



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:45 am BST

PDB ID : 3RMD
Title : Crystal Structure of a replicative DNA polymerase bound to DNA containing
Thymine Glycol
Authors : Aller, P.; Duclos, S.; Wallace, S.S.; Doublié, S.
Deposited on : 2011-04-20
Resolution : 2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

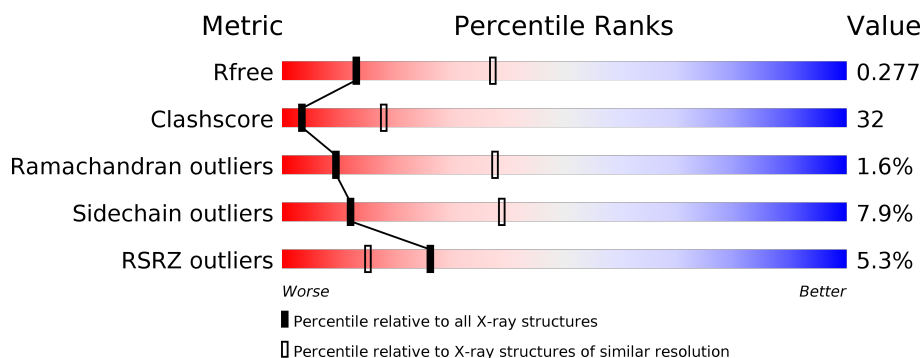
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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.





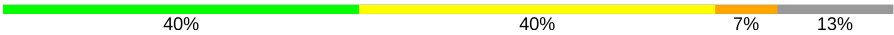
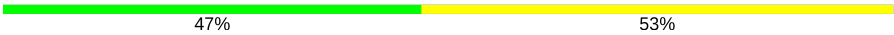
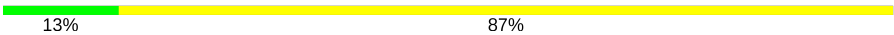
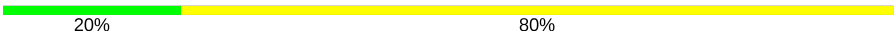
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	906	<div> <div>6%</div> <div> <div></div> <div>56%</div> <div>40%</div> <div>•</div> </div> </div>
1	B	906	<div> <div>7%</div> <div> <div></div> <div>58%</div> <div>37%</div> <div>5%</div> </div> </div>
1	C	906	<div> <div>4%</div> <div> <div></div> <div>49%</div> <div>45%</div> <div>6%</div> <div>•</div> </div> </div>
1	D	906	<div> <div>5%</div> <div> <div></div> <div>40%</div> <div>52%</div> <div>7%</div> <div>•</div> </div> </div>
2	E	18	<div> <div>6%</div> <div> <div></div> <div>22%</div> <div>50%</div> <div>28%</div> </div> </div>
2	G	18	<div> <div></div> <div> <div></div> <div>44%</div> <div>50%</div> <div>6%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	18	 11% 89%
2	K	18	 22% 78%
3	F	15	 40% 40% 7% 13%
3	H	15	 47% 53%
3	J	15	 13% 87%
3	L	15	 20% 80%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31870 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	902	Total	C	N	O	S	0	0	0
			7284	4679	1208	1365	32			
1	B	902	Total	C	N	O	S	0	0	0
			7315	4695	1216	1371	33			
1	C	901	Total	C	N	O	S	0	0	0
			7312	4695	1212	1372	33			
1	D	897	Total	C	N	O	S	3	0	0
			7165	4599	1184	1350	32			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	904	HIS	-	EXPRESSION TAG	UNP Q38087
A	905	HIS	-	EXPRESSION TAG	UNP Q38087
A	906	HIS	-	EXPRESSION TAG	UNP Q38087
B	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	904	HIS	-	EXPRESSION TAG	UNP Q38087
B	905	HIS	-	EXPRESSION TAG	UNP Q38087
B	906	HIS	-	EXPRESSION TAG	UNP Q38087
C	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	904	HIS	-	EXPRESSION TAG	UNP Q38087
C	905	HIS	-	EXPRESSION TAG	UNP Q38087
C	906	HIS	-	EXPRESSION TAG	UNP Q38087
D	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	904	HIS	-	EXPRESSION TAG	UNP Q38087
D	905	HIS	-	EXPRESSION TAG	UNP Q38087
D	906	HIS	-	EXPRESSION TAG	UNP Q38087

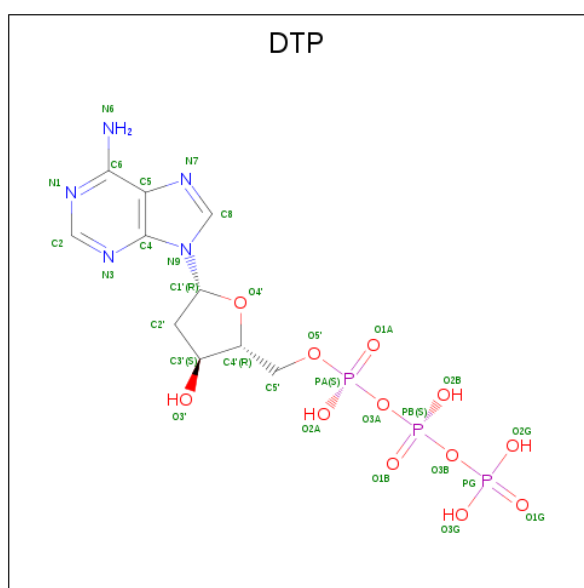
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*TP*(CTG)P*G*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	P	0	0	0
			265	126	54	73	12			
2	G	18	Total	C	N	O	P	0	0	0
			370	175	71	107	17			
2	I	18	Total	C	N	O	P	0	0	0
			370	175	71	107	17			
2	K	18	Total	C	N	O	P	0	0	0
			370	175	71	107	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	13	Total	C	N	O	P	0	0	0
			262	126	45	79	12			
3	H	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
3	J	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
3	L	15	Total	C	N	O	P	0	0	0
			301	143	55	89	14			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	J	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

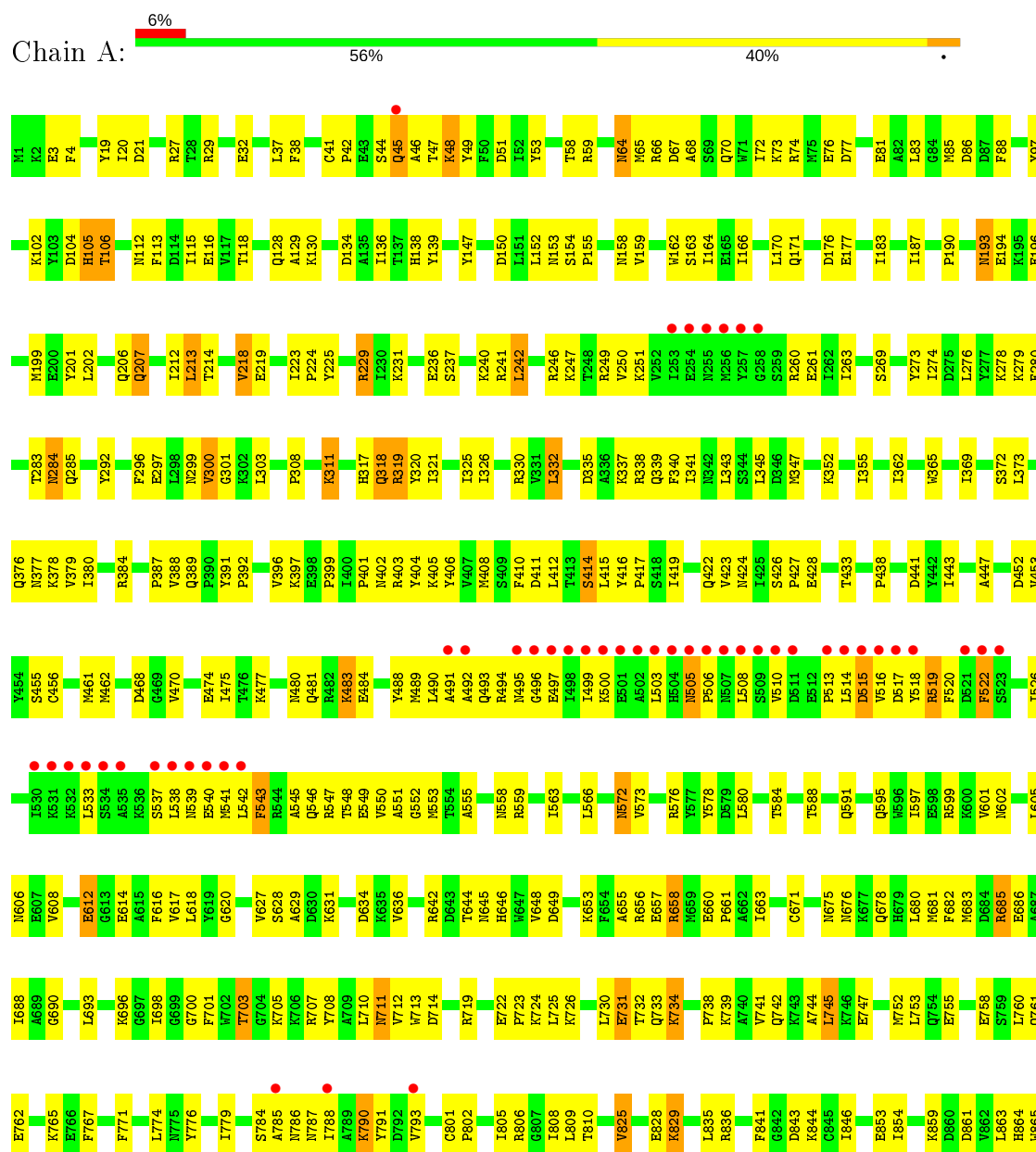
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	50	Total	O	0	0
			50	50		
5	C	40	Total	O	0	0
			40	40		
5	D	27	Total	O	0	0
			27	27		
5	E	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		
5	G	2	Total	O	0	0
			2	2		
5	H	1	Total	O	0	0
			1	1		
5	I	3	Total	O	0	0
			3	3		
5	J	2	Total	O	0	0
			2	2		
5	K	1	Total	O	0	0
			1	1		
5	L	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

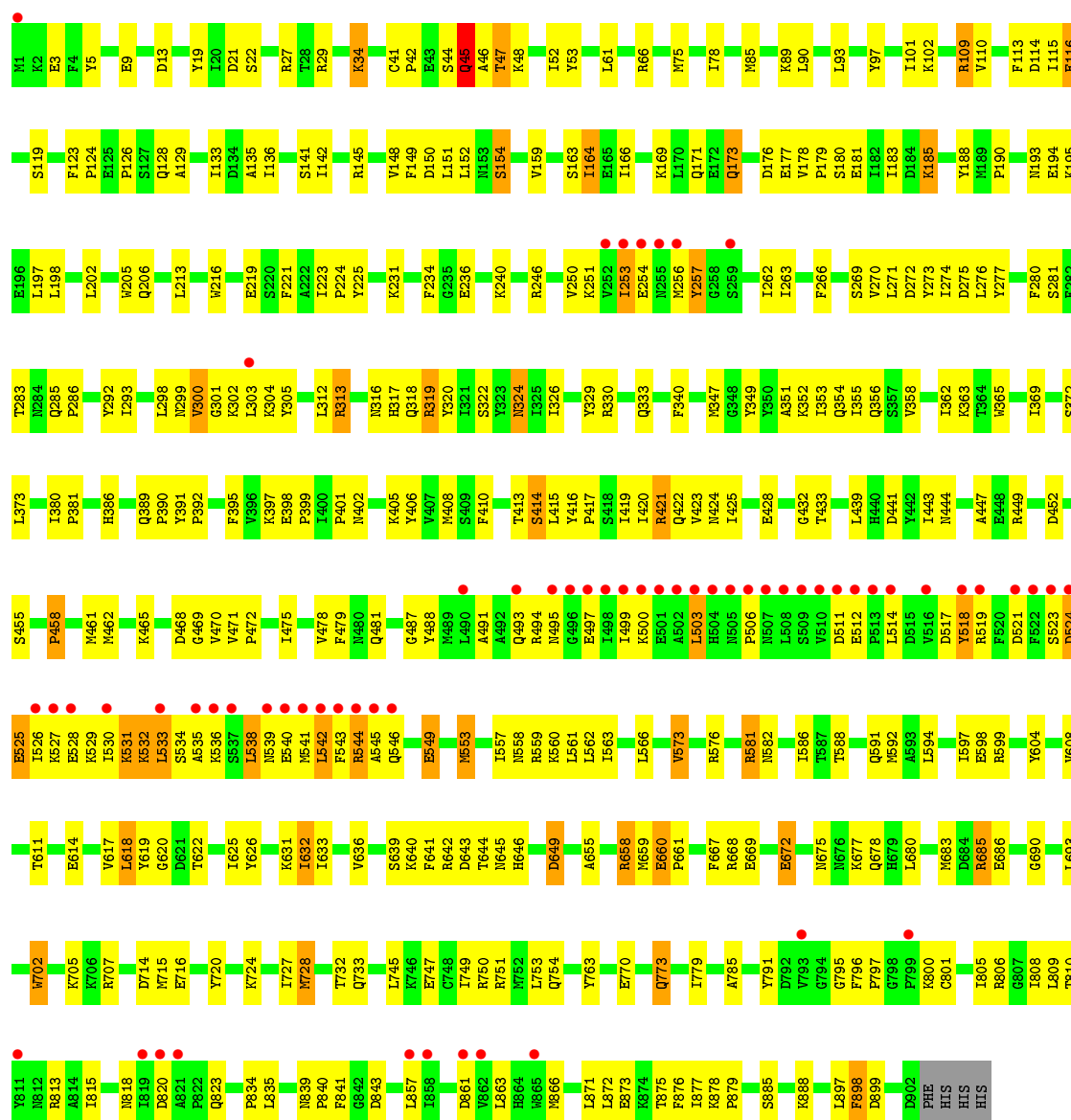
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 polymerase



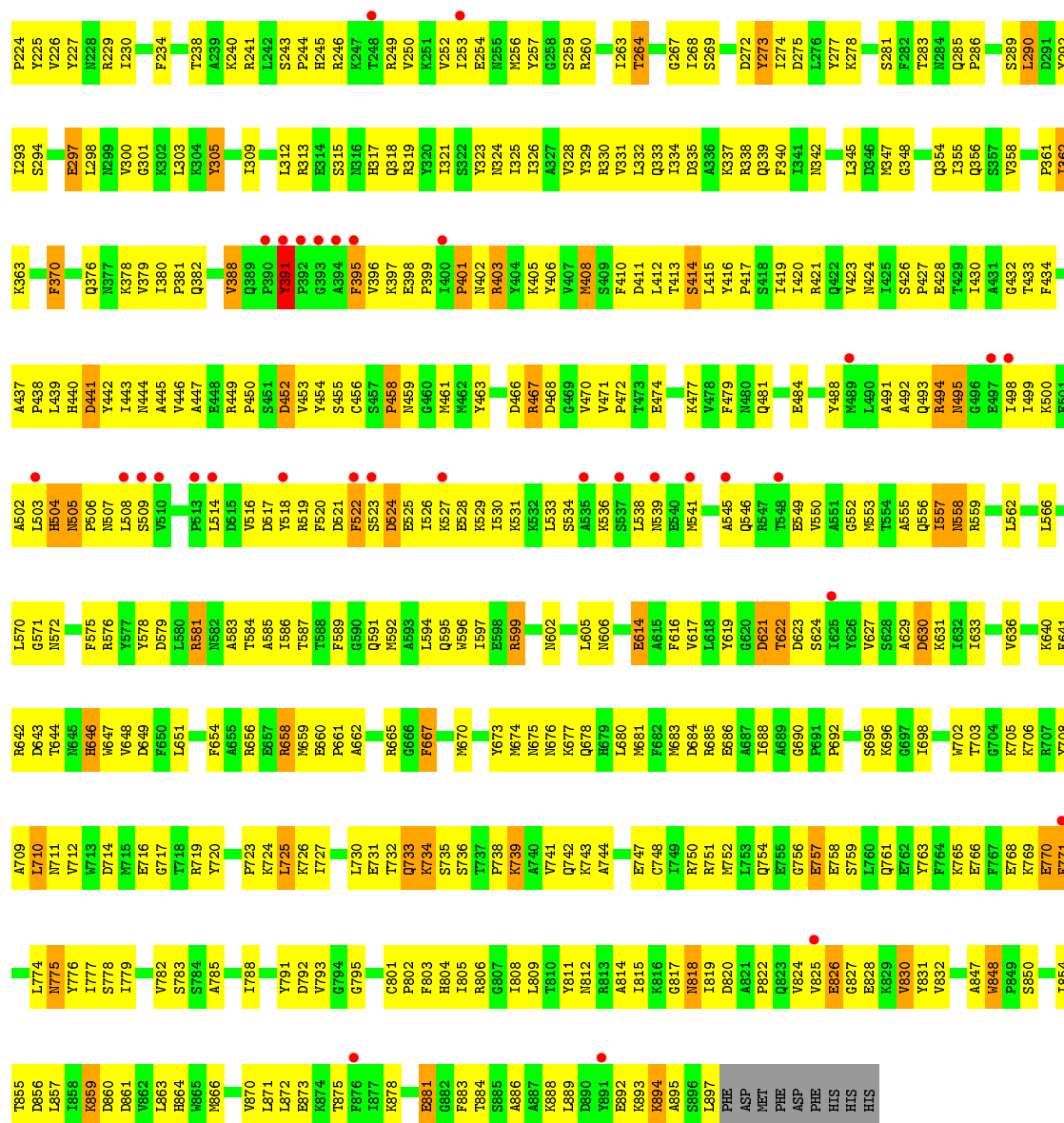


• Molecule 1: DNA polymerase

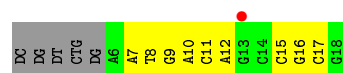


• Molecule 1: DNA polymerase





- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*G*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

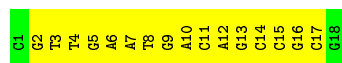


- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*G*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')



- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*G*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:  11% 89%



- Molecule 2: DNA (5'-D(*CP*GP*TP*(CTG)P*G*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:  22% 78%



- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*AP*A)-3')

Chain F:  40% 40% 7% 13%



- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*AP*A)-3')

Chain H:  47% 53%



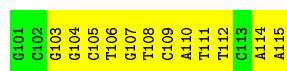
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*AP*A)-3')

Chain J:  13% 87%



- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*AP*A)-3')

Chain L:  20% 80%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.84Å 123.03Å 168.78Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	50.00 – 2.98 49.74 – 2.98	Depositor EDS
% Data completeness (in resolution range)	92.8 (50.00-2.98) 96.6 (49.74-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.275 0.220 , 0.277	Depositor DCC
R_{free} test set	20372 reflections (9.61%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31870	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CTG, DTP

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	0.45	0/7462	0.64	0/10099
1	B	0.44	0/7494	0.63	0/10138
1	C	0.45	0/7491	0.64	0/10134
1	D	0.39	0/7343	0.63	2/9963 (0.0%)
2	E	0.33	0/298	0.68	0/458
2	G	0.40	0/390	0.78	0/598
2	I	0.55	0/390	0.78	0/598
2	K	0.30	0/390	0.65	0/598
3	F	0.57	1/292 (0.3%)	0.71	0/449
3	H	0.39	0/340	0.72	0/523
3	J	0.49	0/340	0.83	0/523
3	L	0.34	0/337	0.68	0/517
All	All	0.43	1/32567 (0.0%)	0.64	2/44598 (0.0%)

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	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	113	DC	N1-C2	5.00	1.45	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	391	TYR	N-CA-CB	-6.65	98.62	110.60
1	D	391	TYR	CA-CB-CG	6.42	125.59	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	12	DA	Sidechain

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	7284	0	7114	388	0
1	B	7315	0	7162	349	0
1	C	7312	0	7157	510	0
1	D	7165	0	6893	607	0
2	E	265	0	146	17	0
2	G	370	0	205	20	0
2	I	370	0	205	29	0
2	K	370	0	205	23	0
3	F	262	0	149	9	0
3	H	304	0	171	10	0
3	J	304	0	171	17	0
3	L	301	0	162	20	0
4	B	30	0	12	3	0
4	J	30	0	12	2	0
5	A	59	0	0	8	0
5	B	50	0	0	3	0
5	C	40	0	0	6	0
5	D	27	0	0	3	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	H	1	0	0	0	0
5	I	3	0	0	1	0
5	J	2	0	0	0	0
5	K	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	1	0	0	0	0
All	All	31870	0	29764	1967	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 32.

