Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:40 PM GMT

PDB ID	:	1PZU
Title	:	An asymmetric NFAT1-RHR homodimer on a pseudo-palindromic, Kappa-B site
Authors	:	Jin, L.; Sliz, P.; Chen, L.; Macian, F.; Rao, A.; Hogan, P.G.; Harrison, S.C.
Deposited on	:	2003-07-14
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/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:

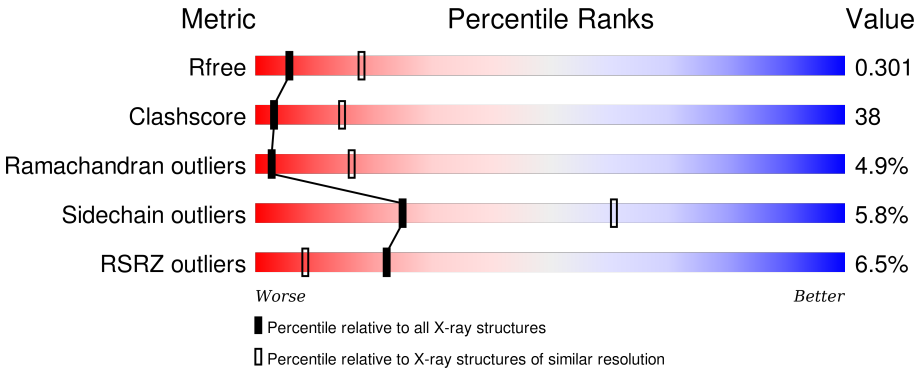
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



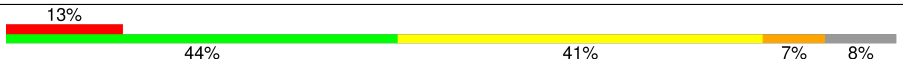
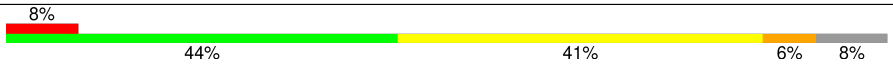
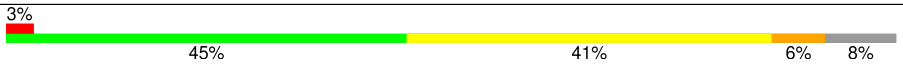
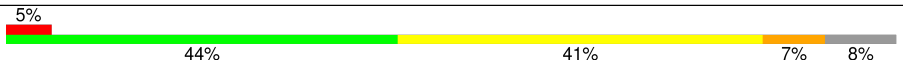
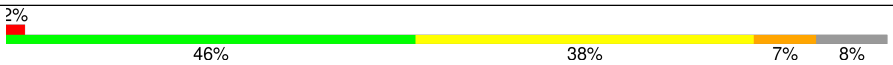
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	14	14% 64% 21%
1	V	14	14% 79% 7%
1	X	14	7% 79% 7% 7%
2	W	14	14% 57% 21% 7%
2	Y	14	36% 57% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Z	14	
3	B	301	
3	D	301	
3	H	301	
3	I	301	
3	L	301	
3	M	301	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14952 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 DNA chain called 5'-D(*TP*TP*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	14	Total	C	N	O	P	0	0	0
			285	138	51	83	13			
1	V	14	Total	C	N	O	P	0	0	0
			285	138	51	83	13			
1	T	14	Total	C	N	O	P	37	0	0
			285	138	51	83	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	14	Total	C	N	O	P	0	0	0
			283	137	52	81	13			
2	Z	14	Total	C	N	O	P	0	0	0
			283	137	52	81	13			
2	W	14	Total	C	N	O	P	0	0	0
			283	137	52	81	13			

- Molecule 3 is a protein called Nuclear factor of activated T-cells, cytoplasmic 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	276	Total	C	N	O	S	0	0	0
			2208	1386	401	412	9			
3	D	276	Total	C	N	O	S	0	0	0
			2208	1386	401	412	9			
3	H	276	Total	C	N	O	S	0	0	0
			2208	1386	401	412	9			
3	I	276	Total	C	N	O	S	0	0	0
			2208	1386	401	412	9			
3	L	276	Total	C	N	O	S	0	0	0
			2208	1386	401	412	9			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	276	Total	C	N	O	S	0	0	0
			2208	1386	401	412	9			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	378	MET	-	CLONING ARTIFACT	UNP Q13469
B	379	ARG	-	CLONING ARTIFACT	UNP Q13469
B	380	GLY	-	CLONING ARTIFACT	UNP Q13469
B	381	SER	-	CLONING ARTIFACT	UNP Q13469
B	382	HIS	-	EXPRESSION TAG	UNP Q13469
B	383	HIS	-	EXPRESSION TAG	UNP Q13469
B	384	HIS	-	EXPRESSION TAG	UNP Q13469
B	385	HIS	-	EXPRESSION TAG	UNP Q13469
B	386	HIS	-	EXPRESSION TAG	UNP Q13469
B	387	HIS	-	EXPRESSION TAG	UNP Q13469
B	388	THR	-	CLONING ARTIFACT	UNP Q13469
B	389	ASP	-	CLONING ARTIFACT	UNP Q13469
B	390	PRO	-	CLONING ARTIFACT	UNP Q13469
B	391	HIS	-	CLONING ARTIFACT	UNP Q13469
B	392	ALA	-	CLONING ARTIFACT	UNP Q13469
B	393	SER	-	CLONING ARTIFACT	UNP Q13469
B	394	SER	-	CLONING ARTIFACT	UNP Q13469
B	395	VAL	-	CLONING ARTIFACT	UNP Q13469
D	378	MET	-	CLONING ARTIFACT	UNP Q13469
D	379	ARG	-	CLONING ARTIFACT	UNP Q13469
D	380	GLY	-	CLONING ARTIFACT	UNP Q13469
D	381	SER	-	CLONING ARTIFACT	UNP Q13469
D	382	HIS	-	EXPRESSION TAG	UNP Q13469
D	383	HIS	-	EXPRESSION TAG	UNP Q13469
D	384	HIS	-	EXPRESSION TAG	UNP Q13469
D	385	HIS	-	EXPRESSION TAG	UNP Q13469
D	386	HIS	-	EXPRESSION TAG	UNP Q13469
D	387	HIS	-	EXPRESSION TAG	UNP Q13469
D	388	THR	-	CLONING ARTIFACT	UNP Q13469
D	389	ASP	-	CLONING ARTIFACT	UNP Q13469
D	390	PRO	-	CLONING ARTIFACT	UNP Q13469
D	391	HIS	-	CLONING ARTIFACT	UNP Q13469
D	392	ALA	-	CLONING ARTIFACT	UNP Q13469
D	393	SER	-	CLONING ARTIFACT	UNP Q13469
D	394	SER	-	CLONING ARTIFACT	UNP Q13469
D	395	VAL	-	CLONING ARTIFACT	UNP Q13469

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	378	MET	-	CLONING ARTIFACT	UNP Q13469
H	379	ARG	-	CLONING ARTIFACT	UNP Q13469
H	380	GLY	-	CLONING ARTIFACT	UNP Q13469
H	381	SER	-	CLONING ARTIFACT	UNP Q13469
H	382	HIS	-	EXPRESSION TAG	UNP Q13469
H	383	HIS	-	EXPRESSION TAG	UNP Q13469
H	384	HIS	-	EXPRESSION TAG	UNP Q13469
H	385	HIS	-	EXPRESSION TAG	UNP Q13469
H	386	HIS	-	EXPRESSION TAG	UNP Q13469
H	387	HIS	-	EXPRESSION TAG	UNP Q13469
H	388	THR	-	CLONING ARTIFACT	UNP Q13469
H	389	ASP	-	CLONING ARTIFACT	UNP Q13469
H	390	PRO	-	CLONING ARTIFACT	UNP Q13469
H	391	HIS	-	CLONING ARTIFACT	UNP Q13469
H	392	ALA	-	CLONING ARTIFACT	UNP Q13469
H	393	SER	-	CLONING ARTIFACT	UNP Q13469
H	394	SER	-	CLONING ARTIFACT	UNP Q13469
H	395	VAL	-	CLONING ARTIFACT	UNP Q13469
I	378	MET	-	CLONING ARTIFACT	UNP Q13469
I	379	ARG	-	CLONING ARTIFACT	UNP Q13469
I	380	GLY	-	CLONING ARTIFACT	UNP Q13469
I	381	SER	-	CLONING ARTIFACT	UNP Q13469
I	382	HIS	-	EXPRESSION TAG	UNP Q13469
I	383	HIS	-	EXPRESSION TAG	UNP Q13469
I	384	HIS	-	EXPRESSION TAG	UNP Q13469
I	385	HIS	-	EXPRESSION TAG	UNP Q13469
I	386	HIS	-	EXPRESSION TAG	UNP Q13469
I	387	HIS	-	EXPRESSION TAG	UNP Q13469
I	388	THR	-	CLONING ARTIFACT	UNP Q13469
I	389	ASP	-	CLONING ARTIFACT	UNP Q13469
I	390	PRO	-	CLONING ARTIFACT	UNP Q13469
I	391	HIS	-	CLONING ARTIFACT	UNP Q13469
I	392	ALA	-	CLONING ARTIFACT	UNP Q13469
I	393	SER	-	CLONING ARTIFACT	UNP Q13469
I	394	SER	-	CLONING ARTIFACT	UNP Q13469
I	395	VAL	-	CLONING ARTIFACT	UNP Q13469
L	378	MET	-	CLONING ARTIFACT	UNP Q13469
L	379	ARG	-	CLONING ARTIFACT	UNP Q13469
L	380	GLY	-	CLONING ARTIFACT	UNP Q13469
L	381	SER	-	CLONING ARTIFACT	UNP Q13469
L	382	HIS	-	EXPRESSION TAG	UNP Q13469
L	383	HIS	-	EXPRESSION TAG	UNP Q13469

Continued on next page...

Continued from previous page...

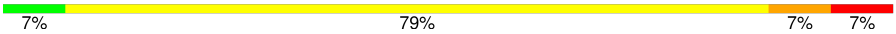
Chain	Residue	Modelled	Actual	Comment	Reference
L	384	HIS	-	EXPRESSION TAG	UNP Q13469
L	385	HIS	-	EXPRESSION TAG	UNP Q13469
L	386	HIS	-	EXPRESSION TAG	UNP Q13469
L	387	HIS	-	EXPRESSION TAG	UNP Q13469
L	388	THR	-	CLONING ARTIFACT	UNP Q13469
L	389	ASP	-	CLONING ARTIFACT	UNP Q13469
L	390	PRO	-	CLONING ARTIFACT	UNP Q13469
L	391	HIS	-	CLONING ARTIFACT	UNP Q13469
L	392	ALA	-	CLONING ARTIFACT	UNP Q13469
L	393	SER	-	CLONING ARTIFACT	UNP Q13469
L	394	SER	-	CLONING ARTIFACT	UNP Q13469
L	395	VAL	-	CLONING ARTIFACT	UNP Q13469
M	378	MET	-	CLONING ARTIFACT	UNP Q13469
M	379	ARG	-	CLONING ARTIFACT	UNP Q13469
M	380	GLY	-	CLONING ARTIFACT	UNP Q13469
M	381	SER	-	CLONING ARTIFACT	UNP Q13469
M	382	HIS	-	EXPRESSION TAG	UNP Q13469
M	383	HIS	-	EXPRESSION TAG	UNP Q13469
M	384	HIS	-	EXPRESSION TAG	UNP Q13469
M	385	HIS	-	EXPRESSION TAG	UNP Q13469
M	386	HIS	-	EXPRESSION TAG	UNP Q13469
M	387	HIS	-	EXPRESSION TAG	UNP Q13469
M	388	THR	-	CLONING ARTIFACT	UNP Q13469
M	389	ASP	-	CLONING ARTIFACT	UNP Q13469
M	390	PRO	-	CLONING ARTIFACT	UNP Q13469
M	391	HIS	-	CLONING ARTIFACT	UNP Q13469
M	392	ALA	-	CLONING ARTIFACT	UNP Q13469
M	393	SER	-	CLONING ARTIFACT	UNP Q13469
M	394	SER	-	CLONING ARTIFACT	UNP Q13469
M	395	VAL	-	CLONING ARTIFACT	UNP Q13469

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

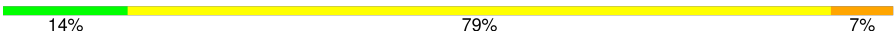
- Molecule 1: 5'-D(*TP*TP*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*A)-3'

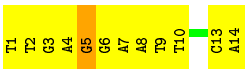
Chain X:



- Molecule 1: 5'-D(*TP*TP*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*A)-3'

Chain V:



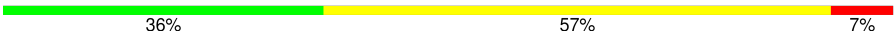


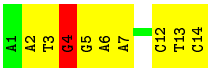
- Molecule 1: 5'-D(*TP*TP*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*A)-3'

Chain T:

- Molecule 2: 5'-D(*AP*AP*TP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3'

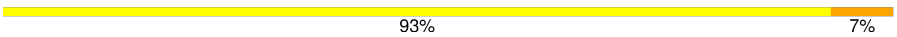
Chain Y:

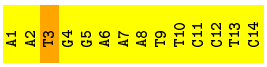




- Molecule 2: 5'-D(*AP*AP*TP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3'

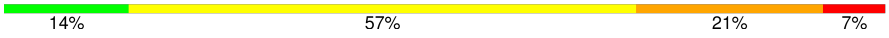
Chain Z:

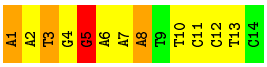




- Molecule 2: 5'-D(*AP*AP*TP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3'

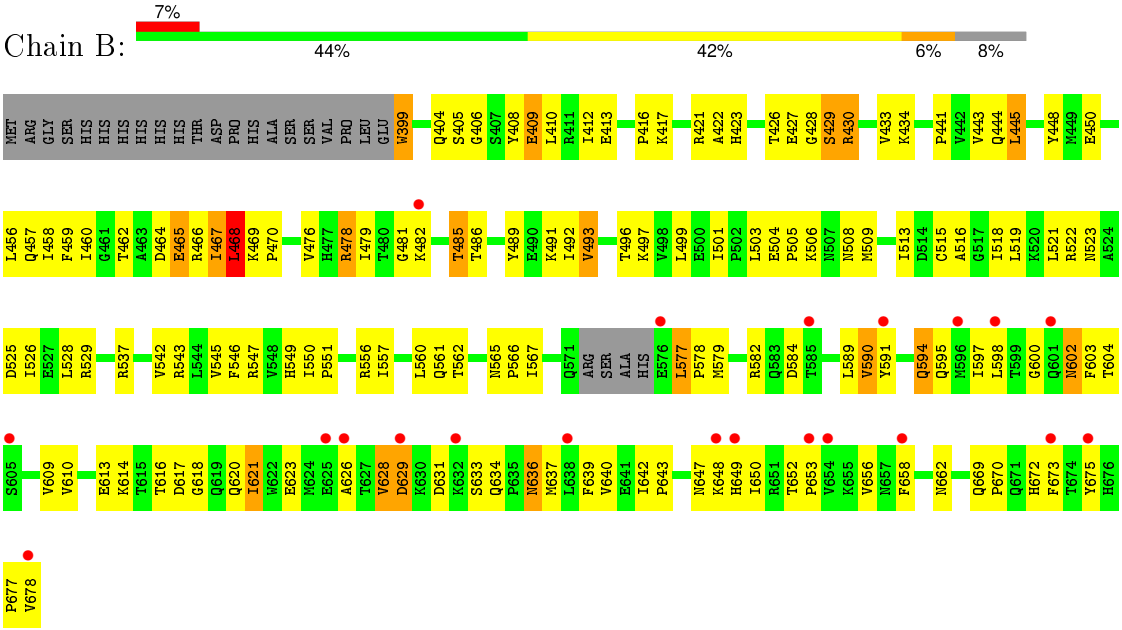
Chain W:





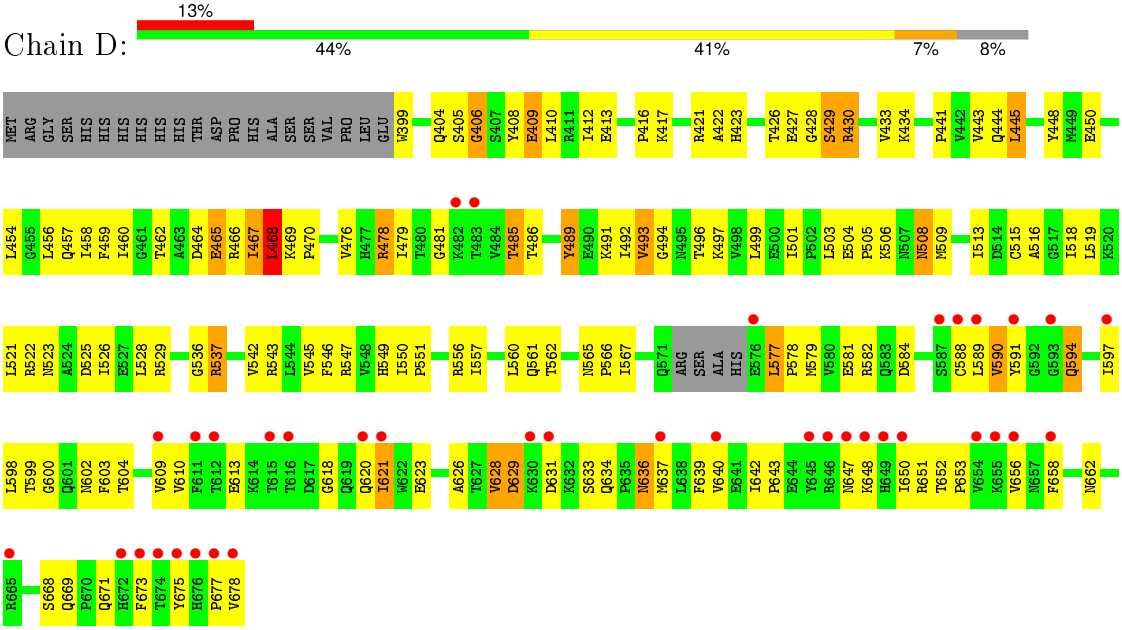
• Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain B:



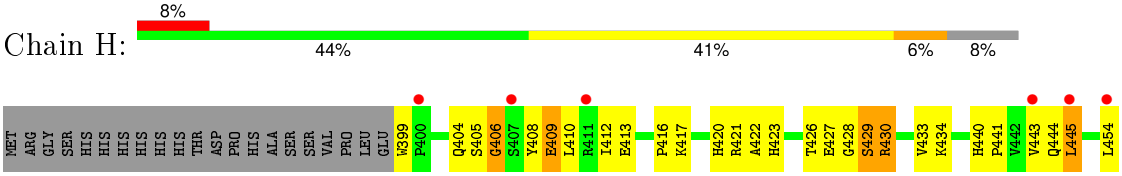
• Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

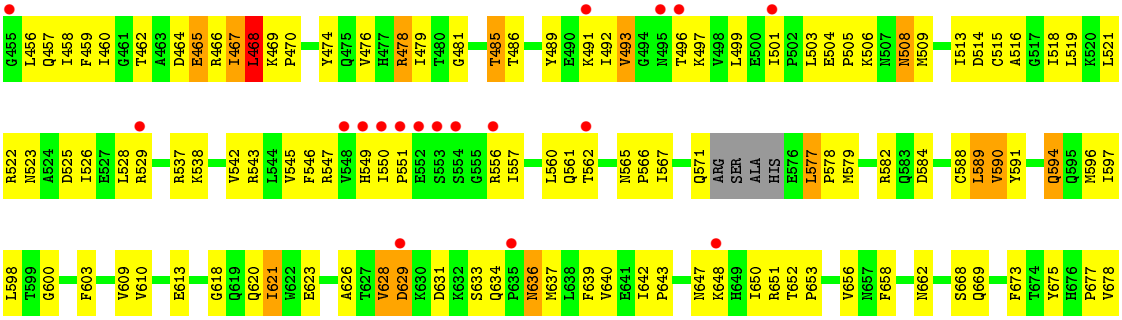
Chain D:



• Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

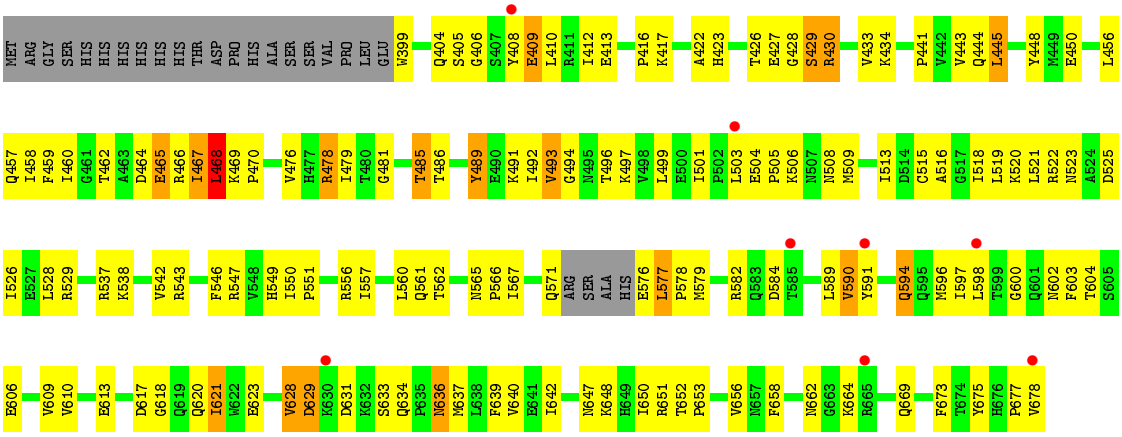
Chain H:





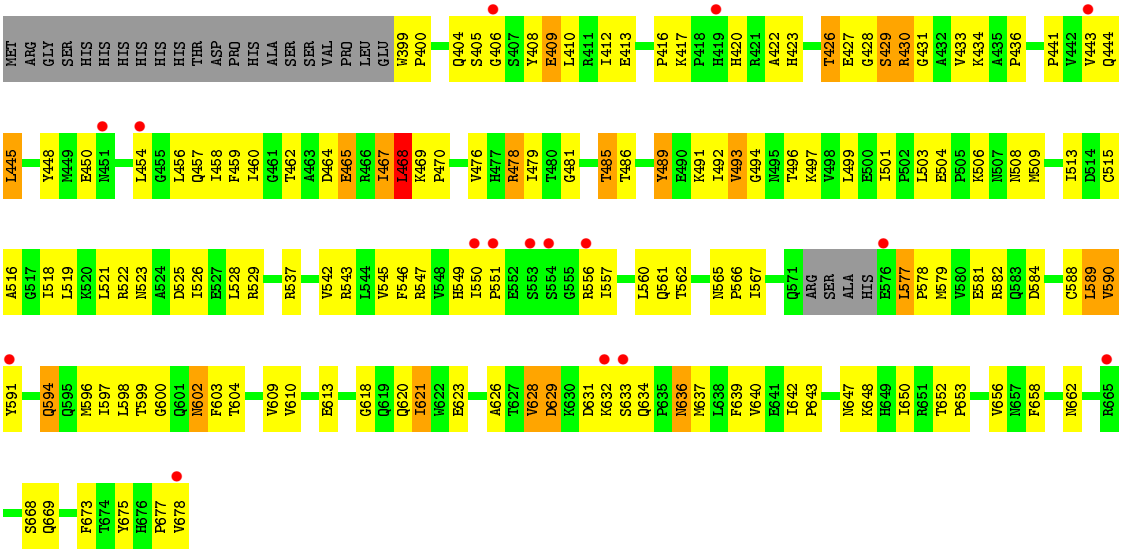
• Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain I:



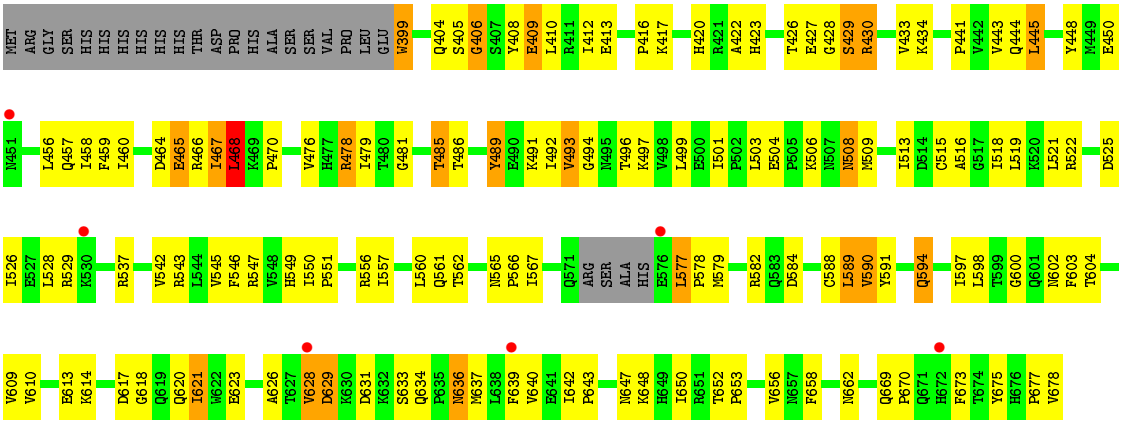
• Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain L:



• Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain M:


MET ARG GLY SER HIS HIS HIS HIS HIS HIS THR ASP PRO HIS ALA SER SER VAL PRO LEU GLU W399 Q404 S405 G406 S407 Y408 E409 L410 R411 I412 E413 P416 K417 H420 R421 A422 H423 T426 E427 G428 S429 R430 V433 K434 P441 V442 V443 Q444 L445 Y448 N449 E450
N451 L456 Q457 I458 F459 I460 D464 E465 R466 I467 L468 K469 P470 V476 H477 R478 I479 T480 G481 T485 T486 Y489 E490 K491 I492 V493 G494 N495 T496 K497 V498 L499 E500 I501 P502 L503 E504 P505 K506 N507 N508 M509 I513 D514 C515 A516 G517 I518 L519 K520 L521 R522 D525
I526 E527 L528 R529 K530 R537 V542 R543 L544 V545 F546 R547 V548 H549 I550 P551 R556 I557 L560 Q561 T562 N565 P566 I567 Q571 ARG SER ALA HIS E576 L577 P578 M579 R582 Q583 D584 C588 L589 V590 Y591 Q594 I597 L598 T599 G600 Q601 N602 F603 T604
V609 V610 E613 K614 D617 G618 Q619 Q620 I621 W622 E623 A626 T627 V628 D629 K630 D631 K632 S633 Q634 K635 N636 M637 L638 F639 V640 E641 I642 P643 N647 K648 H649 I650 R651 T652 P653 V656 M657 F658 N662 Q669 P670 Q671 H672 F673 T674 Y675 H676 P677 V678

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.70Å 122.90Å 241.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 3.10 49.11 – 3.10	Depositor EDS
% Data completeness (in resolution range)	82.4 (29.78-3.10) 82.3 (49.11-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.296 , 0.319 0.284 , 0.301	Depositor DCC
R_{free} test set	1857 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 65.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 37121 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	14952	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	T	0.90	0/319	0.96	2/491 (0.4%)
1	V	0.84	1/319 (0.3%)	0.86	0/491
1	X	0.85	0/319	0.98	2/491 (0.4%)
2	W	0.90	0/317	1.02	1/487 (0.2%)
2	Y	0.84	0/317	0.95	1/487 (0.2%)
2	Z	0.91	0/317	0.96	1/487 (0.2%)
3	B	0.45	0/2255	0.66	0/3048
3	D	0.43	0/2255	0.66	0/3048
3	H	0.42	0/2255	0.66	0/3048
3	I	0.42	0/2255	0.66	0/3048
3	L	0.41	0/2255	0.66	0/3048
3	M	0.42	0/2255	0.66	0/3048
All	All	0.50	1/15438 (0.0%)	0.71	7/21222 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	T	0	1
1	X	0	1
2	W	0	4
2	Y	0	1
2	Z	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	5	DG	C5-C6	-5.68	1.36	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	3	DG	N9-C1'-C2'	5.75	123.52	112.60
1	X	4	DA	N9-C1'-C2'	5.61	123.26	112.60
2	Y	4	DG	C5'-C4'-C3'	-5.44	104.30	114.10
2	W	5	DG	O5'-P-OP1	-5.35	100.88	105.70
1	X	9	DT	OP1-P-O3'	5.16	116.56	105.20
1	T	9	DT	C5'-C4'-C3'	-5.10	104.92	114.10
2	Z	3	DT	C5'-C4'-C3'	-5.06	104.98	114.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	4	DA	Sidechain
2	W	1	DA	Sidechain
2	W	3	DT	Sidechain
2	W	5	DG	Sidechain
2	W	8	DA	Sidechain
1	X	4	DA	Sidechain
2	Y	4	DG	Sidechain
2	Z	14	DC	Sidechain

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	T	285	0	161	18	0
1	V	285	0	161	32	0
1	X	285	0	161	33	0
2	W	283	0	160	28	0
2	Y	283	0	160	20	0
2	Z	283	0	160	25	0
3	B	2208	0	2214	168	1
3	D	2208	0	2214	174	0
3	H	2208	0	2214	163	0
3	I	2208	0	2214	167	1
3	L	2208	0	2214	170	0
3	M	2208	0	2214	163	0
All	All	14952	0	14247	1106	1

