



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:17 AM UTC

PDB ID : 1C9B / pdb_00001c9b
Title : CRYSTAL STRUCTURE OF A HUMAN TBP CORE DOMAIN-HUMAN
TFIIB CORE DOMAIN COMPLEX BOUND TO AN EXTENDED, MODI-
FIED ADENOVIRAL MAJOR LATE PROMOTER (ADMLP)
Authors : Tsai, F.T.F.; Sigler, P.B.
Deposited on : 1999-08-01
Resolution : 2.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

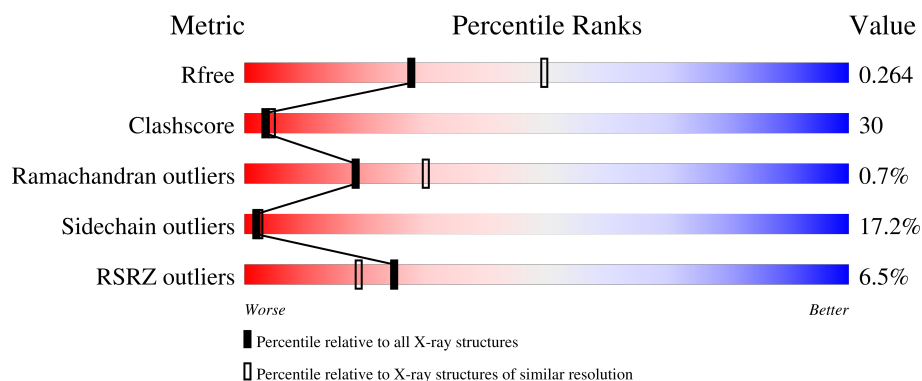
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



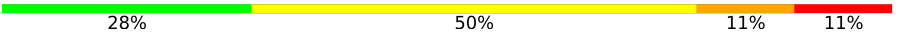
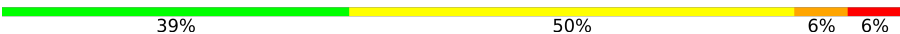
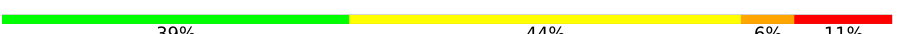
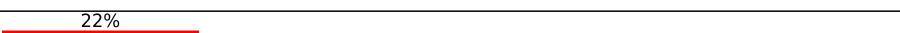
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 of 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	C	18	6% 44% 33% 22%
1	G	18	39% 44% 11% 6%
1	K	18	44% 33% 17% 6%
1	O	18	33% 61% 6%
1	S	18	44% 39% 11% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	18	
2	H	18	
2	L	18	
2	P	18	
2	T	18	
3	A	207	
3	E	207	
3	I	207	
3	M	207	
3	Q	207	
4	B	180	
4	F	180	
4	J	180	
4	N	180	
4	R	180	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19199 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 ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	G	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	K	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	O	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	S	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			

- Molecule 2 is a DNA chain called ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	H	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	L	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	P	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	T	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			

- Molecule 3 is a protein called GENERAL TRANSCRIPTION FACTOR IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			
3	I	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			
3	M	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			
3	Q	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			

- Molecule 4 is a protein called TATA BOX BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	F	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	J	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	N	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	R	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	158	GLY	SER	conflict	UNP P20226
F	158	GLY	SER	conflict	UNP P20226
J	158	GLY	SER	conflict	UNP P20226
N	158	GLY	SER	conflict	UNP P20226
R	158	GLY	SER	conflict	UNP P20226

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	15	Total	O	0	0
			15	15		
5	D	15	Total	O	0	0
			15	15		
5	G	7	Total	O	0	0
			7	7		

Continued on next page...

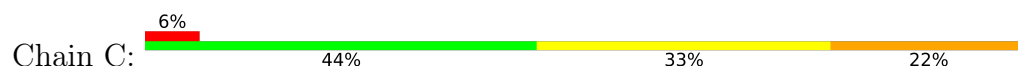
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	14	Total 14	O 14	0	0
5	K	7	Total 7	O 7	0	0
5	L	8	Total 8	O 8	0	0
5	O	7	Total 7	O 7	0	0
5	P	9	Total 9	O 9	0	0
5	S	4	Total 4	O 4	0	0
5	T	4	Total 4	O 4	0	0
5	A	28	Total 28	O 28	0	0
5	B	44	Total 44	O 44	0	0
5	E	56	Total 56	O 56	0	0
5	F	29	Total 29	O 29	0	0
5	I	12	Total 12	O 12	0	0
5	J	22	Total 22	O 22	0	0
5	M	15	Total 15	O 15	0	0
5	N	14	Total 14	O 14	0	0
5	Q	10	Total 10	O 10	0	0
5	R	9	Total 9	O 9	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

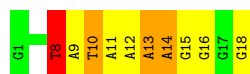
- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT



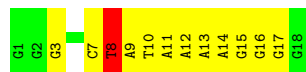
- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT



- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT



- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT



- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

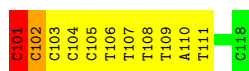


- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

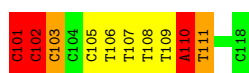




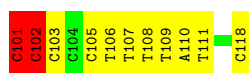
- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT



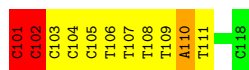
- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT



- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT



- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

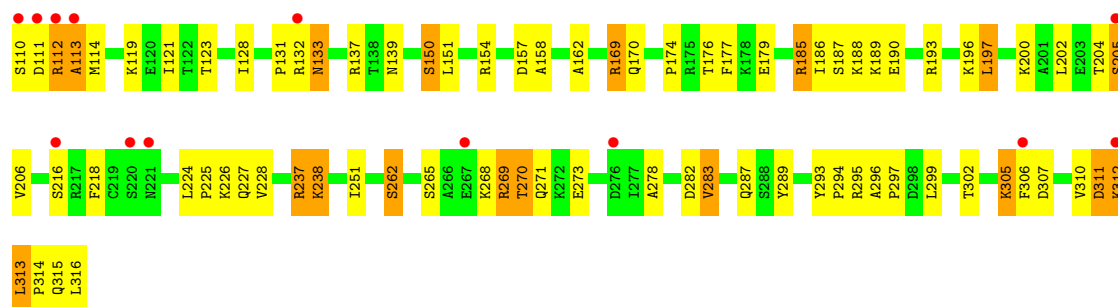


- Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB

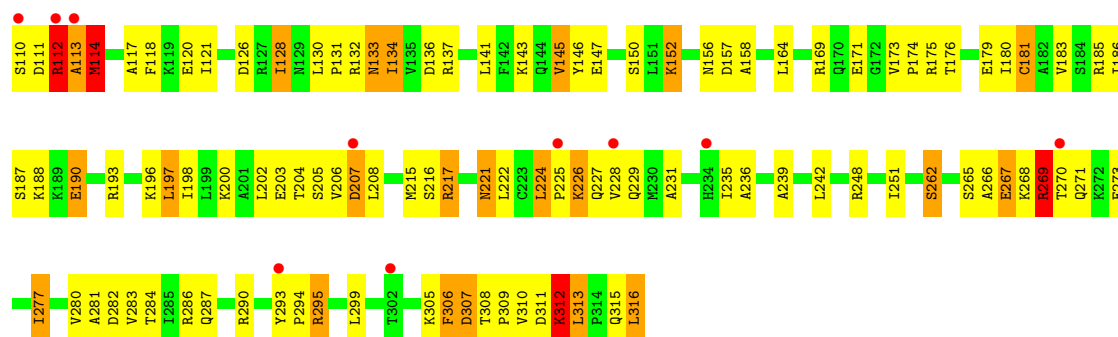


- Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB

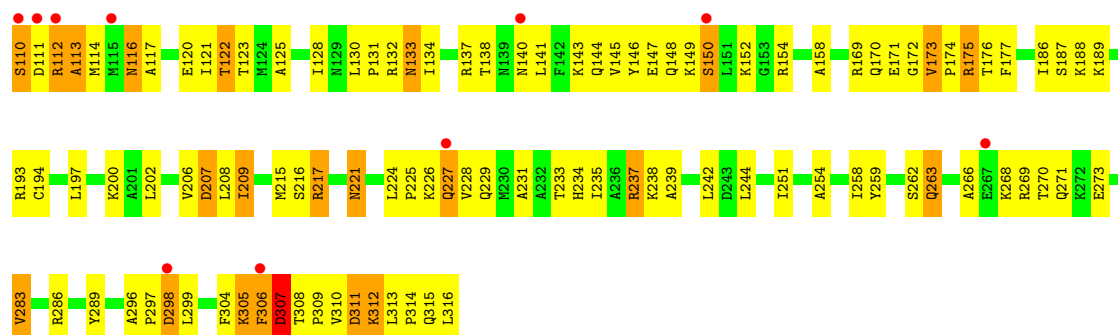




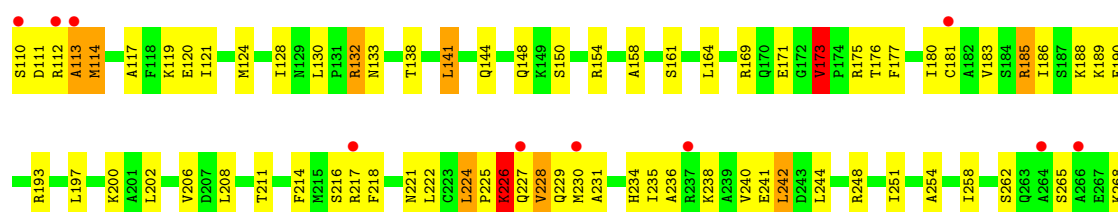
• Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB



• Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB

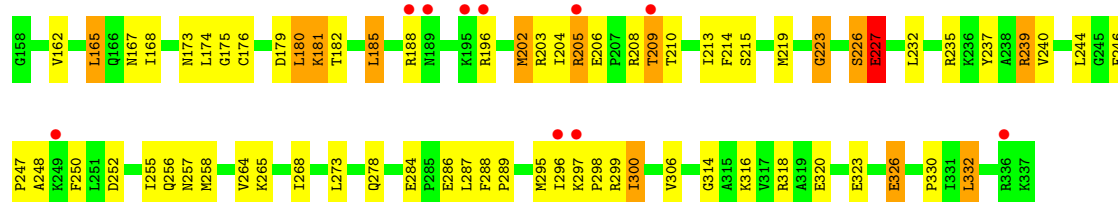


• Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB

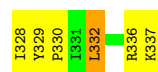
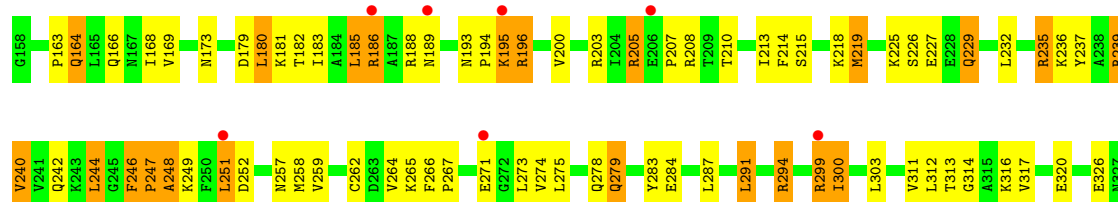