All (1967) 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)
1:C:149:PHE:HB3	1:C:197:LEU:HD11	1.20	1.17
1:B:732:THR:HG23	1:B:733:GLN:HE21	0.98	1.13
1:C:424:ASN:HD22	1:C:677:LYS:HD3	1.01	1.10
1:D:214:THR:HG22	1:D:215:GLY:H	1.10	1.09
3:L:110:DA:H2''	3:L:111:DT:H5'	1.34	1.08
2:E:10:DA:H2''	2:E:11:DC:H5''	1.14	1.07
1:A:422:GLN:HE22	1:A:681:MET:HG2	1.11	1.05
1:D:164:ILE:H	1:D:164:ILE:HD13	1.22	1.05
1:C:511:ASP:HB3	1:C:534:SER:HB2	1.35	1.03
1:D:149:PHE:HB3	1:D:197:LEU:HD21	1.39	1.03
3:L:108:DT:H2''	3:L:109:DC:H5''	1.37	1.02
1:A:642:ARG:H	1:A:646:HIS:CD2	1.77	1.02
1:B:465:LYS:HE3	1:B:677:LYS:HA	1.39	1.01
1:A:493:GLN:HB2	1:A:549:GLU:HG3	1.40	1.01
1:B:668:ARG:HH11	1:B:668:ARG:HB2	1.24	1.01
1:D:116:GLU:HB2	1:D:135:ALA:HB3	1.42	0.99
1:C:25:ARG:NH2	1:C:27:ARG:HH22	1.60	0.98
2:E:8:DT:H1'	2:E:9:DG:H5''	1.44	0.98
1:D:491:ALA:O	1:D:495:ASN:HB2	1.66	0.96
2:E:10:DA:H2''	2:E:11:DC:C5'	1.95	0.95
1:D:606:ASN:HD21	1:D:614:GLU:H	1.04	0.95
1:D:412:LEU:HD12	1:D:623:ASP:HA	1.47	0.95
1:C:25:ARG:HH21	1:C:27:ARG:HH22	1.12	0.94
1:D:517:ASP:HB3	1:D:519:ARG:HG2	1.50	0.94
1:C:512:GLU:HG3	1:C:513:PRO:HD2	1.45	0.94
1:B:732:THR:HG23	1:B:733:GLN:NE2	1.83	0.94
1:B:499:ILE:HG22	1:B:542:LEU:HD22	1.49	0.93
1:C:711:ASN:ND2	1:C:754:GLN:HE21	1.67	0.93
1:C:41:CYS:HB3	1:C:58:THR:HG22	1.49	0.93
1:C:392:PRO:O	1:C:587:THR:HG21	1.69	0.92
1:D:300:VAL:HG23	1:D:301:GLY:H	1.34	0.92
1:C:572:ASN:ND2	1:C:574:TRP:H	1.67	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ARG:H	1:A:646:HIS:HD2	0.98	0.92
2:G:15:DC:H42	3:H:103:DG:H1	1.18	0.92
1:D:82:ALA:H	1:D:382:GLN:HE21	0.92	0.92
1:C:424:ASN:ND2	1:C:677:LYS:HD3	1.84	0.92
3:L:108:DT:H2''	3:L:109:DC:C5'	2.00	0.91
1:C:660:GLU:HB2	1:C:661:PRO:HD3	1.52	0.91
3:F:103:DG:H2''	3:F:104:DG:H5'	1.52	0.90
1:D:136:ILE:HG23	1:D:149:PHE:HB2	1.53	0.90
1:D:97:TYR:HB3	1:D:101:ILE:HD11	1.51	0.90
1:B:636:VAL:O	1:B:640:LYS:HE2	1.71	0.90
1:D:830:VAL:HG23	1:D:848:TRP:O	1.70	0.90
2:E:10:DA:C2'	2:E:11:DC:H5''	2.02	0.90
1:A:752:MET:HG3	1:A:760:LEU:HD13	1.52	0.90
1:D:449:ARG:NH1	1:D:452:ASP:HB3	1.85	0.89
1:D:133:ILE:HD11	1:D:229:ARG:HG2	1.52	0.89
1:B:668:ARG:NH1	1:B:668:ARG:HB2	1.89	0.88
1:C:533:LEU:HD13	1:C:538:LEU:HG	1.53	0.88
1:A:347:MET:HB2	1:A:558:ASN:HD21	1.38	0.88
1:D:347:MET:HG2	1:D:358:VAL:HG13	1.53	0.88
1:D:509:SER:HB3	1:D:534:SER:HB3	1.55	0.88
1:D:443:ILE:HD13	1:D:595:GLN:NE2	1.89	0.87
1:A:516:VAL:HB	1:A:522:PHE:HZ	1.38	0.87
1:D:727:ILE:HG23	1:D:730:LEU:HD12	1.56	0.86
2:I:14:DC:H2''	2:I:15:DC:H5''	1.58	0.86
1:B:732:THR:CG2	1:B:733:GLN:HE21	1.85	0.86
1:D:494:ARG:O	1:D:494:ARG:HG2	1.75	0.86
1:D:751:ARG:NH1	1:D:763:TYR:HB2	1.89	0.85
1:A:176:ASP:HA	1:A:319:ARG:HH21	1.40	0.85
1:D:398:GLU:HB3	1:D:705:LYS:HE3	1.58	0.85
2:I:15:DC:H2''	2:I:16:DG:C8	2.11	0.85
1:D:791:TYR:CE2	1:D:802:PRO:HD3	2.12	0.85
1:C:541:MET:CE	1:C:542:LEU:HB2	2.07	0.85
1:D:395:PHE:HB2	1:D:591:GLN:CD	1.96	0.85
1:C:159:VAL:HG11	1:C:317:HIS:HB3	1.58	0.85
1:C:711:ASN:HD21	1:C:754:GLN:HE21	1.20	0.84
2:G:11:DC:H2''	2:G:12:DA:H5'	1.59	0.84
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.57	0.84
1:A:489:MET:HE1	1:A:553:MET:SD	2.18	0.84
1:D:293:ILE:HD12	1:D:294:SER:N	1.92	0.84
1:A:308:PRO:HG2	1:A:311:LYS:HG3	1.59	0.84
1:B:171:GLN:HE22	1:B:303:LEU:HD13	1.41	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:THR:HG22	1:D:215:GLY:N	1.92	0.84
1:D:82:ALA:N	1:D:382:GLN:HE21	1.74	0.84
1:A:703:THR:HG21	1:A:707:ARG:HD3	1.57	0.83
1:D:82:ALA:H	1:D:382:GLN:NE2	1.76	0.83
1:C:502:ALA:HB1	1:C:533:LEU:HD12	1.59	0.83
1:D:297:GLU:HG2	1:D:334:ILE:HG23	1.61	0.83
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.60	0.82
1:C:206:GLN:HE21	1:C:206:GLN:HA	1.42	0.82
1:C:855:THR:HG22	1:C:857:LEU:H	1.43	0.82
1:D:116:GLU:HG2	1:D:324:ASN:HD22	1.45	0.82
1:A:176:ASP:HA	1:A:319:ARG:NH2	1.94	0.82
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.45	0.82
1:C:611:THR:HG22	1:C:612:GLU:H	1.42	0.82
1:D:224:PRO:HA	1:D:263:ILE:HD12	1.62	0.82
2:E:11:DC:H2''	2:E:12:DA:H5'	1.62	0.82
1:C:818:ASN:ND2	1:C:857:LEU:HD11	1.94	0.81
1:C:180:SER:HA	1:C:183:ILE:HD12	1.61	0.81
1:D:791:TYR:CD2	1:D:801:CYS:HA	2.15	0.81
1:C:412:LEU:HD13	1:C:415:LEU:HD13	1.62	0.81
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.63	0.81
1:D:514:LEU:HD21	1:D:526:ILE:HG23	1.63	0.81
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.63	0.81
1:C:72:ILE:O	1:C:76:GLU:HG3	1.80	0.81
1:C:133:ILE:HD12	1:C:198:LEU:HD21	1.63	0.81
1:A:514:LEU:HD21	1:A:526:ILE:HG22	1.63	0.80
1:D:238:THR:HG23	1:D:241:ARG:HH21	1.45	0.80
1:C:511:ASP:CB	1:C:534:SER:HB2	2.09	0.80
2:I:13:DG:H5''	2:I:13:DG:H8	1.44	0.80
1:A:731:GLU:HG3	1:A:879:PRO:HB3	1.63	0.79
1:D:739:LYS:O	1:D:743:LYS:HG3	1.82	0.79
1:C:491:ALA:HA	1:C:494:ARG:HE	1.47	0.79
1:D:151:LEU:HD12	1:D:153:ASN:O	1.82	0.79
1:A:422:GLN:NE2	1:A:681:MET:HG2	1.95	0.79
1:C:572:ASN:HD22	1:C:574:TRP:H	1.26	0.79
1:A:761:GLN:OE1	1:A:893:LYS:HG2	1.82	0.79
1:D:621:ASP:O	1:D:621:ASP:OD2	2.01	0.79
1:C:254:GLU:HB2	1:C:258:GLY:O	1.83	0.79
1:D:391:TYR:OH	1:D:571:GLY:HA3	1.83	0.79
1:D:442:TYR:HB3	1:D:592:MET:HE3	1.64	0.79
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.19	0.78
1:B:686:GLU:OE2	1:B:716:GLU:HG3	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:NH2	1:A:251:LYS:HZ1	1.82	0.78
1:B:599:ARG:HH11	1:B:599:ARG:HG2	1.47	0.78
1:C:216:TRP:NE1	1:C:274:ILE:HD12	1.98	0.78
1:D:223:ILE:HB	1:D:224:PRO:HD3	1.65	0.78
1:A:642:ARG:N	1:A:646:HIS:HD2	1.80	0.77
1:C:159:VAL:HG12	1:C:160:GLU:H	1.49	0.77
1:D:698:ILE:HG12	1:D:752:MET:O	1.85	0.77
1:C:541:MET:HE3	1:C:542:LEU:HB2	1.66	0.77
1:D:734:LYS:NZ	2:K:7:DA:H4'	1.99	0.77
1:C:495:ASN:ND2	1:C:521:ASP:HA	1.99	0.77
1:D:391:TYR:HE2	1:D:583:ALA:HB1	1.47	0.77
1:D:395:PHE:HB2	1:D:591:GLN:OE1	1.84	0.77
1:D:4:PHE:HB3	5:D:915:HOH:O	1.84	0.77
1:D:391:TYR:CE2	1:D:583:ALA:HB1	2.19	0.77
1:A:97:TYR:O	1:A:352:LYS:HE2	1.85	0.77
1:C:118:THR:OG1	1:C:313:ARG:HG3	1.85	0.77
1:C:312:LEU:HG	1:C:320:TYR:HD1	1.49	0.77
1:C:41:CYS:HB3	1:C:58:THR:CG2	2.13	0.77
1:D:298:LEU:HB2	1:D:300:VAL:HG22	1.67	0.77
1:D:204:PHE:CE1	1:D:208:LYS:HD2	2.20	0.76
1:D:505:ASN:N	1:D:506:PRO:HD3	2.00	0.76
2:I:4:CTG:H2''	2:I:5:DG:H5'	1.67	0.76
1:D:355:ILE:O	1:D:358:VAL:HG23	1.85	0.76
1:B:511:ASP:OD1	1:B:533:LEU:HA	1.84	0.76
1:D:72:ILE:O	1:D:76:GLU:HG3	1.86	0.76
1:A:516:VAL:HB	1:A:522:PHE:CZ	2.22	0.75
1:A:404:TYR:CD1	1:A:618:LEU:HD22	2.22	0.75
1:C:806:ARG:HH11	1:C:806:ARG:HG2	1.51	0.75
3:L:110:DA:H2''	3:L:111:DT:C5'	2.15	0.75
1:C:34:LYS:HE2	1:C:63:ALA:HA	1.68	0.75
1:D:775:ASN:HD22	1:D:776:TYR:H	1.32	0.75
1:C:300:VAL:HG22	1:C:330:ARG:HH12	1.49	0.75
2:K:16:DG:H2''	2:K:17:DC:H5''	1.68	0.75
1:A:493:GLN:HB2	1:A:549:GLU:CG	2.17	0.75
1:D:273:TYR:OH	1:D:335:ASP:HA	1.86	0.75
3:F:104:DG:H2''	3:F:105:DC:O5'	1.86	0.75
2:K:14:DC:H2''	2:K:15:DC:H5'	1.67	0.75
1:A:533:LEU:HD22	1:A:541:MET:HE3	1.69	0.74
1:C:120:PRO:O	1:C:819:ILE:HG21	1.85	0.74
1:D:149:PHE:HB3	1:D:197:LEU:CD2	2.17	0.74
1:B:669:GLU:O	1:B:672:GLU:HG3	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ASP:O	1:C:145:ARG:HG2	1.87	0.74
1:D:398:GLU:CB	1:D:705:LYS:HZ2	2.00	0.74
1:D:441:ASP:HB3	1:D:447:ALA:HB2	1.67	0.74
1:D:440:HIS:CE1	1:D:444:ASN:HD21	2.05	0.74
1:C:424:ASN:HD22	1:C:677:LYS:CD	1.92	0.74
1:D:272:ASP:OD2	1:D:274:ILE:HG22	1.88	0.74
1:A:279:LYS:C	1:A:280:PHE:HD1	1.92	0.73
1:B:514:LEU:HD21	1:B:530:ILE:HG12	1.71	0.73
1:B:397:LYS:HD3	1:B:619:TYR:HA	1.68	0.73
1:B:749:ILE:O	1:B:753:LEU:HD13	1.88	0.73
1:D:711:ASN:OD1	1:D:723:PRO:HB2	1.89	0.73
1:A:703:THR:HG21	1:A:707:ARG:HH11	1.52	0.73
1:C:511:ASP:HB3	1:C:534:SER:CB	2.15	0.73
1:C:572:ASN:HD22	1:C:574:TRP:N	1.86	0.73
1:B:863:LEU:HD12	1:B:866:MET:HE3	1.70	0.73
1:D:686:GLU:OE2	1:D:716:GLU:HG2	1.88	0.73
1:A:213:LEU:CD1	1:A:223:ILE:HD11	2.19	0.73
1:A:48:LYS:HD3	1:A:377:ASN:CG	2.10	0.73
1:B:97:TYR:HB3	1:B:101:ILE:HD11	1.68	0.73
1:D:82:ALA:O	1:D:382:GLN:HG3	1.88	0.73
2:I:3:DT:H2''	2:I:4:CTG:H72	1.71	0.73
1:A:703:THR:CG2	1:A:707:ARG:HD3	2.19	0.72
1:C:507:ASN:HB3	1:C:532:LYS:HA	1.72	0.72
2:I:14:DC:H2''	2:I:15:DC:C5'	2.18	0.72
1:D:163:SER:HB2	1:D:165:GLU:OE2	1.90	0.72
1:A:406:TYR:HB3	1:A:629:ALA:HB3	1.71	0.72
1:D:398:GLU:HB3	1:D:705:LYS:CE	2.19	0.72
1:D:725:LEU:H	1:D:725:LEU:HD12	1.53	0.72
3:L:108:DT:C2'	3:L:109:DC:H5''	2.15	0.72
1:A:825:VAL:HG22	1:A:828:GLU:HG2	1.72	0.72
1:C:534:SER:O	1:C:538:LEU:HB2	1.88	0.71
2:E:11:DC:H2''	2:E:12:DA:C5'	2.18	0.71
1:C:159:VAL:HG11	1:C:317:HIS:CB	2.19	0.71
1:D:238:THR:HG23	1:D:241:ARG:NH2	2.05	0.71
1:A:496:GLY:HA2	1:A:499:ILE:HD12	1.72	0.71
1:C:130:LYS:HE3	1:C:131:HIS:HE1	1.55	0.71
1:D:164:ILE:H	1:D:164:ILE:CD1	1.99	0.71
1:D:442:TYR:HB3	1:D:592:MET:CE	2.20	0.71
2:G:15:DC:N4	3:H:103:DG:H1	1.88	0.71
1:B:152:LEU:HD11	1:B:190:PRO:HB2	1.70	0.71
1:C:872:LEU:HD12	1:C:876:PHE:HB3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:LEU:O	1:B:541:MET:HE3	1.89	0.71
1:D:770:GLU:O	1:D:774:LEU:HG	1.91	0.71
1:A:163:SER:OG	1:A:166:ILE:HD13	1.91	0.71
1:B:163:SER:H	1:B:318:GLN:HE22	1.37	0.71
1:D:648:VAL:HG12	1:D:719:ARG:HH21	1.55	0.70
1:A:338:ARG:HB3	1:A:340:PHE:CE1	2.25	0.70
1:C:451:SER:OG	1:C:453:VAL:HG22	1.90	0.70
1:D:212:ILE:HD11	1:D:345:LEU:HD21	1.73	0.70
1:D:685:ARG:HH11	1:D:688:ILE:HG13	1.56	0.70
2:I:14:DC:C2'	2:I:15:DC:H5''	2.20	0.70
1:B:526:ILE:O	1:B:530:ILE:HG13	1.91	0.70
1:D:514:LEU:HB2	1:D:533:LEU:HD11	1.73	0.70
1:D:449:ARG:HH12	1:D:452:ASP:HB3	1.56	0.70
1:B:495:ASN:OD1	1:B:521:ASP:HA	1.91	0.70
1:B:636:VAL:HG13	1:B:640:LYS:HE3	1.73	0.70
1:C:482:ARG:HH12	1:C:560:LYS:HB2	1.56	0.70
1:C:81:GLU:HG2	1:C:83:LEU:HD22	1.73	0.70
1:C:78:ILE:HG13	1:C:80:LEU:HD23	1.73	0.70
1:D:399:PRO:O	1:D:401:PRO:HD3	1.91	0.70
1:D:696:LYS:O	1:D:756:GLY:HA2	1.92	0.70
1:D:752:MET:HE2	1:D:889:LEU:HD12	1.74	0.70
1:C:162:TRP:HB3	1:C:188:TYR:CE1	2.26	0.70
1:C:509:SER:HB3	1:C:532:LYS:HD2	1.73	0.70
1:D:430:ILE:HD12	1:D:430:ILE:H	1.57	0.70
1:B:253:ILE:HD13	1:B:254:GLU:H	1.57	0.69
1:C:538:LEU:O	1:C:538:LEU:HD23	1.89	0.69
1:C:482:ARG:NH1	1:C:560:LYS:HB2	2.07	0.69
1:C:825:VAL:HB	1:C:828:GLU:CD	2.13	0.69
1:D:15:ILE:HG23	1:D:65:MET:HE1	1.74	0.69
1:C:499:ILE:HG13	1:C:541:MET:SD	2.32	0.69
1:D:109:ARG:HE	1:D:208:LYS:HB3	1.57	0.69
2:G:11:DC:H2''	2:G:12:DA:C5'	2.22	0.69
1:D:809:LEU:HA	1:D:812:ASN:HD22	1.57	0.69
1:C:159:VAL:HG12	1:C:160:GLU:N	2.06	0.69
1:A:397:LYS:HB3	1:A:620:GLY:H	1.58	0.69
1:B:406:TYR:CD2	1:B:633:ILE:HG13	2.28	0.69
1:A:806:ARG:HA	1:A:809:LEU:HD12	1.73	0.69
1:B:523:SER:H	1:B:526:ILE:HD12	1.57	0.69
1:C:104:ASP:OD2	1:C:107:LYS:HG2	1.92	0.69
1:C:318:GLN:HA	1:C:318:GLN:HE21	1.58	0.69
1:C:431:ALA:HA	1:C:464:TYR:CE1	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:PHE:CD1	1:C:197:LEU:HD13	2.28	0.68
1:D:775:ASN:HD22	1:D:776:TYR:N	1.91	0.68
1:B:491:ALA:HA	1:B:494:ARG:NH2	2.09	0.68
1:C:199:MET:HG2	1:C:234:PHE:CZ	2.28	0.68
1:D:214:THR:HG21	1:D:273:TYR:HD2	1.59	0.68
1:A:207:GLN:HA	1:A:207:GLN:HE21	1.58	0.68
1:B:369:ILE:HG22	1:B:373:LEU:HD12	1.76	0.68
1:B:608:VAL:HG13	1:D:897:LEU:HD13	1.73	0.68
1:D:757:GLU:O	1:D:761:GLN:HG3	1.93	0.68
1:C:223:ILE:HB	1:C:224:PRO:HD3	1.74	0.68
1:B:365:TRP:O	1:B:369:ILE:HD12	1.93	0.68
1:C:179:PRO:O	1:C:183:ILE:HG13	1.94	0.68
1:A:642:ARG:NH1	1:A:642:ARG:HB2	2.09	0.67
1:C:727:ILE:HD13	1:C:749:ILE:HD12	1.75	0.67
1:C:322:SER:O	1:C:326:ILE:HG13	1.94	0.67
1:C:14:SER:HB3	1:C:32:GLU:OE2	1.93	0.67
1:C:490:LEU:O	1:C:494:ARG:HG3	1.93	0.67
1:B:421:ARG:HB3	1:B:680:LEU:CD1	2.24	0.67
1:D:493:GLN:HG3	1:D:549:GLU:OE2	1.93	0.67
1:B:303:LEU:HD13	1:B:319:ARG:NH2	2.09	0.67
1:D:153:ASN:HA	1:D:158:ASN:ND2	2.10	0.67
2:K:11:DC:H4'	2:K:11:DC:OP1	1.93	0.67
1:C:171:GLN:HG2	1:C:177:GLU:OE1	1.95	0.67
2:G:12:DA:H2''	2:G:13:DG:C8	2.30	0.67
2:I:13:DG:H2'	2:I:14:DC:C6	2.30	0.67
1:A:410:PHE:HB2	1:A:683:MET:HE1	1.76	0.67
1:A:493:GLN:CB	1:A:549:GLU:HG3	2.22	0.67
1:B:503:LEU:HB2	1:B:542:LEU:HD21	1.77	0.67
1:B:597:ILE:HD13	1:B:683:MET:SD	2.35	0.67
1:C:491:ALA:HA	1:C:494:ARG:NE	2.09	0.67
1:A:280:PHE:HE2	1:A:343:LEU:HD22	1.60	0.67
1:B:303:LEU:HD13	1:B:319:ARG:HH22	1.60	0.67
1:B:416:TYR:O	1:B:420:ILE:HG13	1.94	0.67
1:B:559:ARG:O	1:B:563:ILE:HD12	1.94	0.67
1:C:711:ASN:HD21	1:C:754:GLN:NE2	1.93	0.67
1:D:167:ALA:HA	1:D:176:ASP:HB2	1.77	0.67
1:C:488:TYR:CD2	1:C:519:ARG:HD2	2.29	0.67
1:C:523:SER:HB3	1:C:525:GLU:HG2	1.76	0.67
1:D:412:LEU:HG	1:D:623:ASP:O	1.95	0.67
1:A:171:GLN:NE2	1:A:319:ARG:HH12	1.92	0.66
1:A:597:ILE:O	1:A:601:VAL:HG23	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:ARG:HD3	1:B:646:HIS:CE1	2.30	0.66
1:C:109:ARG:NH1	1:C:142:ILE:HD12	2.11	0.66
2:I:13:DG:H5''	2:I:13:DG:C8	2.29	0.66
1:A:19:TYR:HE1	1:A:29:ARG:HG2	1.61	0.66
1:A:202:LEU:O	1:A:206:GLN:HG2	1.94	0.66
1:C:505:ASN:N	1:C:506:PRO:HD3	2.11	0.66
1:D:197:LEU:O	1:D:197:LEU:HD13	1.94	0.66
1:A:369:ILE:HG12	1:A:474:GLU:HG3	1.78	0.66
1:C:177:GLU:HG3	1:C:303:LEU:HD11	1.76	0.66
1:C:507:ASN:ND2	1:C:508:LEU:H	1.93	0.66
1:D:777:ILE:HD12	1:D:778:SER:N	2.11	0.66
2:G:10:DA:H2''	2:G:11:DC:C5'	2.26	0.66
1:A:411:ASP:OD2	1:A:686:GLU:HG3	1.95	0.66
1:D:416:TYR:CD1	1:D:586:ILE:HG22	2.30	0.66
1:A:231:LYS:HG3	1:A:236:GLU:HA	1.77	0.66
2:K:13:DG:H2''	2:K:14:DC:OP2	1.94	0.66
1:A:752:MET:CG	1:A:760:LEU:HD13	2.26	0.66
1:B:449:ARG:HH12	1:B:452:ASP:HB2	1.61	0.66
1:A:722:GLU:HA	1:A:722:GLU:OE2	1.96	0.65
1:D:140:ASP:OD1	1:D:142:ILE:HG12	1.94	0.65
1:C:808:ILE:HD12	1:C:824:VAL:HG11	1.77	0.65
1:B:119:SER:HB2	1:B:124:PRO:HG3	1.79	0.65
1:B:110:VAL:H	1:B:141:SER:HB3	1.61	0.65
1:D:300:VAL:HG23	1:D:301:GLY:N	2.07	0.65
3:F:103:DG:H2''	3:F:104:DG:C5'	2.25	0.65
1:C:509:SER:OG	1:C:532:LYS:HB3	1.97	0.65
1:D:855:THR:HG22	1:D:857:LEU:HG	1.78	0.65
1:A:48:LYS:HG2	1:A:48:LYS:O	1.95	0.65
1:A:602:ASN:ND2	1:A:616:PHE:H	1.94	0.65
1:C:611:THR:HG22	1:C:612:GLU:N	2.11	0.65
1:C:444:ASN:HA	1:C:599:ARG:HE	1.62	0.65
1:D:503:LEU:O	1:D:503:LEU:HD23	1.97	0.65
1:B:642:ARG:NH1	1:B:646:HIS:ND1	2.41	0.65
1:D:15:ILE:HG13	1:D:31:VAL:HG22	1.79	0.65
1:A:475:ILE:CD1	1:A:566:LEU:HD22	2.27	0.65
1:A:712:VAL:HG22	1:A:724:LYS:O	1.96	0.65
1:C:255:ASN:CG	1:C:256:MET:H	1.98	0.65
1:D:226:VAL:O	1:D:230:ILE:HG13	1.97	0.65
2:E:8:DT:H1'	2:E:9:DG:C5'	2.24	0.64
1:A:499:ILE:HD13	1:A:541:MET:O	1.97	0.64
1:A:171:GLN:HE22	1:A:319:ARG:HH12	1.43	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:VAL:O	1:B:559:ARG:HG3	1.97	0.64
1:D:808:ILE:HG23	1:D:824:VAL:HG21	1.78	0.64
1:A:171:GLN:HE22	1:A:319:ARG:HH22	1.43	0.64
1:C:311:LYS:HA	1:C:314:GLU:OE1	1.98	0.64
1:D:112:ASN:HD21	1:D:331:VAL:HG11	1.63	0.64
1:D:507:ASN:O	1:D:509:SER:N	2.30	0.64
1:D:656:ARG:HB3	1:D:656:ARG:HH11	1.61	0.64
1:A:514:LEU:H	1:A:541:MET:CE	2.10	0.64
1:C:434:PHE:CE1	1:C:460:GLY:HA2	2.31	0.64
1:C:475:ILE:HG23	1:C:476:THR:N	2.12	0.64
1:D:606:ASN:HD21	1:D:614:GLU:N	1.88	0.64
1:D:727:ILE:CG2	1:D:730:LEU:HD12	2.27	0.64
3:L:111:DT:H2''	3:L:112:DT:H5''	1.79	0.64
1:B:468:ASP:OD1	1:B:677:LYS:HE3	1.98	0.64
1:D:499:ILE:HD13	1:D:541:MET:O	1.95	0.64
1:D:660:GLU:HA	1:D:660:GLU:OE1	1.97	0.64
1:B:303:LEU:HB3	1:B:319:ARG:HH21	1.61	0.64
1:C:251:LYS:HG2	1:C:253:ILE:HG23	1.80	0.64
3:H:110:DA:H2''	3:H:111:DT:H5'	1.80	0.64
1:B:326:ILE:O	1:B:330:ARG:HG2	1.97	0.64
1:C:533:LEU:HB3	1:C:538:LEU:HD12	1.80	0.64
3:J:105:DC:H2''	3:J:106:DT:O5'	1.98	0.64
1:B:536:LYS:HA	1:B:539:ASN:HD22	1.63	0.64
1:C:492:ALA:HB3	5:C:940:HOH:O	1.97	0.64
1:D:143:ASP:O	1:D:145:ARG:HG2	1.98	0.64
1:D:526:ILE:HA	1:D:529:LYS:HB2	1.79	0.64
1:A:410:PHE:HB2	1:A:683:MET:CE	2.27	0.63
1:C:525:GLU:CD	1:C:525:GLU:H	2.00	0.63
1:D:3:GLU:HG3	1:D:21:ASP:HA	1.79	0.63
1:D:826:GLU:OE1	1:D:826:GLU:N	2.31	0.63
1:D:825:VAL:CG2	1:D:828:GLU:HB2	2.28	0.63
1:A:128:GLN:HB3	1:A:130:LYS:HE3	1.80	0.63
1:A:343:LEU:O	1:A:343:LEU:HD23	1.99	0.63
1:A:403:ARG:HD2	1:A:887:ALA:O	1.99	0.63
1:B:269:SER:HA	1:B:356:GLN:NE2	2.14	0.63
1:D:159:VAL:HG11	1:D:317:HIS:HB2	1.80	0.63
1:B:416:TYR:CD2	4:B:907:DTP:H2'1	2.33	0.63
1:B:119:SER:CB	1:B:124:PRO:HG3	2.28	0.63
1:B:439:LEU:O	1:B:443:ILE:HG13	1.98	0.63
1:B:503:LEU:HD12	1:B:542:LEU:HG	1.79	0.63
1:C:52:ILE:HD12	1:C:428:GLU:HG3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ASN:HD21	1:D:331:VAL:CG1	2.11	0.63
1:B:685:ARG:HG2	5:B:919:HOH:O	1.98	0.63
1:B:599:ARG:HG2	1:B:599:ARG:NH1	2.14	0.63
1:C:533:LEU:HB3	1:C:538:LEU:CD1	2.28	0.63
1:C:343:LEU:HG	1:C:558:ASN:HD21	1.64	0.63
1:A:308:PRO:HG2	1:A:311:LYS:CG	2.27	0.63
1:C:109:ARG:CZ	1:C:142:ILE:HD12	2.29	0.63
1:C:312:LEU:HG	1:C:320:TYR:CD1	2.33	0.63
1:C:485:HIS:HA	1:C:488:TYR:HB2	1.81	0.63
1:C:505:ASN:N	1:C:506:PRO:CD	2.62	0.63
1:D:606:ASN:ND2	1:D:614:GLU:H	1.88	0.63
1:D:832:VAL:HG22	1:D:847:ALA:HB2	1.81	0.63
1:A:319:ARG:HD3	5:A:907:HOH:O	1.99	0.63
1:B:66:ARG:HB3	5:B:911:HOH:O	1.98	0.63
1:D:204:PHE:HE1	1:D:208:LYS:HD2	1.63	0.63
1:D:791:TYR:HD2	1:D:801:CYS:HA	1.64	0.63
1:A:503:LEU:HA	1:A:538:LEU:HD13	1.80	0.62
1:B:313:ARG:NH1	1:B:313:ARG:HG2	2.12	0.62
1:B:329:TYR:O	1:B:333:GLN:HG3	1.99	0.62
1:C:434:PHE:CE2	1:C:450:PRO:HB3	2.34	0.62
1:A:597:ILE:HD11	1:A:663:ILE:HG23	1.80	0.62
1:B:534:SER:O	1:B:538:LEU:HB2	1.99	0.62
1:C:542:LEU:C	1:C:546:GLN:HE21	2.02	0.62
1:D:136:ILE:HD11	1:D:201:TYR:CE1	2.34	0.62
1:A:280:PHE:HD2	1:A:343:LEU:HD13	1.63	0.62
1:C:144:ASP:O	1:C:145:ARG:HD3	1.99	0.62
1:C:25:ARG:NH2	1:C:27:ARG:NH2	2.43	0.62
1:D:217:ASN:OD1	1:D:220:SER:HB2	1.99	0.62
1:D:658:ARG:HH11	1:D:658:ARG:HG3	1.64	0.62
2:K:10:DA:H2''	2:K:11:DC:O5'	1.99	0.62
1:C:163:SER:OG	1:C:166:ILE:HG13	2.00	0.62
1:A:747:GLU:OE2	1:A:747:GLU:HA	1.99	0.62
2:K:13:DG:H1	3:L:105:DC:H42	1.47	0.62
1:B:305:TYR:CD2	1:B:312:LEU:HD22	2.35	0.62
1:C:188:TYR:CD2	1:C:190:PRO:HD3	2.34	0.62
1:C:193:ASN:OD1	1:C:196:GLU:HG2	2.00	0.62
1:A:412:LEU:HG	1:A:683:MET:HG3	1.80	0.62
1:A:74:ARG:O	1:A:77:ASP:HB2	2.00	0.62
1:A:836:ARG:HG3	1:A:836:ARG:HH11	1.64	0.62
1:B:668:ARG:HH11	1:B:668:ARG:CB	2.08	0.62
1:C:254:GLU:CB	1:C:259:SER:HA	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LYS:HZ3	1:C:302:LYS:HB2	1.65	0.62
1:C:481:GLN:HB3	1:C:559:ARG:HH11	1.63	0.62
1:D:733:GLN:HA	1:D:733:GLN:NE2	2.13	0.62
1:A:249:ARG:HH21	1:A:251:LYS:HZ1	1.45	0.62
1:B:791:TYR:CD2	1:B:801:CYS:HA	2.35	0.62
1:C:477:LYS:O	1:C:481:GLN:HG3	1.99	0.62
1:C:854:ILE:HG22	1:C:859:LYS:HD3	1.82	0.62
1:A:500:LYS:HA	1:A:503:LEU:HD12	1.82	0.61
1:A:685:ARG:NH2	1:A:714:ASP:OD2	2.33	0.61
1:D:145:ARG:HD3	1:D:185:LYS:O	2.00	0.61
1:C:477:LYS:HG2	1:C:481:GLN:HE21	1.63	0.61
1:D:339:GLN:HG2	1:D:342:ASN:HB3	1.80	0.61
1:D:855:THR:CG2	1:D:857:LEU:HG	2.30	0.61
1:C:402:ASN:ND2	1:C:403:ARG:H	1.98	0.61
1:B:270:VAL:C	1:B:271:LEU:HD12	2.20	0.61
1:D:323:TYR:O	1:D:326:ILE:HG13	1.99	0.61
1:D:752:MET:CE	1:D:889:LEU:HD12	2.30	0.61
1:A:475:ILE:HD11	1:A:566:LEU:HD22	1.82	0.61
1:A:602:ASN:HD21	1:A:617:VAL:H	1.46	0.61
1:B:231:LYS:HD2	1:B:236:GLU:OE1	2.01	0.61
1:B:495:ASN:HD21	1:B:521:ASP:HA	1.64	0.61
1:D:206:GLN:NE2	1:D:241:ARG:O	2.34	0.61
1:A:705:LYS:HB2	2:E:8:DT:OP1	2.00	0.61
1:A:19:TYR:CE1	1:A:29:ARG:HG2	2.35	0.61
1:A:513:PRO:HA	1:A:541:MET:HE2	1.83	0.61
1:B:495:ASN:ND2	1:B:521:ASP:HA	2.16	0.61
1:C:431:ALA:HA	1:C:464:TYR:HE1	1.65	0.61
1:D:614:GLU:HB3	1:D:616:PHE:HE2	1.66	0.61
1:C:128:GLN:HB3	5:C:942:HOH:O	2.01	0.61
1:D:804:HIS:O	1:D:808:ILE:HG13	2.01	0.61
1:A:771:PHE:HA	1:A:774:LEU:HD12	1.83	0.61
1:C:49:TYR:CE1	1:C:59:ARG:HB2	2.36	0.61
1:D:621:ASP:O	1:D:623:ASP:N	2.30	0.61
1:A:415:LEU:O	1:A:419:ILE:HG13	2.01	0.61
1:A:642:ARG:N	1:A:646:HIS:CD2	2.59	0.61
1:B:176:ASP:O	1:B:303:LEU:HD12	2.01	0.61
1:C:308:PRO:HG2	1:C:311:LYS:HG2	1.83	0.61
1:C:59:ARG:HH11	1:C:59:ARG:HG3	1.65	0.61
1:D:152:LEU:HD11	1:D:190:PRO:HB2	1.83	0.61
1:C:41:CYS:CB	1:C:58:THR:HG22	2.28	0.61
1:A:422:GLN:HG3	1:A:678:GLN:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:LEU:HD21	1:D:659:MET:HE3	1.81	0.60
1:D:412:LEU:CD1	1:D:623:ASP:HA	2.27	0.60
1:C:36:SER:HB3	1:C:59:ARG:CD	2.31	0.60
1:D:119:SER:HB2	1:D:131:HIS:CD2	2.36	0.60
1:D:499:ILE:O	1:D:503:LEU:HB2	1.99	0.60
1:D:51:ASP:OD1	1:D:53:TYR:N	2.29	0.60
1:D:381:PRO:HG2	1:D:576:ARG:HG2	1.82	0.60
3:H:110:DA:H2''	3:H:111:DT:C5'	2.32	0.60
2:K:16:DG:H2''	2:K:17:DC:C5'	2.32	0.60
1:C:738:PRO:HG2	1:C:741:VAL:HB	1.84	0.60
1:C:797:PRO:HG3	1:C:806:ARG:HE	1.67	0.60
1:D:146:PHE:CE2	1:D:182:ILE:HG13	2.36	0.60
1:B:618:LEU:HD11	1:B:702:TRP:CZ3	2.36	0.60
1:C:164:ILE:HD11	1:C:183:ILE:O	2.01	0.60
1:C:791:TYR:CD2	1:C:801:CYS:HA	2.36	0.60
1:D:416:TYR:HD1	1:D:586:ILE:HG22	1.65	0.60
1:A:139:TYR:CD2	1:A:332:LEU:HD21	2.37	0.60
1:A:588:THR:O	1:A:591:GLN:HB2	2.02	0.60
1:A:802:PRO:CG	3:F:109:DC:H4'	2.31	0.60
1:B:465:LYS:HE3	1:B:677:LYS:CA	2.23	0.60
1:D:214:THR:CG2	1:D:215:GLY:H	1.92	0.60
1:D:599:ARG:HH11	1:D:599:ARG:HB3	1.66	0.60
1:D:648:VAL:HG12	1:D:719:ARG:NH2	2.15	0.60
1:A:738:PRO:HG2	1:A:741:VAL:HB	1.84	0.60
1:A:758:GLU:O	1:A:762:GLU:HG3	2.01	0.60
1:C:34:LYS:HB3	1:C:61:LEU:HD21	1.84	0.60
1:C:858:ILE:O	1:C:862:VAL:HG23	2.02	0.60
1:D:249:ARG:HB3	1:D:264:THR:OG1	2.02	0.60
1:D:356:GLN:N	1:D:356:GLN:OE1	2.26	0.60
1:A:508:LEU:HD22	1:A:508:LEU:N	2.17	0.60
1:A:745:LEU:HD13	1:A:876:PHE:CE1	2.37	0.60
1:B:511:ASP:OD2	1:B:533:LEU:HD23	2.01	0.60
1:B:533:LEU:HD23	1:B:534:SER:H	1.66	0.60
1:C:272:ASP:CG	1:C:274:ILE:HG22	2.22	0.60
1:D:198:LEU:N	1:D:198:LEU:HD22	2.16	0.60
1:D:395:PHE:HB2	1:D:591:GLN:NE2	2.16	0.60
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.31	0.59
1:A:505:ASN:N	1:A:506:PRO:HD3	2.16	0.59
1:C:300:VAL:CG2	1:C:330:ARG:HH12	2.15	0.59
1:C:412:LEU:CD1	1:C:415:LEU:HD13	2.31	0.59
1:D:277:TYR:O	1:D:281:SER:CB	2.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:752:MET:HE3	1:D:884:THR:HG22	1.83	0.59
1:D:403:ARG:HH22	1:D:889:LEU:HD21	1.67	0.59
1:A:176:ASP:O	1:A:303:LEU:HD21	2.02	0.59
1:A:391:TYR:HB2	1:A:392:PRO:HD2	1.83	0.59
1:B:362:ILE:HG12	2:G:2:DG:OP2	2.02	0.59
1:B:660:GLU:HB3	1:B:661:PRO:HD3	1.83	0.59
1:C:176:ASP:O	1:C:177:GLU:HB2	2.02	0.59
1:C:795:GLY:O	1:C:813:ARG:HD3	2.02	0.59
1:C:900:MET:HA	1:C:900:MET:HE2	1.83	0.59
1:D:734:LYS:HG3	1:D:736:SER:H	1.67	0.59
3:J:113:DC:H5'	3:J:113:DC:H6	1.67	0.59
1:B:272:ASP:CG	1:B:274:ILE:HG22	2.21	0.59
1:B:34:LYS:HZ2	1:B:61:LEU:HD11	1.67	0.59
1:D:430:ILE:HD12	1:D:430:ILE:N	2.17	0.59
1:D:792:ASP:OD1	1:D:795:GLY:HA2	2.02	0.59
1:D:830:VAL:HG23	1:D:848:TRP:C	2.22	0.59
1:B:262:ILE:O	1:B:262:ILE:HG13	2.01	0.59
1:D:109:ARG:NH1	1:D:142:ILE:HD11	2.17	0.59
1:D:733:GLN:HA	1:D:733:GLN:HE21	1.67	0.59
1:D:806:ARG:HB3	1:D:806:ARG:NH1	2.16	0.59
1:A:874:LYS:HE2	2:E:11:DC:OP1	2.02	0.59
1:A:495:ASN:C	1:A:497:GLU:H	2.05	0.59
1:A:49:TYR:CE1	1:A:59:ARG:HB2	2.37	0.59
1:B:250:VAL:HG12	1:B:263:ILE:HD13	1.84	0.59
1:C:391:TYR:HB2	1:C:392:PRO:HD2	1.85	0.59
1:D:534:SER:O	1:D:538:LEU:HG	2.03	0.59
1:C:898:PHE:N	1:C:898:PHE:CD2	2.67	0.59
2:E:8:DT:H2''	2:E:9:DG:OP2	2.02	0.59
2:I:9:DG:H2''	2:I:10:DA:H5'	1.84	0.59
1:C:3:GLU:HB2	1:C:20:ILE:O	2.02	0.59
1:B:538:LEU:HD22	1:B:542:LEU:HD23	1.84	0.59
1:D:191:PHE:CD2	1:D:197:LEU:HA	2.37	0.59
1:D:642:ARG:HH21	1:D:646:HIS:CD2	2.21	0.59
1:D:15:ILE:HG23	1:D:65:MET:CE	2.32	0.59
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.83	0.58
1:B:528:GLU:HA	1:B:531:LYS:HD2	1.85	0.58
1:C:898:PHE:HD2	1:C:898:PHE:H	1.50	0.58
1:A:428:GLU:OE1	1:A:470:VAL:HG23	2.03	0.58
1:B:354:GLN:HB3	1:B:356:GLN:OE1	2.02	0.58
1:B:428:GLU:OE1	1:B:470:VAL:HG23	2.02	0.58
1:C:270:VAL:O	1:C:271:LEU:HD23	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ALA:O	1:C:493:GLN:N	2.36	0.58
1:C:557:ILE:O	1:C:561:LEU:HD13	2.02	0.58
1:C:793:VAL:O	1:C:793:VAL:HG12	2.03	0.58
1:D:656:ARG:NH1	1:D:656:ARG:HB3	2.16	0.58
1:D:775:ASN:ND2	1:D:776:TYR:H	2.00	0.58
1:D:85:MET:HA	1:D:380:ILE:HD11	1.85	0.58
2:G:16:DG:H1'	2:G:17:DC:H5''	1.84	0.58
1:A:37:LEU:HD11	1:A:72:ILE:HD11	1.84	0.58
1:A:649:ASP:CG	1:A:719:ARG:HH12	2.05	0.58
1:B:101:ILE:HG21	1:B:349:TYR:HB3	1.85	0.58
1:B:34:LYS:NZ	1:B:61:LEU:HD11	2.19	0.58
3:J:103:DG:H2''	3:J:104:DG:OP2	2.03	0.58
1:D:696:LYS:CB	1:D:756:GLY:HA3	2.34	0.58
1:A:236:GLU:O	1:A:240:LYS:HG2	2.03	0.58
1:A:414:SER:O	1:A:417:PRO:HD2	2.03	0.58
1:B:421:ARG:HB3	1:B:680:LEU:HD12	1.84	0.58
1:D:198:LEU:C	1:D:200:GLU:H	2.07	0.58
1:D:345:LEU:HA	1:D:355:ILE:HD12	1.85	0.58
1:D:686:GLU:HA	1:D:686:GLU:OE2	2.03	0.58
1:B:164:ILE:HD13	1:B:164:ILE:N	2.19	0.58
1:C:18:ARG:NH2	1:C:209:THR:HG22	2.18	0.58
1:C:255:ASN:ND2	1:C:256:MET:H	2.01	0.58
1:C:518:TYR:HB2	1:C:548:THR:HG21	1.85	0.58
1:C:572:ASN:ND2	1:C:574:TRP:N	2.42	0.58
1:D:660:GLU:HB3	1:D:661:PRO:HD3	1.85	0.58
2:K:16:DG:C2'	2:K:17:DC:H5''	2.34	0.58
1:B:380:ILE:HD12	1:B:576:ARG:CZ	2.34	0.58
1:D:405:LYS:O	1:D:690:GLY:HA2	2.03	0.58
1:A:280:PHE:N	1:A:280:PHE:CD1	2.72	0.58
1:A:280:PHE:N	1:A:280:PHE:HD1	2.01	0.58
1:A:653:LYS:HE3	1:A:657:GLU:OE1	2.03	0.58
1:B:101:ILE:HG21	1:B:349:TYR:CD1	2.39	0.58
1:C:113:PHE:CE1	1:C:213:LEU:HD11	2.39	0.58
1:C:461:MET:SD	1:C:581:ARG:HB3	2.43	0.58
1:D:150:ASP:OD2	1:D:321:ILE:HG13	2.04	0.58
1:D:362:ILE:HG22	1:D:363:LYS:N	2.19	0.58
1:A:250:VAL:HG23	1:A:250:VAL:O	2.02	0.58
1:A:64:ASN:HD22	1:A:64:ASN:C	2.06	0.58
1:C:254:GLU:HB3	1:C:259:SER:HA	1.85	0.58
1:D:458:PRO:HG2	1:D:592:MET:SD	2.44	0.58
1:D:81:GLU:HG3	1:D:382:GLN:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ILE:O	1:D:325:ILE:HG13	2.04	0.58
1:D:775:ASN:ND2	1:D:776:TYR:N	2.52	0.58
1:A:105:HIS:HD2	1:A:106:THR:N	2.01	0.57
1:B:405:LYS:O	1:B:690:GLY:HA2	2.04	0.57
1:B:461:MET:SD	1:B:581:ARG:HG2	2.43	0.57
1:C:136:ILE:HB	1:C:149:PHE:HB2	1.86	0.57
1:C:489:MET:HG2	1:C:493:GLN:HE21	1.68	0.57
1:D:523:SER:C	1:D:527:LYS:HG3	2.25	0.57
1:D:256:MET:N	2:K:4:CTG:OP2	2.36	0.57
1:A:387:PRO:O	1:A:389:GLN:HG3	2.04	0.57
1:A:64:ASN:ND2	1:A:67:ASP:H	2.02	0.57
1:C:314:GLU:CD	1:C:314:GLU:H	2.07	0.57
1:D:198:LEU:O	1:D:200:GLU:N	2.38	0.57
1:D:402:ASN:CG	1:D:403:ARG:N	2.57	0.57
1:A:872:LEU:HD12	1:A:876:PHE:HB3	1.85	0.57
1:B:795:GLY:O	1:B:813:ARG:HD3	2.04	0.57
1:C:206:GLN:CA	1:C:206:GLN:HE21	2.15	0.57
1:C:512:GLU:CG	1:C:513:PRO:HD2	2.27	0.57
1:C:611:THR:HG21	1:C:614:GLU:HG3	1.87	0.57
1:D:801:CYS:SG	1:D:806:ARG:HG2	2.45	0.57
2:G:10:DA:H2''	2:G:11:DC:H5''	1.85	0.57
1:C:361:PRO:HD2	2:I:2:DG:OP2	2.03	0.57
1:A:835:LEU:HD11	1:A:846:ILE:HB	1.86	0.57
1:B:727:ILE:HG21	1:B:732:THR:HG21	1.87	0.57
1:D:398:GLU:CA	1:D:705:LYS:HZ2	2.16	0.57
1:D:765:LYS:O	1:D:768:GLU:HB2	2.03	0.57
1:D:830:VAL:HA	1:D:850:SER:HB2	1.87	0.57
2:I:16:DG:H5'	5:I:118:HOH:O	2.04	0.57
1:A:41:CYS:SG	1:A:58:THR:HG23	2.43	0.57
1:A:81:GLU:OE2	1:A:83:LEU:HG	2.05	0.57
1:C:422:GLN:HG3	1:C:678:GLN:O	2.05	0.57
1:D:240:LYS:O	1:D:246:ARG:HA	2.04	0.57
1:D:848:TRP:CD1	1:D:848:TRP:N	2.73	0.57
2:K:11:DC:H2''	2:K:12:DA:H8	1.68	0.57
1:A:112:ASN:HB2	5:A:947:HOH:O	2.04	0.57
1:A:48:LYS:HD3	1:A:377:ASN:OD1	2.04	0.57
1:B:576:ARG:O	1:B:576:ARG:HG3	2.04	0.57
1:C:143:ASP:OD1	1:C:208:LYS:NZ	2.37	0.57
1:A:870:VAL:O	1:A:874:LYS:HG2	2.04	0.57
1:C:162:TRP:HB3	1:C:188:TYR:CZ	2.39	0.57
1:C:163:SER:HB3	1:C:166:ILE:HD12	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:TYR:HB2	1:C:417:PRO:HD3	1.87	0.57
1:D:159:VAL:HG21	1:D:317:HIS:ND1	2.20	0.57
1:D:734:LYS:HZ3	2:K:7:DA:H4'	1.70	0.57
2:E:9:DG:H2''	2:E:10:DA:OP2	2.03	0.57
1:A:802:PRO:HG2	3:F:109:DC:H4'	1.85	0.57
3:F:112:DT:H2''	3:F:113:DC:C6	2.39	0.57
1:A:426:SER:OG	1:A:427:PRO:HD2	2.05	0.57
1:B:668:ARG:O	1:B:672:GLU:HG2	2.05	0.57
1:B:685:ARG:NH2	1:B:714:ASP:OD2	2.31	0.57
1:D:883:PHE:CD2	1:D:883:PHE:N	2.71	0.57
1:A:41:CYS:HB3	1:A:58:THR:HG23	1.87	0.57
1:C:512:GLU:HG3	1:C:513:PRO:CD	2.28	0.57
1:D:165:GLU:CD	1:D:165:GLU:H	2.07	0.57
1:D:330:ARG:O	1:D:334:ILE:HG13	2.05	0.57
1:D:503:LEU:HD11	1:D:539:ASN:OD1	2.04	0.57
1:D:751:ARG:HD3	1:D:759:SER:OG	2.04	0.57
1:A:171:GLN:HE22	1:A:319:ARG:NH1	2.03	0.57
1:A:83:LEU:HD12	1:A:83:LEU:N	2.20	0.57
1:D:468:ASP:OD2	1:D:677:LYS:HE3	2.05	0.57
1:D:602:ASN:HD21	1:D:617:VAL:H	1.52	0.57
1:A:396:VAL:O	1:A:705:LYS:HE2	2.05	0.56
1:C:643:ASP:HA	1:C:693:LEU:HD23	1.87	0.56
1:D:619:TYR:CZ	1:D:621:ASP:HB3	2.40	0.56
1:D:605:LEU:HD11	1:D:659:MET:HE1	1.87	0.56
3:J:113:DC:H2''	3:J:114:DA:C8	2.39	0.56
1:B:560:LYS:HE3	4:B:907:DTP:O3G	2.05	0.56
1:C:533:LEU:CD1	1:C:538:LEU:HG	2.29	0.56
1:C:752:MET:HG2	1:C:889:LEU:CD1	2.35	0.56
1:D:182:ILE:HD12	1:D:329:TYR:CD1	2.40	0.56
1:D:159:VAL:HG21	1:D:317:HIS:CE1	2.39	0.56
1:A:171:GLN:HE22	1:A:319:ARG:NH2	2.04	0.56
1:A:37:LEU:CD1	1:A:72:ILE:HD11	2.34	0.56
1:B:75:MET:O	1:B:78:ILE:HG22	2.05	0.56
1:C:324:ASN:HD22	1:C:324:ASN:C	2.08	0.56
1:C:541:MET:HE1	1:C:542:LEU:HB2	1.85	0.56
1:D:188:TYR:CD2	1:D:190:PRO:HD3	2.40	0.56
1:D:396:VAL:HG23	1:D:396:VAL:O	2.05	0.56
1:D:402:ASN:CG	1:D:403:ARG:H	2.08	0.56
1:D:756:GLY:O	1:D:758:GLU:N	2.38	0.56
2:G:10:DA:H2''	2:G:11:DC:H5'	1.87	0.56
1:A:490:LEU:HD12	1:A:490:LEU:N	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ALA:HA	1:B:494:ARG:CZ	2.36	0.56
1:B:523:SER:O	1:B:527:LYS:HG3	2.04	0.56
1:C:152:LEU:HD11	1:C:190:PRO:HB2	1.87	0.56
1:C:403:ARG:HD3	5:C:937:HOH:O	2.06	0.56
1:D:619:TYR:CE1	1:D:621:ASP:HB3	2.40	0.56
1:D:710:LEU:HD12	1:D:726:LYS:HB3	1.85	0.56
