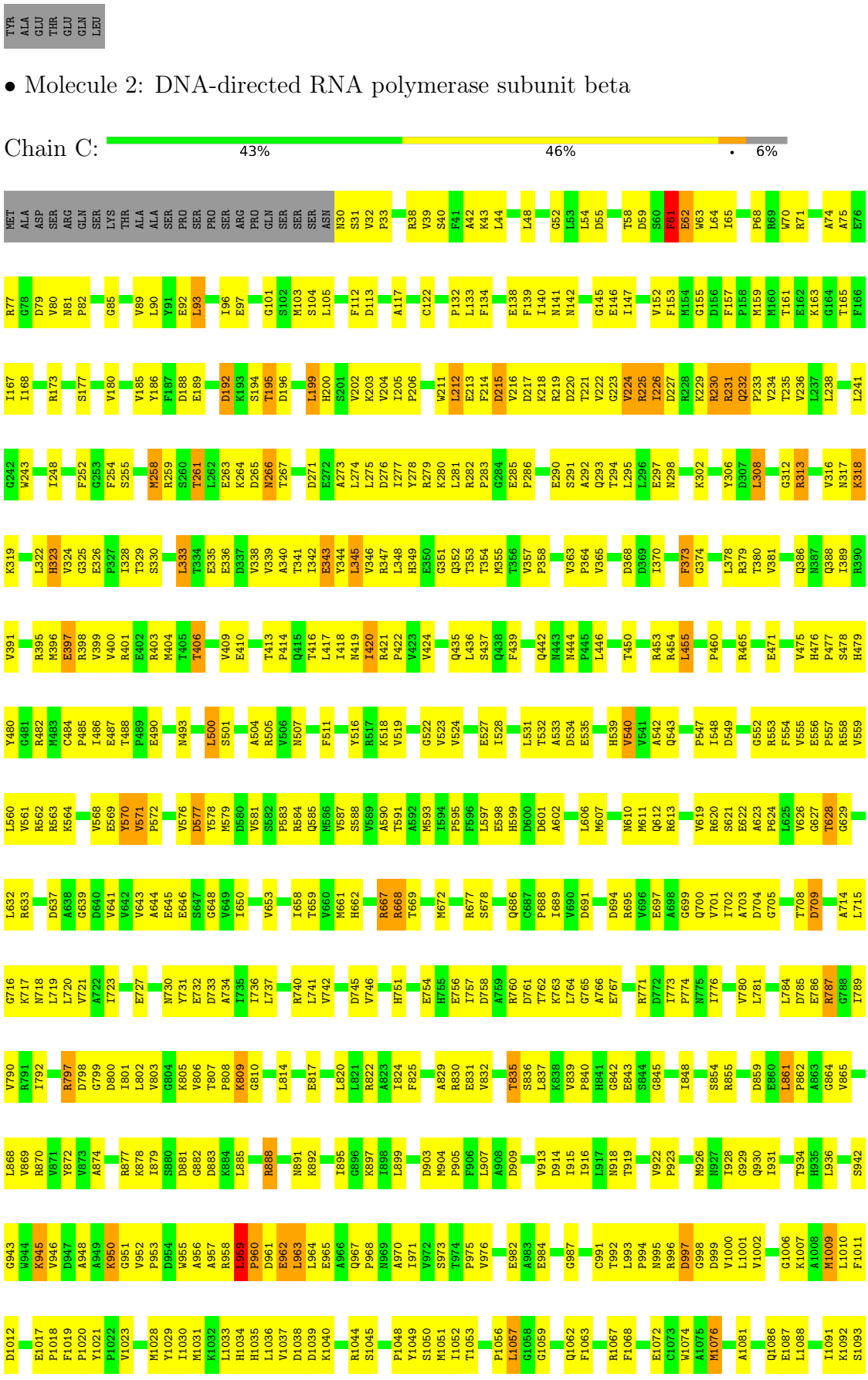


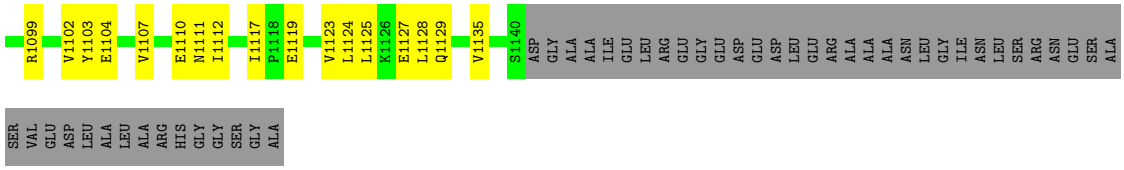
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



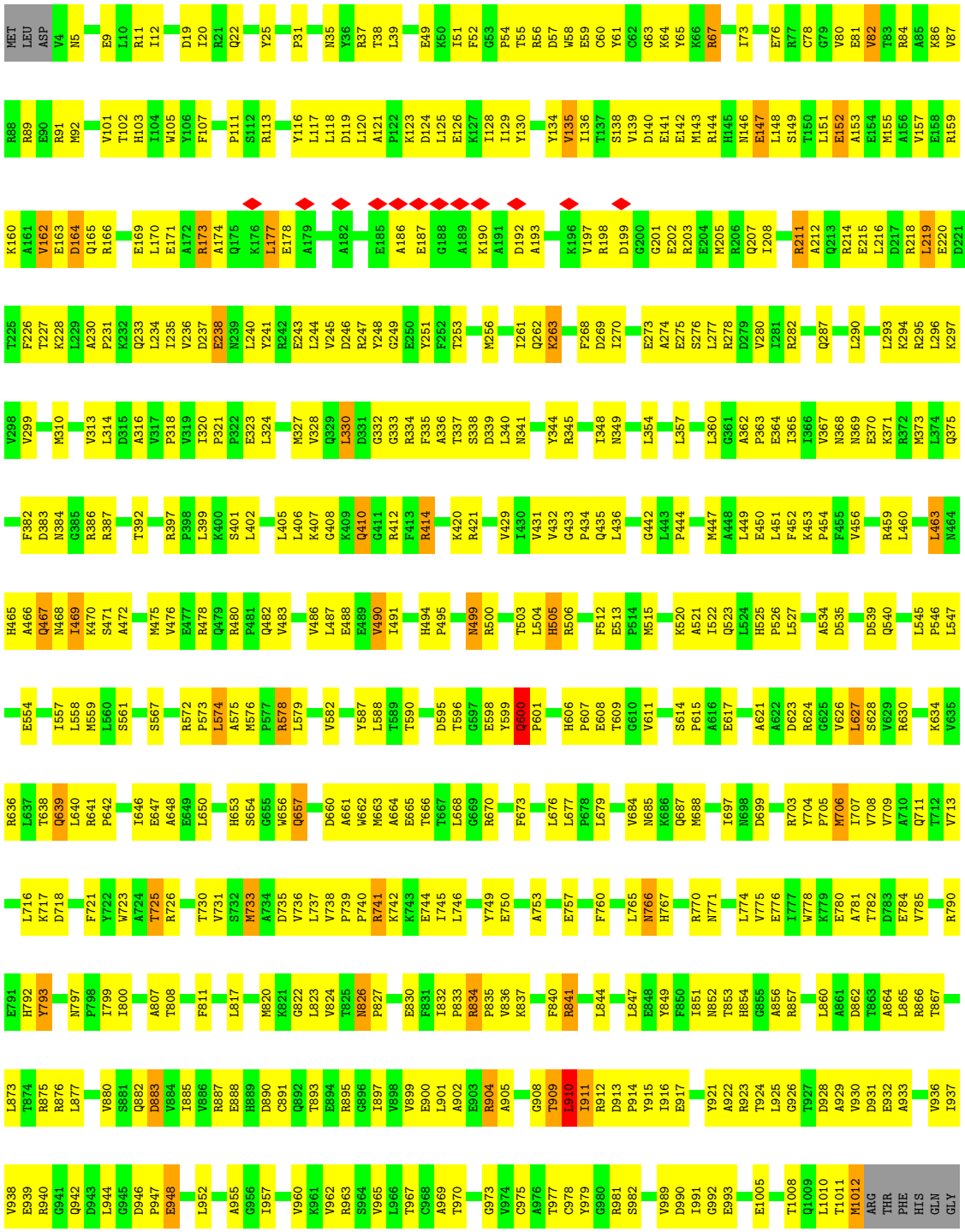


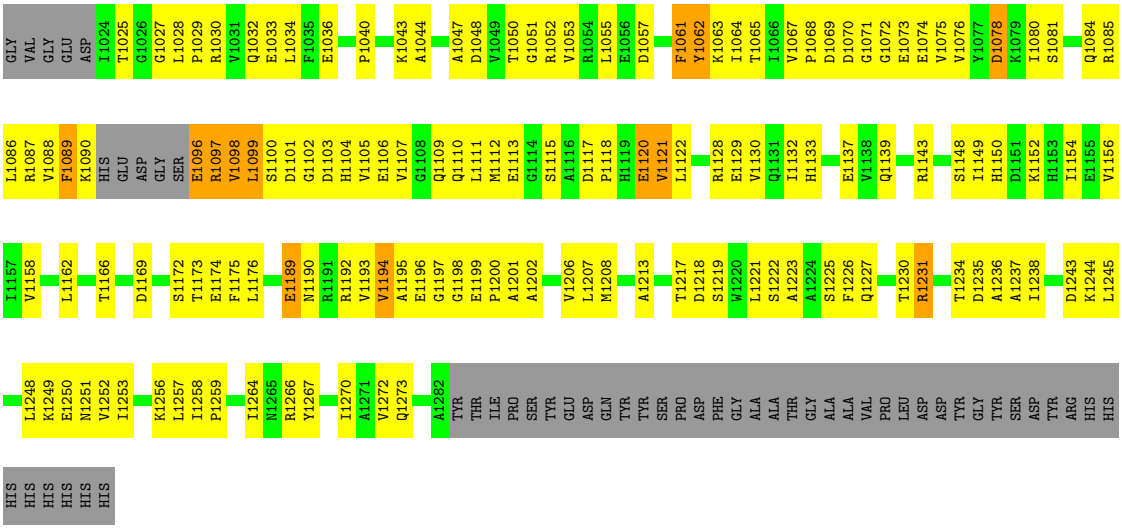

TYR ALA GLU THR GLU GLN LEU
• Molecule 2: DNA-directed RNA polymerase subunit beta
Chain C:
43%
46%
6%



• Molecule 3: DNA-directed RNA polymerase subunit beta'

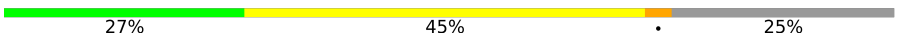
Chain D:

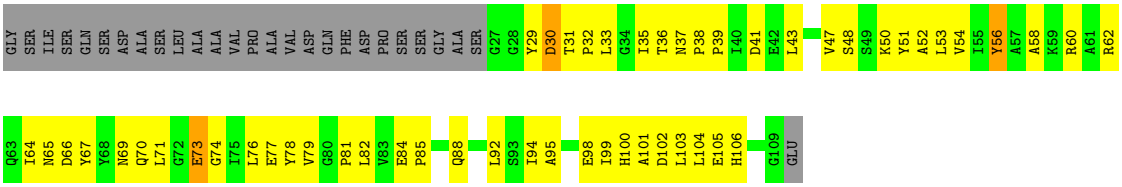




• Molecule 4: DNA-directed RNA polymerase subunit omega

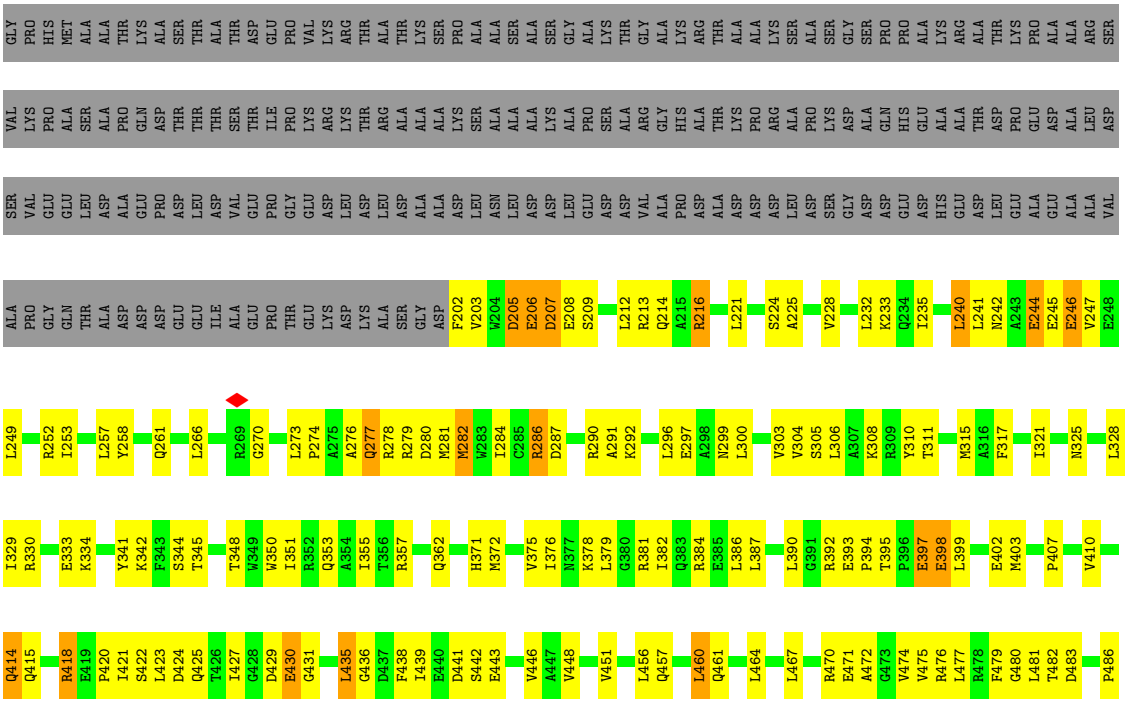
Chain E:





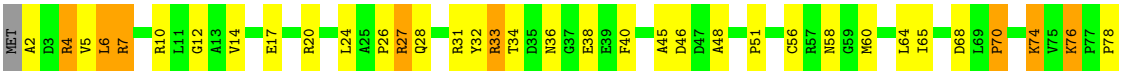
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



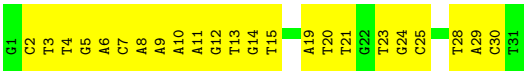
• Molecule 6: RNA polymerase-binding protein RbpA

Chain J:



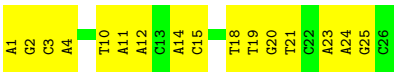
• Molecule 7: DNA (32-MER)

Chain O:



• Molecule 8: DNA (26-MER)

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173509	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	6.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.278	Depositor
Minimum map value	-1.545	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.347	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FI8, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.24	0/1750	0.44	0/2380
1	B	0.24	0/1802	0.43	0/2454
2	C	0.24	0/8714	0.42	0/11824
3	D	0.25	0/10021	0.41	0/13549
4	E	0.24	0/662	0.39	0/901
5	F	0.23	0/2622	0.37	0/3538
6	J	0.35	0/888	0.45	0/1199
7	O	0.49	0/710	0.95	0/1095
8	P	0.54	0/589	0.93	0/906
All	All	0.27	0/27758	0.46	0/37846