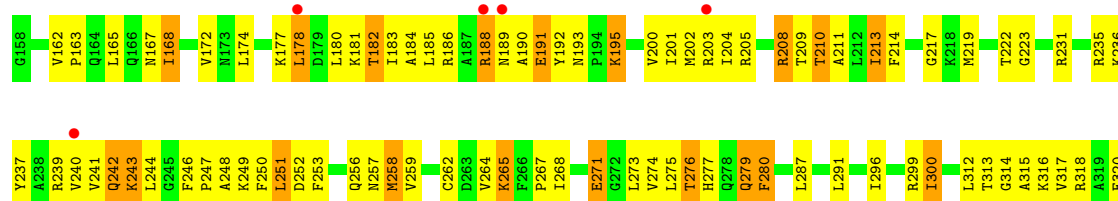
• Molecule 4: TATA BOX BINDING PROTEIN



• Molecule 4: TATA BOX BINDING PROTEIN

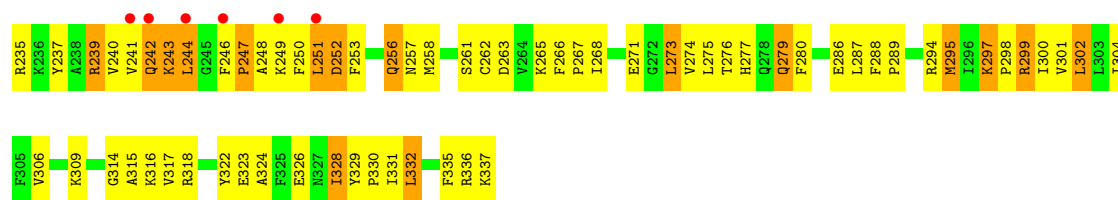


• Molecule 4: TATA BOX BINDING PROTEIN

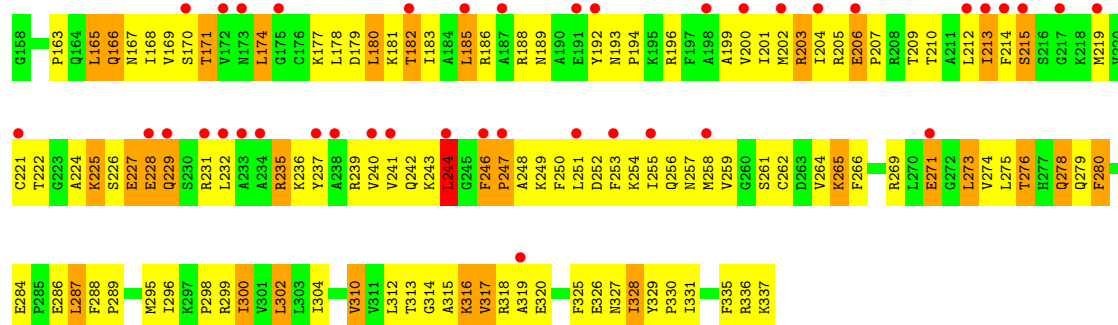


• Molecule 4: TATA BOX BINDING PROTEIN





● Molecule 4: TATA BOX BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.45Å 122.30Å 140.22Å 90.00° 113.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.67	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.65) 94.7 (50.00-2.67)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.65Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.229 , 0.260 0.234 , 0.264	Depositor DCC
R_{free} test set	5030 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19199	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	C	0.56	0/423	1.00	0/653
1	G	0.55	0/423	1.01	1/653 (0.2%)
1	K	0.51	0/423	1.02	2/653 (0.3%)
1	O	0.53	0/423	1.00	1/653 (0.2%)
1	S	0.51	0/423	1.01	2/653 (0.3%)
2	D	0.56	0/397	1.15	3/609 (0.5%)
2	H	0.60	0/397	1.20	3/609 (0.5%)
2	L	0.48	0/397	1.13	4/609 (0.7%)
2	P	0.51	0/397	1.17	2/609 (0.3%)
2	T	0.52	0/397	1.15	2/609 (0.3%)
3	A	0.81	0/1639	1.05	6/2209 (0.3%)
3	E	0.88	0/1639	1.05	5/2209 (0.2%)
3	I	0.75	0/1639	1.04	6/2209 (0.3%)
3	M	0.72	0/1639	1.04	4/2209 (0.2%)
3	Q	0.78	0/1639	1.09	7/2209 (0.3%)
4	B	1.00	3/1453 (0.2%)	1.13	7/1953 (0.4%)
4	F	0.85	0/1453	1.15	8/1953 (0.4%)
4	J	0.77	0/1453	1.09	3/1953 (0.2%)
4	N	0.75	1/1453 (0.1%)	1.08	6/1953 (0.3%)
4	R	0.82	0/1453	1.08	7/1953 (0.4%)
All	All	0.76	4/19560 (0.0%)	1.08	79/27120 (0.3%)