1:D:734:LYS:HG3	1:D:735:SER:N	2.20	0.56
3:J:113:DC:H5'	3:J:113:DC:C6	2.40	0.56
1:A:115:ILE:HG22	1:A:136:ILE:HG12	1.86	0.56
1:C:412:LEU:HD13	1:C:415:LEU:CD1	2.33	0.56
1:D:818:ASN:C	1:D:820:ASP:H	2.09	0.56
3:H:114:DA:H2''	3:H:115:DA:O5'	2.05	0.56
1:A:785:ALA:CB	1:A:808:ILE:HD11	2.35	0.56
1:A:791:TYR:CD2	1:A:801:CYS:HA	2.41	0.56
1:B:720:TYR:CZ	1:B:724:LYS:HD2	2.40	0.56
1:C:579:ASP:HB3	1:C:582:ASN:HD22	1.70	0.56
1:A:876:PHE:O	1:A:879:PRO:HD2	2.04	0.56
1:B:115:ILE:HG22	1:B:136:ILE:HG23	1.87	0.56
1:B:514:LEU:O	1:B:514:LEU:HD12	2.06	0.56
1:C:83:LEU:N	1:C:83:LEU:HD22	2.20	0.56
1:A:475:ILE:HD11	1:A:566:LEU:CD2	2.35	0.56
1:C:302:LYS:CD	1:C:326:ILE:HD12	2.36	0.56
1:D:277:TYR:O	1:D:281:SER:HB3	2.05	0.56
1:D:388:VAL:HG23	1:D:388:VAL:O	2.06	0.56
1:D:791:TYR:CE2	1:D:801:CYS:HA	2.40	0.56
1:D:808:ILE:HG22	1:D:812:ASN:HD21	1.71	0.56
1:A:412:LEU:HD22	1:A:415:LEU:HD13	1.86	0.56
1:C:286:PRO:HB3	1:C:782:VAL:HG21	1.88	0.56
1:C:808:ILE:CD1	1:C:830:VAL:HG11	2.36	0.56
1:A:514:LEU:H	1:A:541:MET:HE2	1.69	0.56
1:A:66:ARG:HG3	1:A:66:ARG:HH11	1.70	0.56
1:B:101:ILE:HD13	1:B:352:LYS:HE2	1.88	0.56
1:B:395:PHE:HB2	1:B:591:GLN:HG3	1.88	0.56
1:C:130:LYS:HG3	1:C:131:HIS:ND1	2.20	0.56
1:C:145:ARG:HB2	1:C:147:TYR:CE1	2.40	0.56
1:C:145:ARG:HB2	1:C:147:TYR:HE1	1.69	0.56
1:C:216:TRP:HE1	1:C:274:ILE:HD12	1.70	0.56
1:C:81:GLU:HG2	1:C:83:LEU:CD2	2.35	0.56
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.88	0.56
1:A:64:ASN:HD21	1:A:67:ASP:CG	2.09	0.56
1:A:739:LYS:HD3	1:A:742:GLN:OE1	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:THR:HB	1:B:614:GLU:HG3	1.88	0.56
1:C:167:ALA:HA	1:C:176:ASP:HB2	1.88	0.56
1:C:891:TYR:CD2	1:C:892:GLU:HG3	2.41	0.56
1:D:444:ASN:HA	1:D:599:ARG:NE	2.21	0.56
1:B:707:ARG:HD2	2:G:7:DA:H4'	1.88	0.56
1:C:305:TYR:OH	1:C:309:ILE:HG12	2.06	0.55
1:C:518:TYR:CD2	1:C:522:PHE:HZ	2.24	0.55
1:C:779:ILE:O	1:C:871:LEU:HD21	2.06	0.55
1:D:505:ASN:N	1:D:506:PRO:CD	2.67	0.55
3:J:110:DA:H2''	3:J:111:DT:H5'	1.87	0.55
1:C:623:ASP:OD2	3:J:115:DA:O3'	2.20	0.55
1:A:213:LEU:HD13	1:A:223:ILE:HD11	1.86	0.55
1:A:373:LEU:HD21	1:A:470:VAL:HG13	1.88	0.55
1:B:475:ILE:HD11	1:B:563:ILE:HG12	1.87	0.55
1:C:298:LEU:O	1:C:299:ASN:HB2	2.06	0.55
1:C:541:MET:O	1:C:545:ALA:N	2.39	0.55
1:D:132:PRO:HB3	1:D:229:ARG:NH2	2.20	0.55
1:D:85:MET:CA	1:D:380:ILE:HD11	2.36	0.55
1:D:825:VAL:HG23	1:D:828:GLU:HB2	1.89	0.55
1:D:274:ILE:HG12	1:D:278:LYS:HE2	1.88	0.55
1:C:587:THR:HG22	1:C:588:THR:N	2.20	0.55
1:D:398:GLU:HA	1:D:705:LYS:HZ2	1.71	0.55
1:A:779:ILE:HG13	1:A:871:LEU:HD21	1.89	0.55
1:B:834:PRO:HD2	1:B:871:LEU:HD13	1.89	0.55
1:B:872:LEU:HD12	1:B:876:PHE:HB3	1.88	0.55
1:D:109:ARG:NH1	1:D:142:ILE:CD1	2.69	0.55
1:A:658:ARG:HH11	1:A:658:ARG:HG3	1.70	0.55
1:A:810:THR:CG2	1:A:841:PHE:HB3	2.36	0.55
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.88	0.55
1:B:753:LEU:N	1:B:753:LEU:HD12	2.21	0.55
1:C:604:TYR:O	1:C:608:VAL:HG23	2.06	0.55
1:D:408:MET:O	1:D:627:VAL:HG22	2.07	0.55
1:D:725:LEU:N	1:D:725:LEU:HD12	2.21	0.55
1:D:817:GLY:HA3	5:D:921:HOH:O	2.07	0.55
1:D:128:GLN:O	1:D:128:GLN:HG3	2.07	0.55
2:K:5:DG:H1'	2:K:6:DA:H5'	1.88	0.55
1:B:285:GLN:HG3	1:B:292:TYR:HE2	1.72	0.55
3:J:107:DG:H2''	3:J:108:DT:H5'	1.89	0.55
1:C:509:SER:O	1:C:511:ASP:N	2.38	0.54
1:C:455:SER:HA	1:C:675:ASN:O	2.07	0.54
1:D:402:ASN:ND2	1:D:403:ARG:O	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:HD23	1:D:61:LEU:O	2.06	0.54
1:D:863:LEU:HA	1:D:866:MET:HE2	1.88	0.54
2:I:13:DG:H2''	2:I:14:DC:H5'	1.89	0.54
1:A:48:LYS:HZ1	2:K:17:DC:P	2.30	0.54
1:A:730:LEU:HD13	1:A:883:PHE:CE1	2.42	0.54
1:B:353:ILE:HG13	1:B:354:GLN:O	2.06	0.54
1:B:779:ILE:HD12	1:B:871:LEU:HD23	1.88	0.54
1:C:498:ILE:HD12	1:C:501:GLU:OE2	2.07	0.54
1:D:105:HIS:CD2	1:D:106:THR:N	2.76	0.54
1:C:308:PRO:HG2	1:C:311:LYS:CG	2.37	0.54
1:C:322:SER:O	1:C:326:ILE:CG1	2.55	0.54
1:D:397:LYS:O	1:D:399:PRO:HD3	2.08	0.54
1:D:776:TYR:CG	1:D:863:LEU:HD11	2.42	0.54
3:L:103:DG:H2''	3:L:104:DG:O5'	2.06	0.54
1:A:129:ALA:O	1:A:229:ARG:NH1	2.41	0.54
1:B:546:GLN:O	1:B:549:GLU:HB3	2.08	0.54
1:C:453:VAL:HG23	1:C:454:TYR:CG	2.42	0.54
1:C:507:ASN:HB3	1:C:532:LYS:HG2	1.87	0.54
1:C:149:PHE:N	1:C:149:PHE:CD1	2.74	0.54
1:D:519:ARG:HB2	1:D:520:PHE:CD2	2.42	0.54
1:D:614:GLU:HB3	1:D:616:PHE:CE2	2.42	0.54
1:A:513:PRO:HG2	1:A:540:GLU:CG	2.38	0.54
1:B:221:PHE:C	1:B:224:PRO:HD2	2.28	0.54
1:B:720:TYR:CE1	1:B:724:LYS:HD2	2.43	0.54
1:C:36:SER:HB3	1:C:59:ARG:HD3	1.89	0.54
1:C:806:ARG:NH1	1:C:844:LYS:HE2	2.22	0.54
1:D:92:TYR:CZ	1:D:96:THR:HG21	2.43	0.54
2:I:9:DG:H2''	2:I:10:DA:C5'	2.38	0.54
2:I:11:DC:H2''	2:I:12:DA:H5'	1.89	0.54
1:A:249:ARG:HH21	1:A:251:LYS:NZ	2.05	0.54
1:A:280:PHE:CE2	1:A:343:LEU:HD22	2.42	0.54
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.89	0.54
1:C:272:ASP:OD1	1:C:274:ILE:HG22	2.08	0.54
1:C:489:MET:HA	5:C:940:HOH:O	2.06	0.54
1:C:78:ILE:CG1	1:C:80:LEU:HD23	2.38	0.54
3:H:105:DC:H2''	3:H:106:DT:O5'	2.08	0.54
3:J:102:DC:H1'	3:J:103:DG:H5'	1.89	0.54
1:B:274:ILE:HG23	1:B:275:ASP:N	2.22	0.54
1:B:835:LEU:HD23	1:B:866:MET:HA	1.90	0.54
1:C:548:THR:HG22	1:C:548:THR:O	2.07	0.54
1:D:191:PHE:HE2	1:D:200:GLU:HG3	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:ILE:O	1:D:530:ILE:HG13	2.08	0.54
1:D:750:ARG:NH2	1:D:751:ARG:HG2	2.22	0.54
1:A:836:ARG:HH12	1:A:865:TRP:HA	1.73	0.54
1:B:597:ILE:HG21	1:B:667:PHE:CE2	2.43	0.54
1:C:41:CYS:HB2	1:C:42:PRO:HD2	1.90	0.54
1:C:458:PRO:HG2	1:C:592:MET:SD	2.48	0.54
1:C:83:LEU:HB3	1:C:379:VAL:HG12	1.90	0.54
1:D:136:ILE:CG2	1:D:149:PHE:HB2	2.31	0.54
1:D:260:ARG:HH11	1:D:260:ARG:HG2	1.73	0.54
1:D:830:VAL:HA	1:D:850:SER:H	1.73	0.54
1:A:696:LYS:HB2	1:A:755:GLU:O	2.07	0.53
1:B:401:PRO:O	1:B:402:ASN:HB2	2.06	0.53
1:B:433:THR:N	1:B:462:MET:HE2	2.24	0.53
1:C:133:ILE:HD12	1:C:198:LEU:CD2	2.37	0.53
1:D:145:ARG:HB2	1:D:147:TYR:CE1	2.42	0.53
1:B:506:PRO:HB3	1:B:538:LEU:HD13	1.89	0.53
1:C:25:ARG:NE	1:C:27:ARG:HH12	2.07	0.53
1:C:302:LYS:HD3	1:C:326:ILE:HD12	1.90	0.53
1:C:518:TYR:HA	1:C:522:PHE:CE1	2.43	0.53
1:D:685:ARG:NH1	1:D:688:ILE:HG13	2.22	0.53
1:D:8:VAL:HG21	1:D:93:LEU:HD13	1.89	0.53
1:B:415:LEU:O	1:B:419:ILE:HG13	2.09	0.53
1:B:526:ILE:HG22	1:B:530:ILE:HD11	1.89	0.53
1:C:33:TYR:HD2	1:C:65:MET:CE	2.21	0.53
1:C:52:ILE:HB	1:C:428:GLU:HG2	1.89	0.53
1:D:528:GLU:OE2	1:D:531:LYS:HD2	2.08	0.53
1:D:826:GLU:O	1:D:828:GLU:HG3	2.08	0.53
2:I:15:DC:H2"	2:I:16:DG:N7	2.23	0.53
1:A:276:LEU:HD21	1:A:341:ILE:HD13	1.91	0.53
1:C:180:SER:HA	1:C:183:ILE:CD1	2.37	0.53
1:C:378:LYS:HE3	5:C:926:HOH:O	2.07	0.53
1:C:870:VAL:HG12	1:C:874:LYS:HE2	1.91	0.53
1:C:752:MET:HG2	1:C:889:LEU:HD12	1.90	0.53
1:D:109:ARG:CZ	1:D:142:ILE:HD11	2.38	0.53
1:D:145:ARG:HB2	1:D:147:TYR:HE1	1.73	0.53
1:D:685:ARG:NH2	1:D:717:GLY:H	2.05	0.53
1:D:826:GLU:CD	1:D:826:GLU:N	2.62	0.53
2:I:3:DT:N3	4:J:2:DTP:N6	2.57	0.53
1:A:725:LEU:HD12	1:A:725:LEU:H	1.73	0.53
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.91	0.53
1:B:495:ASN:CG	1:B:521:ASP:HA	2.29	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:TYR:HB3	1:D:263:ILE:HD13	1.90	0.53
1:D:417:PRO:O	1:D:421:ARG:HG3	2.08	0.53
1:D:444:ASN:HA	1:D:599:ARG:HE	1.72	0.53
1:A:517:ASP:OD2	1:A:519:ARG:HB3	2.09	0.53
1:C:38:PHE:N	1:C:38:PHE:CD1	2.75	0.53
1:D:319:ARG:HH21	1:D:319:ARG:HG2	1.74	0.53
1:D:830:VAL:CA	1:D:850:SER:HB2	2.39	0.53
2:G:16:DG:H2''	2:G:17:DC:C5'	2.39	0.53
1:A:301:GLY:O	1:A:330:ARG:NE	2.25	0.53
1:B:660:GLU:CB	1:B:661:PRO:HD3	2.37	0.53
1:C:271:LEU:HD21	1:C:356:GLN:HA	1.91	0.53
1:C:533:LEU:HD22	1:C:538:LEU:HA	1.90	0.53
1:D:309:ILE:HA	1:D:312:LEU:HB2	1.89	0.53
1:D:441:ASP:OD1	1:D:446:VAL:HB	2.08	0.53
1:D:734:LYS:HG2	1:D:736:SER:HB3	1.91	0.53
1:D:738:PRO:HG2	1:D:741:VAL:HG23	1.91	0.53
1:A:572:ASN:HD22	1:A:573:VAL:N	2.07	0.53
1:B:645:ASN:O	1:B:649:ASP:OD2	2.26	0.53
1:C:549:GLU:HA	5:C:940:HOH:O	2.08	0.53
1:C:83:LEU:CD2	1:C:83:LEU:N	2.72	0.53
1:B:416:TYR:HB2	1:B:417:PRO:HD3	1.91	0.53
1:D:432:GLY:O	1:D:461:MET:HE3	2.08	0.53
1:D:523:SER:O	1:D:527:LYS:HG3	2.09	0.53
1:A:299:ASN:O	1:A:300:VAL:HB	2.09	0.53
1:C:279:LYS:HD2	1:C:280:PHE:CZ	2.43	0.53
1:C:355:ILE:O	1:C:358:VAL:HG13	2.09	0.53
1:C:541:MET:SD	1:C:542:LEU:N	2.82	0.53
1:D:894:LYS:N	1:D:894:LYS:HD2	2.24	0.53
3:L:105:DC:H4'	3:L:105:DC:OP1	2.08	0.53
1:A:713:TRP:CZ3	1:A:723:PRO:HB3	2.42	0.52
1:B:322:SER:O	1:B:326:ILE:HG12	2.09	0.52
1:B:395:PHE:HD2	1:B:594:LEU:HD23	1.74	0.52
1:B:873:GLU:HA	1:B:877:ILE:HG13	1.91	0.52
1:C:172:GLU:H	1:C:172:GLU:CD	2.11	0.52
1:C:560:LYS:HG2	1:C:564:ASN:ND2	2.24	0.52
1:D:403:ARG:NH2	1:D:889:LEU:HD21	2.24	0.52
1:A:433:THR:HG22	1:A:461:MET:HE2	1.91	0.52
1:C:578:TYR:OH	1:C:580:LEU:HD13	2.09	0.52
1:C:791:TYR:CE2	1:C:802:PRO:HD3	2.45	0.52
1:D:791:TYR:CD2	1:D:802:PRO:HD3	2.43	0.52
1:A:503:LEU:HG	1:A:538:LEU:HB3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLU:HA	1:A:734:LYS:HD3	1.92	0.52
1:A:700:GLY:HA2	1:A:753:LEU:HD22	1.92	0.52
1:B:897:LEU:H	1:B:897:LEU:HD12	1.73	0.52
1:C:467:ARG:HG2	1:C:467:ARG:HH11	1.74	0.52
1:D:514:LEU:HD21	1:D:526:ILE:CG2	2.38	0.52
1:D:546:GLN:O	1:D:550:VAL:HG23	2.09	0.52
1:D:621:ASP:O	1:D:622:THR:HG22	2.09	0.52
1:A:105:HIS:CD2	1:A:106:THR:N	2.77	0.52
1:A:153:ASN:HD22	1:A:158:ASN:ND2	2.07	0.52
1:A:362:ILE:HD11	1:A:572:ASN:OD1	2.09	0.52
1:A:405:LYS:O	1:A:690:GLY:HA2	2.10	0.52
1:B:150:ASP:OD2	1:B:188:TYR:OH	2.24	0.52
1:B:47:THR:OG1	1:B:48:LYS:N	2.40	0.52
1:B:514:LEU:HG	1:B:541:MET:CE	2.40	0.52
1:C:109:ARG:HH11	1:C:109:ARG:HG3	1.74	0.52
1:D:260:ARG:HG2	1:D:260:ARG:NH1	2.24	0.52
1:A:365:TRP:CE2	1:A:566:LEU:HD12	2.45	0.52
1:A:599:ARG:HG2	1:A:599:ARG:HH11	1.75	0.52
1:B:149:PHE:HB3	1:B:197:LEU:HD21	1.92	0.52
1:C:48:LYS:HE3	1:C:49:TYR:CE2	2.44	0.52
1:C:533:LEU:HD22	1:C:538:LEU:HG	1.91	0.52
1:C:506:PRO:HG3	1:C:538:LEU:CD1	2.39	0.52
1:D:785:ALA:O	1:D:827:GLY:N	2.42	0.52
1:D:779:ILE:HG22	1:D:871:LEU:HD21	1.90	0.52
1:A:153:ASN:ND2	1:A:158:ASN:ND2	2.57	0.52
1:D:286:PRO:CG	1:D:733:GLN:HG3	2.38	0.52
1:D:741:VAL:HG11	1:D:875:THR:O	2.10	0.52
1:B:231:LYS:HG3	1:B:236:GLU:HA	1.92	0.52
1:B:444:ASN:HA	1:B:599:ARG:HE	1.75	0.52
1:C:130:LYS:HE3	1:C:131:HIS:CE1	2.42	0.52
1:D:105:HIS:CD2	1:D:105:HIS:C	2.83	0.52
1:D:105:HIS:HA	1:D:108:ILE:HD12	1.92	0.52
1:D:140:ASP:HB3	1:D:143:ASP:HB2	1.91	0.52
1:D:198:LEU:C	1:D:200:GLU:N	2.61	0.52
1:D:362:ILE:HD13	1:D:575:PHE:HD1	1.74	0.52
1:D:416:TYR:O	1:D:420:ILE:HG13	2.10	0.52
1:D:685:ARG:HH22	1:D:717:GLY:H	1.57	0.52
1:D:793:VAL:C	1:D:795:GLY:H	2.13	0.52
1:A:397:LYS:O	1:A:399:PRO:HD3	2.10	0.52
1:A:488:TYR:HA	1:A:491:ALA:HB3	1.92	0.52
1:A:785:ALA:HB1	1:A:808:ILE:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ILE:HD13	1:B:254:GLU:N	2.23	0.52
1:B:85:MET:HA	1:B:380:ILE:HD11	1.91	0.52
1:D:362:ILE:CG2	1:D:363:LYS:N	2.73	0.52
1:A:548:THR:O	1:A:551:ALA:N	2.43	0.52
1:C:37:LEU:C	1:C:38:PHE:CD1	2.83	0.52
1:D:202:LEU:O	1:D:202:LEU:HD23	2.09	0.52
1:D:199:MET:HB3	1:D:234:PHE:CE2	2.45	0.52
1:A:284:ASN:HD22	1:A:285:GLN:N	2.07	0.52
1:B:536:LYS:HA	1:B:539:ASN:ND2	2.24	0.52
1:C:461:MET:HB3	1:C:463:TYR:CE1	2.44	0.52
1:D:154:SER:C	1:D:156:TYR:H	2.12	0.52
1:D:286:PRO:HG3	1:D:733:GLN:HG3	1.90	0.52
1:A:339:GLN:HA	1:A:339:GLN:OE1	2.11	0.51
1:A:543:PHE:O	1:A:547:ARG:N	2.42	0.51
1:B:52:ILE:HG13	1:B:53:TYR:CD1	2.44	0.51
1:C:504:HIS:N	1:C:506:PRO:HD3	2.26	0.51
1:C:546:GLN:C	1:C:548:THR:H	2.14	0.51
1:D:398:GLU:HB3	1:D:705:LYS:NZ	2.25	0.51
1:B:164:ILE:HD13	1:B:164:ILE:H	1.75	0.51
1:B:745:LEU:O	1:B:749:ILE:HG13	2.10	0.51
1:B:815:ILE:HD11	1:B:823:GLN:NE2	2.25	0.51
1:C:120:PRO:HD2	1:C:131:HIS:CD2	2.45	0.51
1:D:167:ALA:HB1	1:D:178:VAL:HG21	1.92	0.51
1:D:335:ASP:O	1:D:339:GLN:HA	2.10	0.51
1:D:459:ASN:ND2	1:D:585:ALA:HA	2.25	0.51
1:D:617:VAL:O	1:D:617:VAL:HG23	2.09	0.51
1:D:623:ASP:OD2	1:D:623:ASP:C	2.48	0.51
1:D:622:THR:HG23	1:D:623:ASP:N	2.24	0.51
1:D:739:LYS:HA	1:D:742:GLN:HB3	1.92	0.51
1:D:734:LYS:HZ2	2:K:7:DA:H4'	1.73	0.51
1:A:734:LYS:HE3	5:A:949:HOH:O	2.11	0.51
1:A:864:HIS:HD2	1:A:865:TRP:NE1	2.09	0.51
1:A:898:PHE:N	1:A:898:PHE:CD1	2.78	0.51
1:B:272:ASP:OD2	1:B:274:ILE:HG22	2.10	0.51
1:C:38:PHE:CZ	1:C:59:ARG:HG2	2.45	0.51
1:D:808:ILE:CG2	1:D:824:VAL:HG11	2.40	0.51
1:B:101:ILE:CG2	1:B:349:TYR:HB3	2.40	0.51
1:C:468:ASP:HB3	1:C:677:LYS:HE2	1.93	0.51
1:D:354:GLN:HB3	1:D:356:GLN:OE1	2.10	0.51
1:D:678:GLN:HG3	1:D:680:LEU:HG	1.92	0.51
1:A:428:GLU:CD	1:A:470:VAL:HG23	2.31	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:HG2	1:B:21:ASP:HA	1.93	0.51
1:B:511:ASP:CG	1:B:533:LEU:HD23	2.30	0.51
1:B:611:THR:CB	1:B:614:GLU:HG3	2.41	0.51
1:B:810:THR:CG2	1:B:841:PHE:HB3	2.40	0.51
1:D:274:ILE:HG23	1:D:275:ASP:N	2.26	0.51
1:D:536:LYS:HB2	1:D:536:LYS:NZ	2.25	0.51
1:C:248:THR:HB	1:C:264:THR:O	2.10	0.51
1:C:542:LEU:O	1:C:546:GLN:HG3	2.10	0.51
1:D:227:TYR:CB	1:D:263:ILE:HD13	2.40	0.51
1:A:207:GLN:CA	1:A:207:GLN:HE21	2.22	0.51
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.93	0.51
1:A:685:ARG:NH1	1:A:688:ILE:HG13	2.24	0.51
1:B:163:SER:OG	1:B:166:ILE:HD13	2.09	0.51
1:B:398:GLU:OE2	1:B:705:LYS:HE3	2.10	0.51
4:J:2:DTP:H5'1	4:J:2:DTP:N3	2.26	0.51
3:L:106:DT:H2''	3:L:107:DG:OP2	2.11	0.51
1:A:555:ALA:O	1:A:559:ARG:HG2	2.10	0.51
1:B:277:TYR:O	1:B:281:SER:HB2	2.10	0.51
1:B:159:VAL:HG11	1:B:317:HIS:HB2	1.93	0.51
1:B:347:MET:HE1	1:B:562:LEU:HD11	1.93	0.51
1:B:518:TYR:HD2	1:B:545:ALA:HA	1.74	0.51
1:A:162:TRP:CH2	1:A:164:ILE:HG13	2.45	0.51
1:A:566:LEU:O	1:A:566:LEU:HG	2.11	0.51
1:B:805:ILE:O	1:B:809:LEU:HD13	2.10	0.51
1:C:496:GLY:O	1:C:542:LEU:HD13	2.11	0.51
1:A:345:LEU:HD23	1:A:355:ILE:HG21	1.93	0.51
1:C:634:ASP:C	1:C:636:VAL:H	2.12	0.51
1:D:124:PRO:HB2	1:D:225:TYR:HE1	1.76	0.51
1:D:555:ALA:O	1:D:559:ARG:HG2	2.11	0.51
1:D:416:TYR:HD1	1:D:586:ILE:CG2	2.24	0.51
2:E:16:DG:H2''	2:E:17:DC:C6	2.46	0.51
3:H:110:DA:H1'	3:H:111:DT:H5''	1.91	0.51
1:A:231:LYS:HB3	1:A:231:LYS:NZ	2.26	0.50
1:C:498:ILE:HG23	1:C:499:ILE:HD13	1.93	0.50
1:D:455:SER:OG	1:D:676:ASN:HA	2.11	0.50
1:D:559:ARG:HG2	1:D:559:ARG:HH11	1.76	0.50
1:A:365:TRP:CD2	1:A:566:LEU:HD12	2.46	0.50
1:A:423:VAL:O	1:A:424:ASN:HB3	2.12	0.50
1:A:41:CYS:CB	1:A:58:THR:HG23	2.42	0.50
1:B:180:SER:O	1:B:183:ILE:HG22	2.11	0.50
1:B:529:LYS:HA	1:B:532:LYS:HD3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PHE:CD1	1:C:213:LEU:HD11	2.46	0.50
1:C:273:TYR:OH	1:C:335:ASP:HA	2.11	0.50
1:D:636:VAL:HG21	1:D:641:PHE:HZ	1.76	0.50
1:A:251:LYS:NZ	1:A:251:LYS:HB2	2.26	0.50
1:A:559:ARG:HG2	1:A:559:ARG:HH11	1.76	0.50
1:B:202:LEU:O	1:B:206:GLN:HG2	2.11	0.50
1:B:285:GLN:HG3	1:B:292:TYR:CE2	2.45	0.50
1:C:302:LYS:HE3	1:C:326:ILE:HB	1.92	0.50
1:C:475:ILE:CG2	1:C:476:THR:N	2.74	0.50
1:B:154:SER:HB3	1:B:313:ARG:HH22	1.77	0.50
1:B:493:GLN:O	1:B:497:GLU:HG2	2.11	0.50
1:D:453:VAL:HG23	1:D:454:TYR:CD1	2.47	0.50
1:D:398:GLU:HA	1:D:705:LYS:NZ	2.25	0.50
1:C:233:ILE:HG22	1:C:234:PHE:CD2	2.47	0.50
1:C:453:VAL:HG23	1:C:454:TYR:N	2.26	0.50
1:C:456:CYS:SG	1:C:462:MET:HG2	2.51	0.50
1:D:444:ASN:OD1	1:D:599:ARG:HD2	2.12	0.50
1:D:709:ALA:HB2	1:D:730:LEU:HD11	1.93	0.50
3:F:109:DC:H1'	3:F:110:DA:H5''	1.94	0.50
1:A:249:ARG:NH2	1:A:251:LYS:NZ	2.57	0.50
1:C:477:LYS:HG2	1:C:481:GLN:NE2	2.24	0.50
1:C:878:LYS:HB3	1:C:879:PRO:HD3	1.94	0.50
1:D:410:PHE:HB3	1:D:683:MET:HG2	1.94	0.50
1:D:4:PHE:HA	1:D:97:TYR:HE2	1.77	0.50
1:D:775:ASN:OD1	1:D:777:ILE:HD11	2.12	0.50
3:J:114:DA:H2''	3:J:115:DA:O5'	2.10	0.50
1:B:469:GLY:O	1:B:472:PRO:HG2	2.12	0.50
1:B:499:ILE:HD12	1:B:545:ALA:HB2	1.94	0.50
1:B:597:ILE:CD1	1:B:683:MET:SD	2.99	0.50
1:C:572:ASN:C	1:C:572:ASN:HD22	2.15	0.50
1:D:202:LEU:C	1:D:202:LEU:HD23	2.32	0.50
1:D:224:PRO:HA	1:D:263:ILE:CD1	2.37	0.50
1:D:459:ASN:HD22	1:D:584:THR:HG22	1.75	0.50
1:D:636:VAL:HB	1:D:640:LYS:HD2	1.94	0.50
1:A:163:SER:HB3	1:A:318:GLN:OE1	2.12	0.50
1:A:206:GLN:OE1	1:A:241:ARG:HB3	2.12	0.50
1:A:73:LYS:O	1:A:76:GLU:HB2	2.12	0.50
1:C:109:ARG:HD2	1:C:209:THR:O	2.11	0.50
1:C:553:MET:HA	1:C:553:MET:HE3	1.94	0.50
1:C:878:LYS:HB3	1:C:879:PRO:CD	2.42	0.50
1:D:256:MET:HB2	2:K:4:CTG:OP2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:619:TYR:OH	1:D:621:ASP:HB3	2.11	0.50
1:D:648:VAL:CG1	1:D:719:ARG:NH2	2.75	0.50
1:A:113:PHE:CE1	1:A:218:VAL:CG2	2.95	0.50
1:C:62:PHE:N	1:C:62:PHE:CD1	2.79	0.50
1:D:150:ASP:OD1	1:D:151:LEU:N	2.45	0.50
1:D:428:GLU:N	1:D:428:GLU:OE2	2.45	0.50
1:D:777:ILE:HG22	1:D:848:TRP:HH2	1.77	0.50
1:A:388:VAL:HG22	1:A:573:VAL:HG21	1.94	0.49
1:B:444:ASN:HA	1:B:599:ARG:NE	2.27	0.49
1:B:686:GLU:HG3	1:B:715:MET:SD	2.52	0.49
1:C:493:GLN:HG2	1:C:549:GLU:OE1	2.12	0.49
1:D:15:ILE:CG1	1:D:31:VAL:HG22	2.42	0.49
1:D:221:PHE:O	1:D:224:PRO:HD2	2.12	0.49
1:A:731:GLU:O	1:A:734:LYS:HG2	2.12	0.49
1:B:518:TYR:CD2	1:B:545:ALA:HA	2.47	0.49
1:C:491:ALA:C	1:C:493:GLN:H	2.16	0.49
1:C:499:ILE:HB	1:C:541:MET:CE	2.42	0.49
1:D:455:SER:HA	1:D:675:ASN:O	2.11	0.49
1:B:347:MET:HE2	1:B:562:LEU:HD21	1.95	0.49
1:B:369:ILE:HG22	1:B:373:LEU:CD1	2.41	0.49
1:C:444:ASN:HA	1:C:599:ARG:NE	2.26	0.49
1:C:711:ASN:ND2	1:C:754:GLN:NE2	2.50	0.49
1:C:83:LEU:HB3	1:C:379:VAL:CG1	2.43	0.49
1:C:196:GLU:HA	1:C:196:GLU:OE1	2.12	0.49
1:C:338:ARG:O	1:C:339:GLN:HB2	2.12	0.49
1:C:397:LYS:HB3	1:C:620:GLY:H	1.77	0.49
1:D:105:HIS:HD2	1:D:106:THR:N	2.09	0.49
1:D:170:LEU:HG	1:D:171:GLN:N	2.28	0.49
1:D:16:PHE:HB3	1:D:245:HIS:NE2	2.27	0.49
1:A:711:ASN:HD21	1:A:723:PRO:HB2	1.77	0.49
1:B:471:VAL:N	1:B:472:PRO:HD2	2.28	0.49
1:C:249:ARG:HG3	1:C:249:ARG:HH11	1.78	0.49
1:C:44:SER:O	1:C:46:ALA:N	2.45	0.49
1:C:592:MET:HE2	1:C:670:MET:SD	2.52	0.49
1:D:273:TYR:HH	1:D:335:ASP:HA	1.77	0.49
1:D:416:TYR:HE1	1:D:587:THR:HA	1.77	0.49
1:D:491:ALA:HB1	1:D:520:PHE:HA	1.94	0.49
1:B:164:ILE:CD1	1:B:164:ILE:H	2.26	0.49
1:B:313:ARG:O	1:B:317:HIS:HB2	2.13	0.49
1:B:727:ILE:HG21	1:B:732:THR:CG2	2.42	0.49
1:C:163:SER:H	1:C:318:GLN:HE22	1.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:LEU:HB3	1:C:538:LEU:CG	2.43	0.49
1:C:614:GLU:HB3	1:C:616:PHE:CE1	2.48	0.49
1:C:749:ILE:O	1:C:753:LEU:HG	2.12	0.49
1:D:142:ILE:HG13	1:D:143:ASP:N	2.27	0.49
1:D:204:PHE:O	1:D:207:GLN:HB3	2.12	0.49
2:G:12:DA:H2"	2:G:13:DG:H8	1.76	0.49
1:A:559:ARG:O	1:A:563:ILE:HG13	2.11	0.49
1:B:5:TYR:HB3	1:B:97:TYR:CE2	2.48	0.49
1:C:116:GLU:CB	1:C:135:ALA:HB3	2.37	0.49
1:C:147:TYR:HB3	1:C:149:PHE:HE1	1.78	0.49
1:C:388:VAL:HG23	1:C:388:VAL:O	2.13	0.49
1:C:467:ARG:NH1	1:C:467:ARG:HG2	2.27	0.49
1:C:491:ALA:C	1:C:493:GLN:N	2.66	0.49
1:C:533:LEU:HD13	1:C:538:LEU:CG	2.34	0.49
1:D:180:SER:C	1:D:182:ILE:H	2.14	0.49
1:A:292:TYR:CD2	1:A:292:TYR:C	2.85	0.49
1:A:399:PRO:O	1:A:401:PRO:HD3	2.12	0.49
1:B:19:TYR:CZ	1:B:27:ARG:HB2	2.47	0.49
1:B:3:GLU:HG2	1:B:21:ASP:C	2.33	0.49
1:B:747:GLU:OE1	1:B:747:GLU:HA	2.13	0.49
1:C:508:LEU:O	1:C:509:SER:HB3	2.12	0.49
1:C:533:LEU:HB3	1:C:538:LEU:HG	1.94	0.49
1:C:686:GLU:OE2	1:C:686:GLU:HA	2.13	0.49
1:D:438:PRO:HG2	1:D:441:ASP:HB2	1.94	0.49
1:D:447:ALA:O	1:D:673:TYR:OH	2.28	0.49
2:I:5:DG:H2"	2:I:6:DA:O5'	2.12	0.49
1:B:421:ARG:HG2	1:B:421:ARG:HH11	1.77	0.49
1:C:140:ASP:OD1	1:C:142:ILE:HB	2.12	0.49
1:C:42:PRO:HG2	1:C:45:GLN:HG3	1.94	0.49
1:C:542:LEU:HA	1:C:545:ALA:HB3	1.93	0.49
1:D:297:GLU:HG3	1:D:337:LYS:HD3	1.95	0.49
1:D:748:CYS:O	1:D:752:MET:HG3	2.13	0.49
1:D:815:ILE:C	1:D:815:ILE:HD12	2.33	0.49
2:K:11:DC:H2"	2:K:12:DA:C8	2.48	0.49
1:A:700:GLY:HA3	1:A:710:LEU:HD23	1.95	0.48
1:B:133:ILE:HD12	1:B:198:LEU:HD21	1.95	0.48
1:B:604:TYR:CZ	1:B:608:VAL:HG21	2.47	0.48
1:B:422:GLN:HG3	1:B:678:GLN:O	2.13	0.48
1:D:290:LEU:O	1:D:294:SER:HB2	2.13	0.48
1:D:347:MET:HB2	1:D:558:ASN:OD1	2.11	0.48
2:I:13:DG:H2"	2:I:14:DC:C5'	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:CYS:SG	1:A:462:MET:HG2	2.53	0.48
1:C:219:GLU:O	1:C:219:GLU:HG2	2.11	0.48
1:C:244:PRO:HG2	1:C:267:GLY:HA3	1.95	0.48
1:C:402:ASN:HD22	1:C:403:ARG:H	1.57	0.48
1:D:702:TRP:CD1	1:D:708:TYR:HB3	2.48	0.48
1:A:402:ASN:HA	1:A:886:ALA:O	2.13	0.48
1:A:732:THR:OG1	1:A:733:GLN:NE2	2.26	0.48
1:B:897:LEU:HD12	1:B:897:LEU:N	2.27	0.48
1:C:265:LEU:HD12	1:C:268:ILE:HD12	1.95	0.48
1:C:540:GLU:HA	1:C:540:GLU:OE1	2.13	0.48
1:D:257:TYR:CD2	3:L:112:DT:H72	2.48	0.48
1:D:777:ILE:HG22	1:D:848:TRP:CH2	2.48	0.48
1:A:733:GLN:O	3:F:112:DT:H5"	2.14	0.48
1:A:401:PRO:O	1:A:402:ASN:HB2	2.13	0.48
1:A:543:PHE:C	1:A:543:PHE:CD2	2.86	0.48
1:C:301:GLY:O	1:C:330:ARG:HD2	2.13	0.48
1:C:392:PRO:C	1:C:587:THR:HG21	2.33	0.48
1:D:109:ARG:HH21	1:D:208:LYS:HG2	1.78	0.48
1:D:648:VAL:CG1	1:D:719:ARG:HH21	2.24	0.48
1:D:739:LYS:NZ	1:D:743:LYS:HD2	2.28	0.48
1:B:530:ILE:C	1:B:532:LYS:H	2.16	0.48
1:B:796:PHE:HB3	1:B:797:PRO:HD2	1.95	0.48
1:C:148:VAL:C	1:C:149:PHE:CD1	2.87	0.48
1:D:166:ILE:HG22	1:D:166:ILE:O	2.12	0.48
1:D:313:ARG:HG2	1:D:313:ARG:HH21	1.77	0.48
1:D:466:ASP:CG	1:D:467:ARG:H	2.16	0.48
1:D:654:PHE:CE1	1:D:659:MET:HG3	2.48	0.48
1:D:761:GLN:NE2	1:D:893:LYS:HA	2.28	0.48
1:B:707:ARG:HD2	2:G:7:DA:O3'	2.13	0.48
1:A:760:LEU:HD23	1:A:891:TYR:HA	1.94	0.48
1:B:177:GLU:HB3	1:B:303:LEU:HD11	1.95	0.48
1:B:553:MET:O	1:B:557:ILE:HG12	2.13	0.48
1:C:401:PRO:O	1:C:402:ASN:HB2	2.12	0.48
1:D:52:ILE:O	1:D:428:GLU:HG3	2.14	0.48
1:D:533:LEU:HB2	1:D:538:LEU:HD21	1.96	0.48
1:A:251:LYS:HZ3	1:A:251:LYS:HB2	1.78	0.48
1:B:256:MET:HG2	1:B:257:TYR:CE2	2.48	0.48
1:B:540:GLU:O	1:B:544:ARG:HG3	2.13	0.48
1:B:481:GLN:OE1	1:B:559:ARG:NH1	2.47	0.48
1:C:302:LYS:HZ2	1:C:302:LYS:HA	1.78	0.48
1:C:443:ILE:O	1:C:599:ARG:NH2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:ILE:O	1:C:503:LEU:HG	2.12	0.48
1:C:404:TYR:CD1	1:C:618:LEU:HD22	2.48	0.48
1:C:660:GLU:HB2	1:C:661:PRO:CD	2.35	0.48
1:D:180:SER:O	1:D:182:ILE:N	2.44	0.48
1:D:85:MET:N	1:D:380:ILE:HD11	2.29	0.48
1:D:516:VAL:HG22	1:D:517:ASP:N	2.28	0.48
1:D:654:PHE:CD1	1:D:654:PHE:C	2.87	0.48
2:G:15:DC:H2''	2:G:16:DG:OP2	2.12	0.48
2:K:9:DG:H2''	2:K:10:DA:OP2	2.13	0.48
1:A:3:GLU:HG2	1:A:21:ASP:HA	1.96	0.48
1:B:179:PRO:HB2	1:B:181:GLU:OE1	2.13	0.48
1:C:138:HIS:C	1:C:138:HIS:CD2	2.87	0.48
1:C:506:PRO:HG3	1:C:538:LEU:HD11	1.96	0.48
1:D:309:ILE:HG22	1:D:312:LEU:HD22	1.95	0.48
1:A:326:ILE:O	1:A:330:ARG:HG2	2.14	0.48
1:A:489:MET:HE1	1:A:553:MET:CG	2.44	0.48
1:B:524:ASP:C	1:B:526:ILE:H	2.17	0.48
1:B:878:LYS:HB3	1:B:879:PRO:CD	2.44	0.48
1:C:42:PRO:CG	1:C:45:GLN:HG3	2.44	0.48
1:D:305:TYR:C	1:D:305:TYR:CD2	2.87	0.48
1:D:423:VAL:O	1:D:424:ASN:HB3	2.14	0.48
1:D:758:GLU:HG3	1:D:759:SER:H	1.78	0.48
1:A:870:VAL:O	1:A:874:LYS:CG	2.62	0.48
1:B:538:LEU:O	1:B:542:LEU:HB2	2.14	0.48
1:C:318:GLN:HA	1:C:318:GLN:NE2	2.25	0.48
1:D:370:PHE:C	1:D:370:PHE:CD2	2.87	0.48
1:D:878:LYS:O	1:D:881:GLU:HG3	2.14	0.48
2:I:9:DG:H1'	2:I:10:DA:H5''	1.94	0.48
1:A:104:ASP:OD2	1:A:106:THR:HB	2.14	0.47
1:A:671:CYS:SG	1:A:676:ASN:HB2	2.54	0.47
1:A:829:LYS:HE3	1:A:829:LYS:N	2.28	0.47
1:C:255:ASN:CG	1:C:256:MET:N	2.67	0.47
1:C:68:ALA:O	1:C:72:ILE:HG13	2.14	0.47
1:C:757:GLU:O	1:C:761:GLN:HG3	2.13	0.47
1:D:153:ASN:O	1:D:154:SER:HB2	2.14	0.47
1:D:644:THR:O	1:D:648:VAL:HG23	2.14	0.47
1:B:728:MET:HG3	3:H:114:DA:H3'	1.95	0.47
1:A:343:LEU:HD23	1:A:343:LEU:C	2.35	0.47
1:A:785:ALA:HB1	1:A:788:ILE:HD11	1.95	0.47
1:B:126:PRO:HB2	1:B:224:PRO:HB2	1.96	0.47
1:B:41:CYS:HB2	1:B:42:PRO:HD2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:PHE:CE2	1:C:59:ARG:HG2	2.49	0.47
1:C:482:ARG:O	1:C:483:LYS:C	2.52	0.47
1:D:702:TRP:NE1	1:D:708:TYR:HB3	2.28	0.47
2:I:16:DG:H2''	2:I:17:DC:O5'	2.14	0.47
1:B:270:VAL:O	1:B:271:LEU:HD12	2.12	0.47
1:B:815:ILE:HD11	1:B:823:GLN:HE22	1.79	0.47
1:C:252:VAL:HA	1:C:261:GLU:HA	1.96	0.47
1:D:194:GLU:OE1	1:D:198:LEU:HD21	2.13	0.47
1:D:2:LYS:NZ	1:D:2:LYS:HB3	2.29	0.47
1:D:414:SER:O	1:D:417:PRO:HD2	2.13	0.47
2:E:11:DC:H1'	2:E:12:DA:H5''	1.96	0.47
3:L:111:DT:H2''	3:L:112:DT:C5'	2.43	0.47
1:C:351:ALA:O	1:C:352:LYS:HB2	2.14	0.47
1:C:494:ARG:HH11	1:C:494:ARG:HG2	1.79	0.47
1:C:668:ARG:HG2	1:C:668:ARG:HH11	1.80	0.47
1:D:164:ILE:N	1:D:164:ILE:HD13	2.07	0.47
1:D:411:ASP:OD2	1:D:624:SER:HB3	2.14	0.47
1:D:517:ASP:C	1:D:519:ARG:H	2.17	0.47
1:A:194:GLU:OE1	1:A:229:ARG:NE	2.43	0.47
1:A:406:TYR:CB	1:A:629:ALA:HB3	2.43	0.47
1:B:283:THR:O	1:B:283:THR:HG23	2.15	0.47
1:B:423:VAL:HB	1:B:425:ILE:HG13	1.96	0.47
1:B:797:PRO:HG3	1:B:806:ARG:NH1	2.30	0.47
1:C:373:LEU:HD12	1:C:380:ILE:HG22	1.96	0.47
1:C:450:PRO:HB2	1:C:456:CYS:SG	2.55	0.47
1:C:59:ARG:NH1	1:C:59:ARG:HG3	2.28	0.47
1:D:238:THR:O	1:D:238:THR:HG22	2.14	0.47
1:D:51:ASP:OD1	1:D:53:TYR:HB2	2.15	0.47
1:A:510:VAL:HG23	1:A:510:VAL:O	2.14	0.47
1:B:598:GLU:HG3	1:B:617:VAL:HG11	1.97	0.47
1:C:34:LYS:HD3	1:C:61:LEU:HD21	1.95	0.47
1:D:300:VAL:HG23	1:D:330:ARG:HE	1.79	0.47
1:D:714:ASP:OD2	1:D:719:ARG:HG2	2.15	0.47
2:K:2:DG:N2	5:K:130:HOH:O	2.46	0.47
1:C:302:LYS:HG2	1:C:323:TYR:CE2	2.50	0.47
1:C:553:MET:HA	1:C:553:MET:CE	2.45	0.47
1:A:518:TYR:CE2	1:A:545:ALA:HB2	2.50	0.47
1:A:731:GLU:HG3	1:A:879:PRO:CB	2.40	0.47
1:D:179:PRO:HB2	1:D:182:ILE:CG2	2.44	0.47
3:J:114:DA:H2''	3:J:115:DA:C5'	2.45	0.47
2:K:5:DG:H2''	2:K:6:DA:O5'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HB2	1:A:249:ARG:HE	1.54	0.47
1:A:513:PRO:HG2	1:A:540:GLU:HG2	1.97	0.47
1:C:495:ASN:HB3	1:C:522:PHE:CD1	2.50	0.47
1:C:455:SER:OG	1:C:676:ASN:HA	2.14	0.47
1:D:412:LEU:HD12	1:D:415:LEU:HD22	1.97	0.47
1:D:808:ILE:O	1:D:812:ASN:ND2	2.48	0.47
1:B:197:LEU:HD23	1:B:197:LEU:C	2.34	0.47
1:C:153:ASN:HB3	1:C:158:ASN:OD1	2.15	0.47
1:C:822:PRO:HD2	1:C:855:THR:OG1	2.14	0.47
1:D:413:THR:O	1:D:414:SER:C	2.53	0.47
1:B:488:TYR:CD2	1:B:519:ARG:HD2	2.50	0.47
1:C:163:SER:HB3	1:C:166:ILE:CD1	2.45	0.47
1:C:312:LEU:O	1:C:312:LEU:HD12	2.14	0.47
1:C:497:GLU:O	1:C:497:GLU:HG2	2.15	0.47
1:C:503:LEU:CD2	1:C:538:LEU:HD22	2.45	0.47
1:C:13:ASP:HA	1:C:65:MET:HG3	1.97	0.47
1:A:4:PHE:CZ	1:A:20:ILE:HG13	2.51	0.46
1:A:48:LYS:HB3	1:A:48:LYS:HZ3	1.79	0.46
1:D:553:MET:O	1:D:556:GLN:HG3	2.15	0.46
1:A:297:GLU:OE2	1:A:337:LYS:NZ	2.43	0.46
1:B:3:GLU:HG2	1:B:22:SER:N	2.31	0.46
1:B:413:THR:O	1:B:414:SER:C	2.53	0.46
1:D:19:TYR:CZ	1:D:27:ARG:HB2	2.50	0.46
1:D:470:VAL:HG13	1:D:471:VAL:N	2.30	0.46
1:D:550:VAL:C	1:D:552:GLY:N	2.68	0.46
2:K:5:DG:C6	2:K:6:DA:C2	3.03	0.46
1:A:335:ASP:OD2	1:A:341:ILE:HG12	2.15	0.46
1:A:402:ASN:HB3	1:A:404:TYR:CE2	2.51	0.46
1:A:642:ARG:CZ	1:A:646:HIS:CD2	2.99	0.46
1:B:181:GLU:CD	1:B:181:GLU:H	2.18	0.46
1:B:44:SER:O	1:B:46:ALA:N	2.48	0.46
1:C:384:ARG:HB2	1:C:386:HIS:CE1	2.50	0.46
1:C:490:LEU:O	1:C:494:ARG:CG	2.63	0.46
1:C:507:ASN:CB	1:C:532:LYS:HA	2.44	0.46
1:C:659:MET:O	1:C:663:ILE:HG13	2.16	0.46
1:D:123:PHE:CD1	1:D:124:PRO:HD2	2.49	0.46
1:D:433:THR:HG22	1:D:461:MET:HE1	1.97	0.46
1:A:693:LEU:HA	5:A:929:HOH:O	2.15	0.46
1:A:898:PHE:H	1:A:898:PHE:HD1	1.63	0.46
1:B:415:LEU:HD11	1:B:419:ILE:HD11	1.97	0.46
1:B:423:VAL:O	1:B:424:ASN:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:ILE:HG13	1:B:625:ILE:O	2.15	0.46
1:B:785:ALA:CB	1:B:808:ILE:HD11	2.45	0.46
1:C:120:PRO:HD2	1:C:131:HIS:NE2	2.30	0.46
1:D:151:LEU:HD21	1:D:193:ASN:O	2.15	0.46
1:D:289:SER:O	1:D:293:ILE:HG13	2.15	0.46
1:D:522:PHE:O	1:D:527:LYS:HE3	2.15	0.46
1:A:274:ILE:O	1:A:278:LYS:HG3	2.15	0.46
1:A:805:ILE:HA	1:A:808:ILE:HD12	1.98	0.46
1:A:854:ILE:CG2	1:A:859:LYS:HG3	2.45	0.46
1:B:531:LYS:HB3	1:B:531:LYS:NZ	2.31	0.46
1:B:503:LEU:HD12	1:B:542:LEU:CD2	2.45	0.46
1:C:130:LYS:HG3	1:C:131:HIS:CE1	2.51	0.46
1:C:414:SER:O	1:C:417:PRO:HD2	2.15	0.46
1:C:872:LEU:HD11	1:C:876:PHE:CD2	2.50	0.46
1:D:272:ASP:CG	1:D:274:ILE:HG22	2.36	0.46
1:D:709:ALA:HA	1:D:726:LYS:O	2.16	0.46
1:A:147:TYR:CE2	1:A:187:ILE:HD12	2.50	0.46
1:B:129:ALA:HA	1:B:225:TYR:CZ	2.51	0.46
1:B:299:ASN:O	1:B:300:VAL:HB	2.16	0.46
1:B:163:SER:N	1:B:318:GLN:HE22	2.10	0.46
1:B:523:SER:HA	1:B:527:LYS:HE3	1.98	0.46
1:C:300:VAL:HG22	1:C:330:ARG:NH1	2.23	0.46
1:C:523:SER:HB2	1:C:526:ILE:HG13	1.97	0.46
1:C:546:GLN:C	1:C:548:THR:N	2.68	0.46
1:C:634:ASP:C	1:C:636:VAL:N	2.68	0.46
1:D:33:TYR:HB3	1:D:65:MET:HE1	1.97	0.46
1:D:398:GLU:CB	1:D:705:LYS:HE3	2.39	0.46
1:C:361:PRO:HD2	2:I:2:DG:P	2.55	0.46
1:A:138:HIS:HE1	5:A:919:HOH:O	1.98	0.46
1:A:81:GLU:OE2	1:A:83:LEU:CG	2.64	0.46
1:B:221:PHE:O	1:B:224:PRO:HD2	2.16	0.46
1:B:116:GLU:HG2	1:B:320:TYR:CZ	2.51	0.46
1:B:458:PRO:HB2	1:B:588:THR:HG22	1.97	0.46
1:C:453:VAL:CG2	1:C:454:TYR:N	2.79	0.46
1:D:188:TYR:CE2	1:D:190:PRO:HD3	2.51	0.46
1:D:7:THR:OG1	1:D:18:ARG:HD3	2.15	0.46
1:A:105:HIS:C	1:A:105:HIS:CD2	2.87	0.46
1:A:495:ASN:C	1:A:497:GLU:N	2.69	0.46
1:A:542:LEU:HD12	1:A:542:LEU:C	2.36	0.46
1:A:642:ARG:CZ	1:A:642:ARG:HB2	2.45	0.46
1:A:801:CYS:SG	1:A:805:ILE:HG22	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:MET:HA	1:A:380:ILE:HD11	1.98	0.46
1:D:297:GLU:HA	1:D:297:GLU:OE1	2.15	0.46
1:D:459:ASN:ND2	1:D:585:ALA:CA	2.78	0.46
2:G:16:DG:C2'	2:G:17:DC:H5''	2.46	0.46
1:C:147:TYR:HB3	1:C:149:PHE:CE1	2.51	0.46
1:C:433:THR:O	1:C:462:MET:SD	2.74	0.46
1:C:461:MET:HB3	1:C:463:TYR:HE1	1.80	0.46
1:C:685:ARG:HD2	1:C:685:ARG:C	2.36	0.46
1:C:706:LYS:C	1:C:707:ARG:HG2	2.36	0.46
1:D:426:SER:OG	1:D:427:PRO:HD2	2.16	0.46
1:D:498:ILE:O	1:D:498:ILE:HG22	2.16	0.46