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
3	D	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	61	PHE	Peptide
2	C	958	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	C	960	PRO	Peptide
3	D	1194	VAL	Peptide
3	D	600	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1724	0	1768	120	0
1	B	1775	0	1809	174	0
2	C	8556	0	8459	741	0
3	D	9857	0	9920	774	0
4	E	649	0	645	54	0
5	F	2588	0	2602	222	0
6	J	872	0	852	60	0
7	O	634	0	350	42	0
8	P	526	0	296	37	0
9	C	72	74	0	3	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
12	C	2	0	0	0	0
12	D	4	0	0	3	0
All	All	27262	74	26701	2045	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (2045) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:948:ALA:HB2	2:C:953:PRO:HD3	1.27	1.16
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.33	1.08
2:C:633:ARG:NH1	2:C:637:ASP:OD2	1.87	1.07
2:C:225:ARG:HB2	2:C:231:ARG:HA	1.34	1.06
2:C:960:PRO:HG2	2:C:963:LEU:HD12	1.35	1.04
2:C:959:LEU:HB2	2:C:960:PRO:HD3	1.39	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.40	1.01
3:D:1025:THR:HG21	3:D:1029:PRO:HB2	1.42	1.00
3:D:162:VAL:HG13	3:D:216:LEU:HD22	1.41	1.00
2:C:611:MET:HE1	2:C:892:LYS:HB3	1.42	0.98
2:C:163:LYS:NZ	2:C:639:GLY:O	1.97	0.98
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	1.41	0.98
3:D:750:GLU:OE2	3:D:837:LYS:NZ	1.96	0.97
1:B:183:VAL:HA	1:B:188:ASP:H	1.28	0.97
1:B:104:GLU:HG2	1:B:127:THR:HG22	1.46	0.97
2:C:221:THR:HB	2:C:261:THR:HG22	1.46	0.96
3:D:676:LEU:HD23	3:D:716:LEU:HD23	1.47	0.96
2:C:152:VAL:HG21	2:C:418:ILE:HD12	1.46	0.96
2:C:233:PRO:HB3	5:F:203:VAL:HG11	1.43	0.96
3:D:823:LEU:HD23	3:D:835:PRO:HB3	1.48	0.95
2:C:61:PHE:O	2:C:63:TRP:N	1.98	0.95
2:C:222:VAL:O	2:C:231:ARG:NH1	1.99	0.95
2:C:1135:VAL:HG12	3:D:12:ILE:HG12	1.49	0.94
2:C:220:ASP:HB3	2:C:221:THR:HG22	1.48	0.94
3:D:1089:PHE:CE2	3:D:1103:ASP:OD2	2.20	0.94
1:A:186:ARG:HD2	1:B:147:VAL:HG23	1.49	0.94
2:C:258:MET:HA	2:C:261:THR:HG23	1.49	0.94
2:C:767:GLU:OE1	2:C:805:LYS:NZ	1.99	0.94
3:D:89:ARG:NH1	12:D:1502:HOH:O	1.99	0.94
2:C:825:PHE:HD2	5:F:527:LEU:HD12	1.33	0.93
2:C:1038:ASP:OD1	3:D:520:LYS:NZ	2.01	0.93
2:C:659:THR:HG22	2:C:669:THR:HG22	1.51	0.93
1:B:106:THR:N	1:B:109:ASP:OD2	2.01	0.92
2:C:736:ILE:HD11	2:C:916:ILE:HD12	1.51	0.92
3:D:902:ALA:HB2	3:D:912:ARG:HA	1.50	0.92
2:C:741:LEU:HD22	2:C:746:VAL:HG11	1.51	0.91
1:A:34:LEU:HD11	1:B:218:LEU:HD21	1.50	0.91
2:C:215:ASP:HB2	2:C:223:GLY:HA3	1.53	0.91
2:C:648:GLY:O	2:C:695:ARG:NH1	2.02	0.91
2:C:413:THR:HG22	2:C:416:THR:HG23	1.51	0.91
5:F:502:ARG:NH2	7:O:2:DC:OP2	2.04	0.90
2:C:994:PRO:HB3	2:C:999:ASP:H	1.35	0.90
3:D:1087:ARG:NH1	3:D:1110:GLN:OE1	2.04	0.90
3:D:1067:VAL:HA	3:D:1074:GLU:HG2	1.50	0.90
6:J:27:ARG:HB3	6:J:27:ARG:HH11	1.34	0.90
3:D:1122:LEU:HB2	3:D:1130:VAL:HG21	1.54	0.89
7:O:19:DA:H1'	7:O:20:DT:H5'	1.53	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1127:GLU:OE2	3:D:412:ARG:NH1	2.05	0.89
1:A:40:ARG:HH12	2:C:903:ASP:HB3	1.39	0.88
2:C:400:VAL:HG13	2:C:417:LEU:HB3	1.56	0.88
2:C:230:ARG:NH1	2:C:230:ARG:HA	1.88	0.88
1:B:94:THR:HG22	1:B:139:VAL:HG22	1.53	0.88
2:C:581:VAL:HG22	2:C:585:GLN:HE21	1.38	0.87
3:D:432:VAL:HG22	3:D:434:PRO:HD3	1.56	0.87
2:C:267:THR:HG21	2:C:273:ALA:HB2	1.56	0.87
3:D:1087:ARG:HG3	3:D:1088:VAL:H	1.40	0.86
1:A:40:ARG:NH1	2:C:903:ASP:HB3	1.90	0.86
2:C:1102:VAL:HG23	2:C:1112:ILE:HG23	1.54	0.86
3:D:1128:ARG:HH22	3:D:1132:ILE:HD11	1.41	0.86
5:F:206:GLU:OE1	5:F:207:ASP:N	2.08	0.86
3:D:1128:ARG:HH12	3:D:1132:ILE:HG12	1.39	0.86
2:C:764:LEU:HD22	2:C:810:GLY:HA2	1.56	0.86
3:D:1063:LYS:HZ1	3:D:1078:ASP:HA	1.36	0.86
2:C:221:THR:CB	2:C:261:THR:HG22	2.05	0.85
5:F:386:LEU:HD22	5:F:394:PRO:HG3	1.55	0.85
2:C:229:LYS:HD3	2:C:281:LEU:HA	1.59	0.85
3:D:1097:ARG:HH12	3:D:1100:SER:CB	1.89	0.85
8:P:11:DA:H2"	8:P:12:DA:H5'	1.58	0.85
3:D:323:GLU:OE2	12:D:1501:HOH:O	1.93	0.84
1:B:202:ILE:HD13	1:B:207:ALA:HB2	1.59	0.84
2:C:319:LYS:NZ	2:C:368:ASP:OD1	2.09	0.84
2:C:877:ARG:HH11	2:C:1036:LEU:HD12	1.41	0.84
5:F:502:ARG:NH1	5:F:505:GLN:OE1	2.10	0.84
2:C:285:GLU:HG3	2:C:286:PRO:HD2	1.59	0.84
2:C:233:PRO:HG3	5:F:203:VAL:HG21	1.57	0.84
2:C:959:LEU:HD13	2:C:960:PRO:HD2	1.60	0.84
5:F:240:LEU:HD23	5:F:241:LEU:H	1.43	0.83
3:D:737:LEU:HB2	3:D:793:TYR:HE1	1.43	0.83
2:C:43:LYS:HE3	2:C:959:LEU:HA	1.61	0.83
2:C:231:ARG:HD2	5:F:205:ASP:HB3	1.60	0.83
5:F:306:LEU:HD11	5:F:348:THR:HG23	1.58	0.83
2:C:339:VAL:HA	2:C:342:ILE:HD12	1.58	0.82
5:F:303:VAL:HG22	5:F:351:ILE:HD13	1.62	0.82
2:C:1111:ASN:ND2	4:E:66:ASP:OD1	2.12	0.82
3:D:173:ARG:NH1	3:D:173:ARG:HB2	1.94	0.81
3:D:970:THR:OG1	3:D:973:GLY:O	1.97	0.81
3:D:337:THR:OG1	3:D:341:ASN:ND2	2.14	0.81
3:D:1063:LYS:NZ	3:D:1078:ASP:HA	1.95	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:490:GLU:OE2	2:C:607:MET:HG2	1.81	0.81
3:D:162:VAL:CG1	3:D:216:LEU:HD22	2.11	0.81
3:D:1099:LEU:O	3:D:1099:LEU:HD23	1.79	0.81
3:D:1250:GLU:OE1	3:D:1250:GLU:N	2.14	0.81
2:C:336:GLU:O	2:C:339:VAL:HG22	1.79	0.80
3:D:579:LEU:HD22	3:D:808:THR:HB	1.63	0.80
3:D:1052:ARG:HG2	3:D:1067:VAL:HB	1.63	0.80
5:F:282:MET:O	5:F:286:ARG:HG2	1.80	0.80
3:D:1128:ARG:NH1	3:D:1132:ILE:HG12	1.96	0.80
2:C:487:GLU:OE2	2:C:613:ARG:NH2	2.15	0.80
2:C:909:ASP:OD2	2:C:1001:LEU:HD11	1.81	0.80
2:C:254:PHE:H	2:C:255:SER:HB2	1.44	0.80
3:D:908:GLY:O	3:D:910:LEU:N	2.14	0.80
2:C:213:GLU:OE1	2:C:213:GLU:N	2.15	0.80
1:A:177:LYS:HE2	1:A:193:ILE:HD11	1.64	0.80
1:B:154:ALA:HB3	1:B:158:GLU:HG2	1.62	0.80
3:D:952:LEU:HB3	3:D:957:ILE:HD11	1.64	0.79
3:D:742:LYS:HE2	3:D:746:LEU:HD11	1.65	0.79
3:D:177:LEU:CD1	3:D:201:GLY:HA3	2.12	0.79
5:F:286:ARG:HB2	5:F:290:ARG:HH12	1.45	0.79
5:F:299:ASN:HB2	5:F:328:LEU:HD11	1.63	0.79
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.64	0.79
2:C:945:LYS:N	2:C:991:CYS:SG	2.53	0.79
2:C:347:ARG:NH2	2:C:352:GLN:OE1	2.16	0.79
1:B:182:ARG:NH2	3:D:488:GLU:OE2	2.15	0.79
3:D:1128:ARG:HH12	3:D:1132:ILE:CG1	1.95	0.79
2:C:258:MET:HA	2:C:261:THR:CG2	2.12	0.79
2:C:767:GLU:HG2	2:C:807:THR:HG22	1.64	0.79
3:D:993:GLU:OE2	4:E:51:TYR:OH	2.00	0.79
3:D:144:ARG:NH1	3:D:227:THR:O	2.15	0.79
3:D:911:ILE:H	3:D:911:ILE:HD13	1.48	0.79
2:C:831:GLU:OE1	2:C:831:GLU:N	2.16	0.78
2:C:233:PRO:HG2	2:C:236:VAL:HG23	1.63	0.78
2:C:1045:SER:OG	3:D:453:LYS:NZ	2.16	0.78
3:D:1061:PHE:HB3	3:D:1081:SER:HA	1.65	0.78
2:C:453:ARG:NH2	2:C:501:SER:O	2.15	0.78
3:D:159:ARG:NH2	3:D:220:GLU:OE1	2.15	0.78
2:C:961:ASP:OD1	2:C:962:GLU:N	2.16	0.78
2:C:817:GLU:OE1	2:C:817:GLU:N	2.14	0.78
3:D:190:LYS:NZ	3:D:192:ASP:HB3	1.99	0.78
3:D:909:THR:C	3:D:910:LEU:HG	2.03	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:435:GLN:HG3	2:C:460:PRO:HD3	1.66	0.78
2:C:543:GLN:HE22	3:D:847:LEU:HD13	1.47	0.78
2:C:222:VAL:HG21	2:C:234:VAL:H	1.48	0.78
3:D:64:LYS:NZ	3:D:76:GLU:OE2	2.14	0.78
6:J:106:ARG:O	6:J:108:ARG:NH2	2.17	0.78
3:D:657:GLN:NE2	3:D:660:ASP:O	2.16	0.77
2:C:809:LYS:HB2	2:C:809:LYS:HZ2	1.48	0.77
5:F:439:ILE:HD13	6:J:6:LEU:HD13	1.65	0.77
2:C:797:ARG:O	2:C:839:VAL:HG11	1.85	0.77
2:C:598:GLU:OE1	2:C:598:GLU:N	2.14	0.77
2:C:967:GLN:HG3	2:C:968:PRO:HD2	1.66	0.77
5:F:303:VAL:HG23	5:F:328:LEU:HD12	1.67	0.77
4:E:70:GLN:NE2	4:E:73:GLU:OE2	2.19	0.76
3:D:486:VAL:O	3:D:490:VAL:HG13	1.86	0.76
6:J:27:ARG:HB3	6:J:27:ARG:NH1	1.99	0.76
2:C:254:PHE:CG	2:C:255:SER:HB2	2.20	0.76
3:D:362:ALA:HB1	3:D:363:PRO:HD2	1.66	0.76
3:D:198:ARG:O	3:D:202:GLU:HG2	1.86	0.76
4:E:56:TYR:OH	4:E:104:LEU:HG	1.85	0.76
3:D:641:ARG:HA	3:D:657:GLN:HG2	1.67	0.76
5:F:498:VAL:HB	5:F:502:ARG:HB3	1.67	0.75
7:O:12:DG:H2'	7:O:13:DT:H71	1.68	0.75
3:D:928:ASP:OD1	3:D:940:ARG:N	2.17	0.75
2:C:275:LEU:O	2:C:279:ARG:HG3	1.87	0.75
3:D:1231:ARG:HA	3:D:1234:THR:HG22	1.69	0.75
2:C:809:LYS:HB2	2:C:809:LYS:NZ	2.00	0.75
3:D:736:VAL:HG22	3:D:799:ILE:CD1	2.17	0.75
2:C:252:PHE:HB3	2:C:258:MET:SD	2.27	0.75
3:D:187:GLU:OE1	3:D:187:GLU:N	2.20	0.75
3:D:365:ILE:H	3:D:365:ILE:HD12	1.52	0.75
2:C:233:PRO:HG2	2:C:236:VAL:CG2	2.17	0.75
8:P:11:DA:H4'	8:P:12:DA:OP1	1.85	0.74
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.69	0.74
2:C:231:ARG:CD	5:F:205:ASP:HB3	2.17	0.74
2:C:540:VAL:HG13	2:C:561:VAL:CG2	2.17	0.74
3:D:1128:ARG:HH12	3:D:1132:ILE:CD1	1.99	0.74
3:D:500:ARG:HD2	3:D:534:ALA:HB2	1.69	0.74
6:J:4:ARG:HD3	6:J:5:VAL:H	1.51	0.74
1:B:84:VAL:HB	1:B:199:LYS:HD3	1.70	0.74
2:C:206:PRO:HG3	2:C:306:TYR:CE1	2.23	0.74
1:B:107:ALA:HB3	1:B:121:PRO:HA	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:VAL:HG12	2:C:214:PHE:HB2	1.68	0.74
3:D:263:LYS:HB2	3:D:263:LYS:NZ	2.03	0.74
3:D:31:PRO:HG3	3:D:349:ASN:OD1	1.88	0.73
2:C:803:VAL:O	2:C:836:SER:OG	2.05	0.73
2:C:861:LEU:HB2	2:C:862:PRO:HD2	1.68	0.73
2:C:948:ALA:HB2	2:C:953:PRO:CD	2.15	0.73
3:D:895:ARG:NH1	3:D:967:THR:HB	2.03	0.73
3:D:397:ARG:NH2	5:F:422:SER:OG	2.21	0.73
5:F:216:ARG:HB2	5:F:216:ARG:HH11	1.53	0.73
2:C:259:ARG:O	2:C:263:GLU:HG2	1.88	0.73
3:D:190:LYS:HZ2	3:D:192:ASP:HB3	1.53	0.73
3:D:614:SER:HB2	3:D:615:PRO:HD2	1.69	0.73
1:A:223:ARG:HD2	1:A:224:GLU:H	1.53	0.73
3:D:939:GLU:OE1	3:D:939:GLU:N	2.20	0.73
3:D:908:GLY:C	3:D:910:LEU:H	1.91	0.73
1:B:182:ARG:HA	1:B:182:ARG:HE	1.54	0.73
2:C:277:ILE:O	2:C:281:LEU:HD13	1.88	0.73
3:D:670:ARG:NH1	3:D:685:ASN:OD1	2.20	0.73
3:D:913:ASP:OD1	3:D:914:PRO:HD2	1.89	0.73
3:D:92:MET:HG2	3:D:321:PRO:HD3	1.70	0.72
6:J:89:ARG:HG2	6:J:94:LEU:HD21	1.71	0.72
2:C:177:SER:HB2	2:C:378:LEU:HD11	1.71	0.72
2:C:577:ASP:N	2:C:577:ASP:OD1	2.19	0.72
6:J:51:PRO:O	6:J:64:LEU:HD11	1.88	0.72
2:C:52:GLY:O	2:C:55:ASP:N	2.21	0.72
2:C:540:VAL:HG13	2:C:561:VAL:HG21	1.71	0.72
1:B:128:LEU:HD23	1:B:132:GLY:O	1.88	0.72
2:C:563:ARG:HB2	2:C:563:ARG:HH11	1.54	0.72
3:D:293:LEU:HD22	3:D:1176:LEU:HG	1.70	0.72
3:D:606:HIS:HB2	3:D:607:PRO:HD2	1.71	0.72
2:C:340:ALA:O	2:C:343:GLU:HG3	1.89	0.72
3:D:1193:VAL:HG23	3:D:1199:GLU:HG2	1.70	0.72
5:F:397:GLU:OE1	5:F:398:GLU:N	2.22	0.72
2:C:230:ARG:HA	2:C:230:ARG:HH11	1.51	0.72
2:C:231:ARG:O	2:C:232:GLN:NE2	2.22	0.72
2:C:435:GLN:HE21	2:C:460:PRO:HG3	1.54	0.72
2:C:325:GLY:O	2:C:326:GLU:HG2	1.89	0.72
3:D:1097:ARG:HH12	3:D:1100:SER:HB2	1.54	0.72
2:C:229:LYS:HZ2	2:C:281:LEU:HG	1.53	0.72
2:C:727:GLU:HG2	3:D:725:THR:HG21	1.72	0.72
1:A:9:LEU:HD12	1:A:23:ILE:HD11	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:GLY:HA2	2:C:231:ARG:NH1	2.04	0.71
2:C:1039:ASP:HB2	2:C:1040:LYS:HE3	1.72	0.71
5:F:299:ASN:CB	5:F:328:LEU:HD11	2.20	0.71
5:F:489:LEU:CD1	8:P:20:DG:H2'	2.19	0.71
2:C:959:LEU:HB2	2:C:960:PRO:CD	2.17	0.71
5:F:425:GLN:OE1	5:F:425:GLN:N	2.24	0.71
1:A:186:ARG:HG3	1:B:150:VAL:HB	1.72	0.71
1:B:24:GLU:HG2	1:B:191:LYS:HG3	1.71	0.71
2:C:264:LYS:O	5:F:202:PHE:N	2.24	0.71
2:C:563:ARG:NH1	2:C:569:GLU:OE1	2.23	0.71
5:F:390:LEU:HG	5:F:392:ARG:HG3	1.72	0.71
3:D:54:PRO:HG3	3:D:81:GLU:O	1.90	0.71
3:D:471:SER:HB3	5:F:525:ASP:OD2	1.89	0.71
5:F:446:VAL:HG12	5:F:448:VAL:HG12	1.73	0.71
2:C:787:ARG:HD3	2:C:787:ARG:O	1.91	0.71
3:D:1190:ASN:HD21	3:D:1201:ALA:HB3	1.55	0.71
7:O:19:DA:H4'	7:O:20:DT:OP1	1.89	0.71
1:B:28:PRO:HD3	1:B:189:PHE:HD1	1.55	0.71
1:B:183:VAL:HA	1:B:188:ASP:N	2.05	0.71
5:F:427:ILE:HD11	6:J:2:ALA:N	2.06	0.71
2:C:959:LEU:HD23	2:C:984:GLU:OE1	1.90	0.70
3:D:1198:GLY:O	3:D:1200:PRO:HD3	1.91	0.70
1:B:154:ALA:CB	1:B:158:GLU:HG2	2.20	0.70
3:D:152:GLU:OE2	3:D:153:ALA:N	2.23	0.70
3:D:386:ARG:NH2	3:D:1230:THR:HG21	2.07	0.70
3:D:699:ASP:OD1	3:D:703:ARG:HD3	1.90	0.70
3:D:67:ARG:HA	3:D:67:ARG:NE	2.05	0.70
5:F:507:GLU:O	5:F:511:MET:HG2	1.90	0.70
2:C:63:TRP:O	2:C:85:GLY:N	2.22	0.70
3:D:125:LEU:HD11	3:D:261:ILE:HD11	1.74	0.70
5:F:278:ARG:NH2	5:F:282:MET:SD	2.65	0.70
3:D:460:LEU:HD11	3:D:472:ALA:HB1	1.72	0.70
3:D:1096:GLU:HA	3:D:1096:GLU:OE1	1.91	0.70
5:F:489:LEU:N	8:P:20:DG:OP2	2.15	0.70
2:C:254:PHE:N	2:C:255:SER:HB2	2.06	0.70
3:D:826:ASN:OD1	3:D:832:ILE:HD11	1.92	0.70
3:D:847:LEU:O	3:D:851:ILE:HG12	1.91	0.70
5:F:357:ARG:NH1	7:O:23:DT:H72	2.07	0.70
3:D:269:ASP:O	3:D:273:GLU:HG2	1.92	0.69
2:C:215:ASP:CB	2:C:223:GLY:HA3	2.22	0.69
3:D:237:ASP:OD2	3:D:240:LEU:HB2	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HH12	3:D:623:ASP:HB3	1.58	0.69
3:D:642:PRO:HG2	3:D:647:GLU:HB3	1.74	0.69
3:D:1162:LEU:HD21	3:D:1207:LEU:HD23	1.74	0.69
1:A:177:LYS:CE	1:A:193:ILE:HD11	2.23	0.69
3:D:1010:LEU:HD23	3:D:1028:LEU:HA	1.74	0.69
7:O:5:DG:H2'	7:O:6:DA:C8	2.26	0.69
1:B:15:THR:HG23	1:B:18:ARG:HB2	1.74	0.69
2:C:621:SER:O	2:C:709:ASP:HB2	1.93	0.69
3:D:407:LYS:HG2	3:D:408:GLY:H	1.58	0.69
3:D:1084:GLN:HE21	3:D:1112:MET:HB2	1.57	0.69
5:F:252:ARG:NH2	5:F:287:ASP:OD1	2.22	0.69
1:B:60:LEU:HD22	1:B:60:LEU:H	1.58	0.69
3:D:834:ARG:HA	3:D:834:ARG:HE	1.56	0.69
8:P:1:DA:H5"	8:P:1:DA:H8	1.56	0.69
2:C:39:VAL:HG11	2:C:963:LEU:HG	1.73	0.69
2:C:225:ARG:HB2	2:C:231:ARG:CA	2.19	0.69
8:P:11:DA:H2"	8:P:12:DA:C5'	2.22	0.69
2:C:1044:ARG:HB2	2:C:1063:PHE:HB3	1.74	0.69
2:C:1067:ARG:HA	3:D:421:ARG:HA	1.75	0.69
2:C:229:LYS:CD	2:C:281:LEU:HA	2.23	0.68
3:D:295:ARG:O	3:D:299:VAL:HG23	1.93	0.68
1:B:64:THR:O	1:B:65:THR:OG1	2.07	0.68
3:D:909:THR:HG22	3:D:910:LEU:HG	1.74	0.68
1:B:149:ALA:N	1:B:165:ASP:OD1	2.27	0.68
2:C:959:LEU:HD13	2:C:960:PRO:CD	2.22	0.68
1:A:6:ARG:NH1	1:A:6:ARG:HB3	2.08	0.68
2:C:220:ASP:HB3	2:C:221:THR:CG2	2.21	0.68
3:D:435:GLN:OE1	3:D:435:GLN:N	2.25	0.68
2:C:233:PRO:HB3	5:F:203:VAL:CG1	2.23	0.68
2:C:719:LEU:HD22	2:C:1030:ILE:CD1	2.22	0.68
3:D:926:GLY:O	3:D:940:ARG:NH2	2.27	0.68
2:C:771:ARG:HG2	2:C:781:LEU:HD11	1.75	0.68
3:D:705:PRO:HB2	4:E:41:ASP:OD2	1.93	0.68
2:C:563:ARG:HB2	2:C:563:ARG:NH1	2.07	0.68
2:C:961:ASP:O	2:C:962:GLU:HG3	1.94	0.68
3:D:1070:ASP:N	3:D:1071:GLY:HA2	2.09	0.68
2:C:326:GLU:HB3	2:C:328:ILE:HG23	1.76	0.68
2:C:948:ALA:CB	2:C:953:PRO:HD3	2.16	0.68
3:D:121:ALA:HB3	3:D:124:ASP:OD2	1.94	0.68
3:D:277:LEU:HD11	3:D:295:ARG:NH1	2.09	0.68
3:D:823:LEU:HD23	3:D:835:PRO:CB	2.22	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ARG:NH2	1:B:230:GLU:OE1	2.27	0.68
1:B:81:LYS:NZ	3:D:617:GLU:OE2	2.23	0.68
2:C:338:VAL:O	2:C:342:ILE:HG13	1.94	0.68
2:C:825:PHE:CE2	5:F:524:ARG:HA	2.29	0.68
3:D:749:TYR:CD1	3:D:781:ALA:HB2	2.29	0.68
2:C:230:ARG:O	2:C:231:ARG:HB2	1.94	0.67
2:C:542:ALA:HB2	2:C:576:VAL:CG1	2.24	0.67
2:C:741:LEU:CD2	2:C:746:VAL:HG11	2.24	0.67
3:D:320:ILE:HG13	3:D:321:PRO:HD2	1.76	0.67
3:D:1080:ILE:HG21	3:D:1112:MET:HG3	1.75	0.67
2:C:254:PHE:CD2	2:C:255:SER:HB2	2.29	0.67
3:D:1139:GLN:O	3:D:1143:ARG:HG3	1.94	0.67
5:F:286:ARG:HB2	5:F:290:ARG:NH1	2.09	0.67
2:C:96:ILE:HB	2:C:105:LEU:HB3	1.77	0.67
2:C:343:GLU:O	2:C:346:VAL:HG12	1.94	0.67
1:B:104:GLU:HG2	1:B:127:THR:CG2	2.24	0.67
2:C:584:ARG:HH21	2:C:975:PRO:HB3	1.60	0.67
3:D:163:GLU:OE1	3:D:166:ARG:NH2	2.22	0.67
3:D:737:LEU:HB2	3:D:793:TYR:CE1	2.29	0.67
4:E:43:LEU:HD21	4:E:100:HIS:HB2	1.76	0.67
5:F:441:ASP:OD1	5:F:443:GLU:N	2.24	0.67
2:C:737:LEU:HD11	2:C:895:ILE:HD13	1.76	0.67
2:C:745:ASP:OD1	2:C:878:LYS:HE2	1.95	0.67
5:F:246:GLU:OE1	5:F:247:VAL:N	2.28	0.67
2:C:581:VAL:HG22	2:C:585:GLN:NE2	2.08	0.67
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.76	0.67
3:D:1080:ILE:HG21	3:D:1112:MET:HE3	1.76	0.67
1:A:3:ILE:HD12	1:A:3:ILE:O	1.94	0.67
2:C:785:ASP:OD2	2:C:787:ARG:HD2	1.95	0.67
2:C:967:GLN:CG	2:C:968:PRO:HD2	2.24	0.67
3:D:849:TYR:O	3:D:853:THR:HG23	1.94	0.67
8:P:24:DA:H2'	8:P:25:DG:H8	1.60	0.67
1:A:56:ILE:HB	1:A:59:VAL:CG2	2.24	0.67
1:B:175:THR:HG23	1:B:195:ASP:HB3	1.76	0.67
2:C:233:PRO:CG	5:F:203:VAL:HG21	2.25	0.67
3:D:736:VAL:HG11	3:D:817:LEU:HD22	1.75	0.67
5:F:395:THR:OG1	5:F:398:GLU:HB2	1.94	0.67
3:D:228:LYS:O	3:D:233:GLN:NE2	2.24	0.66
3:D:386:ARG:HH22	3:D:1230:THR:HG21	1.60	0.66
1:A:219:PHE:HE1	1:B:38:LEU:HD22	1.61	0.66
1:B:102:PRO:HB3	1:B:130:ASP:HA	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:GLU:HA	2:C:294:THR:HG23	1.76	0.66
3:D:212:ALA:O	3:D:216:LEU:HG	1.95	0.66
5:F:253:ILE:O	5:F:257:LEU:HD13	1.96	0.66
5:F:281:MET:O	5:F:284:ILE:HG22	1.94	0.66
1:A:176:TYR:HB3	1:A:194:LEU:HD23	1.78	0.66
2:C:950:LYS:HD3	2:C:951:GLY:H	1.59	0.66
2:C:997:ASP:N	2:C:997:ASP:OD1	2.26	0.66
3:D:1173:THR:HG21	3:D:1189:GLU:OE2	1.95	0.66
5:F:303:VAL:CG2	5:F:328:LEU:HD12	2.25	0.66
5:F:489:LEU:HD11	8:P:20:DG:H2'	1.75	0.66
8:P:14:DA:H5'	8:P:14:DA:C8	2.31	0.66
2:C:413:THR:O	2:C:416:THR:OG1	2.13	0.66
3:D:364:GLU:HG3	3:D:368:ASN:OD1	1.95	0.66
5:F:488:THR:OG1	5:F:491:GLU:HB2	1.96	0.66
2:C:192:ASP:OD2	2:C:195:THR:HG23	1.94	0.66
3:D:1043:LYS:HD3	3:D:1044:ALA:N	2.11	0.66
5:F:386:LEU:HD22	5:F:394:PRO:CG	2.23	0.66
2:C:413:THR:HG22	2:C:416:THR:CG2	2.26	0.66
2:C:558:ARG:HH21	2:C:572:PRO:HD3	1.59	0.66
2:C:994:PRO:CB	2:C:998:GLY:HA2	2.26	0.66
3:D:909:THR:O	3:D:910:LEU:HG	1.95	0.66
5:F:446:VAL:CG1	5:F:448:VAL:HG12	2.25	0.66
2:C:825:PHE:CD2	5:F:527:LEU:HD12	2.25	0.66
3:D:155:MET:O	3:D:159:ARG:HG2	1.95	0.66
3:D:201:GLY:O	3:D:205:MET:HG3	1.95	0.66
3:D:447:MET:O	3:D:451:LEU:HD23	1.96	0.66
4:E:105:GLU:OE1	4:E:105:GLU:N	2.25	0.66
2:C:153:PHE:CE2	2:C:155:GLY:HA2	2.31	0.66
2:C:602:ALA:HB3	3:D:856:ALA:CB	2.26	0.66
5:F:228:VAL:O	5:F:232:LEU:HG	1.96	0.66
5:F:257:LEU:HD21	6:J:81:HIS:ND1	2.11	0.66
1:A:21:PHE:CD2	1:A:208:LEU:HD22	2.30	0.66
2:C:180:VAL:HG21	2:C:379:ARG:NH1	2.10	0.66
2:C:757:ILE:HB	2:C:837:LEU:HD22	1.77	0.66
2:C:952:VAL:HG11	2:C:957:ALA:HA	1.78	0.66
3:D:776:GLU:O	3:D:780:GLU:HG2	1.95	0.66
3:D:826:ASN:HB2	3:D:830:GLU:O	1.95	0.66
3:D:946:ASP:HB2	3:D:947:PRO:HD3	1.77	0.66
2:C:861:LEU:HD22	2:C:865:VAL:HG12	1.78	0.65
2:C:186:TYR:CE2	2:C:205:ILE:HD11	2.31	0.65
5:F:261:GLN:HG2	6:J:82:TRP:CZ2	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD13	1:B:7:PRO:HG2	1.78	0.65
1:B:38:LEU:O	1:B:42:LEU:HD13	1.96	0.65
2:C:220:ASP:HB3	2:C:221:THR:HA	1.77	0.65
2:C:960:PRO:HG2	2:C:963:LEU:CD1	2.21	0.65
3:D:749:TYR:HE1	3:D:780:GLU:HB2	1.61	0.65
5:F:317:PHE:CE2	5:F:321:ILE:HD11	2.31	0.65
2:C:771:ARG:HH11	2:C:786:GLU:HA	1.61	0.65
2:C:918:ASN:OD1	2:C:919:THR:N	2.29	0.65
3:D:173:ARG:HB2	3:D:173:ARG:HH11	1.59	0.65
3:D:344:TYR:O	3:D:348:ILE:HG22	1.97	0.65
5:F:516:HIS:ND1	5:F:517:PRO:HD2	2.11	0.65
8:P:24:DA:H2'	8:P:25:DG:C8	2.32	0.65
2:C:524:VAL:HG21	2:C:548:ILE:HD11	1.79	0.65
3:D:1150:HIS:CE1	3:D:1152:LYS:HE3	2.32	0.65
3:D:790:ARG:HB2	3:D:811:PHE:CZ	2.31	0.65
3:D:917:GLU:HA	3:D:921:TYR:CD2	2.31	0.65
3:D:1065:THR:HG23	3:D:1076:VAL:HG22	1.77	0.65
4:E:56:TYR:OH	4:E:104:LEU:O	2.14	0.65
7:O:8:DA:H2"	7:O:9:DA:C8	2.32	0.65
2:C:85:GLY:O	2:C:386:GLN:NE2	2.28	0.65
2:C:152:VAL:HG21	2:C:418:ILE:CD1	2.25	0.65
2:C:357:VAL:CG2	2:C:358:PRO:HD2	2.27	0.65
2:C:610:ASN:OD1	2:C:613:ARG:NH1	2.23	0.65
3:D:595:ASP:OD1	3:D:596:THR:N	2.25	0.65
3:D:885:ILE:HD11	3:D:887:ARG:NH1	2.11	0.65
2:C:790:VAL:HG13	2:C:802:LEU:O	1.97	0.65
3:D:494:HIS:CE1	3:D:545:LEU:HD11	2.31	0.65
3:D:1267:TYR:O	3:D:1270:ILE:HG13	1.96	0.65
6:J:34:THR:OG1	6:J:38:GLU:HB2	1.97	0.65
2:C:232:GLN:HG2	2:C:277:ILE:CD1	2.27	0.65
2:C:442:GLN:O	2:C:678:SER:OG	2.13	0.65
2:C:224:VAL:HG21	2:C:234:VAL:N	2.12	0.64
3:D:84:ARG:HG3	3:D:84:ARG:HH11	1.62	0.64
3:D:314:LEU:HD21	3:D:382:PHE:HE2	1.62	0.64
3:D:923:ARG:HB3	3:D:962:VAL:CG1	2.28	0.64
5:F:306:LEU:CD1	5:F:348:THR:HG23	2.27	0.64
7:O:5:DG:H2"	7:O:6:DA:C5'	2.27	0.64
1:B:28:PRO:HD3	1:B:189:PHE:CD1	2.31	0.64
3:D:662:TRP:CZ3	3:D:664:ALA:HB2	2.33	0.64
1:A:78:LEU:HD13	2:C:620:ARG:HD3	1.78	0.64
1:B:102:PRO:HD3	1:B:131:LYS:H	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:285:GLU:CG	2:C:286:PRO:HD2	2.28	0.64
2:C:786:GLU:OE1	2:C:786:GLU:N	2.30	0.64
3:D:177:LEU:HD12	3:D:201:GLY:HA3	1.80	0.64
3:D:1050:THR:O	3:D:1069:ASP:N	2.23	0.64
7:O:19:DA:C8	7:O:20:DT:H72	2.32	0.64
1:A:40:ARG:HH12	2:C:903:ASP:CB	2.09	0.64
1:A:152:ASN:OD1	1:A:157:ALA:HB3	1.98	0.64
1:B:2:LEU:HD23	1:B:3:ILE:N	2.13	0.64
2:C:760:ARG:HG2	2:C:865:VAL:HG22	1.78	0.64
2:C:774:PRO:HG3	2:C:832:VAL:HG23	1.80	0.64
5:F:249:LEU:O	5:F:253:ILE:HG13	1.97	0.64
8:P:24:DA:H2"	8:P:25:DG:C5'	2.28	0.64
1:B:4:SER:O	1:B:5:GLN:HG2	1.97	0.64
2:C:757:ILE:O	2:C:868:LEU:HD22	1.96	0.64
4:E:73:GLU:OE1	4:E:74:GLY:N	2.31	0.64
5:F:342:LYS:HG2	7:O:30:DC:OP2	1.97	0.64
2:C:622:GLU:O	2:C:714:ALA:HB1	1.96	0.64
3:D:760:PHE:CD1	3:D:770:ARG:HG2	2.33	0.64
3:D:902:ALA:CB	3:D:912:ARG:HA	2.27	0.64
2:C:214:PHE:HE2	2:C:342:ILE:HG12	1.63	0.64
3:D:134:TYR:HE2	3:D:238:GLU:HG3	1.61	0.64
3:D:599:TYR:OH	3:D:608:GLU:OE1	2.09	0.64
5:F:399:LEU:O	5:F:403:MET:N	2.27	0.64
6:J:26:PRO:O	6:J:46:ASP:HB2	1.98	0.64
1:A:183:VAL:HG22	1:A:185:GLN:OE1	1.97	0.64
2:C:202:VAL:CG1	2:C:214:PHE:HB2	2.27	0.64
2:C:357:VAL:HG22	2:C:358:PRO:HD2	1.80	0.64
3:D:940:ARG:NH1	3:D:963:ARG:HH22	1.96	0.64
6:J:24:LEU:HD23	6:J:24:LEU:H	1.63	0.64
3:D:638:THR:O	3:D:639:GLN:NE2	2.31	0.63
3:D:1012:MET:C	3:D:1027:GLY:N	2.52	0.63
1:B:210:SER:O	1:B:214:THR:HG23	1.98	0.63
2:C:399:VAL:O	2:C:403:ARG:HG2	1.98	0.63
2:C:542:ALA:HB2	2:C:576:VAL:HG13	1.80	0.63
2:C:767:GLU:CG	2:C:807:THR:HG22	2.28	0.63
3:D:153:ALA:O	3:D:157:VAL:HG23	1.97	0.63
2:C:737:LEU:CD2	2:C:915:ILE:HG22	2.28	0.63
3:D:721:PHE:O	3:D:725:THR:HG23	1.98	0.63
1:A:6:ARG:HB3	1:A:6:ARG:HH11	1.63	0.63
2:C:363:VAL:CG1	2:C:364:PRO:HD2	2.29	0.63
2:C:396:MET:CE	2:C:418:ILE:HG23	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:413:THR:CG2	2:C:416:THR:HG23	2.28	0.63
3:D:166:ARG:HD3	3:D:216:LEU:HD11	1.81	0.63
1:A:110:ILE:O	1:A:112:PRO:HD3	1.97	0.63
2:C:806:VAL:HG22	2:C:832:VAL:HB	1.80	0.63
3:D:1192:ARG:HG2	3:D:1192:ARG:O	1.98	0.63
3:D:1217:THR:HG22	3:D:1223:ALA:HB2	1.80	0.63
5:F:467:LEU:HD21	5:F:519:ARG:NH1	2.13	0.63
2:C:583:PRO:O	2:C:584:ARG:HG2	1.99	0.63
3:D:1089:PHE:CZ	3:D:1103:ASP:OD2	2.51	0.63
5:F:311:THR:HG21	5:F:317:PHE:HD1	1.64	0.63
5:F:399:LEU:HA	5:F:402:GLU:HB3	1.79	0.63
2:C:950:LYS:HD3	2:C:951:GLY:N	2.13	0.63
5:F:315:MET:CE	5:F:362:GLN:HB2	2.29	0.63
4:E:82:LEU:N	4:E:98:GLU:OE2	2.30	0.62
2:C:697:GLU:OE1	2:C:697:GLU:N	2.32	0.62
3:D:58:TRP:HA	3:D:82:VAL:HG23	1.82	0.62
3:D:219:LEU:O	3:D:222:ILE:HG23	1.99	0.62
5:F:325:ASN:O	5:F:329:ILE:HG13	1.99	0.62
2:C:488:THR:O	2:C:610:ASN:ND2	2.28	0.62
3:D:52:PHE:O	3:D:91:ARG:HD2	1.98	0.62
3:D:73:ILE:HG22	6:J:27:ARG:NH1	2.15	0.62
1:B:152:ASN:ND2	1:B:158:GLU:HG3	2.14	0.62
3:D:642:PRO:HB3	3:D:662:TRP:CD2	2.34	0.62
5:F:317:PHE:HE2	5:F:321:ILE:HD11	1.64	0.62
3:D:888:GLU:OE2	3:D:891:CYS:HA	1.99	0.62
5:F:381:ARG:HD2	5:F:382:ILE:HD12	1.80	0.62
8:P:24:DA:H2"	8:P:25:DG:H5'	1.81	0.62
1:B:41:THR:O	1:B:45:SER:HB3	2.00	0.62
1:B:85:VAL:HG23	1:B:117:THR:O	1.99	0.62
2:C:274:LEU:CD2	2:C:292:ALA:HB1	2.29	0.62
2:C:400:VAL:HG22	2:C:417:LEU:O	2.00	0.62
2:C:101:GLY:O	2:C:142:ASN:ND2	2.28	0.62
2:C:214:PHE:CE2	2:C:342:ILE:HG12	2.34	0.62
2:C:274:LEU:HD11	2:C:292:ALA:O	2.00	0.62
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.64	0.62
2:C:789:ILE:HD12	2:C:789:ILE:O	1.99	0.62
2:C:959:LEU:CB	2:C:960:PRO:HD3	2.25	0.62
5:F:471:GLU:O	5:F:475:VAL:HG23	2.00	0.62
2:C:623:ALA:HA	2:C:714:ALA:HB2	1.81	0.62
2:C:1128:LEU:HD23	3:D:406:LEU:HD21	1.81	0.62
3:D:599:TYR:CZ	3:D:601:PRO:HG3	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:882:GLN:HE22	3:D:1249:LYS:HE2	1.64	0.62