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	C	0	4
1	G	0	3
1	K	0	4
1	O	0	2
1	S	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	3
2	H	0	1
2	L	0	5
2	P	0	2
2	T	0	3
3	I	0	1
4	N	0	1
All	All	0	31

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	MET	SD-CE	-6.14	1.64	1.79
4	B	258	MET	SD-CE	-5.58	1.65	1.79
4	N	295	MET	SD-CE	-5.51	1.65	1.79
4	B	295	MET	SD-CE	-5.32	1.66	1.79

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	113	ALA	N-CA-C	-9.51	101.37	113.16
3	E	113	ALA	N-CA-C	-8.97	102.03	113.16
3	A	113	ALA	N-CA-C	-8.69	102.38	113.16
3	Q	113	ALA	N-CA-C	-8.45	102.69	113.16
2	L	101	DC	N1-C1'-C2'	-7.94	101.59	113.50
3	I	307	ASP	N-CA-C	-7.32	103.24	111.07
2	T	101	DC	N1-C1'-C2'	-7.28	102.58	113.50
2	H	101	DC	N1-C1'-C2'	-7.24	102.64	113.50
3	I	158	ALA	N-CA-C	-6.84	103.75	111.14
2	P	101	DC	N1-C1'-C2'	-6.62	103.57	113.50
4	R	328	ILE	N-CA-C	6.54	118.13	111.00
4	N	316	LYS	N-CA-C	-6.46	105.53	113.41
2	D	101	DC	N1-C1'-C2'	-6.43	103.85	113.50
3	A	173	VAL	CA-C-N	6.29	126.24	119.76
3	A	173	VAL	C-N-CA	6.29	126.24	119.76
3	I	113	ALA	N-CA-C	-6.26	105.39	113.16
3	M	306	PHE	N-CA-C	6.22	118.59	108.63
4	F	252	ASP	N-CA-C	6.16	119.67	111.30
3	Q	307	ASP	N-CA-C	-6.10	104.54	111.07
2	P	102	DC	N1-C1'-C2'	-6.10	104.35	113.50
3	Q	283	VAL	N-CA-C	-6.09	104.57	110.72
4	F	265	LYS	N-CA-C	6.09	120.66	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	235	ARG	CG-CD-NE	-6.04	98.70	112.00
4	R	265	LYS	N-CA-C	6.00	120.54	113.23
4	F	316	LYS	N-CA-C	-5.98	106.11	113.41
2	H	102	DC	N1-C1'-C2'	-5.97	104.55	113.50
3	M	307	ASP	N-CA-C	-5.96	103.96	111.11
3	A	114	MET	N-CA-C	-5.91	104.92	111.36
2	D	109	DT	C5'-C4'-O4'	-5.82	100.67	109.40
3	I	114	MET	N-CA-C	-5.81	105.08	111.82
2	T	102	DC	N1-C1'-C2'	-5.75	104.87	113.50
4	F	246	PHE	CA-C-N	5.75	127.02	119.84
4	F	246	PHE	C-N-CA	5.75	127.02	119.84
4	R	246	PHE	CA-C-N	5.75	127.02	119.84
4	R	246	PHE	C-N-CA	5.75	127.02	119.84
3	I	269	ARG	CG-CD-NE	-5.71	99.44	112.00
4	B	265	LYS	N-CA-C	5.71	120.20	113.23
4	N	252	ASP	N-CA-C	5.69	119.04	111.30
2	L	102	DC	N1-C1'-C2'	-5.67	104.99	113.50
1	K	8	DT	N1-C1'-C2'	-5.67	104.99	113.50
3	E	306	PHE	N-CA-C	5.64	117.65	108.63
1	S	8	DT	N1-C1'-C2'	-5.64	105.04	113.50
3	E	307	ASP	N-CA-C	-5.62	105.06	111.07
4	B	316	LYS	N-CA-C	-5.61	106.57	113.41
3	M	283	VAL	N-CA-C	-5.61	105.06	110.72
3	Q	173	VAL	CA-C-N	5.59	125.60	119.90
3	Q	173	VAL	C-N-CA	5.59	125.60	119.90
3	E	158	ALA	N-CA-C	-5.51	105.19	111.14
1	O	8	DT	N1-C1'-C2'	-5.50	105.25	113.50
4	N	203	ARG	N-CA-C	5.39	117.22	108.26
2	D	102	DC	N1-C1'-C2'	-5.38	105.42	113.50
3	A	307	ASP	N-CA-C	-5.37	105.33	111.07
2	L	110	DA	N9-C1'-C2'	-5.36	105.46	113.50
4	J	252	ASP	N-CA-C	5.36	118.59	111.30
2	L	101	DC	C2'-C3'-O3'	-5.33	103.50	111.50
4	J	316	LYS	N-CA-C	-5.31	106.93	113.41
3	E	162	ALA	N-CA-C	-5.31	105.58	111.36
3	Q	114	MET	N-CA-C	-5.29	105.69	111.82
2	H	101	DC	C2'-C3'-O3'	-5.26	103.61	111.50
4	R	203	ARG	N-CA-C	5.25	116.97	108.26
4	B	223	GLY	N-CA-C	5.24	120.92	114.69
4	B	244	LEU	N-CA-C	-5.22	106.75	113.02
3	Q	132	ARG	CA-CB-CG	5.22	124.53	114.10
1	G	8	DT	N1-C1'-C2'	-5.21	105.68	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	284	THR	N-CA-C	-5.21	105.60	111.28
4	N	265	LYS	N-CA-C	5.20	119.57	113.23
4	N	244	LEU	N-CA-C	-5.18	106.55	112.92
3	I	306	PHE	N-CA-C	5.15	116.87	108.63
4	R	244	LEU	N-CA-C	-5.10	106.65	112.92
4	F	244	LEU	N-CA-C	-5.09	106.91	113.02
4	J	265	LYS	N-CA-C	5.08	120.62	113.56
4	B	252	ASP	N-CA-C	5.07	118.19	111.30
4	R	252	ASP	N-CA-C	5.06	118.19	111.30
4	F	248	ALA	N-CA-C	5.06	117.64	110.10
1	K	10	DT	C5'-C4'-C3'	-5.06	107.31	114.90
1	S	7	DC	N1-C1'-C2'	-5.03	105.96	113.50
4	F	196	ARG	CG-CD-NE	5.01	123.03	112.00
4	B	227	GLU	CA-C-N	5.01	126.95	120.44
4	B	227	GLU	C-N-CA	5.01	126.95	120.44