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

All (1106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:2:DA:H2"	2:W:3:DT:H5"	1.18	1.15
1:X:5:DG:H2"	1:X:6:DG:H5'	1.25	1.12
2:Y:4:DG:H2"	2:Y:5:DG:H5'	1.28	1.11
1:V:3:DG:C2'	1:V:4:DA:H5"	1.82	1.10
2:Y:2:DA:H2"	2:Y:3:DT:H5"	1.29	1.08
1:X:11:DT:H2"	1:X:12:DC:H5'	1.35	1.08
1:V:3:DG:H2"	1:V:4:DA:C5'	1.84	1.08
2:Y:4:DG:H2"	2:Y:5:DG:C5'	1.87	1.04
1:V:2:DT:H2"	1:V:3:DG:C5'	1.88	1.04
2:Z:10:DT:H2"	2:Z:11:DC:H5"	1.35	1.04
1:T:3:DG:H2"	1:T:4:DA:H5"	1.41	1.02
1:V:2:DT:H2"	1:V:3:DG:H5"	1.37	1.02
1:X:5:DG:H2"	1:X:6:DG:C5'	1.89	1.01
1:X:2:DT:H2"	1:X:3:DG:H5'	1.40	1.00
2:Z:1:DA:H2"	2:Z:2:DA:H5'	1.43	1.00
3:D:506:LYS:H	3:D:506:LYS:HD2	1.30	0.96
2:Y:2:DA:C2'	2:Y:3:DT:H5"	1.93	0.96
2:Z:10:DT:H2"	2:Z:11:DC:C5'	1.95	0.96
3:B:506:LYS:H	3:B:506:LYS:HD2	1.33	0.93
3:M:492:ILE:HG22	3:M:493:VAL:H	1.32	0.93
3:I:506:LYS:H	3:I:506:LYS:HD2	1.34	0.93
3:L:492:ILE:HG22	3:L:493:VAL:H	1.34	0.92
3:H:506:LYS:H	3:H:506:LYS:HD2	1.35	0.92
3:H:492:ILE:HG22	3:H:493:VAL:H	1.35	0.91
3:D:492:ILE:HG22	3:D:493:VAL:H	1.35	0.91
3:L:506:LYS:H	3:L:506:LYS:HD2	1.32	0.91
3:M:506:LYS:HD2	3:M:506:LYS:H	1.35	0.91
3:I:492:ILE:HG22	3:I:493:VAL:H	1.34	0.91
2:Y:2:DA:H2"	2:Y:3:DT:C5'	2.00	0.91
2:W:2:DA:C2'	2:W:3:DT:H5"	2.01	0.90
2:W:1:DA:H2"	2:W:2:DA:H5'	1.53	0.90
3:L:399:TRP:HB3	3:L:547:ARG:HH22	1.39	0.88
3:M:628:VAL:HG22	3:M:629:ASP:H	1.39	0.88
2:W:10:DT:H2"	2:W:11:DC:H5'	1.54	0.87
3:B:492:ILE:HG22	3:B:493:VAL:H	1.35	0.87
3:M:399:TRP:HB3	3:M:547:ARG:HH22	1.38	0.86
3:I:628:VAL:HG22	3:I:629:ASP:H	1.38	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1:DT:H2'	1:X:2:DT:H71	1.56	0.86
1:V:5:DG:H2"	1:V:6:DG:H5'	1.58	0.85
3:L:628:VAL:HG22	3:L:629:ASP:H	1.39	0.85
3:D:399:TRP:HB3	3:D:547:ARG:HH22	1.39	0.85
3:B:399:TRP:HB3	3:B:547:ARG:HH22	1.43	0.84
3:B:628:VAL:HG22	3:B:629:ASP:H	1.43	0.83
3:H:565:ASN:HB3	3:H:566:PRO:HD2	1.60	0.83
3:H:399:TRP:HB3	3:H:547:ARG:HH22	1.44	0.83
2:W:4:DG:H2"	2:W:5:DG:H5'	1.60	0.83
3:H:628:VAL:HG22	3:H:629:ASP:H	1.43	0.83
3:I:399:TRP:HB3	3:I:547:ARG:HH22	1.43	0.82
3:D:423:HIS:HB3	3:D:430:ARG:HG3	1.62	0.82
3:D:628:VAL:HG22	3:D:629:ASP:H	1.42	0.82
3:M:565:ASN:HB3	3:M:566:PRO:HD2	1.61	0.82
3:D:405:SER:HA	3:D:560:LEU:HD22	1.61	0.82
3:L:669:GLN:HG3	3:M:669:GLN:OE1	1.78	0.81
3:L:478:ARG:CZ	3:L:491:LYS:HE3	2.11	0.81
2:Z:10:DT:C2'	2:Z:11:DC:H5"	2.11	0.80
3:H:423:HIS:HB3	3:H:430:ARG:HG3	1.63	0.80
3:B:584:ASP:HB3	3:B:597:ILE:H	1.46	0.80
3:L:423:HIS:HB3	3:L:430:ARG:HG3	1.62	0.80
1:X:6:DG:H2"	1:X:7:DA:H5"	1.64	0.80
3:M:423:HIS:HB3	3:M:430:ARG:HG3	1.64	0.80
3:L:584:ASP:HB3	3:L:597:ILE:H	1.47	0.79
1:X:11:DT:H2"	1:X:12:DC:C5'	2.10	0.79
3:M:584:ASP:HB3	3:M:597:ILE:H	1.47	0.79
3:D:565:ASN:HB3	3:D:566:PRO:HD2	1.65	0.79
3:B:478:ARG:CZ	3:B:491:LYS:HE3	2.12	0.79
3:L:669:GLN:H	3:M:669:GLN:HE22	1.26	0.78
3:I:423:HIS:HB3	3:I:430:ARG:HG3	1.64	0.78
1:V:3:DG:H2"	1:V:4:DA:H5"	0.89	0.78
3:B:423:HIS:HB3	3:B:430:ARG:HG3	1.63	0.78
3:I:584:ASP:HB3	3:I:597:ILE:H	1.46	0.78
3:L:460:ILE:HG12	3:L:476:VAL:HG12	1.65	0.78
3:B:504:GLU:HB3	3:B:506:LYS:HD3	1.64	0.78
3:B:460:ILE:HG12	3:B:476:VAL:HG12	1.66	0.78
3:H:478:ARG:CZ	3:H:491:LYS:HE3	2.12	0.78
3:I:460:ILE:HG12	3:I:476:VAL:HG12	1.66	0.78
3:L:621:ILE:HD13	3:L:621:ILE:H	1.48	0.78
3:B:506:LYS:N	3:B:506:LYS:HD2	1.98	0.78
3:I:506:LYS:N	3:I:506:LYS:HD2	1.99	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:565:ASN:HB3	3:L:566:PRO:HD2	1.66	0.78
3:D:584:ASP:HB3	3:D:597:ILE:H	1.49	0.77
3:B:565:ASN:HB3	3:B:566:PRO:HD2	1.65	0.77
3:D:506:LYS:N	3:D:506:LYS:HD2	1.98	0.77
3:H:506:LYS:N	3:H:506:LYS:HD2	1.99	0.77
3:L:506:LYS:N	3:L:506:LYS:HD2	1.98	0.77
3:H:479:ILE:CG1	3:H:515:CYS:HA	2.15	0.77
3:M:479:ILE:HG13	3:M:515:CYS:HA	1.65	0.77
1:V:2:DT:H2"	1:V:3:DG:H5'	1.67	0.77
1:X:1:DT:H2"	1:X:2:DT:C5'	2.13	0.77
3:I:565:ASN:HB3	3:I:566:PRO:HD2	1.67	0.77
3:H:621:ILE:H	3:H:621:ILE:HD13	1.48	0.76
3:M:621:ILE:H	3:M:621:ILE:HD13	1.50	0.76
3:B:621:ILE:HD13	3:B:621:ILE:H	1.50	0.76
1:T:7:DA:H2"	1:T:8:DA:C8	2.20	0.76
3:D:460:ILE:HG12	3:D:476:VAL:HG12	1.67	0.76
3:I:479:ILE:HG13	3:I:515:CYS:HA	1.67	0.76
1:X:9:DT:H2"	1:X:10:DT:H5'	1.66	0.76
3:L:504:GLU:HB3	3:L:506:LYS:HD3	1.67	0.76
3:B:479:ILE:HG13	3:B:515:CYS:HA	1.67	0.76
1:T:3:DG:C2'	1:T:4:DA:H5"	2.16	0.76
3:H:479:ILE:HG13	3:H:515:CYS:HA	1.66	0.76
3:I:504:GLU:HB3	3:I:506:LYS:HD3	1.68	0.76
3:M:506:LYS:N	3:M:506:LYS:HD2	1.99	0.76
3:L:669:GLN:H	3:M:669:GLN:NE2	1.84	0.76
3:I:479:ILE:CG1	3:I:515:CYS:HA	2.16	0.76
3:H:584:ASP:HB3	3:H:597:ILE:H	1.48	0.76
3:D:504:GLU:HB3	3:D:506:LYS:HD3	1.67	0.76
3:M:460:ILE:HG12	3:M:476:VAL:HG12	1.68	0.76
3:M:478:ARG:CZ	3:M:491:LYS:HE3	2.16	0.75
2:W:7:DA:H2"	2:W:8:DA:H5'	1.68	0.75
3:M:405:SER:HA	3:M:560:LEU:HD22	1.67	0.75
3:D:621:ILE:HD13	3:D:621:ILE:H	1.51	0.75
3:L:479:ILE:HG13	3:L:515:CYS:HA	1.69	0.75
3:H:504:GLU:HB3	3:H:506:LYS:HD3	1.67	0.75
1:X:9:DT:H2"	1:X:10:DT:C5'	2.16	0.75
3:I:478:ARG:CZ	3:I:491:LYS:HE3	2.16	0.75
3:L:478:ARG:NE	3:L:491:LYS:HE3	2.02	0.74
3:I:621:ILE:HD13	3:I:621:ILE:H	1.50	0.74
3:H:460:ILE:HG12	3:H:476:VAL:HG12	1.68	0.74
1:T:6:DG:H2"	1:T:7:DA:O5'	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:405:SER:HA	3:H:560:LEU:HD22	1.68	0.74
3:M:504:GLU:HB3	3:M:506:LYS:HD3	1.68	0.74
2:W:2:DA:H2"	2:W:3:DT:C5'	2.09	0.74
3:M:479:ILE:CG1	3:M:515:CYS:HA	2.17	0.74
3:B:405:SER:HA	3:B:560:LEU:HD22	1.69	0.73
3:D:479:ILE:HG13	3:D:515:CYS:HA	1.69	0.73
3:B:669:GLN:HE22	3:D:668:SER:CA	2.01	0.73
3:L:405:SER:HA	3:L:560:LEU:HD22	1.68	0.73
1:V:1:DT:C6	1:V:2:DT:H72	2.23	0.73
3:H:613:GLU:HG2	3:H:621:ILE:HD11	1.71	0.73
3:B:479:ILE:CG1	3:B:515:CYS:HA	2.18	0.73
3:H:528:LEU:HD13	3:H:528:LEU:O	1.89	0.73
3:B:528:LEU:O	3:B:528:LEU:HD13	1.88	0.73
3:D:478:ARG:CZ	3:D:491:LYS:HE3	2.17	0.73
3:D:491:LYS:HZ3	3:D:497:LYS:HD2	1.53	0.73
3:L:479:ILE:CG1	3:L:515:CYS:HA	2.19	0.73
3:I:613:GLU:HG2	3:I:621:ILE:HD11	1.71	0.73
3:B:506:LYS:CD	3:B:506:LYS:H	2.02	0.72
1:V:7:DA:P	3:I:664:LYS:HB3	2.29	0.72
3:B:482:LYS:HB3	3:I:606:GLU:OE2	1.90	0.72
2:Z:2:DA:H2"	2:Z:3:DT:O5'	1.90	0.72
3:H:478:ARG:NE	3:H:491:LYS:HE3	2.05	0.72
3:L:506:LYS:H	3:L:506:LYS:CD	2.03	0.71
3:B:478:ARG:NE	3:B:491:LYS:HE3	2.05	0.71
1:X:1:DT:H2"	1:X:2:DT:H5'	1.72	0.71
3:I:506:LYS:CD	3:I:506:LYS:H	2.03	0.71
3:M:613:GLU:HG2	3:M:621:ILE:HD11	1.73	0.71
3:B:491:LYS:NZ	3:B:497:LYS:HD2	2.06	0.71
3:D:613:GLU:HG2	3:D:621:ILE:HD11	1.72	0.71
3:D:479:ILE:CG1	3:D:515:CYS:HA	2.20	0.71
3:D:491:LYS:NZ	3:D:497:LYS:HD2	2.05	0.71
3:H:460:ILE:HG23	3:H:542:VAL:CG1	2.22	0.70
3:D:399:TRP:HB3	3:D:547:ARG:NH2	2.06	0.70
1:X:11:DT:H5"	3:L:426:THR:HG21	1.74	0.70
2:Z:3:DT:OP1	2:Z:3:DT:H4'	1.91	0.70
3:I:478:ARG:NE	3:I:491:LYS:HE3	2.07	0.70
2:Z:1:DA:H2"	2:Z:2:DA:C5'	2.19	0.70
3:D:506:LYS:H	3:D:506:LYS:CD	2.03	0.70
3:L:669:GLN:N	3:M:669:GLN:HE22	1.90	0.70
3:L:528:LEU:HD13	3:L:528:LEU:O	1.91	0.70
3:M:528:LEU:O	3:M:528:LEU:HD13	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:506:LYS:CD	3:M:506:LYS:H	2.04	0.69
3:H:491:LYS:NZ	3:H:497:LYS:HD2	2.08	0.69
3:L:578:PRO:HD3	3:L:662:ASN:ND2	2.08	0.69
3:L:399:TRP:CB	3:L:547:ARG:HH12	2.04	0.69
1:V:5:DG:H1'	1:V:6:DG:H5"	1.75	0.69
2:Z:11:DC:H2"	2:Z:12:DC:H5'	1.75	0.69
2:Z:5:DG:H2"	2:Z:6:DA:O5'	1.93	0.69
3:I:528:LEU:O	3:I:528:LEU:HD13	1.93	0.69
3:M:399:TRP:HB3	3:M:547:ARG:NH2	2.07	0.68
3:H:399:TRP:CB	3:H:547:ARG:HH12	2.05	0.68
3:L:613:GLU:HG2	3:L:621:ILE:HD11	1.75	0.68
3:M:460:ILE:HG23	3:M:542:VAL:CG1	2.24	0.68
3:I:491:LYS:NZ	3:I:497:LYS:HD2	2.08	0.68
3:M:578:PRO:HD3	3:M:662:ASN:ND2	2.07	0.68
3:L:399:TRP:HB3	3:L:547:ARG:NH2	2.06	0.68
3:D:481:GLY:HA3	3:D:485:THR:HB	1.75	0.68
3:I:628:VAL:HG22	3:I:629:ASP:N	2.08	0.68
3:I:399:TRP:CB	3:I:547:ARG:HH12	2.06	0.68
3:M:478:ARG:NE	3:M:491:LYS:HE3	2.09	0.68
3:H:460:ILE:HG23	3:H:542:VAL:HG11	1.75	0.68
3:L:460:ILE:HG23	3:L:542:VAL:CG1	2.24	0.68
3:I:405:SER:HA	3:I:560:LEU:HD22	1.73	0.68
3:L:481:GLY:HA3	3:L:485:THR:HB	1.75	0.68
3:B:613:GLU:HG2	3:B:621:ILE:HD11	1.74	0.68
3:H:634:GLN:HB2	3:H:637:MET:HB3	1.76	0.67
3:L:399:TRP:HB2	3:L:547:ARG:HH12	1.58	0.67
3:D:578:PRO:HD3	3:D:662:ASN:ND2	2.08	0.67
3:M:481:GLY:HA3	3:M:485:THR:HB	1.75	0.67
3:I:481:GLY:HA3	3:I:485:THR:HB	1.76	0.67
3:B:634:GLN:HB2	3:B:637:MET:HB3	1.75	0.67
2:W:5:DG:H2"	2:W:6:DA:O5'	1.95	0.67
2:Z:12:DC:H2'	2:Z:13:DT:H71	1.75	0.67
3:L:634:GLN:HB2	3:L:637:MET:HB3	1.76	0.67
3:I:399:TRP:HB3	3:I:547:ARG:NH2	2.10	0.67
3:B:669:GLN:NE2	3:D:668:SER:HA	2.09	0.67
3:I:634:GLN:HB2	3:I:637:MET:HB3	1.77	0.67
3:D:634:GLN:HB2	3:D:637:MET:HB3	1.76	0.67
3:H:669:GLN:HG3	3:I:669:GLN:OE1	1.95	0.67
3:M:491:LYS:NZ	3:M:497:LYS:HD2	2.10	0.66
3:D:399:TRP:CB	3:D:547:ARG:HH12	2.07	0.66
3:H:636:ASN:H	3:H:636:ASN:HD22	1.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:399:TRP:CB	3:M:547:ARG:HH12	2.08	0.66
3:B:399:TRP:HB3	3:B:547:ARG:NH2	2.10	0.66
3:L:491:LYS:NZ	3:L:497:LYS:HD2	2.10	0.66
3:H:491:LYS:HZ3	3:H:497:LYS:HD2	1.60	0.66
3:H:459:PHE:HA	3:H:476:VAL:HG11	1.76	0.66
1:V:6:DG:H2"	1:V:7:DA:O5'	1.96	0.66
3:M:399:TRP:HB2	3:M:547:ARG:HH12	1.60	0.66
3:B:399:TRP:CB	3:B:547:ARG:HH12	2.08	0.66
1:X:2:DT:H2"	1:X:3:DG:C5'	2.23	0.66
3:L:628:VAL:HG22	3:L:629:ASP:N	2.10	0.66
3:L:636:ASN:HD22	3:L:636:ASN:H	1.42	0.66
3:B:578:PRO:HD3	3:B:662:ASN:ND2	2.10	0.66
3:H:506:LYS:H	3:H:506:LYS:CD	2.06	0.66
3:B:491:LYS:HZ3	3:B:497:LYS:HD2	1.61	0.66
3:B:481:GLY:HA3	3:B:485:THR:HB	1.77	0.66
3:D:478:ARG:NE	3:D:491:LYS:HE3	2.10	0.66
3:I:636:ASN:HD22	3:I:636:ASN:H	1.43	0.66
2:Y:3:DT:H2"	2:Y:4:DG:C8	2.31	0.65
3:H:399:TRP:HB3	3:H:547:ARG:NH2	2.10	0.65
3:I:399:TRP:HB2	3:I:547:ARG:HH12	1.60	0.65
1:X:1:DT:H2"	1:X:2:DT:H5"	1.79	0.65
3:L:430:ARG:HH11	3:L:430:ARG:HG3	1.61	0.65
3:I:578:PRO:HD3	3:I:662:ASN:ND2	2.10	0.65
3:D:399:TRP:HB2	3:D:547:ARG:HH12	1.61	0.65
1:V:7:DA:OP1	3:I:664:LYS:HB3	1.96	0.65
1:X:6:DG:C2'	1:X:7:DA:H5"	2.27	0.65
3:L:410:LEU:O	3:L:562:THR:HG21	1.97	0.65
2:Y:4:DG:C2'	2:Y:5:DG:C5'	2.72	0.65
3:H:481:GLY:HA3	3:H:485:THR:HB	1.77	0.65
3:M:636:ASN:H	3:M:636:ASN:HD22	1.43	0.65
1:T:9:DT:H2"	1:T:10:DT:H5'	1.78	0.65
3:D:636:ASN:HD22	3:D:636:ASN:H	1.45	0.64
2:W:1:DA:HO5'	2:W:1:DA:H8	1.43	0.64
3:M:634:GLN:HB2	3:M:637:MET:HB3	1.78	0.64
3:B:460:ILE:HG23	3:B:542:VAL:CG1	2.27	0.64
1:T:5:DG:H2"	1:T:6:DG:H5'	1.78	0.64
3:D:628:VAL:HG22	3:D:629:ASP:N	2.12	0.64
3:L:542:VAL:CG1	3:L:543:ARG:N	2.61	0.64
3:D:598:LEU:HD21	3:D:658:PHE:HE1	1.63	0.64
3:H:399:TRP:HB2	3:H:547:ARG:HH12	1.62	0.64
3:M:479:ILE:HD12	3:M:479:ILE:O	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:460:ILE:HG23	3:D:542:VAL:CG1	2.28	0.64
3:H:542:VAL:CG1	3:H:543:ARG:N	2.61	0.64
3:L:581:GLU:OE1	3:M:614:LYS:HD2	1.97	0.64
3:B:598:LEU:HD21	3:B:658:PHE:HE1	1.63	0.64
2:W:10:DT:H2"	2:W:11:DC:C5'	2.26	0.63
3:M:410:LEU:O	3:M:562:THR:HG21	1.98	0.63
3:D:528:LEU:O	3:D:528:LEU:HD13	1.98	0.63
3:M:628:VAL:HG22	3:M:629:ASP:N	2.10	0.63
3:H:628:VAL:HG22	3:H:629:ASP:N	2.13	0.63
1:V:2:DT:C2'	1:V:3:DG:C5'	2.71	0.63
3:B:479:ILE:HD12	3:B:481:GLY:H	1.64	0.63
2:Y:4:DG:H2"	2:Y:5:DG:H5"	1.75	0.63
3:H:598:LEU:HD21	3:H:658:PHE:HE1	1.64	0.62
3:L:459:PHE:HA	3:L:476:VAL:HG11	1.81	0.62
2:Z:10:DT:H2"	2:Z:11:DC:H5'	1.82	0.62
3:B:636:ASN:HD22	3:B:636:ASN:H	1.48	0.62
3:L:542:VAL:HG12	3:L:543:ARG:N	2.14	0.62
2:Z:3:DT:H2"	2:Z:4:DG:C8	2.35	0.62
3:B:628:VAL:HG22	3:B:629:ASP:N	2.13	0.62
3:L:479:ILE:HD12	3:L:481:GLY:H	1.64	0.62
3:D:459:PHE:HA	3:D:476:VAL:HG11	1.80	0.62
3:I:479:ILE:O	3:I:479:ILE:HD12	2.00	0.62
3:L:598:LEU:HD21	3:L:658:PHE:HE1	1.64	0.62
3:I:460:ILE:HG23	3:I:542:VAL:CG1	2.30	0.61
3:B:399:TRP:HB2	3:B:547:ARG:HH12	1.63	0.61
3:I:491:LYS:HZ3	3:I:497:LYS:HD2	1.65	0.61
3:H:578:PRO:HD3	3:H:662:ASN:ND2	2.15	0.61
3:B:459:PHE:HA	3:B:476:VAL:HG11	1.81	0.61
3:I:584:ASP:CB	3:I:597:ILE:H	2.13	0.61
3:H:478:ARG:HB3	3:H:499:LEU:HD21	1.82	0.61
3:I:636:ASN:N	3:I:636:ASN:HD22	1.98	0.61
3:L:598:LEU:HD21	3:L:658:PHE:CE1	2.35	0.61
3:I:459:PHE:HA	3:I:476:VAL:HG11	1.83	0.61
3:D:542:VAL:CG1	3:D:543:ARG:N	2.62	0.61
2:W:4:DG:H2"	2:W:5:DG:C5'	2.30	0.61
3:B:542:VAL:CG1	3:B:543:ARG:N	2.64	0.61