3:D:1231:ARG:HA	3:D:1234:THR:CG2	2.29	0.62
2:C:507:ASN:HB2	2:C:511:PHE:O	1.99	0.61
3:D:1033:GLU:OE2	3:D:1040:PRO:HB3	1.99	0.61
2:C:220:ASP:CB	2:C:221:THR:HG22	2.27	0.61
3:D:453:LYS:NZ	3:D:453:LYS:HB3	2.15	0.61
3:D:143:MET:HA	3:D:146:ASN:OD1	2.00	0.61
3:D:741:ARG:HB2	3:D:744:GLU:OE2	1.98	0.61
3:D:913:ASP:O	3:D:916:ILE:HG13	2.01	0.61
3:D:1064:ILE:HD11	3:D:1112:MET:HE2	1.83	0.61
3:D:1219:SER:HB2	3:D:1243:ASP:OD2	1.99	0.61
5:F:486:PRO:O	5:F:487:ARG:HD3	1.99	0.61
2:C:220:ASP:CB	2:C:221:THR:HA	2.30	0.61
2:C:222:VAL:HG21	2:C:234:VAL:N	2.14	0.61
2:C:278:TYR:CD1	2:C:291:SER:HB2	2.35	0.61
1:A:153:ARG:CZ	2:C:797:ARG:HG2	2.30	0.61
2:C:922:VAL:HB	2:C:923:PRO:HD3	1.82	0.61
3:D:873:LEU:O	3:D:877:LEU:HD23	2.00	0.61
7:O:5:DG:H2"	7:O:6:DA:H5'	1.82	0.61
1:B:96:TYR:CD1	1:B:137:GLU:HG2	2.35	0.61
2:C:140:ILE:HG12	2:C:146:GLU:O	2.00	0.61
3:D:709:VAL:O	3:D:713:VAL:HG23	2.00	0.61
2:C:103:MET:HB2	2:C:139:PHE:CE1	2.36	0.61
2:C:646:GLU:HB3	2:C:662:HIS:CE1	2.36	0.61
2:C:855:ARG:HH11	2:C:861:LEU:HD12	1.66	0.61
2:C:1040:LYS:HD3	3:D:540:GLN:HE22	1.65	0.61
3:D:460:LEU:HD11	3:D:472:ALA:CB	2.30	0.61
3:D:1067:VAL:HG22	3:D:1074:GLU:CD	2.21	0.61
2:C:58:THR:O	2:C:62:GLU:HB2	2.00	0.61
2:C:599:HIS:HB3	2:C:928:ILE:CD1	2.31	0.61
2:C:1044:ARG:HB2	2:C:1063:PHE:CB	2.31	0.61
3:D:467:GLN:HA	3:D:467:GLN:HE21	1.65	0.61
3:D:963:ARG:HD3	3:D:978:CYS:SG	2.41	0.61
4:E:85:PRO:HB3	4:E:94:ILE:CD1	2.31	0.61
2:C:400:VAL:O	2:C:404:MET:HB2	2.00	0.61
4:E:47:VAL:CG1	4:E:52:ALA:HB3	2.31	0.61
2:C:290:GLU:HG2	2:C:294:THR:OG1	2.01	0.60
3:D:767:HIS:O	3:D:770:ARG:HG3	2.00	0.60
1:B:182:ARG:HA	1:B:182:ARG:NE	2.13	0.60
2:C:225:ARG:HD3	2:C:230:ARG:CA	2.30	0.60
9:C:1201:FI8:O8	9:C:1201:FI8:O11	2.19	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:305:SER:O	5:F:308:LYS:HG2	2.01	0.60
2:C:531:LEU:HD11	2:C:578:TYR:CE2	2.36	0.60
2:C:993:LEU:HD22	2:C:993:LEU:H	1.64	0.60
3:D:155:MET:HE3	3:D:219:LEU:HD12	1.84	0.60
5:F:429:ASP:OD1	5:F:430:GLU:N	2.27	0.60
1:A:18:ARG:NH1	1:A:195:ASP:OD2	2.33	0.60
1:A:105:VAL:HG23	1:A:128:LEU:HD13	1.81	0.60
2:C:205:ILE:HG22	2:C:211:TRP:CE2	2.36	0.60
3:D:111:PRO:HB2	3:D:116:TYR:CE2	2.36	0.60
3:D:929:ALA:O	3:D:937:ILE:HG22	2.01	0.60
3:D:931:ASP:HB3	3:D:955:ALA:HB1	1.83	0.60
3:D:1139:GLN:HG3	3:D:1143:ARG:HE	1.66	0.60
6:J:7:ARG:HD2	6:J:7:ARG:O	2.01	0.60
7:O:3:DT:C6	7:O:4:DT:H72	2.36	0.60
1:A:10:SER:OG	1:A:22:VAL:HG13	2.02	0.60
2:C:1044:ARG:CZ	2:C:1056:PRO:HB3	2.30	0.60
1:A:40:ARG:CD	1:B:33:THR:HG22	2.30	0.60
1:B:95:MET:HG2	1:B:113:PRO:CD	2.32	0.60
1:B:202:ILE:HD12	1:B:202:ILE:O	2.01	0.60
2:C:103:MET:SD	2:C:404:MET:HG2	2.41	0.60
2:C:721:VAL:HG23	2:C:915:ILE:HG13	1.83	0.60
2:C:797:ARG:HG3	2:C:800:ASP:OD2	2.01	0.60
3:D:1122:LEU:CB	3:D:1130:VAL:HG21	2.31	0.60
2:C:323:HIS:HB3	2:C:326:GLU:HG3	1.82	0.60
3:D:215:GLU:HG2	3:D:218:ARG:HH21	1.64	0.60
6:J:101:ARG:HA	6:J:101:ARG:HH11	1.65	0.60
1:A:105:VAL:O	1:A:125:ILE:HB	2.02	0.60
2:C:905:PRO:O	2:C:913:VAL:HG13	2.02	0.60
3:D:1087:ARG:CG	3:D:1088:VAL:H	2.11	0.60
2:C:200:HIS:O	2:C:345:LEU:HD21	2.01	0.60
2:C:290:GLU:OE1	2:C:291:SER:N	2.35	0.60
2:C:1110:GLU:HG2	4:E:69:ASN:HD21	1.67	0.59
3:D:219:LEU:HA	3:D:222:ILE:CG2	2.32	0.59
3:D:1098:VAL:O	3:D:1098:VAL:HG22	2.01	0.59
5:F:516:HIS:CG	5:F:517:PRO:HD2	2.37	0.59
8:P:23:DA:H2"	8:P:24:DA:C5'	2.31	0.59
2:C:482:ARG:HH11	2:C:532:THR:C	2.06	0.59
2:C:602:ALA:HB3	3:D:856:ALA:HB1	1.84	0.59
3:D:22:GLN:O	3:D:22:GLN:HG2	2.02	0.59
1:A:186:ARG:HD2	1:B:147:VAL:CG2	2.27	0.59
7:O:19:DA:H2'	7:O:20:DT:C7	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:TYR:CG	2:C:291:SER:HB2	2.37	0.59
2:C:946:VAL:HB	2:C:964:LEU:HB3	1.84	0.59
5:F:492:ILE:O	5:F:495:VAL:HG12	2.02	0.59
6:J:40:PHE:CD2	6:J:56:CYS:HB3	2.36	0.59
6:J:102:LEU:O	6:J:105:ILE:HG22	2.01	0.59
8:P:23:DA:H2"	8:P:24:DA:H5'	1.85	0.59
1:A:144:ARG:NE	1:B:232:ILE:HD11	2.17	0.59
2:C:241:LEU:HD21	2:C:335:GLU:CB	2.33	0.59
3:D:925:LEU:HD21	3:D:944:LEU:HD11	1.84	0.59
3:D:711:GLN:OE1	4:E:30:ASP:HB2	2.02	0.59
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.85	0.59
1:A:218:LEU:O	1:A:221:LEU:HD22	2.02	0.59
1:B:71:GLU:OE1	1:B:71:GLU:N	2.28	0.59
2:C:220:ASP:HB3	2:C:221:THR:CA	2.33	0.59
2:C:338:VAL:O	2:C:341:THR:HG22	2.02	0.59
1:A:105:VAL:HG23	1:A:128:LEU:CD1	2.33	0.59
1:B:55:ARG:NH1	1:B:55:ARG:HB2	2.18	0.59
2:C:77:ARG:NH2	2:C:505:ARG:HH12	2.00	0.59
2:C:446:LEU:O	2:C:446:LEU:HD23	2.02	0.59
3:D:125:LEU:O	3:D:129:ILE:HG23	2.03	0.59
3:D:725:THR:OG1	3:D:726:ARG:HD2	2.03	0.59
2:C:231:ARG:HB2	5:F:205:ASP:HB3	1.84	0.59
2:C:1050:SER:HB3	2:C:1053:THR:O	2.03	0.59
3:D:638:THR:HG22	3:D:661:ALA:HB2	1.85	0.59
3:D:1172:SER:HB3	3:D:1199:GLU:CB	2.33	0.59
5:F:390:LEU:HG	5:F:392:ARG:CG	2.32	0.59
1:B:124:HIS:CE1	1:B:127:THR:HG23	2.38	0.59
2:C:267:THR:HG21	2:C:273:ALA:CB	2.31	0.59
2:C:559:VAL:HG12	2:C:560:LEU:O	2.03	0.59
2:C:737:LEU:CD1	2:C:895:ILE:HD13	2.33	0.59
2:C:1059:GLY:H	2:C:1062:GLN:CB	2.16	0.59
3:D:666:THR:HG22	3:D:685:ASN:ND2	2.18	0.59
3:D:1221:LEU:HD23	3:D:1221:LEU:H	1.68	0.59
5:F:490:ASP:HB2	5:F:500:ARG:HD3	1.85	0.59
2:C:224:VAL:O	2:C:226:ILE:HG22	2.02	0.58
2:C:1048:PRO:HG2	2:C:1057:LEU:O	2.01	0.58
3:D:297:LYS:NZ	3:D:1176:LEU:HD11	2.18	0.58
3:D:740:PRO:HD3	3:D:792:HIS:CD2	2.38	0.58
3:D:1053:VAL:HG12	3:D:1103:ASP:O	2.04	0.58
3:D:1067:VAL:HG22	3:D:1074:GLU:OE2	2.03	0.58
3:D:1128:ARG:NH2	3:D:1132:ILE:HD11	2.14	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.84	0.58
5:F:334:LYS:HE3	7:O:25:DC:P	2.43	0.58
5:F:418:ARG:HB2	5:F:418:ARG:NH2	2.18	0.58
5:F:474:VAL:HG22	5:F:496:TYR:HE2	1.66	0.58
1:B:84:VAL:HG22	1:B:119:HIS:HB2	1.85	0.58
2:C:519:VAL:N	2:C:577:ASP:O	2.31	0.58
2:C:789:ILE:HG21	2:C:869:VAL:HG21	1.85	0.58
3:D:866:ARG:HD2	3:D:1010:LEU:O	2.03	0.58
3:D:1150:HIS:ND1	3:D:1152:LYS:HG2	2.18	0.58
3:D:902:ALA:H	3:D:913:ASP:HB2	1.68	0.58
3:D:1162:LEU:CD2	3:D:1207:LEU:HD23	2.33	0.58
1:B:136:VAL:HG12	1:B:138:LEU:HD12	1.85	0.58
2:C:267:THR:CG2	2:C:273:ALA:HB2	2.29	0.58
2:C:328:ILE:HD12	2:C:328:ILE:O	2.03	0.58
2:C:539:HIS:HD1	2:C:578:TYR:HE2	1.49	0.58
9:C:1201:FI8:O14	3:D:412:ARG:NH2	2.36	0.58
3:D:245:VAL:O	3:D:249:GLY:HA3	2.04	0.58
3:D:354:LEU:HB2	3:D:370:GLU:CG	2.33	0.58
2:C:715:LEU:N	2:C:1029:TYR:OH	2.37	0.58
2:C:1044:ARG:NH1	2:C:1056:PRO:HB3	2.18	0.58
3:D:707:ILE:HD12	4:E:39:PRO:HB3	1.85	0.58
3:D:766:ASN:HD22	3:D:766:ASN:H	1.51	0.58
3:D:899:VAL:HG12	3:D:900:GLU:H	1.68	0.58
2:C:217:ASP:OD1	2:C:231:ARG:NH2	2.37	0.58
3:D:273:GLU:O	3:D:277:LEU:HD13	2.04	0.58
3:D:1068:PRO:HG2	3:D:1072:GLY:N	2.19	0.58
1:A:95:MET:HE3	1:A:112:PRO:HB3	1.85	0.58
2:C:646:GLU:HB3	2:C:662:HIS:ND1	2.18	0.58
3:D:930:VAL:HG12	3:D:936:VAL:HA	1.86	0.58
1:B:62:GLU:OE2	1:B:65:THR:HB	2.04	0.58
2:C:222:VAL:CB	2:C:234:VAL:HG13	2.34	0.58
2:C:1002:VAL:CG1	2:C:1006:GLY:HA2	2.34	0.58
3:D:991:ILE:HG22	3:D:991:ILE:O	2.02	0.58
2:C:1081:ALA:HB1	3:D:554:GLU:OE1	2.03	0.58
1:A:40:ARG:HG2	1:B:33:THR:HG22	1.85	0.57
3:D:31:PRO:HB3	3:D:348:ILE:CG2	2.34	0.57
3:D:226:PHE:CE1	3:D:248:TYR:HB3	2.38	0.57
3:D:369:ASN:O	3:D:373:MET:HG3	2.04	0.57
5:F:296:LEU:O	5:F:300:LEU:HG	2.03	0.57
5:F:386:LEU:HD11	5:F:398:GLU:CD	2.25	0.57
1:A:182:ARG:HH11	3:D:624:ARG:NH1	2.02	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:VAL:HG12	2:C:81:ASN:OD1	2.05	0.57
2:C:584:ARG:NH2	2:C:975:PRO:HB3	2.19	0.57
2:C:1087:GLU:OE2	3:D:547:LEU:HB2	2.03	0.57
2:C:623:ALA:HA	2:C:714:ALA:CB	2.34	0.57
3:D:736:VAL:HG22	3:D:799:ILE:HD11	1.87	0.57
3:D:1010:LEU:HD23	3:D:1028:LEU:CA	2.35	0.57
2:C:152:VAL:HG11	2:C:418:ILE:HG21	1.87	0.57
2:C:524:VAL:N	2:C:552:GLY:O	2.27	0.57
5:F:379:LEU:HD11	5:F:410:VAL:HG23	1.87	0.57
5:F:514:LEU:O	5:F:519:ARG:HB2	2.03	0.57
2:C:231:ARG:CB	5:F:205:ASP:HB3	2.35	0.57
2:C:313:ARG:HG3	2:C:330:SER:O	2.05	0.57
2:C:982:GLU:OE1	3:D:841:ARG:NH2	2.37	0.57
3:D:1084:GLN:HE21	3:D:1112:MET:CB	2.17	0.57
7:O:6:DA:H1'	7:O:7:DC:H5'	1.87	0.57
1:B:3:ILE:HD11	1:B:27:GLU:HG2	1.87	0.57
3:D:447:MET:HE3	3:D:522:ILE:HD11	1.85	0.57
3:D:557:ILE:HD12	4:E:54:VAL:HG22	1.87	0.57
3:D:668:LEU:HD23	3:D:668:LEU:O	2.05	0.57
5:F:511:MET:HB3	5:F:515:ARG:HH12	1.70	0.57
2:C:293:GLN:NE2	2:C:297:GLU:OE2	2.38	0.57
2:C:531:LEU:HD11	2:C:578:TYR:CD2	2.40	0.57
2:C:899:LEU:H	2:C:899:LEU:HD22	1.68	0.57
3:D:125:LEU:HD11	3:D:261:ILE:CD1	2.35	0.57
3:D:981:ARG:HG2	3:D:982:SER:O	2.05	0.57
3:D:1050:THR:HG22	3:D:1106:GLU:HA	1.86	0.57
4:E:58:ALA:O	4:E:62:ARG:HG3	2.05	0.57
2:C:215:ASP:O	2:C:223:GLY:N	2.37	0.57
3:D:136:ILE:HD11	3:D:235:ILE:CD1	2.35	0.57
3:D:738:VAL:HG13	3:D:739:PRO:HD2	1.86	0.57
3:D:1087:ARG:HG3	3:D:1088:VAL:N	2.17	0.57
1:A:102:PRO:HG3	1:A:130:ASP:OD1	2.04	0.57
6:J:101:ARG:NH1	6:J:101:ARG:HB3	2.19	0.57
2:C:650:ILE:HG21	2:C:691:ASP:O	2.04	0.56
2:C:727:GLU:CG	3:D:725:THR:HG21	2.35	0.56
3:D:665:GLU:HG3	3:D:665:GLU:O	2.05	0.56
3:D:910:LEU:HD12	3:D:910:LEU:O	2.05	0.56
5:F:395:THR:HB	5:F:397:GLU:OE2	2.04	0.56
1:B:153:ARG:HA	1:B:153:ARG:NE	2.20	0.56
2:C:882:GLY:HA3	2:C:1037:VAL:HG11	1.87	0.56
1:A:89:GLU:OE2	1:A:93:VAL:HG11	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:CD1	1:B:7:PRO:HG2	2.35	0.56
2:C:40:SER:HA	2:C:973:SER:OG	2.05	0.56
2:C:388:GLN:O	2:C:391:VAL:HG12	2.04	0.56
2:C:742:VAL:HG22	2:C:879:ILE:HG22	1.87	0.56
3:D:162:VAL:HG13	3:D:216:LEU:CD2	2.27	0.56
3:D:1061:PHE:HB3	3:D:1081:SER:CA	2.35	0.56
3:D:1068:PRO:HD3	3:D:1074:GLU:HA	1.86	0.56
3:D:1195:ALA:O	3:D:1197:GLY:N	2.38	0.56
5:F:415:GLN:O	5:F:418:ARG:NH2	2.38	0.56
5:F:498:VAL:HG23	5:F:503:ILE:HG12	1.87	0.56
7:O:19:DA:H2"	7:O:20:DT:O5'	2.05	0.56
1:B:96:TYR:O	1:B:110:ILE:HG13	2.04	0.56
3:D:101:VAL:HG13	3:D:375:GLN:OE1	2.05	0.56
3:D:146:ASN:OD1	3:D:147:GLU:N	2.36	0.56
3:D:797:ASN:O	3:D:800:ILE:HG22	2.06	0.56
3:D:909:THR:O	3:D:910:LEU:CG	2.53	0.56
5:F:328:LEU:O	5:F:328:LEU:HD23	2.05	0.56
2:C:548:ILE:HD11	2:C:579:MET:HE1	1.88	0.56
5:F:213:ARG:N	5:F:213:ARG:HD2	2.20	0.56
5:F:213:ARG:O	5:F:216:ARG:HG3	2.06	0.56
2:C:848:ILE:CD1	2:C:874:ALA:HB2	2.35	0.56
2:C:885:LEU:HD23	2:C:1030:ILE:HD12	1.86	0.56
3:D:276:SER:O	3:D:280:VAL:HG23	2.05	0.56
3:D:1235:ASP:OD1	3:D:1236:ALA:N	2.38	0.56
1:A:34:LEU:HD11	1:B:218:LEU:CD2	2.28	0.56
3:D:35:ASN:OD1	3:D:38:THR:HG22	2.05	0.56
3:D:480:ARG:O	3:D:483:VAL:HG13	2.06	0.56
3:D:599:TYR:CE2	3:D:601:PRO:HG3	2.40	0.56
3:D:736:VAL:HG11	3:D:817:LEU:CD2	2.35	0.56
3:D:866:ARG:NH1	3:D:1011:THR:HA	2.21	0.56
3:D:963:ARG:CD	3:D:978:CYS:HA	2.36	0.56
3:D:1133:HIS:O	3:D:1137:GLU:HG2	2.06	0.56
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.88	0.56
3:D:330:LEU:HD11	5:F:439:ILE:HD12	1.87	0.56
3:D:733:MET:O	3:D:733:MET:HG2	2.06	0.56
5:F:414:GLN:HE21	5:F:414:GLN:HA	1.69	0.56
2:C:173:ARG:NH2	2:C:437:SER:O	2.37	0.56
2:C:203:LYS:HG2	2:C:205:ILE:HG23	1.87	0.56
2:C:727:GLU:H	3:D:725:THR:HG22	1.71	0.56
3:D:222:ILE:HD13	3:D:223:TRP:N	2.21	0.56
3:D:1080:ILE:HG21	3:D:1112:MET:CE	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:334:LYS:HG2	5:F:334:LYS:O	2.06	0.56
2:C:258:MET:CA	2:C:261:THR:HG23	2.31	0.55
2:C:355:MET:HB2	2:C:365:VAL:CG2	2.36	0.55
2:C:899:LEU:HB2	2:C:904:MET:HE1	1.88	0.55
3:D:599:TYR:CD1	3:D:601:PRO:HD3	2.41	0.55
3:D:1173:THR:HA	3:D:1174:GLU:OE1	2.07	0.55
4:E:37:ASN:OD1	4:E:38:PRO:HA	2.06	0.55
8:P:1:DA:H5"	8:P:1:DA:C8	2.40	0.55
3:D:1052:ARG:CG	3:D:1067:VAL:HB	2.36	0.55
5:F:305:SER:HA	5:F:308:LYS:HD2	1.88	0.55
5:F:489:LEU:HG	8:P:20:DG:P	2.46	0.55
1:B:70:LYS:HE3	1:B:127:THR:OG1	2.06	0.55
2:C:224:VAL:HG21	2:C:234:VAL:HA	1.88	0.55
2:C:622:GLU:HB3	2:C:717:LYS:HD3	1.87	0.55
2:C:773:ILE:HG23	2:C:774:PRO:HD2	1.87	0.55
1:A:221:LEU:HD12	1:B:7:PRO:O	2.07	0.55
1:B:182:ARG:HB3	1:B:186:ARG:CB	2.36	0.55
2:C:222:VAL:HG11	2:C:234:VAL:CG2	2.36	0.55
2:C:842:GLY:O	2:C:843:GLU:HG3	2.06	0.55
3:D:218:ARG:O	3:D:222:ILE:HG22	2.05	0.55
3:D:452:PHE:O	3:D:456:VAL:HG12	2.05	0.55
3:D:760:PHE:CE1	3:D:767:HIS:HA	2.41	0.55
3:D:913:ASP:HB3	3:D:916:ILE:CG1	2.36	0.55
2:C:322:LEU:C	2:C:324:VAL:H	2.10	0.55
2:C:569:GLU:HG2	2:C:570:TYR:H	1.72	0.55
2:C:595:PRO:HG3	2:C:888:ARG:NH2	2.21	0.55
2:C:992:THR:HG23	2:C:1000:VAL:HG13	1.88	0.55
3:D:320:ILE:CG1	3:D:321:PRO:HD2	2.36	0.55
3:D:598:GLU:HG2	3:D:599:TYR:N	2.22	0.55
3:D:684:VAL:HG11	3:D:688:MET:HE1	1.87	0.55
3:D:765:LEU:HD23	3:D:765:LEU:H	1.72	0.55
3:D:1190:ASN:ND2	3:D:1201:ALA:HB3	2.21	0.55
3:D:1217:THR:CG2	3:D:1223:ALA:HB2	2.36	0.55
6:J:40:PHE:CZ	6:J:58:ASN:HB2	2.42	0.55
2:C:322:LEU:O	2:C:324:VAL:N	2.38	0.55
2:C:522:GLY:O	2:C:553:ARG:HA	2.07	0.55
2:C:919:THR:HG23	3:D:731:VAL:CG2	2.36	0.55
2:C:982:GLU:HB2	3:D:841:ARG:HH22	1.72	0.55
3:D:173:ARG:HE	3:D:205:MET:HG2	1.70	0.55
1:A:94:THR:O	1:A:113:PRO:HG3	2.07	0.55
1:B:97:LEU:HB2	1:B:110:ILE:HD12	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:222:VAL:HG21	2:C:234:VAL:HG13	1.87	0.55
2:C:454:ARG:C	2:C:455:LEU:HD23	2.27	0.55
3:D:876:ARG:NH1	3:D:1036:GLU:OE1	2.40	0.55
3:D:1099:LEU:HD23	3:D:1099:LEU:C	2.27	0.55
6:J:103:GLU:OE1	6:J:104:LEU:N	2.40	0.55
1:B:24:GLU:CG	1:B:191:LYS:HG3	2.36	0.55
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.87	0.55
2:C:224:VAL:HG21	2:C:234:VAL:CA	2.37	0.55
2:C:542:ALA:HB3	2:C:579:MET:HB2	1.89	0.55
2:C:820:LEU:CD2	5:F:481:LEU:HD11	2.37	0.55
3:D:944:LEU:HA	3:D:948:GLU:HG3	1.88	0.55
3:D:1064:ILE:HD12	3:D:1080:ILE:HD12	1.89	0.55
3:D:1118:PRO:HA	3:D:1121:VAL:CG1	2.37	0.55
5:F:266:LEU:O	5:F:266:LEU:HD13	2.06	0.55
5:F:311:THR:HG21	5:F:317:PHE:CD1	2.41	0.55
5:F:490:ASP:HB2	5:F:500:ARG:CD	2.36	0.55
2:C:224:VAL:O	2:C:224:VAL:HG12	2.07	0.55
2:C:475:VAL:HG23	3:D:854:HIS:CE1	2.42	0.55
2:C:764:LEU:HD23	2:C:808:PRO:CB	2.37	0.55
2:C:959:LEU:HD12	2:C:959:LEU:N	2.22	0.55
3:D:31:PRO:HB3	3:D:348:ILE:HG23	1.88	0.55
3:D:49:GLU:OE2	3:D:55:THR:OG1	2.23	0.55
5:F:315:MET:HE2	5:F:362:GLN:HB2	1.89	0.55
2:C:281:LEU:HD23	2:C:295:LEU:HD21	1.88	0.55
2:C:500:LEU:CD2	2:C:504:ALA:HB3	2.36	0.55
2:C:1034:HIS:O	2:C:1035:HIS:ND1	2.40	0.55
3:D:915:TYR:CZ	3:D:1143:ARG:HD3	2.42	0.55
5:F:372:MET:O	5:F:376:ILE:HG13	2.07	0.55
2:C:133:LEU:HD23	2:C:134:PHE:N	2.22	0.54
2:C:686:GLN:HG3	2:C:704:ASP:O	2.08	0.54
2:C:1068:PHE:HZ	2:C:1076:MET:HG3	1.72	0.54
3:D:193:ALA:O	3:D:197:VAL:HG23	2.07	0.54
3:D:459:ARG:HH12	3:D:463:LEU:HD23	1.71	0.54
3:D:706:MET:N	4:E:41:ASP:OD2	2.37	0.54
1:B:38:LEU:HD12	1:B:42:LEU:CD1	2.37	0.54
2:C:103:MET:HG3	2:C:404:MET:HE1	1.87	0.54
2:C:413:THR:OG1	2:C:414:PRO:HD2	2.07	0.54
2:C:554:PHE:CD1	2:C:559:VAL:HG21	2.43	0.54
3:D:107:PHE:CE2	3:D:129:ILE:HD11	2.42	0.54
3:D:170:LEU:O	3:D:173:ARG:HG3	2.07	0.54
3:D:778:TRP:CD1	3:D:835:PRO:HD3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:895:ARG:HH11	3:D:967:THR:HB	1.71	0.54
1:A:25:PRO:O	1:A:26:LEU:HD23	2.08	0.54
1:B:89:GLU:OE1	1:B:89:GLU:N	2.41	0.54
2:C:163:LYS:HG3	2:C:639:GLY:HA3	1.89	0.54
2:C:549:ASP:HB2	2:C:555:VAL:CG2	2.38	0.54
3:D:641:ARG:HA	3:D:657:GLN:CG	2.35	0.54
3:D:923:ARG:HB3	3:D:962:VAL:HG11	1.88	0.54
3:D:1025:THR:CG2	3:D:1029:PRO:HB2	2.26	0.54
8:P:14:DA:H2"	8:P:15:DC:O5'	2.06	0.54
2:C:32:VAL:HG21	2:C:632:LEU:HD11	1.88	0.54
2:C:587:VAL:HG13	2:C:591:THR:HB	1.88	0.54
2:C:632:LEU:O	2:C:632:LEU:HD22	2.07	0.54
2:C:959:LEU:CB	2:C:960:PRO:CD	2.84	0.54
3:D:57:ASP:OD2	6:J:14:VAL:HA	2.06	0.54
5:F:371:HIS:NE2	7:O:21:DT:OP2	2.39	0.54
6:J:85:LEU:HA	6:J:88:ARG:NH1	2.21	0.54
1:B:107:ALA:HB3	1:B:121:PRO:CA	2.38	0.54
2:C:134:PHE:HE1	2:C:153:PHE:HB2	1.72	0.54
2:C:543:GLN:OE1	2:C:543:GLN:HA	2.08	0.54
2:C:754:GLU:OE2	2:C:870:ARG:HD2	2.07	0.54
2:C:799:GLY:H	2:C:839:VAL:HG13	1.73	0.54
2:C:822:ARG:NH1	2:C:829:ALA:HB2	2.23	0.54
2:C:1093:SER:CB	3:D:420:LYS:HD3	2.37	0.54
3:D:113:ARG:NH2	3:D:1235:ASP:HB3	2.22	0.54
3:D:297:LYS:HZ3	3:D:1176:LEU:HD11	1.71	0.54
3:D:948:GLU:O	3:D:952:LEU:HG	2.08	0.54
3:D:1064:ILE:HD11	3:D:1112:MET:CE	2.37	0.54
6:J:28:GLN:NE2	6:J:46:ASP:O	2.41	0.54
2:C:519:VAL:HG11	2:C:576:VAL:HG12	1.90	0.54
3:D:190:LYS:HG2	3:D:192:ASP:H	1.72	0.54
2:C:561:VAL:HG22	2:C:562:ARG:H	1.72	0.54
3:D:873:LEU:HD22	3:D:1028:LEU:HD11	1.89	0.54
3:D:925:LEU:HD22	3:D:960:VAL:HG12	1.89	0.54
4:E:76:LEU:HG	4:E:77:GLU:H	1.71	0.54
5:F:378:LYS:HG2	5:F:403:MET:HE3	1.88	0.54
1:A:71:GLU:HB3	1:A:75:GLU:HB3	1.89	0.54
2:C:485:PRO:O	3:D:857:ARG:NH2	2.41	0.54
2:C:518:LYS:HA	2:C:578:TYR:HD1	1.73	0.54
3:D:78:CYS:O	3:D:80:VAL:HG23	2.07	0.54
3:D:199:ASP:O	3:D:203:ARG:HG2	2.08	0.54
3:D:1244:LYS:HE2	3:D:1244:LYS:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1264:ILE:CG2	3:D:1266:ARG:HG2	2.38	0.54
4:E:85:PRO:HB3	4:E:94:ILE:HD13	1.90	0.54
5:F:342:LYS:HG2	7:O:29:DA:H3'	1.90	0.54
5:F:476:ARG:O	5:F:480:GLY:N	2.40	0.54
8:P:14:DA:H1'	8:P:15:DC:H5'	1.89	0.54
1:A:147:VAL:HG12	1:A:168:TYR:HE2	1.73	0.54
1:A:221:LEU:HD23	1:A:222:ALA:N	2.22	0.54
2:C:177:SER:HB2	2:C:378:LEU:CD1	2.37	0.54
2:C:532:THR:CG2	2:C:535:GLU:HG2	2.38	0.54
2:C:571:VAL:HG13	2:C:572:PRO:O	2.07	0.54
2:C:805:LYS:HB3	2:C:836:SER:HA	1.90	0.54
3:D:174:ALA:O	3:D:178:GLU:HG3	2.07	0.54
3:D:410:GLN:HA	3:D:410:GLN:HE21	1.73	0.54
3:D:504:LEU:HB3	3:D:1005:GLU:HG2	1.89	0.54
4:E:32:PRO:HB2	4:E:36:THR:HG23	1.90	0.54
2:C:705:GLY:N	2:C:708:THR:OG1	2.31	0.54
2:C:885:LEU:HD13	2:C:895:ILE:HD11	1.89	0.54
2:C:1044:ARG:HD2	2:C:1063:PHE:HB2	1.90	0.54
3:D:314:LEU:HD21	3:D:382:PHE:CE2	2.43	0.54
5:F:334:LYS:HD2	5:F:350:TRP:CZ2	2.42	0.54
8:P:18:DT:H2'	8:P:19:DT:H72	1.88	0.54
1:A:185:GLN:OE1	1:A:185:GLN:N	2.42	0.53
2:C:192:ASP:O	2:C:196:ASP:HA	2.07	0.53
2:C:225:ARG:HD3	2:C:230:ARG:N	2.23	0.53
2:C:318:LYS:HZ3	2:C:318:LYS:HB2	1.72	0.53
3:D:1063:LYS:HD3	3:D:1064:ILE:N	2.23	0.53
3:D:1105:VAL:HG13	3:D:1109:GLN:HB3	1.89	0.53
3:D:1219:SER:OG	3:D:1222:SER:HB3	2.07	0.53
5:F:489:LEU:HD12	8:P:20:DG:H2'	1.90	0.53
6:J:89:ARG:HG2	6:J:94:LEU:CD2	2.37	0.53
2:C:771:ARG:CG	2:C:781:LEU:HD11	2.39	0.53
3:D:1097:ARG:HH12	3:D:1100:SER:N	2.06	0.53
3:D:1097:ARG:NH1	3:D:1100:SER:CB	2.66	0.53
5:F:303:VAL:HG22	5:F:351:ILE:CD1	2.36	0.53
6:J:68:ASP:OD2	6:J:70:PRO:HD3	2.09	0.53
1:B:55:ARG:HD3	1:B:137:GLU:OE1	2.08	0.53
2:C:271:ASP:HA	2:C:274:LEU:HB3	1.89	0.53
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.91	0.53
2:C:1110:GLU:HG2	4:E:69:ASN:ND2	2.23	0.53
3:D:354:LEU:HB2	3:D:370:GLU:HG3	1.89	0.53
3:D:1068:PRO:HG3	3:D:1073:GLU:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1070:ASP:HB2	3:D:1071:GLY:CA	2.39	0.53
2:C:254:PHE:HE1	2:C:347:ARG:HH11	1.56	0.53
2:C:1125:LEU:O	2:C:1129:GLN:HG3	2.08	0.53
3:D:119:ASP:C	3:D:120:LEU:HD12	2.29	0.53
3:D:241:TYR:O	3:D:245:VAL:HG23	2.08	0.53
2:C:547:PRO:O	2:C:555:VAL:HG23	2.08	0.53
2:C:1117:ILE:CD1	3:D:5:ASN:HA	2.38	0.53
3:D:1208:MET:HG3	3:D:1213:ALA:HB2	1.89	0.53
5:F:498:VAL:CG2	5:F:503:ILE:HG12	2.38	0.53
1:B:218:LEU:O	1:B:218:LEU:HD23	2.07	0.53
2:C:718:ASN:C	2:C:719:LEU:HD12	2.29	0.53
3:D:383:ASP:OD2	3:D:386:ARG:HB2	2.08	0.53
3:D:957:ILE:HD12	3:D:957:ILE:O	2.09	0.53
3:D:1086:LEU:HD23	3:D:1112:MET:HE1	1.91	0.53
3:D:1272:VAL:HG13	4:E:56:TYR:HE1	1.73	0.53
5:F:407:PRO:HA	5:F:410:VAL:HG12	1.90	0.53
2:C:222:VAL:HG23	2:C:224:VAL:HG23	1.90	0.53
2:C:397:GLU:OE1	2:C:398:ARG:N	2.41	0.53
2:C:756:GLU:OE1	2:C:870:ARG:HD3	2.08	0.53
3:D:12:ILE:HG22	3:D:1237:ALA:HA	1.90	0.53
3:D:73:ILE:HG22	6:J:27:ARG:HH11	1.72	0.53
3:D:277:LEU:HD23	3:D:296:LEU:CA	2.38	0.53
3:D:866:ARG:CD	3:D:1010:LEU:O	2.56	0.53
5:F:276:ALA:HA	5:F:279:ARG:NH2	2.24	0.53
1:A:40:ARG:CG	1:B:33:THR:HG22	2.38	0.53
2:C:486:ILE:HD11	3:D:849:TYR:CE2	2.43	0.53
2:C:1007:LYS:NZ	3:D:735:ASP:OD2	2.38	0.53
3:D:128:ILE:HD13	3:D:135:VAL:HG21	1.90	0.53
4:E:101:ALA:HB3	4:E:103:LEU:HD13	1.89	0.53
1:B:182:ARG:HG3	1:B:185:GLN:HB3	1.90	0.53
2:C:216:VAL:HG11	2:C:349:HIS:HD2	1.74	0.53
2:C:252:PHE:HB3	2:C:258:MET:CE	2.39	0.53
2:C:338:VAL:HG12	2:C:342:ILE:HD11	1.91	0.53
2:C:1117:ILE:HD13	3:D:5:ASN:HA	1.90	0.53
3:D:263:LYS:HB2	3:D:263:LYS:HZ3	1.74	0.53
3:D:657:GLN:NE2	3:D:660:ASP:OD1	2.41	0.53
3:D:1190:ASN:O	3:D:1193:VAL:HB	2.08	0.53
5:F:498:VAL:HB	5:F:502:ARG:CB	2.35	0.53
2:C:518:LYS:HD3	2:C:527:GLU:OE1	2.09	0.53
2:C:1037:VAL:HG21	3:D:520:LYS:HB2	1.91	0.53
3:D:782:THR:O	3:D:785:VAL:HG12	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1086:LEU:CD2	3:D:1112:MET:HE1	2.39	0.53
3:D:1175:PHE:CE2	3:D:1189:GLU:HG2	2.43	0.53
7:O:14:DG:C8	7:O:15:DT:H72	2.43	0.53
2:C:420:ILE:HD13	2:C:421:ARG:N	2.23	0.52
2:C:727:GLU:H	3:D:725:THR:CG2	2.22	0.52
3:D:965:VAL:HG13	3:D:979:TYR:HA	1.90	0.52
3:D:1097:ARG:NH1	3:D:1100:SER:OG	2.42	0.52
6:J:99:LYS:HZ3	6:J:99:LYS:HB2	1.74	0.52
3:D:134:TYR:CE2	3:D:238:GLU:HG3	2.42	0.52
3:D:525:HIS:CG	3:D:526:PRO:HD2	2.43	0.52
1:B:147:VAL:HG13	1:B:166:SER:HB2	1.91	0.52
2:C:275:LEU:CD1	2:C:279:ARG:HE	2.22	0.52
2:C:1011:PHE:CD1	2:C:1018:PRO:HB3	2.44	0.52
3:D:797:ASN:HB3	3:D:800:ILE:HG22	1.90	0.52
6:J:40:PHE:CE2	6:J:58:ASN:HB2	2.44	0.52
1:A:138:LEU:HD12	1:A:138:LEU:N	2.24	0.52
1:B:66:VAL:HB	1:B:69:VAL:CG2	2.39	0.52
3:D:155:MET:CE	3:D:219:LEU:HD12	2.40	0.52
3:D:433:GLY:O	3:D:435:GLN:N	2.43	0.52
2:C:764:LEU:HD23	2:C:808:PRO:HB2	1.90	0.52
3:D:136:ILE:HD11	3:D:235:ILE:HD12	1.92	0.52
3:D:268:PHE:HE2	3:D:270:ILE:HG12	1.75	0.52
3:D:387:ARG:CZ	5:F:225:ALA:HA	2.40	0.52
3:D:876:ARG:O	3:D:880:VAL:HG12	2.09	0.52
3:D:913:ASP:HB3	3:D:916:ILE:HG13	1.91	0.52
3:D:1086:LEU:HD23	3:D:1112:MET:SD	2.49	0.52
3:D:1176:LEU:H	3:D:1176:LEU:HD12	1.74	0.52
2:C:203:LYS:HD2	2:C:211:TRP:CE3	2.45	0.52
2:C:225:ARG:O	2:C:225:ARG:HG2	2.10	0.52
2:C:500:LEU:HD22	2:C:504:ALA:HB3	1.92	0.52
3:D:1064:ILE:HD12	3:D:1080:ILE:CD1	2.39	0.52
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.45	0.52
3:D:39:LEU:HD22	3:D:335:PHE:HZ	1.75	0.52
3:D:736:VAL:HG22	3:D:799:ILE:HD12	1.91	0.52
3:D:750:GLU:HA	3:D:750:GLU:OE1	2.09	0.52
1:A:60:LEU:H	1:A:60:LEU:HD12	1.75	0.52
2:C:232:GLN:HG2	2:C:277:ILE:HD13	1.92	0.52
2:C:1104:GLU:HB2	5:F:451:VAL:HG22	1.92	0.52
3:D:924:THR:HA	3:D:942:GLN:O	2.10	0.52
4:E:95:ALA:O	4:E:99:ILE:HG13	2.09	0.52
6:J:74:LYS:O	6:J:74:LYS:HD3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:519:VAL:HG23	2:C:523:VAL:C	2.30	0.52
3:D:138:SER:HB3	3:D:253:THR:OG1	2.10	0.52
3:D:634:LYS:HE2	3:D:663:MET:CE	2.40	0.52
3:D:826:ASN:CG	3:D:827:PRO:HD2	2.30	0.52
3:D:908:GLY:C	3:D:910:LEU:N	2.59	0.52
3:D:913:ASP:H	3:D:916:ILE:HD11	1.74	0.52
3:D:1044:ALA:HA	3:D:1084:GLN:HE22	1.73	0.52
3:D:1174:GLU:OE1	3:D:1174:GLU:N	2.42	0.52
1:A:193:ILE:HG13	1:A:193:ILE:O	2.10	0.52
2:C:39:VAL:CG1	2:C:963:LEU:HG	2.38	0.52
2:C:516:TYR:CD2	2:C:531:LEU:HD12	2.45	0.52
2:C:928:ILE:HD11	3:D:840:PHE:O	2.09	0.52
3:D:224:SER:O	3:D:227:THR:OG1	2.27	0.52
3:D:891:CYS:HB2	3:D:969:ALA:HB3	1.92	0.52
3:D:938:VAL:HG13	3:D:942:GLN:OE1	2.10	0.52
3:D:1088:VAL:HG13	3:D:1098:VAL:HA	1.92	0.52
1:B:11:GLU:OE1	1:B:12:ASP:N	2.42	0.51
1:B:192:LEU:HD12	1:B:193:ILE:H	1.74	0.51
2:C:43:LYS:HE3	2:C:959:LEU:CA	2.37	0.51
2:C:89:VAL:O	2:C:92:GLU:HG2	2.09	0.51
2:C:254:PHE:HE1	2:C:347:ARG:HG2	1.74	0.51
2:C:282:ARG:HB2	2:C:283:PRO:HA	1.91	0.51
2:C:689:ILE:O	2:C:689:ILE:HG13	2.08	0.51
2:C:773:ILE:HG22	2:C:774:PRO:O	2.09	0.51