1:D:572:ASN:O	1:D:578:TYR:HB2	2.16	0.46
1:D:4:PHE:HA	1:D:97:TYR:CE2	2.51	0.46
1:B:487:GLY:O	1:B:491:ALA:HB2	2.15	0.46
1:C:475:ILE:HD13	1:C:566:LEU:HD22	1.98	0.46
1:C:49:TYR:HE1	1:C:59:ARG:HB2	1.81	0.46
3:L:111:DT:C2'	3:L:112:DT:H5''	2.45	0.46
1:A:376:GLN:NE2	1:A:378:LYS:HD2	2.31	0.45
1:A:490:LEU:HD23	1:A:494:ARG:HD3	1.98	0.45
1:A:713:TRP:CE3	1:A:723:PRO:HB3	2.51	0.45
1:A:745:LEU:HD13	1:A:876:PHE:CD1	2.51	0.45
1:B:145:ARG:HD3	1:B:185:LYS:O	2.17	0.45
1:B:597:ILE:HG21	1:B:667:PHE:CZ	2.51	0.45
1:B:876:PHE:O	1:B:879:PRO:HG2	2.15	0.45
1:C:159:VAL:CG1	1:C:160:GLU:N	2.76	0.45
1:D:188:TYR:CE2	1:D:190:PRO:HB3	2.51	0.45
1:D:221:PHE:HE2	1:D:225:TYR:HD1	1.64	0.45
1:D:254:GLU:HB3	1:D:259:SER:HB3	1.98	0.45
1:D:491:ALA:O	1:D:495:ASN:CB	2.52	0.45
1:D:504:HIS:C	1:D:506:PRO:HD3	2.35	0.45
1:A:303:LEU:HB3	5:A:907:HOH:O	2.15	0.45
1:A:599:ARG:HG2	1:A:599:ARG:NH1	2.32	0.45
1:C:250:VAL:HG22	1:C:263:ILE:CD1	2.47	0.45
1:D:191:PHE:CD1	1:D:197:LEU:HD23	2.51	0.45
1:D:19:TYR:CE1	1:D:27:ARG:HB2	2.51	0.45
1:D:776:TYR:CD2	1:D:863:LEU:HD11	2.50	0.45
1:D:883:PHE:N	1:D:883:PHE:HD2	2.13	0.45
1:B:622:THR:HB	3:H:115:DA:O3'	2.15	0.45
1:A:412:LEU:HG	1:A:683:MET:CG	2.45	0.45
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.98	0.45
1:B:432:GLY:C	1:B:462:MET:HE2	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:PHE:HB3	1:B:683:MET:HG2	1.98	0.45
1:B:750:ARG:HG2	1:B:754:GLN:NE2	2.31	0.45
1:D:348:GLY:HA3	1:D:355:ILE:HD13	1.99	0.45
1:D:599:ARG:HH11	1:D:599:ARG:CG	2.30	0.45
1:D:631:LYS:HA	1:D:631:LYS:HE2	1.97	0.45
1:D:84:GLY:C	1:D:380:ILE:HD11	2.37	0.45
3:L:103:DG:OP2	3:L:103:DG:H8	2.00	0.45
1:A:455:SER:OG	1:A:676:ASN:HA	2.17	0.45
1:B:89:LYS:HE3	1:B:89:LYS:HB2	1.62	0.45
1:C:395:PHE:CE2	1:C:595:GLN:HG3	2.52	0.45
1:C:397:LYS:HE2	1:C:598:GLU:OE1	2.16	0.45
1:C:700:GLY:HA2	1:C:753:LEU:HD22	1.98	0.45
1:C:854:ILE:HG22	1:C:859:LYS:CD	2.47	0.45
1:C:894:LYS:HD3	1:C:894:LYS:HA	1.68	0.45
1:D:198:LEU:N	1:D:198:LEU:CD2	2.79	0.45
1:D:811:TYR:O	1:D:814:ALA:HB3	2.15	0.45
1:D:771:PHE:CE2	1:D:872:LEU:HB2	2.52	0.45
1:A:152:LEU:HD11	1:A:190:PRO:HB2	1.99	0.45
1:A:644:THR:O	1:A:648:VAL:HG23	2.17	0.45
1:A:836:ARG:HG3	1:A:836:ARG:NH1	2.31	0.45
1:B:535:ALA:O	1:B:539:ASN:ND2	2.49	0.45
1:B:800:LYS:O	1:B:800:LYS:HG2	2.16	0.45
1:C:279:LYS:HD2	1:C:280:PHE:CE2	2.52	0.45
1:C:542:LEU:C	1:C:546:GLN:NE2	2.68	0.45
1:D:153:ASN:ND2	1:D:192:ASP:O	2.50	0.45
1:D:208:LYS:O	1:D:209:THR:C	2.54	0.45
1:D:227:TYR:CD2	1:D:263:ILE:HD13	2.51	0.45
1:D:227:TYR:HB3	1:D:263:ILE:CD1	2.47	0.45
1:D:283:THR:O	1:D:283:THR:HG23	2.16	0.45
1:A:112:ASN:ND2	1:A:214:THR:HG23	2.31	0.45
1:A:337:LYS:HE3	1:A:338:ARG:HD3	1.97	0.45
1:C:149:PHE:HD1	1:C:149:PHE:N	2.13	0.45
1:D:109:ARG:HH21	1:D:208:LYS:CG	2.30	0.45
1:D:194:GLU:OE2	1:D:229:ARG:NH2	2.48	0.45
1:D:268:ILE:HG22	1:D:269:SER:N	2.31	0.45
2:I:12:DA:H1'	2:I:13:DG:C8	2.52	0.45
1:A:193:ASN:HD21	1:A:196:GLU:CD	2.20	0.45
1:A:38:PHE:N	1:A:38:PHE:CD1	2.85	0.45
1:A:48:LYS:NZ	1:A:48:LYS:HB3	2.32	0.45
1:A:785:ALA:C	1:A:786:ASN:HD22	2.20	0.45
1:B:303:LEU:HB3	1:B:319:ARG:NH2	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:ALA:HB2	1:B:808:ILE:HD11	1.98	0.45
1:D:292:TYR:C	1:D:292:TYR:CD1	2.90	0.45
1:D:326:ILE:O	1:D:330:ARG:HG2	2.16	0.45
1:A:237:SER:HB2	5:A:918:HOH:O	2.17	0.45
1:A:513:PRO:HG3	1:A:537:SER:HA	1.97	0.45
1:C:15:ILE:HD13	1:C:92:TYR:CD1	2.52	0.45
1:C:254:GLU:HB2	1:C:259:SER:HA	1.98	0.45
1:C:779:ILE:HD11	1:C:866:MET:HE1	1.99	0.45
1:D:138:HIS:CD2	1:D:138:HIS:C	2.90	0.45
1:D:243:SER:C	1:D:245:HIS:H	2.20	0.45
1:D:642:ARG:HB3	1:D:646:HIS:ND1	2.32	0.45
1:D:651:LEU:HA	1:D:651:LEU:HD23	1.86	0.45
1:A:276:LEU:CD2	1:A:341:ILE:HD13	2.47	0.45
1:A:376:GLN:HB2	1:A:378:LYS:HG3	1.99	0.45
1:B:313:ARG:CG	1:B:313:ARG:NH1	2.78	0.45
1:B:818:ASN:OD1	1:B:857:LEU:HD11	2.16	0.45
1:C:405:LYS:O	1:C:690:GLY:HA2	2.16	0.45
1:C:52:ILE:HD12	1:C:428:GLU:CG	2.46	0.45
1:C:78:ILE:CD1	1:C:80:LEU:HD23	2.46	0.45
1:D:297:GLU:O	1:D:298:LEU:HD23	2.16	0.45
1:D:50:PHE:HD2	1:D:54:GLY:O	2.00	0.45
1:D:642:ARG:NH2	1:D:646:HIS:NE2	2.65	0.45
1:D:658:ARG:NH1	1:D:658:ARG:HG3	2.31	0.45
1:D:806:ARG:HB3	1:D:806:ARG:HH11	1.82	0.45
2:I:13:DG:O6	3:J:104:DG:O6	2.35	0.45
1:C:167:ALA:HA	1:C:176:ASP:OD1	2.17	0.45
1:D:41:CYS:HB2	1:D:42:PRO:HD2	1.99	0.45
1:D:471:VAL:HB	1:D:472:PRO:CD	2.42	0.45
1:D:776:TYR:OH	1:D:854:ILE:HG22	2.17	0.45
1:A:412:LEU:HD22	1:A:415:LEU:CD1	2.46	0.44
1:A:347:MET:CB	1:A:558:ASN:HD21	2.22	0.44
1:A:725:LEU:HD12	1:A:725:LEU:N	2.32	0.44
1:C:295:GLU:HA	1:C:300:VAL:H	1.82	0.44
1:C:302:LYS:HD2	1:C:323:TYR:CD2	2.52	0.44
1:C:431:ALA:HB1	1:C:454:TYR:CE2	2.52	0.44
1:C:61:LEU:HD23	1:C:62:PHE:N	2.32	0.44
1:C:900:MET:HA	1:C:900:MET:CE	2.46	0.44
1:D:406:TYR:HE2	1:D:647:TRP:CE2	2.36	0.44
1:D:434:PHE:CE2	1:D:450:PRO:HB3	2.52	0.44
1:D:44:SER:O	1:D:46:ALA:N	2.49	0.44
1:D:484:GLU:HG2	1:D:488:TYR:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:705:LYS:H	1:D:705:LYS:HG2	1.65	0.44
1:A:218:VAL:HG13	1:A:223:ILE:HD12	2.00	0.44
1:A:321:ILE:O	1:A:325:ILE:HG13	2.16	0.44
1:A:658:ARG:NH1	1:A:658:ARG:HG3	2.32	0.44
1:B:347:MET:CE	1:B:562:LEU:HD21	2.47	0.44
1:B:751:ARG:NE	1:B:763:TYR:HB2	2.33	0.44
1:C:457:SER:O	1:C:459:ASN:N	2.50	0.44
1:C:525:GLU:OE2	1:C:525:GLU:N	2.50	0.44
1:D:198:LEU:O	1:D:201:TYR:N	2.51	0.44
1:D:116:GLU:CG	1:D:324:ASN:HD22	2.22	0.44
3:L:114:DA:C2	3:L:115:DA:N1	2.85	0.44
1:A:499:ILE:O	1:A:503:LEU:HG	2.17	0.44
1:A:731:GLU:HA	1:A:734:LYS:HG2	2.00	0.44
1:B:352:LYS:HB2	5:B:923:HOH:O	2.18	0.44
1:B:750:ARG:HH11	1:B:754:GLN:NE2	2.15	0.44
1:C:313:ARG:HG2	1:C:320:TYR:CE1	2.53	0.44
1:D:727:ILE:HG23	1:D:730:LEU:CD1	2.39	0.44
1:D:758:GLU:CG	1:D:759:SER:H	2.29	0.44
1:D:886:ALA:C	1:D:888:LYS:H	2.20	0.44
3:L:114:DA:H2''	3:L:115:DA:OP2	2.18	0.44
1:A:44:SER:O	1:A:46:ALA:N	2.51	0.44
1:A:489:MET:HE1	1:A:553:MET:HG2	1.99	0.44
1:B:116:GLU:CB	1:B:135:ALA:HB3	2.48	0.44
1:B:503:LEU:HD12	1:B:542:LEU:CG	2.44	0.44
1:C:118:THR:HG1	1:C:313:ARG:HG3	1.81	0.44
1:C:453:VAL:HG23	1:C:454:TYR:CD2	2.52	0.44
1:D:197:LEU:C	1:D:197:LEU:HD13	2.37	0.44
1:D:398:GLU:CB	1:D:705:LYS:NZ	2.74	0.44
1:D:519:ARG:HH11	1:D:519:ARG:HG3	1.82	0.44
1:D:499:ILE:HD12	1:D:545:ALA:HB2	2.00	0.44
1:A:505:ASN:C	1:A:505:ASN:HD22	2.20	0.44
1:B:523:SER:N	1:B:526:ILE:HD12	2.30	0.44
1:B:397:LYS:HB3	1:B:620:GLY:H	1.83	0.44
1:B:636:VAL:HG13	1:B:640:LYS:CE	2.44	0.44
1:B:408:MET:CE	1:B:655:ALA:HB2	2.47	0.44
1:C:218:VAL:HG23	1:C:222:ALA:HB3	1.99	0.44
1:C:252:VAL:HG12	1:C:252:VAL:O	2.17	0.44
1:C:291:ASP:OD1	1:C:301:GLY:HA3	2.18	0.44
1:C:302:LYS:HB2	1:C:302:LYS:NZ	2.31	0.44
1:C:800:LYS:HA	2:I:11:DC:O3'	2.16	0.44
1:C:831:TYR:CD2	1:C:850:SER:HA	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ASP:OD1	1:D:141:SER:N	2.50	0.44
1:D:556:GLN:HE21	1:D:557:ILE:HG12	1.82	0.44
1:D:7:THR:HG21	1:D:267:GLY:O	2.18	0.44
1:A:138:HIS:HD2	1:A:201:TYR:OH	1.99	0.44
1:A:443:ILE:HD13	1:A:595:GLN:HB2	2.00	0.44
1:A:480:ASN:O	1:A:483:LYS:HG2	2.17	0.44
1:A:492:ALA:HB3	1:A:549:GLU:HB2	2.00	0.44
1:A:546:GLN:O	1:A:550:VAL:HG13	2.17	0.44
1:A:787:ASN:O	1:A:790:LYS:HB3	2.17	0.44
1:B:355:ILE:O	1:B:358:VAL:HG13	2.18	0.44
1:B:797:PRO:HG3	1:B:806:ARG:HH12	1.83	0.44
1:B:839:ASN:HA	1:B:840:PRO:HD3	1.85	0.44
1:B:871:LEU:O	1:B:875:THR:HG23	2.18	0.44
1:C:163:SER:CB	1:C:166:ILE:HG13	2.48	0.44
1:C:324:ASN:C	1:C:324:ASN:ND2	2.70	0.44
1:B:644:THR:HG21	1:C:77:ASP:OD2	2.18	0.44
1:D:445:ALA:HA	1:D:673:TYR:CE1	2.53	0.44
1:D:42:PRO:HG2	1:D:45:GLN:HB2	2.00	0.44
1:A:27:ARG:HH11	1:A:27:ARG:HG3	1.82	0.44
1:A:490:LEU:O	1:A:494:ARG:HB3	2.17	0.44
1:B:298:LEU:CD1	1:B:333:GLN:HB2	2.48	0.44
1:C:189:MET:HB3	1:C:191:PHE:HE1	1.82	0.44
1:C:34:LYS:HD3	1:C:61:LEU:CD2	2.48	0.44
1:C:481:GLN:HB3	1:C:559:ARG:NH1	2.32	0.44
1:A:483:LYS:NZ	1:A:483:LYS:HB2	2.33	0.44
1:A:656:ARG:HA	1:A:660:GLU:CG	2.48	0.44
1:C:109:ARG:NH1	1:C:140:ASP:OD2	2.51	0.44
1:C:133:ILE:HD13	1:C:226:VAL:HG22	2.00	0.44
1:C:399:PRO:HB3	1:C:619:TYR:HB2	1.99	0.44
1:C:725:LEU:HD11	1:C:750:ARG:HB2	1.99	0.44
1:D:133:ILE:HD11	1:D:229:ARG:CG	2.35	0.44
1:D:149:PHE:N	1:D:149:PHE:CD1	2.86	0.44
1:D:570:LEU:HA	1:D:570:LEU:HD23	1.81	0.44
1:D:419:ILE:HD13	1:D:589:PHE:HB3	2.00	0.44
1:A:113:PHE:CE1	1:A:218:VAL:HG21	2.53	0.44
1:B:123:PHE:HA	1:B:124:PRO:HD3	1.86	0.44
1:B:171:GLN:NE2	1:B:303:LEU:HD13	2.20	0.44
1:C:19:TYR:CE1	1:C:27:ARG:HB2	2.53	0.44
1:C:249:ARG:HG3	1:C:249:ARG:NH1	2.31	0.44
1:C:33:TYR:OH	1:C:95:ASP:OD2	2.18	0.44
1:D:596:TRP:CE2	1:D:670:MET:HB2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:114:DA:H2"	3:J:115:DA:H5"	2.00	0.44
2:K:5:DG:N3	2:K:6:DA:O4'	2.51	0.44
1:A:744:ALA:HB2	1:A:767:PHE:CE2	2.53	0.43
1:B:152:LEU:CD1	1:B:190:PRO:HB2	2.44	0.43
1:B:351:ALA:O	1:B:352:LYS:HB2	2.18	0.43
1:B:491:ALA:HB3	1:B:519:ARG:O	2.18	0.43
1:C:62:PHE:CD2	1:C:68:ALA:HA	2.53	0.43
1:D:305:TYR:HD2	1:D:305:TYR:C	2.21	0.43
1:D:491:ALA:CB	1:D:520:PHE:HA	2.49	0.43
1:D:832:VAL:HG22	1:D:847:ALA:CB	2.48	0.43
1:A:612:GLU:OE1	1:A:612:GLU:N	2.43	0.43
1:D:126:PRO:HB2	1:D:224:PRO:HB2	2.00	0.43
1:D:182:ILE:O	1:D:186:ILE:HG23	2.18	0.43
1:D:453:VAL:HG23	1:D:454:TYR:CG	2.53	0.43
1:D:622:THR:CG2	1:D:623:ASP:N	2.81	0.43
1:D:782:VAL:HG12	1:D:783:SER:N	2.33	0.43
1:D:892:GLU:O	1:D:894:LYS:HE3	2.18	0.43
1:A:503:LEU:HD21	1:A:539:ASN:OD1	2.18	0.43
1:A:51:ASP:OD2	1:A:53:TYR:N	2.46	0.43
1:A:627:VAL:HG12	1:A:628:SER:N	2.33	0.43
1:A:776:TYR:OH	1:A:853:GLU:HG3	2.17	0.43
1:B:582:ASN:O	1:B:586:ILE:HG13	2.19	0.43
1:C:431:ALA:HB1	1:C:454:TYR:CZ	2.53	0.43
1:C:611:THR:CG2	1:C:612:GLU:N	2.81	0.43
1:D:122:GLY:HA3	1:D:826:GLU:HB2	2.00	0.43
1:D:290:LEU:HD23	1:D:290:LEU:O	2.19	0.43
1:D:581:ARG:HH11	1:D:581:ARG:HG2	1.83	0.43
1:D:86:ASP:OD2	1:D:86:ASP:N	2.43	0.43
1:A:701:PHE:CE2	1:A:752:MET:HE2	2.53	0.43
1:B:727:ILE:HD13	1:B:749:ILE:HD13	2.00	0.43
1:C:121:ASP:C	1:C:819:ILE:HG12	2.39	0.43
1:C:6:LEU:HD11	1:C:26:GLU:HG2	2.00	0.43
1:C:499:ILE:CG2	1:C:541:MET:HE2	2.48	0.43
1:C:65:MET:HB3	1:C:88:PHE:CD2	2.53	0.43
1:D:152:LEU:HD12	1:D:152:LEU:N	2.32	0.43
1:D:206:GLN:NE2	1:D:241:ARG:HB3	2.33	0.43
1:D:595:GLN:HB3	1:D:595:GLN:HE21	1.62	0.43
1:D:599:ARG:HH11	1:D:599:ARG:CB	2.29	0.43
1:A:492:ALA:CB	1:A:549:GLU:HB2	2.49	0.43
1:A:65:MET:HB3	1:A:88:PHE:CD1	2.53	0.43
1:A:738:PRO:HG2	1:A:741:VAL:CB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLU:CG	1:A:879:PRO:HB3	2.40	0.43
1:A:97:TYR:O	1:A:352:LYS:CE	2.61	0.43
1:B:129:ALA:HA	1:B:225:TYR:CE1	2.54	0.43
1:B:19:TYR:HE1	1:B:29:ARG:HG2	1.82	0.43
1:B:391:TYR:HB2	1:B:392:PRO:HD2	2.00	0.43
1:B:503:LEU:HD23	1:B:506:PRO:HD3	2.00	0.43
1:B:541:MET:O	1:B:545:ALA:HB2	2.19	0.43
1:B:898:PHE:HE2	1:D:654:PHE:HB2	1.82	0.43
1:C:425:ILE:HG23	1:C:463:TYR:CE2	2.54	0.43
1:C:502:ALA:HB1	1:C:533:LEU:CD1	2.41	0.43
1:D:182:ILE:HD12	1:D:329:TYR:CG	2.53	0.43
1:D:252:VAL:O	1:D:252:VAL:HG23	2.19	0.43
1:D:338:ARG:HD2	1:D:340:PHE:CZ	2.52	0.43
1:D:803:PHE:C	1:D:803:PHE:CD2	2.91	0.43
1:D:826:GLU:H	1:D:826:GLU:CD	2.21	0.43
3:J:107:DG:H2''	3:J:108:DT:C5'	2.48	0.43
1:A:547:ARG:O	1:A:550:VAL:HG22	2.18	0.43
1:B:455:SER:HA	1:B:675:ASN:O	2.18	0.43
1:C:455:SER:OG	1:C:676:ASN:ND2	2.51	0.43
1:D:199:MET:O	1:D:203:ASN:HB2	2.18	0.43
1:D:319:ARG:O	1:D:323:TYR:N	2.48	0.43
1:D:440:HIS:NE2	1:D:444:ASN:ND2	2.66	0.43
1:D:733:GLN:CA	1:D:733:GLN:HE21	2.26	0.43
1:A:102:LYS:HD3	1:A:102:LYS:C	2.39	0.43
1:A:410:PHE:CD1	1:A:410:PHE:N	2.87	0.43
1:A:518:TYR:O	1:A:519:ARG:C	2.57	0.43
1:A:49:TYR:CE1	1:A:59:ARG:HD3	2.54	0.43
1:A:73:LYS:HA	1:A:76:GLU:OE2	2.18	0.43
1:B:875:THR:O	1:B:879:PRO:HG3	2.18	0.43
1:D:194:GLU:O	1:D:198:LEU:HD23	2.19	0.43
1:D:241:ARG:HG2	1:D:246:ARG:HE	1.84	0.43
1:D:440:HIS:HA	1:D:443:ILE:HD12	2.01	0.43
1:D:662:ALA:HA	1:D:665:ARG:NH1	2.33	0.43
1:D:667:PHE:HD1	1:D:681:MET:O	2.01	0.43
1:D:677:LYS:HE2	5:D:924:HOH:O	2.18	0.43
1:A:452:ASP:OD1	1:A:453:VAL:HG23	2.18	0.43
1:A:552:GLY:O	1:A:555:ALA:N	2.51	0.43
1:A:790:LYS:HG2	1:A:791:TYR:CE1	2.53	0.43
1:B:301:GLY:O	1:B:330:ARG:NE	2.46	0.43
1:B:538:LEU:HD22	1:B:542:LEU:CD2	2.49	0.43
1:C:486:LYS:HG2	1:C:556:GLN:HG3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:LYS:HE2	1:C:561:LEU:HD12	2.01	0.43
1:C:565:SER:HA	2:I:2:DG:N2	2.33	0.43
1:C:742:GLN:O	1:C:746:LYS:HB2	2.18	0.43
1:C:362:ILE:HG12	2:I:2:DG:C5'	2.49	0.43
3:J:101:DG:H2"	3:J:102:DC:C6	2.54	0.43
1:A:392:PRO:HG2	1:A:584:THR:HG23	2.00	0.43
1:A:438:PRO:O	1:A:441:ASP:HB2	2.18	0.43
1:A:514:LEU:O	1:A:516:VAL:N	2.50	0.43
1:A:537:SER:O	1:A:540:GLU:N	2.51	0.43
1:A:455:SER:HA	1:A:675:ASN:O	2.19	0.43
1:B:173:GLN:HE21	1:B:173:GLN:HB2	1.53	0.43
1:B:206:GLN:HE22	1:B:246:ARG:NH2	2.17	0.43
1:B:236:GLU:O	1:B:240:LYS:HG3	2.18	0.43
1:C:5:TYR:HE1	1:C:101:ILE:CD1	2.32	0.43
1:C:475:ILE:HG23	1:C:476:THR:H	1.84	0.43
1:C:503:LEU:HD21	1:C:538:LEU:HD22	1.99	0.43
1:C:824:VAL:HG22	1:C:849:PRO:HD3	2.00	0.43
1:D:153:ASN:HA	1:D:158:ASN:HD21	1.83	0.43
1:D:332:LEU:N	1:D:332:LEU:CD1	2.82	0.43
1:D:439:LEU:HD12	1:D:439:LEU:HA	1.89	0.43
1:D:524:ASP:HA	1:D:527:LYS:HB2	2.01	0.43
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.19	0.43
1:B:251:LYS:HE3	1:B:262:ILE:HD11	2.01	0.43
1:C:159:VAL:CG1	1:C:160:GLU:H	2.23	0.43
1:C:234:PHE:HB3	1:C:238:THR:OG1	2.19	0.43
1:C:243:SER:HB2	1:C:248:THR:HG22	2.01	0.43
1:C:314:GLU:HG2	1:C:315:SER:H	1.83	0.43
1:C:489:MET:C	1:C:491:ALA:N	2.72	0.43
1:C:572:ASN:HD21	1:C:574:TRP:HB2	1.83	0.43
1:C:597:ILE:HD12	1:C:597:ILE:HA	1.91	0.43
1:D:170:LEU:HG	1:D:171:GLN:H	1.82	0.43
1:D:112:ASN:O	1:D:328:VAL:HG13	2.18	0.43
1:D:48:LYS:HE3	1:D:49:TYR:CZ	2.53	0.43
1:D:550:VAL:C	1:D:552:GLY:H	2.21	0.43
1:A:708:TYR:CE2	1:A:726:LYS:HE2	2.53	0.42
1:A:786:ASN:N	1:A:786:ASN:HD22	2.17	0.42
1:A:793:VAL:HG12	1:A:793:VAL:O	2.19	0.42
1:B:365:TRP:CD2	1:B:566:LEU:HD13	2.53	0.42
1:C:527:LYS:C	1:C:529:LYS:H	2.22	0.42
1:C:667:PHE:HB3	1:C:679:HIS:HE1	1.83	0.42
1:C:745:LEU:HD23	1:C:745:LEU:HA	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ASP:CG	1:D:104:ASP:O	2.57	0.42
1:D:147:TYR:N	1:D:147:TYR:CD1	2.87	0.42
1:D:202:LEU:HD21	1:D:241:ARG:NH1	2.33	0.42
1:D:362:ILE:HD11	1:D:575:PHE:HA	2.01	0.42
1:D:830:VAL:HG22	1:D:847:ALA:HB1	2.01	0.42
1:B:197:LEU:HD23	1:B:197:LEU:O	2.18	0.42
1:B:271:LEU:HB3	1:B:276:LEU:HD11	2.00	0.42
1:B:641:PHE:HA	1:B:646:HIS:HD2	1.84	0.42
1:B:658:ARG:HG3	1:B:658:ARG:HH11	1.83	0.42
1:B:873:GLU:HA	1:B:877:ILE:CG1	2.49	0.42
1:C:806:ARG:NH1	1:C:806:ARG:HG2	2.25	0.42
1:D:456:CYS:HB2	1:D:674:MET:HE3	2.00	0.42
1:D:723:PRO:C	1:D:724:LYS:HD2	2.40	0.42
1:A:273:TYR:HE1	1:A:335:ASP:OD2	2.02	0.42
1:A:497:GLU:OE2	1:A:497:GLU:HA	2.20	0.42
1:B:13:ASP:OD2	1:B:66:ARG:HB2	2.19	0.42
1:B:178:VAL:HA	1:B:326:ILE:HD11	2.01	0.42
1:B:386:HIS:HB2	1:B:573:VAL:HG22	2.01	0.42
1:C:269:SER:HB3	1:C:356:GLN:HG3	2.01	0.42
1:C:656:ARG:HA	1:C:660:GLU:HG3	2.01	0.42
1:D:135:ALA:C	1:D:136:ILE:HG22	2.38	0.42
1:D:234:PHE:CD2	1:D:238:THR:HG21	2.54	0.42
1:D:376:GLN:HB2	1:D:378:LYS:HG3	2.01	0.42
1:D:48:LYS:HE3	1:D:49:TYR:OH	2.19	0.42
1:A:150:ASP:OD1	1:A:317:HIS:CE1	2.73	0.42
1:A:416:TYR:CD2	1:A:416:TYR:N	2.87	0.42
1:A:785:ALA:HB1	1:A:808:ILE:CD1	2.48	0.42
1:A:784:SER:OG	1:A:829:LYS:HE2	2.19	0.42
1:B:779:ILE:HD12	1:B:871:LEU:CD2	2.48	0.42
1:C:132:PRO:HB3	1:C:194:GLU:OE1	2.19	0.42
1:C:33:TYR:HD2	1:C:65:MET:HE1	1.83	0.42
1:C:36:SER:HB3	1:C:59:ARG:HD2	2.01	0.42
1:C:441:ASP:HB3	1:C:447:ALA:HB2	2.00	0.42
1:D:406:TYR:HB3	1:D:629:ALA:HB3	2.02	0.42
1:D:660:GLU:CB	1:D:661:PRO:HD3	2.48	0.42
1:B:362:ILE:HG12	2:G:2:DG:H5'	2.02	0.42
1:A:212:ILE:HD13	1:A:269:SER:HB2	2.02	0.42
1:A:403:ARG:C	1:A:404:TYR:CD2	2.93	0.42
1:A:415:LEU:HG	1:A:419:ILE:HD11	2.02	0.42
1:A:572:ASN:C	1:A:572:ASN:HD22	2.23	0.42
1:B:416:TYR:CD2	4:B:907:DTP:C2'	3.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:MET:O	1:B:660:GLU:C	2.57	0.42
1:B:643:ASP:HA	1:B:693:LEU:HD23	2.01	0.42
1:C:154:SER:C	1:C:156:TYR:H	2.23	0.42
1:C:462:MET:HE2	1:C:462:MET:HB2	1.84	0.42
1:C:641:PHE:CE2	1:C:647:TRP:HA	2.54	0.42
1:D:187:ILE:O	1:D:187:ILE:HG22	2.19	0.42
1:D:199:MET:HB3	1:D:234:PHE:HE2	1.84	0.42
1:D:290:LEU:O	1:D:294:SER:CB	2.68	0.42
1:D:401:PRO:HG3	1:D:703:THR:O	2.20	0.42
1:D:499:ILE:CD1	1:D:545:ALA:HB2	2.49	0.42
1:D:362:ILE:HD11	1:D:575:PHE:CA	2.49	0.42
1:D:734:LYS:HG3	1:D:735:SER:H	1.84	0.42
1:D:856:ASP:HA	1:D:859:LYS:HB3	2.00	0.42
3:L:109:DC:H4'	3:L:109:DC:OP1	2.18	0.42
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.34	0.42
1:A:605:LEU:HA	1:A:608:VAL:HG22	2.00	0.42
1:A:785:ALA:HB2	1:A:808:ILE:HD11	2.01	0.42
1:B:195:LYS:HG2	1:B:234:PHE:CZ	2.54	0.42
1:B:85:MET:HE1	1:B:90:LEU:HD23	2.02	0.42
1:C:518:TYR:C	1:C:520:PHE:H	2.21	0.42
1:C:62:PHE:HE2	1:C:71:TRP:HB2	1.84	0.42
1:C:65:MET:HG2	1:C:65:MET:H	1.58	0.42
1:C:656:ARG:HA	1:C:660:GLU:CG	2.50	0.42
1:C:680:LEU:HA	1:C:682:PHE:CZ	2.54	0.42
1:D:440:HIS:CE1	1:D:444:ASN:ND2	2.83	0.42
1:D:741:VAL:O	1:D:744:ALA:N	2.52	0.42
2:E:7:DA:H4'	2:E:8:DT:OP1	2.19	0.42
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.55	0.42
1:A:656:ARG:HA	1:A:660:GLU:HG3	2.02	0.42
1:A:682:PHE:HA	5:A:924:HOH:O	2.19	0.42
1:A:68:ALA:O	1:A:72:ILE:HG13	2.20	0.42
1:A:844:LYS:HB3	1:A:844:LYS:HE2	1.86	0.42
1:B:524:ASP:O	1:B:526:ILE:N	2.52	0.42
1:B:649:ASP:OD2	1:B:649:ASP:N	2.52	0.42
1:C:362:ILE:HA	1:C:362:ILE:HD13	1.90	0.42
1:C:556:GLN:C	1:C:556:GLN:NE2	2.73	0.42
1:C:703:THR:OG1	1:C:707:ARG:HB2	2.20	0.42
1:C:876:PHE:O	1:C:879:PRO:HG2	2.20	0.42
1:D:161:GLU:HG2	1:D:162:TRP:H	1.85	0.42
1:D:401:PRO:O	1:D:402:ASN:HB2	2.19	0.42
1:D:62:PHE:N	1:D:62:PHE:CD1	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:ALA:O	1:D:630:ASP:C	2.57	0.42
1:A:518:TYR:CD2	1:A:545:ALA:HB2	2.55	0.42
1:A:66:ARG:HH11	1:A:66:ARG:CG	2.33	0.42
1:B:101:ILE:HG21	1:B:349:TYR:CG	2.55	0.42
1:B:525:GLU:O	1:B:525:GLU:HG2	2.19	0.42
1:B:625:ILE:HG12	1:B:683:MET:HE1	2.02	0.42
1:C:597:ILE:HB	1:C:667:PHE:CZ	2.54	0.42
1:C:768:GLU:HG2	1:C:872:LEU:HD21	2.02	0.42
1:D:202:LEU:O	1:D:205:TRP:HB3	2.20	0.42
1:D:254:GLU:HA	1:D:259:SER:HA	2.00	0.42
1:D:329:TYR:O	1:D:333:GLN:HG3	2.20	0.42
1:D:15:ILE:HD11	1:D:92:TYR:CE2	2.54	0.42
1:A:410:PHE:CB	1:A:683:MET:HE2	2.50	0.42
1:A:550:VAL:HG23	1:A:551:ALA:N	2.35	0.42
1:A:411:ASP:CG	1:A:686:GLU:HG3	2.40	0.42
1:A:396:VAL:HG12	1:A:705:LYS:HG2	2.01	0.42
1:B:197:LEU:CD2	1:B:197:LEU:C	2.88	0.42
1:B:216:TRP:HZ2	1:B:293:ILE:HG13	1.84	0.42
1:B:395:PHE:HB2	1:B:591:GLN:CG	2.50	0.42
1:B:506:PRO:HB3	1:B:538:LEU:CD1	2.50	0.42
1:B:770:GLU:O	1:B:773:GLN:HG2	2.19	0.42
1:C:139:TYR:CD1	1:C:139:TYR:C	2.93	0.42
1:C:233:ILE:HG22	1:C:234:PHE:CE2	2.55	0.42
1:C:426:SER:OG	1:C:427:PRO:HD2	2.20	0.42
1:C:407:VAL:HA	1:C:627:VAL:O	2.20	0.42
1:C:850:SER:O	1:C:852:THR:HG23	2.19	0.42
1:D:137:THR:O	1:D:328:VAL:HG21	2.20	0.42
1:D:605:LEU:HD11	1:D:659:MET:CE	2.49	0.42
1:D:739:LYS:CE	1:D:743:LYS:HD2	2.50	0.42
1:D:863:LEU:HG	1:D:866:MET:HE2	2.01	0.42
1:A:118:THR:N	1:A:134:ASP:OD2	2.52	0.42
1:A:508:LEU:CD2	1:A:508:LEU:N	2.82	0.42
1:A:606:ASN:OD1	1:A:616:PHE:HE1	2.02	0.42
1:A:787:ASN:HB3	1:A:790:LYS:HB3	2.00	0.42
1:A:810:THR:OG1	1:A:843:ASP:HB2	2.20	0.42
1:B:9:GLU:HG2	1:B:266:PHE:CD2	2.55	0.42
1:B:632:ILE:HA	1:B:632:ILE:HD13	1.83	0.42
1:B:727:ILE:HD13	1:B:749:ILE:CD1	2.49	0.42
1:C:510:VAL:O	1:C:510:VAL:HG12	2.19	0.42
1:C:592:MET:CE	1:C:670:MET:SD	3.08	0.42
1:C:877:ILE:O	1:C:878:LYS:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:SER:C	1:D:156:TYR:N	2.74	0.42
1:D:253:ILE:HG23	1:D:260:ARG:NH1	2.35	0.42
1:D:380:ILE:HB	1:D:576:ARG:HD3	2.02	0.42
1:D:449:ARG:HH11	1:D:452:ASP:HB3	1.76	0.42
1:D:492:ALA:HA	1:D:495:ASN:HB3	2.00	0.42
1:D:579:ASP:C	1:D:579:ASP:OD2	2.58	0.42
1:D:445:ALA:HB2	1:D:596:TRP:CZ3	2.54	0.42
1:D:633:ILE:HA	1:D:633:ILE:HD13	1.90	0.42
2:E:15:DC:O2	3:F:104:DG:N2	2.53	0.42
1:A:171:GLN:HE22	1:A:319:ARG:CZ	2.33	0.41
1:C:423:VAL:HB	1:C:425:ILE:HG13	2.02	0.41
1:C:402:ASN:HA	1:C:886:ALA:O	2.19	0.41
1:D:493:GLN:C	1:D:495:ASN:H	2.23	0.41
1:D:500:LYS:C	1:D:502:ALA:H	2.22	0.41
1:D:734:LYS:HE2	1:D:734:LYS:HB2	1.89	0.41
1:B:185:LYS:HG2	1:B:185:LYS:H	1.62	0.41
1:B:45:GLN:O	1:B:47:THR:HG22	2.20	0.41
1:B:678:GLN:HG2	1:B:680:LEU:HG	2.02	0.41
1:B:625:ILE:HG12	1:B:683:MET:CE	2.50	0.41
1:C:299:ASN:O	1:C:300:VAL:HB	2.20	0.41
1:C:420:ILE:HG12	1:C:586:ILE:HD11	2.01	0.41
1:C:727:ILE:CG2	1:C:730:LEU:HB2	2.51	0.41
1:C:887:ALA:O	1:C:888:LYS:HB2	2.20	0.41
1:D:194:GLU:O	1:D:195:LYS:C	2.58	0.41
1:D:642:ARG:HG2	1:D:643:ASP:OD2	2.19	0.41
1:D:777:ILE:HD12	1:D:778:SER:H	1.81	0.41
1:A:405:LYS:HA	1:A:698:ILE:O	2.21	0.41
1:B:164:ILE:CD1	1:B:164:ILE:N	2.81	0.41
1:C:425:ILE:HA	1:C:463:TYR:CD2	2.55	0.41
1:C:682:PHE:CD1	1:C:682:PHE:N	2.86	0.41
1:D:277:TYR:O	1:D:281:SER:HB2	2.19	0.41
1:D:788:ILE:HD11	1:D:809:LEU:HD23	2.02	0.41
1:D:97:TYR:HB3	1:D:101:ILE:CD1	2.37	0.41
2:G:16:DG:H2''	2:G:17:DC:H5'	2.01	0.41
1:A:616:PHE:HE2	1:A:631:LYS:HB3	1.86	0.41
1:B:517:ASP:O	1:B:519:ARG:N	2.54	0.41
1:C:308:PRO:HG3	1:C:311:LYS:HE3	2.01	0.41
1:C:413:THR:O	1:C:414:SER:C	2.59	0.41
1:C:415:LEU:HD22	1:C:623:ASP:HB3	2.03	0.41
1:C:452:ASP:O	1:C:452:ASP:OD2	2.38	0.41
1:C:500:LYS:HA	1:C:503:LEU:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:LEU:H	1:C:561:LEU:CD1	2.33	0.41
1:D:362:ILE:HD13	1:D:575:PHE:CD1	2.55	0.41
1:D:398:GLU:HA	1:D:705:LYS:CE	2.51	0.41
1:D:596:TRP:NE1	1:D:670:MET:HB2	2.35	0.41
1:D:720:TYR:CD2	1:D:724:LYS:HG2	2.56	0.41
1:D:860:ASP:O	1:D:864:HIS:HB2	2.21	0.41
1:D:779:ILE:HG22	1:D:871:LEU:CD2	2.50	0.41
3:L:105:DC:H2'	3:L:106:DT:C6	2.55	0.41
1:A:518:TYR:O	1:A:520:PHE:N	2.54	0.41
1:A:711:ASN:ND2	1:A:723:PRO:HB2	2.36	0.41
1:A:786:ASN:O	1:A:805:ILE:HD11	2.20	0.41
1:B:171:GLN:HE22	1:B:303:LEU:CD1	2.23	0.41
1:B:500:LYS:HA	1:B:542:LEU:HD11	2.03	0.41
1:C:217:ASN:HD22	1:C:274:ILE:HD13	1.84	0.41
1:C:283:THR:O	1:C:283:THR:HG23	2.20	0.41
1:C:397:LYS:O	1:C:399:PRO:HD3	2.21	0.41
1:C:542:LEU:C	1:C:544:ARG:N	2.74	0.41
1:D:227:TYR:CG	1:D:263:ILE:HD13	2.54	0.41
1:D:283:THR:O	1:D:285:GLN:N	2.53	0.41
1:D:815:ILE:HD12	1:D:815:ILE:O	2.21	0.41
1:D:808:ILE:HG23	1:D:824:VAL:HG11	2.02	0.41
2:G:4:CTG:H2'	2:G:4:CTG:O6	2.21	0.41
3:J:104:DG:H2''	3:J:105:DC:C6	2.56	0.41
3:L:108:DT:C1'	3:L:109:DC:H5''	2.51	0.41
1:A:338:ARG:HB3	1:A:340:PHE:CZ	2.55	0.41
1:A:518:TYR:OH	1:A:541:MET:HB3	2.21	0.41
1:B:749:ILE:O	1:B:753:LEU:CD1	2.63	0.41
1:C:193:ASN:OD1	1:C:196:GLU:CG	2.67	0.41
1:C:518:TYR:HA	1:C:522:PHE:HE1	1.84	0.41
1:D:179:PRO:HB2	1:D:182:ILE:HG21	2.02	0.41
1:D:305:TYR:HD2	1:D:305:TYR:O	2.02	0.41
1:D:411:ASP:O	1:D:683:MET:HA	2.21	0.41
1:D:771:PHE:CE2	1:D:872:LEU:HD13	2.56	0.41
3:L:108:DT:H2''	3:L:109:DC:O5'	2.15	0.41
1:A:183:ILE:HD12	1:A:183:ILE:HA	1.88	0.41
1:A:202:LEU:CD1	1:A:242:LEU:HD13	2.51	0.41
1:B:423:VAL:O	1:B:424:ASN:CB	2.69	0.41
1:C:542:LEU:C	1:C:544:ARG:H	2.24	0.41
1:D:477:LYS:O	1:D:481:GLN:HG3	2.20	0.41
1:A:285:GLN:OE1	1:A:296:PHE:CE1	2.74	0.41
1:A:642:ARG:HB2	1:A:646:HIS:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ARG:NH1	1:B:142:ILE:HD12	2.36	0.41
1:B:280:PHE:HB2	1:B:340:PHE:CE1	2.55	0.41
1:B:626:TYR:CD1	1:B:626:TYR:N	2.89	0.41
1:C:166:ILE:HB	1:C:318:GLN:OE1	2.20	0.41
1:D:136:ILE:HD11	1:D:201:TYR:CZ	2.55	0.41
1:D:461:MET:HB3	1:D:463:TYR:CE1	2.56	0.41
1:D:710:LEU:HD13	1:D:712:VAL:HG22	2.02	0.41
1:D:692:PRO:CD	1:D:754:GLN:HA	2.50	0.41
1:D:831:TYR:CD1	1:D:848:TRP:CZ3	3.09	0.41
1:A:481:GLN:O	1:A:484:GLU:HB3	2.20	0.41
1:A:578:TYR:OH	1:A:580:LEU:HD13	2.21	0.41
1:A:731:GLU:HA	1:A:734:LYS:CD	2.51	0.41
1:B:402:ASN:OD1	1:B:888:LYS:HE2	2.20	0.41
1:C:221:PHE:C	1:C:224:PRO:HD2	2.41	0.41
1:C:494:ARG:NH1	1:C:494:ARG:HG2	2.36	0.41
1:C:659:MET:O	1:C:660:GLU:C	2.59	0.41
1:D:423:VAL:O	1:D:424:ASN:CB	2.69	0.41
1:D:566:LEU:HG	1:D:566:LEU:O	2.19	0.41
1:D:802:PRO:O	1:D:805:ILE:N	2.53	0.41
1:D:831:TYR:HD1	1:D:848:TRP:CZ3	2.38	0.41
1:D:83:LEU:HB3	1:D:379:VAL:HG12	2.02	0.41
1:D:870:VAL:O	1:D:870:VAL:HG12	2.21	0.41
2:G:16:DG:C1'	2:G:17:DC:H5''	2.49	0.41
1:D:731:GLU:HG2	2:K:7:DA:H5''	2.02	0.41
1:A:170:LEU:HA	1:A:177:GLU:HG2	2.03	0.41
1:A:231:LYS:HB3	1:A:231:LYS:HZ2	1.86	0.41
1:A:48:LYS:CB	1:A:48:LYS:NZ	2.84	0.41
1:A:408:MET:SD	1:A:655:ALA:HB2	2.61	0.41
1:B:524:ASP:C	1:B:526:ILE:N	2.75	0.41
1:B:514:LEU:CD2	1:B:530:ILE:HG12	2.48	0.41
1:C:486:LYS:CG	1:C:556:GLN:HG3	2.51	0.41
1:C:640:LYS:HE3	1:C:640:LYS:HB2	1.92	0.41
1:D:10:GLN:NE2	1:D:88:PHE:HD2	2.18	0.41
1:D:257:TYR:N	1:D:257:TYR:CD1	2.89	0.41
1:D:818:ASN:N	1:D:818:ASN:OD1	2.54	0.41
2:I:14:DC:H2''	2:I:15:DC:H5'	2.00	0.41
3:J:107:DG:H1'	3:J:108:DT:H5''	2.03	0.41
1:A:64:ASN:ND2	1:A:67:ASP:CG	2.74	0.41
1:A:741:VAL:CG1	1:A:745:LEU:HD22	2.51	0.41
1:B:497:GLU:HA	1:B:497:GLU:OE2	2.21	0.41
1:B:872:LEU:HD11	1:B:876:PHE:HD2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HA	1:B:93:LEU:HD12	1.84	0.41
1:C:505:ASN:H	1:C:506:PRO:HD3	1.85	0.41
1:C:561:LEU:N	1:C:561:LEU:HD12	2.36	0.41
1:C:608:VAL:HG12	1:C:608:VAL:O	2.21	0.41
1:C:818:ASN:ND2	1:C:857:LEU:CD1	2.76	0.41
1:D:19:TYR:CD1	1:D:19:TYR:N	2.89	0.41
1:D:191:PHE:CE2	1:D:200:GLU:HG3	2.54	0.41
1:D:437:ALA:HB1	1:D:438:PRO:HD2	2.02	0.41
1:D:747:GLU:CD	1:D:750:ARG:HE	2.24	0.41
1:A:113:PHE:CE1	1:A:218:VAL:HG22	2.56	0.40
1:A:548:THR:O	1:A:551:ALA:HB3	2.20	0.40
1:A:422:GLN:NE2	1:A:680:LEU:H	2.18	0.40
1:B:202:LEU:HD12	1:B:202:LEU:HA	1.80	0.40
1:B:286:PRO:HG2	1:B:292:TYR:CZ	2.56	0.40
1:B:324:ASN:C	1:B:324:ASN:HD22	2.23	0.40
1:B:381:PRO:O	1:B:576:ARG:HD2	2.21	0.40
1:B:872:LEU:HD11	1:B:876:PHE:CD2	2.56	0.40
1:C:302:LYS:HD3	1:C:303:LEU:H	1.86	0.40
1:C:474:GLU:O	1:C:478:VAL:HG23	2.22	0.40
1:C:498:ILE:HG23	1:C:499:ILE:CD1	2.51	0.40
1:C:507:ASN:CB	1:C:531:LYS:O	2.68	0.40
1:C:533:LEU:CG	1:C:538:LEU:HG	2.51	0.40
1:C:53:TYR:CD1	1:C:428:GLU:HB3	2.56	0.40
1:C:558:ASN:N	1:C:558:ASN:HD22	2.17	0.40
1:C:580:LEU:HD12	1:C:580:LEU:HA	1.78	0.40
1:D:665:ARG:NH2	1:D:665:ARG:HB2	2.36	0.40
1:D:802:PRO:HD2	1:D:805:ILE:HG13	2.02	0.40
1:A:492:ALA:O	1:A:545:ALA:HB1	2.20	0.40
1:A:634:ASP:C	1:A:636:VAL:H	2.23	0.40
1:A:784:SER:CB	1:A:829:LYS:HE2	2.51	0.40
1:B:151:LEU:HD13	1:B:194:GLU:HA	2.03	0.40
1:B:205:TRP:HH2	1:B:213:LEU:CD2	2.34	0.40
1:B:517:ASP:C	1:B:519:ARG:H	2.25	0.40
1:C:193:ASN:HD21	1:C:195:LYS:HB2	1.85	0.40
1:C:302:LYS:CB	1:C:302:LYS:NZ	2.85	0.40
1:C:507:ASN:ND2	1:C:508:LEU:N	2.67	0.40
1:C:362:ILE:HD13	1:C:569:ALA:HB1	2.03	0.40
1:C:458:PRO:CG	1:C:592:MET:SD	3.10	0.40
1:D:105:HIS:CD2	1:D:106:THR:HG23	2.55	0.40
1:D:194:GLU:O	1:D:197:LEU:N	2.50	0.40
1:D:412:LEU:CD1	1:D:415:LEU:HD22	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:ILE:HA	1:D:597:ILE:HD12	1.88	0.40
1:D:649:ASP:CG	1:D:719:ARG:HH12	2.23	0.40
1:D:758:GLU:CG	1:D:759:SER:N	2.85	0.40
1:D:791:TYR:HD2	1:D:801:CYS:CA	2.32	0.40
3:H:103:DG:H2"	3:H:104:DG:C8	2.56	0.40
1:A:250:VAL:HG12	1:A:263:ILE:HD12	2.03	0.40
1:A:493:GLN:O	1:A:496:GLY:N	2.52	0.40
1:B:166:ILE:O	1:B:169:LYS:HB2	2.21	0.40
1:B:219:GLU:OE1	1:B:262:ILE:HD12	2.21	0.40
1:B:389:GLN:HA	1:B:390:PRO:HD3	1.87	0.40
1:B:512:GLU:O	1:B:533:LEU:HD21	2.22	0.40
1:B:52:ILE:HG13	1:B:53:TYR:CE1	2.56	0.40
1:B:897:LEU:O	1:B:899:ASP:N	2.54	0.40
1:C:249:ARG:HH12	1:C:251:LYS:HB2	1.87	0.40
1:C:393:GLY:O	1:C:587:THR:HG23	2.21	0.40
1:D:173:GLN:HE21	1:D:173:GLN:HB3	1.56	0.40
1:D:4:PHE:CE2	1:D:20:ILE:HG13	2.57	0.40
1:D:517:ASP:O	1:D:519:ARG:N	2.47	0.40
1:D:769:LYS:O	1:D:771:PHE:N	2.53	0.40
2:E:7:DA:H1'	2:E:8:DT:C6	2.57	0.40
2:E:7:DA:H1'	2:E:8:DT:H5'	2.04	0.40
2:I:7:DA:C8	2:I:8:DT:H72	2.56	0.40
1:B:274:ILE:CG2	1:B:275:ASP:N	2.83	0.40
1:B:397:LYS:O	1:B:399:PRO:HD3	2.21	0.40
1:B:52:ILE:O	1:B:428:GLU:HG3	2.22	0.40
1:B:458:PRO:HG3	1:B:592:MET:SD	2.61	0.40
1:B:425:ILE:O	1:B:472:PRO:HD3	2.22	0.40
1:C:109:ARG:HG3	1:C:109:ARG:NH1	2.36	0.40
1:C:191:PHE:CD2	1:C:197:LEU:HA	2.57	0.40
1:C:511:ASP:CA	1:C:534:SER:HB2	2.51	0.40
1:C:560:LYS:HG2	1:C:564:ASN:HD21	1.86	0.40
1:C:589:PHE:C	1:C:589:PHE:CD1	2.94	0.40
1:C:645:ASN:OD1	1:C:719:ARG:NH1	2.52	0.40
1:D:461:MET:HG2	1:D:463:TYR:OH	2.21	0.40
1:D:503:LEU:C	1:D:503:LEU:HD23	2.41	0.40
1:D:619:TYR:C	1:D:619:TYR:CD1	2.94	0.40
1:D:771:PHE:CD2	1:D:872:LEU:HD13	2.56	0.40
1:A:129:ALA:HA	1:A:225:TYR:CE1	2.56	0.40
1:A:273:TYR:CE1	1:A:335:ASP:OD2	2.74	0.40
1:A:279:LYS:C	1:A:280:PHE:CD1	2.82	0.40
1:A:284:ASN:ND2	1:A:285:GLN:N	2.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLN:HE21	1:A:378:LYS:HE3	1.87	0.40
1:A:765:LYS:HB2	1:A:765:LYS:HE3	1.91	0.40
1:A:825:VAL:HG22	1:A:828:GLU:CG	2.45	0.40
1:B:471:VAL:O	1:B:475:ILE:HG22	2.22	0.40
1:C:161:GLU:HG2	1:C:161:GLU:H	1.70	0.40
1:C:507:ASN:HD22	1:C:508:LEU:H	1.63	0.40
1:D:283:THR:OG1	1:D:285:GLN:NE2	2.55	0.40
1:D:176:ASP:OD1	1:D:318:GLN:HG3	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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	900/906 (99%)	824 (92%)	71 (8%)	5 (1%)	25	61
1	B	900/906 (99%)	822 (91%)	68 (8%)	10 (1%)	14	47
1	C	899/906 (99%)	803 (89%)	83 (9%)	13 (1%)	11	41
1	D	895/906 (99%)	764 (85%)	103 (12%)	28 (3%)	4	20
All	All	3594/3624 (99%)	3213 (89%)	325 (9%)	56 (2%)	9	38