2:Y:5:DG:H2"	2:Y:6:DA:O5'	2.00	0.61
3:B:427:GLU:CD	3:B:430:ARG:HH12	2.04	0.61
3:D:410:LEU:O	3:D:562:THR:HG21	2.00	0.61
3:M:631:ASP:C	3:M:633:SER:H	2.04	0.61
3:I:479:ILE:HD12	3:I:481:GLY:H	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:459:PHE:HA	3:M:476:VAL:HG11	1.83	0.61
3:H:542:VAL:HG12	3:H:543:ARG:N	2.15	0.61
3:L:584:ASP:CB	3:L:597:ILE:H	2.14	0.60
3:B:479:ILE:HD12	3:B:479:ILE:O	2.01	0.60
3:M:492:ILE:HG22	3:M:493:VAL:N	2.11	0.60
3:L:636:ASN:N	3:L:636:ASN:HD22	1.97	0.60
3:I:542:VAL:CG1	3:I:543:ARG:N	2.65	0.60
3:H:459:PHE:HA	3:H:476:VAL:CG1	2.31	0.60
3:D:598:LEU:HD21	3:D:658:PHE:CE1	2.37	0.60
3:L:460:ILE:HG23	3:L:542:VAL:HG11	1.82	0.60
2:Z:11:DC:H2"	2:Z:12:DC:C5'	2.32	0.60
2:W:11:DC:H2"	2:W:12:DC:H5'	1.84	0.60
3:D:479:ILE:HD12	3:D:481:GLY:H	1.66	0.60
3:H:636:ASN:N	3:H:636:ASN:HD22	1.99	0.60
3:B:598:LEU:HD21	3:B:658:PHE:CE1	2.36	0.60
3:L:413:GLU:HG3	3:L:444:GLN:HE21	1.65	0.60
3:H:445:LEU:HD11	3:H:550:ILE:HD11	1.84	0.60
1:X:2:DT:C2'	1:X:3:DG:H5'	2.23	0.60
3:H:479:ILE:HD12	3:H:481:GLY:H	1.66	0.60
3:D:556:ARG:HG2	3:D:557:ILE:H	1.64	0.60
3:M:584:ASP:CB	3:M:597:ILE:H	2.14	0.60
3:M:478:ARG:HB3	3:M:499:LEU:HD21	1.84	0.60
3:L:478:ARG:HB3	3:L:499:LEU:HD21	1.83	0.59
3:I:478:ARG:HB3	3:I:499:LEU:HD21	1.83	0.59
3:H:410:LEU:O	3:H:562:THR:HG21	2.00	0.59
3:I:598:LEU:HD21	3:I:658:PHE:HE1	1.66	0.59
2:Z:6:DA:H2"	2:Z:7:DA:C8	2.38	0.59
3:D:479:ILE:O	3:D:479:ILE:HD12	2.02	0.59
3:B:614:LYS:HD2	3:D:581:GLU:OE1	2.02	0.59
3:L:436:PRO:HG3	3:L:632:LYS:HE2	1.84	0.59
3:D:478:ARG:HB3	3:D:499:LEU:HD21	1.84	0.59
3:I:427:GLU:CD	3:I:430:ARG:HH12	2.05	0.59
3:L:556:ARG:HG2	3:L:557:ILE:H	1.67	0.59
3:M:479:ILE:HD12	3:M:481:GLY:H	1.67	0.59
3:H:598:LEU:HD21	3:H:658:PHE:CE1	2.38	0.59
3:I:410:LEU:O	3:I:562:THR:HG21	2.02	0.59
3:H:628:VAL:HG13	3:H:629:ASP:N	2.17	0.59
3:M:636:ASN:N	3:M:636:ASN:HD22	1.98	0.59
3:M:542:VAL:CG1	3:M:543:ARG:N	2.66	0.59
3:H:441:PRO:HG2	3:H:513:ILE:HB	1.84	0.59
3:H:413:GLU:HG3	3:H:444:GLN:HE21	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:460:ILE:HG23	3:M:542:VAL:HG11	1.84	0.59
3:B:669:GLN:HE22	3:D:668:SER:HB2	1.67	0.59
3:M:556:ARG:HG2	3:M:557:ILE:H	1.68	0.59
3:I:571:GLN:O	3:I:576:GLU:OE2	2.20	0.59
1:X:7:DA:H2"	1:X:8:DA:C8	2.38	0.58
3:L:430:ARG:HH11	3:L:430:ARG:CG	2.16	0.58
3:I:598:LEU:HD21	3:I:658:PHE:CE1	2.38	0.58
1:V:2:DT:C2'	1:V:3:DG:H5"	2.23	0.58
3:D:542:VAL:HG12	3:D:543:ARG:N	2.16	0.58
3:M:491:LYS:HZ3	3:M:497:LYS:HD2	1.68	0.58
3:B:410:LEU:O	3:B:562:THR:HG21	2.02	0.58
3:L:631:ASP:C	3:L:633:SER:H	2.07	0.58
3:M:430:ARG:HH11	3:M:430:ARG:HG3	1.68	0.58
3:H:479:ILE:HD12	3:H:479:ILE:O	2.03	0.58
3:M:413:GLU:HG3	3:M:444:GLN:HE21	1.67	0.58
3:L:423:HIS:HB3	3:L:430:ARG:CG	2.31	0.58
3:B:459:PHE:HA	3:B:476:VAL:CG1	2.34	0.58
3:H:584:ASP:CB	3:H:597:ILE:H	2.16	0.58
3:B:669:GLN:HE22	3:D:668:SER:CB	2.15	0.58
3:D:636:ASN:HD22	3:D:636:ASN:N	2.00	0.58
3:I:413:GLU:HG3	3:I:444:GLN:HE21	1.69	0.58
3:M:598:LEU:HD21	3:M:658:PHE:HE1	1.68	0.58
3:B:556:ARG:HG2	3:B:557:ILE:H	1.68	0.58
3:B:669:GLN:HE22	3:D:668:SER:HA	1.64	0.58
3:L:445:LEU:HD11	3:L:550:ILE:HD11	1.85	0.58
3:H:631:ASP:C	3:H:633:SER:H	2.06	0.58
1:X:8:DA:H2"	1:X:9:DT:OP2	2.03	0.58
3:B:636:ASN:HD22	3:B:636:ASN:N	2.01	0.58
3:D:413:GLU:HG3	3:D:444:GLN:HE21	1.69	0.58
3:L:478:ARG:HG2	3:L:491:LYS:HD2	1.85	0.58
3:B:584:ASP:CB	3:B:597:ILE:H	2.15	0.57
3:B:542:VAL:HG12	3:B:543:ARG:N	2.18	0.57
3:H:408:TYR:O	3:H:409:GLU:HB2	2.04	0.57
3:L:491:LYS:HZ3	3:L:497:LYS:HD2	1.69	0.57
3:I:526:ILE:O	3:I:529:ARG:HG2	2.04	0.57
3:M:526:ILE:O	3:M:529:ARG:HG2	2.04	0.57
1:V:2:DT:C2'	1:V:3:DG:H5'	2.33	0.57
3:I:631:ASP:C	3:I:633:SER:H	2.07	0.57
3:H:427:GLU:CD	3:H:430:ARG:HH12	2.08	0.57
3:D:460:ILE:HG23	3:D:542:VAL:HG11	1.86	0.57
3:M:542:VAL:HG12	3:M:543:ARG:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:492:ILE:HG22	3:I:493:VAL:N	2.13	0.57
3:B:650:ILE:HG13	3:B:677:PRO:HB3	1.87	0.57
3:B:430:ARG:HH11	3:B:430:ARG:HG3	1.69	0.57
3:I:503:LEU:HB3	3:I:509:MET:CE	2.35	0.57
1:V:5:DG:H1'	1:V:6:DG:C5'	2.34	0.57
3:H:417:LYS:HG3	3:H:434:LYS:O	2.04	0.57
3:B:460:ILE:HG23	3:B:542:VAL:HG11	1.85	0.57
3:I:467:ILE:O	3:I:468:LEU:C	2.42	0.57
3:B:413:GLU:HG3	3:B:444:GLN:HE21	1.68	0.57
3:L:427:GLU:CD	3:L:430:ARG:HH12	2.08	0.57
3:B:467:ILE:O	3:B:468:LEU:C	2.43	0.57
3:M:459:PHE:HA	3:M:476:VAL:CG1	2.34	0.57
3:D:459:PHE:HA	3:D:476:VAL:CG1	2.35	0.56
3:B:408:TYR:O	3:B:409:GLU:HB2	2.05	0.56
3:I:628:VAL:HG13	3:I:629:ASP:N	2.20	0.56
2:W:12:DC:H5'	2:W:12:DC:H6	1.69	0.56
3:D:628:VAL:HG13	3:D:629:ASP:N	2.20	0.56
3:D:631:ASP:C	3:D:633:SER:H	2.07	0.56
3:B:478:ARG:HB3	3:B:499:LEU:HD21	1.87	0.56
3:M:648:LYS:C	3:M:648:LYS:HD3	2.26	0.56
3:D:613:GLU:O	3:D:621:ILE:HD13	2.06	0.56
3:M:503:LEU:HB3	3:M:509:MET:HE3	1.87	0.56
3:D:650:ILE:HG13	3:D:677:PRO:HB3	1.87	0.56
3:D:427:GLU:CD	3:D:430:ARG:HH12	2.07	0.56
3:H:423:HIS:HB3	3:H:430:ARG:CG	2.34	0.56
2:Z:7:DA:H1'	2:Z:8:DA:H5'	1.87	0.56
3:M:427:GLU:CD	3:M:430:ARG:HH12	2.09	0.56
3:M:598:LEU:HD21	3:M:658:PHE:CE1	2.41	0.56
2:Y:12:DC:H1'	2:Y:13:DT:H5"	1.87	0.56
3:I:408:TYR:O	3:I:409:GLU:HB2	2.05	0.56
3:B:526:ILE:O	3:B:529:ARG:HG2	2.06	0.56
3:H:478:ARG:HG2	3:H:491:LYS:HD2	1.88	0.56
3:I:441:PRO:HG2	3:I:513:ILE:HB	1.88	0.56
3:I:556:ARG:HG2	3:I:557:ILE:H	1.71	0.56
3:M:478:ARG:H	3:M:478:ARG:HD2	1.71	0.56
3:D:478:ARG:HG2	3:D:491:LYS:HD2	1.87	0.56
3:H:556:ARG:HG2	3:H:557:ILE:H	1.71	0.56
3:D:620:GLN:OE1	3:D:623:GLU:HB2	2.06	0.56
3:B:670:PRO:HD3	3:D:579:MET:HB3	1.88	0.56
3:M:501:ILE:C	3:M:501:ILE:HD12	2.26	0.56
3:I:430:ARG:HG3	3:I:430:ARG:HH11	1.69	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:526:ILE:O	3:H:529:ARG:HG2	2.06	0.55
1:V:5:DG:C2'	1:V:6:DG:H5'	2.35	0.55
3:B:423:HIS:HB3	3:B:430:ARG:CG	2.35	0.55
3:L:417:LYS:HG3	3:L:434:LYS:O	2.05	0.55
3:D:467:ILE:O	3:D:468:LEU:C	2.45	0.55
3:I:566:PRO:O	3:I:567:ILE:HD13	2.06	0.55
3:D:526:ILE:O	3:D:529:ARG:HG2	2.06	0.55
3:L:526:ILE:O	3:L:529:ARG:HG2	2.06	0.55
3:I:459:PHE:HA	3:I:476:VAL:CG1	2.37	0.55
3:M:408:TYR:O	3:M:409:GLU:HB2	2.06	0.55
3:D:423:HIS:HB3	3:D:430:ARG:CG	2.33	0.55
3:I:460:ILE:HG23	3:I:542:VAL:HG11	1.88	0.55
3:M:441:PRO:HG2	3:M:513:ILE:HB	1.89	0.55
3:L:459:PHE:HA	3:L:476:VAL:CG1	2.36	0.55
3:H:492:ILE:HG22	3:H:493:VAL:N	2.15	0.55
3:M:399:TRP:HB2	3:M:547:ARG:NH1	2.22	0.55
3:L:628:VAL:HG13	3:L:629:ASP:N	2.22	0.55
3:I:648:LYS:HD3	3:I:648:LYS:C	2.26	0.55
3:L:441:PRO:HG2	3:L:513:ILE:HB	1.89	0.55
3:B:492:ILE:HG22	3:B:493:VAL:N	2.15	0.55
3:M:417:LYS:HG3	3:M:434:LYS:O	2.07	0.55
3:L:408:TYR:O	3:L:409:GLU:HB2	2.06	0.55
3:B:648:LYS:HD3	3:B:648:LYS:C	2.27	0.55
1:V:2:DT:O2	2:W:1:DA:H2	1.90	0.54
3:I:417:LYS:HG3	3:I:434:LYS:O	2.06	0.54
3:L:479:ILE:O	3:L:479:ILE:HD12	2.06	0.54
3:I:445:LEU:HD11	3:I:550:ILE:HD11	1.89	0.54
3:H:648:LYS:C	3:H:648:LYS:HD3	2.27	0.54
3:D:648:LYS:HD3	3:D:648:LYS:C	2.26	0.54
3:B:427:GLU:OE1	3:B:430:ARG:NH1	2.40	0.54
3:I:542:VAL:HG12	3:I:543:ARG:N	2.22	0.54
3:H:613:GLU:O	3:H:621:ILE:HD13	2.05	0.54
3:H:650:ILE:HG13	3:H:677:PRO:HB3	1.88	0.54
3:B:582:ARG:NH1	3:B:582:ARG:HB2	2.23	0.54
1:T:13:DC:H2"	1:T:14:DA:C8	2.42	0.54
2:W:12:DC:H5'	2:W:12:DC:C6	2.42	0.54
3:I:399:TRP:HB2	3:I:547:ARG:NH1	2.23	0.54
3:D:584:ASP:CB	3:D:597:ILE:H	2.17	0.54
3:M:620:GLN:OE1	3:M:623:GLU:HB2	2.07	0.54
3:H:430:ARG:HG3	3:H:430:ARG:HH11	1.72	0.54
3:H:620:GLN:OE1	3:H:623:GLU:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:584:ASP:HB2	3:M:597:ILE:HB	1.88	0.54
3:D:422:ALA:HB1	3:D:518:ILE:O	2.07	0.54
1:V:4:DA:H4'	1:V:4:DA:OP1	2.08	0.54
3:M:547:ARG:HG2	3:M:561:GLN:HB2	1.90	0.54
3:M:417:LYS:O	3:M:567:ILE:HD12	2.08	0.54
3:B:441:PRO:HG2	3:B:513:ILE:HB	1.90	0.54
3:D:582:ARG:HB2	3:D:582:ARG:NH1	2.23	0.54
3:L:620:GLN:OE1	3:L:623:GLU:HB2	2.07	0.54
3:B:631:ASP:C	3:B:633:SER:H	2.09	0.54
3:D:417:LYS:O	3:D:567:ILE:HD12	2.07	0.54
1:X:9:DT:H2"	1:X:10:DT:H5"	1.89	0.54
3:D:399:TRP:HB2	3:D:547:ARG:NH1	2.23	0.54
3:B:547:ARG:HG2	3:B:561:GLN:HB2	1.90	0.54
3:M:478:ARG:N	3:M:478:ARG:HD2	2.22	0.54
3:I:503:LEU:HB3	3:I:509:MET:HE3	1.90	0.54
3:L:648:LYS:HD3	3:L:648:LYS:C	2.28	0.54
1:X:7:DA:H2"	1:X:8:DA:H8	1.71	0.54
3:H:547:ARG:HG2	3:H:561:GLN:HB2	1.90	0.54
3:H:478:ARG:H	3:H:478:ARG:HD2	1.73	0.54
3:H:501:ILE:HD12	3:H:501:ILE:C	2.28	0.54
3:D:445:LEU:HD11	3:D:550:ILE:HD11	1.89	0.54
3:H:503:LEU:HB3	3:H:509:MET:CE	2.38	0.54
1:X:12:DC:H2"	1:X:13:DC:H5'	1.90	0.53
3:I:464:ASP:O	3:I:465:GLU:HG2	2.09	0.53
3:L:578:PRO:HD3	3:L:662:ASN:HD22	1.72	0.53
3:I:571:GLN:O	3:I:576:GLU:OE1	2.27	0.53
3:L:549:HIS:O	3:L:551:PRO:HD3	2.08	0.53
3:I:522:ARG:HB2	3:I:525:ASP:OD2	2.09	0.53
3:D:501:ILE:HD12	3:D:501:ILE:C	2.29	0.53
3:D:430:ARG:HH11	3:D:430:ARG:HG3	1.73	0.53
3:H:669:GLN:H	3:I:669:GLN:HE22	1.56	0.53
3:I:571:GLN:O	3:I:576:GLU:CD	2.47	0.53
3:I:501:ILE:HD12	3:I:501:ILE:C	2.28	0.53
3:I:650:ILE:HG13	3:I:677:PRO:HB3	1.89	0.53
1:X:3:DG:H2"	1:X:4:DA:OP2	2.09	0.53
3:M:478:ARG:HG2	3:M:491:LYS:HD2	1.90	0.53
3:M:578:PRO:HD3	3:M:662:ASN:HD22	1.70	0.53
3:L:456:LEU:HD23	3:L:501:ILE:HD11	1.91	0.53
3:D:408:TYR:O	3:D:409:GLU:HB2	2.07	0.53
3:B:620:GLN:OE1	3:B:623:GLU:HB2	2.09	0.53
3:B:628:VAL:HG13	3:B:629:ASP:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:441:PRO:HG2	3:D:513:ILE:HB	1.89	0.53
3:I:584:ASP:HB2	3:I:597:ILE:HB	1.90	0.53
3:L:399:TRP:HB2	3:L:547:ARG:NH1	2.22	0.53
3:B:617:ASP:HA	3:D:637:MET:SD	2.48	0.53
3:I:478:ARG:N	3:I:478:ARG:HD2	2.24	0.53
3:H:467:ILE:O	3:H:468:LEU:C	2.47	0.53
2:Z:8:DA:H2"	2:Z:9:DT:H5'	1.90	0.53
3:D:478:ARG:HD2	3:D:478:ARG:H	1.73	0.53
3:B:600:GLY:N	3:B:603:PHE:HE2	2.06	0.53
2:Y:14:DC:H2"	2:Z:1:DA:C8	2.43	0.53
3:H:399:TRP:HB2	3:H:547:ARG:NH1	2.23	0.53
3:B:478:ARG:N	3:B:478:ARG:HD2	2.24	0.53
3:L:503:LEU:HB3	3:L:509:MET:CE	2.38	0.53
2:W:4:DG:C2'	2:W:5:DG:H5'	2.35	0.53
3:M:628:VAL:HG13	3:M:629:ASP:N	2.23	0.53
3:H:566:PRO:O	3:H:567:ILE:HD13	2.09	0.53
3:I:423:HIS:HB3	3:I:430:ARG:CG	2.37	0.53
3:H:458:ILE:HG12	3:H:546:PHE:CD1	2.44	0.53
3:L:467:ILE:O	3:L:468:LEU:C	2.48	0.53
3:M:479:ILE:HD12	3:M:479:ILE:C	2.30	0.53
3:B:501:ILE:C	3:B:501:ILE:HD12	2.30	0.53
3:L:650:ILE:HG13	3:L:677:PRO:HB3	1.91	0.53
3:D:578:PRO:HD3	3:D:662:ASN:HD22	1.72	0.52
3:H:458:ILE:HD11	3:H:513:ILE:HD12	1.91	0.52
3:L:458:ILE:HD11	3:L:513:ILE:HD12	1.91	0.52
3:M:423:HIS:HB3	3:M:430:ARG:CG	2.35	0.52
3:H:584:ASP:HB2	3:H:597:ILE:HB	1.91	0.52
3:I:478:ARG:HG2	3:I:491:LYS:HD2	1.91	0.52
3:B:456:LEU:HD23	3:B:501:ILE:HD11	1.91	0.52
3:L:582:ARG:HB2	3:L:582:ARG:NH1	2.24	0.52
3:D:547:ARG:HG2	3:D:561:GLN:HB2	1.92	0.52
3:M:650:ILE:HG13	3:M:677:PRO:HB3	1.90	0.52
2:Y:6:DA:H2"	2:Y:7:DA:C8	2.43	0.52
3:H:427:GLU:OE1	3:H:430:ARG:NH1	2.42	0.52
3:M:613:GLU:O	3:M:621:ILE:HD13	2.09	0.52
2:Y:14:DC:H2"	2:Z:1:DA:H8	1.74	0.52
3:M:565:ASN:HB3	3:M:566:PRO:CD	2.37	0.52
3:D:478:ARG:HD2	3:D:478:ARG:N	2.25	0.52
3:M:600:GLY:N	3:M:603:PHE:HE2	2.07	0.52
3:M:427:GLU:OE1	3:M:430:ARG:NH1	2.43	0.52
3:M:503:LEU:HB3	3:M:509:MET:CE	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:582:ARG:NH1	3:I:582:ARG:HB2	2.24	0.52
2:Y:4:DG:C2'	2:Y:5:DG:H5"	2.37	0.52
3:M:430:ARG:CG	3:M:430:ARG:HH11	2.22	0.52
3:L:417:LYS:O	3:L:567:ILE:HD12	2.09	0.52
3:B:613:GLU:O	3:B:621:ILE:HD13	2.10	0.52
3:I:578:PRO:HD3	3:I:662:ASN:HD22	1.73	0.52
3:M:458:ILE:HG12	3:M:546:PHE:CD1	2.44	0.52
3:I:422:ALA:HB1	3:I:518:ILE:O	2.10	0.52
2:W:11:DC:N4	3:D:427:GLU:OE2	2.43	0.52
3:B:584:ASP:HB2	3:B:597:ILE:HB	1.92	0.52
1:V:1:DT:H5"	1:T:14:DA:H1'	1.91	0.52
3:L:547:ARG:HG2	3:L:561:GLN:HB2	1.91	0.52
3:L:478:ARG:H	3:L:478:ARG:HD2	1.74	0.52
3:L:427:GLU:OE1	3:L:430:ARG:NH1	2.43	0.52
3:L:416:PRO:HG2	3:L:567:ILE:HD11	1.92	0.52
3:I:478:ARG:HD2	3:I:478:ARG:H	1.75	0.52
1:X:2:DT:H1'	1:X:3:DG:H5"	1.91	0.52
1:X:4:DA:OP2	1:X:4:DA:H2'	2.10	0.52
3:B:399:TRP:HB2	3:B:547:ARG:NH1	2.25	0.52
3:D:522:ARG:HB2	3:D:525:ASP:OD2	2.10	0.52
3:B:486:THR:HG22	3:B:486:THR:O	2.10	0.52
1:V:9:DT:H1'	1:V:10:DT:H5"	1.92	0.51
3:H:549:HIS:O	3:H:551:PRO:HD3	2.10	0.51
1:T:3:DG:H2"	1:T:4:DA:C5'	2.26	0.51
3:L:478:ARG:HD2	3:L:478:ARG:N	2.25	0.51
3:I:427:GLU:OE1	3:I:430:ARG:NH1	2.43	0.51
3:M:636:ASN:N	3:M:636:ASN:ND2	2.59	0.51
