



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:52 pm BST

PDB ID : 4G7Z
Title : Crystal structure of Thermus thermophilus transcription initiation complex containing 5-BrU at template-strand position +1
Authors : Zhang, Y.; Ebright, R.H.
Deposited on : 2012-07-20
Resolution : 3.81 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
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

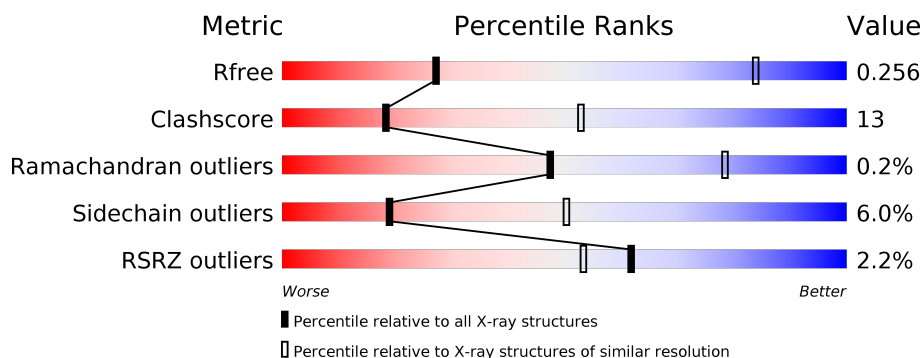
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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	315	<div> <div>42%</div> <div>27%</div> <div>•</div> <div>28%</div> </div>
1	B	315	<div> <div>43%</div> <div>26%</div> <div>•</div> <div>30%</div> </div>
1	K	315	<div> <div>5%</div> <div>55%</div> <div>16%</div> <div>•</div> <div>28%</div> </div>
1	L	315	<div> <div>54%</div> <div>17%</div> <div>•</div> <div>29%</div> </div>
2	C	1119	<div> <div>5%</div> <div>60%</div> <div>36%</div> <div>• •</div> </div>
2	M	1119	<div> <div>5%</div> <div>70%</div> <div>27%</div> <div>• •</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	443	
5	P	443	
6	H	27	
6	R	27	
7	G	21	
7	Q	21	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BRU	Q	15	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 56872 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			
1	K	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	L	225	Total	C	N	O	S	0	0	0
			1773	1133	308	330	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			
2	M	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1482	Total	C	N	O	S	0	0	0
			11704	7421	2059	2189	35			
3	N	1489	Total	C	N	O	S	0	0	0
			11746	7446	2066	2198	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			
5	P	347	Total	C	N	O	S	0	0	0
			2814	1774	510	526	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	EXPRESSION TAG	UNP Q5SKW1
F	-18	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-17	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-16	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-15	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-14	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-13	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-12	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-11	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-10	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-9	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-8	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-7	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-6	LEU	-	EXPRESSION TAG	UNP Q5SKW1
F	-5	VAL	-	EXPRESSION TAG	UNP Q5SKW1
F	-4	PRO	-	EXPRESSION TAG	UNP Q5SKW1
F	-3	ARG	-	EXPRESSION TAG	UNP Q5SKW1
F	-2	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-1	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	0	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-19	MET	-	EXPRESSION TAG	UNP Q5SKW1
P	-18	GLY	-	EXPRESSION TAG	UNP Q5SKW1
P	-17	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-16	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-15	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-14	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-13	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-12	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-11	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-10	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-9	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-8	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-7	GLY	-	EXPRESSION TAG	UNP Q5SKW1
P	-6	LEU	-	EXPRESSION TAG	UNP Q5SKW1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	VAL	-	EXPRESSION TAG	UNP Q5SKW1
P	-4	PRO	-	EXPRESSION TAG	UNP Q5SKW1
P	-3	ARG	-	EXPRESSION TAG	UNP Q5SKW1
P	-2	GLY	-	EXPRESSION TAG	UNP Q5SKW1
P	-1	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	0	HIS	-	EXPRESSION TAG	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*C
P*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			
6	R	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 7 is a DNA chain called 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*G
P*AP*GP*(BRU)P*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	16	Total	Br	C	N	O	P	0	0
			328	1	155	63	94	15		
7	Q	16	Total	Br	C	N	O	P	0	0
			328	1	155	63	94	15		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	N	2	Total	Zn	0	0
			2	2		

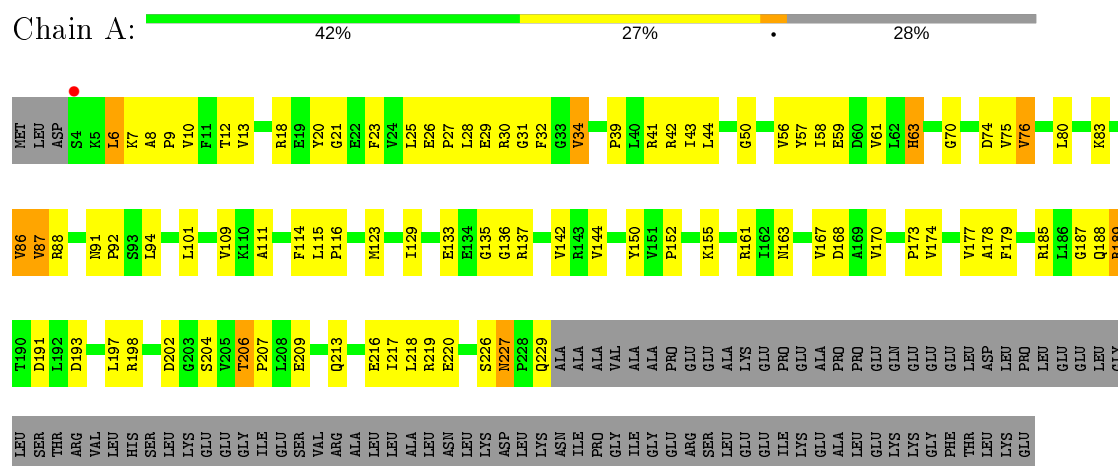
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		
9	N	1	Total	Mg	0	0
			1	1		

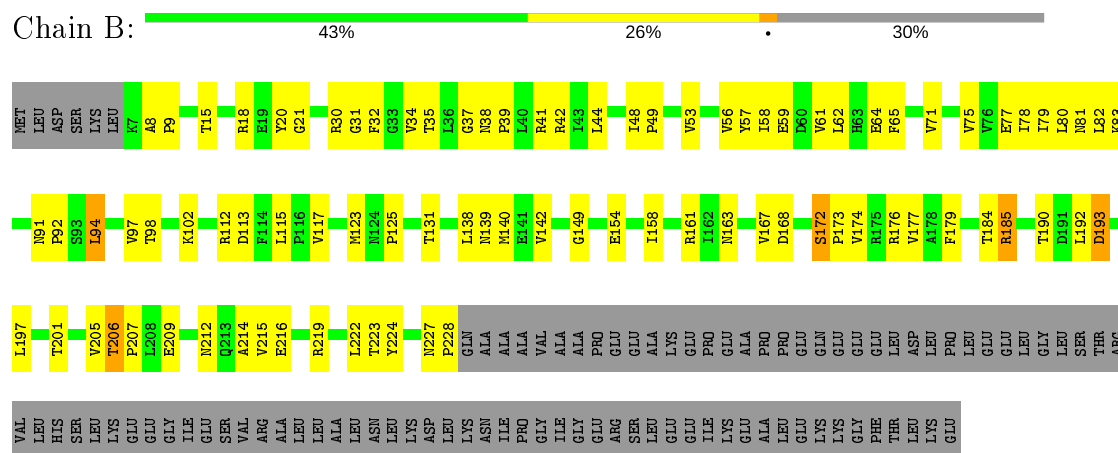
3 Residue-property plots

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.

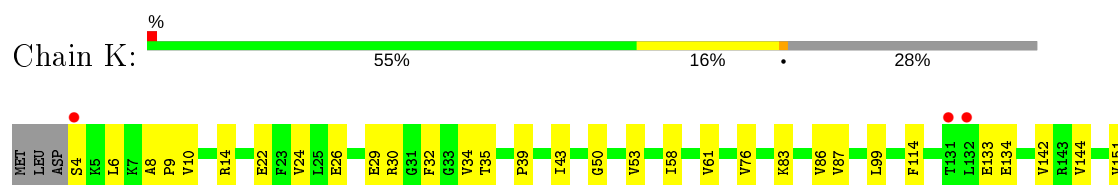
• Molecule 1: DNA-directed RNA polymerase subunit alpha

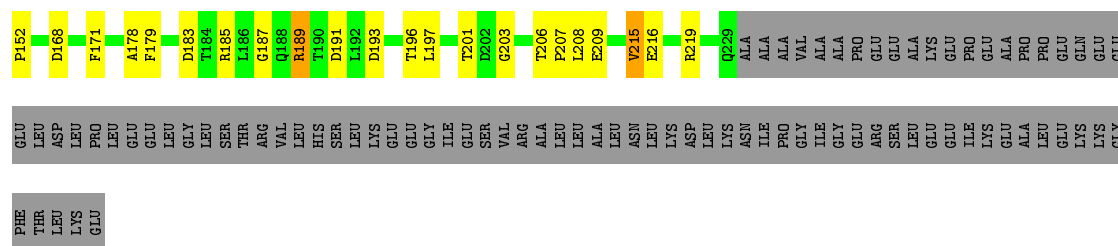


• Molecule 1: DNA-directed RNA polymerase subunit alpha



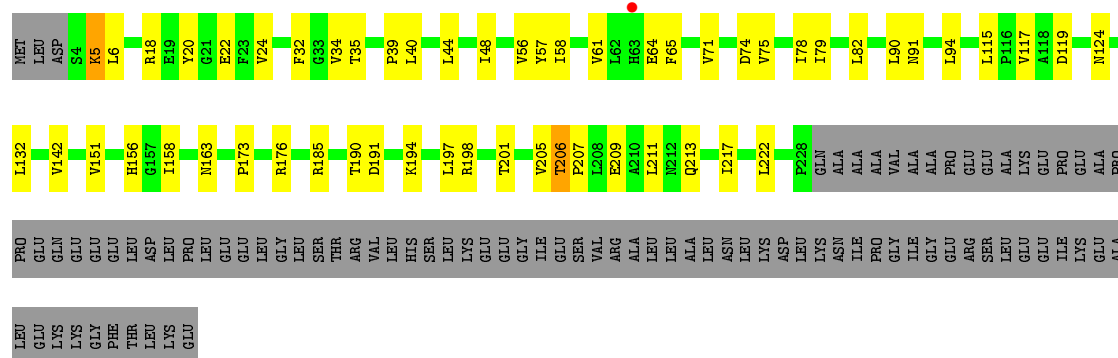
• Molecule 1: DNA-directed RNA polymerase subunit alpha





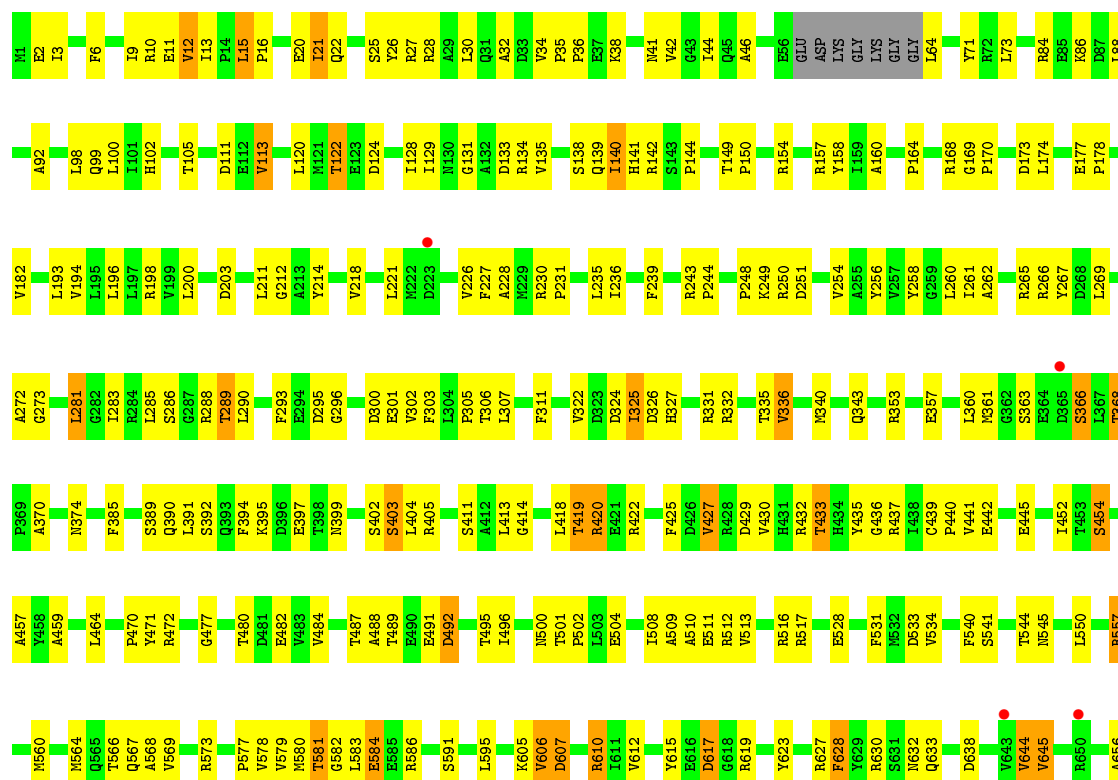
- Molecule 1: DNA-directed RNA polymerase subunit alpha

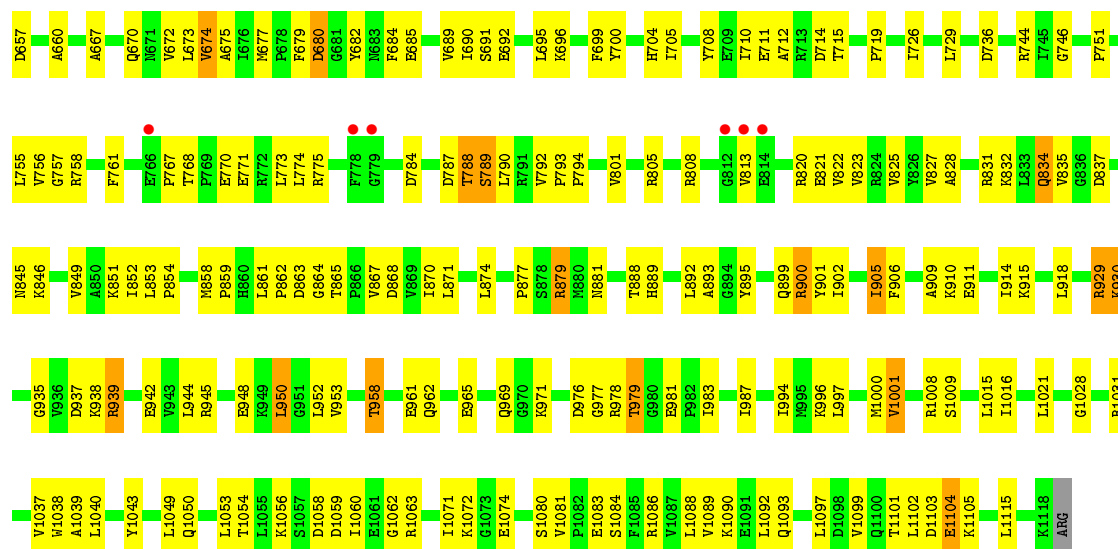
Chain L: 54% 17% 29%



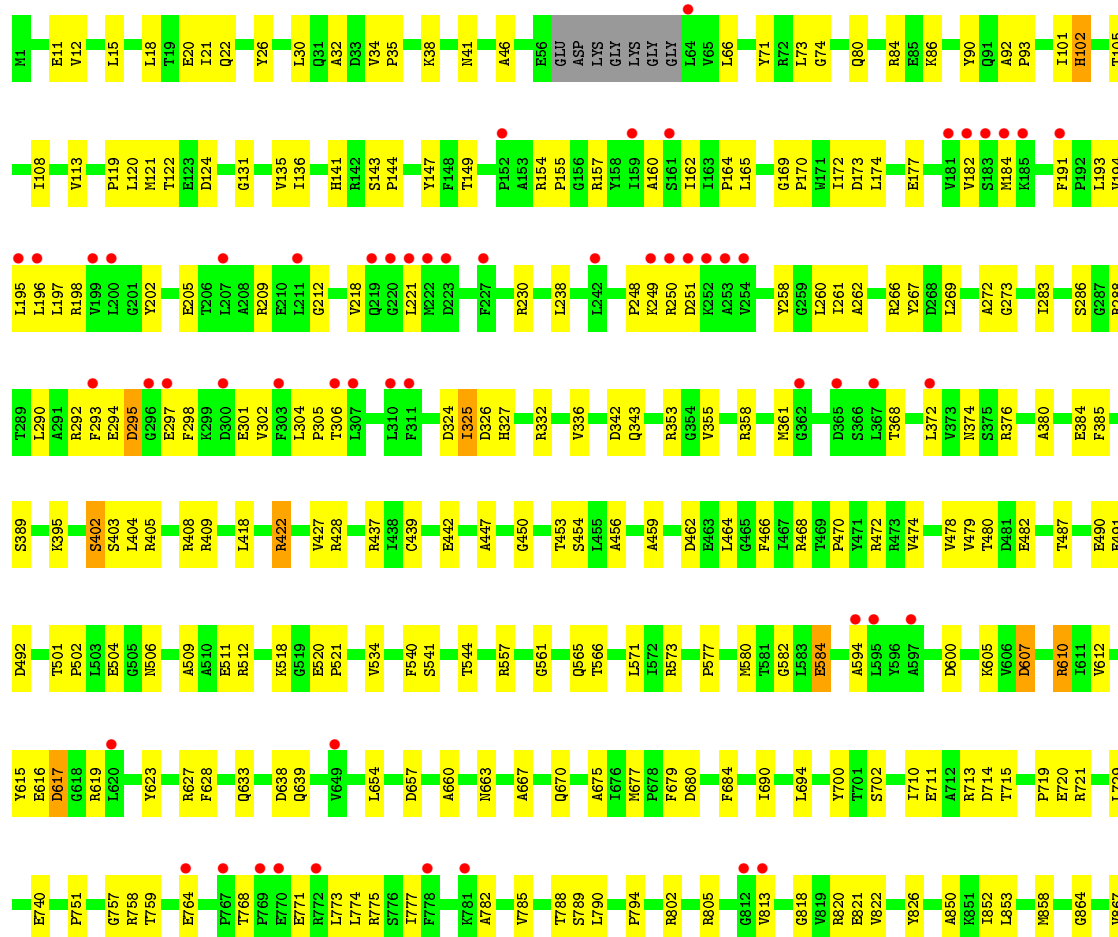
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 60% 36%