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	12	DA	Sidechain
1	C	14	DA	Sidechain
1	C	18	DG	Sidechain
1	C	8	DT	Sidechain
2	D	101	DC	Sidechain
2	D	102	DC	Sidechain
2	D	111	DT	Sidechain
1	G	12	DA	Sidechain
1	G	18	DG	Sidechain
1	G	8	DT	Sidechain
2	H	101	DC	Sidechain
3	I	269	ARG	Sidechain
1	K	13	DA	Sidechain
1	K	14	DA	Sidechain
1	K	18	DG	Sidechain
1	K	8	DT	Sidechain
2	L	101	DC	Sidechain
2	L	102	DC	Sidechain
2	L	103	DC	Sidechain
2	L	110	DA	Sidechain
2	L	111	DT	Sidechain
4	N	299	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	O	13	DA	Sidechain
1	O	8	DT	Sidechain
2	P	101	DC	Sidechain
2	P	102	DC	Sidechain
1	S	14	DA	Sidechain
1	S	8	DT	Sidechain
2	T	101	DC	Sidechain
2	T	102	DC	Sidechain
2	T	110	DA	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	375	0	202	17	0
1	G	375	0	202	20	0
1	K	375	0	202	9	0
1	O	375	0	202	14	0
1	S	375	0	202	13	0
2	D	357	0	205	13	0
2	H	357	0	205	13	0
2	L	357	0	205	14	0
2	P	357	0	205	19	0
2	T	357	0	205	24	0
3	A	1615	0	1670	95	0
3	E	1615	0	1670	65	0
3	I	1615	0	1670	119	0
3	M	1615	0	1670	121	0
3	Q	1615	0	1670	93	0
4	B	1427	0	1517	52	0
4	F	1427	0	1517	101	0
4	J	1427	0	1517	97	0
4	N	1427	0	1517	114	0
4	R	1427	0	1517	138	0
5	A	28	0	0	4	0
5	B	44	0	0	2	0
5	C	15	0	0	2	0
5	D	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	56	0	0	2	0
5	F	29	0	0	1	0
5	G	7	0	0	1	0
5	H	14	0	0	0	0
5	I	12	0	0	2	0
5	J	22	0	0	0	0
5	K	7	0	0	1	0
5	L	8	0	0	0	0
5	M	15	0	0	1	0
5	N	14	0	0	3	0
5	O	7	0	0	1	0
5	P	9	0	0	0	0
5	Q	10	0	0	0	0
5	R	9	0	0	1	0
5	S	4	0	0	0	0
5	T	4	0	0	0	0
All	All	19199	0	17970	1100	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 30.