3:L:522:ARG:HB2	3:L:525:ASP:OD2	2.11	0.51
2:W:1:DA:H2"	2:W:2:DA:C5'	2.35	0.51
2:Y:2:DA:C1'	2:Y:3:DT:H5"	2.40	0.51
3:L:492:ILE:HG22	3:L:493:VAL:N	2.13	0.51
3:L:584:ASP:HB2	3:L:597:ILE:HB	1.91	0.51
3:H:478:ARG:N	3:H:478:ARG:HD2	2.23	0.51
3:L:613:GLU:O	3:L:621:ILE:HD13	2.10	0.51
3:L:636:ASN:N	3:L:636:ASN:ND2	2.58	0.51
3:H:636:ASN:N	3:H:636:ASN:ND2	2.58	0.51
3:H:503:LEU:HB3	3:H:509:MET:HE3	1.91	0.51
3:H:422:ALA:HB1	3:H:518:ILE:O	2.10	0.51
3:I:430:ARG:HH11	3:I:430:ARG:CG	2.24	0.51
3:H:501:ILE:HD12	3:H:501:ILE:O	2.11	0.51
3:M:422:ALA:HB1	3:M:518:ILE:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:7:DA:H2"	2:Z:8:DA:H5'	1.92	0.51
3:B:478:ARG:HG2	3:B:491:LYS:HD2	1.92	0.51
3:L:412:ILE:HD11	3:L:546:PHE:HD2	1.75	0.51
3:D:503:LEU:HB3	3:D:509:MET:CE	2.40	0.51
3:B:478:ARG:H	3:B:478:ARG:HD2	1.74	0.51
3:B:479:ILE:C	3:B:479:ILE:HD12	2.30	0.51
3:H:459:PHE:CZ	3:H:545:VAL:HG11	2.46	0.51
2:Z:6:DA:OP1	2:Z:6:DA:H4'	2.11	0.51
3:M:460:ILE:HG23	3:M:542:VAL:HG13	1.90	0.51
1:X:5:DG:H2"	1:X:6:DG:H5"	1.83	0.51
3:M:416:PRO:HG2	3:M:567:ILE:HD11	1.93	0.51
3:B:416:PRO:HG2	3:B:567:ILE:HD11	1.92	0.51
3:I:636:ASN:N	3:I:636:ASN:ND2	2.58	0.51
3:L:503:LEU:HB3	3:L:509:MET:HE3	1.91	0.51
3:B:609:VAL:HG21	3:B:640:VAL:HG21	1.93	0.51
3:B:464:ASP:O	3:B:465:GLU:HG2	2.10	0.51
3:H:582:ARG:HB2	3:H:582:ARG:NH1	2.26	0.51
3:D:492:ILE:HG22	3:D:493:VAL:N	2.15	0.50
3:H:417:LYS:O	3:H:567:ILE:HD12	2.10	0.50
3:I:549:HIS:O	3:I:551:PRO:HD3	2.10	0.50
3:L:412:ILE:HD13	3:L:443:VAL:HG22	1.93	0.50
3:H:522:ARG:HB2	3:H:525:ASP:OD2	2.11	0.50
3:I:620:GLN:OE1	3:I:623:GLU:HB2	2.10	0.50
3:B:670:PRO:HD3	3:D:579:MET:CE	2.42	0.50
3:B:578:PRO:HD3	3:B:662:ASN:HD22	1.74	0.50
3:D:647:ASN:O	3:D:650:ILE:HG23	2.10	0.50
3:I:458:ILE:HD11	3:I:513:ILE:HD12	1.93	0.50
3:B:503:LEU:HB3	3:B:509:MET:HE3	1.92	0.50
3:H:428:GLY:O	3:H:429:SER:C	2.50	0.50
3:L:464:ASP:O	3:L:465:GLU:HG2	2.11	0.50
3:L:399:TRP:CB	3:L:547:ARG:NH1	2.74	0.50
3:L:423:HIS:HB3	3:L:430:ARG:HB2	1.92	0.50
3:I:417:LYS:O	3:I:567:ILE:HD12	2.11	0.50
3:M:459:PHE:CZ	3:M:545:VAL:HG11	2.46	0.50
3:D:636:ASN:ND2	3:D:636:ASN:N	2.60	0.50
3:I:458:ILE:HG12	3:I:546:PHE:CD1	2.47	0.50
3:I:416:PRO:HG2	3:I:567:ILE:HD11	1.94	0.50
3:M:468:LEU:HD23	3:M:543:ARG:NH2	2.27	0.50
3:D:412:ILE:HD13	3:D:443:VAL:HG22	1.91	0.50
3:D:584:ASP:HB2	3:D:597:ILE:HB	1.93	0.50
3:I:613:GLU:O	3:I:621:ILE:HD13	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:412:ILE:HD11	3:L:546:PHE:CD2	2.46	0.50
3:L:501:ILE:HD12	3:L:501:ILE:C	2.32	0.50
3:D:549:HIS:O	3:D:551:PRO:HD3	2.11	0.50
2:Z:12:DC:C2'	2:Z:13:DT:H71	2.42	0.50
3:B:430:ARG:CG	3:B:430:ARG:HH11	2.24	0.50
3:H:668:SER:HB2	3:I:669:GLN:HE22	1.76	0.50
3:I:577:LEU:HB2	3:I:578:PRO:HD2	1.94	0.50
3:B:458:ILE:HD11	3:B:513:ILE:HD12	1.93	0.50
3:H:464:ASP:O	3:H:465:GLU:HG2	2.11	0.50
2:Y:2:DA:H1'	2:Y:3:DT:H5"	1.93	0.50
3:M:566:PRO:O	3:M:567:ILE:HD13	2.12	0.50
3:B:491:LYS:NZ	3:B:497:LYS:CD	2.75	0.50
3:H:479:ILE:C	3:H:479:ILE:HD12	2.32	0.50
3:D:479:ILE:C	3:D:479:ILE:HD12	2.31	0.50
3:D:633:SER:HA	3:D:639:PHE:HE1	1.77	0.50
3:M:501:ILE:HD12	3:M:501:ILE:O	2.12	0.50
3:L:599:THR:HG23	3:M:617:ASP:O	2.11	0.49
3:B:633:SER:HA	3:B:639:PHE:HE1	1.77	0.49
3:L:430:ARG:NH1	3:L:430:ARG:CG	2.72	0.49
3:I:479:ILE:C	3:I:479:ILE:HD12	2.32	0.49
3:D:399:TRP:CB	3:D:547:ARG:NH1	2.76	0.49
1:T:7:DA:H2"	1:T:8:DA:H8	1.72	0.49
3:B:417:LYS:HG3	3:B:434:LYS:O	2.12	0.49
3:H:647:ASN:O	3:H:650:ILE:HG23	2.12	0.49
3:B:412:ILE:HD13	3:B:443:VAL:HG22	1.94	0.49
3:M:445:LEU:HD11	3:M:550:ILE:HD11	1.94	0.49
3:D:590:VAL:HG23	3:D:591:TYR:H	1.78	0.49
3:D:430:ARG:CG	3:D:430:ARG:HH11	2.25	0.49
3:H:423:HIS:HB3	3:H:430:ARG:HB2	1.95	0.49
3:I:609:VAL:HG21	3:I:640:VAL:HG21	1.94	0.49
1:V:5:DG:H2"	1:V:6:DG:C5'	2.37	0.49
3:D:565:ASN:HB3	3:D:566:PRO:CD	2.40	0.49
3:L:460:ILE:HG23	3:L:542:VAL:HG13	1.92	0.49
3:M:578:PRO:O	3:M:579:MET:HG3	2.12	0.49
3:I:594:GLN:HB2	3:I:642:ILE:HD12	1.94	0.49
1:T:5:DG:H1'	1:T:6:DG:C5'	2.43	0.49
3:I:600:GLY:N	3:I:603:PHE:HE2	2.11	0.49
3:H:412:ILE:HD13	3:H:443:VAL:HG22	1.94	0.49
3:M:456:LEU:HD11	3:M:546:PHE:HB3	1.95	0.49
3:I:648:LYS:HE2	3:I:678:VAL:HB	1.95	0.49
3:B:445:LEU:HD11	3:B:550:ILE:HD11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:7:DA:OP2	3:I:664:LYS:HB3	2.11	0.49
3:L:468:LEU:HD23	3:L:543:ARG:NH2	2.27	0.49
3:H:433:VAL:HG23	3:H:516:ALA:O	2.12	0.49
3:L:428:GLY:O	3:L:429:SER:C	2.50	0.49
3:M:522:ARG:HB2	3:M:525:ASP:OD2	2.13	0.49
3:I:547:ARG:HG2	3:I:561:GLN:HB2	1.93	0.49
3:H:600:GLY:N	3:H:603:PHE:HE2	2.11	0.49
3:D:521:LEU:HD13	3:D:526:ILE:HD11	1.95	0.49
3:B:503:LEU:HB3	3:B:509:MET:CE	2.43	0.49
3:H:486:THR:O	3:H:486:THR:HG22	2.12	0.49
3:M:467:ILE:O	3:M:468:LEU:C	2.50	0.49
3:I:456:LEU:HD23	3:I:501:ILE:HD11	1.94	0.49
1:X:6:DG:H2"	1:X:7:DA:C5'	2.38	0.49
3:D:417:LYS:HG3	3:D:434:LYS:O	2.12	0.49
3:B:566:PRO:O	3:B:567:ILE:HD13	2.13	0.49
3:B:670:PRO:CD	3:D:579:MET:HB3	2.43	0.49
3:M:456:LEU:HD23	3:M:501:ILE:HD11	1.95	0.49
3:B:609:VAL:HG21	3:B:640:VAL:CG2	2.43	0.49
3:I:423:HIS:O	3:I:519:LEU:HD12	2.13	0.48
3:L:579:MET:CE	3:M:670:PRO:HD3	2.43	0.48
3:D:594:GLN:HB2	3:D:642:ILE:HD12	1.95	0.48
3:L:590:VAL:HG23	3:L:591:TYR:H	1.78	0.48
3:M:582:ARG:NH1	3:M:582:ARG:HB2	2.27	0.48
3:L:633:SER:HA	3:L:639:PHE:HE1	1.77	0.48
3:L:600:GLY:N	3:L:603:PHE:HE2	2.10	0.48
3:M:464:ASP:O	3:M:465:GLU:HG2	2.13	0.48
3:L:668:SER:CA	3:M:669:GLN:HE22	2.26	0.48
3:D:460:ILE:HG23	3:D:542:VAL:HG13	1.95	0.48
3:H:577:LEU:HB2	3:H:578:PRO:HD2	1.96	0.48
3:B:636:ASN:ND2	3:B:636:ASN:N	2.61	0.48
3:I:412:ILE:HD11	3:I:546:PHE:CD2	2.48	0.48
2:W:4:DG:H1'	2:W:5:DG:C5'	2.44	0.48
1:X:5:DG:C2'	1:X:6:DG:C5'	2.78	0.48
3:H:460:ILE:HG23	3:H:542:VAL:HG13	1.94	0.48
3:M:412:ILE:HD13	3:M:443:VAL:HG22	1.94	0.48
3:M:458:ILE:HG12	3:M:546:PHE:HD1	1.79	0.48
3:M:647:ASN:O	3:M:650:ILE:HG23	2.13	0.48
3:I:633:SER:HA	3:I:639:PHE:HE1	1.78	0.48
3:H:565:ASN:HB3	3:H:566:PRO:CD	2.37	0.48
3:L:668:SER:HA	3:M:669:GLN:NE2	2.28	0.48
2:Z:10:DT:C2'	2:Z:11:DC:C5'	2.80	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:647:ASN:HD22	3:D:650:ILE:HG22	1.79	0.48
2:W:12:DC:H2"	2:W:13:DT:O5'	2.14	0.48
3:H:479:ILE:HG13	3:H:515:CYS:CA	2.39	0.48
3:I:479:ILE:HG13	3:I:515:CYS:CA	2.40	0.48
3:L:669:GLN:H	3:M:669:GLN:CD	2.15	0.48
3:I:481:GLY:CA	3:I:485:THR:HB	2.43	0.48
3:B:669:GLN:HE22	3:D:669:GLN:H	1.61	0.48
3:I:521:LEU:HD13	3:I:526:ILE:HD11	1.96	0.48
3:D:456:LEU:HD23	3:D:501:ILE:HD11	1.96	0.48
3:L:566:PRO:O	3:L:567:ILE:HD13	2.13	0.48
3:B:669:GLN:NE2	3:D:668:SER:HB2	2.28	0.48
3:I:412:ILE:HD13	3:I:443:VAL:HG22	1.95	0.48
3:M:412:ILE:HD11	3:M:546:PHE:HD2	1.79	0.48
3:L:486:THR:O	3:L:486:THR:HG22	2.13	0.48
3:B:594:GLN:HB2	3:B:642:ILE:HD12	1.94	0.48
3:D:416:PRO:HG2	3:D:567:ILE:HD11	1.94	0.48
1:T:5:DG:H1'	1:T:6:DG:H5"	1.96	0.48
3:H:578:PRO:HD3	3:H:662:ASN:HD22	1.79	0.48
3:M:428:GLY:O	3:M:429:SER:C	2.52	0.48
3:M:633:SER:HA	3:M:639:PHE:HE1	1.78	0.47
3:H:416:PRO:HG2	3:H:567:ILE:HD11	1.96	0.47
3:B:460:ILE:HG23	3:B:542:VAL:HG13	1.95	0.47
3:D:459:PHE:CZ	3:D:545:VAL:HG11	2.49	0.47
3:I:412:ILE:HD11	3:I:546:PHE:HD2	1.79	0.47
3:M:458:ILE:HD11	3:M:513:ILE:HD12	1.96	0.47
3:M:647:ASN:HD22	3:M:650:ILE:HG22	1.79	0.47
3:D:464:ASP:O	3:D:465:GLU:HG2	2.14	0.47
3:L:479:ILE:HD12	3:L:479:ILE:C	2.34	0.47
3:L:521:LEU:HD13	3:L:526:ILE:HD11	1.95	0.47
3:H:647:ASN:HD22	3:H:650:ILE:HG22	1.77	0.47
3:D:501:ILE:HD12	3:D:501:ILE:O	2.14	0.47
3:M:631:ASP:C	3:M:633:SER:N	2.67	0.47
3:M:521:LEU:HD13	3:M:526:ILE:HD11	1.97	0.47
3:L:458:ILE:HG12	3:L:546:PHE:CD1	2.49	0.47
3:H:503:LEU:HD22	3:H:509:MET:C	2.34	0.47
3:D:423:HIS:O	3:D:519:LEU:HD12	2.15	0.47
3:B:417:LYS:O	3:B:567:ILE:HD12	2.14	0.47
3:H:481:GLY:CA	3:H:485:THR:HB	2.44	0.47
3:D:481:GLY:CA	3:D:485:THR:HB	2.43	0.47
3:I:503:LEU:HD13	3:I:509:MET:HE3	1.95	0.47
3:D:458:ILE:HD11	3:D:513:ILE:HD12	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:652:THR:HG23	3:L:653:PRO:HD2	1.97	0.47
3:B:590:VAL:HG23	3:B:591:TYR:H	1.79	0.47
3:M:481:GLY:CA	3:M:485:THR:HB	2.42	0.47
3:B:579:MET:O	3:B:600:GLY:HA3	2.14	0.47
3:L:422:ALA:HB1	3:L:518:ILE:O	2.14	0.47
3:I:399:TRP:CB	3:I:547:ARG:NH1	2.75	0.47
3:I:460:ILE:HG23	3:I:542:VAL:HG13	1.96	0.47
3:I:609:VAL:HG21	3:I:640:VAL:CG2	2.44	0.47
3:D:566:PRO:O	3:D:567:ILE:HD13	2.14	0.47
3:B:468:LEU:HD23	3:B:543:ARG:NH2	2.30	0.47
3:B:565:ASN:HB3	3:B:566:PRO:CD	2.42	0.47
3:D:468:LEU:HD23	3:D:543:ARG:NH2	2.30	0.47
3:M:491:LYS:NZ	3:M:497:LYS:CD	2.77	0.47
3:H:412:ILE:HD11	3:H:546:PHE:HD2	1.80	0.47
3:B:647:ASN:O	3:B:650:ILE:HG23	2.14	0.47
3:B:501:ILE:HD12	3:B:501:ILE:O	2.14	0.47
3:M:590:VAL:HG23	3:M:591:TYR:H	1.79	0.47
3:B:428:GLY:O	3:B:429:SER:C	2.52	0.47
3:M:549:HIS:O	3:M:551:PRO:HD3	2.13	0.47
3:H:609:VAL:HG21	3:H:640:VAL:HG21	1.97	0.47
3:B:522:ARG:HB2	3:B:525:ASP:OD2	2.15	0.47
3:I:428:GLY:O	3:I:429:SER:C	2.52	0.47
3:L:433:VAL:HG23	3:L:516:ALA:O	2.14	0.47
2:W:7:DA:C2	2:W:8:DA:C4	3.02	0.47
3:D:600:GLY:N	3:D:603:PHE:HE2	2.12	0.47
3:B:549:HIS:O	3:B:551:PRO:HD3	2.15	0.47
3:L:594:GLN:HB2	3:L:642:ILE:HD12	1.95	0.47
3:M:656:VAL:HG22	3:M:673:PHE:O	2.15	0.47
3:B:423:HIS:O	3:B:519:LEU:HD12	2.15	0.47
3:B:669:GLN:NE2	3:D:669:GLN:H	2.13	0.47
3:D:486:THR:O	3:D:486:THR:HG22	2.14	0.47
1:X:9:DT:C2'	1:X:10:DT:H5"	2.45	0.47
2:W:12:DC:H1'	2:W:13:DT:H5'	1.96	0.47
3:H:399:TRP:CB	3:H:547:ARG:NH1	2.74	0.47
3:B:577:LEU:HB2	3:B:578:PRO:HD2	1.97	0.47
3:I:458:ILE:HG12	3:I:546:PHE:HD1	1.80	0.47
3:B:648:LYS:HE2	3:B:678:VAL:HB	1.96	0.47
2:W:4:DG:H1'	2:W:5:DG:H5"	1.98	0.46
3:I:579:MET:O	3:I:600:GLY:HA3	2.15	0.46
3:I:501:ILE:O	3:I:501:ILE:HD12	2.15	0.46
3:D:470:PRO:HB3	3:D:496:THR:HG21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:628:VAL:CG2	3:M:629:ASP:H	2.17	0.46
3:L:579:MET:HB3	3:M:670:PRO:HD3	1.98	0.46
3:H:669:GLN:H	3:I:669:GLN:NE2	2.12	0.46
3:D:610:VAL:O	3:D:658:PHE:HA	2.15	0.46
3:H:412:ILE:HD11	3:H:546:PHE:CD2	2.49	0.46
3:B:458:ILE:HG12	3:B:546:PHE:CD1	2.50	0.46
3:H:466:ARG:HA	3:H:466:ARG:HD2	1.80	0.46
1:V:13:DC:H2"	1:V:14:DA:C8	2.51	0.46
3:D:626:ALA:HB2	3:D:643:PRO:HD3	1.97	0.46
2:Z:9:DT:C6	2:Z:10:DT:H72	2.50	0.46
3:M:399:TRP:CB	3:M:547:ARG:NH1	2.77	0.46
3:M:479:ILE:HG13	3:M:515:CYS:CA	2.39	0.46
3:H:445:LEU:HD11	3:H:550:ILE:CD1	2.46	0.46
3:L:647:ASN:O	3:L:650:ILE:HG23	2.15	0.46
3:L:470:PRO:HB3	3:L:496:THR:HG21	1.96	0.46
3:B:399:TRP:CB	3:B:547:ARG:NH1	2.77	0.46
2:W:7:DA:H2"	2:W:8:DA:C5'	2.41	0.46
3:M:610:VAL:O	3:M:658:PHE:HA	2.16	0.46
3:M:412:ILE:HD11	3:M:546:PHE:CD2	2.50	0.46
3:D:412:ILE:HD11	3:D:546:PHE:CD2	2.50	0.46
3:H:505:PRO:HD2	3:H:506:LYS:HZ3	1.81	0.46
3:L:668:SER:HB2	3:M:669:GLN:HE22	1.81	0.46
3:B:610:VAL:O	3:B:658:PHE:HA	2.16	0.46
3:L:503:LEU:HD22	3:L:509:MET:C	2.36	0.46
3:L:626:ALA:HB2	3:L:643:PRO:HD3	1.98	0.46
3:B:433:VAL:HG23	3:B:516:ALA:O	2.16	0.46
3:H:590:VAL:HG23	3:H:591:TYR:H	1.79	0.46
3:H:421:ARG:HG2	3:H:430:ARG:HD2	1.97	0.46
3:H:631:ASP:C	3:H:633:SER:N	2.69	0.46
3:I:433:VAL:HG23	3:I:516:ALA:O	2.16	0.46
3:D:609:VAL:HG21	3:D:640:VAL:HG21	1.98	0.46
3:D:556:ARG:HG2	3:D:557:ILE:N	2.30	0.46
3:D:458:ILE:HG12	3:D:546:PHE:CD1	2.51	0.46
3:H:609:VAL:HG21	3:H:640:VAL:CG2	2.46	0.46
3:D:428:GLY:O	3:D:429:SER:C	2.53	0.46
3:I:462:THR:HG23	3:I:469:LYS:O	2.16	0.46
3:B:462:THR:HG23	3:B:469:LYS:O	2.16	0.46
3:I:656:VAL:HG22	3:I:673:PHE:O	2.15	0.46
3:M:430:ARG:NH1	3:M:430:ARG:CG	2.78	0.46
3:I:491:LYS:NZ	3:I:497:LYS:CD	2.76	0.46
3:L:600:GLY:O	3:L:636:ASN:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:577:LEU:HB2	3:D:578:PRO:HD2	1.97	0.46
3:B:412:ILE:HD11	3:B:546:PHE:CD2	2.51	0.46
1:T:11:DT:H1'	1:T:12:DC:H5"	1.98	0.46
1:V:7:DA:H2"	1:V:8:DA:C8	2.51	0.45
3:D:427:GLU:OE1	3:D:430:ARG:NH1	2.49	0.45
3:H:491:LYS:NZ	3:H:497:LYS:CD	2.77	0.45
3:B:479:ILE:HG13	3:B:515:CYS:CA	2.41	0.45
3:H:457:GLN:O	3:H:546:PHE:HA	2.16	0.45
1:X:11:DT:C2'	1:X:12:DC:C5'	2.89	0.45
3:L:423:HIS:HB3	3:L:430:ARG:CB	2.46	0.45
3:L:459:PHE:CZ	3:L:545:VAL:HG11	2.51	0.45
3:H:468:LEU:HD23	3:H:543:ARG:NH2	2.32	0.45
3:M:577:LEU:HB2	3:M:578:PRO:HD2	1.98	0.45
3:H:600:GLY:O	3:H:636:ASN:HB2	2.17	0.45
3:B:653:PRO:HA	3:B:675:TYR:O	2.16	0.45