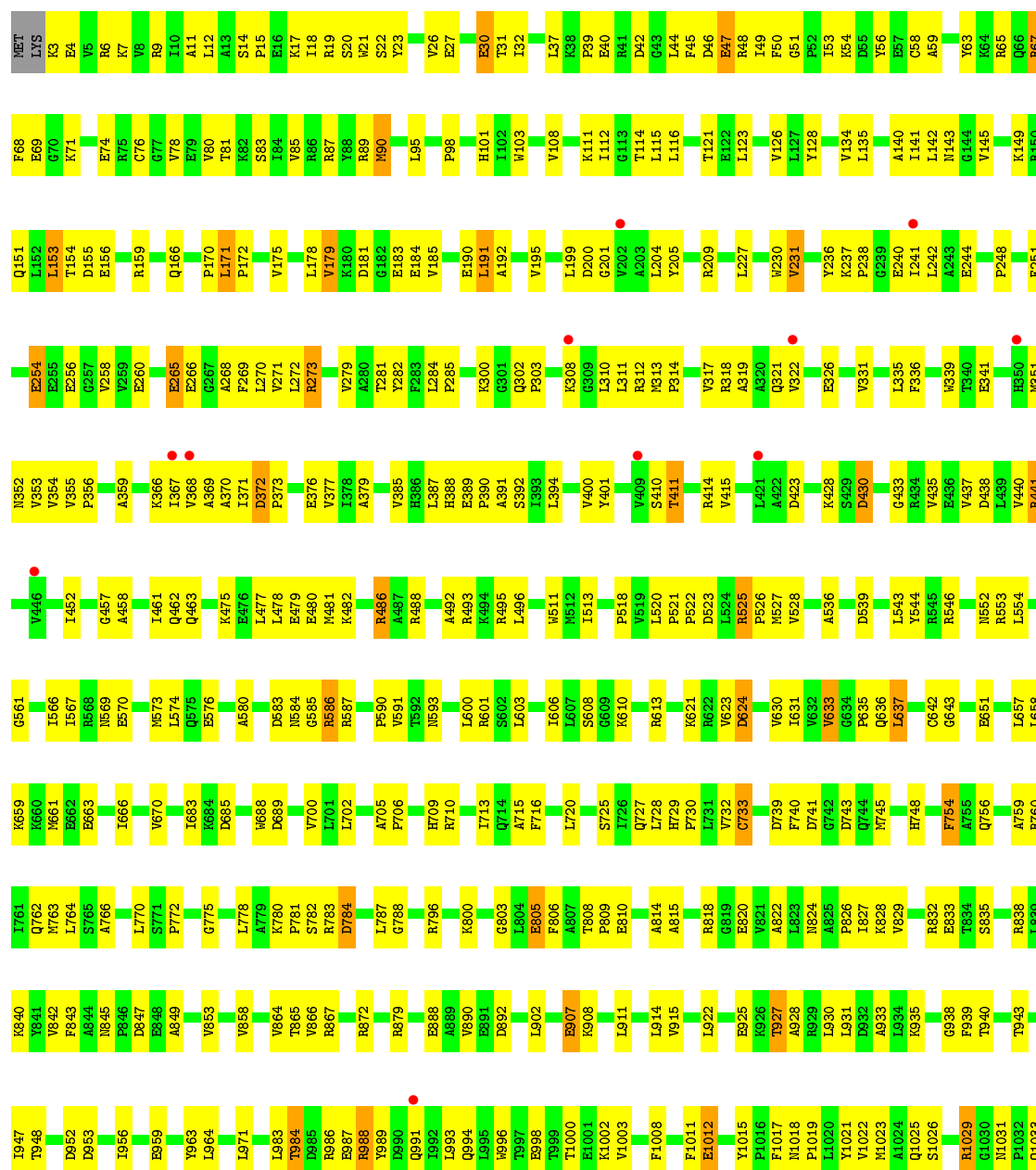


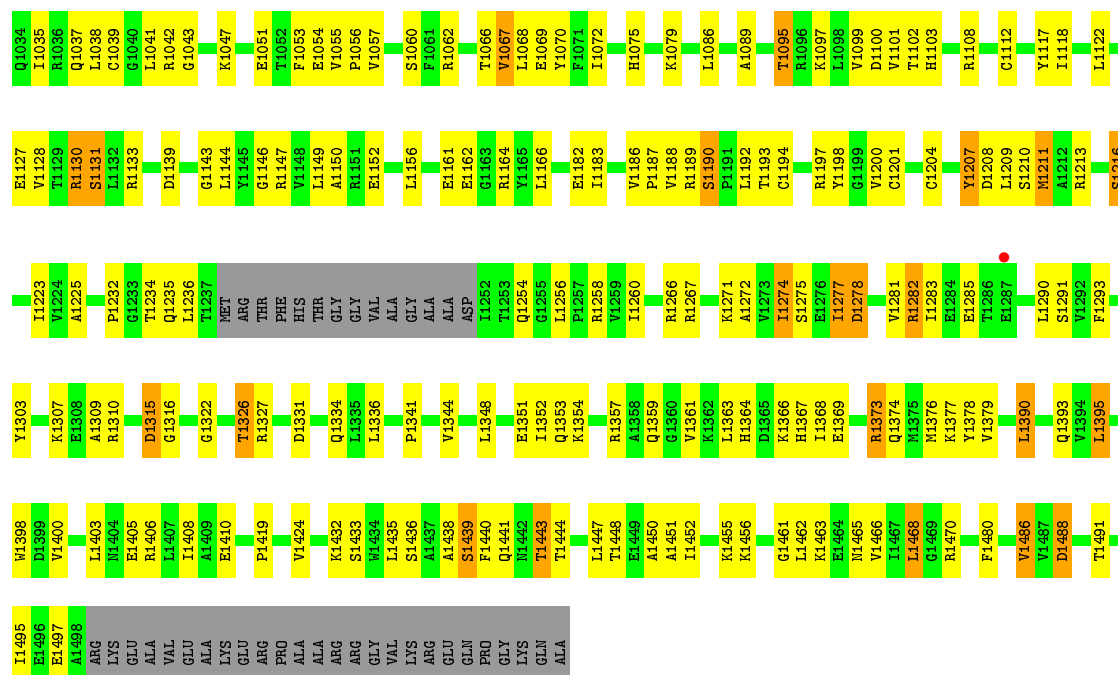
• Molecule 2: DNA-directed RNA polymerase subunit beta



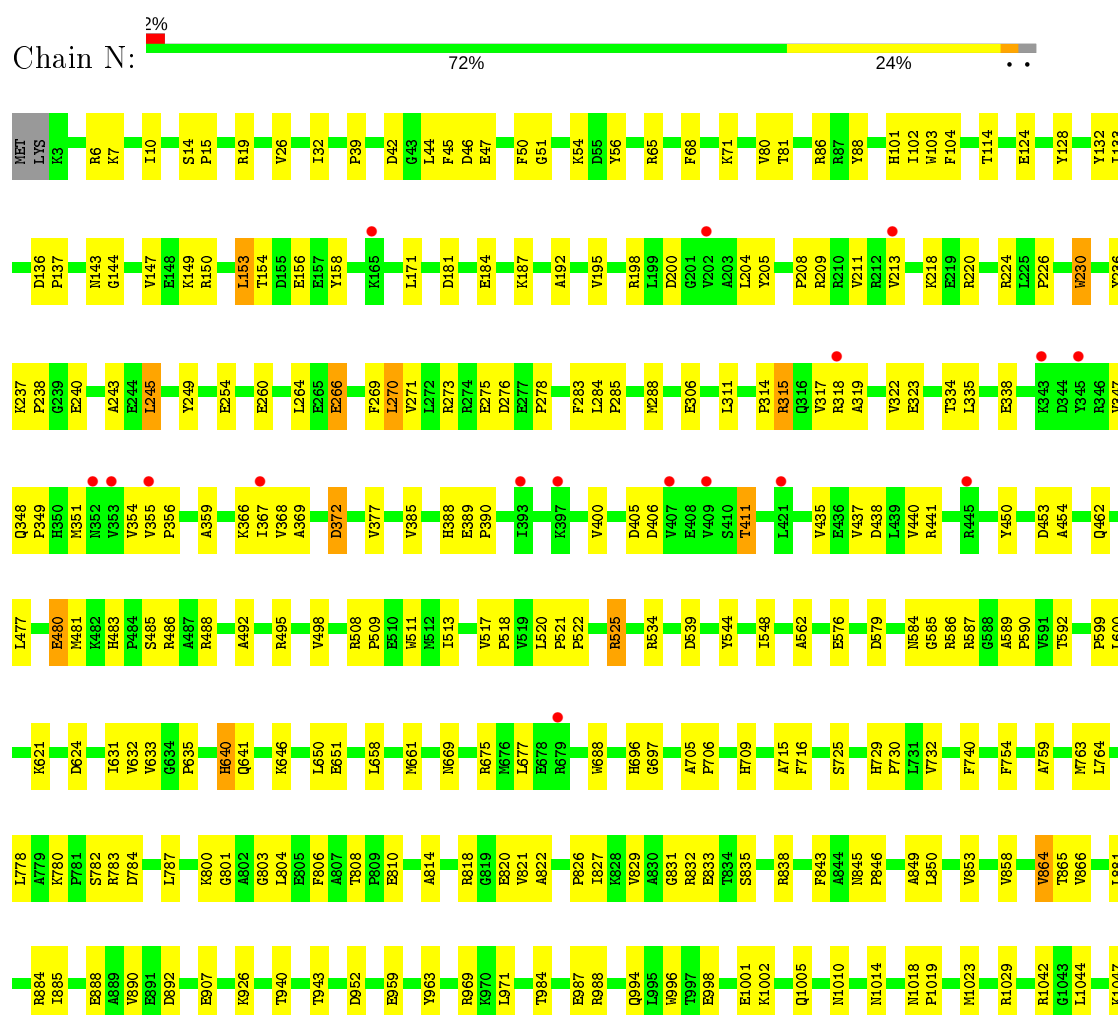


• Molecule 3: DNA-directed RNA polymerase subunit beta'

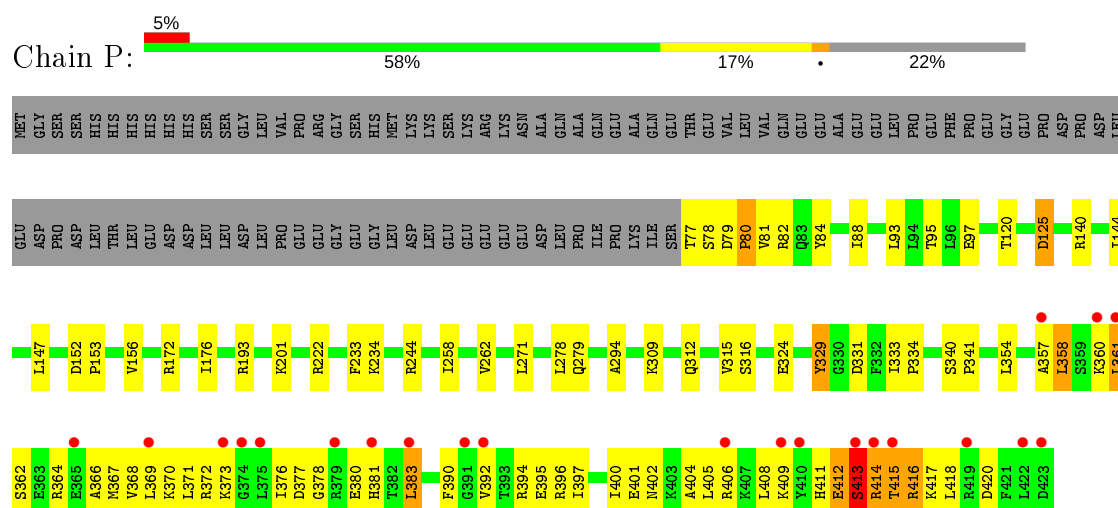




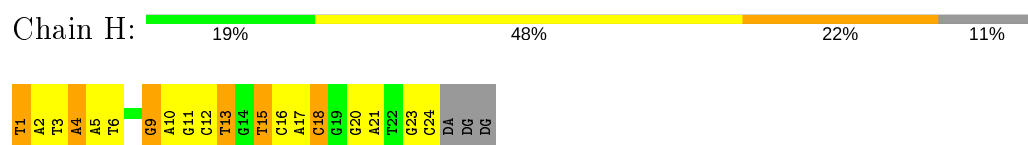
• Molecule 3: DNA-directed RNA polymerase subunit beta'



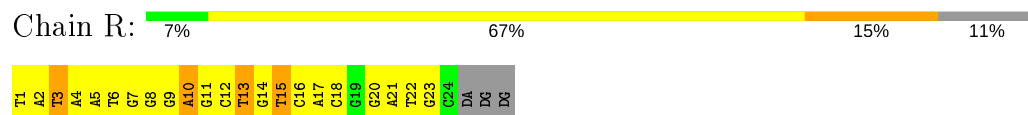
WORLDWIDE
 **PDB**
PROTEIN DATA BANK



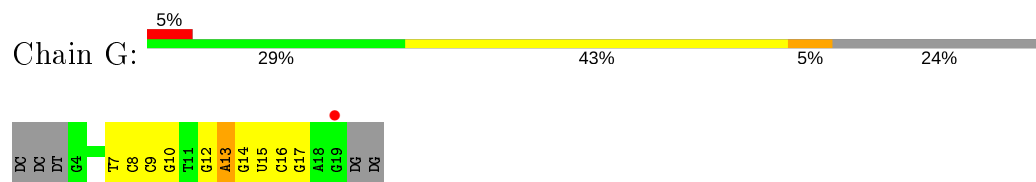
- Molecule 6: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'



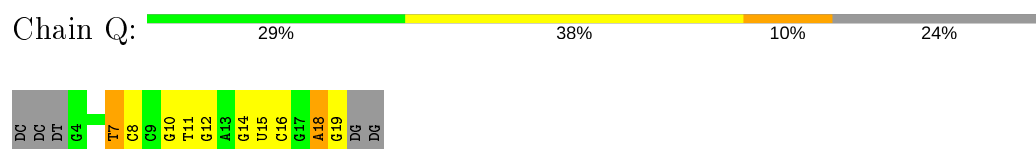
- Molecule 6: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'



- Molecule 7: 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*(BRU)P*CP*GP*AP*GP*GP*G)-3'



- Molecule 7: 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*(BRU)P*CP*GP*AP*GP*GP*G)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	185.47Å 103.59Å 296.51Å 90.00° 98.53° 90.00°	Depositor
Resolution (Å)	49.85 – 3.81 49.85 – 3.81	Depositor EDS
% Data completeness (in resolution range)	51.6 (49.85-3.81) 82.2 (49.85-3.81)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.176 , 0.232 0.192 , 0.256	Depositor DCC
R_{free} test set	1776 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	120.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 99.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	56872	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5249e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.46	0/1814	0.66	0/2466
1	B	0.45	0/1782	0.67	0/2424
1	K	0.26	0/1814	0.45	0/2466
1	L	0.26	0/1805	0.47	0/2454
2	C	0.47	0/8937	0.70	0/12087
2	M	0.26	0/8937	0.48	1/12087 (0.0%)
3	D	0.48	0/11910	0.69	1/16105 (0.0%)
3	N	0.25	0/11952	0.47	0/16162
4	E	0.45	0/775	0.66	0/1045
4	O	0.24	0/775	0.43	0/1045
5	F	0.25	0/2852	0.44	0/3837
5	P	0.26	0/2859	0.45	0/3847
6	H	0.89	0/556	1.73	20/858 (2.3%)
6	R	1.00	2/556 (0.4%)	1.66	15/858 (1.7%)
7	G	0.82	0/345	1.34	4/529 (0.8%)
7	Q	0.79	0/345	1.37	6/529 (1.1%)
All	All	0.39	2/58014 (0.0%)	0.64	47/78799 (0.1%)

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	M	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	5	DA	N9-C4	5.04	1.40	1.37
6	R	12	DC	C1'-N1	5.01	1.55	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	12	DC	O4'-C1'-N1	10.39	115.27	108.00
6	R	17	DA	O4'-C1'-N9	9.91	114.94	108.00
6	H	18	DC	O4'-C4'-C3'	-9.12	100.53	106.00
2	M	422	ARG	NE-CZ-NH2	-8.82	115.89	120.30
6	R	23	DG	O4'-C1'-N9	8.35	113.84	108.00
7	Q	8	DC	O4'-C1'-N1	8.08	113.65	108.00
6	H	23	DG	O4'-C1'-N9	8.06	113.64	108.00
6	H	20	DG	O4'-C1'-N9	7.36	113.15	108.00
6	H	17	DA	O4'-C1'-N9	6.95	112.86	108.00
6	R	12	DC	O4'-C1'-N1	6.82	112.77	108.00
6	H	9	DG	C3'-C2'-C1'	-6.46	94.75	102.50
7	G	13	DA	O4'-C4'-C3'	-6.42	101.93	104.50
6	R	20	DG	C1'-O4'-C4'	-6.35	103.75	110.10
6	R	10	DA	O4'-C1'-N9	6.31	112.41	108.00
6	H	15	DT	O4'-C1'-N1	6.20	112.34	108.00
6	H	12	DC	C4'-C3'-C2'	-6.17	97.55	103.10
6	H	20	DG	C1'-O4'-C4'	-6.16	103.94	110.10
7	G	8	DC	O4'-C1'-N1	6.02	112.22	108.00
6	R	16	DC	O4'-C1'-N1	5.99	112.19	108.00
7	G	10	DG	O4'-C1'-N9	5.95	112.17	108.00
6	R	13	DT	C5-C4-O4	-5.95	120.74	124.90
6	R	15	DT	O4'-C1'-N1	5.93	112.15	108.00
6	R	4	DA	O4'-C1'-N9	5.91	112.14	108.00
7	Q	11	DT	N3-C4-O4	5.82	123.39	119.90
6	H	13	DT	C4-C5-C7	5.81	122.49	119.00
6	R	15	DT	N3-C4-O4	5.80	123.38	119.90
3	D	1468	LEU	CA-CB-CG	5.79	128.62	115.30
6	R	13	DT	O4'-C1'-N1	5.76	112.03	108.00
6	R	1	DT	O4'-C1'-N1	5.72	112.01	108.00
6	H	13	DT	O4'-C1'-N1	5.72	112.01	108.00
7	G	9	DC	O4'-C1'-N1	5.71	112.00	108.00
6	H	1	DT	O4'-C1'-N1	5.67	111.97	108.00
6	H	4	DA	N1-C6-N6	5.63	121.98	118.60
7	Q	18	DA	O4'-C1'-N9	5.31	111.72	108.00
7	Q	7	DT	O4'-C1'-N1	5.30	111.71	108.00
6	H	24	DC	O4'-C1'-N1	5.23	111.66	108.00
6	H	13	DT	C5-C4-O4	-5.19	121.27	124.90
6	R	22	DT	O4'-C1'-N1	5.17	111.62	108.00
6	H	18	DC	P-O5'-C5'	-5.16	112.64	120.90
6	H	9	DG	O4'-C1'-N9	5.16	111.61	108.00
7	Q	12	DG	C8-N9-C4	-5.12	104.35	106.40
6	R	18	DC	O4'-C1'-N1	5.11	111.57	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	20	DG	O4'-C1'-C2'	-5.07	101.84	105.90
7	Q	10	DG	O4'-C1'-N9	5.07	111.55	108.00
6	H	15	DT	N3-C4-O4	5.06	122.93	119.90
6	R	3	DT	C4-C5-C7	5.05	122.03	119.00
6	H	1	DT	N3-C4-O4	5.04	122.93	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	294	GLU	Peptide

5.2 Too-close contacts

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	1782	0	1834	69	0
1	B	1750	0	1797	63	0
1	K	1782	0	1834	32	0
1	L	1773	0	1826	35	0
2	C	8770	0	8874	308	0
2	M	8770	0	8874	214	0
3	D	11704	0	11934	397	0
3	N	11746	0	11974	270	0
4	E	761	0	778	31	0
4	O	761	0	778	18	0
5	F	2807	0	2882	74	0
5	P	2814	0	2889	120	0
6	H	495	0	272	18	0
6	R	495	0	272	15	0
7	G	328	0	178	7	0
7	Q	328	0	178	13	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	D	1	0	0	0	0
9	N	1	0	0	0	0
All	All	56872	0	57174	1519	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 13.