All (1100) 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)
4:N:193:ASN:HB3	4:N:196:ARG:NE	1.37	1.35
4:N:193:ASN:CB	4:N:196:ARG:HE	1.47	1.26
3:Q:224:LEU:CD2	3:Q:228:VAL:HG21	1.67	1.23
4:N:188:ARG:HG3	4:N:189:ASN:H	1.04	1.20
1:G:11:DA:H2''	1:G:12:DA:H5'	1.22	1.16
1:O:11:DA:H2''	1:O:12:DA:H5'	1.23	1.16
4:N:295:MET:HE1	4:N:324:ALA:HA	1.23	1.16
3:Q:295:ARG:HH11	3:Q:295:ARG:HG2	1.11	1.16
4:R:259:VAL:HG22	4:R:313:THR:HG22	1.20	1.13
3:I:309:PRO:HG2	3:I:312:LYS:HG2	1.22	1.12
3:A:270:THR:HG22	3:A:273:GLU:H	1.05	1.11
4:B:181:LYS:H	4:B:181:LYS:HD2	1.02	1.11
1:S:11:DA:H2''	1:S:12:DA:H5'	1.30	1.10
4:N:229:GLN:HA	4:N:229:GLN:HE21	1.17	1.09
4:N:229:GLN:HA	4:N:229:GLN:NE2	1.66	1.09
1:K:11:DA:H2''	1:K:12:DA:H5'	1.17	1.08
4:F:181:LYS:H	4:F:181:LYS:HD2	0.96	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:193:ASN:ND2	4:F:195:LYS:HD2	1.68	1.08
4:R:269:ARG:HG2	4:R:337:LYS:HG2	1.35	1.06
4:N:180:LEU:HD21	4:N:215:SER:HB3	1.37	1.05
3:Q:224:LEU:HD22	3:Q:228:VAL:HG21	1.09	1.04
4:R:242:GLN:HG2	4:R:248:ALA:HB3	1.07	1.04
4:N:188:ARG:HG3	4:N:189:ASN:N	1.68	1.03
4:F:180:LEU:HD21	4:F:215:SER:HB3	1.36	1.02
4:F:188:ARG:HG3	4:F:189:ASN:H	1.23	1.02
3:I:133:ASN:H	3:I:133:ASN:HD22	1.07	1.02
3:Q:128:ILE:CG2	3:Q:183:VAL:HG11	1.89	1.02
4:J:188:ARG:HG2	4:J:189:ASN:N	1.75	1.01
4:R:213:ILE:HD13	4:R:219:MET:HB3	1.40	1.01
4:F:193:ASN:HD21	4:F:195:LYS:HD2	1.15	1.00
3:M:125:ALA:HA	3:M:130:LEU:HD12	1.39	1.00
3:M:209:ILE:HD12	3:M:209:ILE:H	1.24	1.00
4:F:229:GLN:HA	4:F:229:GLN:HE21	1.26	1.00
3:M:305:LYS:H	3:M:305:LYS:CD	1.71	0.99
4:F:180:LEU:H	4:F:180:LEU:HD22	1.26	0.99
4:R:207:PRO:HB3	4:R:229:GLN:OE1	1.64	0.98
3:M:175:ARG:HH11	3:M:175:ARG:HG2	1.27	0.97
4:R:286:GLU:HG3	5:R:338:HOH:O	1.62	0.97
3:I:312:LYS:HD3	3:I:312:LYS:N	1.79	0.97
3:I:270:THR:HG23	3:I:273:GLU:H	1.29	0.97
4:N:243:LYS:HD3	4:N:243:LYS:O	1.64	0.97
4:R:259:VAL:HG22	4:R:313:THR:CG2	1.94	0.96
4:F:181:LYS:HD2	4:F:181:LYS:N	1.82	0.95
4:F:205:ARG:H	4:F:205:ARG:HD2	1.31	0.95
3:Q:224:LEU:HD23	3:Q:228:VAL:HG11	1.47	0.95
4:J:279:GLN:HG3	4:J:280:PHE:CE2	2.02	0.95
4:R:181:LYS:O	4:R:185:LEU:HD13	1.67	0.94
4:F:205:ARG:H	4:F:205:ARG:CD	1.77	0.94
3:Q:242:LEU:HB3	3:Q:244:LEU:HD13	1.46	0.94
2:D:108:DT:H2''	2:D:109:DT:H5'	1.50	0.94
2:T:110:DA:H2''	2:T:111:DT:H5'	1.49	0.94
4:N:193:ASN:O	4:N:196:ARG:HG3	1.66	0.94
2:P:110:DA:H5'	4:N:166:GLN:HG2	1.48	0.94
2:T:110:DA:H5'	4:R:166:GLN:HG2	1.48	0.94
4:R:271:GLU:CD	4:R:271:GLU:H	1.76	0.94
3:Q:128:ILE:HG23	3:Q:183:VAL:HG11	1.50	0.94
3:I:295:ARG:HG3	3:I:295:ARG:HH11	1.32	0.93
1:C:11:DA:H2''	1:C:12:DA:H5'	1.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:242:GLN:HG2	4:R:248:ALA:CB	1.99	0.93
2:H:108:DT:H2''	2:H:109:DT:H5'	1.49	0.93
4:R:213:ILE:CD1	4:R:219:MET:HB3	1.98	0.93
3:I:204:THR:HG22	3:I:205:SER:H	1.35	0.92
4:N:229:GLN:HE21	4:N:229:GLN:CA	1.82	0.92
4:R:188:ARG:NH2	4:R:189:ASN:HD21	1.68	0.91
4:J:193:ASN:ND2	4:J:195:LYS:HG3	1.85	0.91
3:I:312:LYS:HD3	3:I:312:LYS:H	1.32	0.91
4:N:229:GLN:HE22	4:N:232:LEU:HD12	1.34	0.90