2:C:855:ARG:HH11	2:C:861:LEU:CD1	2.22	0.51
3:D:500:ARG:CD	3:D:534:ALA:HB2	2.39	0.51
3:D:1062:TYR:HB2	3:D:1080:ILE:HB	1.93	0.51
12:D:1501:HOH:O	6:J:10:ARG:NH1	2.43	0.51
6:J:4:ARG:HA	6:J:4:ARG:NE	2.24	0.51
1:A:60:LEU:HD12	1:A:60:LEU:N	2.25	0.51
2:C:628:THR:OG1	2:C:629:GLY:N	2.43	0.51
2:C:672:MET:SD	2:C:688:PRO:HD3	2.50	0.51
2:C:955:TRP:NE1	2:C:987:GLY:HA3	2.24	0.51
2:C:167:ILE:O	2:C:168:ILE:HD13	2.09	0.51
2:C:716:GLY:N	2:C:1029:TYR:OH	2.35	0.51
3:D:240:LEU:O	3:D:240:LEU:HD23	2.10	0.51
3:D:600:GLN:HA	3:D:600:GLN:NE2	2.25	0.51
5:F:273:LEU:HB3	5:F:274:PRO:HD2	1.92	0.51
1:B:68:GLY:O	1:B:128:LEU:HA	2.09	0.51
2:C:189:GLU:HB2	2:C:200:HIS:CD2	2.46	0.51
2:C:1086:GLN:OE1	3:D:1257:LEU:HD13	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:277:LEU:HD11	3:D:295:ARG:HH11	1.73	0.51
3:D:923:ARG:HB3	3:D:962:VAL:HG13	1.93	0.51
3:D:1012:MET:C	3:D:1027:GLY:HA3	2.30	0.51
2:C:153:PHE:CZ	2:C:155:GLY:HA2	2.46	0.51
3:D:897:ILE:HB	3:D:1128:ARG:HH21	1.76	0.51
6:J:24:LEU:HD23	6:J:24:LEU:N	2.26	0.51
1:A:42:LEU:O	1:A:171:VAL:HG11	2.11	0.51
2:C:396:MET:HE2	2:C:418:ILE:HG23	1.93	0.51
2:C:549:ASP:HB2	2:C:555:VAL:HG22	1.91	0.51
3:D:1169:ASP:HB2	3:D:1202:ALA:HB3	1.91	0.51
2:C:33:PRO:HG2	2:C:700:GLN:HA	1.92	0.51
2:C:641:VAL:O	2:C:643:VAL:HG23	2.10	0.51
5:F:244:GLU:HA	5:F:247:VAL:HG23	1.92	0.51
2:C:64:LEU:HA	2:C:85:GLY:HA3	1.93	0.51
2:C:177:SER:CB	2:C:378:LEU:HD11	2.40	0.51
2:C:1099:ARG:O	2:C:1102:VAL:HG12	2.10	0.51
3:D:103:HIS:CE1	3:D:105:TRP:HB2	2.46	0.51
3:D:134:TYR:HA	3:D:256:MET:HG2	1.93	0.51
3:D:736:VAL:CG1	3:D:817:LEU:HD22	2.41	0.51
5:F:266:LEU:O	5:F:270:GLY:N	2.44	0.51
5:F:415:GLN:HE22	5:F:418:ARG:HH12	1.59	0.51
2:C:809:LYS:N	2:C:831:GLU:O	2.29	0.51
2:C:948:ALA:CB	2:C:952:VAL:HA	2.41	0.51
2:C:1023:VAL:HA	3:D:730:THR:HG21	1.92	0.51
3:D:468:ASN:HD21	3:D:470:LYS:HB3	1.76	0.51
3:D:1064:ILE:CD1	3:D:1112:MET:HE2	2.41	0.51
3:D:1173:THR:O	3:D:1175:PHE:N	2.44	0.51
5:F:467:LEU:HD11	5:F:514:LEU:HD21	1.92	0.51
1:B:154:ALA:HB1	1:B:157:ALA:HB3	1.93	0.51
2:C:200:HIS:CD2	2:C:348:LEU:HG	2.46	0.51
2:C:409:VAL:O	2:C:410:GLU:HB3	2.11	0.51
3:D:9:GLU:OE2	3:D:1244:LYS:NZ	2.44	0.51
3:D:61:TYR:HB2	3:D:80:VAL:HG21	1.93	0.51
3:D:567:SER:OG	3:D:574:LEU:HD13	2.11	0.51
3:D:749:TYR:CG	3:D:781:ALA:HB2	2.46	0.51
5:F:387:LEU:HB2	5:F:394:PRO:HD3	1.93	0.51
1:B:134:LEU:HD21	1:B:136:VAL:HG23	1.93	0.50
2:C:380:THR:OG1	2:C:381:VAL:N	2.44	0.50
2:C:644:ALA:HB2	2:C:702:ILE:HD11	1.93	0.50
3:D:1221:LEU:H	3:D:1221:LEU:CD2	2.23	0.50
5:F:344:SER:OG	7:O:30:DC:OP2	2.28	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:14:DA:H5'	8:P:14:DA:H8	1.74	0.50
2:C:157:PHE:CE1	2:C:389:ILE:HD11	2.45	0.50
2:C:312:GLY:O	2:C:316:VAL:HG23	2.10	0.50
2:C:593:MET:HA	2:C:628:THR:CG2	2.41	0.50
2:C:907:LEU:HD23	2:C:1010:LEU:CD2	2.41	0.50
3:D:129:ILE:HG13	3:D:130:TYR:CD2	2.46	0.50
3:D:475:MET:HG3	3:D:480:ARG:CG	2.41	0.50
3:D:607:PRO:O	3:D:609:THR:HG23	2.11	0.50
4:E:33:LEU:O	4:E:36:THR:HG22	2.10	0.50
5:F:208:GLU:O	5:F:212:LEU:HG	2.12	0.50
5:F:249:LEU:HD22	5:F:291:ALA:HB1	1.93	0.50
1:B:102:PRO:HB3	1:B:129:ASN:O	2.11	0.50
2:C:281:LEU:HD23	2:C:295:LEU:CD2	2.41	0.50
2:C:737:LEU:HD22	2:C:915:ILE:HG22	1.93	0.50
2:C:801:ILE:N	2:C:801:ILE:HD12	2.26	0.50
2:C:943:GLY:O	2:C:993:LEU:HD23	2.10	0.50
2:C:1011:PHE:CE1	2:C:1018:PRO:HB3	2.46	0.50
3:D:35:ASN:CG	3:D:38:THR:HG22	2.32	0.50
3:D:360:LEU:HD12	3:D:360:LEU:H	1.75	0.50
3:D:407:LYS:HG2	3:D:408:GLY:N	2.26	0.50
3:D:1128:ARG:HH12	3:D:1132:ILE:HD11	1.77	0.50
5:F:206:GLU:O	5:F:208:GLU:N	2.44	0.50
5:F:334:LYS:HD2	5:F:350:TRP:HZ2	1.76	0.50
5:F:341:TYR:CE1	7:O:28:DT:H5"	2.47	0.50
1:A:225:LEU:O	1:A:225:LEU:HD22	2.11	0.50
1:B:201:SER:O	1:B:202:ILE:HG23	2.10	0.50
2:C:370:ILE:HD12	2:C:370:ILE:N	2.26	0.50
2:C:822:ARG:NE	5:F:527:LEU:HD21	2.27	0.50
3:D:151:LEU:HD21	3:D:251:TYR:CE2	2.46	0.50
3:D:588:LEU:HD23	3:D:723:TRP:CE2	2.47	0.50
8:P:20:DG:H2"	8:P:21:DT:O5'	2.12	0.50
1:A:219:PHE:CE1	1:B:38:LEU:HD22	2.43	0.50
1:B:3:ILE:CD1	1:B:27:GLU:HG2	2.42	0.50
2:C:363:VAL:HG12	2:C:364:PRO:HD2	1.94	0.50
2:C:1117:ILE:HD12	2:C:1117:ILE:N	2.26	0.50
3:D:113:ARG:HG2	3:D:1238:ILE:CD1	2.42	0.50
3:D:611:VAL:HG12	3:D:634:LYS:HB2	1.93	0.50
3:D:634:LYS:HG2	3:D:665:GLU:HB3	1.93	0.50
3:D:639:GLN:O	3:D:640:LEU:HD23	2.11	0.50
3:D:1226:PHE:O	3:D:1227:GLN:HG3	2.11	0.50
5:F:209:SER:O	5:F:213:ARG:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:ILE:O	2:C:147:ILE:HG22	2.12	0.50
2:C:274:LEU:HG	2:C:292:ALA:HB1	1.93	0.50
2:C:274:LEU:HD21	2:C:292:ALA:O	2.11	0.50
2:C:363:VAL:HG13	2:C:364:PRO:HD2	1.93	0.50
2:C:450:THR:HG21	2:C:590:ALA:HB2	1.93	0.50
2:C:524:VAL:HG21	2:C:548:ILE:CD1	2.40	0.50
2:C:691:ASP:HB2	2:C:694:ASP:OD1	2.12	0.50
5:F:216:ARG:HB2	5:F:216:ARG:NH1	2.24	0.50
8:P:19:DT:H2"	8:P:20:DG:H8	1.77	0.50
1:A:186:ARG:HG3	1:B:150:VAL:CB	2.41	0.50
2:C:192:ASP:OD1	2:C:194:SER:OG	2.21	0.50
2:C:290:GLU:HA	2:C:294:THR:CG2	2.41	0.50
3:D:468:ASN:HD22	3:D:470:LYS:H	1.59	0.50
3:D:590:THR:HG23	3:D:630:ARG:HE	1.77	0.50
1:B:15:THR:CG2	1:B:18:ARG:HB2	2.39	0.50
2:C:653:VAL:HG12	2:C:658:ILE:HG23	1.94	0.50
3:D:84:ARG:HG3	3:D:84:ARG:NH1	2.24	0.50
3:D:1086:LEU:HA	3:D:1112:MET:SD	2.51	0.50
3:D:1264:ILE:HG22	3:D:1266:ARG:HG2	1.93	0.50
4:E:60:ARG:NH1	4:E:64:ILE:HG13	2.26	0.50
5:F:244:GLU:HA	5:F:247:VAL:CG2	2.42	0.50
7:O:19:DA:C1'	7:O:20:DT:H5'	2.32	0.50
2:C:70:TRP:CH2	2:C:82:PRO:HB2	2.47	0.50
2:C:736:ILE:HD11	2:C:916:ILE:CD1	2.33	0.50
3:D:1103:ASP:OD1	3:D:1104:HIS:N	2.45	0.50
4:E:104:LEU:HD23	4:E:104:LEU:N	2.27	0.50
1:A:42:LEU:HD23	1:A:211:ALA:HB2	1.93	0.49
1:B:2:LEU:CD2	1:B:4:SER:H	2.24	0.49
2:C:180:VAL:HG21	2:C:379:ARG:HH11	1.77	0.49
2:C:771:ARG:NH1	2:C:786:GLU:HA	2.27	0.49
2:C:781:LEU:O	2:C:781:LEU:HD23	2.12	0.49
3:D:832:ILE:HG22	3:D:834:ARG:H	1.77	0.49
3:D:891:CYS:SG	3:D:893:THR:HG22	2.52	0.49
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.76	0.49
2:C:33:PRO:HG2	2:C:700:GLN:CA	2.42	0.49
2:C:96:ILE:N	2:C:105:LEU:O	2.45	0.49
2:C:212:LEU:N	2:C:212:LEU:HD23	2.26	0.49
2:C:224:VAL:O	2:C:226:ILE:N	2.45	0.49
2:C:406:THR:O	2:C:406:THR:OG1	2.30	0.49
2:C:756:GLU:OE2	2:C:868:LEU:HD11	2.12	0.49
3:D:164:ASP:N	3:D:164:ASP:OD1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:240:LEU:O	3:D:244:LEU:HG	2.12	0.49
5:F:242:ASN:OD1	5:F:245:GLU:HG3	2.12	0.49
5:F:427:ILE:HG23	5:F:427:ILE:O	2.12	0.49
7:O:28:DT:H2"	7:O:29:DA:C8	2.47	0.49
8:P:24:DA:H2"	8:P:25:DG:O4'	2.12	0.49
1:B:6:ARG:HG3	1:B:234:ILE:HG23	1.94	0.49
2:C:97:GLU:O	2:C:401:ARG:NH2	2.42	0.49
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.47	0.49
2:C:1074:TRP:HH2	3:D:875:ARG:HG3	1.77	0.49
3:D:287:GLN:N	3:D:287:GLN:OE1	2.46	0.49
3:D:588:LEU:O	3:D:588:LEU:HD22	2.12	0.49
5:F:496:TYR:O	5:F:498:VAL:HG13	2.12	0.49
5:F:501:GLU:O	5:F:505:GLN:HG2	2.12	0.49
7:O:5:DG:H2'	7:O:6:DA:H8	1.74	0.49
2:C:65:ILE:HD11	2:C:159:MET:SD	2.52	0.49
2:C:216:VAL:HG23	2:C:345:LEU:HD11	1.94	0.49
2:C:222:VAL:CG2	2:C:234:VAL:HG13	2.43	0.49
2:C:806:VAL:CG2	2:C:832:VAL:HB	2.43	0.49
5:F:386:LEU:HD11	5:F:398:GLU:OE1	2.12	0.49
2:C:199:LEU:HD23	2:C:199:LEU:N	2.27	0.49
2:C:418:ILE:HG22	2:C:420:ILE:HG22	1.93	0.49
2:C:568:VAL:HG13	3:D:847:LEU:HD23	1.94	0.49
2:C:659:THR:HG22	2:C:669:THR:CG2	2.32	0.49
3:D:449:LEU:O	3:D:449:LEU:HD13	2.12	0.49
5:F:221:LEU:O	5:F:224:SER:OG	2.22	0.49
1:B:7:PRO:HA	1:B:24:GLU:O	2.13	0.49
1:B:136:VAL:HG12	1:B:138:LEU:CD1	2.42	0.49
2:C:421:ARG:O	2:C:424:VAL:HG12	2.11	0.49
3:D:333:GLY:O	5:F:415:GLN:NE2	2.45	0.49
3:D:579:LEU:CD2	3:D:808:THR:HB	2.40	0.49
3:D:745:ILE:HD13	3:D:784:GLU:HG2	1.95	0.49
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.93	0.49
3:D:876:ARG:HH22	3:D:1032:GLN:HG3	1.78	0.49
5:F:280:ASP:OD1	5:F:281:MET:N	2.46	0.49
1:B:233:GLU:OE1	1:B:233:GLU:HA	2.13	0.49
2:C:44:LEU:N	2:C:44:LEU:HD12	2.28	0.49
2:C:222:VAL:HB	2:C:234:VAL:HG13	1.94	0.49
2:C:223:GLY:O	2:C:225:ARG:N	2.43	0.49
2:C:275:LEU:HD13	2:C:279:ARG:HE	1.77	0.49
2:C:741:LEU:HA	2:C:746:VAL:HG12	1.94	0.49
2:C:948:ALA:HB1	2:C:952:VAL:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:277:LEU:HD23	3:D:296:LEU:HB2	1.95	0.49
3:D:527:LEU:CD1	3:D:713:VAL:HG12	2.42	0.49
3:D:642:PRO:HB3	3:D:662:TRP:CE3	2.48	0.49
3:D:1189:GLU:O	3:D:1192:ARG:HB3	2.12	0.49
3:D:1193:VAL:O	3:D:1193:VAL:HG22	2.13	0.49
3:D:1230:THR:O	3:D:1234:THR:HG22	2.13	0.49
1:A:223:ARG:CD	1:A:224:GLU:H	2.23	0.49
1:B:183:VAL:O	1:B:187:THR:HA	2.12	0.49
2:C:93:LEU:CD1	2:C:96:ILE:HD11	2.43	0.49
3:D:173:ARG:HB2	3:D:173:ARG:CZ	2.42	0.49
2:C:396:MET:HE3	2:C:418:ILE:HG23	1.94	0.49
2:C:771:ARG:NE	2:C:781:LEU:HD21	2.27	0.49
3:D:25:TYR:HD2	3:D:91:ARG:HD3	1.78	0.49
3:D:55:THR:HG22	6:J:12:GLY:CA	2.43	0.49
3:D:436:LEU:HD22	3:D:515:MET:CE	2.43	0.49
5:F:328:LEU:HD23	5:F:328:LEU:C	2.33	0.49
1:B:105:VAL:HG12	1:B:125:ILE:HG21	1.94	0.49
2:C:500:LEU:HD23	2:C:501:SER:H	1.78	0.49
2:C:532:THR:OG1	2:C:533:ALA:N	2.46	0.49
2:C:719:LEU:CD2	2:C:1030:ILE:HD11	2.28	0.49
3:D:67:ARG:NE	6:J:17:GLU:OE2	2.45	0.49
3:D:717:LYS:HG3	3:D:718:ASP:N	2.28	0.49
3:D:822:GLY:O	3:D:835:PRO:HB2	2.13	0.49
3:D:885:ILE:HD11	3:D:887:ARG:HH12	1.76	0.49
6:J:45:ALA:HB3	6:J:48:ALA:HB2	1.95	0.49
1:A:161:ARG:NH1	1:A:161:ARG:HB2	2.26	0.48
2:C:1009:MET:HA	2:C:1009:MET:HE3	1.95	0.48
3:D:899:VAL:HG12	3:D:900:GLU:N	2.27	0.48
2:C:222:VAL:CG2	2:C:224:VAL:HG23	2.43	0.48
2:C:230:ARG:HH11	2:C:230:ARG:CA	2.23	0.48
2:C:238:LEU:HD11	2:C:243:TRP:CD2	2.48	0.48
2:C:601:ASP:OD1	2:C:602:ALA:N	2.45	0.48
2:C:992:THR:CG2	2:C:1000:VAL:HG13	2.44	0.48
3:D:237:ASP:OD2	3:D:240:LEU:N	2.37	0.48
3:D:513:GLU:HG3	3:D:513:GLU:O	2.13	0.48
3:D:642:PRO:HD3	3:D:657:GLN:HG2	1.94	0.48
3:D:1050:THR:HG23	3:D:1107:VAL:CG2	2.42	0.48
3:D:1225:SER:O	3:D:1225:SER:OG	2.31	0.48
1:A:59:VAL:CG1	1:A:66:VAL:HG22	2.44	0.48
1:A:97:LEU:HD21	1:A:105:VAL:HG11	1.94	0.48
1:B:146:TYR:CE2	3:D:621:ALA:HB2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:HG13	1:B:150:VAL:O	2.14	0.48
2:C:238:LEU:CD2	2:C:248:ILE:HG12	2.43	0.48
2:C:396:MET:HB2	2:C:422:PRO:HG2	1.94	0.48
2:C:995:ASN:OD1	2:C:995:ASN:N	2.46	0.48
3:D:1070:ASP:HB2	3:D:1071:GLY:O	2.13	0.48
3:D:1243:ASP:OD1	3:D:1244:LYS:N	2.45	0.48
5:F:505:GLN:HG3	5:F:506:ILE:N	2.29	0.48
1:A:95:MET:CE	1:A:112:PRO:HB3	2.44	0.48
1:B:170:PRO:HB2	1:B:202:ILE:HD11	1.96	0.48
2:C:215:ASP:CA	2:C:223:GLY:HA3	2.43	0.48
2:C:723:ILE:O	2:C:723:ILE:HG22	2.14	0.48
2:C:767:GLU:HB3	2:C:805:LYS:HZ2	1.78	0.48
5:F:286:ARG:CZ	5:F:286:ARG:HA	2.42	0.48
5:F:306:LEU:O	5:F:306:LEU:HD23	2.13	0.48
6:J:78:PRO:O	6:J:80:THR:HG23	2.13	0.48
1:A:2:LEU:HD12	1:A:2:LEU:O	2.13	0.48
1:B:42:LEU:HD12	1:B:211:ALA:CB	2.43	0.48
2:C:224:VAL:HG21	2:C:233:PRO:C	2.33	0.48
2:C:1040:LYS:HD3	3:D:540:GLN:NE2	2.28	0.48
3:D:148:LEU:O	3:D:152:GLU:HG3	2.14	0.48
3:D:463:LEU:O	3:D:465:HIS:N	2.43	0.48
2:C:465:ARG:HD2	2:C:493:ASN:OD1	2.13	0.48
2:C:556:GLU:HB2	2:C:557:PRO:HD2	1.96	0.48
3:D:992:GLY:HA2	3:D:1264:ILE:HD11	1.95	0.48
3:D:1106:GLU:HA	3:D:1106:GLU:OE1	2.14	0.48
3:D:1249:LYS:O	3:D:1253:ILE:HG13	2.13	0.48
7:O:8:DA:H2"	7:O:9:DA:H8	1.76	0.48
1:A:144:ARG:CZ	1:B:232:ILE:HD11	2.43	0.48
1:B:19:SER:OG	1:B:204:PRO:HG2	2.13	0.48
1:B:102:PRO:CB	1:B:130:ASP:HA	2.44	0.48
2:C:274:LEU:HD23	2:C:292:ALA:HB1	1.94	0.48
2:C:945:LYS:HB2	2:C:945:LYS:NZ	2.29	0.48
3:D:25:TYR:HE2	3:D:91:ARG:HG2	1.79	0.48
3:D:263:LYS:HB2	3:D:263:LYS:HZ2	1.74	0.48
3:D:1012:MET:C	3:D:1027:GLY:H	2.16	0.48
3:D:1154:ILE:O	3:D:1158:VAL:HG23	2.13	0.48
1:B:3:ILE:HD11	1:B:27:GLU:CG	2.43	0.48
2:C:117:ALA:HB3	2:C:122:CYS:SG	2.54	0.48
2:C:167:ILE:N	2:C:167:ILE:HD12	2.29	0.48
2:C:222:VAL:HG11	2:C:234:VAL:HG22	1.96	0.48
2:C:254:PHE:H	2:C:255:SER:CB	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:587:VAL:HG12	2:C:588:SER:O	2.14	0.48
2:C:1040:LYS:HA	2:C:1040:LYS:HE2	1.95	0.48
2:C:1135:VAL:CG1	3:D:12:ILE:HG12	2.34	0.48
3:D:598:GLU:HG2	3:D:599:TYR:H	1.77	0.48
3:D:608:GLU:O	3:D:609:THR:OG1	2.19	0.48
3:D:641:ARG:HA	3:D:657:GLN:CB	2.43	0.48
3:D:1052:ARG:NH2	3:D:1102:GLY:HA2	2.28	0.48
3:D:1080:ILE:CG2	3:D:1112:MET:HG3	2.42	0.48
5:F:395:THR:HG1	5:F:398:GLU:HB2	1.78	0.48
5:F:483:ASP:N	5:F:483:ASP:OD1	2.45	0.48
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.96	0.48
3:D:141:GLU:OE1	3:D:141:GLU:HA	2.14	0.48
3:D:323:GLU:OE1	3:D:323:GLU:HA	2.13	0.48
3:D:475:MET:HG3	3:D:480:ARG:HG3	1.95	0.48
3:D:545:LEU:HD12	3:D:546:PRO:HD2	1.96	0.48
3:D:834:ARG:CB	3:D:835:PRO:HA	2.44	0.48
5:F:474:VAL:HG22	5:F:496:TYR:CE2	2.48	0.48
7:O:7:DC:H2"	7:O:8:DA:C8	2.48	0.48
2:C:1037:VAL:HG12	3:D:429:VAL:HG11	1.96	0.48
3:D:459:ARG:NH1	3:D:463:LEU:HD23	2.29	0.48
7:O:4:DT:H2"	7:O:5:DG:H8	1.79	0.48
2:C:317:ASN:HA	2:C:322:LEU:HB2	1.96	0.47
2:C:763:LYS:NZ	3:D:332:GLY:H	2.11	0.47
3:D:117:LEU:O	3:D:117:LEU:HD13	2.13	0.47
3:D:578:ARG:O	3:D:582:VAL:HG23	2.13	0.47
3:D:1047:ALA:HB2	3:D:1111:LEU:HD11	1.95	0.47
3:D:1251:ASN:ND2	3:D:1259:PRO:HD3	2.29	0.47
5:F:386:LEU:HD22	5:F:394:PRO:HB3	1.96	0.47
2:C:206:PRO:HG3	2:C:306:TYR:CZ	2.49	0.47
2:C:584:ARG:HG3	2:C:584:ARG:O	2.14	0.47
2:C:814:LEU:HD22	2:C:814:LEU:H	1.79	0.47
3:D:240:LEU:HD23	3:D:244:LEU:HG	1.95	0.47
3:D:627:LEU:HD22	3:D:628:SER:O	2.14	0.47
3:D:965:VAL:CG1	3:D:979:TYR:HA	2.44	0.47
4:E:85:PRO:HB3	4:E:94:ILE:HD11	1.94	0.47
1:A:27:GLU:OE1	1:A:27:GLU:HA	2.13	0.47
1:B:96:TYR:CE1	1:B:137:GLU:HG2	2.48	0.47
2:C:223:GLY:C	2:C:225:ARG:H	2.18	0.47
2:C:308:LEU:H	2:C:308:LEU:CD2	2.26	0.47
2:C:560:LEU:HD23	2:C:569:GLU:O	2.15	0.47
3:D:357:LEU:HD23	3:D:357:LEU:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1118:PRO:O	3:D:1121:VAL:HG13	2.13	0.47
5:F:244:GLU:O	5:F:247:VAL:HB	2.14	0.47
6:J:92:GLU:OE1	6:J:92:GLU:HA	2.14	0.47
2:C:542:ALA:HB2	2:C:576:VAL:HG11	1.94	0.47
2:C:737:LEU:HD11	2:C:895:ILE:CD1	2.44	0.47
2:C:861:LEU:HB2	2:C:862:PRO:CD	2.41	0.47
2:C:1040:LYS:HE2	2:C:1040:LYS:CA	2.44	0.47
3:D:149:SER:O	3:D:152:GLU:HG3	2.14	0.47
3:D:940:ARG:NH1	3:D:963:ARG:NH2	2.62	0.47
3:D:1051:GLY:CA	3:D:1069:ASP:HB2	2.44	0.47
1:B:70:LYS:NZ	1:B:70:LYS:CB	2.78	0.47
2:C:30:ASN:O	2:C:31:SER:OG	2.28	0.47
2:C:741:LEU:HA	2:C:746:VAL:CG1	2.44	0.47
3:D:431:VAL:HG13	3:D:521:ALA:HB1	1.97	0.47
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.14	0.47
4:E:47:VAL:HG21	4:E:53:LEU:HB2	1.95	0.47
5:F:467:LEU:CD2	5:F:519:ARG:NH1	2.78	0.47
2:C:374:GLY:HA3	2:C:534:ASP:OD1	2.14	0.47
2:C:419:ASN:O	2:C:422:PRO:HD2	2.15	0.47
2:C:776:ILE:HD11	2:C:780:VAL:HG21	1.95	0.47
2:C:928:ILE:HD12	2:C:929:GLY:N	2.30	0.47
3:D:157:VAL:HA	3:D:160:LYS:HG2	1.95	0.47
3:D:360:LEU:H	3:D:360:LEU:CD1	2.28	0.47
3:D:387:ARG:NH1	5:F:225:ALA:HB1	2.30	0.47
3:D:704:TYR:HB3	3:D:705:PRO:HD2	1.96	0.47
5:F:482:THR:HG23	5:F:483:ASP:N	2.30	0.47
1:A:9:LEU:HD23	1:A:9:LEU:O	2.15	0.47
1:A:18:ARG:HH21	2:C:996:ARG:HH12	1.61	0.47
1:A:128:LEU:HD12	1:A:128:LEU:N	2.29	0.47
2:C:105:LEU:HD12	2:C:138:GLU:O	2.14	0.47
2:C:329:THR:O	2:C:329:THR:HG23	2.14	0.47
2:C:395:ARG:O	2:C:399:VAL:HG23	2.14	0.47
2:C:486:ILE:CD1	3:D:849:TYR:HE2	2.27	0.47
2:C:623:ALA:HB2	2:C:709:ASP:OD2	2.14	0.47
2:C:771:ARG:HE	2:C:781:LEU:HD21	1.79	0.47
2:C:792:ILE:HD12	2:C:792:ILE:H	1.79	0.47
2:C:905:PRO:HD2	2:C:916:ILE:HD11	1.96	0.47
2:C:942:SER:O	2:C:968:PRO:HB3	2.15	0.47
2:C:1045:SER:HB3	3:D:450:GLU:O	2.14	0.47
2:C:1088:LEU:HD23	2:C:1092:LYS:HD2	1.97	0.47
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:ARG:HG3	3:D:212:ALA:CB	2.44	0.47
3:D:230:ALA:O	3:D:233:GLN:HG3	2.14	0.47
3:D:557:ILE:CD1	4:E:54:VAL:HG22	2.44	0.47
3:D:757:GLU:OE1	3:D:770:ARG:HD3	2.15	0.47
4:E:47:VAL:HG12	4:E:48:SER:N	2.30	0.47
5:F:378:LYS:O	5:F:382:ILE:HD13	2.15	0.47
5:F:386:LEU:HD23	5:F:386:LEU:O	2.15	0.47
5:F:387:LEU:HG	5:F:392:ARG:O	2.15	0.47
6:J:4:ARG:HA	6:J:4:ARG:HE	1.80	0.47
7:O:20:DT:H2"	7:O:21:DT:H71	1.96	0.47
1:A:106:THR:HB	1:A:123:MET:O	2.15	0.47
2:C:265:ASP:OD1	2:C:266:ASN:N	2.48	0.47
2:C:736:ILE:HG12	2:C:916:ILE:HB	1.96	0.47
3:D:340:LEU:HD21	3:D:402:LEU:HD23	1.95	0.47
3:D:360:LEU:HD12	3:D:360:LEU:N	2.29	0.47
3:D:579:LEU:HD23	3:D:807:ALA:O	2.14	0.47
3:D:823:LEU:CD2	3:D:835:PRO:HB3	2.33	0.47
3:D:1252:VAL:HG23	3:D:1258:ILE:HG22	1.97	0.47
1:A:66:VAL:O	1:A:69:VAL:HG22	2.13	0.47
2:C:235:THR:HG21	2:C:265:ASP:HB3	1.96	0.47
3:D:207:GLN:OE1	3:D:208:ILE:HD12	2.15	0.47
3:D:1189:GLU:HG3	3:D:1190:ASN:N	2.30	0.47
3:D:1243:ASP:OD1	3:D:1245:LEU:N	2.25	0.47
5:F:281:MET:HG3	5:F:282:MET:N	2.30	0.47
5:F:460:LEU:O	5:F:464:LEU:HD13	2.15	0.47
2:C:205:ILE:HG22	2:C:211:TRP:CD2	2.50	0.47
2:C:279:ARG:O	2:C:283:PRO:HA	2.15	0.47
2:C:561:VAL:HG22	2:C:562:ARG:N	2.30	0.47
2:C:1051:MET:SD	3:D:328:VAL:HG21	2.54	0.47
3:D:19:ASP:O	3:D:22:GLN:N	2.33	0.47
3:D:1272:VAL:HG13	4:E:56:TYR:CE1	2.50	0.47
5:F:241:LEU:HA	5:F:245:GLU:OE1	2.14	0.47
5:F:482:THR:HG23	5:F:483:ASP:H	1.80	0.47
1:A:153:ARG:NE	2:C:797:ARG:HG2	2.31	0.46
1:B:60:LEU:H	1:B:60:LEU:CD2	2.28	0.46
1:B:68:GLY:O	1:B:129:ASN:N	2.38	0.46
2:C:141:ASN:OD1	2:C:142:ASN:N	2.48	0.46
2:C:646:GLU:HB3	2:C:662:HIS:HD1	1.81	0.46
3:D:384:ASN:HB2	3:D:401:SER:HB3	1.97	0.46
3:D:765:LEU:HD23	3:D:765:LEU:N	2.29	0.46
5:F:386:LEU:HD22	5:F:394:PRO:CB	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:19:DA:H2'	7:O:20:DT:H72	1.97	0.46
1:A:49:ALA:CB	1:A:87:SER:H	2.28	0.46
1:B:100:GLN:HA	1:B:133:LYS:HA	1.97	0.46
2:C:480:TYR:CD2	2:C:562:ARG:NH1	2.83	0.46
2:C:814:LEU:HD22	2:C:814:LEU:N	2.30	0.46
3:D:173:ARG:NE	3:D:205:MET:HG2	2.29	0.46
4:E:64:ILE:O	4:E:67:TYR:HB3	2.16	0.46
5:F:372:MET:O	5:F:375:VAL:HG22	2.16	0.46
6:J:99:LYS:O	6:J:102:LEU:HB3	2.16	0.46
8:P:10:DT:H2"	8:P:11:DA:H8	1.79	0.46
1:A:84:VAL:HG13	1:A:84:VAL:O	2.16	0.46
1:A:220:GLY:HA2	1:A:223:ARG:HB2	1.97	0.46
2:C:677:ARG:HG2	2:C:678:SER:O	2.15	0.46
2:C:883:ASP:O	2:C:895:ILE:HG13	2.16	0.46
2:C:1009:MET:HA	2:C:1009:MET:CE	2.45	0.46
2:C:1049:TYR:CD1	2:C:1099:ARG:NH1	2.83	0.46
3:D:73:ILE:CG2	6:J:27:ARG:NH1	2.78	0.46
3:D:1089:PHE:CD2	3:D:1099:LEU:HB2	2.49	0.46
3:D:1110:GLN:NE2	3:D:1112:MET:O	2.48	0.46
5:F:333:GLU:HA	6:J:81:HIS:NE2	2.31	0.46
8:P:11:DA:C2'	8:P:12:DA:H5'	2.38	0.46
1:A:24:GLU:OE1	1:A:191:LYS:HD2	2.15	0.46
2:C:351:GLY:O	2:C:352:GLN:HG2	2.15	0.46
2:C:633:ARG:O	2:C:633:ARG:HG3	2.15	0.46
3:D:39:LEU:HD22	3:D:335:PHE:CZ	2.50	0.46
3:D:186:ALA:HB3	3:D:187:GLU:OE1	2.15	0.46
3:D:246:ASP:OD1	3:D:247:ARG:N	2.49	0.46
3:D:262:GLN:HE21	3:D:310:MET:CE	2.29	0.46
3:D:453:LYS:HG3	3:D:476:VAL:HG11	1.97	0.46
3:D:1176:LEU:HD12	3:D:1176:LEU:N	2.29	0.46
2:C:185:VAL:HG12	2:C:204:VAL:HG22	1.96	0.46
2:C:854:SER:H	2:C:859:ASP:HB2	1.79	0.46
3:D:587:TYR:HE1	3:D:630:ARG:NH1	2.14	0.46
3:D:1030:ARG:NH2	3:D:1034:LEU:HD21	2.31	0.46
3:D:1089:PHE:HE2	3:D:1103:ASP:OD2	1.91	0.46
5:F:489:LEU:HG	8:P:20:DG:OP2	2.15	0.46
2:C:48:LEU:HB2	2:C:528:ILE:CD1	2.46	0.46
2:C:532:THR:HG23	2:C:535:GLU:HG2	1.98	0.46
2:C:792:ILE:HD12	2:C:792:ILE:N	2.30	0.46
2:C:922:VAL:HG22	2:C:930:GLN:HE21	1.80	0.46
3:D:339:ASP:OD2	5:F:424:ASP:OD2	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:453:LYS:HB3	3:D:453:LYS:HZ2	1.80	0.46
3:D:572:ARG:HB2	3:D:573:PRO:HD2	1.98	0.46
3:D:708:VAL:HG22	4:E:29:TYR:HB3	1.97	0.46
5:F:407:PRO:O	5:F:410:VAL:HG12	2.16	0.46
1:B:162:ILE:CG2	3:D:607:PRO:HG3	2.46	0.46
2:C:344:TYR:OH	2:C:365:VAL:HA	2.16	0.46
2:C:571:VAL:HG13	2:C:572:PRO:N	2.30	0.46
3:D:139:VAL:HG12	3:D:231:PRO:HD3	1.98	0.46
3:D:963:ARG:HD2	3:D:978:CYS:HA	1.96	0.46
5:F:292:LYS:O	5:F:296:LEU:HG	2.14	0.46
5:F:381:ARG:HA	5:F:384:ARG:NH2	2.30	0.46
1:A:218:LEU:HD21	1:B:34:LEU:CD2	2.46	0.46
3:D:165:GLN:O	3:D:169:GLU:HG2	2.15	0.46
5:F:257:LEU:HD21	6:J:81:HIS:CE1	2.50	0.46
7:O:5:DG:H2"	7:O:6:DA:O4'	2.14	0.46
1:B:3:ILE:HG23	1:B:5:GLN:O	2.15	0.46
1:B:96:TYR:HD1	1:B:137:GLU:HG2	1.78	0.46
1:B:107:ALA:HB3	1:B:121:PRO:C	2.36	0.46
1:B:151:GLN:HE22	1:B:155:SER:HA	1.81	0.46
2:C:278:TYR:CE1	2:C:291:SER:HB2	2.51	0.46
2:C:400:VAL:O	2:C:404:MET:N	2.49	0.46
3:D:57:ASP:HB3	3:D:58:TRP:CE3	2.50	0.46
3:D:414:ARG:HB2	3:D:414:ARG:HH21	1.80	0.46
3:D:449:LEU:O	3:D:449:LEU:HD22	2.16	0.46
3:D:1128:ARG:NH1	3:D:1132:ILE:CG1	2.67	0.46
1:A:35:GLY:HA2	1:A:192:LEU:HD21	1.98	0.46
2:C:421:ARG:N	2:C:422:PRO:HD2	2.31	0.46
2:C:484:CYS:HB2	2:C:588:SER:HB3	1.97	0.46
2:C:737:LEU:HD23	2:C:915:ILE:HG22	1.97	0.46
2:C:877:ARG:NH1	2:C:1036:LEU:HD12	2.20	0.46
2:C:1135:VAL:HA	3:D:11:ARG:O	2.16	0.46
3:D:1055:LEU:H	3:D:1101:ASP:CG	2.20	0.46
4:E:84:GLU:H	4:E:84:GLU:CD	2.20	0.46
5:F:300:LEU:O	5:F:304:VAL:HG23	2.16	0.46
6:J:32:TYR:OH	6:J:51:PRO:HG2	2.15	0.46
6:J:76:LYS:H	6:J:76:LYS:HD2	1.80	0.46
6:J:101:ARG:HH11	6:J:101:ARG:CA	2.29	0.46
1:A:184:GLU:OE1	1:A:184:GLU:HA	2.16	0.45
1:A:187:THR:O	1:A:187:THR:HG23	2.16	0.45
1:B:80:LEU:CD2	1:B:125:ILE:HD13	2.46	0.45
1:B:196:VAL:O	1:B:196:VAL:HG22	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:GLN:O	2:C:442:GLN:HG3	2.16	0.45
2:C:444:ASN:HD22	2:C:715:LEU:HD22	1.81	0.45
2:C:643:VAL:HG13	2:C:699:GLY:O	2.16	0.45
2:C:1068:PHE:CE1	2:C:1072:GLU:HB3	2.51	0.45
3:D:234:LEU:HD23	3:D:235:ILE:N	2.31	0.45
3:D:243:GLU:O	3:D:247:ARG:HB3	2.17	0.45
3:D:778:TRP:NE1	3:D:835:PRO:HD3	2.31	0.45
3:D:1012:MET:C	3:D:1027:GLY:CA	2.85	0.45
4:E:81:PRO:HB3	4:E:94:ILE:HG21	1.98	0.45
6:J:6:LEU:H	6:J:6:LEU:HD12	1.81	0.45
1:A:147:VAL:HG12	1:A:168:TYR:CE2	2.50	0.45
1:B:14:LEU:HB2	1:B:18:ARG:O	2.16	0.45
1:B:218:LEU:HD23	1:B:218:LEU:C	2.37	0.45
2:C:298:ASN:HA	2:C:302:LYS:HE3	1.99	0.45
2:C:581:VAL:H	2:C:585:GLN:NE2	2.14	0.45
3:D:405:LEU:C	3:D:406:LEU:HD12	2.36	0.45
1:B:2:LEU:HD22	1:B:4:SER:H	1.80	0.45
2:C:482:ARG:NH1	2:C:533:ALA:HA	2.32	0.45
2:C:606:LEU:HD23	2:C:606:LEU:C	2.36	0.45
2:C:661:MET:HE2	2:C:667:ARG:HG2	1.99	0.45
2:C:959:LEU:HD12	2:C:959:LEU:H	1.81	0.45
3:D:466:ALA:HB1	3:D:471:SER:OG	2.16	0.45
5:F:274:PRO:HD2	5:F:277:GLN:HG2	1.98	0.45
2:C:694:ASP:OD1	2:C:694:ASP:N	2.50	0.45
3:D:263:LYS:NZ	3:D:263:LYS:CB	2.78	0.45
3:D:557:ILE:HD13	4:E:53:LEU:HD23	1.98	0.45
3:D:1085:ARG:HG2	3:D:1113:GLU:OE1	2.17	0.45
5:F:350:TRP:HH2	7:O:25:DC:OP2	1.99	0.45
1:B:95:MET:HG2	1:B:113:PRO:HD3	1.99	0.45
1:B:107:ALA:HB3	1:B:121:PRO:O	2.16	0.45
2:C:211:TRP:O	2:C:227:ASP:N	2.44	0.45
2:C:254:PHE:N	2:C:255:SER:CB	2.77	0.45
2:C:571:VAL:CG2	2:C:572:PRO:HD2	2.29	0.45
3:D:453:LYS:HB3	3:D:454:PRO:HD3	1.98	0.45
3:D:915:TYR:CE1	3:D:1143:ARG:HD3	2.51	0.45
1:A:127:THR:C	1:A:128:LEU:HD12	2.37	0.45
1:A:144:ARG:HG2	1:B:1:MET:CE	2.46	0.45
1:B:59:VAL:HG12	1:B:59:VAL:O	2.17	0.45
1:B:70:LYS:NZ	1:B:70:LYS:HB2	2.31	0.45
2:C:71:ARG:O	2:C:75:ALA:HB2	2.16	0.45
2:C:622:GLU:OE2	2:C:718:ASN:ND2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:668:ARG:HD3	2:C:669:THR:N	2.32	0.45
2:C:1012:ASP:HB2	2:C:1019:PHE:CE1	2.52	0.45
3:D:387:ARG:NH2	5:F:225:ALA:HA	2.32	0.45
3:D:1129:GLU:HA	3:D:1129:GLU:OE1	2.16	0.45
1:B:65:THR:HG22	1:B:66:VAL:N	2.32	0.45
1:B:84:VAL:CG2	1:B:119:HIS:HB2	2.45	0.45
2:C:757:ILE:HG22	2:C:869:VAL:HG13	1.98	0.45
2:C:805:LYS:HB3	2:C:835:THR:O	2.17	0.45
3:D:151:LEU:HD21	3:D:251:TYR:HE2	1.82	0.45
3:D:365:ILE:HD12	3:D:365:ILE:N	2.26	0.45