All (1519) 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)
5:P:408:LEU:O	5:P:412:GLU:CB	1.72	1.37
5:P:408:LEU:O	5:P:412:GLU:HB2	1.07	1.23
5:P:408:LEU:HD23	5:P:412:GLU:CG	1.69	1.21
7:Q:14:DG:H2''	7:Q:15:BRU:O5'	1.43	1.15
3:N:1238:MET:SD	3:N:1359:GLN:OE1	2.07	1.12
3:N:1238:MET:O	3:N:1246:VAL:HA	1.50	1.10
3:N:1238:MET:CE	3:N:1238:MET:HA	1.84	1.07
3:D:1194:CYS:HB2	3:D:1204:CYS:SG	2.01	1.01
5:P:415:THR:HG22	5:P:416:ARG:HG2	1.40	1.00
3:N:1238:MET:HA	3:N:1238:MET:HE3	1.44	0.99
5:P:77:THR:CG2	5:P:78:SER:N	2.30	0.95
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.33	0.91
5:P:408:LEU:HD23	5:P:412:GLU:HG3	1.50	0.90
5:P:408:LEU:HA	5:P:412:GLU:HG2	1.50	0.90
5:P:77:THR:CG2	5:P:78:SER:H	1.83	0.90
5:P:415:THR:CG2	5:P:416:ARG:HG2	2.03	0.88
5:P:416:ARG:O	5:P:417:LYS:HG2	1.72	0.88
2:C:757:GLY:HA2	2:C:789:SER:HB3	1.57	0.87
5:P:77:THR:HG22	5:P:78:SER:N	1.87	0.87
5:P:412:GLU:OE1	5:P:412:GLU:HA	1.74	0.86
5:P:77:THR:HG23	5:P:78:SER:H	1.39	0.85
5:P:408:LEU:O	5:P:412:GLU:CG	2.25	0.84
1:L:90:LEU:HB2	1:L:119:ASP:HB3	1.59	0.84
5:P:408:LEU:HD23	5:P:412:GLU:CB	2.07	0.83
2:C:441:VAL:HG21	2:C:544:THR:HG21	1.58	0.83
2:M:764:GLU:HG2	3:N:54:LYS:HE2	1.60	0.83
3:N:592:THR:HB	3:N:600:LEU:HD21	1.59	0.83
3:N:800:LYS:HB3	3:N:822:ALA:HB2	1.60	0.83
5:P:408:LEU:HD23	5:P:412:GLU:HG2	1.60	0.83
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.12	0.83
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.12	0.82
7:Q:14:DG:H2''	7:Q:15:BRU:C5'	2.08	0.82
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.12	0.82
5:P:411:HIS:O	5:P:415:THR:HG21	1.80	0.82
1:B:58:ILE:HB	1:B:61:VAL:HB	1.62	0.81
3:N:520:LEU:O	3:N:525:ARG:NH1	2.13	0.81
5:P:408:LEU:CA	5:P:412:GLU:HG2	2.10	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:628:PHE:H	2:M:638:ASP:HB3	1.47	0.80
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.61	0.79
3:D:984:THR:HB	3:D:987:GLU:H	1.46	0.79
2:C:1050:GLN:O	2:C:1054:THR:OG1	1.99	0.79
5:P:411:HIS:O	5:P:415:THR:CB	2.30	0.79
2:M:266:ARG:NH1	6:R:11:DG:N7	2.31	0.79
1:B:206:THR:HG22	1:B:209:GLU:H	1.47	0.79
3:D:1353:GLN:HE22	3:D:1363:LEU:HB3	1.48	0.78
3:D:520:LEU:O	3:D:525:ARG:NH1	2.17	0.77
5:P:408:LEU:C	5:P:412:GLU:HB2	2.04	0.77
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.65	0.77
3:N:1238:MET:O	3:N:1246:VAL:CA	2.30	0.77
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.64	0.77
2:M:212:GLY:HA2	2:M:218:VAL:HG21	1.67	0.77
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.66	0.76
2:C:573:ARG:O	2:C:670:GLN:NE2	2.17	0.76
3:D:576:GLU:OE2	3:D:587:ARG:NH1	2.17	0.76
5:P:412:GLU:OE1	5:P:412:GLU:CA	2.34	0.76
7:Q:15:BRU:N3	7:Q:16:DC:C5	2.54	0.76
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.52	0.75
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.68	0.75
3:N:39:PRO:HG2	3:N:47:GLU:HG3	1.68	0.75
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.68	0.75
3:D:739:ASP:OD1	3:D:741:ASP:CG	2.24	0.75
1:L:206:THR:HG22	1:L:209:GLU:H	1.50	0.75
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.69	0.74
5:F:386:VAL:HB	5:F:397:ILE:HG12	1.67	0.74
3:D:372:ASP:N	3:D:372:ASP:OD1	2.20	0.74
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.68	0.74
3:N:1404:ASN:HD21	3:N:1415:VAL:H	1.33	0.74
2:M:950:LEU:HB3	2:M:952:LEU:HD13	1.70	0.74
2:C:394:PHE:HE2	2:C:632:ASN:HB3	1.53	0.73
2:C:353:ARG:HH22	6:H:9:DG:H3'	1.54	0.73
5:P:79:ASP:OD2	6:R:8:DG:N1	2.20	0.73
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.71	0.73
2:C:660:ALA:HB1	2:C:667:ALA:O	1.88	0.73
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.70	0.73
5:F:364:ARG:HH11	5:F:400:ILE:HD12	1.52	0.73
2:C:15:LEU:HD21	2:C:457:ALA:HB1	1.68	0.73
3:D:1435:LEU:O	3:D:1439:SER:OG	2.07	0.73
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:21:DA:H61	7:G:7:DT:H3	1.37	0.73
2:C:86:LYS:HD3	2:C:813:VAL:HB	1.70	0.72
2:C:615:TYR:OH	2:C:623:TYR:OH	2.05	0.72
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.71	0.72
1:B:53:VAL:HG11	1:B:82:LEU:HD22	1.71	0.72
3:D:438:ASP:OD1	3:D:441:ARG:NH2	2.23	0.71
3:N:1404:ASN:ND2	3:N:1415:VAL:H	1.86	0.71
2:M:160:ALA:HB3	2:M:174:LEU:HB2	1.71	0.71
3:D:1315:ASP:OD1	3:D:1315:ASP:N	2.23	0.71
3:D:1406:ARG:O	3:D:1410:GLU:HB2	1.90	0.71
2:C:708:TYR:HE1	2:C:827:VAL:HB	1.55	0.71
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.26	0.71
3:N:1395:LEU:HD11	3:N:1400:VAL:HB	1.71	0.71
2:C:1081:VAL:HB	2:C:1086:ARG:HH21	1.56	0.71
3:D:1047:LYS:HB2	3:D:1051:GLU:O	1.90	0.71
3:N:1123:PHE:HB3	3:N:1132:LEU:HD21	1.73	0.71
3:N:411:THR:HB	3:N:437:VAL:H	1.54	0.71
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.73	0.71
5:P:392:VAL:HG21	5:P:397:ILE:HD13	1.73	0.71
1:A:42:ARG:NH2	1:B:31:GLY:O	2.23	0.70
2:C:134:ARG:NH1	2:C:392:SER:O	2.23	0.70
3:D:1152:GLU:HG2	3:D:1161:GLU:HA	1.72	0.70
3:N:1435:LEU:O	3:N:1439:SER:OG	2.09	0.70
3:D:411:THR:HB	3:D:437:VAL:H	1.56	0.70
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.25	0.70
3:N:669:ASN:HD22	5:P:417:LYS:HD2	1.55	0.70
1:K:30:ARG:HD3	1:K:191:ASP:HB2	1.72	0.70
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.74	0.70
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.71	0.70
2:M:615:TYR:HH	2:M:623:TYR:HH	1.22	0.70
5:P:411:HIS:O	5:P:415:THR:CG2	2.39	0.70
3:N:1232:PRO:O	3:N:1235:GLN:HB2	1.91	0.69
3:D:1341:PRO:HB3	3:D:1376:MET:HE1	1.74	0.69
5:P:408:LEU:CD2	5:P:412:GLU:CG	2.62	0.69
7:Q:14:DG:C2'	7:Q:15:BRU:O5'	2.30	0.69
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.25	0.69
1:B:80:LEU:HD23	3:D:867:ARG:HD3	1.75	0.69
6:R:21:DA:H61	7:Q:7:DT:H3	1.38	0.69
1:K:39:PRO:HG3	1:L:39:PRO:HG3	1.75	0.69
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.74	0.69
5:P:408:LEU:O	5:P:412:GLU:CA	2.40	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:714:ASP:OD1	2:M:820:ARG:NH2	2.22	0.68
3:N:372:ASP:N	3:N:372:ASP:OD1	2.25	0.68
2:M:102:HIS:HB3	2:M:105:THR:HB	1.74	0.68
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.75	0.68
3:D:864:VAL:HG12	3:D:865:THR:H	1.58	0.68
3:N:1237:THR:O	3:N:1238:MET:HB2	1.94	0.68
3:D:68:PHE:HB3	3:D:71:LYS:HB3	1.75	0.68
3:D:843:PHE:HB2	3:D:866:VAL:HG22	1.75	0.68
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.76	0.68
2:M:66:LEU:HD22	2:M:372:LEU:HD23	1.75	0.68
3:N:323:GLU:HB2	3:N:334:THR:HB	1.75	0.68
3:N:988:ARG:NH2	3:N:1054:GLU:OE2	2.27	0.68
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.74	0.68
5:P:144:ILE:HB	5:P:147:LEU:HB2	1.75	0.67
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.74	0.67
2:C:950:LEU:HB3	2:C:952:LEU:HD13	1.74	0.67
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.27	0.67
2:C:30:LEU:O	2:C:71:TYR:OH	2.12	0.67
2:M:893:ALA:HB2	2:M:918:LEU:HD23	1.76	0.67
2:C:15:LEU:O	2:C:586:ARG:NH2	2.22	0.67
2:M:521:PRO:HB3	3:N:1068:LEU:HD21	1.76	0.67
1:A:30:ARG:HD3	1:A:191:ASP:HB2	1.74	0.67
1:B:77:GLU:O	1:B:81:ASN:ND2	2.28	0.67
3:D:994:GLN:NE2	3:D:998:GLU:OE2	2.26	0.67
3:N:1238:MET:HG3	3:N:1253:THR:HB	1.77	0.67
3:D:1128:VAL:HG23	3:D:1133:ARG:HD3	1.76	0.66
3:N:1083:ASP:O	3:N:1087:ARG:CG	2.43	0.66
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.77	0.66
5:P:412:GLU:O	5:P:413:SER:C	2.33	0.66
3:D:496:LEU:HD23	3:D:1390:LEU:HD13	1.77	0.66
2:M:395:LYS:HE2	2:M:403:SER:HB2	1.78	0.66
2:C:617:ASP:OD1	2:C:617:ASP:N	2.28	0.66
2:C:266:ARG:NH2	6:H:11:DG:O6	2.28	0.66
5:P:79:ASP:O	5:P:81:VAL:N	2.29	0.66
2:M:577:PRO:HG2	2:M:580:MET:HG2	1.78	0.66
3:N:347:VAL:HG13	3:N:351:MET:HG3	1.77	0.66
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.78	0.66
1:L:56:VAL:HG21	1:L:82:LEU:HD13	1.77	0.66
5:P:367:MET:HB3	5:P:390:PHE:HZ	1.60	0.66
1:A:43:ILE:HD11	1:A:218:LEU:HD13	1.78	0.65
2:C:1104:GLU:HB3	3:D:6:ARG:HG3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:14:DG:C2'	7:Q:15:BRU:H6	2.26	0.65
2:M:511:GLU:HG3	2:M:512:ARG:HG2	1.78	0.65
3:D:835:SER:HB3	3:D:838:ARG:HG3	1.77	0.65
2:M:573:ARG:O	2:M:670:GLN:NE2	2.30	0.65
3:D:155:ASP:OD2	3:D:159:ARG:NH1	2.29	0.65
3:D:553:ARG:HD2	3:D:570:GLU:OE2	1.97	0.65
2:M:802:ARG:HB2	2:M:826:TYR:HB2	1.79	0.65
1:B:185:ARG:HH11	1:B:190:THR:HG23	1.62	0.65
3:N:1233:GLY:O	3:N:1235:GLN:N	2.30	0.65
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.79	0.65
5:P:368:VAL:HG11	5:P:397:ILE:HD11	1.79	0.64
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.30	0.64
1:L:185:ARG:HH11	1:L:190:THR:HG23	1.61	0.64
3:D:285:PRO:HG2	3:D:311:LEU:HD12	1.78	0.64
3:D:1309:ALA:HB1	3:D:1326:THR:HG23	1.80	0.64
3:D:326:GLU:HG2	3:D:331:VAL:HG22	1.79	0.64
2:C:425:PHE:HD1	3:D:1079:LYS:HG3	1.62	0.64
5:P:408:LEU:CD2	5:P:412:GLU:HG3	2.24	0.64
3:D:1290:LEU:HD12	3:D:1307:LYS:HA	1.79	0.64
5:F:367:MET:HB3	5:F:390:PHE:HZ	1.62	0.64
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.79	0.63
1:L:44:LEU:HA	1:L:48:ILE:HD13	1.79	0.63
2:M:164:PRO:HA	2:M:269:LEU:HD12	1.80	0.63
2:M:492:ASP:HB3	2:M:518:LYS:HG2	1.79	0.63
2:C:770:GLU:OE2	5:F:351:SER:OG	2.16	0.63
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.79	0.63
2:C:1054:THR:O	2:C:1059:ASP:HB3	1.99	0.63
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.79	0.63
5:F:144:ILE:HB	5:F:147:LEU:HB2	1.81	0.63
3:N:1310:ARG:HD3	3:N:1327:ARG:HH11	1.64	0.63
2:M:1104:GLU:HB3	3:N:6:ARG:HG3	1.81	0.63
5:P:415:THR:HG22	5:P:416:ARG:N	2.13	0.63
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.81	0.63
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	1.81	0.63
1:B:201:THR:HG21	1:B:205:VAL:O	1.99	0.62
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.33	0.62
2:M:1008:ARG:HH11	2:M:1028:GLY:HA2	1.63	0.62
2:C:937:ASP:OD2	2:C:939:ARG:NH1	2.32	0.62
4:E:59:ASN:HB3	4:E:62:THR:OG1	1.99	0.62
5:P:408:LEU:O	5:P:412:GLU:N	2.31	0.62
6:R:2:DA:H5'	6:R:2:DA:C8	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1103:ASP:HB3	2:C:1105:LYS:H	1.63	0.62
2:C:283:ILE:HD13	2:C:305:PRO:HG2	1.81	0.62
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.64	0.62
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.15	0.62
3:N:835:SER:HB3	3:N:838:ARG:HG3	1.82	0.62
5:P:79:ASP:OD2	5:P:82:ARG:HB2	1.98	0.62
1:L:58:ILE:HB	1:L:61:VAL:HB	1.82	0.62
3:N:266:GLU:OE2	3:N:315:ARG:NH2	2.33	0.62
2:C:168:ARG:NH2	2:C:265:ARG:O	2.29	0.62
3:D:154:THR:HG22	3:D:156:GLU:H	1.64	0.62
3:N:260:GLU:OE1	3:N:273:ARG:NH1	2.33	0.62
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.82	0.62
1:B:212:ASN:HA	1:B:215:VAL:HG22	1.82	0.62
3:D:9:ARG:HG3	3:D:1456:LYS:HG3	1.81	0.62
6:H:15:DT:H2''	6:H:16:DC:H5'	1.81	0.62
3:N:1127:GLU:HG3	3:N:1133:ARG:HB3	1.81	0.62
3:N:438:ASP:OD1	3:N:441:ARG:NH2	2.28	0.62
3:D:590:PRO:HB2	3:D:600:LEU:HD12	1.82	0.61
1:A:58:ILE:HB	1:A:61:VAL:HB	1.82	0.61
2:C:607:ASP:HB3	2:C:610:ARG:H	1.65	0.61
3:D:39:PRO:HB3	3:D:45:PHE:O	2.00	0.61
2:C:404:LEU:HD13	2:C:591:SER:HB2	1.80	0.61
3:D:890:VAL:HG23	3:D:892:ASP:H	1.65	0.61
2:M:258:TYR:HB2	2:M:298:PHE:HZ	1.65	0.61
7:Q:14:DG:C4	7:Q:15:BRU:BR	3.08	0.61
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.82	0.61
3:N:224:ARG:NE	3:N:254:GLU:OE2	2.25	0.61
1:A:135:GLY:O	1:A:137:ARG:HG3	2.01	0.61
3:D:15:PRO:HA	3:D:18:ILE:HD12	1.83	0.61
1:B:59:GLU:OE1	1:B:139:ASN:ND2	2.26	0.61
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.81	0.61
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.81	0.61
2:C:893:ALA:HB2	2:C:918:LEU:HD23	1.82	0.61
3:D:1353:GLN:NE2	3:D:1363:LEU:HB3	2.15	0.61
3:D:1405:GLU:HA	3:D:1408:ILE:HG22	1.82	0.61
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.82	0.60
2:C:394:PHE:CE2	2:C:632:ASN:HB3	2.36	0.60
3:D:1127:GLU:HB3	3:D:1133:ARG:HE	1.65	0.60
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	1.83	0.60
1:A:133:GLU:OE2	2:C:605:LYS:HA	2.01	0.60
5:F:238:TYR:HH	6:H:1:DT:H6	1.50	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLU:HB2	3:D:872:ARG:NH1	2.16	0.60
3:N:832:ARG:HG3	3:N:833:GLU:HG2	1.83	0.60
5:P:364:ARG:O	5:P:368:VAL:HG13	2.01	0.60
3:D:1285:GLU:HA	3:D:1290:LEU:HD23	1.83	0.60
3:N:1083:ASP:OD1	3:N:1087:ARG:NH1	2.35	0.60
3:D:716:PHE:HZ	3:D:732:VAL:HG21	1.67	0.60
3:D:988:ARG:HB3	3:D:988:ARG:HH11	1.65	0.60
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.33	0.60
3:N:808:THR:HG22	3:N:810:GLU:H	1.66	0.60
5:P:415:THR:CG2	5:P:416:ARG:N	2.64	0.60
5:P:409:LYS:HG2	5:P:413:SER:HB2	1.84	0.60
3:D:112:ILE:HB	3:D:123:LEU:HD21	1.84	0.60
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.83	0.60
3:N:1130:ARG:HD3	3:N:1131:SER:H	1.67	0.60
5:P:408:LEU:O	5:P:412:GLU:HG2	2.01	0.60
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.83	0.60
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.84	0.60
1:A:206:THR:HB	1:A:209:GLU:HG3	1.84	0.60
2:C:690:ILE:HB	2:C:852:ILE:HD13	1.84	0.60
3:N:1429:LEU:HG	3:N:1440:PHE:HD1	1.66	0.60
3:N:270:LEU:HD23	3:N:284:LEU:HD11	1.83	0.60
2:C:540:PHE:HE1	2:C:906:PHE:HE2	1.50	0.59
2:M:198:ARG:HH11	2:M:230:ARG:HA	1.67	0.59
2:M:617:ASP:OD1	2:M:617:ASP:N	2.35	0.59
2:C:704:HIS:HD2	2:C:831:ARG:HG3	1.67	0.59
3:D:580:ALA:O	3:D:584:ASN:HB2	2.02	0.59
3:D:268:ALA:HB3	3:D:284:LEU:HB2	1.82	0.59
1:L:71:VAL:HG22	1:L:132:LEU:HG	1.84	0.59
2:M:402:SER:HA	2:M:566:THR:HG23	1.83	0.59
3:N:1100:ASP:OD1	3:N:1463:LYS:NZ	2.28	0.59
3:D:1216:SER:HB3	4:E:16:LYS:H	1.66	0.59
2:M:86:LYS:HD2	2:M:813:VAL:HB	1.84	0.59
2:M:1001:VAL:HG11	3:N:725:SER:HB3	1.83	0.59
1:A:83:LYS:HE2	1:A:168:ASP:HB2	1.84	0.59
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.82	0.59
2:C:691:SER:HA	2:C:858:MET:HE3	1.84	0.59
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.85	0.59
1:A:10:VAL:HG22	1:A:26:GLU:O	2.03	0.59
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.66	0.59
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.68	0.59
2:C:677:MET:HB3	2:C:987:ILE:HD13	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1012:GLU:HB2	3:D:1021:TYR:OH	2.03	0.59
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.83	0.59
3:D:808:THR:HG22	3:D:810:GLU:H	1.67	0.59
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.85	0.59
3:N:994:GLN:NE2	3:N:998:GLU:OE2	2.36	0.59
3:N:1252:ILE:HG23	3:N:1253:THR:HG23	1.84	0.58
2:C:627:ARG:NH1	2:C:638:ASP:OD2	2.36	0.58
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.84	0.58
2:C:711:GLU:O	2:C:758:ARG:NH1	2.36	0.58
2:C:853:LEU:HB2	2:C:858:MET:CE	2.33	0.58
2:C:484:VAL:HG21	2:C:531:PHE:HE2	1.68	0.58
3:D:142:LEU:HG	3:D:143:ASN:H	1.66	0.58
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.85	0.58
3:N:1010:ASN:OD1	3:N:1014:ASN:ND2	2.35	0.58
3:N:1083:ASP:OD1	3:N:1087:ARG:CG	2.51	0.58
1:A:185:ARG:HB2	1:A:189:ARG:O	2.04	0.58
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.84	0.58
3:N:658:LEU:HD23	3:N:661:MET:HE1	1.85	0.58
2:C:758:ARG:HE	2:C:788:THR:HB	1.68	0.58
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.36	0.58
3:N:1189:ARG:HB3	3:N:1204:CYS:HA	1.84	0.58
3:N:1094:LEU:HD22	3:N:1260:ILE:HG12	1.86	0.58
3:N:1290:LEU:HD12	3:N:1307:LYS:HA	1.83	0.58
1:K:83:LYS:HE3	1:K:168:ASP:HB2	1.84	0.58
3:N:14:SER:HB3	3:N:511:TRP:CE2	2.39	0.58
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.85	0.58
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.84	0.58
2:M:660:ALA:HB1	2:M:667:ALA:O	2.04	0.58
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.38	0.57
2:C:582:GLY:HA2	2:C:902:ILE:HD13	1.85	0.57
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.18	0.57
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.04	0.57
3:N:237:LYS:O	3:N:240:GLU:HB3	2.04	0.57
2:C:169:GLY:HA3	2:C:267:TYR:CD1	2.39	0.57
2:C:402:SER:HA	2:C:566:THR:HG23	1.85	0.57
2:C:736:ASP:O	2:C:744:ARG:HG2	2.04	0.57
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.38	0.57
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.86	0.57
2:M:353:ARG:HH22	6:R:9:DG:H3'	1.69	0.57
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.86	0.57
2:M:775:ARG:HD3	2:M:782:ALA:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:404:ALA:O	5:P:408:LEU:HB2	2.03	0.57
5:P:411:HIS:O	5:P:415:THR:HB	2.03	0.57
3:N:273:ARG:HB3	3:N:278:PRO:HA	1.85	0.57
5:P:78:SER:O	5:P:79:ASP:C	2.43	0.57
1:A:70:GLY:HA3	1:A:136:GLY:HA3	1.86	0.57
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.87	0.57
3:N:1083:ASP:OD1	3:N:1087:ARG:CZ	2.53	0.57
3:N:368:VAL:HB	3:N:377:VAL:HB	1.87	0.57
2:C:714:ASP:OD1	2:C:820:ARG:NH2	2.36	0.57
2:M:35:PRO:HG2	2:M:38:LYS:HD3	1.86	0.57
3:N:1143:GLY:O	3:N:1147:ARG:HD2	2.04	0.57
3:D:204:LEU:HD23	3:D:441:ARG:CZ	2.35	0.57
3:D:539:ASP:OD1	5:F:316:SER:OG	2.18	0.57
2:M:162:ILE:HB	2:M:172:ILE:HB	1.86	0.57
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.05	0.57
2:M:751:PRO:HB3	2:M:794:PRO:HA	1.86	0.57
3:N:1258:ARG:NH2	3:N:1351:GLU:HG2	2.13	0.57
2:C:420:ARG:HB2	2:C:420:ARG:NH1	2.19	0.57
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.86	0.57
2:M:437:ARG:NH1	2:M:491:GLU:OE2	2.35	0.57
2:M:911:GLU:OE2	3:N:1062:ARG:NH1	2.38	0.57
4:O:40:LEU:HG	4:O:67:GLU:HG2	1.87	0.57
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.87	0.56
5:F:113:ILE:HD13	5:F:128:ARG:HG3	1.86	0.56
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.38	0.56
1:A:74:ASP:OD1	1:A:76:VAL:HG12	2.05	0.56
2:C:272:ALA:HA	2:C:464:LEU:HD12	1.87	0.56
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	1.87	0.56
3:N:1233:GLY:C	3:N:1235:GLN:H	2.08	0.56
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.35	0.56
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.87	0.56
5:P:414:ARG:HG2	5:P:415:THR:N	2.19	0.56
1:K:133:GLU:HG2	1:K:134:GLU:H	1.70	0.56
2:M:1053:LEU:HA	3:N:621:LYS:HD2	1.87	0.56
2:M:684:PHE:HB3	3:N:633:VAL:HG21	1.86	0.56
7:Q:14:DG:H2'	7:Q:15:BRU:BR	2.61	0.56
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.88	0.56
3:D:1000:THR:HA	3:D:1041:LEU:HD11	1.88	0.56
1:B:32:PHE:HA	1:B:35:THR:HB	1.88	0.56
3:D:141:ILE:HG13	3:D:145:VAL:O	2.06	0.56
2:M:1103:ASP:HB3	2:M:1105:LYS:H	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1101:VAL:HG21	3:N:1424:VAL:HB	1.87	0.56
3:D:1373:ARG:HG3	3:D:1374:GLN:N	2.20	0.56
3:N:562:ALA:O	5:P:140:ARG:NH2	2.33	0.56
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.88	0.56