1:G:3:DG:N3	5:G:147:HOH:O	2.03	0.90
3:M:289:TYR:CE2	3:M:316:LEU:HD12	2.07	0.90
4:J:279:GLN:HG3	4:J:280:PHE:HE2	1.37	0.89
3:Q:189:LYS:HE2	3:Q:193:ARG:HH21	1.35	0.89
3:Q:189:LYS:HE2	3:Q:193:ARG:NH2	1.87	0.89
3:A:189:LYS:HE2	3:A:193:ARG:NH2	1.86	0.89
3:M:224:LEU:HB3	3:M:228:VAL:HG21	1.52	0.89
4:R:165:LEU:O	4:R:225:LYS:HD3	1.72	0.89
4:N:193:ASN:CG	4:N:196:ARG:HG2	1.98	0.89
4:N:295:MET:HE1	4:N:324:ALA:CA	2.02	0.89
3:I:133:ASN:H	3:I:133:ASN:ND2	1.68	0.89
3:I:185:ARG:HG2	5:I:318:HOH:O	1.71	0.88
3:Q:224:LEU:HD22	3:Q:228:VAL:CG2	2.01	0.88
4:F:259:VAL:HG22	4:F:313:THR:HG22	1.52	0.88
4:B:181:LYS:H	4:B:181:LYS:CD	1.87	0.88
2:P:110:DA:H2''	2:P:111:DT:H5'	1.54	0.88
4:R:288:PHE:CD2	4:R:289:PRO:HD2	2.08	0.87
1:G:9:DA:H2''	1:G:10:DT:H5'	1.57	0.87
3:A:267:GLU:OE2	3:A:267:GLU:HA	1.69	0.87
4:B:181:LYS:HD2	4:B:181:LYS:N	1.87	0.87
4:J:167:ASN:HD21	4:J:223:GLY:H	1.22	0.87
3:E:133:ASN:HD22	3:E:133:ASN:H	1.17	0.87
3:M:209:ILE:HD12	3:M:209:ILE:N	1.89	0.87
3:A:270:THR:HG22	3:A:273:GLU:N	1.89	0.86
4:F:235:ARG:HH21	4:F:235:ARG:HG3	1.38	0.86
4:R:242:GLN:CG	4:R:248:ALA:HB3	2.01	0.86
4:J:193:ASN:HD21	4:J:195:LYS:HG3	1.38	0.85
4:R:179:ASP:OD1	4:R:182:THR:HG22	1.76	0.85
3:I:270:THR:HG22	3:I:273:GLU:CG	2.05	0.85
3:I:221:ASN:N	3:I:221:ASN:HD22	1.73	0.85
3:I:270:THR:HG22	3:I:273:GLU:HG3	1.57	0.85
4:N:256:GLN:HE21	4:N:256:GLN:HA	1.42	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:121:ILE:HD13	3:Q:138:THR:HG22	1.58	0.84
3:M:224:LEU:HD21	3:M:269:ARG:HE	1.43	0.84
3:E:112:ARG:HH22	3:E:114:MET:HE3	1.43	0.84
3:M:305:LYS:H	3:M:305:LYS:HD2	1.41	0.84
4:N:178:LEU:HD11	4:N:217:GLY:HA2	1.58	0.84
3:A:133:ASN:HD22	3:A:133:ASN:H	1.26	0.83
3:Q:225:PRO:O	3:Q:228:VAL:HG13	1.78	0.83
3:M:189:LYS:HE2	3:M:193:ARG:NH1	1.93	0.83
4:R:207:PRO:HB3	4:R:229:GLN:CD	2.04	0.82
3:A:133:ASN:HD22	3:A:133:ASN:N	1.77	0.82
2:P:108:DT:H2''	2:P:109:DT:H5'	1.61	0.82
4:R:224:ALA:HA	4:R:229:GLN:HE22	1.42	0.82
1:O:8:DT:H2''	1:O:9:DA:H5'	1.61	0.82
4:F:229:GLN:HE21	4:F:229:GLN:CA	1.93	0.82
3:A:226:LYS:HG2	3:A:230:MET:HE2	1.61	0.81
3:M:140:ASN:O	3:M:144:GLN:HG3	1.79	0.81
4:N:231:ARG:HA	4:N:253:PHE:CE2	2.15	0.81
4:N:257:ASN:HD21	4:N:314:GLY:H	1.28	0.81
1:G:11:DA:H2''	1:G:12:DA:C5'	2.08	0.81
4:F:188:ARG:HG3	4:F:189:ASN:N	1.94	0.81
1:C:8:DT:H2''	1:C:9:DA:H5'	1.63	0.81
2:L:110:DA:H2''	2:L:111:DT:H5'	1.62	0.81
3:I:306:PHE:CE1	3:I:310:VAL:HG22	2.16	0.81
4:F:299:ARG:O	4:F:300:ILE:HD13	1.81	0.80
3:Q:231:ALA:O	3:Q:235:ILE:HG13	1.80	0.80
4:N:202:MET:HE3	4:N:213:ILE:HD11	1.60	0.80
1:K:9:DA:H2''	1:K:10:DT:H5'	1.64	0.80
3:M:263:GLN:HG2	3:M:314:PRO:HG2	1.64	0.80
2:T:107:DT:OP1	4:R:196:ARG:NH2	2.15	0.80
4:J:205:ARG:O	4:J:205:ARG:HD3	1.81	0.80
3:M:305:LYS:CD	3:M:305:LYS:N	2.42	0.80
1:G:18:DG:O3'	3:M:316:LEU:HD23	1.81	0.79
4:B:179:ASP:OD1	4:B:182:THR:HG23	1.82	0.79
3:I:295:ARG:HH11	3:I:295:ARG:CG	1.94	0.79
4:J:186:ARG:NH1	4:J:244:LEU:HD22	1.96	0.79
4:B:257:ASN:HD21	4:B:314:GLY:H	1.31	0.79
3:I:270:THR:CG2	3:I:273:GLU:H	1.95	0.79
1:K:11:DA:H2''	1:K:12:DA:C5'	2.07	0.79