3:B:481:GLY:CA	3:B:485:THR:HB	2.44	0.45
3:M:600:GLY:O	3:M:636:ASN:HB2	2.16	0.45
3:H:456:LEU:HD11	3:H:546:PHE:HB3	1.97	0.45
3:I:648:LYS:HE2	3:I:678:VAL:CB	2.46	0.45
3:B:412:ILE:HD11	3:B:546:PHE:HD2	1.80	0.45
3:I:647:ASN:O	3:I:650:ILE:HG23	2.16	0.45
3:D:609:VAL:HG21	3:D:640:VAL:CG2	2.46	0.45
3:D:653:PRO:HA	3:D:675:TYR:O	2.15	0.45
3:H:423:HIS:O	3:H:519:LEU:HD12	2.16	0.45
1:T:9:DT:H2"	1:T:10:DT:C5'	2.45	0.45
3:D:648:LYS:HE2	3:D:678:VAL:HB	1.98	0.45
3:L:609:VAL:HG21	3:L:640:VAL:HG21	1.99	0.45
3:H:521:LEU:HD13	3:H:526:ILE:HD11	1.99	0.45
3:H:648:LYS:HE2	3:H:678:VAL:HB	1.99	0.45
1:V:4:DA:H2"	1:V:5:DG:C8	2.51	0.45
3:H:503:LEU:HD13	3:H:509:MET:HE3	1.98	0.45
3:L:637:MET:SD	3:M:617:ASP:HA	2.57	0.45
3:H:456:LEU:HD23	3:H:501:ILE:HD11	1.99	0.45
3:I:653:PRO:HA	3:I:675:TYR:O	2.17	0.45
3:H:610:VAL:O	3:H:658:PHE:HA	2.17	0.45
3:B:652:THR:HG23	3:B:653:PRO:HD2	1.99	0.45
3:B:672:HIS:NE2	3:D:671:GLN:OE1	2.46	0.45
3:M:594:GLN:HB2	3:M:642:ILE:HD12	1.98	0.45
2:Y:4:DG:C2'	2:Y:5:DG:H5'	2.21	0.45
3:L:565:ASN:HB3	3:L:566:PRO:CD	2.41	0.45
3:H:458:ILE:HG12	3:H:546:PHE:HD1	1.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:648:LYS:HE2	3:M:678:VAL:HB	1.99	0.45
3:H:594:GLN:HB2	3:H:642:ILE:HD12	1.99	0.45
2:W:7:DA:H1'	2:W:8:DA:H5"	1.98	0.45
3:I:423:HIS:HB3	3:I:430:ARG:HB2	1.99	0.45
3:H:633:SER:HA	3:H:639:PHE:HE1	1.80	0.45
3:L:412:ILE:CD1	3:L:443:VAL:HG22	2.47	0.45
3:D:456:LEU:HD11	3:D:546:PHE:HB3	1.98	0.45
3:L:656:VAL:HG22	3:L:673:PHE:O	2.17	0.45
3:H:470:PRO:HB3	3:H:496:THR:HG21	1.98	0.45
3:B:423:HIS:HB3	3:B:430:ARG:HB2	1.98	0.44
1:T:6:DG:C2'	1:T:7:DA:O5'	2.63	0.44
3:L:445:LEU:HD11	3:L:550:ILE:CD1	2.47	0.44
3:D:491:LYS:NZ	3:D:497:LYS:CD	2.76	0.44
3:D:579:MET:O	3:D:600:GLY:HA3	2.17	0.44
3:B:600:GLY:O	3:B:636:ASN:HB2	2.18	0.44
3:I:578:PRO:O	3:I:579:MET:HG3	2.17	0.44
3:H:412:ILE:CD1	3:H:443:VAL:HG22	2.47	0.44
3:L:448:TYR:CZ	3:L:450:GLU:HB2	2.52	0.44
3:L:436:PRO:HB2	3:L:632:LYS:CB	2.47	0.44
3:B:521:LEU:HD13	3:B:526:ILE:HD11	1.99	0.44
3:D:412:ILE:HD11	3:D:546:PHE:HD2	1.81	0.44
3:D:629:ASP:HB2	3:D:639:PHE:HB2	1.99	0.44
3:I:430:ARG:NH1	3:I:430:ARG:CG	2.77	0.44
3:B:430:ARG:NH1	3:B:430:ARG:CG	2.78	0.44
1:X:10:DT:H2"	1:X:11:DT:O5'	2.17	0.44
3:D:505:PRO:HD2	3:D:506:LYS:HZ3	1.83	0.44
3:I:633:SER:O	3:I:634:GLN:HG2	2.18	0.44
3:L:481:GLY:CA	3:L:485:THR:HB	2.43	0.44
3:B:456:LEU:HD11	3:B:546:PHE:HB3	2.00	0.44
3:M:609:VAL:HG21	3:M:640:VAL:HG21	1.99	0.44
3:I:486:THR:HG22	3:I:486:THR:O	2.17	0.44
3:H:656:VAL:HG22	3:H:673:PHE:O	2.17	0.44
3:B:656:VAL:HG22	3:B:673:PHE:O	2.18	0.44
3:D:631:ASP:C	3:D:633:SER:N	2.71	0.44
3:H:430:ARG:CG	3:H:430:ARG:HH11	2.28	0.44
3:I:465:GLU:O	3:I:466:ARG:HB2	2.16	0.44
3:H:579:MET:O	3:H:600:GLY:HA3	2.18	0.44
3:B:578:PRO:O	3:B:579:MET:HG3	2.17	0.44
3:B:470:PRO:HB3	3:B:496:THR:HG21	1.99	0.44
3:D:462:THR:HG23	3:D:469:LYS:O	2.18	0.44
3:D:503:LEU:HB3	3:D:509:MET:HE3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:422:ALA:HB1	3:B:518:ILE:O	2.18	0.44
3:D:656:VAL:HG22	3:D:673:PHE:O	2.18	0.44
3:D:423:HIS:HB3	3:D:430:ARG:HB2	2.00	0.44
3:L:479:ILE:HG13	3:L:515:CYS:CA	2.43	0.44
3:D:578:PRO:O	3:D:579:MET:HG3	2.17	0.44
3:B:648:LYS:HE2	3:B:678:VAL:CB	2.48	0.44
1:T:5:DG:C2'	1:T:6:DG:H5'	2.45	0.44
3:L:610:VAL:O	3:L:658:PHE:HA	2.17	0.44
3:L:458:ILE:HG12	3:L:546:PHE:HD1	1.82	0.44
3:D:503:LEU:HD22	3:D:509:MET:C	2.38	0.44
3:D:503:LEU:HD13	3:D:509:MET:HE3	2.00	0.44
3:M:508:ASN:HD22	3:M:508:ASN:HA	1.60	0.44
2:W:4:DG:C2'	2:W:5:DG:C5'	2.93	0.43
3:M:423:HIS:O	3:M:519:LEU:HD12	2.17	0.43
3:L:556:ARG:HG2	3:L:557:ILE:N	2.33	0.43
3:I:503:LEU:HD22	3:I:509:MET:C	2.38	0.43
3:L:501:ILE:HD12	3:L:501:ILE:O	2.18	0.43
3:H:653:PRO:HA	3:H:675:TYR:O	2.17	0.43
3:I:470:PRO:HB3	3:I:496:THR:HG21	1.99	0.43
3:D:590:VAL:HG23	3:D:591:TYR:N	2.34	0.43
3:I:652:THR:HG23	3:I:653:PRO:HD2	2.00	0.43
3:L:462:THR:HG23	3:L:469:LYS:O	2.18	0.43
3:M:633:SER:O	3:M:634:GLN:HG2	2.18	0.43
3:M:423:HIS:HB3	3:M:430:ARG:HB2	2.00	0.43
3:L:577:LEU:HB2	3:L:578:PRO:HD2	1.99	0.43
3:H:579:MET:HG2	3:I:669:GLN:HG2	2.00	0.43
3:B:647:ASN:HD22	3:B:650:ILE:HG22	1.83	0.43
3:M:433:VAL:HG23	3:M:516:ALA:O	2.18	0.43
1:X:9:DT:C2'	1:X:10:DT:C5'	2.94	0.43
3:I:631:ASP:C	3:I:633:SER:N	2.70	0.43
3:L:668:SER:HB2	3:M:669:GLN:NE2	2.33	0.43
3:H:478:ARG:H	3:H:478:ARG:CD	2.31	0.43
3:D:600:GLY:O	3:D:636:ASN:HB2	2.18	0.43
3:M:470:PRO:HB3	3:M:496:THR:HG21	1.98	0.43
3:M:486:THR:HG22	3:M:486:THR:O	2.17	0.43
3:I:590:VAL:HG23	3:I:591:TYR:H	1.82	0.43
3:I:505:PRO:HD2	3:I:506:LYS:HZ3	1.82	0.43
3:I:464:ASP:O	3:I:465:GLU:CG	2.66	0.43
3:I:457:GLN:O	3:I:546:PHE:HA	2.17	0.43
3:H:508:ASN:HA	3:H:508:ASN:HD22	1.58	0.43
1:V:7:DA:OP1	3:I:664:LYS:CB	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:8:DA:H1'	1:V:9:DT:H5'	1.99	0.43
3:B:633:SER:O	3:B:634:GLN:HG2	2.18	0.43
3:D:633:SER:HA	3:D:639:PHE:CE1	2.53	0.43
3:H:423:HIS:HB3	3:H:430:ARG:CB	2.48	0.43
3:B:459:PHE:CZ	3:B:545:VAL:HG11	2.53	0.43
3:L:456:LEU:HD11	3:L:546:PHE:HB3	2.00	0.43
3:I:647:ASN:HD22	3:I:650:ILE:HG22	1.83	0.43
3:I:468:LEU:HD23	3:I:543:ARG:NH2	2.34	0.43
3:M:579:MET:O	3:M:600:GLY:HA3	2.17	0.43
3:D:412:ILE:CD1	3:D:443:VAL:HG22	2.48	0.43
3:B:503:LEU:HD13	3:B:509:MET:HE3	2.01	0.43
3:M:609:VAL:HG21	3:M:640:VAL:CG2	2.48	0.43
3:D:421:ARG:HG2	3:D:430:ARG:HD2	2.01	0.43
3:I:633:SER:HA	3:I:639:PHE:CE1	2.54	0.43
3:L:631:ASP:C	3:L:633:SER:N	2.70	0.43
3:H:406:GLY:H	3:H:560:LEU:CD2	2.30	0.43
3:L:579:MET:O	3:L:600:GLY:HA3	2.18	0.43
3:I:412:ILE:CD1	3:I:443:VAL:HG22	2.49	0.43
3:D:652:THR:HG23	3:D:653:PRO:HD2	2.00	0.43
2:Y:12:DC:H2"	2:Y:13:DT:H5'	2.00	0.43
2:Y:13:DT:H2"	2:Y:14:DC:C6	2.54	0.43
3:B:669:GLN:OE1	3:D:669:GLN:HG3	2.18	0.43
3:L:647:ASN:HD22	3:L:650:ILE:HG22	1.84	0.43
3:B:465:GLU:O	3:B:466:ARG:HB2	2.19	0.43
3:M:464:ASP:O	3:M:465:GLU:C	2.57	0.43
3:L:609:VAL:HG21	3:L:640:VAL:CG2	2.49	0.43
2:Y:3:DT:OP2	3:L:431:GLY:HA3	2.19	0.43
3:M:547:ARG:NE	3:M:561:GLN:OE1	2.38	0.43
3:L:653:PRO:HA	3:L:675:TYR:O	2.18	0.43
3:M:588:CYS:SG	3:M:589:LEU:N	2.92	0.43
3:L:633:SER:HA	3:L:639:PHE:CE1	2.54	0.42
3:I:600:GLY:O	3:I:636:ASN:HB2	2.18	0.42
3:M:457:GLN:O	3:M:546:PHE:HA	2.19	0.42
3:M:626:ALA:HB2	3:M:643:PRO:HD3	2.01	0.42
3:B:631:ASP:C	3:B:633:SER:N	2.73	0.42
3:M:503:LEU:HD13	3:M:509:MET:HE3	2.00	0.42
3:B:590:VAL:HG23	3:B:591:TYR:N	2.34	0.42
3:B:503:LEU:HD22	3:B:509:MET:C	2.39	0.42
3:H:588:CYS:SG	3:H:589:LEU:N	2.92	0.42
3:L:633:SER:O	3:L:634:GLN:HG2	2.19	0.42
3:D:479:ILE:HG13	3:D:515:CYS:CA	2.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:464:ASP:O	3:L:465:GLU:CG	2.68	0.42
3:D:536:GLY:O	3:D:537:ARG:C	2.58	0.42
3:D:458:ILE:HG12	3:D:546:PHE:HD1	1.83	0.42
3:D:465:GLU:O	3:D:466:ARG:HB2	2.20	0.42
3:B:448:TYR:CZ	3:B:450:GLU:HB2	2.55	0.42
3:M:652:THR:HG23	3:M:653:PRO:HD2	2.01	0.42
3:M:653:PRO:HA	3:M:675:TYR:O	2.20	0.42
3:H:462:THR:HG23	3:H:469:LYS:O	2.19	0.42
3:D:430:ARG:CG	3:D:430:ARG:NH1	2.80	0.42
3:B:617:ASP:O	3:D:599:THR:HG23	2.20	0.42
3:D:478:ARG:HB2	3:D:489:TYR:CE2	2.55	0.42
3:M:412:ILE:CD1	3:M:443:VAL:HG22	2.50	0.42
3:L:590:VAL:HG23	3:L:591:TYR:N	2.34	0.42
1:X:10:DT:OP1	3:L:523:ASN:N	2.53	0.42
3:H:578:PRO:O	3:H:579:MET:HG3	2.19	0.42
3:L:648:LYS:HE2	3:L:678:VAL:HB	2.01	0.42
3:B:522:ARG:O	3:B:523:ASN:C	2.58	0.42
3:H:590:VAL:HG23	3:H:591:TYR:N	2.34	0.42
3:H:652:THR:HG23	3:H:653:PRO:HD2	2.01	0.42
2:Z:7:DA:C2'	2:Z:8:DA:H5'	2.48	0.42
3:L:423:HIS:O	3:L:519:LEU:HD12	2.20	0.42
3:B:458:ILE:HG12	3:B:546:PHE:HD1	1.84	0.42
3:D:457:GLN:O	3:D:546:PHE:HA	2.20	0.42
3:L:588:CYS:SG	3:L:589:LEU:N	2.93	0.42
3:M:633:SER:HA	3:M:639:PHE:CE1	2.54	0.42
3:I:629:ASP:HB2	3:I:639:PHE:HB2	2.02	0.42
3:L:629:ASP:HB2	3:L:639:PHE:HB2	2.01	0.42
3:L:621:ILE:HD13	3:L:621:ILE:N	2.25	0.42
3:I:522:ARG:O	3:I:523:ASN:C	2.56	0.42
3:B:464:ASP:O	3:B:465:GLU:CG	2.67	0.42
3:M:590:VAL:HG23	3:M:591:TYR:N	2.35	0.42
3:L:668:SER:CA	3:M:669:GLN:NE2	2.82	0.42
3:I:610:VAL:O	3:I:658:PHE:HA	2.19	0.42
3:M:494:GLY:C	3:M:496:THR:H	2.23	0.42
3:I:448:TYR:CZ	3:I:450:GLU:HB2	2.54	0.42
2:W:3:DT:H2"	2:W:4:DG:C8	2.54	0.41
2:Z:6:DA:N7	3:H:571:GLN:NE2	2.52	0.41
3:B:633:SER:HA	3:B:639:PHE:CE1	2.54	0.41
3:L:478:ARG:H	3:L:478:ARG:CD	2.32	0.41
3:I:456:LEU:HD11	3:I:546:PHE:HB3	2.01	0.41
3:M:448:TYR:CZ	3:M:450:GLU:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:651:ARG:HD3	3:I:651:ARG:HA	1.86	0.41
3:L:503:LEU:HD13	3:L:509:MET:HE3	2.01	0.41
3:D:448:TYR:CZ	3:D:454:LEU:HD21	2.55	0.41
2:W:6:DA:H2"	2:W:7:DA:C8	2.55	0.41
3:B:629:ASP:HB2	3:B:639:PHE:HB2	2.03	0.41
3:I:621:ILE:HD13	3:I:621:ILE:N	2.28	0.41
3:L:436:PRO:HB2	3:L:632:LYS:HB3	2.03	0.41
3:D:493:VAL:HB	3:D:494:GLY:H	1.62	0.41
3:I:485:THR:CG2	3:I:485:THR:O	2.68	0.41
3:B:485:THR:O	3:B:485:THR:CG2	2.66	0.41
3:I:478:ARG:HB2	3:I:489:TYR:CE2	2.56	0.41
3:B:600:GLY:H	3:B:603:PHE:HE2	1.68	0.41
3:L:596:MET:HE3	3:L:598:LEU:HD11	2.02	0.41
3:D:454:LEU:HD23	3:D:509:MET:HE2	2.03	0.41
3:D:588:CYS:SG	3:D:594:GLN:CD	2.99	0.41
3:B:421:ARG:HG2	3:B:430:ARG:HD2	2.02	0.41
3:H:485:THR:CG2	3:H:485:THR:O	2.67	0.41
3:B:669:GLN:HE22	3:D:669:GLN:N	2.17	0.41
3:B:556:ARG:HG2	3:B:557:ILE:N	2.34	0.41
3:L:457:GLN:O	3:L:546:PHE:HA	2.21	0.41
3:H:464:ASP:O	3:H:465:GLU:CG	2.68	0.41
1:V:7:DA:OP1	3:I:664:LYS:HD3	2.20	0.41
3:H:547:ARG:NE	3:H:561:GLN:OE1	2.36	0.41
3:D:633:SER:O	3:D:634:GLN:HG2	2.21	0.41
3:I:596:MET:HE3	3:I:598:LEU:HD11	2.01	0.41
3:M:503:LEU:HD22	3:M:509:MET:C	2.40	0.41
3:I:464:ASP:C	3:I:465:GLU:HG2	2.41	0.41
3:I:466:ARG:O	3:I:467:ILE:CG1	2.69	0.41
3:H:668:SER:CA	3:I:669:GLN:HE22	2.34	0.41
3:D:582:ARG:CB	3:D:582:ARG:HH11	2.33	0.41
3:H:465:GLU:O	3:H:466:ARG:HB2	2.21	0.41
1:V:8:DA:H2"	1:V:9:DT:OP2	2.20	0.41
3:D:406:GLY:H	3:D:560:LEU:CD2	2.34	0.41
3:I:445:LEU:HD11	3:I:550:ILE:CD1	2.51	0.41
3:B:457:GLN:O	3:B:546:PHE:HA	2.21	0.41
3:H:454:LEU:HD23	3:H:509:MET:CE	2.51	0.41
3:L:602:ASN:O	3:L:604:THR:HG23	2.21	0.41
3:B:505:PRO:HG2	3:B:506:LYS:HD2	2.03	0.41
3:I:493:VAL:HB	3:I:494:GLY:H	1.66	0.41
3:L:399:TRP:HA	3:L:400:PRO:HD3	1.94	0.41
3:L:478:ARG:HB2	3:L:489:TYR:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:577:LEU:O	3:M:577:LEU:HD12	2.21	0.41
3:B:464:ASP:O	3:B:465:GLU:C	2.59	0.41
3:M:465:GLU:O	3:M:466:ARG:HB2	2.20	0.41
3:D:464:ASP:O	3:D:465:GLU:C	2.59	0.41
3:L:494:GLY:C	3:L:496:THR:H	2.25	0.41
1:X:12:DC:H2"	1:X:13:DC:C5'	2.51	0.41
3:L:578:PRO:O	3:L:579:MET:HG3	2.21	0.41
3:D:648:LYS:HE2	3:D:678:VAL:CB	2.51	0.41
3:B:412:ILE:CD1	3:B:443:VAL:HG22	2.51	0.41
3:M:602:ASN:O	3:M:604:THR:HG23	2.21	0.41
3:H:621:ILE:H	3:H:621:ILE:CD1	2.27	0.40
3:H:637:MET:SD	3:I:617:ASP:HA	2.62	0.40
3:H:596:MET:HE3	3:H:598:LEU:HD11	2.02	0.40
3:H:408:TYR:O	3:H:409:GLU:CB	2.69	0.40
3:I:602:ASN:O	3:I:604:THR:HG23	2.21	0.40
3:H:440:HIS:CG	3:H:514:ASP:HB3	2.56	0.40
3:D:433:VAL:HG23	3:D:516:ALA:O	2.20	0.40
3:B:626:ALA:HB2	3:B:643:PRO:HD3	2.03	0.40
3:D:508:ASN:HD22	3:D:508:ASN:HA	1.62	0.40
3:I:565:ASN:HB3	3:I:566:PRO:CD	2.43	0.40
3:H:460:ILE:HG21	3:H:474:TYR:HB3	2.03	0.40
3:H:633:SER:O	3:H:634:GLN:HG2	2.22	0.40
3:I:556:ARG:HG2	3:I:557:ILE:N	2.36	0.40
3:D:448:TYR:CZ	3:D:450:GLU:HB2	2.56	0.40
3:H:522:ARG:O	3:H:523:ASN:C	2.59	0.40
3:D:602:ASN:O	3:D:604:THR:HG23	2.22	0.40
3:H:430:ARG:CG	3:H:430:ARG:NH1	2.81	0.40
3:M:478:ARG:HB2	3:M:489:TYR:CE2	2.56	0.40
3:D:651:ARG:HD3	3:D:651:ARG:HA	1.81	0.40
3:M:629:ASP:HB2	3:M:639:PHE:HB2	2.03	0.40
3:I:519:LEU:HD12	3:I:520:LYS:H	1.86	0.40
3:M:406:GLY:H	3:M:560:LEU:CD2	2.33	0.40
3:B:600:GLY:N	3:B:603:PHE:CE2	2.88	0.40
3:D:445:LEU:HD11	3:D:550:ILE:CD1	2.50	0.40
3:M:466:ARG:HA	3:M:466:ARG:HD2	1.81	0.40
3:B:602:ASN:O	3:B:604:THR:HG23	2.21	0.40
3:H:626:ALA:HB2	3:H:643:PRO:HD3	2.03	0.40
3:B:595:GLN:HB3	3:B:595:GLN:HE21	1.70	0.40
3:H:651:ARG:HA	3:H:651:ARG:HD3	1.84	0.40
1:T:13:DC:H2"	1:T:14:DA:H8	1.85	0.40
1:V:1:DT:C5'	1:T:14:DA:O3'	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1:DT:H2"	1:V:2:DT:OP2	2.22	0.40
3:L:454:LEU:HD23	3:L:509:MET:HE2	2.03	0.40
3:D:522:ARG:O	3:D:523:ASN:C	2.59	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:649:HIS:NE2	3:I:602:ASN:ND2[4_556]	2.09	0.11