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.19	0.56
2:M:136:ILE:HB	2:M:336:VAL:HG12	1.86	0.56
3:D:814:ALA:O	3:D:818:ARG:HG3	2.05	0.56
5:F:368:VAL:HG22	5:F:397:ILE:HD11	1.87	0.56
1:K:50:GLY:HA3	1:K:171:PHE:O	2.06	0.56
3:D:242:LEU:HD23	3:D:285:PRO:HG3	1.88	0.55
3:N:56:TYR:HB3	3:N:65:ARG:O	2.05	0.55
2:M:1064:ASN:HA	5:P:341:PRO:HB3	1.88	0.55
2:C:944:LEU:HD22	2:C:962:GLN:HB3	1.88	0.55
2:M:628:PHE:H	2:M:638:ASP:CB	2.19	0.55
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.89	0.55
3:D:759:ALA:HA	3:D:763:MET:HB2	1.88	0.55
1:K:201:THR:HG22	1:K:203:GLY:H	1.70	0.55
2:C:477:GLY:O	2:C:508:ILE:HG12	2.05	0.55
2:C:773:LEU:HD23	5:F:354:LEU:HD13	1.88	0.55
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.88	0.55
2:C:540:PHE:CE1	2:C:906:PHE:HE2	2.24	0.55
3:D:209:ARG:N	3:D:389:GLU:O	2.28	0.55
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.42	0.55
3:D:584:ASN:HD21	3:D:590:PRO:HD2	1.71	0.55
3:D:845:ASN:OD1	3:D:847:ASP:HB2	2.07	0.55
3:N:1198:TYR:OH	3:N:1432:LYS:NZ	2.35	0.55
3:N:1460:ILE:HG13	3:N:1461:GLY:H	1.72	0.55
5:P:79:ASP:OD1	5:P:81:VAL:HB	2.07	0.55
6:R:10:DA:H2"	6:R:11:DG:H5"	1.89	0.55
2:C:953:VAL:HB	2:C:962:GLN:HG2	1.87	0.55
3:D:959:GLU:HB3	3:D:963:TYR:HE1	1.71	0.55
1:B:112:ARG:HG3	1:B:113:ASP:OD1	2.07	0.55
1:K:206:THR:HB	1:K:209:GLU:HG3	1.89	0.55
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.22	0.55
2:C:290:LEU:HD22	2:C:302:VAL:HG11	1.89	0.55
2:M:580:MET:SD	2:M:584:GLU:HG3	2.45	0.55
3:N:45:PHE:HB3	3:N:86:ARG:HH22	1.71	0.55
2:C:399:ASN:ND2	2:C:568:ALA:O	2.37	0.55
2:C:689:VAL:HB	2:C:870:ILE:HD12	1.88	0.55
3:N:1083:ASP:O	3:N:1087:ARG:HG2	2.07	0.55
2:C:1053:LEU:HD11	3:D:1466:VAL:HG13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:169:GLY:HA3	2:C:267:TYR:HD1	1.72	0.54
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.88	0.54
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.71	0.54
2:M:911:GLU:HG3	2:M:912:PRO:HD3	1.90	0.54
2:M:850:ALA:HA	3:N:632:VAL:CG2	2.38	0.54
1:A:219:ARG:HG3	1:A:220:GLU:N	2.22	0.54
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.89	0.54
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.89	0.54
3:D:1021:TYR:O	3:D:1025:GLN:HG2	2.07	0.54
3:D:237:LYS:N	3:D:240:GLU:OE1	2.35	0.54
2:M:690:ILE:HB	2:M:852:ILE:HD13	1.89	0.54
5:P:383:LEU:H	5:P:383:LEU:HD23	1.71	0.54
2:C:25:SER:OG	2:C:335:THR:OG1	2.12	0.54
1:A:178:ALA:HB2	2:C:864:GLY:N	2.23	0.54
3:D:1194:CYS:CB	3:D:1204:CYS:SG	2.80	0.54
3:D:1275:SER:HA	3:D:1303:TYR:HE1	1.71	0.54
2:M:1102:LEU:HB2	3:N:7:LYS:HB2	1.89	0.54
3:N:1233:GLY:C	3:N:1235:GLN:N	2.60	0.54
3:N:1254:GLN:HB3	3:N:1258:ARG:HB2	1.89	0.54
2:C:787:ASP:OD1	2:C:789:SER:OG	2.26	0.54
2:C:889:HIS:O	2:C:892:LEU:HB3	2.07	0.54
3:D:1439:SER:HB2	3:D:1463:LYS:NZ	2.23	0.54
2:M:269:LEU:HB2	2:M:288:ARG:O	2.07	0.54
2:M:853:LEU:HB2	2:M:858:MET:CE	2.37	0.54
3:N:952:ASP:HA	3:N:1062:ARG:HH21	1.72	0.54
3:N:864:VAL:HG12	3:N:865:THR:H	1.71	0.54
7:Q:14:DG:H2'	7:Q:15:BRU:H6	1.89	0.54
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.88	0.54
1:K:206:THR:HG22	1:K:208:LEU:H	1.73	0.54
2:M:1106:ASP:OD1	3:N:7:LYS:NZ	2.24	0.54
2:M:41:ASN:O	2:M:46:ALA:HB2	2.08	0.54
3:N:584:ASN:HD21	3:N:590:PRO:HD2	1.72	0.54
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.07	0.54
2:C:862:PRO:HB3	2:C:929:ARG:HH21	1.73	0.54
3:N:154:THR:HG22	3:N:156:GLU:H	1.72	0.54
2:C:420:ARG:HB2	2:C:420:ARG:CZ	2.38	0.54
3:D:368:VAL:HB	3:D:377:VAL:HB	1.90	0.54
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.90	0.54
3:D:630:VAL:O	3:D:725:SER:HB2	2.07	0.54
3:D:760:ARG:NH2	4:E:3:GLU:OE1	2.26	0.54
4:E:3:GLU:O	4:E:6:ILE:HB	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:843:PHE:HB2	3:N:866:VAL:HG22	1.89	0.54
5:P:401:GLU:O	5:P:405:LEU:HB2	2.08	0.54
1:A:41:ARG:HG3	1:A:177:VAL:HG12	1.90	0.54
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.72	0.54
7:G:12:DG:H2'	7:G:13:DA:C8	2.42	0.54
2:M:1009:SER:HB3	3:N:651:GLU:O	2.06	0.54
3:N:1233:GLY:O	3:N:1236:LEU:N	2.30	0.54
3:N:45:PHE:HD1	3:N:522:PRO:HB3	1.72	0.54
3:N:584:ASN:OD1	3:N:590:PRO:HD2	2.07	0.54
5:P:79:ASP:O	5:P:82:ARG:N	2.40	0.54
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.89	0.53
2:M:144:PRO:HB2	2:M:273:GLY:HA3	1.90	0.53
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.90	0.53
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.91	0.53
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.90	0.53
1:A:70:GLY:N	2:C:607:ASP:OD1	2.36	0.53
3:D:1225:ALA:HA	3:D:1367:HIS:ND1	2.24	0.53
2:C:768:THR:HG21	5:F:347:GLN:NE2	2.23	0.53
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.91	0.53
1:A:18:ARG:O	1:A:207:PRO:HD3	2.09	0.53
2:C:154:ARG:HG3	2:C:177:GLU:OE2	2.09	0.53
3:D:1152:GLU:HG3	3:D:1162:GLU:HG3	1.89	0.53
3:D:1488:ASP:HA	4:E:73:LEU:HD23	1.90	0.53
3:N:1083:ASP:OD2	3:N:1087:ARG:NH1	2.41	0.53
3:N:1277:ILE:HG22	3:N:1278:ASP:H	1.73	0.53
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.24	0.53
3:N:171:LEU:HD22	3:N:390:PRO:HG2	1.91	0.53
3:D:486:ARG:H	3:D:486:ARG:HD2	1.72	0.53
3:D:739:ASP:OD1	3:D:741:ASP:OD1	2.27	0.53
2:M:1090:LYS:HD3	2:M:1112:PHE:CZ	2.43	0.53
2:M:409:ARG:HH22	2:M:442:GLU:HG2	1.74	0.53
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.71	0.53
2:C:230:ARG:HG2	2:C:231:PRO:HD2	1.90	0.53
3:D:815:ALA:O	3:D:820:GLU:HB2	2.08	0.53
3:D:780:LYS:HE3	3:D:908:LYS:HE2	1.90	0.53
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.44	0.53
2:C:437:ARG:NH1	2:C:491:GLU:OE2	2.38	0.53
3:D:236:TYR:H	3:D:319:ALA:HB3	1.74	0.53
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.90	0.53
3:N:103:TRP:CE2	3:N:1444:THR:HG22	2.44	0.53
5:P:369:LEU:HD12	5:P:401:GLU:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:211:LEU:HD23	2:C:218:VAL:HG22	1.90	0.53
6:H:3:DT:H2"	6:H:4:DA:C8	2.44	0.53
2:M:713:ARG:H	2:M:720:GLU:HB2	1.74	0.53
2:C:877:PRO:HG3	3:D:1023:MET:CE	2.39	0.53
3:D:87:ARG:HG2	3:D:523:ASP:HB3	1.90	0.53
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.89	0.53
3:N:260:GLU:HB3	3:N:271:VAL:HB	1.90	0.53
1:A:91:ASN:O	1:A:94:LEU:HB3	2.09	0.52
2:C:198:ARG:NH2	2:C:203:ASP:OD2	2.42	0.52
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.09	0.52
3:N:204:LEU:HD23	3:N:441:ARG:CZ	2.39	0.52
1:A:44:LEU:O	1:A:174:VAL:HG21	2.09	0.52
3:D:1035:ILE:HA	3:D:1038:LEU:HD12	1.91	0.52
3:D:788:GLY:HA3	3:D:938:GLY:O	2.10	0.52
3:N:1127:GLU:HB2	3:N:1133:ARG:HB3	1.91	0.52
1:B:123:MET:O	1:B:125:PRO:HD3	2.09	0.52
2:C:582:GLY:N	2:C:584:GLU:OE2	2.42	0.52
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.44	0.52
2:M:474:VAL:HG22	2:M:479:VAL:HG22	1.91	0.52
2:M:690:ILE:HG23	2:M:694:LEU:HD12	1.89	0.52
1:A:63:HIS:HD2	2:C:746:GLY:HA2	1.74	0.52
3:D:835:SER:H	3:D:838:ARG:HD2	1.74	0.52
2:M:283:ILE:HD13	2:M:305:PRO:HG2	1.92	0.52
1:K:178:ALA:HB2	2:M:864:GLY:N	2.25	0.52
3:D:1089:ALA:O	7:G:14:DG:H5"	2.08	0.52
1:L:205:VAL:HG12	1:L:206:THR:H	1.75	0.52
2:M:84:ARG:HA	2:M:131:GLY:HA2	1.90	0.52
2:M:15:LEU:HD23	2:M:18:LEU:HD21	1.91	0.52
5:P:396:ARG:NH2	5:P:400:ILE:HD12	2.24	0.52
2:C:128:ILE:O	2:C:129:ILE:HD13	2.10	0.52
3:D:1047:LYS:HG2	3:D:1053:PHE:CE1	2.45	0.52
3:D:1149:LEU:HD21	3:D:1166:LEU:HD21	1.92	0.52
5:P:79:ASP:CG	5:P:79:ASP:O	2.47	0.52
2:C:331:ARG:NH2	2:C:427:VAL:HG12	2.25	0.52
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.92	0.52
3:D:254:GLU:O	3:D:300:LYS:HG3	2.09	0.52
3:D:803:GLY:HA2	3:D:826:PRO:O	2.10	0.52
3:N:759:ALA:HA	3:N:763:MET:HB2	1.92	0.52
5:P:394:ARG:HG2	5:P:395:GLU:HG2	1.90	0.52
5:P:414:ARG:O	5:P:415:THR:C	2.48	0.52
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:502:PRO:HG2	2:C:510:ALA:HB2	1.92	0.52
3:D:1395:LEU:HD11	3:D:1400:VAL:HB	1.90	0.52
3:D:231:VAL:O	3:D:236:TYR:OH	2.26	0.52
3:D:689:ASP:HB3	4:E:51:LEU:HD11	1.91	0.52
5:F:397:ILE:HA	5:F:400:ILE:HG12	1.92	0.52
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.44	0.52
3:D:879:ARG:O	3:D:902:LEU:HD11	2.09	0.52
2:M:879:ARG:HD2	2:M:879:ARG:N	2.24	0.52
3:N:576:GLU:OE2	3:N:587:ARG:NH1	2.43	0.52
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.91	0.51
3:D:236:TYR:HB3	3:D:313:MET:HG3	1.91	0.51
3:D:42:ASP:OD1	3:D:48:ARG:NH2	2.43	0.51
1:B:83:LYS:NZ	3:D:842:VAL:O	2.43	0.51
5:F:95:THR:HG22	5:F:96:LEU:H	1.75	0.51
1:K:215:VAL:HG12	1:L:222:LEU:HD22	1.91	0.51
3:N:137:PRO:HB3	3:N:147:VAL:HG12	1.90	0.51
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.92	0.51
2:C:214:TYR:O	2:C:218:VAL:HG23	2.10	0.51
2:C:437:ARG:CZ	2:C:488:ALA:HA	2.39	0.51
2:C:874:LEU:HD22	3:D:1029:ARG:HB2	1.92	0.51
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.10	0.51
2:C:262:ALA:HA	2:C:289:THR:CG2	2.41	0.51
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.75	0.51
2:M:32:ALA:HB2	2:M:73:LEU:HD12	1.91	0.51
3:N:539:ASP:OD1	5:P:316:SER:OG	2.27	0.51
5:P:125:ASP:OD1	5:P:125:ASP:N	2.27	0.51
2:C:1060:ILE:HD11	2:C:1083:GLU:HG2	1.93	0.51
3:D:1117:TYR:HA	3:D:1193:THR:HG21	1.93	0.51
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.30	0.51
1:L:124:ASN:OD1	1:L:124:ASN:N	2.43	0.51
3:N:132:TYR:HB2	3:N:153:LEU:HD12	1.91	0.51
3:N:534:ARG:HH12	5:P:312:GLN:HB3	1.76	0.51
3:D:1103:HIS:HA	3:D:1223:ILE:HD11	1.93	0.51
5:F:218:GLN:O	5:F:222:ARG:HG2	2.10	0.51
3:N:314:PRO:HG2	3:N:317:VAL:CG1	2.40	0.51
2:C:198:ARG:NH2	2:C:228:ALA:O	2.44	0.51
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.30	0.51
3:D:27:GLU:O	3:D:552:ASN:ND2	2.43	0.51
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.92	0.51
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.26	0.51
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:181:ASP:HB2	3:N:205:TYR:CD1	2.45	0.51
3:N:355:VAL:HG11	3:N:385:VAL:HG21	1.93	0.51
3:N:483:HIS:CD2	3:N:485:SER:H	2.29	0.51
5:P:360:LYS:NZ	5:P:416:ARG:HD3	2.25	0.51
2:C:942:GLU:OE2	2:C:945:ARG:NH2	2.37	0.51
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.93	0.51
4:O:32:ARG:O	4:O:95:VAL:HG21	2.10	0.51
2:M:376:ARG:NH2	5:P:279:GLN:OE1	2.43	0.51
2:C:389:SER:OG	2:C:390:GLN:N	2.43	0.51
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.92	0.51
1:A:61:VAL:HG21	1:A:75:VAL:HG21	1.93	0.51
1:L:213:GLN:O	1:L:217:ILE:HG13	2.11	0.51
2:M:355:VAL:HG13	2:M:372:LEU:HG	1.92	0.51
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.25	0.51
4:O:95:VAL:O	4:O:95:VAL:HG12	2.11	0.51
3:D:134:VAL:HG22	3:D:151:GLN:O	2.11	0.51
3:D:475:LYS:HA	3:D:478:LEU:HD12	1.92	0.51
3:D:543:LEU:O	3:D:546:ARG:HG2	2.11	0.51
3:D:683:ILE:HG21	3:D:688:TRP:CZ2	2.46	0.51
2:C:256:TYR:HE1	6:H:10:DA:H61	1.57	0.51
2:M:326:ASP:OD1	6:R:14:DG:N2	2.34	0.51
2:M:487:THR:HG23	2:M:490:GLU:H	1.75	0.51
2:M:677:MET:HB3	2:M:987:ILE:HD13	1.93	0.51
3:D:569:ASN:O	3:D:573:MET:HG3	2.11	0.50
2:M:768:THR:HB	2:M:771:GLU:HB2	1.92	0.50
3:N:1083:ASP:O	3:N:1087:ARG:HG3	2.11	0.50
1:B:80:LEU:HB3	3:D:867:ARG:NH2	2.27	0.50
3:D:256:GLU:OE2	3:D:300:LYS:HE3	2.12	0.50
2:M:1094:ALA:HA	3:N:518:PRO:HB2	1.92	0.50
1:A:193:ASP:HB3	2:C:938:LYS:HD2	1.92	0.50
2:C:139:GLN:HB2	2:C:391:LEU:HD11	1.92	0.50
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.32	0.50
4:E:17:TYR:O	4:E:21:VAL:HG23	2.11	0.50
2:M:358:ARG:HH12	2:M:374:ASN:HB2	1.75	0.50
2:M:1090:LYS:HE2	3:N:88:TYR:O	2.12	0.50
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.46	0.50
3:D:702:LEU:O	3:D:713:ILE:HA	2.12	0.50
2:M:561:GLY:O	2:M:565:GLN:HG3	2.11	0.50
5:P:416:ARG:C	5:P:417:LYS:HG2	2.32	0.50
1:B:48:ILE:HD11	1:B:214:ALA:HB2	1.92	0.50
3:D:1156:LEU:HD23	3:D:1182:GLU:OE2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:322:VAL:HG22	3:D:335:LEU:HD11	1.94	0.50
1:K:43:ILE:HG12	1:L:32:PHE:CZ	2.47	0.50
1:L:91:ASN:HB3	1:L:94:LEU:HB2	1.94	0.50
2:M:267:TYR:CE2	2:M:290:LEU:HG	2.45	0.50
2:C:1059:ASP:OD1	2:C:1080:SER:OG	2.25	0.50
2:C:236:ILE:HG23	2:C:248:PRO:HB3	1.94	0.50
2:C:244:PRO:HD2	5:F:82:ARG:NH1	2.26	0.50
2:C:290:LEU:HB3	2:C:303:PHE:HE1	1.77	0.50
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.93	0.50
3:D:56:TYR:HB3	3:D:65:ARG:O	2.11	0.50
4:E:19:LEU:O	4:E:23:VAL:HG23	2.12	0.50
4:E:46:PRO:HB2	4:E:57:ASP:HB3	1.93	0.50
1:K:58:ILE:HB	1:K:61:VAL:HB	1.92	0.50
3:N:275:GLU:HG2	3:N:276:ASP:H	1.76	0.50
3:N:814:ALA:O	3:N:818:ARG:HG3	2.10	0.50
4:O:88:GLU:OE2	4:O:91:ARG:NH1	2.37	0.50
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.94	0.50
3:D:808:THR:HG22	3:D:810:GLU:N	2.27	0.50
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.45	0.50
6:H:10:DA:H2"	6:H:11:DG:O4'	2.12	0.50
2:M:910:LYS:HB3	2:M:912:PRO:HD2	1.93	0.50
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.94	0.50
5:F:364:ARG:O	5:F:368:VAL:HG23	2.11	0.50
1:K:4:SER:HA	1:K:189:ARG:HH12	1.77	0.50
1:L:5:LYS:HE3	1:L:6:LEU:H	1.77	0.50
3:N:1238:MET:O	3:N:1246:VAL:O	2.29	0.50
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.93	0.50
2:C:430:VAL:HG12	3:D:1075:HIS:CE1	2.47	0.50
2:C:644:VAL:HG22	2:C:645:VAL:H	1.76	0.50
3:D:890:VAL:HB	3:D:922:LEU:HD22	1.93	0.50
2:M:1051:GLU:HB3	2:M:1056:LYS:HE3	1.93	0.50
2:C:808:ARG:NH1	5:F:305:GLU:OE2	2.43	0.49
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.92	0.49
2:C:987:ILE:HA	3:D:948:THR:HG21	1.94	0.49
2:M:874:LEU:HD13	3:N:783:ARG:HB3	1.94	0.49
3:D:1236:LEU:HB2	3:D:1256:LEU:HB2	1.94	0.49
3:D:477:LEU:O	3:D:481:MET:HG2	2.12	0.49
3:D:142:LEU:HG	3:D:143:ASN:N	2.27	0.49
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.13	0.49
5:F:88:ILE:HD11	5:F:192:LEU:HD13	1.93	0.49
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.94	0.49
3:D:339:TRP:CZ3	3:D:341:GLU:HB2	2.46	0.49
3:N:801:GLY:O	3:N:804:LEU:HG	2.12	0.49
5:P:79:ASP:O	5:P:79:ASP:OD1	2.30	0.49
3:D:15:PRO:O	3:D:19:ARG:HG3	2.13	0.49
3:D:705:ALA:HA	3:D:706:PRO:C	2.33	0.49
3:N:42:ASP:N	3:N:46:ASP:OD2	2.39	0.49
3:N:890:VAL:HG23	3:N:892:ASP:H	1.77	0.49
3:D:1066:THR:H	3:D:1069:GLU:HB2	1.78	0.49
3:D:1118:ILE:HD12	3:D:1192:LEU:HD12	1.95	0.49
3:D:1267:ARG:HG2	3:D:1331:ASP:OD1	2.12	0.49
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.95	0.49
3:D:806:PHE:O	3:D:829:VAL:HA	2.13	0.49
2:C:580:MET:SD	2:C:584:GLU:HG3	2.53	0.49
3:D:1101:VAL:HG21	3:D:1424:VAL:HB	1.95	0.49
3:D:47:GLU:HA	3:D:51:GLY:O	2.12	0.49
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.46	0.49
2:M:157:ARG:NH1	2:M:177:GLU:HG3	2.27	0.49
1:B:115:LEU:O	1:B:117:VAL:HG23	2.13	0.49
3:D:1208:ASP:OD1	3:D:1210:SER:OG	2.29	0.49
2:M:170:PRO:HA	6:R:13:DT:O4	2.13	0.49
2:M:358:ARG:HH22	2:M:374:ASN:HB2	1.78	0.49
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.95	0.49
1:A:56:VAL:HG23	1:A:167:VAL:HG21	1.95	0.49
2:C:672:VAL:CG2	2:C:994:ILE:HD12	2.42	0.49
2:C:425:PHE:CD1	3:D:1079:LYS:HG3	2.46	0.49
5:F:212:LEU:HD22	5:F:247:ILE:HG23	1.94	0.49
1:L:32:PHE:HA	1:L:35:THR:HB	1.94	0.49
2:M:777:ILE:O	5:P:409:LYS:HG3	2.12	0.49
3:N:15:PRO:O	3:N:19:ARG:HG3	2.13	0.49
3:N:236:TYR:HB2	3:N:319:ALA:HB3	1.95	0.49
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.27	0.49
2:C:413:LEU:HD12	2:C:452:ILE:HD11	1.94	0.48
2:C:564:MET:HE1	2:C:846:LYS:HB3	1.95	0.48
2:C:98:LEU:HD12	2:C:113:VAL:HG21	1.95	0.48
3:D:1310:ARG:HD3	3:D:1327:ARG:HH11	1.78	0.48
2:M:520:GLU:HG3	2:M:521:PRO:HD2	1.94	0.48
5:P:358:LEU:HD23	5:P:370:LYS:HE2	1.95	0.48
5:P:408:LEU:C	5:P:412:GLU:HG2	2.33	0.48
7:Q:15:BRU:C2	7:Q:16:DC:C5	2.96	0.48
2:M:422:ARG:NH2	6:R:14:DG:OP1	2.35	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:HA	1:B:138:LEU:O	2.13	0.48
3:D:185:VAL:N	3:D:201:GLY:O	2.35	0.48
5:F:162:LYS:HE3	5:F:162:LYS:HB2	1.71	0.48
3:D:67:ARG:HH11	5:F:379:ARG:HB2	1.79	0.48
2:M:428:ARG:NH2	2:M:447:ALA:O	2.45	0.48
3:N:584:ASN:OD1	3:N:585:GLY:N	2.46	0.48
1:A:111:ALA:O	1:A:114:PHE:HD1	1.96	0.48
2:C:1089:VAL:HG13	2:C:1099:VAL:HB	1.96	0.48
5:F:110:MET:HA	5:F:113:ILE:HD12	1.96	0.48
5:F:363:GLU:O	5:F:367:MET:HB2	2.13	0.48
2:M:197:LEU:O	2:M:202:TYR:HB2	2.12	0.48
3:N:1283:ILE:HG13	3:N:1315:ASP:HB3	1.94	0.48
1:B:65:PHE:HE1	3:D:809:PRO:HG2	1.77	0.48
2:C:1059:ASP:OD2	2:C:1062:GLY:HA3	2.13	0.48
2:C:397:GLU:HB3	2:C:403:SER:HB3	1.94	0.48
2:C:540:PHE:HB3	2:C:544:THR:HB	1.96	0.48
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.95	0.48
3:D:46:ASP:HB3	3:D:49:ILE:HG13	1.95	0.48
3:D:657:LEU:HG	3:D:661:MET:HE2	1.95	0.48
2:M:607:ASP:HB3	2:M:610:ARG:H	1.79	0.48
3:N:1380:GLU:HB2	3:N:1420:LEU:HD22	1.95	0.48
3:N:853:VAL:HG22	3:N:858:VAL:HG23	1.96	0.48
5:P:411:HIS:O	5:P:412:GLU:OE1	2.30	0.48
2:C:258:TYR:CE2	2:C:293:PHE:HB2	2.49	0.48
3:D:828:LYS:HA	3:D:832:ARG:HA	1.94	0.48
2:M:957:LYS:HG2	2:M:961:GLU:OE1	2.13	0.48
3:N:187:LYS:HG3	3:N:198:ARG:O	2.13	0.48
3:D:171:LEU:HD11	3:D:192:ALA:HB2	1.94	0.48
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.95	0.48
4:E:37:ASN:N	4:E:37:ASN:OD1	2.38	0.48
2:M:184:MET:HE1	2:M:191:PHE:CZ	2.49	0.48
1:A:202:ASP:OD1	1:A:204:SER:OG	2.22	0.48
2:C:1009:SER:HB3	3:D:651:GLU:O	2.14	0.48
2:C:20:GLU:HG3	2:C:21:ILE:N	2.28	0.48
2:M:1054:THR:HG22	2:M:1082:PRO:HG3	1.94	0.48
2:M:286:SER:OG	2:M:301:GLU:OE2	2.18	0.48
2:M:456:ALA:HB3	2:M:459:ALA:HB2	1.96	0.48
3:N:959:GLU:HB3	3:N:963:TYR:CE1	2.49	0.48
5:P:411:HIS:C	5:P:415:THR:HB	2.33	0.48
2:C:700:TYR:HD2	2:C:996:LYS:HB2	1.78	0.48
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:927:THR:O	3:D:931:LEU:HG	2.13	0.48
2:M:30:LEU:O	2:M:71:TYR:OH	2.29	0.48
2:C:102:HIS:HB3	2:C:105:THR:HB	1.95	0.48
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.95	0.48
3:D:1376:MET:HE3	3:D:1376:MET:HB3	1.66	0.48
3:D:573:MET:SD	5:F:210:LEU:HB3	2.54	0.48
2:M:292:ARG:O	2:M:298:PHE:HD2	1.96	0.48
2:M:943:VAL:HG21	2:M:973:VAL:HG13	1.96	0.48
3:N:143:ASN:OD1	3:N:144:GLY:N	2.45	0.48
3:N:675:ARG:HH12	5:P:420:ASP:HB3	1.78	0.48
5:P:413:SER:O	5:P:417:LYS:O	2.32	0.48
1:B:161:ARG:HE	1:B:161:ARG:HB2	1.44	0.48
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.96	0.48
3:D:1211:MET:HB3	3:D:1213:ARG:HE	1.77	0.48
3:D:171:LEU:HD12	3:D:195:VAL:HG21	1.95	0.48
5:P:367:MET:O	5:P:371:LEU:HG	2.13	0.48
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.96	0.47
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.96	0.47
2:C:1060:ILE:O	2:C:1063:ARG:HG2	2.14	0.47
2:C:182:VAL:HG23	2:C:193:LEU:HB3	1.94	0.47