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	VAL
1	A	515	ASP
1	B	300	VAL
1	B	518	TYR
1	C	45	GLN
1	C	300	VAL
1	C	534	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	161	GLU
1	D	315	SER
1	D	622	THR
1	D	732	THR
1	D	757	GLU
1	D	895	ALA
1	A	45	GLN
1	B	45	GLN
1	B	304	LYS
1	B	898	PHE
1	C	304	LYS
1	C	458	PRO
1	C	492	ALA
1	C	509	SER
1	C	510	VAL
1	C	896	SER
1	D	45	GLN
1	D	136	ILE
1	D	181	GLU
1	D	508	LEU
1	D	733	GLN
1	D	819	ILE
1	D	859	LYS
1	A	900	MET
1	B	524	ASP
1	B	525	GLU
1	C	415	LEU
1	C	494	ARG
1	D	199	MET
1	D	522	PHE
1	D	822	PRO
1	A	519	ARG
1	B	414	SER
1	C	522	PHE
1	D	179	PRO
1	D	414	SER
1	D	458	PRO
1	D	518	TYR
1	D	734	LYS
1	D	770	GLU
1	D	771	PHE
1	B	458	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	388	VAL
1	D	524	ASP
1	B	561	LEU
1	D	222	ALA
1	D	244	PRO
1	C	505	ASN
1	D	187	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	781/803 (97%)	726 (93%)	55 (7%)	15	45
1	B	788/803 (98%)	732 (93%)	56 (7%)	14	44
1	C	788/803 (98%)	726 (92%)	62 (8%)	12	39
1	D	758/803 (94%)	684 (90%)	74 (10%)	8	29
All	All	3115/3212 (97%)	2868 (92%)	247 (8%)	12	39