3:D:1101:ASP:OD1	3:D:1102:GLY:N	2.50	0.45
5:F:429:ASP:O	5:F:431:GLY:HA2	2.16	0.45
1:B:66:VAL:HG23	1:B:73:VAL:HG22	1.99	0.45
2:C:400:VAL:CG1	2:C:417:LEU:HB3	2.37	0.45
2:C:471:GLU:OE1	2:C:471:GLU:N	2.50	0.45
3:D:177:LEU:HD23	3:D:178:GLU:N	2.32	0.45
3:D:313:VAL:O	3:D:313:VAL:HG23	2.16	0.45
3:D:900:GLU:N	3:D:900:GLU:OE1	2.50	0.45
5:F:329:ILE:O	5:F:333:GLU:HG3	2.17	0.45
6:J:36:ASN:ND2	6:J:60:MET:SD	2.90	0.45
8:P:1:DA:H2"	8:P:2:DG:O4'	2.17	0.45
2:C:188:ASP:OD1	2:C:188:ASP:N	2.50	0.45
2:C:203:LYS:HB2	2:C:203:LYS:NZ	2.32	0.45
3:D:641:ARG:HA	3:D:657:GLN:HB2	1.98	0.45
3:D:864:ALA:O	3:D:867:THR:HG22	2.17	0.45
5:F:232:LEU:O	5:F:235:ILE:HG12	2.16	0.45
5:F:379:LEU:HD23	5:F:379:LEU:C	2.37	0.45
5:F:511:MET:CB	5:F:515:ARG:HH12	2.30	0.45
6:J:101:ARG:HH11	6:J:101:ARG:CB	2.29	0.45
1:A:102:PRO:HD3	1:A:130:ASP:HA	1.98	0.45
1:B:77:ILE:HG23	1:B:164:VAL:CG1	2.47	0.45
2:C:225:ARG:HD3	2:C:230:ARG:C	2.37	0.45
2:C:848:ILE:HD12	2:C:874:ALA:HB2	1.98	0.45
3:D:574:LEU:HD12	3:D:574:LEU:HA	1.81	0.45
3:D:865:LEU:HD13	3:D:865:LEU:C	2.38	0.45
3:D:930:VAL:HA	3:D:937:ILE:HG22	1.98	0.45
3:D:1051:GLY:O	3:D:1104:HIS:HA	2.17	0.45
3:D:1070:ASP:HB2	3:D:1071:GLY:C	2.38	0.45
3:D:1148:SER:O	3:D:1149:ILE:HD13	2.17	0.45
3:D:1175:PHE:CZ	3:D:1189:GLU:HG2	2.52	0.45
5:F:279:ARG:NH2	5:F:279:ARG:HB3	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:516:HIS:HD2	5:F:518:SER:OG	1.99	0.45
1:A:55:ARG:HH21	1:A:161:ARG:HH12	1.64	0.44
1:A:97:LEU:HD21	1:A:105:VAL:CG1	2.47	0.44
1:B:166:SER:HB3	1:B:168:TYR:CE1	2.52	0.44
2:C:1076:MET:HE1	3:D:559:MET:SD	2.57	0.44
3:D:113:ARG:HG2	3:D:1238:ILE:HD11	1.99	0.44
3:D:487:LEU:HD12	3:D:491:ILE:HG13	1.99	0.44
3:D:576:MET:HG3	3:D:697:ILE:HD12	1.99	0.44
3:D:1062:TYR:CD2	3:D:1112:MET:HE3	2.52	0.44
1:A:215:LEU:HG	1:B:219:PHE:CE1	2.52	0.44
2:C:952:VAL:CG1	2:C:957:ALA:HA	2.44	0.44
3:D:111:PRO:HB2	3:D:116:TYR:HE2	1.79	0.44
1:A:11:GLU:CD	1:A:205:ARG:HE	2.20	0.44
1:A:56:ILE:HG12	1:A:136:VAL:HB	1.98	0.44
2:C:231:ARG:CG	2:C:232:GLN:N	2.80	0.44
3:D:1226:PHE:CE2	3:D:1249:LYS:NZ	2.85	0.44
5:F:438:PHE:HB3	6:J:4:ARG:O	2.17	0.44
6:J:33:ARG:HD3	6:J:34:THR:O	2.17	0.44
1:A:62:GLU:O	1:A:62:GLU:HG2	2.17	0.44
2:C:323:HIS:O	2:C:326:GLU:HB2	2.17	0.44
4:E:31:THR:HG23	4:E:31:THR:O	2.18	0.44
1:A:40:ARG:NE	1:B:33:THR:HG22	2.32	0.44
2:C:224:VAL:HG22	2:C:234:VAL:HG12	1.98	0.44
2:C:274:LEU:HG	2:C:292:ALA:CB	2.48	0.44
3:D:211:ARG:HA	3:D:214:ARG:NH2	2.33	0.44
3:D:456:VAL:O	3:D:460:LEU:HG	2.18	0.44
3:D:1053:VAL:CG1	3:D:1103:ASP:H	2.31	0.44
3:D:1063:LYS:HZ2	3:D:1076:VAL:CG1	2.30	0.44
7:O:23:DT:H2"	7:O:24:DG:H8	1.83	0.44
1:A:95:MET:HE1	1:A:110:ILE:HG21	1.98	0.44
3:D:58:TRP:CA	3:D:82:VAL:HG23	2.46	0.44
3:D:223:TRP:O	3:D:227:THR:HG23	2.17	0.44
3:D:341:ASN:O	3:D:345:ARG:HG3	2.18	0.44
3:D:1069:ASP:OD2	3:D:1104:HIS:HE1	2.01	0.44
4:E:43:LEU:HB3	4:E:53:LEU:HD11	1.99	0.44
1:A:226:ASN:HB2	1:B:9:LEU:HD23	1.99	0.44
1:B:38:LEU:HD13	1:B:38:LEU:HA	1.74	0.44
1:B:74:THR:OG1	3:D:608:GLU:OE2	2.33	0.44
1:B:112:PRO:HB2	1:B:116:VAL:HG23	2.00	0.44
2:C:219:ARG:HG3	2:C:220:ASP:O	2.17	0.44
3:D:860:LEU:HD12	3:D:860:LEU:HA	1.88	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:909:THR:O	3:D:910:LEU:CB	2.66	0.44
3:D:952:LEU:HB3	3:D:957:ILE:CD1	2.43	0.44
3:D:1064:ILE:CD1	3:D:1080:ILE:HD12	2.48	0.44
3:D:1221:LEU:HD23	3:D:1221:LEU:N	2.33	0.44
1:A:1:MET:O	1:A:2:LEU:HD12	2.18	0.44
1:B:161:ARG:O	1:B:161:ARG:HG3	2.18	0.44
2:C:568:VAL:CG1	3:D:847:LEU:HD23	2.48	0.44
2:C:619:VAL:HG23	2:C:620:ARG:HG2	2.00	0.44
3:D:20:ILE:HG21	3:D:316:ALA:O	2.18	0.44
3:D:148:LEU:O	3:D:148:LEU:HD22	2.18	0.44
3:D:1063:LYS:HZ1	3:D:1078:ASP:CA	2.19	0.44
5:F:246:GLU:OE1	5:F:247:VAL:HG23	2.17	0.44
8:P:18:DT:H2"	8:P:19:DT:C6	2.53	0.44
1:B:107:ALA:O	1:B:110:ILE:HG22	2.17	0.44
2:C:476:HIS:H	2:C:479:HIS:CD2	2.36	0.44
2:C:611:MET:HE2	2:C:1033:LEU:HD21	2.00	0.44
2:C:730:ASN:HA	2:C:734:ALA:HB3	2.00	0.44
2:C:845:GLY:HA3	2:C:874:ALA:O	2.17	0.44
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.99	0.44
3:D:460:LEU:C	3:D:460:LEU:HD12	2.38	0.44
3:D:463:LEU:HD23	3:D:463:LEU:H	1.82	0.44
1:B:55:ARG:HB2	1:B:55:ARG:CZ	2.47	0.43
2:C:278:TYR:CD2	2:C:291:SER:HB2	2.52	0.43
4:E:76:LEU:HG	4:E:77:GLU:N	2.33	0.43
5:F:477:LEU:O	5:F:487:ARG:HG2	2.18	0.43
1:A:9:LEU:HD12	1:A:23:ILE:CD1	2.44	0.43
1:B:78:LEU:C	1:B:78:LEU:HD12	2.39	0.43
2:C:542:ALA:HB3	2:C:579:MET:CB	2.47	0.43
2:C:612:GLN:HE21	2:C:888:ARG:HG3	1.81	0.43
2:C:817:GLU:HG2	5:F:457:GLN:HG2	2.00	0.43
3:D:236:VAL:O	3:D:236:VAL:HG12	2.19	0.43
3:D:647:GLU:HG3	3:D:648:ALA:N	2.33	0.43
3:D:1050:THR:HG23	3:D:1107:VAL:HG22	2.00	0.43
3:D:1097:ARG:NH1	3:D:1100:SER:HB2	2.26	0.43
5:F:394:PRO:HB2	5:F:399:LEU:HD11	2.00	0.43
2:C:202:VAL:HG22	2:C:203:LYS:N	2.34	0.43
2:C:761:ASP:HA	2:C:766:ALA:HA	1.99	0.43
3:D:25:TYR:CD2	3:D:91:ARG:HD3	2.54	0.43
3:D:136:ILE:HD11	3:D:235:ILE:HD11	2.00	0.43
3:D:290:LEU:O	3:D:294:LYS:HG3	2.18	0.43
3:D:495:PRO:HA	3:D:512:PHE:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:535:ASP:OD1	3:D:539:ASP:OD2	2.36	0.43
5:F:233:LYS:HE2	5:F:233:LYS:HB3	1.79	0.43
5:F:258:TYR:CE2	6:J:98:LEU:HD13	2.54	0.43
5:F:492:ILE:HD11	5:F:503:ILE:HG21	2.01	0.43
8:P:3:DC:H2"	8:P:4:DA:O5'	2.18	0.43
2:C:524:VAL:HB	2:C:552:GLY:HA2	1.99	0.43
2:C:641:VAL:CG1	2:C:701:VAL:HG13	2.48	0.43
2:C:760:ARG:HB3	2:C:864:GLY:O	2.18	0.43
1:A:35:GLY:CA	1:A:192:LEU:HD21	2.49	0.43
1:A:97:LEU:HB2	1:A:110:ILE:HG12	2.00	0.43
2:C:103:MET:HG3	2:C:404:MET:CE	2.48	0.43
2:C:215:ASP:N	2:C:223:GLY:HA3	2.33	0.43
2:C:519:VAL:HG23	2:C:524:VAL:N	2.33	0.43
2:C:754:GLU:HB2	2:C:872:TYR:CE1	2.53	0.43
2:C:762:THR:HG23	2:C:765:GLY:H	1.83	0.43
2:C:774:PRO:O	2:C:776:ILE:HG22	2.19	0.43
3:D:102:THR:HG22	3:D:313:VAL:HG12	2.00	0.43
3:D:505:HIS:H	3:D:505:HIS:CD2	2.36	0.43
3:D:1256:LYS:HG2	3:D:1257:LEU:N	2.34	0.43
5:F:278:ARG:NH2	5:F:278:ARG:O	2.52	0.43
5:F:491:GLU:O	5:F:494:GLN:HB3	2.18	0.43
1:B:128:LEU:N	1:B:128:LEU:HD12	2.33	0.43
2:C:781:LEU:HA	2:C:784:LEU:HD13	2.01	0.43
2:C:994:PRO:HB3	2:C:999:ASP:N	2.16	0.43
2:C:994:PRO:CG	2:C:998:GLY:HA2	2.48	0.43
3:D:118:LEU:HB3	3:D:120:LEU:HD13	2.01	0.43
3:D:513:GLU:HB2	4:E:35:ILE:HG13	2.01	0.43
3:D:646:ILE:CG2	3:D:650:LEU:HD12	2.49	0.43
3:D:1097:ARG:NH1	3:D:1100:SER:N	2.66	0.43
4:E:50:LYS:O	4:E:54:VAL:HG23	2.19	0.43
5:F:273:LEU:HB3	5:F:274:PRO:CD	2.48	0.43
5:F:430:GLU:HA	5:F:431:GLY:HA3	1.63	0.43
7:O:7:DC:H2"	7:O:8:DA:H8	1.83	0.43
7:O:19:DA:H2"	7:O:20:DT:C5'	2.48	0.43
1:B:74:THR:HG21	3:D:608:GLU:OE2	2.18	0.43
2:C:113:ASP:HB2	2:C:132:PRO:HD2	2.00	0.43
2:C:946:VAL:HG12	2:C:948:ALA:H	1.83	0.43
2:C:967:GLN:CD	2:C:968:PRO:HD2	2.39	0.43
3:D:125:LEU:CD1	3:D:261:ILE:HD11	2.44	0.43
3:D:336:ALA:HA	5:F:421:ILE:O	2.18	0.43
3:D:1055:LEU:HD23	3:D:1055:LEU:C	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1087:ARG:CG	3:D:1088:VAL:N	2.78	0.43
7:O:11:DA:H2"	7:O:12:DG:H5"	2.01	0.43
1:A:9:LEU:HD21	1:B:225:LEU:HD11	2.00	0.43
1:A:65:THR:HG22	1:A:72:ASP:CB	2.48	0.43
1:A:219:PHE:CG	1:B:215:LEU:HD22	2.54	0.43
1:B:78:LEU:HD12	3:D:636:ARG:HH21	1.83	0.43
2:C:77:ARG:HG3	2:C:77:ARG:O	2.18	0.43
2:C:195:THR:HG21	2:C:218:LYS:HG3	1.99	0.43
2:C:593:MET:HA	2:C:628:THR:HG21	2.01	0.43
2:C:597:LEU:HD23	2:C:976:VAL:CG1	2.48	0.43
3:D:60:CYS:SG	3:D:63:GLY:N	2.89	0.43
3:D:834:ARG:HA	3:D:834:ARG:NE	2.29	0.43
3:D:1251:ASN:CG	3:D:1259:PRO:HD3	2.39	0.43
4:E:92:LEU:O	4:E:92:LEU:HD13	2.19	0.43
5:F:442:SER:HB3	6:J:7:ARG:CG	2.48	0.43
1:A:225:LEU:C	1:A:225:LEU:HD13	2.38	0.43
1:B:182:ARG:HG3	1:B:186:ARG:H	1.84	0.43
2:C:79:ASP:N	2:C:79:ASP:OD1	2.51	0.43
2:C:112:PHE:CD1	2:C:159:MET:HE1	2.54	0.43
2:C:205:ILE:O	2:C:205:ILE:HG13	2.18	0.43
2:C:624:PRO:HB3	2:C:1029:TYR:CE1	2.54	0.43
2:C:626:VAL:O	2:C:888:ARG:NH2	2.50	0.43
2:C:830:ARG:HD2	2:C:832:VAL:HG22	2.01	0.43
2:C:897:LYS:HG3	2:C:899:LEU:HD13	2.00	0.43
2:C:982:GLU:HB2	3:D:841:ARG:NH2	2.33	0.43
2:C:1128:LEU:CD2	3:D:406:LEU:HD21	2.48	0.43
3:D:117:LEU:HD13	3:D:117:LEU:C	2.39	0.43
3:D:274:ALA:O	3:D:278:ARG:HD3	2.19	0.43
3:D:294:LYS:O	3:D:297:LYS:HB3	2.18	0.43
3:D:482:GLN:OE1	3:D:482:GLN:N	2.43	0.43
3:D:905:ALA:HB2	3:D:911:ILE:HD12	2.00	0.43
5:F:472:ALA:O	5:F:476:ARG:HG3	2.19	0.43
1:A:47:PRO:HG3	1:B:230:GLU:O	2.18	0.43
1:A:54:ILE:HD11	1:A:77:ILE:CD1	2.49	0.43
1:B:181:THR:HG21	1:B:191:LYS:HD3	2.00	0.43
2:C:38:ARG:HG2	2:C:973:SER:HB3	2.01	0.43
2:C:762:THR:N	2:C:765:GLY:O	2.48	0.43
2:C:820:LEU:HA	5:F:479:PHE:CE1	2.53	0.43
2:C:1119:GLU:O	2:C:1119:GLU:HG2	2.19	0.43
3:D:121:ALA:HB3	3:D:124:ASP:CG	2.38	0.43
3:D:436:LEU:HD22	3:D:515:MET:HE1	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:596:THR:HG22	3:D:626:VAL:O	2.19	0.43
3:D:901:LEU:HD12	3:D:960:VAL:CG2	2.49	0.43
3:D:975:CYS:SG	3:D:978:CYS:HB2	2.58	0.43
4:E:101:ALA:CB	4:E:103:LEU:HD13	2.49	0.43
5:F:418:ARG:HB2	5:F:418:ARG:CZ	2.49	0.43
7:O:6:DA:H2"	7:O:7:DC:C5'	2.49	0.43
1:A:46:ILE:HD12	1:A:210:SER:OG	2.18	0.42
1:B:3:ILE:O	1:B:4:SER:OG	2.29	0.42
2:C:196:ASP:N	2:C:196:ASP:OD1	2.50	0.42
2:C:343:GLU:HA	2:C:346:VAL:HG12	2.00	0.42
2:C:809:LYS:NZ	2:C:832:VAL:O	2.52	0.42
2:C:881:ASP:OD1	2:C:881:ASP:N	2.52	0.42
3:D:55:THR:HG22	6:J:12:GLY:HA2	2.01	0.42
3:D:459:ARG:HH21	4:E:88:GLN:NE2	2.17	0.42
3:D:753:ALA:HB1	3:D:774:LEU:CD2	2.48	0.42
3:D:866:ARG:HH11	3:D:1011:THR:HA	1.81	0.42
3:D:1008:THR:HG22	3:D:1008:THR:O	2.19	0.42
3:D:1053:VAL:HG12	3:D:1103:ASP:N	2.34	0.42
3:D:1070:ASP:HB2	3:D:1071:GLY:HA2	2.00	0.42
5:F:456:LEU:HD13	5:F:526:TYR:CD2	2.54	0.42
6:J:108:ARG:HD3	6:J:108:ARG:N	2.34	0.42
1:B:50:ALA:HB3	1:B:168:TYR:CD1	2.54	0.42
1:B:69:VAL:HG23	1:B:71:GLU:O	2.20	0.42
2:C:93:LEU:HD12	2:C:96:ILE:HD11	2.01	0.42
2:C:221:THR:OG1	2:C:261:THR:HG22	2.18	0.42
2:C:476:HIS:HD2	2:C:478:SER:H	1.67	0.42
2:C:820:LEU:HB2	5:F:479:PHE:CD1	2.53	0.42
3:D:37:ARG:HB3	3:D:37:ARG:NH1	2.34	0.42
3:D:433:GLY:O	3:D:436:LEU:HG	2.19	0.42
3:D:684:VAL:HG11	3:D:688:MET:CE	2.49	0.42
3:D:771:ASN:OD1	3:D:833:PRO:HG3	2.19	0.42
3:D:1080:ILE:CG2	3:D:1112:MET:HE3	2.46	0.42
8:P:2:DG:H2"	8:P:3:DC:O5'	2.19	0.42
1:B:100:GLN:CB	1:B:133:LYS:HB2	2.49	0.42
2:C:230:ARG:O	2:C:231:ARG:CB	2.64	0.42
2:C:357:VAL:HG22	2:C:358:PRO:CD	2.49	0.42
2:C:658:ILE:HD11	2:C:688:PRO:CB	2.25	0.42
3:D:932:GLU:O	3:D:933:ALA:C	2.56	0.42
1:A:183:VAL:HG13	1:A:185:GLN:OE1	2.20	0.42
2:C:141:ASN:O	2:C:145:GLY:HA2	2.19	0.42
2:C:353:THR:HG23	2:C:354:THR:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:518:LYS:HG3	2:C:518:LYS:O	2.19	0.42
2:C:548:ILE:HD11	2:C:579:MET:CE	2.50	0.42
3:D:151:LEU:HD21	3:D:251:TYR:OH	2.18	0.42
3:D:268:PHE:CZ	3:D:273:GLU:HG3	2.54	0.42
3:D:444:PRO:HD2	3:D:447:MET:CE	2.49	0.42
3:D:588:LEU:O	3:D:588:LEU:HD13	2.19	0.42
3:D:952:LEU:CB	3:D:957:ILE:HD11	2.43	0.42
3:D:989:VAL:HG22	3:D:990:ASP:N	2.34	0.42
3:D:1040:PRO:HB2	3:D:1115:SER:HB2	2.01	0.42
3:D:1048:ASP:OD2	3:D:1075:VAL:HG11	2.20	0.42
3:D:1166:THR:HB	3:D:1206:VAL:CG2	2.48	0.42
1:A:57:ASP:N	1:A:57:ASP:OD1	2.52	0.42
1:A:217:GLU:O	1:B:234:ILE:HD12	2.19	0.42
2:C:173:ARG:NH1	2:C:439:PHE:CZ	2.87	0.42
2:C:436:LEU:HD13	2:C:460:PRO:HD2	2.02	0.42
3:D:834:ARG:HB2	3:D:835:PRO:HA	2.02	0.42
3:D:913:ASP:N	3:D:916:ILE:HD11	2.35	0.42
3:D:1117:ASP:OD1	3:D:1120:GLU:HB2	2.19	0.42
1:B:6:ARG:CZ	1:B:237:SER:HA	2.49	0.42
2:C:353:THR:O	2:C:365:VAL:N	2.24	0.42
2:C:967:GLN:O	2:C:970:ALA:HB2	2.20	0.42
3:D:64:LYS:NZ	3:D:65:TYR:OH	2.52	0.42
3:D:91:ARG:O	3:D:321:PRO:HG3	2.19	0.42
3:D:216:LEU:N	3:D:216:LEU:HD23	2.35	0.42
3:D:657:GLN:HA	3:D:660:ASP:OD1	2.19	0.42
3:D:1044:ALA:HA	3:D:1084:GLN:NE2	2.35	0.42
5:F:395:THR:OG1	5:F:397:GLU:OE1	2.30	0.42
5:F:470:ARG:O	5:F:474:VAL:HG23	2.19	0.42
6:J:31:ARG:O	6:J:65:ILE:HB	2.19	0.42
1:B:118:VAL:HG12	1:B:120:ASN:H	1.84	0.42
1:B:177:LYS:O	1:B:177:LYS:HD3	2.19	0.42
2:C:213:GLU:O	2:C:223:GLY:O	2.37	0.42
2:C:231:ARG:HB3	5:F:205:ASP:OD2	2.19	0.42
2:C:274:LEU:CG	2:C:292:ALA:HB1	2.48	0.42
2:C:282:ARG:HB3	2:C:283:PRO:O	2.19	0.42
2:C:308:LEU:H	2:C:308:LEU:HD23	1.84	0.42
2:C:587:VAL:HG13	2:C:591:THR:CG2	2.49	0.42
2:C:797:ARG:HD3	2:C:798:ASP:N	2.35	0.42
2:C:1076:MET:HA	2:C:1076:MET:CE	2.50	0.42
3:D:363:PRO:HD3	5:F:296:LEU:HD12	2.02	0.42
3:D:429:VAL:HG23	3:D:539:ASP:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1061:PHE:CB	3:D:1081:SER:HA	2.41	0.42
3:D:1221:LEU:CD2	3:D:1243:ASP:OD2	2.68	0.42
5:F:435:LEU:O	5:F:435:LEU:HD23	2.19	0.42
6:J:98:LEU:O	6:J:102:LEU:HB2	2.20	0.42
1:B:80:LEU:O	1:B:83:LEU:HB3	2.20	0.42
1:B:102:PRO:HB3	1:B:130:ASP:CA	2.48	0.42
2:C:161:THR:OG1	2:C:165:THR:O	2.33	0.42
2:C:326:GLU:CB	2:C:328:ILE:HG13	2.50	0.42
2:C:519:VAL:HG13	2:C:576:VAL:O	2.20	0.42
2:C:822:ARG:NH1	2:C:829:ALA:CB	2.83	0.42
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.52	0.42
2:C:926:MET:HE1	3:D:817:LEU:CA	2.50	0.42
2:C:955:TRP:CD1	2:C:956:ALA:HB2	2.54	0.42
2:C:1135:VAL:HG23	2:C:1135:VAL:O	2.20	0.42
5:F:299:ASN:HB3	5:F:328:LEU:HD11	2.00	0.42
1:A:54:ILE:HD11	1:A:77:ILE:HD11	2.02	0.42
1:A:61:HIS:H	1:A:61:HIS:CD2	2.38	0.42
2:C:68:PRO:O	2:C:71:ARG:HB3	2.20	0.42
2:C:134:PHE:CE1	2:C:153:PHE:HD1	2.37	0.42
2:C:180:VAL:HG11	2:C:379:ARG:NH1	2.34	0.42
2:C:540:VAL:O	2:C:540:VAL:HG12	2.20	0.42
2:C:720:LEU:HD23	2:C:913:VAL:HA	2.02	0.42
2:C:1044:ARG:NH2	2:C:1048:PRO:O	2.52	0.42
3:D:144:ARG:O	3:D:144:ARG:HD2	2.20	0.42
3:D:844:LEU:HD12	3:D:844:LEU:N	2.35	0.42
3:D:1194:VAL:O	3:D:1195:ALA:C	2.58	0.42
5:F:345:THR:HA	7:O:30:DC:H41	1.85	0.42
1:A:95:MET:HG2	1:A:113:PRO:HD2	2.01	0.42
1:A:186:ARG:HA	1:A:186:ARG:HD3	1.82	0.42
2:C:225:ARG:CB	2:C:231:ARG:HA	2.25	0.42
2:C:275:LEU:HD12	2:C:276:ASP:N	2.35	0.42
2:C:731:TYR:OH	3:D:578:ARG:HD3	2.19	0.42
2:C:1017:GLU:HB3	2:C:1018:PRO:HD2	2.02	0.42
2:C:1052:ILE:HB	5:F:436:GLY:O	2.20	0.42
3:D:140:ASP:O	3:D:142:GLU:N	2.52	0.42
3:D:320:ILE:HD11	3:D:324:LEU:CD1	2.50	0.42
3:D:824:VAL:HG21	3:D:836:VAL:HG21	2.02	0.42
8:P:10:DT:H2"	8:P:11:DA:C8	2.54	0.42
1:A:181:THR:HG21	1:A:189:PHE:CZ	2.55	0.41
2:C:71:ARG:O	2:C:75:ALA:CB	2.67	0.41
2:C:264:LYS:HB3	5:F:202:PHE:N	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:LEU:HD21	2:C:292:ALA:C	2.40	0.41
2:C:558:ARG:NH2	2:C:572:PRO:HD3	2.32	0.41
2:C:861:LEU:CB	2:C:862:PRO:HD2	2.44	0.41
2:C:1093:SER:HB2	3:D:420:LYS:HD3	2.02	0.41
3:D:64:LYS:HZ2	3:D:65:TYR:HE2	1.60	0.41
3:D:130:TYR:OH	3:D:387:ARG:HG2	2.20	0.41
3:D:345:ARG:HA	3:D:348:ILE:HG22	2.01	0.41
3:D:707:ILE:O	3:D:707:ILE:HG12	2.20	0.41
3:D:749:TYR:CE1	3:D:780:GLU:HB2	2.49	0.41
8:P:1:DA:H2"	8:P:2:DG:C5'	2.50	0.41
1:A:218:LEU:HD21	1:B:34:LEU:HD22	2.02	0.41
1:B:208:LEU:HD12	1:B:208:LEU:O	2.20	0.41
2:C:254:PHE:CA	2:C:255:SER:HB2	2.50	0.41
2:C:326:GLU:C	2:C:328:ILE:H	2.24	0.41
2:C:672:MET:CE	2:C:703:ALA:HB2	2.50	0.41
2:C:946:VAL:HG23	2:C:964:LEU:O	2.20	0.41
2:C:946:VAL:N	2:C:964:LEU:O	2.31	0.41
2:C:1103:TYR:CE2	2:C:1107:VAL:HG21	2.55	0.41
2:C:1124:LEU:O	2:C:1128:LEU:HG	2.20	0.41
3:D:25:TYR:CE2	3:D:91:ARG:HG2	2.56	0.41
3:D:56:ARG:HB2	3:D:59:GLU:HB2	2.02	0.41
3:D:118:LEU:CB	3:D:120:LEU:HD13	2.49	0.41
3:D:207:GLN:NE2	3:D:211:ARG:NH1	2.67	0.41
3:D:499:ASN:ND2	3:D:503:THR:OG1	2.49	0.41
3:D:740:PRO:HG2	3:D:741:ARG:HG3	2.01	0.41
3:D:1053:VAL:HG12	3:D:1103:ASP:H	1.85	0.41
3:D:1122:LEU:HD22	3:D:1207:LEU:HB2	2.02	0.41
4:E:56:TYR:CE2	4:E:106:HIS:HD2	2.37	0.41
5:F:278:ARG:HH22	5:F:282:MET:CG	2.34	0.41
5:F:297:GLU:HA	5:F:300:LEU:HG	2.03	0.41
5:F:439:ILE:CD1	6:J:6:LEU:HD13	2.45	0.41
1:B:111:VAL:O	1:B:111:VAL:HG13	2.20	0.41
1:B:179:ASP:HB2	1:B:191:LYS:HB3	2.02	0.41
2:C:38:ARG:NH1	2:C:971:ILE:CG2	2.84	0.41
1:A:223:ARG:O	1:A:225:LEU:N	2.53	0.41
1:B:2:LEU:HD23	1:B:3:ILE:H	1.83	0.41
1:B:69:VAL:HA	1:B:127:THR:O	2.21	0.41
2:C:267:THR:HG21	2:C:273:ALA:CA	2.50	0.41
2:C:455:LEU:HD23	2:C:455:LEU:N	2.36	0.41
2:C:824:ILE:HG22	2:C:825:PHE:CD1	2.54	0.41
3:D:244:LEU:O	3:D:249:GLY:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:337:THR:OG1	3:D:338:SER:N	2.53	0.41
3:D:527:LEU:HD13	3:D:713:VAL:CG1	2.50	0.41
5:F:415:GLN:NE2	5:F:418:ARG:HH12	2.18	0.41
5:F:456:LEU:HD13	5:F:526:TYR:HD2	1.85	0.41
5:F:487:ARG:HB2	5:F:492:ILE:HG23	2.02	0.41
5:F:495:VAL:HG22	5:F:495:VAL:O	2.20	0.41
8:P:23:DA:H2'	8:P:24:DA:H8	1.85	0.41
1:B:21:PHE:HE2	1:B:196:VAL:HG11	1.85	0.41
1:B:34:LEU:C	1:B:34:LEU:HD12	2.41	0.41
2:C:317:ASN:HB3	2:C:324:VAL:HG12	2.01	0.41
2:C:658:ILE:HG22	2:C:659:THR:N	2.35	0.41
3:D:335:PHE:O	5:F:420:PRO:HA	2.21	0.41
3:D:468:ASN:ND2	3:D:470:LYS:H	2.19	0.41
3:D:627:LEU:HD23	3:D:628:SER:H	1.84	0.41
3:D:923:ARG:CB	3:D:962:VAL:HG11	2.51	0.41
6:J:76:LYS:HD2	6:J:76:LYS:O	2.20	0.41
7:O:10:DA:H5'	7:O:10:DA:C8	2.56	0.41
7:O:12:DG:H5"	7:O:12:DG:H8	1.85	0.41
1:B:143:GLY:HA3	1:B:168:TYR:CD2	2.55	0.41
2:C:345:LEU:O	2:C:345:LEU:HD22	2.20	0.41
3:D:84:ARG:O	3:D:87:VAL:HG22	2.20	0.41
3:D:370:GLU:HA	3:D:370:GLU:OE1	2.20	0.41
3:D:392:THR:HA	3:D:399:LEU:HD12	2.01	0.41
3:D:679:LEU:O	3:D:679:LEU:HD23	2.21	0.41
3:D:939:GLU:OE1	3:D:942:GLN:NE2	2.54	0.41
3:D:1097:ARG:HD2	3:D:1098:VAL:N	2.36	0.41
5:F:493:GLY:O	5:F:497:GLY:N	2.54	0.41
1:A:14:LEU:HD12	1:A:18:ARG:HD2	2.02	0.41
1:A:177:LYS:CG	1:A:193:ILE:HD11	2.50	0.41
1:B:21:PHE:HZ	1:B:204:PRO:O	2.04	0.41
1:B:38:LEU:HD12	1:B:42:LEU:HD13	2.01	0.41
2:C:52:GLY:O	2:C:54:LEU:N	2.53	0.41
2:C:721:VAL:HG11	2:C:1028:MET:HB2	2.03	0.41
2:C:862:PRO:HG2	2:C:865:VAL:HG21	2.01	0.41
2:C:1020:PRO:HG2	2:C:1021:TYR:CD2	2.55	0.41
3:D:123:LYS:HE3	3:D:123:LYS:HB2	1.83	0.41
3:D:453:LYS:NZ	3:D:453:LYS:CB	2.83	0.41
3:D:512:PHE:CE1	3:D:561:SER:HB2	2.56	0.41
3:D:557:ILE:HD13	4:E:53:LEU:CD2	2.50	0.41
3:D:882:GLN:HB2	3:D:1248:LEU:HD11	2.02	0.41
3:D:915:TYR:CD2	3:D:1143:ARG:NH1	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1207:LEU:HD13	3:D:1207:LEU:C	2.41	0.41
4:E:102:ASP:C	4:E:103:LEU:HD12	2.41	0.41
5:F:371:HIS:CE1	7:O:21:DT:OP2	2.74	0.41
7:O:4:DT:H2"	7:O:5:DG:C8	2.54	0.41
8:P:14:DA:C1'	8:P:15:DC:H5'	2.50	0.41
8:P:19:DT:H2"	8:P:20:DG:C8	2.54	0.41
1:A:216:VAL:HG13	1:B:216:VAL:HG22	2.03	0.41
2:C:627:GLY:O	2:C:973:SER:HA	2.20	0.41
2:C:961:ASP:C	2:C:962:GLU:HG3	2.41	0.41
3:D:170:LEU:C	3:D:170:LEU:HD13	2.41	0.41
3:D:638:THR:HG22	3:D:661:ALA:CB	2.50	0.41
3:D:882:GLN:HG3	3:D:883:ASP:OD1	2.21	0.41
3:D:1172:SER:HB3	3:D:1199:GLU:HB3	2.00	0.41
6:J:104:LEU:HD23	6:J:104:LEU:C	2.41	0.41
1:A:84:VAL:HG12	1:A:120:ASN:CG	2.42	0.41
1:B:95:MET:SD	1:B:113:PRO:HD2	2.61	0.41
1:B:138:LEU:HD12	1:B:138:LEU:N	2.36	0.41
1:B:215:LEU:O	1:B:215:LEU:HD23	2.20	0.41
2:C:222:VAL:HG11	2:C:234:VAL:CG1	2.50	0.41
2:C:254:PHE:CE1	2:C:347:ARG:NH1	2.85	0.41
2:C:282:ARG:CB	2:C:283:PRO:CA	2.98	0.41
2:C:410:GLU:HA	2:C:410:GLU:OE1	2.21	0.41
2:C:519:VAL:HG12	2:C:577:ASP:C	2.41	0.41
2:C:563:ARG:CG	2:C:564:LYS:H	2.34	0.41
2:C:645:GLU:HA	2:C:645:GLU:OE1	2.20	0.41
2:C:741:LEU:CA	2:C:746:VAL:HG12	2.51	0.41
2:C:1123:VAL:O	2:C:1127:GLU:HG3	2.21	0.41
9:C:1201:FI8:C24	9:C:1201:FI8:C25	2.98	0.41
3:D:527:LEU:HD22	3:D:575:ALA:O	2.21	0.41
3:D:527:LEU:HD11	3:D:713:VAL:HG12	2.02	0.41
3:D:778:TRP:CE2	3:D:835:PRO:HD3	2.55	0.41
3:D:922:ALA:HB1	3:D:981:ARG:HB3	2.03	0.41
3:D:981:ARG:HG2	3:D:982:SER:N	2.34	0.41
3:D:1068:PRO:HG2	3:D:1072:GLY:H	1.86	0.41
3:D:1089:PHE:HD2	3:D:1099:LEU:HB2	1.85	0.41
3:D:1217:THR:OG1	3:D:1218:ASP:N	2.54	0.41
4:E:32:PRO:CB	4:E:36:THR:HG23	2.50	0.41
5:F:509:LYS:HD2	5:F:509:LYS:HA	1.90	0.41
1:B:3:ILE:HG22	1:B:233:GLU:O	2.20	0.41
1:B:90:ASP:OD1	1:B:142:ARG:HD3	2.20	0.41
2:C:339:VAL:HA	2:C:342:ILE:CD1	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:809:LYS:HZ2	2:C:809:LYS:CB	2.27	0.41
2:C:840:PRO:HD2	2:C:843:GLU:OE1	2.21	0.41
3:D:345:ARG:HA	3:D:348:ILE:CG2	2.51	0.41
2:C:435:GLN:CG	2:C:460:PRO:HD3	2.44	0.40
2:C:607:MET:O	2:C:611:MET:HG3	2.21	0.40
2:C:1040:LYS:HB3	3:D:540:GLN:NE2	2.35	0.40
3:D:293:LEU:HD23	3:D:293:LEU:O	2.20	0.40
3:D:367:VAL:HG12	3:D:371:LYS:HE3	2.02	0.40
3:D:606:HIS:HB2	3:D:607:PRO:CD	2.46	0.40
3:D:744:GLU:HG3	3:D:745:ILE:N	2.35	0.40
3:D:910:LEU:O	3:D:910:LEU:CD1	2.69	0.40
4:E:32:PRO:HG2	4:E:37:ASN:HB2	2.02	0.40
1:A:41:THR:OG1	1:A:215:LEU:HD21	2.22	0.40
1:A:133:LYS:HD3	1:A:133:LYS:C	2.42	0.40
2:C:74:ALA:HB1	2:C:79:ASP:OD2	2.21	0.40
2:C:224:VAL:HB	2:C:232:GLN:O	2.20	0.40
2:C:231:ARG:HD2	5:F:205:ASP:CB	2.39	0.40
2:C:254:PHE:CE1	2:C:347:ARG:HG2	2.54	0.40
2:C:333:LEU:HD22	2:C:338:VAL:HG23	2.02	0.40
2:C:339:VAL:CG2	2:C:340:ALA:N	2.85	0.40
2:C:542:ALA:N	2:C:578:TYR:O	2.48	0.40
2:C:558:ARG:HH21	2:C:572:PRO:CD	2.30	0.40
2:C:732:GLU:O	2:C:733:ASP:HB2	2.21	0.40
2:C:754:GLU:HB2	2:C:872:TYR:CD1	2.56	0.40
3:D:55:THR:HG22	3:D:55:THR:O	2.22	0.40
3:D:327:MET:HG3	3:D:337:THR:HB	2.03	0.40
3:D:449:LEU:HD13	3:D:449:LEU:C	2.41	0.40
3:D:467:GLN:HA	3:D:467:GLN:NE2	2.34	0.40
3:D:673:PHE:O	3:D:676:LEU:HB2	2.21	0.40
3:D:746:LEU:HD23	3:D:746:LEU:HA	1.94	0.40
3:D:780:GLU:HA	3:D:780:GLU:OE1	2.21	0.40
3:D:820:MET:HG2	3:D:822:GLY:N	2.36	0.40
3:D:1122:LEU:CA	3:D:1130:VAL:HG21	2.51	0.40
5:F:386:LEU:HD11	5:F:398:GLU:OE2	2.20	0.40
1:B:15:THR:O	1:B:17:ASN:N	2.54	0.40
1:B:95:MET:HG2	1:B:113:PRO:HD2	2.03	0.40
2:C:96:ILE:O	2:C:104:SER:HA	2.21	0.40
2:C:1074:TRP:CH2	3:D:875:ARG:HG3	2.55	0.40
3:D:170:LEU:HA	3:D:173:ARG:HG2	2.04	0.40
3:D:287:GLN:CD	3:D:287:GLN:H	2.25	0.40
3:D:469:ILE:C	3:D:469:ILE:HD13	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:890:ASP:HA	3:D:977:THR:OG1	2.21	0.40
3:D:1063:LYS:HD3	3:D:1064:ILE:H	1.87	0.40
3:D:1063:LYS:CE	3:D:1078:ASP:HA	2.52	0.40
5:F:274:PRO:HD2	5:F:277:GLN:HB2	2.03	0.40
5:F:310:TYR:HD2	5:F:355:ILE:HG21	1.86	0.40
5:F:415:GLN:HA	5:F:418:ARG:NH2	2.36	0.40
7:O:19:DA:H2'	7:O:20:DT:H73	2.04	0.40
2:C:252:PHE:O	2:C:255:SER:O	2.40	0.40
2:C:373:PHE:HD2	2:C:482:ARG:CD	2.34	0.40
2:C:740:ARG:HH21	2:C:914:ASP:CG	2.23	0.40
2:C:756:GLU:HB2	2:C:870:ARG:HG2	2.03	0.40
2:C:868:LEU:C	2:C:868:LEU:HD13	2.42	0.40
3:D:211:ARG:HA	3:D:214:ARG:HH21	1.84	0.40
3:D:558:LEU:HD13	4:E:54:VAL:HG21	2.03	0.40
3:D:653:HIS:CD2	3:D:654:SER:H	2.39	0.40
3:D:660:ASP:OD1	3:D:660:ASP:N	2.54	0.40
3:D:771:ASN:O	3:D:775:VAL:HG23	2.22	0.40
3:D:834:ARG:CB	3:D:835:PRO:CA	3.00	0.40
3:D:1139:GLN:HG3	3:D:1143:ARG:NE	2.34	0.40
4:E:32:PRO:HB2	4:E:37:ASN:HB2	2.02	0.40
5:F:488:THR:HB	8:P:19:DT:H3'	2.02	0.40
1:B:179:ASP:HB2	1:B:191:LYS:HE2	2.03	0.40
2:C:280:LYS:HD3	2:C:280:LYS:HA	1.94	0.40
2:C:931:ILE:O	2:C:934:THR:HB	2.21	0.40
3:D:76:GLU:H	3:D:76:GLU:CD	2.23	0.40
3:D:406:LEU:HD12	3:D:406:LEU:N	2.37	0.40
3:D:627:LEU:HD23	3:D:628:SER:N	2.36	0.40
3:D:911:ILE:H	3:D:911:ILE:CD1	2.26	0.40
3:D:981:ARG:O	3:D:1152:LYS:NZ	2.54	0.40
5:F:387:LEU:HD12	5:F:393:GLU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/347 (65%)	206 (92%)	18 (8%)	0	100	100
1	B	235/347 (68%)	200 (85%)	35 (15%)	0	100	100
2	C	1109/1181 (94%)	961 (87%)	141 (13%)	7 (1%)	25	59
3	D	1257/1324 (95%)	1148 (91%)	105 (8%)	4 (0%)	41	73
4	E	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
5	F	324/531 (61%)	306 (94%)	18 (6%)	0	100	100
6	J	105/111 (95%)	89 (85%)	15 (14%)	1 (1%)	15	48
All	All	3335/3951 (84%)	2985 (90%)	338 (10%)	12 (0%)	38	68