2:M:1031:ARG:NE	7:Q:16:DC:OP1	2.46	0.47
2:M:1054:THR:O	2:M:1059:ASP:HB3	2.14	0.47
2:M:504:GLU:HG2	2:M:509:ALA:HB2	1.96	0.47
2:M:627:ARG:HA	2:M:638:ASP:HB2	1.96	0.47
3:N:661:MET:HE2	3:N:677:LEU:HD11	1.95	0.47
2:C:385:PHE:O	2:C:389:SER:HB3	2.14	0.47
3:D:1211:MET:SD	4:E:16:LYS:HD3	2.54	0.47
2:M:249:LYS:C	2:M:251:ASP:H	2.17	0.47
3:N:1194:CYS:O	3:N:1373:ARG:NH2	2.46	0.47
5:P:371:LEU:HD23	5:P:376:ILE:HD11	1.96	0.47
2:C:300:ASP:OD1	2:C:301:GLU:N	2.47	0.47
2:C:965:GLU:O	2:C:969:GLN:HG3	2.14	0.47
3:D:636:GLN:NE2	3:D:727:GLN:OE1	2.48	0.47
2:M:248:PRO:C	2:M:250:ARG:H	2.17	0.47
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.49	0.47
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.66	0.47
2:C:489:THR:O	2:C:492:ASP:HB2	2.14	0.47
2:C:682:TYR:CD1	2:C:851:LYS:HB2	2.47	0.47
2:C:834:GLN:O	2:C:837:ASP:HB2	2.14	0.47
2:C:243:ARG:NH2	6:H:9:DG:O6	2.45	0.47
2:M:439:CYS:HB2	2:M:541:SER:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:911:GLU:O	2:M:915:LYS:HG2	2.13	0.47
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.96	0.47
4:E:57:ASP:O	4:E:63:TRP:NE1	2.38	0.47
5:F:268:ILE:HD13	5:F:311:ALA:HB2	1.96	0.47
2:M:540:PHE:HB3	2:M:544:THR:HB	1.94	0.47
3:N:1044:LEU:HD12	3:N:1044:LEU:H	1.78	0.47
2:C:1056:LYS:O	3:D:624:ASP:N	2.47	0.47
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.29	0.47
3:D:1390:LEU:O	3:D:1393:GLN:HG2	2.15	0.47
3:D:251:PHE:HZ	3:D:282:TYR:CD1	2.32	0.47
2:C:1071:ILE:HG23	3:D:670:VAL:HG21	1.96	0.47
1:K:8:ALA:HA	1:K:9:PRO:HD3	1.63	0.47
2:M:182:VAL:HG23	2:M:193:LEU:HB3	1.97	0.47
2:M:385:PHE:O	2:M:389:SER:HB3	2.13	0.47
3:N:1156:LEU:HD23	3:N:1182:GLU:OE2	2.14	0.47
3:N:1236:LEU:CD1	3:N:1355:VAL:CG1	2.93	0.47
3:N:187:LYS:N	3:N:200:ASP:HB3	2.30	0.47
2:C:692:GLU:O	2:C:696:LYS:HG3	2.14	0.47
3:D:1101:VAL:HB	3:D:1102:THR:HG23	1.96	0.47
3:D:554:LEU:HD23	3:D:574:LEU:HD22	1.97	0.47
3:D:760:ARG:NH1	4:E:59:ASN:OD1	2.47	0.47
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.45	0.47
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.97	0.47
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.80	0.47
3:N:1086:LEU:O	3:N:1088:THR:N	2.48	0.47
1:A:206:THR:HG22	1:A:209:GLU:H	1.80	0.47
2:C:586:ARG:O	2:C:586:ARG:HG3	2.15	0.47
3:D:642:CYS:HB3	3:D:716:PHE:CD1	2.50	0.47
2:M:169:GLY:HA3	2:M:267:TYR:CD1	2.50	0.47
3:N:1384:PRO:HB3	3:N:1389:LEU:O	2.15	0.47
1:A:13:VAL:HG13	1:A:23:PHE:CE1	2.50	0.47
2:C:1058:ASP:OD2	2:C:1084:SER:HB2	2.14	0.47
2:C:286:SER:OG	2:C:301:GLU:OE2	2.31	0.47
2:C:41:ASN:O	2:C:46:ALA:HB2	2.15	0.47
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.96	0.47
3:D:1440:PHE:O	3:D:1441:GLN:HG3	2.15	0.47
3:D:170:PRO:HA	3:D:392:SER:HB3	1.97	0.47
5:F:181:GLU:O	5:F:185:GLN:HG2	2.15	0.47
1:L:18:ARG:O	1:L:207:PRO:HD3	2.14	0.47
2:M:205:GLU:O	2:M:209:ARG:HG2	2.15	0.47
2:M:944:LEU:HD22	2:M:962:GLN:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.35	0.47
1:B:64:GLU:HG2	1:B:75:VAL:CG1	2.45	0.47
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.97	0.47
2:C:892:LEU:O	2:C:895:TYR:HB3	2.15	0.47
2:M:1116:ALA:HB2	3:N:88:TYR:HB3	1.97	0.47
3:N:640:HIS:ND1	3:N:641:GLN:HG3	2.29	0.47
2:C:258:TYR:HE2	2:C:293:PHE:HB2	1.79	0.46
2:C:480:THR:HB	2:C:482:GLU:HG2	1.97	0.46
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.50	0.46
3:D:373:PRO:O	3:D:376:GLU:HG2	2.15	0.46
3:D:583:ASP:CG	3:D:586:ARG:HG3	2.35	0.46
2:M:594:ALA:HB1	2:M:654:LEU:HD11	1.97	0.46
3:N:1481:VAL:HB	4:O:18:ARG:HA	1.96	0.46
2:C:673:LEU:HD22	2:C:895:TYR:CE1	2.50	0.46
3:D:601:ARG:NH1	3:D:606:ILE:HG12	2.30	0.46
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.80	0.46
3:N:1083:ASP:CG	3:N:1087:ARG:NH1	2.69	0.46
3:N:1404:ASN:HD21	3:N:1415:VAL:HG23	1.80	0.46
2:C:26:TYR:CE2	2:C:30:LEU:HD11	2.50	0.46
2:C:140:ILE:HD11	2:C:331:ARG:NE	2.30	0.46
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.30	0.46
3:D:68:PHE:HB2	3:D:80:VAL:HG21	1.98	0.46
3:D:959:GLU:O	3:D:963:TYR:HD1	1.98	0.46
4:E:37:ASN:HB3	4:E:93:TYR:CD1	2.50	0.46
2:M:615:TYR:OH	2:M:623:TYR:OH	2.05	0.46
3:N:1282:ARG:HB3	3:N:1293:PHE:HB2	1.97	0.46
5:P:364:ARG:HG2	5:P:390:PHE:CE2	2.50	0.46
2:C:283:ILE:HG21	2:C:305:PRO:CG	2.46	0.46
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.98	0.46
3:D:135:LEU:O	3:D:149:LYS:HG3	2.16	0.46
3:D:17:LYS:O	3:D:20:SER:HB3	2.15	0.46
1:L:24:VAL:HG11	1:L:194:LYS:HE3	1.97	0.46
2:M:480:THR:HB	2:M:482:GLU:HG2	1.96	0.46
2:M:930:LYS:HA	2:M:930:LYS:HD2	1.67	0.46
3:N:658:LEU:HA	3:N:661:MET:HE3	1.98	0.46
1:A:191:ASP:N	1:A:191:ASP:OD1	2.36	0.46
2:C:1090:LYS:HA	2:C:1090:LYS:HD2	1.75	0.46
1:A:150:TYR:OH	2:C:832:LYS:HE2	2.15	0.46
2:C:987:ILE:HG23	3:D:948:THR:HB	1.97	0.46
3:D:1008:PHE:O	3:D:1012:GLU:HB3	2.15	0.46
3:D:134:VAL:HG13	3:D:153:LEU:HD21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.97	0.46
2:C:680:ASP:H	3:D:943:THR:HB	1.80	0.46
4:E:33:HIS:HB2	4:E:37:ASN:OD1	2.16	0.46
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.51	0.46
5:P:358:LEU:O	5:P:366:ALA:HB2	2.16	0.46
1:A:70:GLY:HA3	1:A:136:GLY:CA	2.45	0.46
2:C:170:PRO:HA	6:H:13:DT:O4	2.16	0.46
2:C:281:LEU:HD22	2:C:306:THR:HA	1.98	0.46
3:D:19:ARG:HA	3:D:22:SER:HB3	1.98	0.46
3:N:136:ASP:H	3:N:453:ASP:HB3	1.80	0.46
4:O:48:MET:N	4:O:55:PHE:O	2.47	0.46
5:P:358:LEU:HA	5:P:358:LEU:HD12	1.78	0.46
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.97	0.46
1:A:191:ASP:O	2:C:938:LYS:NZ	2.49	0.46
2:C:1015:LEU:HD23	5:F:335:ASP:HA	1.97	0.46
2:C:1040:LEU:HA	2:C:1040:LEU:HD23	1.60	0.46
2:C:295:ASP:OD1	2:C:295:ASP:N	2.49	0.46
3:D:1053:PHE:CE1	3:D:1072:ILE:HG23	2.50	0.46
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.97	0.46
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.97	0.46
3:D:700:VAL:O	3:D:715:ALA:HA	2.15	0.46
3:D:911:LEU:O	3:D:915:VAL:HG23	2.16	0.46
2:M:774:LEU:HD12	2:M:777:ILE:HD12	1.98	0.46
1:B:37:GLY:HA3	1:B:179:PHE:CE1	2.50	0.46
2:C:581:THR:N	2:C:584:GLU:OE2	2.49	0.46
2:C:630:ARG:HB2	2:C:705:ILE:HB	1.97	0.46
2:C:500:ASN:OD1	3:D:1067:VAL:HG12	2.15	0.46
2:C:1088:LEU:HD13	3:D:613:ARG:HG2	1.98	0.46
2:M:874:LEU:HD23	3:N:1023:MET:SD	2.55	0.46
1:K:183:ASP:HA	2:M:938:LYS:HE3	1.98	0.46
3:N:1276:GLU:OE2	3:N:1301:LYS:HE2	2.16	0.46
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.98	0.46
2:C:685:GLU:OE1	2:C:685:GLU:HA	2.16	0.46
2:C:699:PHE:HB3	2:C:700:TYR:HD1	1.81	0.46
3:D:689:ASP:CB	4:E:51:LEU:HD11	2.46	0.46
3:D:964:LEU:HA	3:D:964:LEU:HD23	1.77	0.46
2:M:22:GLN:HB3	2:M:121:MET:HE1	1.98	0.46
3:N:963:TYR:CE2	3:N:1002:LYS:HD3	2.51	0.46
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.51	0.46
3:N:1236:LEU:HD13	3:N:1355:VAL:CG1	2.46	0.46
3:N:114:THR:HG23	3:N:495:ARG:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:14:ASP:OD1	4:O:18:ARG:NH1	2.49	0.46
3:D:1161:GLU:CD	3:D:1164:ARG:HB2	2.36	0.46
3:D:178:LEU:HD12	3:D:190:GLU:HB3	1.97	0.46
3:N:1124:GLN:HG3	3:N:1127:GLU:CD	2.37	0.46
1:A:31:GLY:O	1:B:42:ARG:NH2	2.45	0.45
2:C:194:VAL:HG13	2:C:221:LEU:HD23	1.97	0.45
2:C:877:PRO:HG3	3:D:1023:MET:HE3	1.98	0.45
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.97	0.45
3:D:351:MET:HB3	3:D:370:ALA:HB2	1.98	0.45
3:D:849:ALA:O	3:D:853:VAL:HG23	2.15	0.45
2:M:501:THR:HA	2:M:502:PRO:HD3	1.77	0.45
2:M:758:ARG:HH21	2:M:788:THR:HB	1.81	0.45
1:K:191:ASP:O	2:M:938:LYS:NZ	2.49	0.45
3:N:827:ILE:HG22	3:N:829:VAL:HG23	1.97	0.45
3:N:1211:MET:SD	4:O:16:LYS:HE2	2.56	0.45
1:A:34:VAL:HG22	1:B:42:ARG:NH2	2.30	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.58	0.45
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.99	0.45
2:C:930:LYS:HE3	2:C:935:GLY:HA2	1.98	0.45
2:C:937:ASP:OD1	2:C:938:LYS:N	2.49	0.45
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.16	0.45
3:D:796:ARG:HB2	3:D:824:ASN:ND2	2.31	0.45
4:E:83:ASP:N	4:E:83:ASP:OD1	2.50	0.45
2:M:195:LEU:HD23	2:M:238:LEU:HD13	1.98	0.45
1:A:179:PHE:HB3	1:A:197:LEU:CD2	2.47	0.45
2:C:419:THR:HG22	2:C:420:ARG:H	1.80	0.45
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.99	0.45
3:D:1274:ILE:HB	3:D:1322:GLY:HA2	1.99	0.45
2:M:577:PRO:HB3	2:M:993:PHE:CG	2.52	0.45
2:M:700:TYR:HD2	2:M:996:LYS:HB2	1.82	0.45
5:P:84:TYR:O	5:P:88:ILE:HG12	2.16	0.45
1:B:177:VAL:HG13	1:B:197:LEU:HD11	1.99	0.45
3:D:781:PRO:HG2	3:D:911:LEU:HB3	1.99	0.45
3:N:1429:LEU:HG	3:N:1440:PHE:CD1	2.49	0.45
3:N:705:ALA:HA	3:N:706:PRO:C	2.37	0.45
5:P:354:LEU:O	5:P:358:LEU:HB2	2.15	0.45
5:P:412:GLU:O	5:P:413:SER:O	2.35	0.45
2:C:605:LYS:HD3	2:C:610:ARG:NE	2.31	0.45
3:D:71:LYS:O	3:D:80:VAL:HG22	2.17	0.45
3:N:477:LEU:O	3:N:481:MET:HG2	2.16	0.45
5:P:153:PRO:O	5:P:156:VAL:HG22	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:628:PHE:N	2:C:628:PHE:CD2	2.84	0.45
2:C:704:HIS:CD2	2:C:831:ARG:HG3	2.50	0.45
2:M:571:LEU:HD22	2:M:700:TYR:HA	1.98	0.45
3:N:1353:GLN:O	3:N:1357:ARG:HG3	2.16	0.45
3:N:890:VAL:O	3:N:926:LYS:NZ	2.38	0.45
5:P:402:ASN:O	5:P:406:ARG:HG3	2.16	0.45
1:B:18:ARG:O	1:B:207:PRO:HD3	2.16	0.45
2:C:939:ARG:H	2:C:939:ARG:HG2	1.47	0.45
3:D:1041:LEU:HD13	3:D:1043:GLY:HA2	1.99	0.45
3:D:1491:THR:HG22	3:D:1495:ILE:HD11	1.98	0.45
3:D:805:GLU:HB3	3:D:828:LYS:HB2	1.99	0.45
3:D:989:TYR:O	3:D:993:LEU:HG	2.17	0.45
3:N:1130:ARG:O	3:N:1131:SER:OG	2.27	0.45
5:P:383:LEU:HD12	5:P:395:GLU:OE1	2.17	0.45
5:P:411:HIS:C	5:P:412:GLU:OE1	2.55	0.45
1:A:29:GLU:O	1:A:32:PHE:HB2	2.16	0.45
1:B:71:VAL:HG13	1:B:131:THR:O	2.17	0.45
3:D:126:VAL:O	3:D:457:GLY:N	2.41	0.45
3:D:1336:LEU:HD13	3:D:1344:VAL:HG21	1.99	0.45
3:D:166:GLN:HB3	3:D:394:LEU:HD11	1.99	0.45
3:D:178:LEU:HG	3:D:192:ALA:HA	1.99	0.45
3:D:367:ILE:HG13	3:D:379:ALA:HB2	1.99	0.45
3:D:371:ILE:HG21	5:F:232:ARG:NH1	2.31	0.45
2:C:971:LYS:NZ	3:D:953:ASP:OD1	2.49	0.45
2:C:374:ASN:HD21	5:F:276:ARG:NH1	2.14	0.45
5:F:383:LEU:O	5:F:397:ILE:HG21	2.17	0.45
1:L:201:THR:HG21	1:L:205:VAL:O	2.16	0.45
2:M:719:PRO:HB2	2:M:721:ARG:HD3	1.98	0.45
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.98	0.45
2:M:853:LEU:HB2	2:M:858:MET:HE1	1.98	0.45
2:M:1056:LYS:O	3:N:624:ASP:N	2.49	0.45
3:N:633:VAL:C	3:N:635:PRO:HD3	2.37	0.45
3:N:803:GLY:HA2	3:N:826:PRO:O	2.17	0.45
5:P:233:PHE:CE1	6:R:3:DT:H5"	2.52	0.45
2:C:595:LEU:HB2	2:C:656:ALA:HB3	1.99	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.45
3:D:53:ILE:HG22	3:D:54:LYS:HG3	1.99	0.45
5:F:367:MET:HB3	5:F:390:PHE:CZ	2.48	0.45
2:M:1008:ARG:NH1	2:M:1028:GLY:HA2	2.32	0.45
3:N:101:HIS:HB3	3:N:104:PHE:HD2	1.81	0.45
3:N:520:LEU:HD23	3:N:525:ARG:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:849:ALA:O	3:N:853:VAL:HG23	2.16	0.45
7:Q:18:DA:H2"	7:Q:19:DG:H5"	1.98	0.45
1:A:9:PRO:HB3	1:A:27:PRO:O	2.16	0.45
2:C:550:LEU:HD23	2:C:905:ILE:CG2	2.46	0.45
3:D:730:PRO:O	3:D:733:CYS:HB2	2.16	0.45
3:D:832:ARG:HG3	3:D:833:GLU:HG2	1.98	0.45
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.50	0.45
4:E:14:ASP:OD2	4:E:18:ARG:HD2	2.17	0.45
5:F:361:LEU:HB2	5:F:366:ALA:HB2	1.97	0.45
5:F:370:LYS:O	5:F:376:ILE:HG12	2.17	0.45
2:M:154:ARG:HA	2:M:155:PRO:HD3	1.81	0.45
2:M:462:ASP:OD2	2:M:468:ARG:NH1	2.45	0.45
1:A:185:ARG:CZ	1:A:187:GLY:HA2	2.47	0.44
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.75	0.44
2:C:1043:TYR:HE1	3:D:710:ARG:O	2.00	0.44
2:C:177:GLU:HB3	2:C:178:PRO:HA	1.98	0.44
3:D:1271:LYS:HG3	3:D:1272:ALA:O	2.17	0.44
2:M:26:TYR:OH	2:M:119:PRO:O	2.30	0.44
2:M:122:THR:OG1	2:M:124:ASP:OD1	2.35	0.44
5:P:368:VAL:CG1	5:P:397:ILE:HD11	2.44	0.44
1:A:87:VAL:HG11	1:A:144:VAL:HG11	1.98	0.44
2:C:258:TYR:CD2	2:C:262:ALA:HB3	2.52	0.44
2:C:433:THR:O	2:C:437:ARG:HD2	2.16	0.44
2:C:679:PHE:HB2	2:C:870:ILE:HG21	1.99	0.44
3:D:480:GLU:HG2	3:D:492:ALA:HB2	1.99	0.44
3:D:925:GLU:HG3	4:E:2:ALA:HB3	1.99	0.44
3:D:1486:VAL:HG21	4:E:22:VAL:HG13	1.99	0.44
2:M:80:GLN:HG2	2:M:90:TYR:CE1	2.52	0.44
2:M:874:LEU:HD21	3:N:787:LEU:HD22	2.00	0.44
3:N:285:PRO:O	3:N:288:MET:HB3	2.16	0.44
3:N:213:VAL:HG21	3:N:367:ILE:HD13	2.00	0.44
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.98	0.44
2:C:976:ASP:OD1	2:C:977:GLY:N	2.50	0.44
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.17	0.44
3:D:1103:HIS:HE2	3:D:1436:SER:HG	1.65	0.44
3:D:1235:GLN:O	3:D:1359:GLN:HG2	2.17	0.44
2:M:805:ARG:NH2	2:M:821:GLU:OE1	2.47	0.44
3:N:1042:ARG:HB3	3:N:1057:VAL:HB	1.99	0.44
3:N:208:PRO:HA	3:N:390:PRO:HA	1.98	0.44
1:B:138:LEU:HD11	1:B:140:MET:HE2	1.98	0.44
2:C:239:PHE:CZ	2:C:243:ARG:HD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.52	0.44
5:F:163:LEU:HB3	5:F:174:LEU:HD22	1.98	0.44
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.99	0.44
2:M:202:TYR:CE1	2:M:304:LEU:HD22	2.52	0.44
2:M:450:GLY:HA2	3:N:1078:ARG:NH1	2.32	0.44
3:N:238:PRO:HD3	3:N:318:ARG:HG3	1.98	0.44
3:N:388:HIS:O	3:N:390:PRO:HD3	2.17	0.44
1:A:43:ILE:HG12	1:B:32:PHE:CZ	2.52	0.44
2:C:34:VAL:HA	2:C:35:PRO:HD2	1.83	0.44
2:C:679:PHE:HA	3:D:943:THR:HB	1.99	0.44
3:D:463:GLN:HA	3:D:463:GLN:OE1	2.17	0.44
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.99	0.44
3:D:764:LEU:HD23	3:D:766:ALA:HB3	2.00	0.44
5:F:374:GLY:HA2	5:F:379:ARG:O	2.17	0.44
2:M:657:ASP:OD2	2:M:663:ASN:N	2.47	0.44
3:N:348:GLN:HB3	3:N:349:PRO:HD2	1.99	0.44
1:A:213:GLN:O	1:A:217:ILE:HG13	2.18	0.44
2:C:1072:LYS:HD3	2:C:1074:GLU:OE2	2.17	0.44
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.33	0.44
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.81	0.44
5:F:237:THR:HA	6:H:5:DA:N7	2.32	0.44
2:M:135:VAL:HG23	2:M:395:LYS:HG3	1.99	0.44
3:N:646:LYS:HB3	3:N:688:TRP:CZ3	2.53	0.44
3:N:696:HIS:HD2	3:N:697:GLY:N	2.15	0.44
2:C:511:GLU:HG3	2:C:512:ARG:HG2	1.98	0.44
2:C:674:VAL:HG21	2:C:871:LEU:HG	1.99	0.44
3:D:18:ILE:CG2	3:D:518:PRO:HG3	2.48	0.44
3:D:209:ARG:NH2	3:D:391:ALA:HA	2.33	0.44
3:D:643:GLY:HA3	3:D:727:GLN:HB2	2.00	0.44
2:M:679:PHE:CE2	2:M:853:LEU:HD11	2.53	0.44
3:N:1127:GLU:CG	3:N:1133:ARG:HB3	2.46	0.44
1:B:20:TYR:C	1:B:207:PRO:HG2	2.39	0.44
2:C:38:LYS:HE2	2:C:38:LYS:HB3	1.71	0.44
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.17	0.44
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.79	0.44
3:D:271:VAL:HG22	3:D:281:THR:HG23	2.00	0.44
3:D:567:ILE:HA	3:D:567:ILE:HD13	1.58	0.44
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.83	0.44
5:F:188:ILE:HD13	5:F:221:ILE:HG12	2.00	0.44
1:K:193:ASP:HB3	2:M:938:LYS:HD2	1.99	0.44
2:M:1097:LEU:HD13	3:N:10:ILE:HD11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.99	0.44
2:M:853:LEU:HB2	2:M:858:MET:HE2	1.99	0.44
2:M:74:GLY:HA3	2:M:93:PRO:HG2	2.00	0.44
2:M:976:ASP:OD2	2:M:978:ARG:NH1	2.50	0.44
3:N:32:ILE:O	5:P:258:ILE:HG23	2.17	0.44
2:C:212:GLY:HA2	2:C:218:VAL:HG21	2.00	0.44
3:D:1128:VAL:CG2	3:D:1133:ARG:HD3	2.43	0.44
3:D:772:PRO:O	3:D:1209:LEU:HD12	2.17	0.44
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.53	0.44
3:D:242:LEU:HA	3:D:242:LEU:HD12	1.78	0.44
1:L:48:ILE:HG22	1:L:173:PRO:HD2	2.00	0.44
2:M:173:ASP:O	2:M:184:MET:HA	2.17	0.44
2:M:34:VAL:HA	2:M:35:PRO:HD2	1.83	0.44
2:M:759:THR:HB	2:M:785:VAL:HB	1.99	0.44
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.18	0.44
3:N:405:ASP:CG	3:N:406:ASP:H	2.21	0.44
3:N:821:VAL:HG11	3:N:827:ILE:HD11	2.00	0.44
5:P:222:ARG:HE	5:P:222:ARG:HA	1.82	0.44
1:A:80:LEU:HD23	2:C:573:ARG:HD2	2.00	0.43
1:B:38:ASN:O	1:B:41:ARG:N	2.50	0.43
1:B:57:TYR:CZ	1:B:161:ARG:HD2	2.53	0.43
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.68	0.43
2:C:363:SER:HB3	2:C:366:SER:H	1.82	0.43
2:C:99:GLN:HG3	2:C:99:GLN:O	2.18	0.43
3:D:1352:ILE:HD12	3:D:1368:ILE:HG23	2.00	0.43
5:F:371:LEU:O	5:F:381:HIS:HD2	2.01	0.43
2:M:965:GLU:O	2:M:969:GLN:HG3	2.18	0.43
3:N:1144:LEU:O	3:N:1147:ARG:HG3	2.18	0.43
3:N:209:ARG:N	3:N:389:GLU:O	2.28	0.43
4:O:14:ASP:N	4:O:14:ASP:OD2	2.43	0.43
5:P:373:LYS:HA	5:P:373:LYS:HD3	1.88	0.43
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.88	0.43
3:D:265:GLU:HB3	3:D:266:GLU:H	1.51	0.43
5:F:157:GLU:O	5:F:161:GLN:HG2	2.18	0.43
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.77	0.43
2:M:258:TYR:CD2	2:M:262:ALA:HB3	2.52	0.43
2:M:719:PRO:HB3	2:M:820:ARG:NH2	2.34	0.43
3:N:1147:ARG:HD3	3:N:1188:VAL:HG11	1.99	0.43
3:N:715:ALA:HB3	3:N:764:LEU:HA	2.00	0.43
4:O:49:GLN:NE2	4:O:50:THR:O	2.51	0.43
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:372:ARG:O	5:P:380:GLU:HB2	2.18	0.43
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.59	0.43
3:D:128:TYR:OH	3:D:587:ARG:HD2	2.17	0.43
3:D:815:ALA:HA	3:D:818:ARG:CZ	2.48	0.43
3:D:963:TYR:HE2	3:D:1002:LYS:HD3	1.83	0.43
1:L:115:LEU:O	1:L:117:VAL:HG23	2.19	0.43
2:M:1019:GLN:HG2	2:M:1058:ASP:HB3	2.00	0.43
2:M:258:TYR:CE2	2:M:293:PHE:HB2	2.53	0.43
3:N:589:ALA:HB1	3:N:599:PRO:HB3	2.00	0.43
3:N:68:PHE:HB2	3:N:80:VAL:HG21	2.01	0.43
2:M:1021:LEU:HD22	5:P:331:ASP:O	2.19	0.43
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.33	0.43
2:C:835:VAL:HG13	2:C:849:VAL:O	2.18	0.43
3:D:998:GLU:O	3:D:1002:LYS:HG3	2.18	0.43
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.18	0.43
3:D:179:VAL:HG21	3:D:191:LEU:HD12	2.00	0.43
3:D:561:GLY:HA3	5:F:132:ARG:HD3	2.00	0.43
3:D:728:LEU:HD12	3:D:729:HIS:H	1.84	0.43
5:F:152:ASP:HB2	5:F:153:PRO:HD2	2.01	0.43
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.00	0.43
5:P:372:ARG:HD2	5:P:381:HIS:O	2.19	0.43
5:P:79:ASP:O	5:P:80:PRO:C	2.57	0.43
2:C:144:PRO:HD2	2:C:332:ARG:HD3	2.00	0.43
2:C:767:PRO:HB2	2:C:771:GLU:HB3	2.00	0.43
3:D:1351:GLU:O	3:D:1354:LYS:HB2	2.19	0.43
7:G:14:DG:H2'	7:G:15:BRU:H6	2.00	0.43
1:L:20:TYR:C	1:L:207:PRO:HG2	2.38	0.43
1:L:75:VAL:O	1:L:79:ILE:HG23	2.17	0.43
2:M:976:ASP:CG	2:M:978:ARG:HH11	2.22	0.43
2:C:283:ILE:HG21	2:C:305:PRO:HG2	2.00	0.43
2:C:888:THR:O	2:C:892:LEU:N	2.51	0.43
3:D:787:LEU:HD21	3:D:947:ILE:HG13	2.01	0.43
3:D:1266:ARG:CZ	6:H:18:DC:H5"	2.49	0.43
2:M:905:ILE:HG22	2:M:906:PHE:CD2	2.53	0.43
3:N:158:TYR:CE1	3:N:454:ALA:HB3	2.53	0.43
3:N:411:THR:HA	3:N:435:VAL:HG12	1.99	0.43
3:N:881:LEU:O	3:N:885:ILE:HG13	2.17	0.43
5:P:361:LEU:HD12	5:P:362:SER:H	1.84	0.43
1:A:6:LEU:HD13	1:A:7:LYS:H	1.82	0.43
1:B:149:GLY:HA2	1:B:172:SER:HB2	2.01	0.43
3:D:140:ALA:CB	3:D:452:ILE:HD12	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:422:ARG:HB3	6:H:15:DT:OP2	2.19	0.43