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	45	GLN
1	A	47	THR
1	A	48	LYS
1	A	64	ASN
1	A	70	GLN
1	A	86	ASP
1	A	105	HIS
1	A	106	THR
1	A	193	ASN
1	A	199	MET
1	A	207	GLN
1	A	213	LEU
1	A	218	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	219	GLU
1	A	229	ARG
1	A	242	LEU
1	A	246	ARG
1	A	247	LYS
1	A	260	ARG
1	A	261	GLU
1	A	283	THR
1	A	284	ASN
1	A	311	LYS
1	A	318	GLN
1	A	319	ARG
1	A	332	LEU
1	A	372	SER
1	A	379	VAL
1	A	384	ARG
1	A	414	SER
1	A	468	ASP
1	A	477	LYS
1	A	483	LYS
1	A	505	ASN
1	A	515	ASP
1	A	522	PHE
1	A	543	PHE
1	A	572	ASN
1	A	612	GLU
1	A	614	GLU
1	A	645	ASN
1	A	658	ARG
1	A	685	ARG
1	A	703	THR
1	A	711	ASN
1	A	731	GLU
1	A	734	LYS
1	A	745	LEU
1	A	790	LYS
1	A	825	VAL
1	A	829	LYS
1	A	861	ASP
1	A	863	LEU
1	A	878	LYS
1	B	34	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	45	GLN
1	B	47	THR
1	B	102	LYS
1	B	109	ARG
1	B	113	PHE
1	B	114	ASP
1	B	116	GLU
1	B	128	GLN
1	B	148	VAL
1	B	154	SER
1	B	164	ILE
1	B	173	GLN
1	B	185	LYS
1	B	193	ASN
1	B	253	ILE
1	B	257	TYR
1	B	273	TYR
1	B	302	LYS
1	B	313	ARG
1	B	316	ASN
1	B	319	ARG
1	B	324	ASN
1	B	363	LYS
1	B	372	SER
1	B	421	ARG
1	B	479	PHE
1	B	503	LEU
1	B	531	LYS
1	B	532	LYS
1	B	533	LEU
1	B	538	LEU
1	B	542	LEU
1	B	543	PHE
1	B	544	ARG
1	B	549	GLU
1	B	553	MET
1	B	558	ASN
1	B	573	VAL
1	B	581	ARG
1	B	618	LEU
1	B	631	LYS
1	B	632	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	639	SER
1	B	649	ASP
1	B	658	ARG
1	B	660	GLU
1	B	672	GLU
1	B	685	ARG
1	B	702	TRP
1	B	728	MET
1	B	773	GLN
1	B	820	ASP
1	B	843	ASP
1	B	861	ASP
1	B	885	SER
1	C	18	ARG
1	C	26	GLU
1	C	38	PHE
1	C	43	GLU
1	C	58	THR
1	C	59	ARG
1	C	64	ASN
1	C	65	MET
1	C	73	LYS
1	C	77	ASP
1	C	83	LEU
1	C	127	SER
1	C	149	PHE
1	C	185	LYS
1	C	203	ASN
1	C	206	GLN
1	C	238	THR
1	C	273	TYR
1	C	302	LYS
1	C	313	ARG
1	C	314	GLU
1	C	324	ASN
1	C	326	ILE
1	C	330	ARG
1	C	356	GLN
1	C	375	GLU
1	C	402	ASN
1	C	408	MET
1	C	414	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	426	SER
1	C	428	GLU
1	C	429	THR
1	C	440	HIS
1	C	456	CYS
1	C	461	MET
1	C	466	ASP
1	C	467	ARG
1	C	474	GLU
1	C	479	PHE
1	C	494	ARG
1	C	507	ASN
1	C	517	ASP
1	C	518	TYR
1	C	525	GLU
1	C	533	LEU
1	C	541	MET
1	C	547	ARG
1	C	556	GLN
1	C	562	LEU
1	C	572	ASN
1	C	581	ARG
1	C	587	THR
1	C	614	GLU
1	C	686	GLU
1	C	702	TRP
1	C	760	LEU
1	C	781	SER
1	C	806	ARG
1	C	843	ASP
1	C	880	LEU
1	C	898	PHE
1	C	900	MET
1	D	2	LYS
1	D	8	VAL
1	D	10	GLN
1	D	32	GLU
1	D	36	SER
1	D	45	GLN
1	D	61	LEU
1	D	104	ASP
1	D	105	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	113	PHE
1	D	121	ASP
1	D	133	ILE
1	D	136	ILE
1	D	147	TYR
1	D	151	LEU
1	D	164	ILE
1	D	173	GLN
1	D	181	GLU
1	D	194	GLU
1	D	213	LEU
1	D	250	VAL
1	D	264	THR
1	D	273	TYR
1	D	290	LEU
1	D	297	GLU
1	D	303	LEU
1	D	305	TYR
1	D	361	PRO
1	D	362	ILE
1	D	370	PHE
1	D	391	TYR
1	D	395	PHE
1	D	401	PRO
1	D	403	ARG
1	D	408	MET
1	D	441	ASP
1	D	452	ASP
1	D	467	ARG
1	D	474	GLU
1	D	479	PHE
1	D	494	ARG
1	D	495	ASN
1	D	504	HIS
1	D	505	ASN
1	D	521	ASP
1	D	525	GLU
1	D	557	ILE
1	D	558	ASN
1	D	562	LEU
1	D	581	ARG
1	D	594	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	599	ARG
1	D	614	GLU
1	D	621	ASP
1	D	630	ASP
1	D	646	HIS
1	D	658	ARG
1	D	667	PHE
1	D	684	ASP
1	D	695	SER
1	D	706	LYS
1	D	710	LEU
1	D	725	LEU
1	D	739	LYS
1	D	766	GLU
1	D	775	ASN
1	D	818	ASN
1	D	826	GLU
1	D	830	VAL
1	D	848	TRP
1	D	861	ASP
1	D	873	GLU
1	D	881	GLU
1	D	894	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	40	HIS
1	A	64	ASN
1	A	98	ASN
1	A	112	ASN
1	A	138	HIS
1	A	153	ASN
1	A	158	ASN
1	A	171	GLN
1	A	193	ASN
1	A	207	GLN
1	A	284	ASN
1	A	285	GLN
1	A	376	GLN
1	A	386	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	389	GLN
1	A	422	GLN
1	A	505	ASN
1	A	556	GLN
1	A	558	ASN
1	A	572	ASN
1	A	602	ASN
1	A	645	ASN
1	A	646	HIS
1	A	678	GLN
1	A	711	ASN
1	A	733	GLN
1	A	786	ASN
1	A	864	HIS
1	B	171	GLN
1	B	173	GLN
1	B	316	ASN
1	B	318	GLN
1	B	324	ASN
1	B	389	GLN
1	B	504	HIS
1	B	505	ASN
1	B	539	ASN
1	B	558	ASN
1	B	645	ASN
1	B	733	GLN
1	B	754	GLN
1	B	823	GLN
1	C	10	GLN
1	C	40	HIS
1	C	131	HIS
1	C	203	ASN
1	C	206	GLN
1	C	207	GLN
1	C	255	ASN
1	C	284	ASN
1	C	285	GLN
1	C	318	GLN
1	C	324	ASN
1	C	402	ASN
1	C	424	ASN
1	C	493	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	507	ASN
1	C	546	GLN
1	C	556	GLN
1	C	558	ASN
1	C	564	ASN
1	C	572	ASN
1	C	675	ASN
1	C	676	ASN
1	C	678	GLN
1	C	679	HIS
1	C	711	ASN
1	C	775	ASN
1	C	787	ASN
1	C	818	ASN
1	C	823	GLN
1	D	10	GLN
1	D	105	HIS
1	D	112	ASN
1	D	206	GLN
1	D	285	GLN
1	D	318	GLN
1	D	333	GLN
1	D	382	GLN
1	D	424	ASN
1	D	444	ASN
1	D	480	ASN
1	D	505	ASN
1	D	546	GLN
1	D	556	GLN
1	D	558	ASN
1	D	595	GLN
1	D	602	ASN
1	D	606	ASN
1	D	675	ASN
1	D	733	GLN
1	D	754	GLN
1	D	761	GLN
1	D	773	GLN
1	D	775	ASN
1	D	812	ASN
1	D	823	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	CTG	I	4	3,2	19,23,24	0.88	1 (5%)	21,35,38	0.64	1 (4%)
2	CTG	G	4	3,2	19,23,24	0.81	0	21,35,38	0.73	1 (4%)
2	CTG	K	4	2	19,23,24	0.83	1 (5%)	21,35,38	0.59	0