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	62	GLU
2	C	323	HIS
3	D	909	THR
3	D	910	LEU
3	D	904	ARG
2	C	61	PHE
2	C	225	ARG
2	C	231	ARG
2	C	959	LEU
3	D	1196	GLU
2	C	224	VAL
6	J	70	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/297 (66%)	185 (95%)	10 (5%)	24	55
1	B	197/297 (66%)	186 (94%)	11 (6%)	21	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	924/997 (93%)	872 (94%)	52 (6%)	21	52
3	D	1041/1103 (94%)	969 (93%)	72 (7%)	15	46
4	E	69/89 (78%)	62 (90%)	7 (10%)	7	28
5	F	272/429 (63%)	246 (90%)	26 (10%)	8	30
6	J	93/97 (96%)	79 (85%)	14 (15%)	3	12
All	All	2791/3309 (84%)	2599 (93%)	192 (7%)	19	46

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	22	VAL
1	A	34	LEU
1	A	51	VAL
1	A	61	HIS
1	A	88	GLU
1	A	138	LEU
1	A	144	ARG
1	A	146	TYR
1	A	221	LEU
1	B	11	GLU
1	B	27	GLU
1	B	38	LEU
1	B	61	HIS
1	B	84	VAL
1	B	117	THR
1	B	153	ARG
1	B	175	THR
1	B	177	LYS
1	B	182	ARG
1	B	196	VAL
2	C	59	ASP
2	C	90	LEU
2	C	93	LEU
2	C	192	ASP
2	C	195	THR
2	C	199	LEU
2	C	212	LEU
2	C	215	ASP
2	C	226	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	230	ARG
2	C	232	GLN
2	C	258	MET
2	C	261	THR
2	C	266	ASN
2	C	308	LEU
2	C	313	ARG
2	C	318	LYS
2	C	333	LEU
2	C	343	GLU
2	C	345	LEU
2	C	373	PHE
2	C	397	GLU
2	C	406	THR
2	C	420	ILE
2	C	455	LEU
2	C	500	LEU
2	C	540	VAL
2	C	570	TYR
2	C	571	VAL
2	C	577	ASP
2	C	628	THR
2	C	667	ARG
2	C	668	ARG
2	C	709	ASP
2	C	787	ARG
2	C	797	ARG
2	C	809	LYS
2	C	835	THR
2	C	861	LEU
2	C	888	ARG
2	C	936	LEU
2	C	945	LYS
2	C	950	LYS
2	C	959	LEU
2	C	962	GLU
2	C	963	LEU
2	C	965	GLU
2	C	997	ASP
2	C	1009	MET
2	C	1031	MET
2	C	1057	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1076	MET
3	D	51	ILE
3	D	67	ARG
3	D	82	VAL
3	D	86	LYS
3	D	126	GLU
3	D	135	VAL
3	D	147	GLU
3	D	152	GLU
3	D	162	VAL
3	D	164	ASP
3	D	171	GLU
3	D	173	ARG
3	D	177	LEU
3	D	211	ARG
3	D	219	LEU
3	D	222	ILE
3	D	238	GLU
3	D	263	LYS
3	D	275	GLU
3	D	282	ARG
3	D	330	LEU
3	D	334	ARG
3	D	410	GLN
3	D	414	ARG
3	D	463	LEU
3	D	467	GLN
3	D	469	ILE
3	D	478	ARG
3	D	490	VAL
3	D	499	ASN
3	D	505	HIS
3	D	506	ARG
3	D	574	LEU
3	D	578	ARG
3	D	600	GLN
3	D	627	LEU
3	D	639	GLN
3	D	656	TRP
3	D	657	GLN
3	D	677	LEU
3	D	687	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	706	MET
3	D	725	THR
3	D	733	MET
3	D	741	ARG
3	D	766	ASN
3	D	793	TYR
3	D	826	ASN
3	D	834	ARG
3	D	841	ARG
3	D	862	ASP
3	D	883	ASP
3	D	904	ARG
3	D	910	LEU
3	D	911	ILE
3	D	948	GLU
3	D	1012	MET
3	D	1057	ASP
3	D	1061	PHE
3	D	1062	TYR
3	D	1078	ASP
3	D	1089	PHE
3	D	1090	LYS
3	D	1096	GLU
3	D	1097	ARG
3	D	1098	VAL
3	D	1099	LEU
3	D	1120	GLU
3	D	1121	VAL
3	D	1189	GLU
3	D	1231	ARG
3	D	1273	GLN
4	E	30	ASP
4	E	56	TYR
4	E	65	ASN
4	E	71	LEU
4	E	73	GLU
4	E	78	TYR
4	E	79	VAL
5	F	205	ASP
5	F	206	GLU
5	F	207	ASP
5	F	214	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	216	ARG
5	F	240	LEU
5	F	244	GLU
5	F	246	GLU
5	F	277	GLN
5	F	282	MET
5	F	286	ARG
5	F	330	ARG
5	F	353	GLN
5	F	397	GLU
5	F	398	GLU
5	F	414	GLN
5	F	418	ARG
5	F	423	LEU
5	F	430	GLU
5	F	435	LEU
5	F	460	LEU
5	F	461	GLN
5	F	491	GLU
5	F	492	ILE
5	F	500	ARG
5	F	527	LEU
6	J	4	ARG
6	J	6	LEU
6	J	7	ARG
6	J	20	ARG
6	J	27	ARG
6	J	33	ARG
6	J	74	LYS
6	J	76	LYS
6	J	86	LEU
6	J	97	LEU
6	J	99	LYS
6	J	101	ARG
6	J	103	GLU
6	J	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	B	5	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	79	ASN
1	B	124	HIS
1	B	151	GLN
1	B	226	ASN
2	C	57	GLN
2	C	200	HIS
2	C	317	ASN
2	C	349	HIS
2	C	388	GLN
2	C	435	GLN
2	C	442	GLN
2	C	476	HIS
2	C	479	HIS
2	C	585	GLN
2	C	612	GLN
2	C	751	HIS
2	C	920	HIS
2	C	969	ASN
2	C	986	GLN
2	C	1066	GLN
3	D	175	GLN
3	D	262	GLN
3	D	341	ASN
3	D	369	ASN
3	D	410	GLN
3	D	439	HIS
3	D	467	GLN
3	D	468	ASN
3	D	499	ASN
3	D	540	GLN
3	D	600	GLN
3	D	639	GLN
3	D	693	GLN
3	D	766	ASN
3	D	854	HIS
3	D	1084	GLN
3	D	1104	HIS
3	D	1139	GLN
3	D	1227	GLN
3	D	1251	ASN
4	E	65	ASN
4	E	69	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	106	HIS
5	F	214	GLN
5	F	299	ASN
5	F	322	GLN
5	F	325	ASN
5	F	353	GLN
5	F	388	GLN
5	F	414	GLN
5	F	457	GLN
5	F	516	HIS
6	J	36	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	FI8	C	1201	-	74,75,75	1.86	19 (25%)	88,109,109	1.62	17 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FI8	C	1201	-	-	20/75/118/118	0/3/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	FI8	C1-C3	5.17	1.57	1.50
9	C	1201	FI8	C14-C15	4.31	1.54	1.45
9	C	1201	FI8	O1-C18	-4.14	1.39	1.46
9	C	1201	FI8	O1-C2	3.82	1.43	1.34
9	C	1201	FI8	O17-C49	3.76	1.43	1.34
9	C	1201	FI8	O10-C29	-3.75	1.39	1.44
9	C	1201	FI8	C14-C13	3.13	1.38	1.33
9	C	1201	FI8	O10-C33	2.94	1.40	1.34
9	C	1201	FI8	C38-CL2	2.93	1.79	1.72
9	C	1201	FI8	C5-C4	2.76	1.52	1.43
9	C	1201	FI8	C10-C9	2.63	1.38	1.33
9	C	1201	FI8	C36-CL1	2.62	1.78	1.72
9	C	1201	FI8	C11-C10	2.58	1.54	1.50
9	C	1201	FI8	C2-C3	2.40	1.53	1.49
9	C	1201	FI8	C17-C16	2.30	1.54	1.50
9	C	1201	FI8	C11-C12	-2.16	1.51	1.53
9	C	1201	FI8	O14-C46	-2.16	1.43	1.45
9	C	1201	FI8	O13-C35	2.03	1.41	1.37
9	C	1201	FI8	C7-C6	2.03	1.56	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1201	FI8	C18-C17-C16	-5.23	104.00	113.02
9	C	1201	FI8	O14-C46-C45	4.60	115.06	107.67
9	C	1201	FI8	C31-C30-C29	-4.25	106.94	113.41
9	C	1201	FI8	O1-C2-C3	3.73	117.40	112.14
9	C	1201	FI8	C7-C6-C5	-3.66	120.69	125.41
9	C	1201	FI8	O17-C49-C50	3.21	117.32	111.19
9	C	1201	FI8	C38-C37-C36	3.12	120.93	117.81
9	C	1201	FI8	C29-O10-C33	-3.01	112.40	117.21
9	C	1201	FI8	C35-C36-CL1	2.64	121.04	118.08
9	C	1201	FI8	C5-C4-C3	-2.63	123.84	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1201	FI8	O2-C2-C3	-2.53	120.30	124.12
9	C	1201	FI8	C24-C13-C12	2.51	120.03	115.68
9	C	1201	FI8	C4-C5-C6	-2.50	117.78	123.63
9	C	1201	FI8	C28-C29-C30	2.46	113.92	110.30
9	C	1201	FI8	C45-O17-C49	-2.34	114.39	117.92
9	C	1201	FI8	C11-C12-C13	-2.24	109.43	113.89
9	C	1201	FI8	C41-C40-C39	-2.14	106.83	112.27