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	
3	B	272/301 (90%)	213 (78%)	45 (16%)	14 (5%)	2	15
3	D	272/301 (90%)	212 (78%)	48 (18%)	12 (4%)	3	18
3	H	272/301 (90%)	215 (79%)	43 (16%)	14 (5%)	2	15
3	I	272/301 (90%)	212 (78%)	47 (17%)	13 (5%)	3	17
3	L	272/301 (90%)	211 (78%)	47 (17%)	14 (5%)	2	15
3	M	272/301 (90%)	214 (79%)	45 (16%)	13 (5%)	3	17
All	All	1632/1806 (90%)	1277 (78%)	275 (17%)	80 (5%)	3	16

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	406	GLY
3	B	467	ILE
3	B	590	VAL
3	B	628	VAL
3	D	406	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	467	ILE
3	D	590	VAL
3	D	628	VAL
3	H	406	GLY
3	H	590	VAL
3	H	628	VAL
3	I	406	GLY
3	I	467	ILE
3	I	590	VAL
3	I	628	VAL
3	L	406	GLY
3	L	467	ILE
3	L	590	VAL
3	L	628	VAL
3	M	406	GLY
3	M	467	ILE
3	M	590	VAL
3	M	628	VAL
3	B	409	GLU
3	D	409	GLU
3	D	465	GLU
3	H	409	GLU
3	H	429	SER
3	H	467	ILE
3	I	409	GLU
3	I	429	SER
3	I	594	GLN
3	L	409	GLU
3	L	429	SER
3	M	409	GLU
3	M	465	GLU
3	M	594	GLN
3	B	404	GLN
3	B	429	SER
3	B	465	GLU
3	B	468	LEU
3	B	594	GLN
3	D	404	GLN
3	D	429	SER
3	D	468	LEU
3	D	594	GLN
3	H	404	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	465	GLU
3	H	468	LEU
3	H	594	GLN
3	I	404	GLN
3	I	465	GLU
3	I	468	LEU
3	L	404	GLN
3	L	465	GLU
3	L	468	LEU
3	L	594	GLN
3	M	404	GLN
3	M	429	SER
3	M	468	LEU
3	H	420	HIS
3	L	420	HIS
3	M	420	HIS
3	B	602	ASN
3	B	616	THR
3	H	538	LYS
3	D	493	VAL
3	I	538	LYS
3	L	602	ASN
3	M	493	VAL
3	H	493	VAL
3	I	493	VAL
3	L	493	VAL
3	B	493	VAL
3	B	618	GLY
3	H	618	GLY
3	D	618	GLY
3	I	618	GLY
3	L	618	GLY
3	M	618	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
3	B	247/269 (92%)	232 (94%)	15 (6%)	23	59
3	D	247/269 (92%)	233 (94%)	14 (6%)	25	62
3	H	247/269 (92%)	233 (94%)	14 (6%)	25	62
3	I	247/269 (92%)	233 (94%)	14 (6%)	25	62
3	L	247/269 (92%)	233 (94%)	14 (6%)	25	62
3	M	247/269 (92%)	232 (94%)	15 (6%)	23	59
All	All	1482/1614 (92%)	1396 (94%)	86 (6%)	25	61