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
2	CTG	I	4	3,2	-	0/7/45/46	0/2/2/2
2	CTG	G	4	3,2	-	0/7/45/46	0/2/2/2
2	CTG	K	4	2	-	0/7/45/46	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	CTG	C1'-N1	2.89	1.49	1.45
2	K	4	CTG	C1'-N1	2.36	1.48	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	CTG	N3-C2-N1	-2.57	114.02	116.69
2	G	4	CTG	N3-C2-N1	-2.12	114.50	116.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	4	CTG	2	0
2	G	4	CTG	1	0
2	K	4	CTG	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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
4	DTP	J	2	-	26,32,32	0.75	0	30,50,50	0.87	2 (6%)
4	DTP	B	907	-	26,32,32	0.68	0	30,50,50	1.00	2 (6%)

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
4	DTP	J	2	-	-	3/18/34/34	0/3/3/3
4	DTP	B	907	-	-	5/18/34/34	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	907	DTP	C5-C6-N6	2.46	124.10	120.35
4	B	907	DTP	O2G-PG-O1G	2.22	119.38	110.68
4	J	2	DTP	O2G-PG-O1G	2.18	119.22	110.68
4	J	2	DTP	C5-C6-N6	2.02	123.43	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

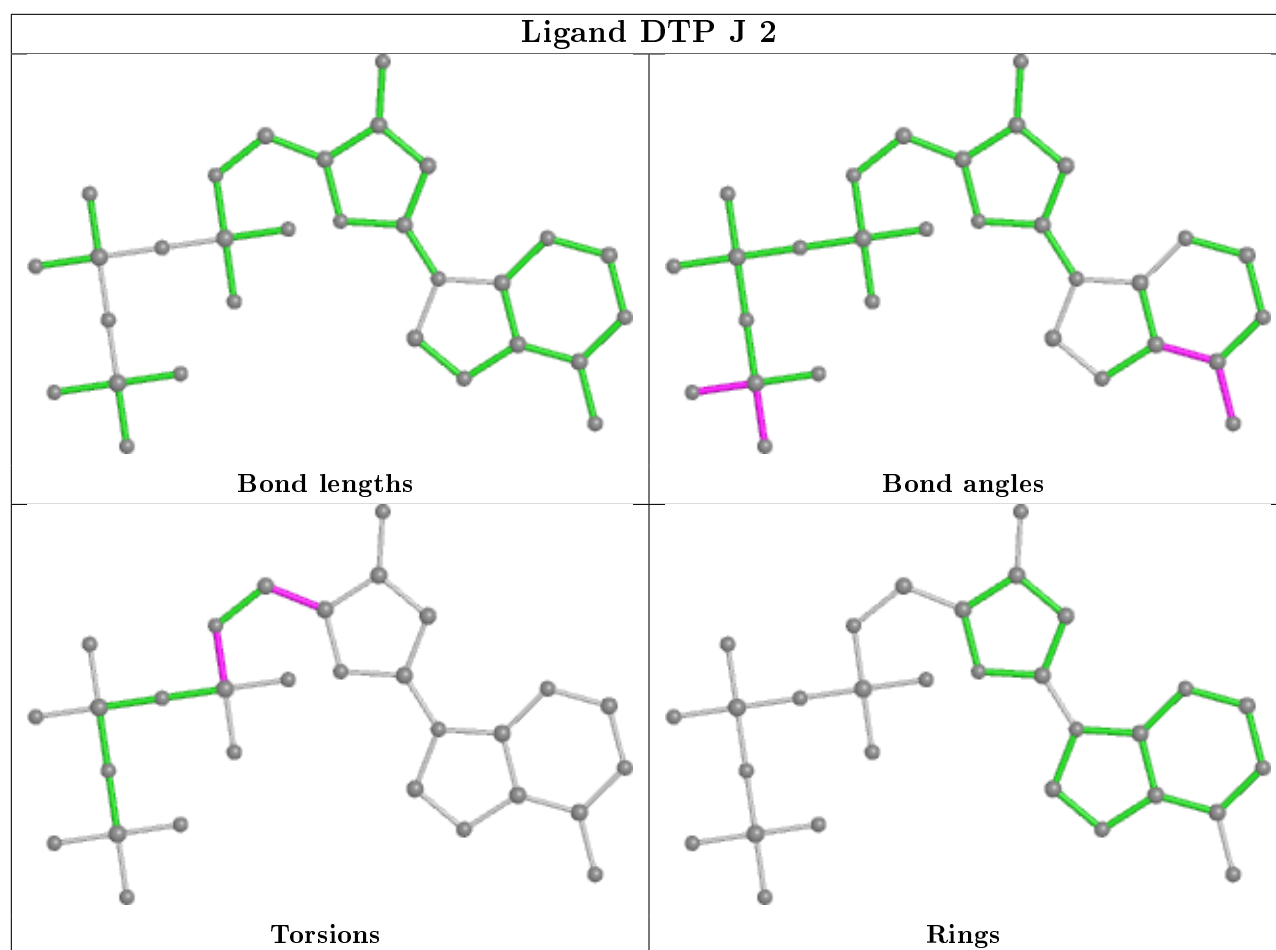
Mol	Chain	Res	Type	Atoms
4	J	2	DTP	C5'-O5'-PA-O3A
4	B	907	DTP	C5'-O5'-PA-O2A
4	B	907	DTP	C5'-O5'-PA-O3A
4	B	907	DTP	PG-O3B-PB-O1B
4	J	2	DTP	C5'-O5'-PA-O1A
4	B	907	DTP	C5'-O5'-PA-O1A
4	B	907	DTP	PG-O3B-PB-O2B
4	J	2	DTP	O4'-C4'-C5'-O5'