2:C:353:ARG:NH2	6:H:9:DG:H3'	2.29	0.43
1:K:185:ARG:NH1	1:K:187:GLY:HA2	2.33	0.43
1:L:65:PHE:HZ	3:N:810:GLU:HB2	1.82	0.43
2:M:952:LEU:HB3	2:M:966:LEU:HD21	2.01	0.43
3:N:1377:LYS:HE3	3:N:1378:TYR:CZ	2.53	0.43
3:N:818:ARG:HB2	3:N:820:GLU:HG3	2.01	0.43
5:P:201:LYS:NZ	5:P:244:ARG:HH21	2.17	0.43
2:C:260:LEU:C	2:C:261:ILE:HD12	2.39	0.43
2:C:281:LEU:HD22	2:C:305:PRO:O	2.19	0.43
2:C:628:PHE:HD2	2:C:628:PHE:N	2.17	0.43
2:C:899:GLN:HE21	2:C:901:TYR:HE2	1.66	0.43
2:C:958:THR:HG23	2:C:961:GLU:OE1	2.18	0.43
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.54	0.43
3:D:23:TYR:CD2	3:D:89:ARG:HD3	2.54	0.43
3:D:98:PRO:O	3:D:458:ALA:HB3	2.18	0.43
3:D:87:ARG:HG2	3:D:523:ASP:CB	2.49	0.43
5:F:166:LEU:HD13	5:F:170:HIS:HB3	2.01	0.43
1:L:40:LEU:HD13	1:L:211:LEU:HD11	2.00	0.43
1:A:6:LEU:HD22	1:A:6:LEU:HA	1.86	0.43
2:C:979:THR:HB	2:C:981:GLU:HG3	2.01	0.43
3:D:1348:LEU:O	3:D:1352:ILE:HG13	2.18	0.43
3:D:1432:LYS:O	3:D:1455:LYS:NZ	2.52	0.43
3:D:272:LEU:O	3:D:279:VAL:N	2.44	0.43
1:L:64:GLU:HG2	1:L:75:VAL:HG11	2.01	0.43
2:M:164:PRO:HB3	2:M:267:TYR:CZ	2.54	0.43
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.82	0.43
1:A:150:TYR:HD1	1:A:170:VAL:HG22	1.84	0.43
2:C:164:PRO:HB2	2:C:168:ARG:O	2.19	0.43
2:C:569:VAL:HG11	2:C:704:HIS:HE1	1.84	0.43
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.19	0.43
3:D:116:LEU:HD11	3:D:461:ILE:HG23	2.01	0.43
3:D:566:ILE:HD13	5:F:217:ASN:HB3	2.00	0.43
3:D:984:THR:HG22	3:D:986:ARG:H	1.82	0.43
7:G:17:DG:O5'	7:G:17:DG:H8	2.01	0.43
1:K:53:VAL:HG22	1:K:144:VAL:HG22	2.01	0.43
1:K:39:PRO:O	1:K:43:ILE:HG13	2.19	0.43
2:M:1095:LEU:HD13	3:N:103:TRP:CH2	2.54	0.43
2:M:818:GLY:HA3	5:P:309:LYS:HD2	2.00	0.43
3:N:544:TYR:O	3:N:548:ILE:HG12	2.19	0.43
3:N:806:PHE:O	3:N:829:VAL:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:413:SER:HB3	5:P:414:ARG:H	1.56	0.43
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.84	0.42
3:D:1281:VAL:O	3:D:1316:GLY:N	2.36	0.42
2:C:1001:VAL:HG11	3:D:725:SER:HB3	2.01	0.42
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.85	0.42
3:N:521:PRO:HA	3:N:522:PRO:HD3	1.79	0.42
3:N:1216:SER:HB3	4:O:16:LYS:H	1.84	0.42
4:O:80:VAL:HG22	4:O:81:PRO:O	2.18	0.42
1:A:57:TYR:CE1	1:A:163:ASN:HB2	2.53	0.42
2:C:139:GLN:HG2	2:C:140:ILE:N	2.34	0.42
2:C:142:ARG:NH2	2:C:325:ILE:HD13	2.33	0.42
2:C:3:ILE:CD1	2:C:900:ARG:HG3	2.50	0.42
2:C:501:THR:HG21	2:C:513:VAL:HB	2.01	0.42
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.53	0.42
3:D:183:GLU:O	3:D:185:VAL:HG23	2.20	0.42
3:D:827:ILE:HG22	3:D:829:VAL:HG23	2.00	0.42
1:K:14:ARG:HB2	1:K:22:GLU:HB2	2.01	0.42
1:K:206:THR:HG23	1:K:207:PRO:HD2	2.01	0.42
1:L:22:GLU:HG2	1:L:198:ARG:HG2	2.01	0.42
2:M:290:LEU:HD23	2:M:302:VAL:HG21	1.99	0.42
4:O:95:VAL:O	4:O:95:VAL:CG1	2.66	0.42
5:P:368:VAL:HG12	5:P:390:PHE:CE1	2.54	0.42
1:B:91:ASN:HA	1:B:92:PRO:HD2	1.79	0.42
2:C:249:LYS:C	2:C:251:ASP:H	2.23	0.42
2:C:906:PHE:HZ	3:D:1070:TYR:CD2	2.38	0.42
3:D:1130:ARG:CD	3:D:1131:SER:H	2.32	0.42
3:D:623:VAL:HG21	3:D:748:HIS:ND1	2.34	0.42
6:H:15:DT:C2'	6:H:16:DC:H5'	2.46	0.42
1:L:79:ILE:HA	1:L:82:LEU:HD12	2.01	0.42
3:N:1413:THR:HG22	3:N:1414:PRO:HD2	2.01	0.42
4:O:42:PRO:HA	4:O:45:ARG:HD2	2.01	0.42
5:P:357:ALA:HA	5:P:360:LYS:HG2	2.01	0.42
5:P:372:ARG:HA	5:P:381:HIS:O	2.18	0.42
6:R:14:DG:H2''	6:R:15:DT:H5'	2.01	0.42
1:A:88:ARG:HB2	1:A:123:MET:SD	2.59	0.42
1:A:25:LEU:HD21	1:B:224:TYR:CB	2.48	0.42
2:C:111:ASP:OD1	2:C:370:ALA:HB2	2.19	0.42
2:C:495:THR:HG23	2:C:517:ARG:HG3	2.02	0.42
2:C:557:ARG:NH1	2:C:879:ARG:HG3	2.34	0.42
2:C:719:PRO:O	2:C:761:PHE:HD1	2.02	0.42
3:D:30:GLU:HG2	5:F:259:ARG:CD	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:264:LEU:HD12	3:N:264:LEU:O	2.19	0.42
3:N:273:ARG:HB2	3:N:275:GLU:O	2.19	0.42
5:P:408:LEU:CD2	5:P:412:GLU:HG2	2.40	0.42
5:P:415:THR:CG2	5:P:416:ARG:CG	2.88	0.42
2:C:1092:LEU:HA	2:C:1092:LEU:HD23	1.84	0.42
2:C:605:LYS:HB2	2:C:612:VAL:HB	2.02	0.42
3:D:1341:PRO:HG3	3:D:1419:PRO:CB	2.50	0.42
3:D:554:LEU:CD2	3:D:574:LEU:HD22	2.49	0.42
5:F:372:ARG:HE	5:F:383:LEU:HG	1.85	0.42
3:N:1083:ASP:OD1	3:N:1087:ARG:HG3	2.19	0.42
3:N:245:LEU:HD22	3:N:249:TYR:HB3	2.01	0.42
4:O:8:LYS:HB2	4:O:8:LYS:HE3	1.79	0.42
5:P:193:ARG:HB2	6:R:6:DT:H1'	2.01	0.42
5:P:79:ASP:C	5:P:81:VAL:N	2.71	0.42
5:P:79:ASP:C	5:P:79:ASP:OD1	2.57	0.42
2:C:1039:ALA:HB3	3:D:713:ILE:HD12	2.02	0.42
2:C:368:THR:HB	2:C:370:ALA:H	1.84	0.42
2:C:710:ILE:HD12	2:C:790:LEU:HB2	2.02	0.42
2:C:881:ASN:N	2:C:881:ASN:OD1	2.46	0.42
2:C:910:LYS:O	2:C:914:ILE:HG13	2.20	0.42
3:D:925:GLU:O	3:D:928:ALA:HB3	2.20	0.42
5:F:128:ARG:NH2	5:F:129:GLU:OE1	2.53	0.42
1:K:83:LYS:CE	1:K:168:ASP:HB2	2.47	0.42
3:N:1236:LEU:CD1	3:N:1355:VAL:HG11	2.50	0.42
3:N:517:VAL:HA	3:N:518:PRO:HD3	1.89	0.42
6:R:13:DT:H2''	6:R:14:DG:OP2	2.19	0.42
1:A:114:PHE:HE1	1:A:129:ILE:HD11	1.85	0.42
1:A:155:LYS:HD3	1:A:155:LYS:HA	1.82	0.42
1:B:97:VAL:HG12	1:B:98:THR:N	2.34	0.42
2:C:226:VAL:HG13	2:C:227:PHE:CD1	2.55	0.42
2:C:269:LEU:HB2	2:C:288:ARG:O	2.19	0.42
2:C:326:ASP:HA	2:C:331:ARG:HD2	2.02	0.42
2:C:805:ARG:NH2	2:C:821:GLU:OE1	2.53	0.42
3:D:236:TYR:HB2	3:D:319:ALA:HB3	2.01	0.42
3:D:584:ASN:OD1	3:D:585:GLY:N	2.53	0.42
7:G:16:DC:H6	7:G:16:DC:H5''	1.84	0.42
2:M:332:ARG:HB3	2:M:466:PHE:CE2	2.55	0.42
3:N:1086:LEU:C	3:N:1088:THR:N	2.71	0.42
3:N:1280:VAL:HA	3:N:1317:ASP:O	2.20	0.42
3:N:462:GLN:HB2	3:N:513:ILE:HG21	2.01	0.42
3:N:71:LYS:O	3:N:80:VAL:HG22	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:193:ARG:HB3	6:R:7:DG:H5'	2.01	0.42
5:P:357:ALA:HB1	5:P:408:LEU:HD21	2.02	0.42
1:A:86:VAL:HG22	1:A:123:MET:HG3	2.01	0.42
2:C:248:PRO:C	2:C:250:ARG:H	2.23	0.42
2:C:28:ARG:HH11	2:C:42:VAL:HG21	1.84	0.42
2:C:942:GLU:O	2:C:945:ARG:HB3	2.19	0.42
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	2.01	0.42
3:D:1275:SER:O	3:D:1322:GLY:N	2.35	0.42
3:D:227:LEU:HD13	3:D:331:VAL:HG21	2.01	0.42
3:D:241:ILE:HA	3:D:312:ARG:CB	2.50	0.42
3:D:754:PHE:HA	4:E:24:ALA:HB1	2.00	0.42
2:M:768:THR:O	2:M:771:GLU:N	2.53	0.42
3:N:1001:GLU:O	3:N:1005:GLN:HG2	2.20	0.42
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.80	0.42
3:N:1238:MET:O	3:N:1246:VAL:C	2.58	0.42
3:N:315:ARG:H	3:N:315:ARG:HD3	1.85	0.42
5:P:93:LEU:HD21	5:P:193:ARG:HD3	2.02	0.42
5:P:324:GLU:OE2	5:P:324:GLU:N	2.50	0.42
1:B:172:SER:HA	1:B:173:PRO:HD2	1.88	0.42
1:B:8:ALA:HA	1:B:9:PRO:HD3	1.71	0.42
2:C:22:GLN:OE1	2:C:336:VAL:HG11	2.20	0.42
2:C:295:ASP:HA	2:C:296:GLY:HA2	1.49	0.42
2:C:390:GLN:OE1	2:C:414:GLY:HA2	2.19	0.42
3:D:11:ALA:HA	3:D:1451:ALA:O	2.20	0.42
3:D:237:LYS:HB3	3:D:237:LYS:HE2	1.80	0.42
3:D:475:LYS:O	3:D:478:LEU:HB2	2.20	0.42
3:D:479:GLU:OE1	3:D:482:LYS:NZ	2.48	0.42
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.79	0.42
3:D:930:LEU:O	3:D:933:ALA:HB3	2.20	0.42
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.55	0.42
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.52	0.42
2:M:582:GLY:N	2:M:584:GLU:OE2	2.46	0.42
2:M:600:ASP:O	2:M:616:GLU:HG2	2.20	0.42
1:B:44:LEU:O	1:B:174:VAL:HG21	2.19	0.42
2:C:1097:LEU:HD11	3:D:103:TRP:HZ3	1.84	0.42
3:D:907:GLU:HB3	3:D:1026:SER:HA	2.02	0.42
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.55	0.42
3:D:313:MET:HA	3:D:314:PRO:HD3	1.74	0.42
4:E:14:ASP:N	4:E:14:ASP:OD2	2.50	0.42
4:E:80:VAL:HG22	4:E:81:PRO:O	2.20	0.42
2:M:304:LEU:HB3	2:M:305:PRO:HD3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:380:ALA:O	2:M:384:GLU:HB2	2.19	0.42
3:N:356:PRO:HG2	3:N:359:ALA:HB2	2.01	0.42
2:C:243:ARG:HA	2:C:244:PRO:HD3	1.81	0.41
2:C:672:VAL:HB	2:C:868:ASP:HB2	2.02	0.41
3:D:1438:ALA:O	3:D:1443:THR:HG23	2.20	0.41
2:C:1093:GLN:HB3	3:D:21:TRP:CZ3	2.55	0.41
5:F:291:ILE:HG22	5:F:295:MET:HG3	2.02	0.41
6:H:21:DA:N6	7:G:7:DT:H3	2.12	0.41
1:K:29:GLU:O	1:K:32:PHE:HB2	2.20	0.41
2:M:260:LEU:HA	2:M:260:LEU:HD12	1.94	0.41
2:C:15:LEU:HA	2:C:16:PRO:HD3	1.91	0.41
2:C:44:ILE:HD13	2:C:44:ILE:HA	1.71	0.41
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	2.01	0.41
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.00	0.41
3:D:3:LYS:HA	3:D:3:LYS:HD2	1.56	0.41
3:D:3:LYS:HE3	3:D:4:GLU:H	1.85	0.41
3:D:659:LYS:HE3	3:D:663:GLU:OE2	2.19	0.41
3:D:95:LEU:HD22	3:D:574:LEU:HD21	2.02	0.41
5:F:271:LEU:HD11	5:F:304:VAL:HG13	2.01	0.41
2:M:20:GLU:HG3	2:M:21:ILE:N	2.35	0.41
2:M:272:ALA:HA	2:M:464:LEU:HD12	2.02	0.41
3:N:1018:ASN:HA	3:N:1019:PRO:HD3	1.87	0.41
3:N:1190:SER:OG	3:N:1369:GLU:OE1	2.33	0.41
2:M:680:ASP:OD1	3:N:943:THR:HG21	2.20	0.41
1:A:168:ASP:OD2	2:C:832:LYS:NZ	2.34	0.41
2:C:439:CYS:HA	2:C:440:PRO:HD3	1.69	0.41
3:D:411:THR:HA	3:D:435:VAL:HG12	2.02	0.41
2:M:324:ASP:O	2:M:325:ILE:HB	2.20	0.41
2:M:442:GLU:OE1	2:M:541:SER:OG	2.20	0.41
3:N:1236:LEU:CD1	3:N:1355:VAL:HG12	2.51	0.41
3:N:65:ARG:HG3	5:P:378:GLY:O	2.21	0.41
7:Q:14:DG:C2'	7:Q:15:BRU:C5'	2.92	0.41
1:A:227:ASN:N	1:A:227:ASN:OD1	2.54	0.41
2:C:150:PRO:HD3	2:C:322:VAL:HG11	2.02	0.41
2:C:899:GLN:NE2	2:C:901:TYR:HE2	2.19	0.41
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.20	0.41
3:D:388:HIS:O	3:D:390:PRO:HD3	2.20	0.41
3:D:739:ASP:O	3:D:743:ASP:HB2	2.20	0.41
5:F:309:LYS:HA	5:F:312:GLN:HE21	1.86	0.41
2:M:143:SER:O	2:M:147:TYR:OH	2.22	0.41
2:M:302:VAL:O	2:M:306:THR:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:47:GLU:HA	3:N:51:GLY:O	2.20	0.41
3:N:729:HIS:HA	3:N:730:PRO:HD3	1.90	0.41
4:O:57:ASP:HA	4:O:58:PRO:HD3	1.86	0.41
5:P:152:ASP:HB2	5:P:153:PRO:HD2	2.01	0.41
5:P:415:THR:HG22	5:P:416:ARG:H	1.84	0.41
1:B:167:VAL:HG12	1:B:168:ASP:O	2.21	0.41
2:C:756:VAL:HG21	2:C:823:VAL:HG11	2.02	0.41
3:D:111:LYS:HD3	3:D:111:LYS:HA	1.84	0.41
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.32	0.41
3:D:1258:ARG:NH2	3:D:1351:GLU:HG2	2.34	0.41
3:D:172:PRO:HB2	3:D:175:VAL:CG2	2.50	0.41
3:D:353:VAL:HG11	3:D:387:LEU:HD11	2.03	0.41
3:D:603:LEU:HD23	3:D:603:LEU:HA	1.69	0.41
5:F:193:ARG:HB2	6:H:6:DT:H1'	2.03	0.41
1:K:206:THR:HG22	1:K:208:LEU:N	2.35	0.41
1:L:151:VAL:HG11	1:L:156:HIS:HB3	2.01	0.41
2:M:639:GLN:HA	2:M:657:ASP:O	2.21	0.41
3:N:114:THR:HG21	3:N:498:VAL:HG21	2.02	0.41
3:N:230:TRP:HA	3:N:243:ALA:HA	2.02	0.41
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.89	0.41
5:P:79:ASP:CG	5:P:82:ARG:H	2.22	0.41
2:C:122:THR:OG1	2:C:124:ASP:OD1	2.39	0.41
2:C:569:VAL:HG21	2:C:1000:MET:HE3	2.02	0.41
2:C:9:ILE:HD11	2:C:500:ASN:HD22	1.86	0.41
3:D:1256:LEU:HD12	3:D:1256:LEU:O	2.20	0.41
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	2.03	0.41
3:D:76:CYS:HB2	3:D:78:VAL:HG23	2.01	0.41
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.84	0.41
5:F:120:THR:HG22	5:F:122:LEU:HD13	2.01	0.41
5:F:372:ARG:HD3	5:F:401:GLU:OE2	2.20	0.41
1:L:64:GLU:HG2	1:L:75:VAL:CG1	2.50	0.41
3:N:1127:GLU:CB	3:N:1133:ARG:HB3	2.51	0.41
3:N:1492:LEU:HD12	3:N:1493:LYS:HD2	2.03	0.41
3:N:508:ARG:HA	3:N:509:PRO:HD3	1.93	0.41
3:N:45:PHE:CD1	3:N:522:PRO:HB3	2.53	0.41
2:M:361:MET:SD	5:P:201:LYS:HD2	2.61	0.41
5:P:234:LYS:HB3	5:P:234:LYS:HE2	1.91	0.41
1:B:30:ARG:HA	1:B:193:ASP:OD1	2.21	0.41
1:B:205:VAL:HG12	1:B:206:THR:H	1.86	0.41
3:D:956:ILE:HG12	3:D:1039:CYS:O	2.20	0.41
3:D:1352:ILE:HD12	3:D:1368:ILE:CG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:302:GLN:HB2	3:D:303:PRO:HD2	2.03	0.41
3:D:401:TYR:OH	3:D:430:ASP:HB2	2.21	0.41
3:D:59:ALA:HB3	3:D:76:CYS:HB2	2.03	0.41
3:D:610:LYS:HB3	3:D:610:LYS:HE2	1.68	0.41
2:C:361:MET:SD	5:F:201:LYS:HE3	2.61	0.41
2:M:101:ILE:HG12	2:M:108:ILE:HG22	2.02	0.41
2:M:261:ILE:HG23	2:M:290:LEU:HB2	2.02	0.41
2:M:580:MET:HB3	2:M:584:GLU:CD	2.41	0.41
3:N:1238:MET:HG3	3:N:1253:THR:CB	2.48	0.41
3:N:1386:ASP:OD2	3:N:1413:THR:OG1	2.31	0.41
3:N:1434:TRP:NE1	3:N:1457:ASP:HB2	2.36	0.41
3:N:50:PHE:CD2	3:N:522:PRO:HD3	2.54	0.41
5:P:278:LEU:HD11	5:P:294:ALA:HB3	2.03	0.41
1:A:34:VAL:HG22	1:B:42:ARG:CZ	2.51	0.41
2:C:861:LEU:HD12	2:C:865:THR:OG1	2.20	0.41
3:D:115:LEU:HA	3:D:115:LEU:HD23	1.75	0.41
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.56	0.41
3:D:637:LEU:O	3:D:729:HIS:HD2	2.03	0.41
3:D:631:ILE:CG2	3:D:745:MET:HB2	2.51	0.41
5:F:304:VAL:O	5:F:308:LEU:HG	2.20	0.41
2:M:719:PRO:HB3	2:M:820:ARG:CZ	2.51	0.41
3:N:1133:ARG:HG2	3:N:1134:LEU:N	2.34	0.41
5:P:411:HIS:O	5:P:415:THR:OG1	2.38	0.41
5:P:95:THR:OG1	5:P:97:GLU:OE1	2.28	0.41
2:C:150:PRO:HA	2:C:158:TYR:CD1	2.56	0.41
2:C:712:ALA:O	2:C:820:ARG:HB3	2.20	0.41
2:C:88:LEU:HD23	2:C:813:VAL:HG23	2.03	0.41
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.21	0.41
3:D:1447:LEU:HD23	3:D:1447:LEU:HA	1.75	0.41
3:D:959:GLU:HB3	3:D:963:TYR:CD1	2.55	0.41
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.85	0.41
5:F:233:PHE:CD2	6:H:2:DA:H1'	2.56	0.41
2:M:404:LEU:O	2:M:408:ARG:HG3	2.21	0.41
2:M:627:ARG:HA	2:M:627:ARG:HD3	1.94	0.41
2:M:878:SER:HB2	3:N:1029:ARG:HD2	2.03	0.41
3:N:269:PHE:CE2	3:N:283:PHE:HD1	2.38	0.41
3:N:631:ILE:HG13	3:N:740:PHE:HD2	1.85	0.41
3:N:831:GLY:O	3:N:832:ARG:HB3	2.21	0.41
2:C:397:GLU:HB3	2:C:403:SER:CB	2.51	0.41
2:C:411:SER:OG	2:C:413:LEU:HB2	2.21	0.41
2:C:436:GLY:O	2:C:459:ALA:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:502:PRO:HB2	2:C:509:ALA:HB3	2.02	0.41
2:C:550:LEU:HD23	2:C:905:ILE:HG21	2.02	0.41
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.56	0.41
2:M:936:VAL:HG11	2:M:959:PRO:HB2	2.03	0.41
3:N:226:PRO:HD3	3:N:249:TYR:CE1	2.56	0.41
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.54	0.41
5:P:412:GLU:O	5:P:415:THR:N	2.54	0.41
1:B:173:PRO:O	1:B:201:THR:HG23	2.21	0.41
1:B:20:TYR:CG	1:B:21:GLY:N	2.88	0.41
2:C:160:ALA:O	2:C:173:ASP:HA	2.21	0.41
2:C:644:VAL:HG22	2:C:645:VAL:HG23	2.02	0.41
3:D:591:VAL:HB	3:D:593:ASN:O	2.21	0.41
5:F:223:ALA:HB2	5:F:242:TRP:HB2	2.02	0.41
2:M:974:LEU:HD12	2:M:974:LEU:HA	1.95	0.41
3:N:102:ILE:HB	3:N:579:ASP:OD1	2.21	0.41
3:N:480:GLU:HG2	3:N:492:ALA:HB2	2.03	0.41
3:N:658:LEU:HD23	3:N:661:MET:CE	2.51	0.41
3:N:778:LEU:HA	3:N:778:LEU:HD23	1.89	0.41
3:N:984:THR:HB	3:N:987:GLU:H	1.86	0.41
1:A:50:GLY:HA3	1:A:173:PRO:HD3	2.04	0.40
1:A:20:TYR:CD2	1:A:21:GLY:N	2.89	0.40
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.89	0.40
2:C:200:LEU:HD22	2:C:300:ASP:HB2	2.02	0.40
2:C:628:PHE:H	2:C:638:ASP:CB	2.34	0.40
2:C:755:LEU:HD22	2:C:825:VAL:HG11	2.03	0.40
3:D:1033:GLN:O	3:D:1037:GLN:HG3	2.21	0.40
3:D:1495:ILE:HG21	4:E:84:ARG:HB3	2.03	0.40
3:D:31:THR:OG1	3:D:32:ILE:N	2.54	0.40
3:D:366:LYS:HD3	3:D:369:ALA:HB2	2.03	0.40
3:D:415:VAL:N	3:D:433:GLY:O	2.37	0.40
1:K:151:VAL:HA	1:K:152:PRO:HD3	1.86	0.40
1:L:74:ASP:O	1:L:78:ILE:HG13	2.20	0.40
4:O:87:LYS:HA	4:O:87:LYS:HD3	1.88	0.40
2:C:454:SER:HB3	2:C:541:SER:HB2	2.03	0.40
2:C:859:PRO:O	2:C:867:VAL:HG22	2.22	0.40
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.36	0.40
3:D:90:MET:HB3	3:D:90:MET:HE2	1.87	0.40
5:F:125:ASP:O	5:F:129:GLU:HG2	2.21	0.40
2:M:368:THR:O	2:M:372:LEU:HB2	2.22	0.40
2:M:478:VAL:HG13	2:M:506:ASN:HB3	2.02	0.40
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:220:ARG:HH11	3:N:334:THR:HG21	1.86	0.40
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.85	0.40
3:D:1232:PRO:CB	3:D:1361:VAL:HG11	2.52	0.40
3:D:1282:ARG:HB3	3:D:1293:PHE:HB2	2.03	0.40
3:D:1307:LYS:HG2	3:D:1307:LYS:O	2.22	0.40
3:D:204:LEU:HD23	3:D:441:ARG:NH1	2.36	0.40
4:E:49:GLN:NE2	4:E:50:THR:O	2.55	0.40
5:F:95:THR:HG22	5:F:96:LEU:N	2.36	0.40
1:K:10:VAL:HG22	1:K:26:GLU:O	2.21	0.40
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.56	0.40
2:M:1071:ILE:HA	2:M:1071:ILE:HD13	1.96	0.40
2:M:194:VAL:HG22	2:M:221:LEU:HG	2.03	0.40
3:N:996:TRP:CE2	3:N:1056:PRO:HG3	2.56	0.40
3:N:128:TYR:OH	3:N:587:ARG:HD2	2.21	0.40
3:N:1353:GLN:NE2	3:N:1363:LEU:O	2.48	0.40
3:N:1379:VAL:HG21	3:N:1400:VAL:HG11	2.03	0.40
3:N:322:VAL:HG12	3:N:335:LEU:HD23	2.02	0.40
3:N:845:ASN:HB2	3:N:846:PRO:HD2	2.03	0.40
5:P:172:ARG:O	5:P:176:ILE:HG12	2.20	0.40
6:R:10:DA:H2''	6:R:11:DG:O4'	2.21	0.40
2:C:606:VAL:HB	2:C:645:VAL:HG22	2.03	0.40
2:C:705:ILE:HG13	2:C:828:ALA:HB2	2.03	0.40
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.92	0.40
3:D:1197:ARG:HG3	3:D:1398:TRP:CE2	2.56	0.40
3:D:111:LYS:HG3	3:D:1452:ILE:HD11	2.04	0.40
3:D:536:ALA:HA	5:F:315:VAL:O	2.21	0.40
3:D:756:GLN:HB3	4:E:61:VAL:HG21	2.02	0.40
5:F:126:LEU:O	5:F:130:VAL:HG23	2.21	0.40
5:F:394:ARG:HG3	5:F:395:GLU:N	2.35	0.40
1:K:32:PHE:HA	1:K:35:THR:HB	2.02	0.40
2:M:1050:GLN:O	2:M:1054:THR:OG1	2.26	0.40
2:M:729:LEU:HA	2:M:729:LEU:HD23	1.82	0.40
3:N:633:VAL:HG13	3:N:635:PRO:HD3	2.03	0.40
1:B:154:GLU:HG2	3:D:840:LYS:NZ	2.36	0.40
2:C:1021:LEU:O	2:C:1028:GLY:HA3	2.21	0.40
2:C:690:ILE:HD13	2:C:690:ILE:HA	1.84	0.40
3:D:1139:ASP:OD1	3:D:1357:ARG:HD3	2.22	0.40
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.03	0.40
3:D:631:ILE:HG13	3:D:740:PHE:HD2	1.86	0.40
3:D:756:GLN:O	3:D:760:ARG:HG3	2.22	0.40
2:M:165:LEU:HA	2:M:165:LEU:HD23	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:963:TYR:HE2	3:N:1002:LYS:HD3	1.86	0.40
3:N:1277:ILE:HG22	3:N:1278:ASP:N	2.36	0.40
3:N:1315:ASP:OD1	3:N:1315:ASP:N	2.54	0.40
3:N:1406:ARG:O	3:N:1410:GLU:HB2	2.22	0.40
3:N:149:LYS:O	3:N:150:ARG:HB2	2.21	0.40
3:N:716:PHE:HZ	3:N:732:VAL:HG21	1.86	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	224/315 (71%)	219 (98%)	3 (1%)	2 (1%)	17	54
1	B	220/315 (70%)	209 (95%)	11 (5%)	0	100	100
1	K	224/315 (71%)	220 (98%)	4 (2%)	0	100	100
1	L	223/315 (71%)	214 (96%)	9 (4%)	0	100	100
2	C	1107/1119 (99%)	1066 (96%)	40 (4%)	1 (0%)	51	83
2	M	1107/1119 (99%)	1065 (96%)	40 (4%)	2 (0%)	47	78
3	D	1478/1524 (97%)	1418 (96%)	59 (4%)	1 (0%)	51	83
3	N	1485/1524 (97%)	1423 (96%)	59 (4%)	3 (0%)	47	78
4	E	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
4	O	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
5	F	344/443 (78%)	337 (98%)	7 (2%)	0	100	100
5	P	345/443 (78%)	331 (96%)	12 (4%)	2 (1%)	25	62
All	All	6941/7630 (91%)	6678 (96%)	252 (4%)	11 (0%)	47	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	325	ILE
2	M	295	ASP
2	M	325	ILE
5	P	413	SER
3	N	1234	THR
5	P	80	PRO
3	N	1087	ARG
3	D	440	VAL
1	A	59	GLU
1	A	226	SER
3	N	440	VAL