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1201	FI8	C9-C10-C11-C12
9	C	1201	FI8	C9-C10-C11-C22
9	C	1201	FI8	C10-C11-C22-C23
9	C	1201	FI8	C17-C18-C19-O5A
9	C	1201	FI8	O1-C18-C19-O5A
9	C	1201	FI8	C50-C49-O17-C45
9	C	1201	FI8	O18-C49-O17-C45
9	C	1201	FI8	C34-C33-O10-C29
9	C	1201	FI8	O11-C33-O10-C29
9	C	1201	FI8	C17-C18-O1-C2
9	C	1201	FI8	C7-C8-C9-C21
9	C	1201	FI8	C19-C18-O1-C2
9	C	1201	FI8	C17-C18-C19-C20
9	C	1201	FI8	O1-C18-C19-C20
9	C	1201	FI8	C5-C6-C7-C8
9	C	1201	FI8	C12-C11-C22-C23
9	C	1201	FI8	C11-C12-O4-C42
9	C	1201	FI8	O3-C8-C9-C21
9	C	1201	FI8	O17-C49-C50-C51
9	C	1201	FI8	C3-C4-C5-C6

There are no ring outliers.

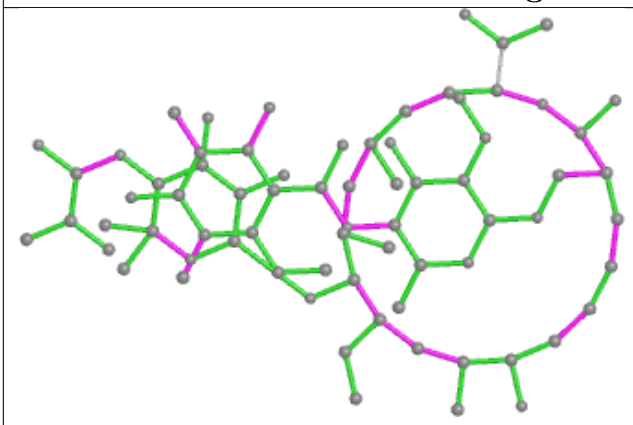
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1201	FI8	3	0

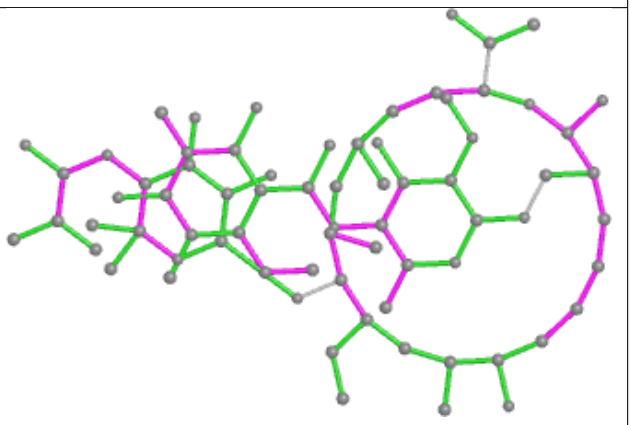
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

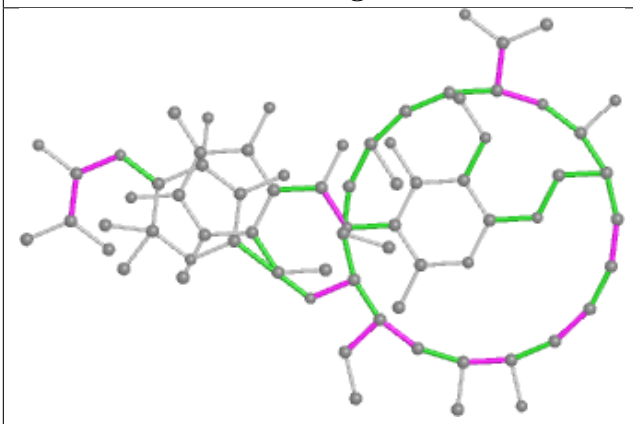
Ligand FI8 C 1201



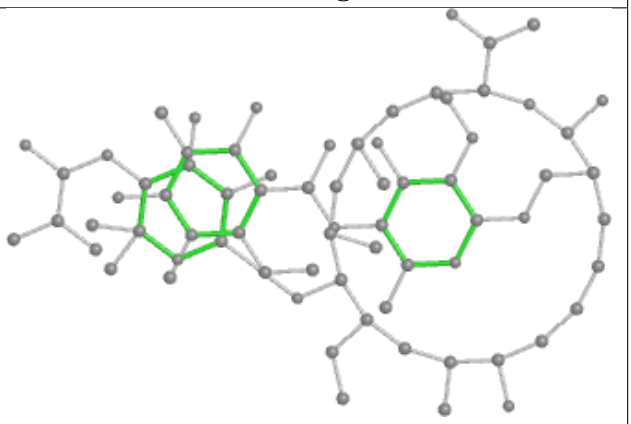
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

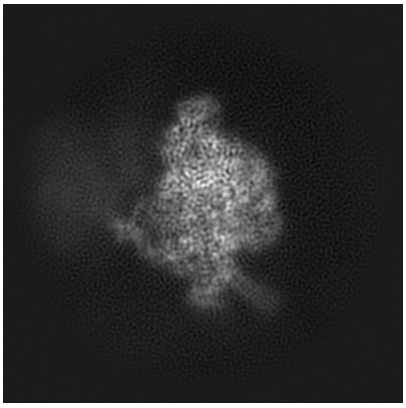
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7319. These allow visual inspection of the internal detail of the map and identification of artifacts.