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	399	TRP
3	B	426	THR
3	B	430	ARG
3	B	445	LEU
3	B	468	LEU
3	B	478	ARG
3	B	485	THR
3	B	489	TYR
3	B	508	ASN
3	B	537	ARG
3	B	577	LEU
3	B	589	LEU
3	B	621	ILE
3	B	629	ASP
3	B	636	ASN
3	D	426	THR
3	D	430	ARG
3	D	445	LEU
3	D	468	LEU
3	D	478	ARG
3	D	485	THR
3	D	489	TYR
3	D	508	ASN
3	D	537	ARG
3	D	577	LEU
3	D	589	LEU
3	D	621	ILE
3	D	629	ASP
3	D	636	ASN
3	H	426	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	430	ARG
3	H	445	LEU
3	H	468	LEU
3	H	478	ARG
3	H	485	THR
3	H	489	TYR
3	H	508	ASN
3	H	537	ARG
3	H	577	LEU
3	H	589	LEU
3	H	621	ILE
3	H	629	ASP
3	H	636	ASN
3	I	426	THR
3	I	430	ARG
3	I	445	LEU
3	I	468	LEU
3	I	478	ARG
3	I	485	THR
3	I	489	TYR
3	I	508	ASN
3	I	537	ARG
3	I	577	LEU
3	I	589	LEU
3	I	621	ILE
3	I	629	ASP
3	I	636	ASN
3	L	426	THR
3	L	430	ARG
3	L	445	LEU
3	L	468	LEU
3	L	478	ARG
3	L	485	THR
3	L	489	TYR
3	L	508	ASN
3	L	537	ARG
3	L	577	LEU
3	L	589	LEU
3	L	621	ILE
3	L	629	ASP
3	L	636	ASN
3	M	399	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	426	THR
3	M	430	ARG
3	M	445	LEU
3	M	468	LEU
3	M	478	ARG
3	M	485	THR
3	M	489	TYR
3	M	508	ASN
3	M	537	ARG
3	M	577	LEU
3	M	589	LEU
3	M	621	ILE
3	M	629	ASP
3	M	636	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	420	HIS
3	B	444	GLN
3	B	446	HIS
3	B	451	ASN
3	B	477	HIS
3	B	495	ASN
3	B	508	ASN
3	B	523	ASN
3	B	583	GLN
3	B	594	GLN
3	B	595	GLN
3	B	601	GLN
3	B	636	ASN
3	B	647	ASN
3	B	669	GLN
3	B	671	GLN
3	D	420	HIS
3	D	444	GLN
3	D	446	HIS
3	D	451	ASN
3	D	477	HIS
3	D	495	ASN
3	D	508	ASN
3	D	523	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	583	GLN
3	D	594	GLN
3	D	595	GLN
3	D	601	GLN
3	D	636	ASN
3	D	647	ASN
3	H	420	HIS
3	H	444	GLN
3	H	451	ASN
3	H	477	HIS
3	H	495	ASN
3	H	508	ASN
3	H	523	ASN
3	H	583	GLN
3	H	594	GLN
3	H	595	GLN
3	H	601	GLN
3	H	636	ASN
3	H	647	ASN
3	I	420	HIS
3	I	444	GLN
3	I	451	ASN
3	I	477	HIS
3	I	495	ASN
3	I	508	ASN
3	I	523	ASN
3	I	583	GLN
3	I	594	GLN
3	I	595	GLN
3	I	601	GLN
3	I	636	ASN
3	I	647	ASN
3	L	420	HIS
3	L	444	GLN
3	L	446	HIS
3	L	451	ASN
3	L	477	HIS
3	L	495	ASN
3	L	508	ASN
3	L	523	ASN
3	L	583	GLN
3	L	594	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	595	GLN
3	L	636	ASN
3	L	647	ASN
3	M	420	HIS
3	M	444	GLN
3	M	446	HIS
3	M	451	ASN
3	M	477	HIS
3	M	495	ASN
3	M	508	ASN
3	M	523	ASN
3	M	583	GLN
3	M	594	GLN
3	M	595	GLN
3	M	601	GLN
3	M	636	ASN
3	M	647	ASN
3	M	669	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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	T	12/14 (85%)	-0.22	0 100 100	18, 23, 30, 31	0
1	V	14/14 (100%)	-0.15	0 100 100	25, 30, 38, 38	0
1	X	14/14 (100%)	-0.14	0 100 100	21, 28, 34, 47	0
2	W	14/14 (100%)	-0.20	0 100 100	19, 26, 33, 38	0
2	Y	14/14 (100%)	-0.03	0 100 100	21, 27, 42, 48	0
2	Z	14/14 (100%)	-0.07	0 100 100	22, 31, 41, 41	0
3	B	276/301 (91%)	0.51	21 (7%) 17 6	8, 60, 142, 160	0
3	D	276/301 (91%)	0.72	38 (13%) 4 2	14, 68, 153, 172	0
3	H	276/301 (91%)	0.61	24 (8%) 13 4	45, 72, 106, 114	0
3	I	276/301 (91%)	0.33	8 (2%) 55 31	21, 70, 90, 107	0
3	L	276/301 (91%)	0.43	16 (5%) 26 11	33, 79, 98, 112	0
3	M	276/301 (91%)	0.31	6 (2%) 65 42	14, 66, 87, 106	0
All	All	1738/1890 (91%)	0.45	113 (6%) 22 8	8, 69, 141, 172	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	678	VAL	8.8
3	D	647	ASN	8.3
3	B	596	MET	5.6
3	D	656	VAL	5.4
3	D	649	HIS	5.3
3	H	454	LEU	5.2
3	H	553	SER	5.2
3	H	552	GLU	5.0
3	H	501	ILE	5.0
3	L	553	SER	4.9
3	B	675	TYR	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	649	HIS	4.5
3	D	677	PRO	4.5
3	B	678	VAL	4.4
3	H	529	ARG	4.3
3	D	674	THR	4.2
3	D	654	VAL	4.1
3	B	629	ASP	4.1
3	H	548	VAL	4.1
3	L	550	ILE	4.0
3	D	676	HIS	4.0
3	H	551	PRO	3.9
3	B	626	ALA	3.9
3	D	616	THR	3.8
3	D	576	GLU	3.7
3	D	620	GLN	3.5
3	D	482	LYS	3.5
3	D	675	TYR	3.5
3	D	673	PHE	3.4
3	L	551	PRO	3.4
3	H	411	ARG	3.4
3	D	597	ILE	3.3
3	D	672	HIS	3.3
3	H	407	SER	3.2
3	B	601	GLN	3.2
3	B	654	VAL	3.2
3	D	646	ARG	3.2
3	D	640	VAL	3.1
3	H	562	THR	3.1
3	M	639	PHE	3.1
3	B	576	GLU	3.0
3	B	598	LEU	3.0
3	M	576	GLU	3.0
3	D	630	LYS	2.9
3	L	678	VAL	2.9
3	M	628	VAL	2.9
3	H	556	ARG	2.9
3	D	589	LEU	2.8
3	D	650	ILE	2.8
3	B	638	LEU	2.8
3	H	495	ASN	2.8
3	H	635	PRO	2.8
3	D	621	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	455	GLY	2.7
3	D	591	TYR	2.7
3	D	611	PHE	2.7
3	B	605	SER	2.7
3	D	609	VAL	2.7
3	L	633	SER	2.7
3	D	631	ASP	2.6
3	L	632	LYS	2.6
3	L	576	GLU	2.6
3	I	585	THR	2.6
3	D	665	ARG	2.6
3	D	615	THR	2.6
3	B	482	LYS	2.6
3	I	665	ARG	2.6
3	B	658	PHE	2.6
3	H	554	SER	2.6
3	D	648	LYS	2.5
3	H	496	THR	2.5
3	M	672	HIS	2.5
3	D	637	MET	2.5
3	D	593	GLY	2.5
3	H	491	LYS	2.5
3	L	554	SER	2.4
3	D	483	THR	2.4
3	H	550	ILE	2.4
3	M	451	ASN	2.4
3	D	587	SER	2.3
3	B	591	TYR	2.3
3	L	443	VAL	2.3
3	H	549	HIS	2.3
3	H	445	LEU	2.3
3	H	629	ASP	2.3
3	B	653	PRO	2.3
3	B	585	THR	2.3
3	D	645	TYR	2.2
3	H	443	VAL	2.2
3	L	406	GLY	2.2
3	D	612	THR	2.2
3	B	648	LYS	2.2
3	L	451	ASN	2.2
3	M	530	LYS	2.2
3	I	503	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	556	ARG	2.2
3	D	658	PHE	2.1
3	B	632	LYS	2.1
3	L	454	LEU	2.1
3	I	630	LYS	2.1
3	L	665	ARG	2.1
3	I	598	LEU	2.1
3	B	625	GLU	2.1
3	I	591	TYR	2.1
3	D	655	LYS	2.1
3	H	648	LYS	2.1
3	D	588	CYS	2.0
3	H	400	PRO	2.0
3	I	678	VAL	2.0
3	L	419	HIS	2.0
3	B	673	PHE	2.0
3	L	591	TYR	2.0
3	I	408	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.