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	199/273 (73%)	185 (93%)	14 (7%)	15	45
1	B	195/273 (71%)	182 (93%)	13 (7%)	16	47
1	K	199/273 (73%)	191 (96%)	8 (4%)	31	59
1	L	198/273 (72%)	192 (97%)	6 (3%)	41	66
2	C	936/941 (100%)	854 (91%)	82 (9%)	10	38
2	M	936/941 (100%)	903 (96%)	33 (4%)	36	63
3	D	1250/1279 (98%)	1139 (91%)	111 (9%)	9	37
3	N	1253/1279 (98%)	1197 (96%)	56 (4%)	27	57
4	E	83/88 (94%)	76 (92%)	7 (8%)	11	40
4	O	83/88 (94%)	81 (98%)	2 (2%)	49	71
5	F	301/388 (78%)	291 (97%)	10 (3%)	38	64
5	P	302/388 (78%)	285 (94%)	17 (6%)	21	52
All	All	5935/6484 (92%)	5576 (94%)	359 (6%)	19	50

All (359) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	12	THR
1	A	34	VAL
1	A	63	HIS
1	A	76	VAL
1	A	86	VAL
1	A	87	VAL
1	A	142	VAL
1	A	188	GLN
1	A	189	ARG
1	A	198	ARG
1	A	206	THR
1	A	227	ASN
1	A	229	GLN
1	B	15	THR
1	B	34	VAL
1	B	62	LEU
1	B	78	ILE
1	B	94	LEU
1	B	158	ILE
1	B	172	SER
1	B	184	THR
1	B	185	ARG
1	B	192	LEU
1	B	193	ASP
1	B	206	THR
1	B	223	THR
2	C	2	GLU
2	C	10	ARG
2	C	11	GLU
2	C	12	VAL
2	C	13	ILE
2	C	15	LEU
2	C	21	ILE
2	C	27	ARG
2	C	113	VAL
2	C	122	THR
2	C	133	ASP
2	C	138	SER
2	C	140	ILE
2	C	141	HIS
2	C	149	THR
2	C	196	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	281	LEU
2	C	285	LEU
2	C	289	THR
2	C	311	PHE
2	C	336	VAL
2	C	340	MET
2	C	357	GLU
2	C	360	LEU
2	C	366	SER
2	C	368	THR
2	C	403	SER
2	C	418	LEU
2	C	419	THR
2	C	420	ARG
2	C	427	VAL
2	C	429	ASP
2	C	432	ARG
2	C	433	THR
2	C	445	GLU
2	C	454	SER
2	C	487	THR
2	C	492	ASP
2	C	516	ARG
2	C	528	GLU
2	C	557	ARG
2	C	560	MET
2	C	581	THR
2	C	584	GLU
2	C	606	VAL
2	C	607	ASP
2	C	610	ARG
2	C	617	ASP
2	C	628	PHE
2	C	633	GLN
2	C	644	VAL
2	C	645	VAL
2	C	657	ASP
2	C	674	VAL
2	C	680	ASP
2	C	695	LEU
2	C	715	THR
2	C	729	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	774	LEU
2	C	775	ARG
2	C	784	ASP
2	C	788	THR
2	C	789	SER
2	C	801	VAL
2	C	834	GLN
2	C	845	ASN
2	C	863	ASP
2	C	879	ARG
2	C	900	ARG
2	C	905	ILE
2	C	929	ARG
2	C	930	LYS
2	C	939	ARG
2	C	950	LEU
2	C	958	THR
2	C	978	ARG
2	C	979	THR
2	C	1001	VAL
2	C	1016	ILE
2	C	1031	ARG
2	C	1101	THR
2	C	1104	GLU
3	D	12	LEU
3	D	30	GLU
3	D	37	LEU
3	D	47	GLU
3	D	67	ARG
3	D	69	GLU
3	D	81	THR
3	D	83	SER
3	D	90	MET
3	D	101	HIS
3	D	108	VAL
3	D	121	THR
3	D	153	LEU
3	D	171	LEU
3	D	179	VAL
3	D	184	GLU
3	D	191	LEU
3	D	199	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	200	ASP
3	D	230	TRP
3	D	231	VAL
3	D	254	GLU
3	D	258	VAL
3	D	265	GLU
3	D	269	PHE
3	D	273	ARG
3	D	352	ASN
3	D	354	VAL
3	D	372	ASP
3	D	400	VAL
3	D	410	SER
3	D	411	THR
3	D	414	ARG
3	D	423	ASP
3	D	428	LYS
3	D	430	ASP
3	D	441	ARG
3	D	486	ARG
3	D	488	ARG
3	D	493	ARG
3	D	525	ARG
3	D	527	MET
3	D	544	TYR
3	D	586	ARG
3	D	608	SER
3	D	624	ASP
3	D	633	VAL
3	D	637	LEU
3	D	666	ILE
3	D	685	ASP
3	D	709	HIS
3	D	720	LEU
3	D	733	CYS
3	D	754	PHE
3	D	762	GLN
3	D	778	LEU
3	D	782	SER
3	D	784	ASP
3	D	805	GLU
3	D	858	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	907	GLU
3	D	914	LEU
3	D	927	THR
3	D	940	THR
3	D	971	LEU
3	D	983	LEU
3	D	984	THR
3	D	988	ARG
3	D	991	GLN
3	D	1011	PHE
3	D	1012	GLU
3	D	1015	TYR
3	D	1017	PHE
3	D	1029	ARG
3	D	1031	ASN
3	D	1055	VAL
3	D	1060	SER
3	D	1067	VAL
3	D	1086	LEU
3	D	1095	THR
3	D	1112	CYS
3	D	1130	ARG
3	D	1131	SER
3	D	1183	ILE
3	D	1190	SER
3	D	1200	VAL
3	D	1201	CYS
3	D	1207	TYR
3	D	1211	MET
3	D	1216	SER
3	D	1234	THR
3	D	1274	ILE
3	D	1277	ILE
3	D	1278	ASP
3	D	1282	ARG
3	D	1283	ILE
3	D	1291	SER
3	D	1315	ASP
3	D	1326	THR
3	D	1373	ARG
3	D	1390	LEU
3	D	1395	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1403	LEU
3	D	1433	SER
3	D	1439	SER
3	D	1443	THR
3	D	1444	THR
3	D	1468	LEU
3	D	1486	VAL
3	D	1488	ASP
3	D	1497	GLU
4	E	15	SER
4	E	19	LEU
4	E	37	ASN
4	E	50	THR
4	E	68	LEU
4	E	83	ASP
4	E	92	LEU
5	F	88	ILE
5	F	117	SER
5	F	120	THR
5	F	125	ASP
5	F	138	SER
5	F	193	ARG
5	F	209	PHE
5	F	295	MET
5	F	338	LEU
5	F	376	ILE
1	K	6	LEU
1	K	34	VAL
1	K	76	VAL
1	K	86	VAL
1	K	87	VAL
1	K	142	VAL
1	K	189	ARG
1	K	215	VAL
1	L	5	LYS
1	L	34	VAL
1	L	158	ILE
1	L	191	ASP
1	L	197	LEU
1	L	206	THR
2	M	11	GLU
2	M	102	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	113	VAL
2	M	141	HIS
2	M	149	THR
2	M	196	LEU
2	M	295	ASP
2	M	297	GLU
2	M	342	ASP
2	M	402	SER
2	M	418	LEU
2	M	427	VAL
2	M	453	THR
2	M	454	SER
2	M	557	ARG
2	M	584	GLU
2	M	607	ASP
2	M	610	ARG
2	M	617	ASP
2	M	633	GLN
2	M	702	SER
2	M	715	THR
2	M	879	ARG
2	M	905	ILE
2	M	930	LYS
2	M	939	ARG
2	M	957	LYS
2	M	968	LEU
2	M	978	ARG
2	M	1001	VAL
2	M	1010	THR
2	M	1080	SER
2	M	1104	GLU
3	N	81	THR
3	N	133	ILE
3	N	153	LEU
3	N	184	GLU
3	N	211	VAL
3	N	230	TRP
3	N	245	LEU
3	N	266	GLU
3	N	270	LEU
3	N	306	GLU
3	N	311	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	N	315	ARG
3	N	354	VAL
3	N	372	ASP
3	N	400	VAL
3	N	411	THR
3	N	450	TYR
3	N	480	GLU
3	N	486	ARG
3	N	488	ARG
3	N	525	ARG
3	N	586	ARG
3	N	640	HIS
3	N	650	LEU
3	N	709	HIS
3	N	754	PHE
3	N	780	LYS
3	N	782	SER
3	N	784	ASP
3	N	864	VAL
3	N	907	GLU
3	N	940	THR
3	N	969	ARG
3	N	971	LEU
3	N	1055	VAL
3	N	1067	VAL
3	N	1087	ARG
3	N	1127	GLU
3	N	1130	ARG
3	N	1188	VAL
3	N	1194	CYS
3	N	1196	THR
3	N	1216	SER
3	N	1219	GLU
3	N	1236	LEU
3	N	1237	THR
3	N	1238	MET
3	N	1315	ASP
3	N	1326	THR
3	N	1373	ARG
3	N	1382	THR
3	N	1389	LEU
3	N	1390	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	N	1413	THR
3	N	1433	SER
3	N	1439	SER
4	O	16	LYS
4	O	50	THR
5	P	120	THR
5	P	125	ASP
5	P	262	VAL
5	P	271	LEU
5	P	315	VAL
5	P	329	TYR
5	P	340	SER
5	P	358	LEU
5	P	361	LEU
5	P	377	ASP
5	P	383	LEU
5	P	412	GLU
5	P	413	SER
5	P	414	ARG
5	P	415	THR
5	P	416	ARG
5	P	418	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	639	GLN
2	C	704	HIS
3	D	762	GLN
3	D	824	ASN
3	D	1172	HIS
3	D	1353	GLN
4	E	33	HIS
2	M	704	HIS
3	N	483	HIS
3	N	1404	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
7	BRU	G	15	7	15,21,22	3.20	6 (40%)	17,30,33	1.67	2 (11%)
7	BRU	Q	15	7	15,21,22	3.20	6 (40%)	17,30,33	1.70	2 (11%)