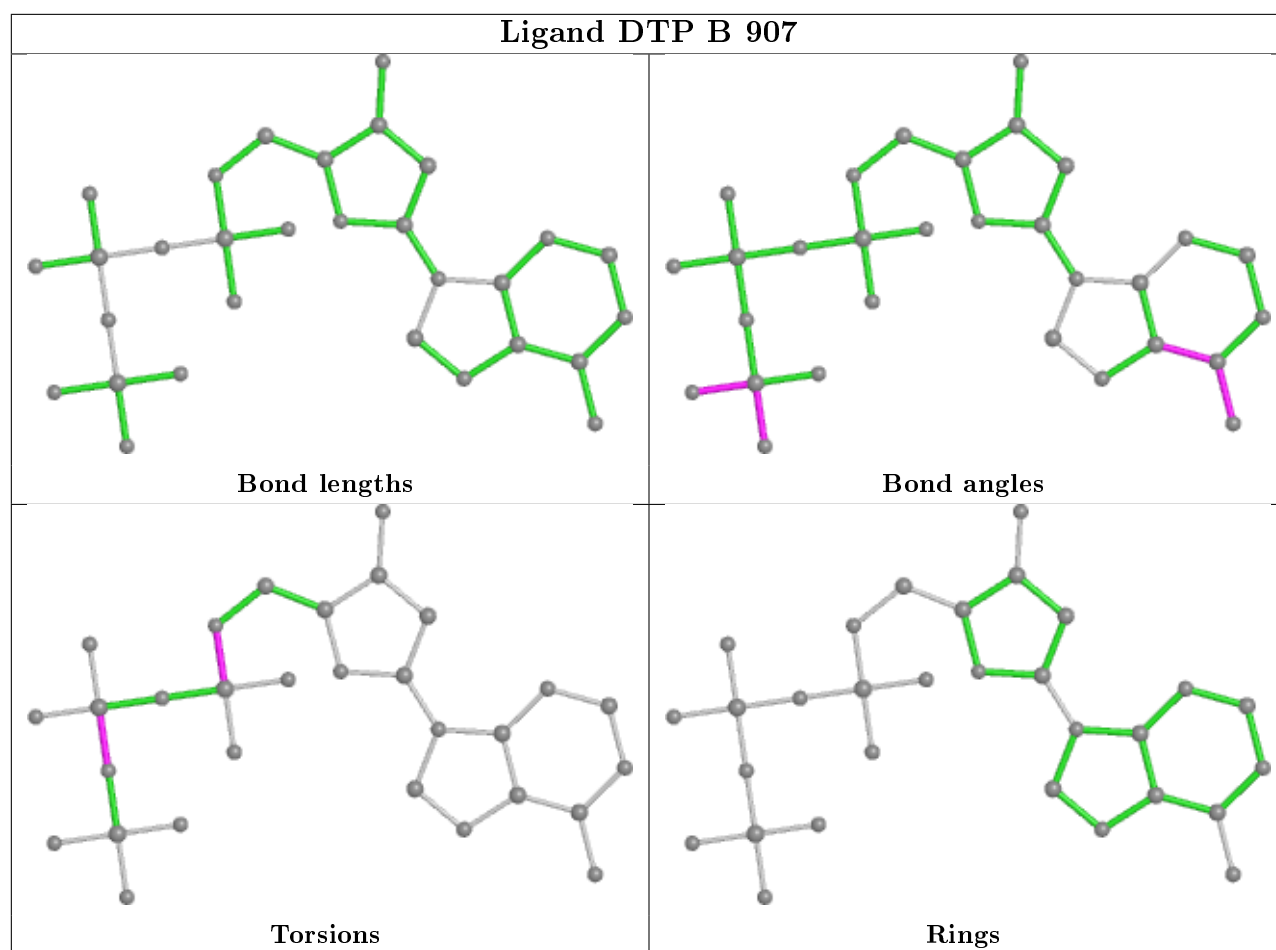
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	2	DTP	2	0
4	B	907	DTP	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 than 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.





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	902/906 (99%)	0.36	51 (5%)	23	13	23, 52, 158, 200	0
1	B	902/906 (99%)	0.36	64 (7%)	16	8	27, 53, 146, 170	0
1	C	901/906 (99%)	0.32	40 (4%)	34	20	21, 55, 145, 173	0
1	D	897/906 (99%)	0.40	43 (4%)	30	18	37, 70, 126, 170	1 (0%)
2	E	13/18 (72%)	0.58	1 (7%)	13	6	69, 110, 130, 135	0
2	G	17/18 (94%)	0.14	0	100	100	52, 72, 106, 106	0
2	I	17/18 (94%)	-0.15	0	100	100	36, 53, 88, 96	0
2	K	17/18 (94%)	0.37	0	100	100	39, 105, 142, 145	0
3	F	13/15 (86%)	0.91	0	100	100	94, 121, 139, 140	0
3	H	15/15 (100%)	0.06	0	100	100	45, 79, 149, 150	0
3	J	15/15 (100%)	-0.27	0	100	100	36, 63, 121, 124	0
3	L	15/15 (100%)	0.14	0	100	100	82, 116, 141, 145	0
All	All	3724/3756 (99%)	0.35	199 (5%)	26	15	21, 57, 140, 200	1 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	535	ALA	10.9
1	D	394	ALA	9.4
1	B	545	ALA	9.2
1	A	498	ILE	8.5
1	B	499	ILE	7.9
1	C	530	ILE	7.8
1	D	393	GLY	7.6
1	D	391	TYR	7.3
1	A	533	LEU	7.2
1	A	504	HIS	7.2
1	B	508	LEU	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	542	LEU	6.7
1	B	502	ALA	6.6
1	C	500	LYS	6.7
1	B	530	ILE	6.6
1	A	508	LEU	6.4
1	C	503	LEU	6.3
1	C	513	PRO	6.2
1	D	498	ILE	6.2
1	A	502	ALA	6.0
1	D	395	PHE	5.9
1	C	508	LEU	5.8
1	B	510	VAL	5.8
1	C	504	HIS	5.7
1	A	516	VAL	5.6
1	D	392	PRO	5.4
1	A	501	GLU	5.4
1	A	517	ASP	5.4
1	A	541	MET	5.3
1	B	507	ASN	5.3
1	B	522	PHE	5.3
1	A	542	LEU	5.2
1	B	503	LEU	5.2
1	A	256	MET	5.1
1	B	509	SER	4.9
1	C	256	MET	4.9
1	B	259	SER	4.9
1	B	504	HIS	4.8
1	A	530	ILE	4.8
1	A	497	GLU	4.8
1	B	253	ILE	4.7
1	B	496	GLY	4.6
1	A	518	TYR	4.6
1	C	257	TYR	4.6
1	C	510	VAL	4.6
1	B	514	LEU	4.5
1	D	510	VAL	4.5
1	A	515	ASP	4.5
1	B	506	PRO	4.4
1	A	509	SER	4.4
1	A	499	ILE	4.4
1	B	255	ASN	4.4
1	A	505	ASN	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	546	GLN	4.3
1	D	390	PRO	4.2
1	B	523	SER	4.1
1	A	785	ALA	4.1
1	B	505	ASN	4.1
1	A	506	PRO	4.1
1	B	537	SER	4.1
1	C	534	SER	4.0
1	A	534	SER	4.0
1	A	793	VAL	4.0
1	B	526	ILE	4.0
1	B	500	LYS	4.0
1	B	793	VAL	3.9
1	C	505	ASN	3.9
1	B	524	ASP	3.8
1	C	522	PHE	3.7
1	A	539	ASN	3.7
1	A	491	ALA	3.7
1	B	252	VAL	3.7
1	B	533	LEU	3.7
1	D	825	VAL	3.7
1	A	537	SER	3.6
1	B	511	ASP	3.6
1	A	532	LYS	3.6
1	D	541	MET	3.6
1	B	501	GLU	3.6
1	B	535	ALA	3.6
1	A	503	LEU	3.6
1	D	625	ILE	3.6
1	A	535	ALA	3.5
1	B	512	GLU	3.5
1	D	184	ASP	3.5
1	C	303	LEU	3.5
1	B	541	MET	3.4
1	D	539	ASN	3.4
1	C	512	GLU	3.4
1	B	490	LEU	3.4
1	A	511	ASP	3.4
1	C	541	MET	3.4
1	C	258	GLY	3.3
1	B	858	ILE	3.3
1	A	507	ASN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	513	PRO	3.3
1	B	497	GLU	3.3
1	D	513	PRO	3.3
1	D	45	GLN	3.3
1	B	256	MET	3.2
1	B	303	LEU	3.2
1	A	522	PHE	3.2
1	B	495	ASN	3.2
1	B	254	GLU	3.2
1	B	527	LYS	3.2
1	C	532	LYS	3.2
1	C	253	ILE	3.1
1	B	521	ASP	3.1
1	C	506	PRO	3.0
1	B	516	VAL	3.0
1	C	252	VAL	3.0
1	C	495	ASN	3.0
1	C	531	LYS	3.0
1	A	514	LEU	2.9
1	D	514	LEU	2.9
1	B	498	ILE	2.9
1	D	173	GLN	2.9
1	B	518	TYR	2.9
1	A	538	LEU	2.9
1	B	821	ALA	2.8
1	D	508	LEU	2.8
1	B	865	TRP	2.8
1	B	493	GLN	2.8
1	D	518	TYR	2.8
1	A	523	SER	2.8
1	D	535	ALA	2.7
1	C	542	LEU	2.7
1	B	536	LYS	2.7
1	D	522	PHE	2.7
1	C	514	LEU	2.7
1	D	157	GLY	2.7
1	C	499	ILE	2.7
1	A	45	GLN	2.6
1	A	510	VAL	2.6
1	D	545	ALA	2.6
1	C	301	GLY	2.6
1	A	900	MET	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	503	LEU	2.6
1	A	255	ASN	2.6
1	A	788	ILE	2.6
1	C	901	PHE	2.6
1	A	253	ILE	2.6
1	C	78	ILE	2.5
1	B	519	ARG	2.5
1	B	862	VAL	2.5
1	D	537	SER	2.5
1	C	543	PHE	2.5
1	B	528	GLU	2.5
1	A	496	GLY	2.5
1	A	500	LYS	2.5
1	B	1	MET	2.5
1	C	255	ASN	2.5
1	B	543	PHE	2.5
1	A	521	ASP	2.4
1	D	527	LYS	2.4
1	B	811	TYR	2.4
1	B	539	ASN	2.4
1	A	495	ASN	2.4
1	D	164	ILE	2.4
1	B	820	ASP	2.4
1	A	257	TYR	2.3
1	C	502	ALA	2.3
2	E	13	DG	2.3
1	A	258	GLY	2.3
1	C	511	ASP	2.3
1	D	523	SER	2.3
1	A	492	ALA	2.3
1	A	531	LYS	2.3
1	D	253	ILE	2.2
1	C	496	GLY	2.2
1	D	400	ILE	2.2
1	C	300	VAL	2.2
1	B	857	LEU	2.2
1	D	205	TRP	2.2
1	C	521	ASP	2.2
1	B	819	ILE	2.2
1	D	248	THR	2.2
1	A	513	PRO	2.2
1	D	162	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	254	GLU	2.2
1	D	891	TYR	2.2
1	D	548	THR	2.1
1	B	540	GLU	2.1
1	A	540	GLU	2.1
1	B	861	ASP	2.1
1	C	60	LYS	2.1
1	C	539	ASN	2.1
1	D	179	PRO	2.1
1	D	489	MET	2.1
1	D	509	SER	2.1
1	C	497	GLU	2.1
1	D	152	LEU	2.1
1	D	876	PHE	2.1
1	D	175	GLY	2.1
1	C	507	ASN	2.1
1	B	799	PRO	2.0
1	B	544	ARG	2.0
1	D	771	PHE	2.0
1	D	497	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CTG	K	4	22/23	0.81	0.24	134,145,148,148	0
2	CTG	I	4	22/23	0.88	0.21	79,88,93,95	0
2	CTG	G	4	22/23	0.94	0.19	71,76,79,80	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

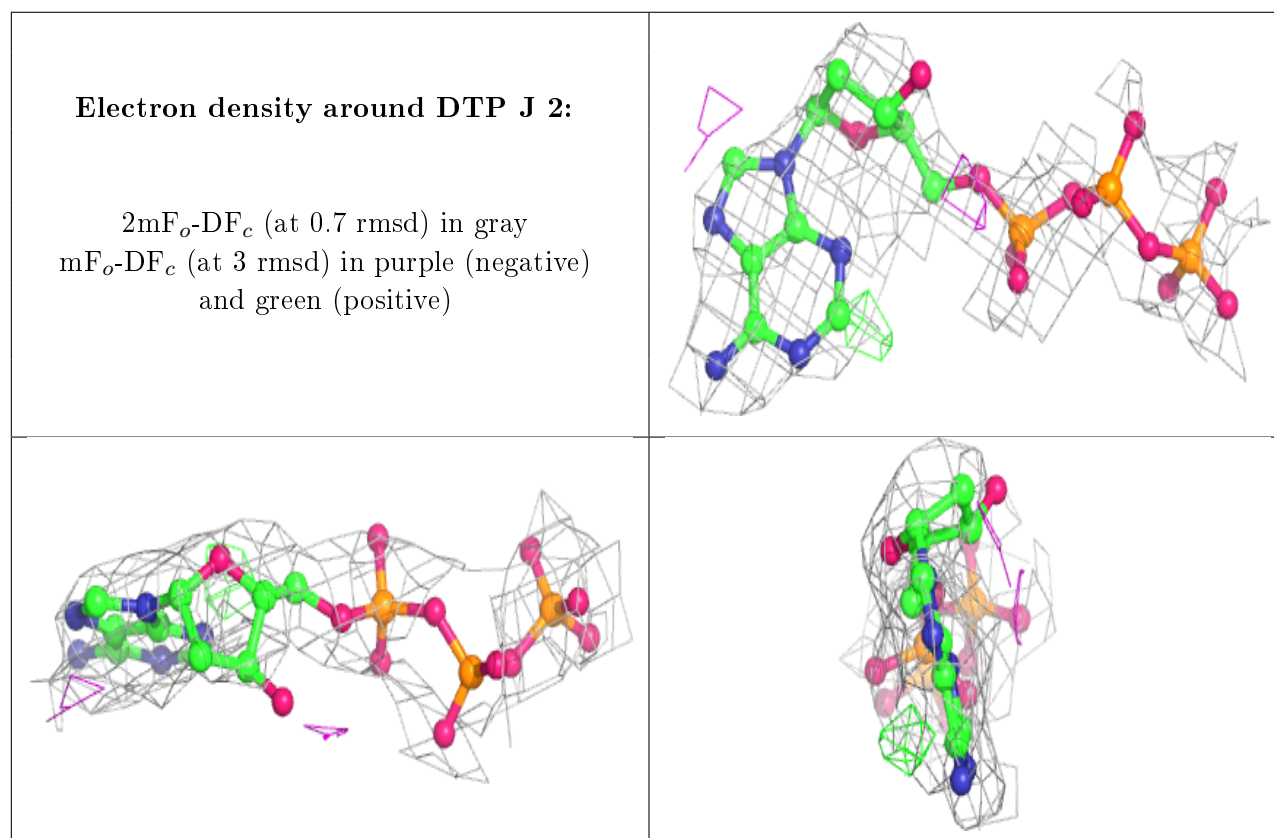
6.4 Ligands [i](#)

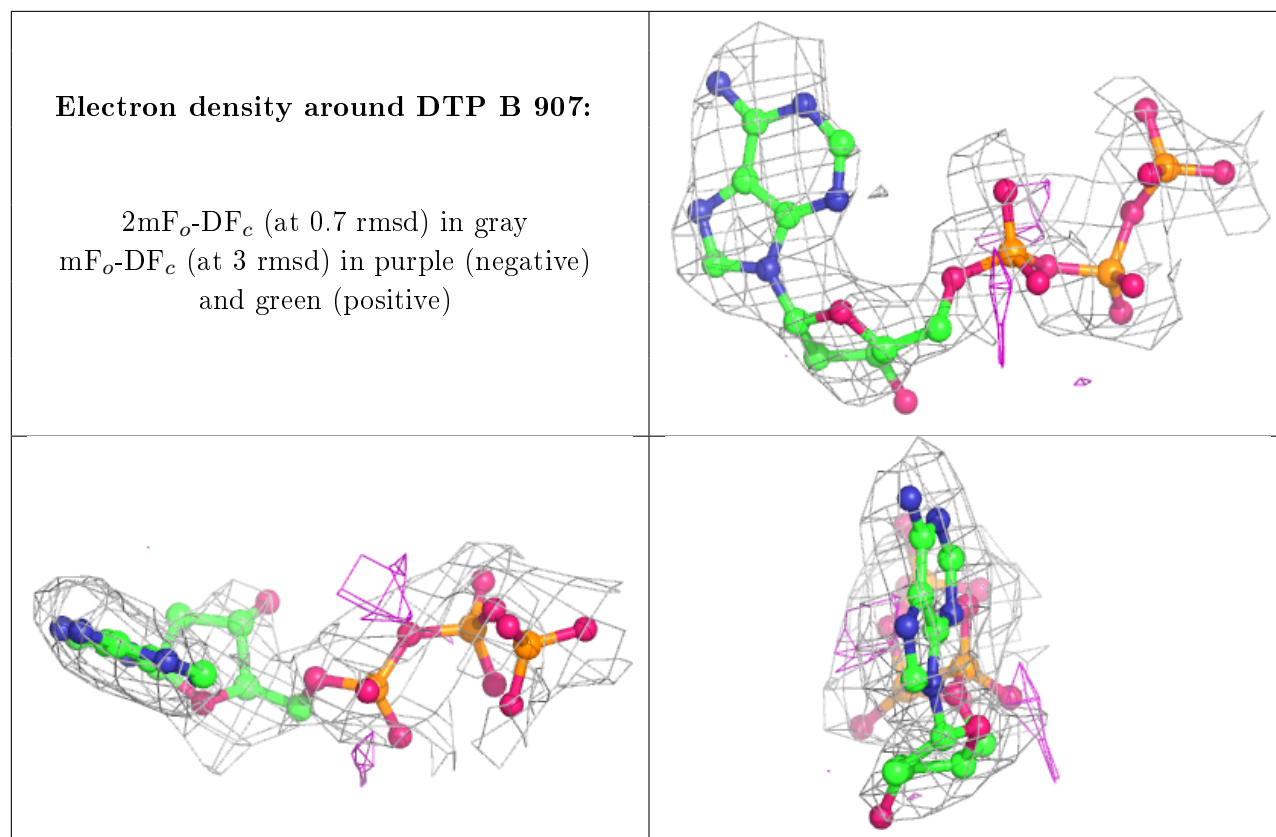
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DTP	J	2	30/30	0.72	0.29	140,147,166,166	0
4	DTP	B	907	30/30	0.75	0.28	133,137,151,151	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.