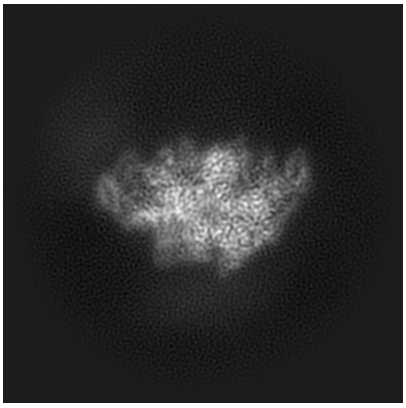
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

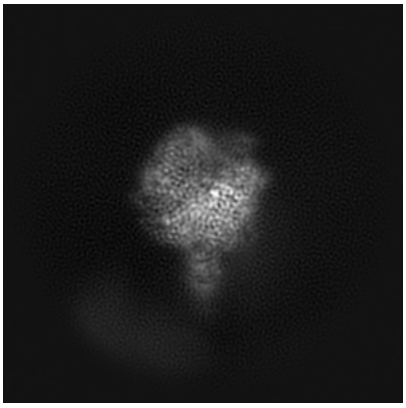
6.1.1 Primary map



X



Y

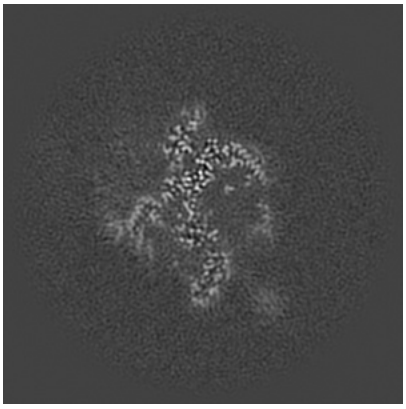


Z

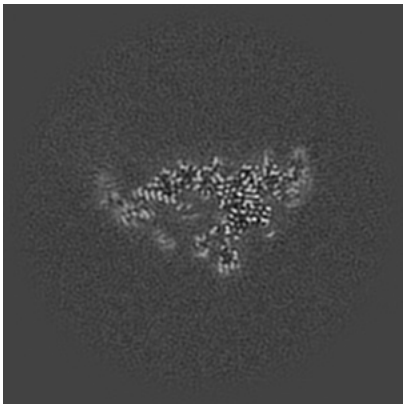
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

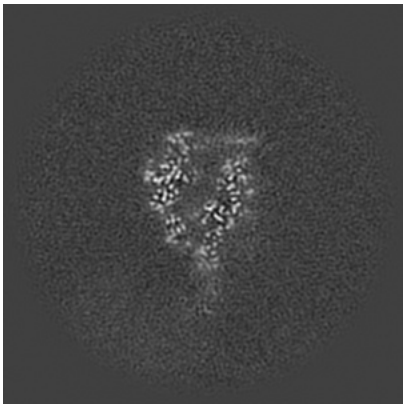
6.2.1 Primary map



X Index: 150



Y Index: 150

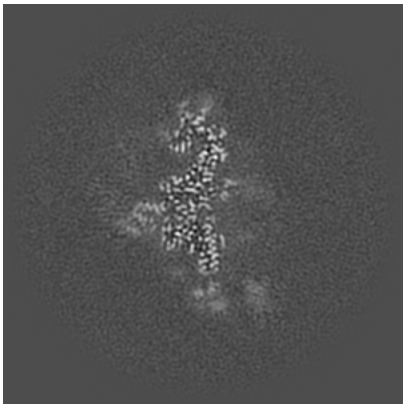


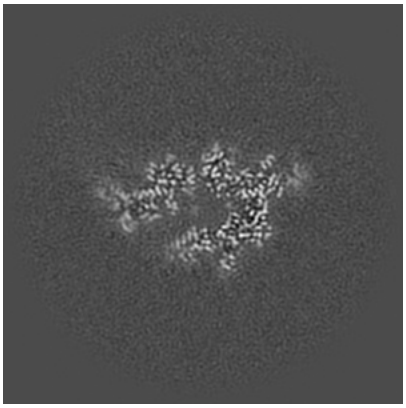
Z Index: 150

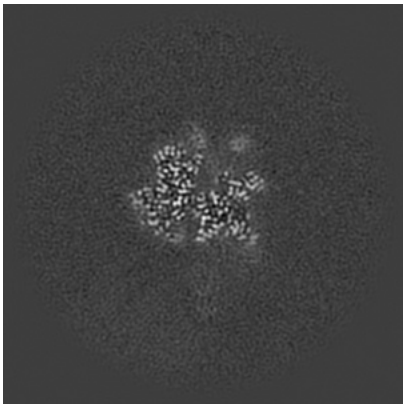
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 159

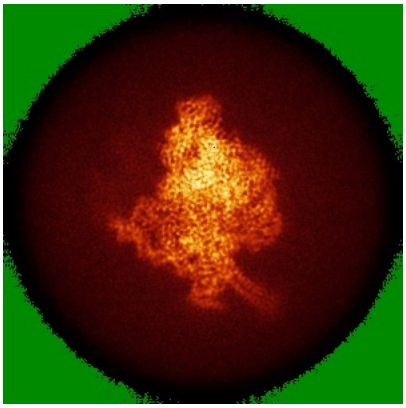

Y Index: 158

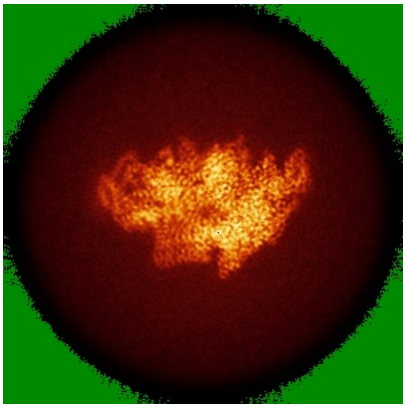

Z Index: 168

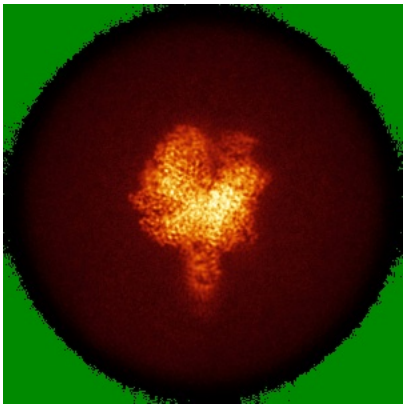
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

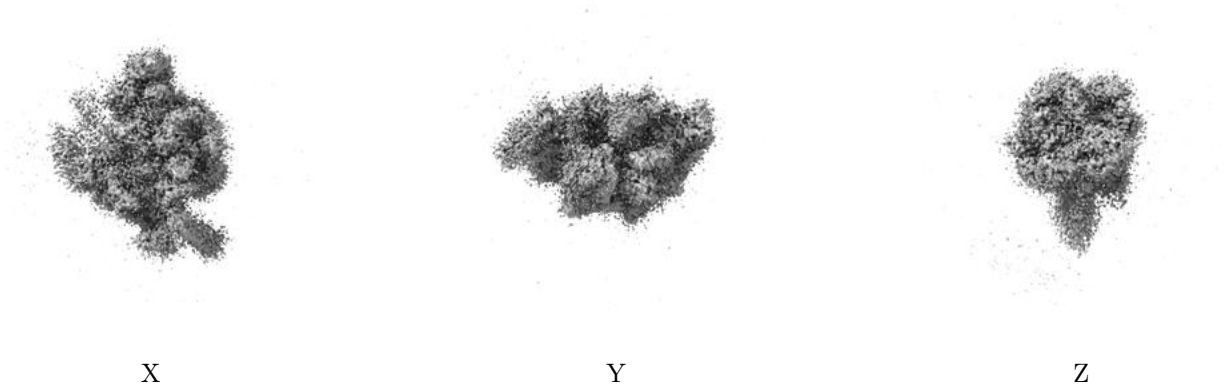

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.347. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

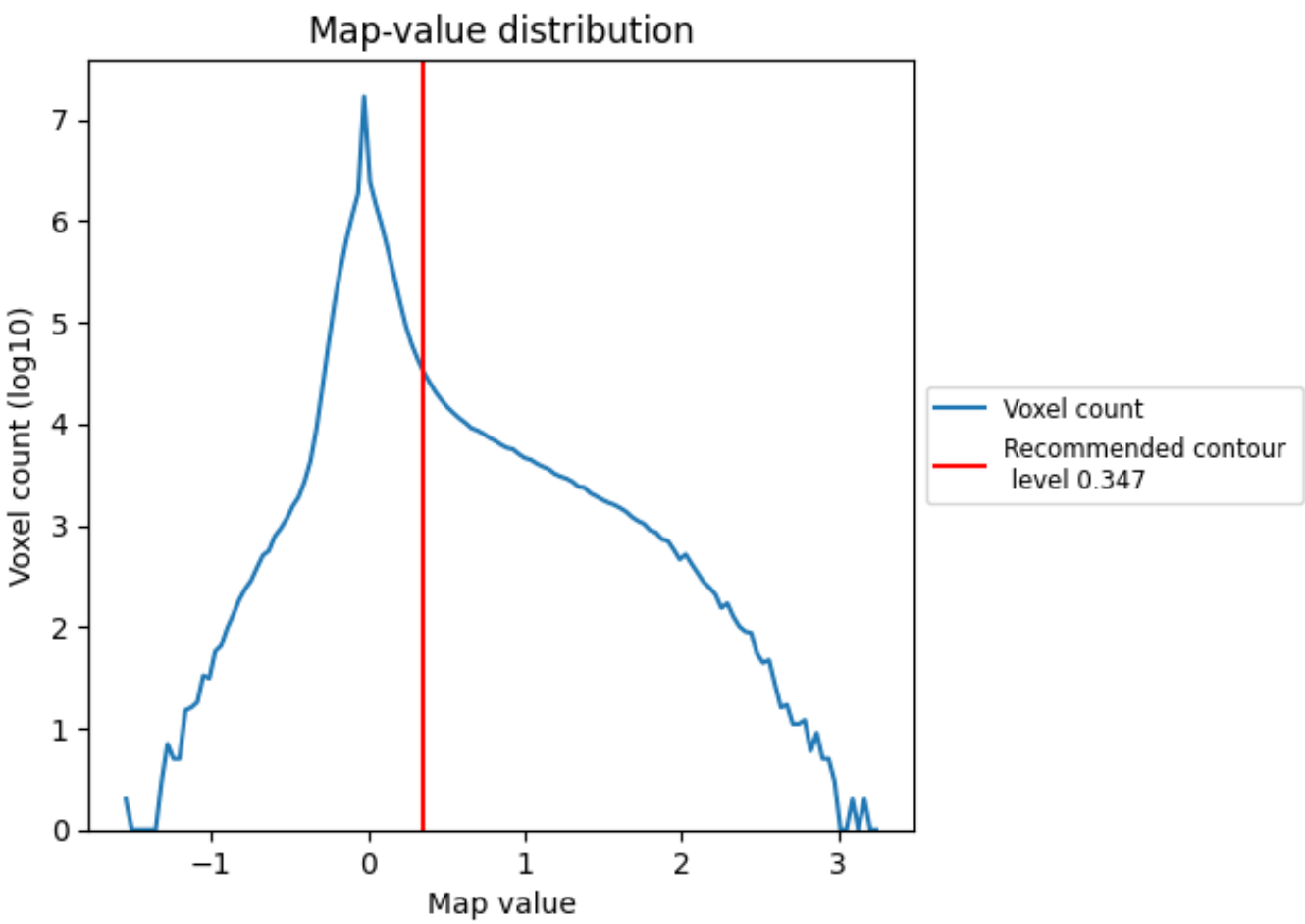
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

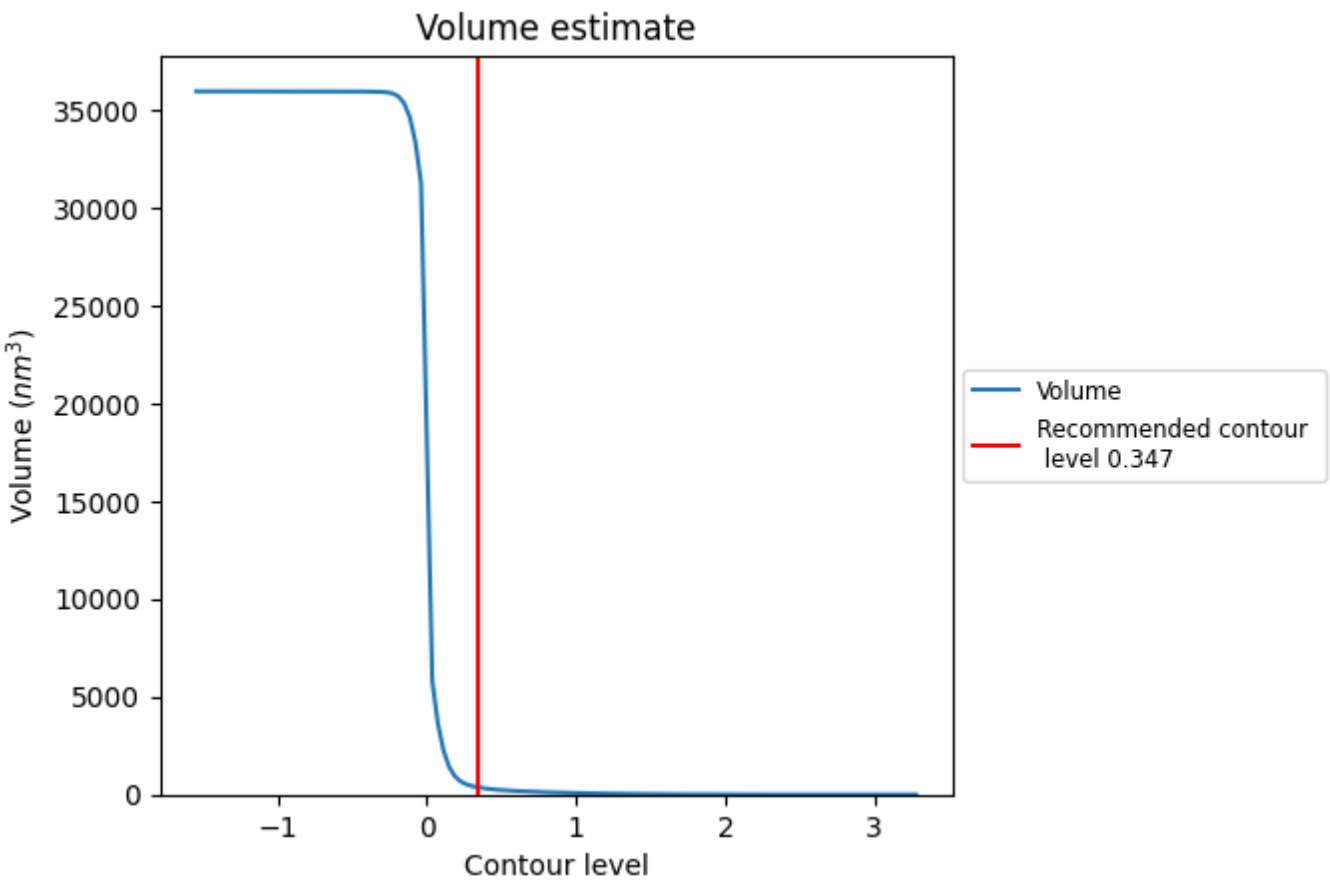
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

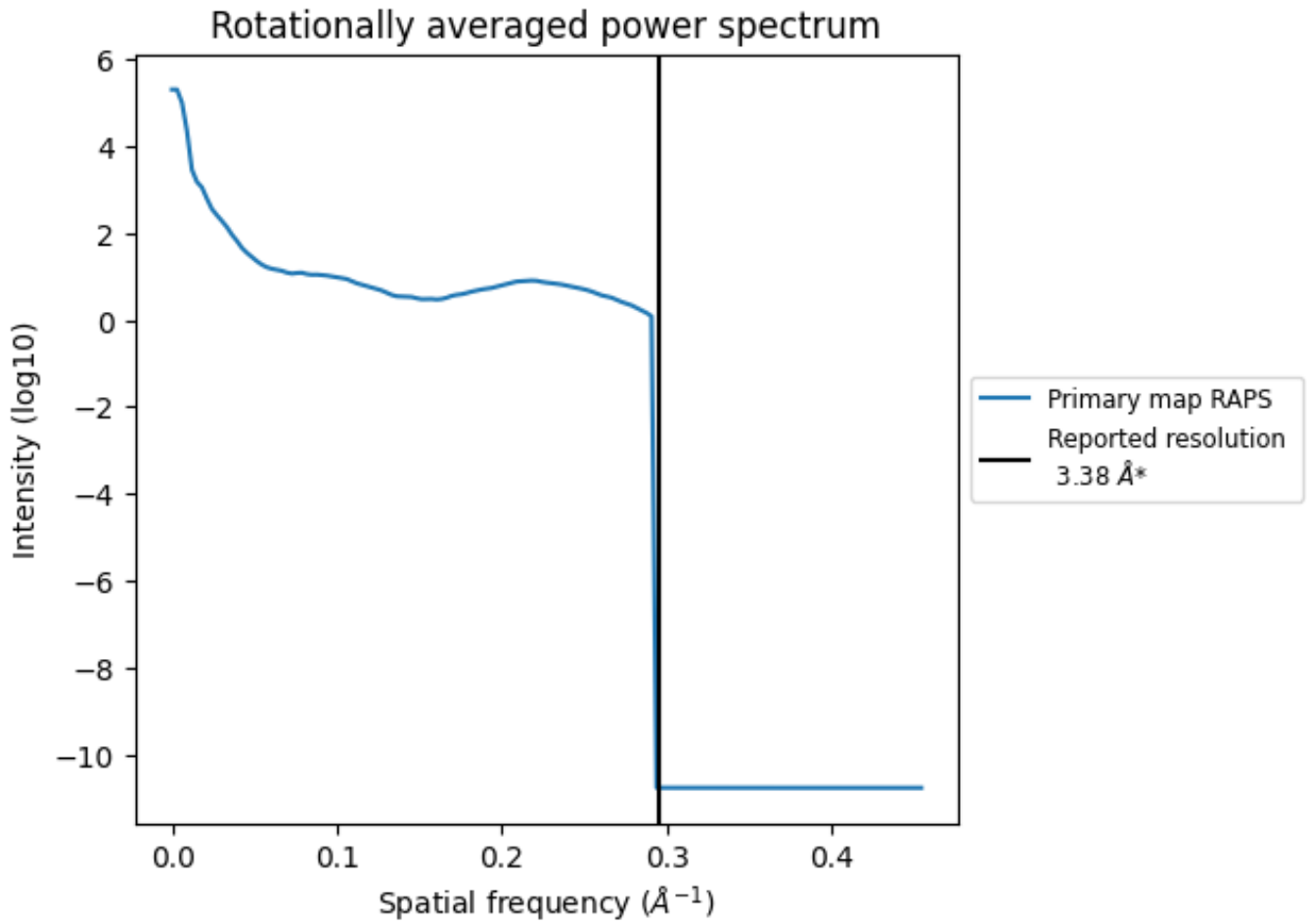
7.2 Volume estimate (i)



The volume at the recommended contour level is 365 nm^3; this corresponds to an approximate mass of 329 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.296 Å^{-1}

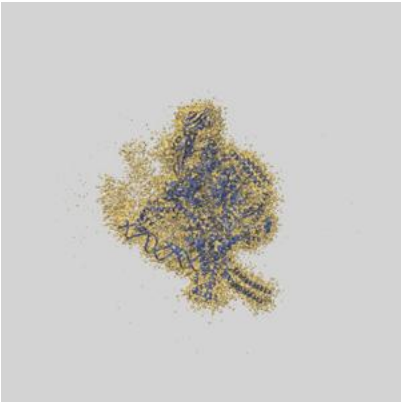
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

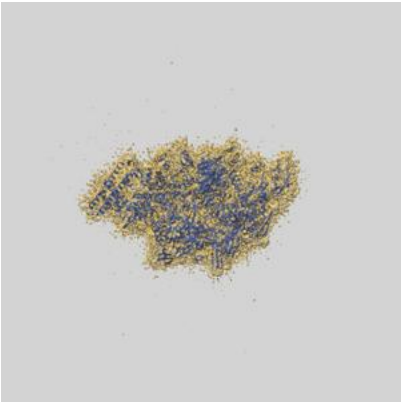
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7319 and PDB model 6BZO. Per-residue inclusion information can be found in section 3 on page 8.

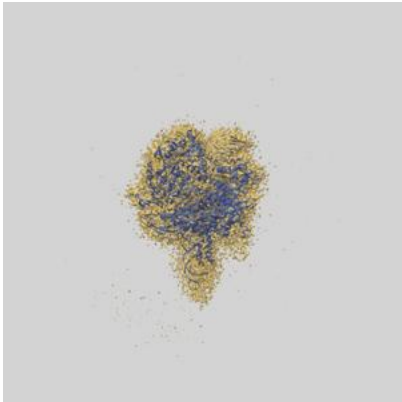
9.1 Map-model overlay (i)



X



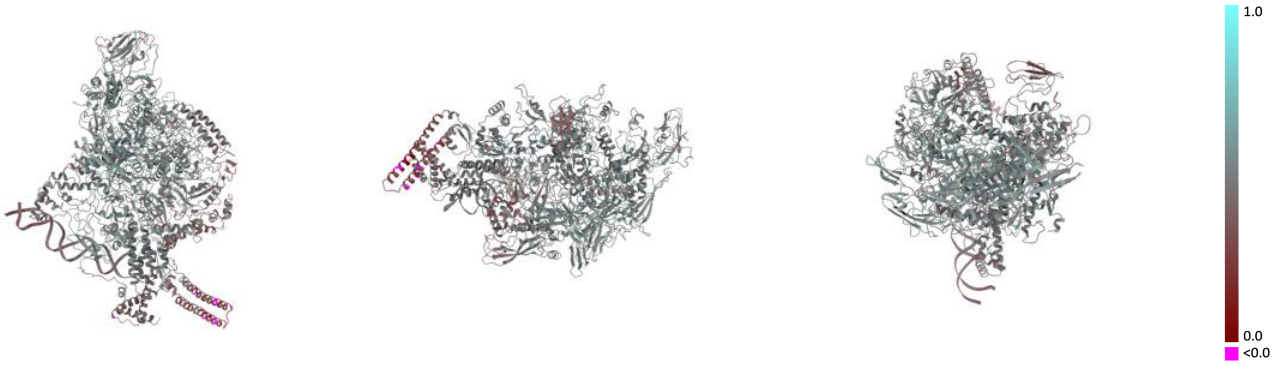
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.347 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

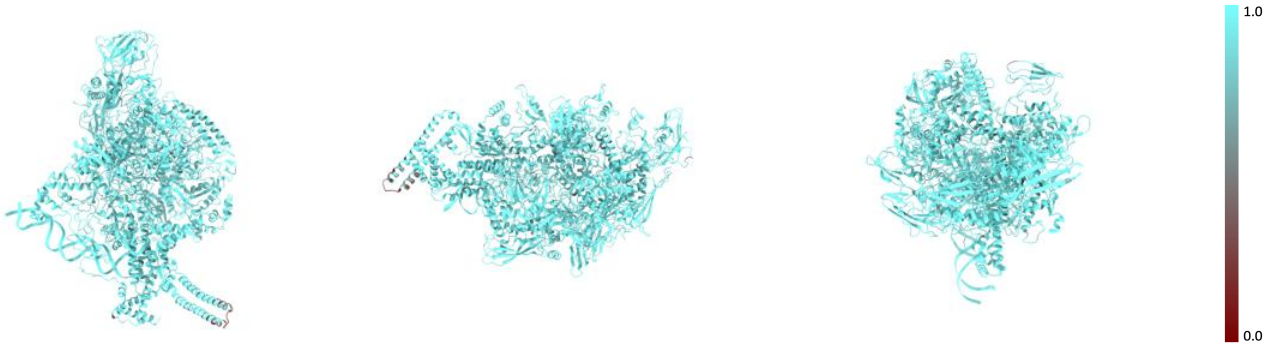
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

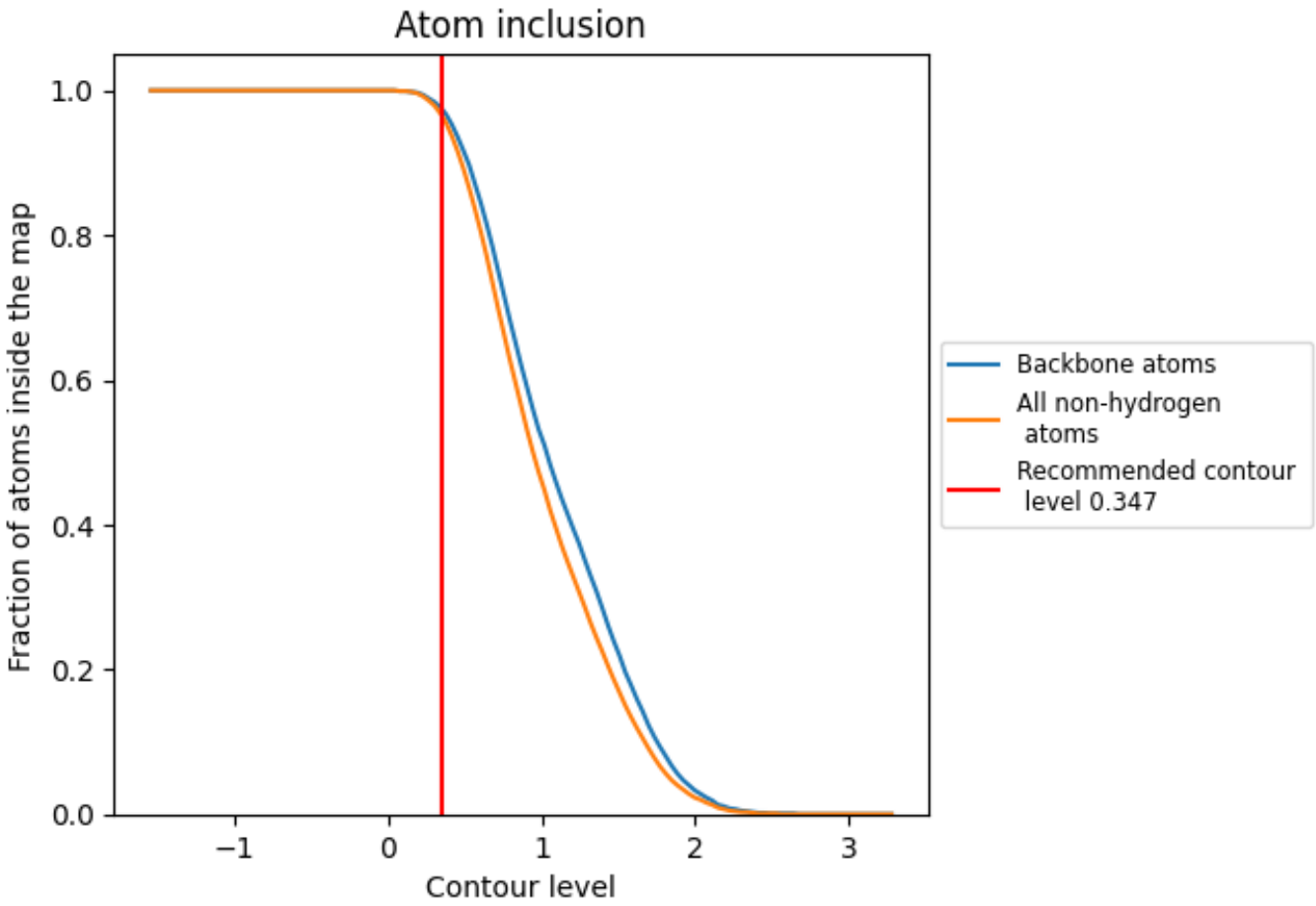
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.347).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.347) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9660	0.4890
A	0.9750	0.5130
B	0.9680	0.4960
C	0.9710	0.5050
D	0.9640	0.4910
E	0.9610	0.5010
F	0.9600	0.4520
J	0.9510	0.4750
O	0.9970	0.4080
P	0.9910	0.3890