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
7	BRU	G	15	7	-	3/4/21/22	0/2/2/2
7	BRU	Q	15	7	-	0/4/21/22	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	15	BRU	C4-C5	8.60	1.49	1.38
7	G	15	BRU	C4-C5	8.54	1.49	1.38
7	G	15	BRU	C4-N3	4.93	1.41	1.33
7	Q	15	BRU	C4-N3	4.92	1.41	1.33
7	G	15	BRU	O4-C4	4.75	1.36	1.24
7	Q	15	BRU	O4-C4	4.73	1.36	1.24
7	G	15	BRU	C2-N3	2.84	1.43	1.38
7	G	15	BRU	O4'-C4'	-2.82	1.38	1.45
7	Q	15	BRU	C2-N3	2.81	1.43	1.38
7	Q	15	BRU	O4'-C4'	-2.79	1.38	1.45
7	G	15	BRU	C2'-C3'	-2.05	1.47	1.52
7	Q	15	BRU	C2'-C3'	-2.04	1.47	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	Q	15	BRU	C4-N3-C2	5.78	120.02	115.14
7	G	15	BRU	C4-N3-C2	5.68	119.94	115.14
7	Q	15	BRU	C5-C4-N3	-3.08	119.95	123.64
7	G	15	BRU	C5-C4-N3	-3.00	120.05	123.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	15	BRU	O4'-C1'-N1-C6
7	G	15	BRU	C3'-C4'-C5'-O5'
7	G	15	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	15	BRU	1	0
7	Q	15	BRU	10	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	226/315 (71%)	-0.28	1 (0%) 92 88	112, 138, 163, 174	0
1	B	222/315 (70%)	-0.34	0 100 100	111, 145, 190, 215	0
1	K	226/315 (71%)	-0.23	3 (1%) 77 70	114, 145, 171, 193	0
1	L	225/315 (71%)	-0.23	1 (0%) 92 88	114, 150, 198, 222	0
2	C	1111/1119 (99%)	-0.18	10 (0%) 84 78	89, 136, 212, 240	0
2	M	1111/1119 (99%)	0.04	56 (5%) 28 24	98, 154, 239, 269	0
3	D	1482/1524 (97%)	-0.21	12 (0%) 86 81	86, 136, 196, 258	1 (0%)
3	N	1489/1524 (97%)	-0.12	26 (1%) 70 62	84, 139, 199, 263	1 (0%)
4	E	94/99 (94%)	-0.08	1 (1%) 80 74	107, 138, 175, 185	0
4	O	94/99 (94%)	0.03	4 (4%) 35 29	109, 141, 191, 201	0
5	F	346/443 (78%)	-0.03	20 (5%) 23 18	112, 152, 238, 251	0
5	P	347/443 (78%)	-0.02	22 (6%) 20 15	117, 161, 253, 290	0
6	H	24/27 (88%)	-0.36	0 100 100	144, 191, 241, 247	0
6	R	24/27 (88%)	-0.38	0 100 100	142, 204, 241, 254	0
7	G	15/21 (71%)	-0.29	1 (6%) 17 13	146, 181, 229, 233	0
7	Q	15/21 (71%)	-0.36	0 100 100	160, 197, 234, 235	0
All	All	7051/7726 (91%)	-0.13	157 (2%) 62 53	84, 144, 219, 290	2 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1247	ALA	5.2
2	M	207	LEU	5.0
3	N	1238	MET	5.0
2	M	221	LEU	4.9
2	M	181	VAL	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	P	413	SER	4.9
5	P	375	LEU	4.9
2	M	311	PHE	4.7
5	P	414	ARG	4.4
2	M	251	ASP	4.3
2	M	196	LEU	4.3
3	N	1248	GLY	4.3
2	M	307	LEU	4.1
2	M	769	PRO	4.1
2	M	594	ALA	4.1
2	M	306	THR	4.0
2	M	249	LYS	3.9
2	M	211	LEU	3.8
3	N	1246	VAL	3.8
3	N	1307	LYS	3.7
5	P	365	GLU	3.7
2	M	191	PHE	3.7
4	O	95	VAL	3.6
2	M	64	LEU	3.6
3	N	1312	LEU	3.6
5	F	373	LYS	3.6
2	M	200	LEU	3.5
2	C	812	GLY	3.5
2	M	184	MET	3.5
2	M	770	GLU	3.5
2	C	778	PHE	3.4
2	C	813	VAL	3.4
2	M	253	ALA	3.4
5	F	381	HIS	3.3
2	M	223	ASP	3.3
2	C	814	GLU	3.2
1	A	4	SER	3.2
5	P	406	ARG	3.2
2	M	185	LYS	3.2
3	D	322	VAL	3.2
2	M	300	ASP	3.1
4	O	89	MET	3.1
3	N	352	ASN	3.1
5	P	392	VAL	3.0
2	M	365	ASP	3.0
5	P	391	GLY	3.0
2	M	159	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	182	VAL	3.0
2	M	303	PHE	3.0
3	N	353	VAL	2.8
2	M	161	SER	2.8
2	M	367	LEU	2.8
2	M	772	ARG	2.8
5	P	369	LEU	2.8
3	D	367	ILE	2.8
1	K	4	SER	2.7
3	N	1495	ILE	2.7
2	M	767	PRO	2.7
5	P	361	LEU	2.7
5	F	419	ARG	2.7
5	P	410	TYR	2.7
5	F	372	ARG	2.6
2	M	227	PHE	2.6
2	M	199	VAL	2.6
3	N	355	VAL	2.6
2	C	365	ASP	2.6
3	N	421	LEU	2.6
2	M	242	LEU	2.6
5	F	375	LEU	2.6
2	M	296	GLY	2.6
5	P	357	ALA	2.6
3	N	679	ARG	2.6
2	C	766	GLU	2.5
2	M	195	LEU	2.5
2	M	220	GLY	2.5
3	N	213	VAL	2.5
2	M	219	GLN	2.5
4	E	85	LEU	2.5
5	F	380	GLU	2.4
5	F	418	LEU	2.4
5	F	404	ALA	2.4
5	P	422	LEU	2.4
2	M	250	ARG	2.4
3	N	202	VAL	2.4
5	F	400	ILE	2.4
3	D	368	VAL	2.4
2	M	781	LYS	2.4
2	M	372	LEU	2.4
3	N	407	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	P	415	THR	2.4
5	P	383	LEU	2.4
3	N	1308	GLU	2.3
4	O	86	GLN	2.3
5	F	407	LYS	2.3
2	M	293	PHE	2.3
3	D	202	VAL	2.3
1	K	131	THR	2.3
2	M	297	GLU	2.3
5	F	416	ARG	2.3
5	P	379	ARG	2.3
5	P	419	ARG	2.3
3	D	1287	GLU	2.3
2	M	778	PHE	2.3
5	F	379	ARG	2.3
2	M	310	LEU	2.3
2	C	223	ASP	2.3
2	C	643	VAL	2.3
2	C	650	ARG	2.3
3	N	345	TYR	2.3
2	M	222	MET	2.3
3	N	397	LYS	2.3
5	P	373	LYS	2.3
2	M	595	LEU	2.3
3	N	393	ILE	2.3
5	P	423	ASP	2.3
5	F	390	PHE	2.3
2	M	252	LYS	2.2
5	P	374	GLY	2.2
5	F	399	GLN	2.2
4	O	85	LEU	2.2
1	K	132	LEU	2.2
5	F	408	LEU	2.2
3	D	308	LYS	2.2
5	P	409	LYS	2.2
5	P	381	HIS	2.2
2	M	812	GLY	2.2
5	P	360	LYS	2.2
5	F	423	ASP	2.2
2	C	779	GLY	2.2
2	M	620	LEU	2.2
2	M	813	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	318	ARG	2.2
3	N	445	ARG	2.2
3	D	421	LEU	2.1
2	M	597	ALA	2.1
3	D	446	VAL	2.1
3	D	991	GLN	2.1
1	L	63	HIS	2.1
3	N	1253	THR	2.1
5	F	361	LEU	2.1
5	F	393	THR	2.1
2	M	183	SER	2.1
2	M	254	VAL	2.1
3	N	343	LYS	2.1
2	M	362	GLY	2.1
3	D	409	VAL	2.0
2	M	764	GLU	2.0
5	F	389	PHE	2.0
3	D	350	HIS	2.0
3	N	367	ILE	2.0
3	D	241	ILE	2.0
2	M	649	VAL	2.0
3	N	409	VAL	2.0
3	N	165	LYS	2.0
7	G	19	DG	2.0
2	M	152	PRO	2.0
5	F	396	ARG	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
7	BRU	Q	15	20/21	0.83	0.24	177,196,247,303	1
7	BRU	G	15	20/21	0.89	0.25	138,145,192,257	1

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
9	MG	D	2003	1/1	0.94	0.23	111,111,111,111	0
9	MG	N	2003	1/1	0.98	0.22	127,127,127,127	0
8	ZN	D	2002	1/1	0.99	0.09	164,164,164,164	0
8	ZN	N	2002	1/1	0.99	0.06	138,138,138,138	0
8	ZN	N	2001	1/1	0.99	0.22	166,166,166,166	0
8	ZN	D	2001	1/1	1.00	0.17	168,168,168,168	0

6.5 Other polymers [i](#)

There are no such residues in this entry.