2:T:108:DT:H1'	4:R:167:ASN:HD21	1.47	0.79
2:T:108:DT:H2''	2:T:109:DT:H5'	1.64	0.79
3:M:141:LEU:O	3:M:145:VAL:HG23	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:239:ARG:HG2	4:N:242:GLN:HE22	1.48	0.79
4:N:180:LEU:CD2	4:N:215:SER:HB3	2.13	0.78
4:N:328:ILE:HG23	4:N:332:LEU:HD22	1.66	0.78
4:J:276:THR:OG1	4:J:277:HIS:HD2	1.65	0.78
4:F:181:LYS:H	4:F:181:LYS:CD	1.83	0.78
4:R:213:ILE:HD13	4:R:219:MET:CB	2.14	0.78
3:Q:295:ARG:HG2	3:Q:295:ARG:NH1	1.85	0.78
4:N:178:LEU:CD1	4:N:217:GLY:HA2	2.13	0.77
4:F:179:ASP:O	4:F:182:THR:HG22	1.83	0.77
2:T:109:DT:H5''	4:R:167:ASN:HD22	1.49	0.77
3:I:267:GLU:HB2	3:I:269:ARG:HH11	1.49	0.77
3:I:248:ARG:HH22	3:I:287:GLN:NE2	1.83	0.77
3:I:190:GLU:OE2	3:I:193:ARG:NH1	2.17	0.77
2:T:109:DT:H5''	4:R:167:ASN:ND2	1.99	0.77
4:N:318:ARG:HG2	4:N:322:TYR:CE2	2.20	0.77
4:N:193:ASN:O	4:N:196:ARG:CG	2.32	0.77
3:I:157:ASP:HB2	3:I:185:ARG:NH2	1.99	0.76
1:G:15:DG:H2''	1:G:16:DG:H5''	1.66	0.76
4:F:259:VAL:HG22	4:F:313:THR:CG2	2.16	0.76
4:F:193:ASN:HD21	4:F:195:LYS:CD	1.97	0.76
3:I:309:PRO:HG2	3:I:312:LYS:CG	2.11	0.76
4:J:186:ARG:HH11	4:J:244:LEU:HD22	1.50	0.76
3:Q:295:ARG:HH11	3:Q:295:ARG:CG	1.95	0.76
4:R:186:ARG:CZ	4:R:244:LEU:HG	2.15	0.76
3:M:270:THR:HG23	3:M:273:GLU:H	1.51	0.76
4:J:259:VAL:HG22	4:J:313:THR:HG22	1.67	0.76
3:M:131:PRO:HG2	3:M:134:ILE:HG12	1.67	0.76
3:M:173:VAL:HG23	3:M:173:VAL:O	1.84	0.76
4:R:186:ARG:NH1	4:R:244:LEU:O	2.15	0.76
4:R:257:ASN:HD21	4:R:314:GLY:H	1.31	0.75
1:G:11:DA:C2'	1:G:12:DA:H5'	2.12	0.75
1:S:14:DA:H1'	4:R:214:PHE:CZ	2.22	0.75
3:I:131:PRO:HB2	3:I:133:ASN:HD21	1.49	0.75
4:J:204:ILE:HD12	4:J:236:LYS:HD2	1.68	0.75
4:J:188:ARG:HG2	4:J:189:ASN:H	1.46	0.75
3:A:221:ASN:N	3:A:221:ASN:HD22	1.84	0.74
4:F:266:PHE:CD1	4:F:336:ARG:HG3	2.21	0.74
4:N:295:MET:CE	4:N:324:ALA:HA	2.12	0.74
3:I:286:ARG:O	3:I:290:ARG:HG3	1.86	0.74
3:Q:226:LYS:HD3	3:Q:226:LYS:H	1.53	0.74
3:I:267:GLU:N	3:I:267:GLU:OE2	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:7:DC:H2''	1:S:8:DT:H5'	1.68	0.74
3:I:176:THR:OG1	3:I:179:GLU:HG3	1.87	0.74
4:J:181:LYS:O	4:J:185:LEU:HG	1.87	0.74
2:L:108:DT:H2''	2:L:109:DT:H5'	1.70	0.74
4:F:226:SER:OG	4:F:229:GLN:HB2	1.86	0.74
3:Q:224:LEU:CD2	3:Q:228:VAL:CG2	2.58	0.74
4:N:188:ARG:CG	4:N:189:ASN:H	1.94	0.73
3:M:112:ARG:HG3	3:M:112:ARG:O	1.88	0.73
4:F:188:ARG:CG	4:F:189:ASN:H	2.00	0.73
3:I:111:ASP:C	3:I:113:ALA:H	1.95	0.73
4:N:247:PRO:O	4:N:249:LYS:HE2	1.89	0.73
2:T:110:DA:C5'	4:R:166:GLN:HG2	2.19	0.73
3:I:176:THR:HG22	3:I:251:ILE:HD13	1.70	0.73
3:M:125:ALA:CA	3:M:130:LEU:HD12	2.18	0.73
3:M:137:ARG:HE	3:M:170:GLN:NE2	1.86	0.73
3:Q:235:ILE:HG23	3:Q:299:LEU:HB3	1.71	0.73
3:E:133:ASN:H	3:E:133:ASN:ND2	1.87	0.73
4:N:202:MET:HE3	4:N:213:ILE:CD1	2.17	0.73
4:N:240:VAL:O	4:N:244:LEU:HG	1.89	0.73
2:H:110:DA:H2''	2:H:111:DT:H5'	1.71	0.73
4:R:209:THR:HG23	4:R:222:THR:O	1.88	0.72
4:F:229:GLN:HA	4:F:229:GLN:NE2	2.01	0.72
3:Q:173:VAL:CG1	3:Q:175:ARG:NH2	2.53	0.72
3:E:270:THR:HG23	3:E:273:GLU:OE1	1.89	0.72
4:N:186:ARG:HG2	4:N:244:LEU:HD22	1.71	0.72
3:I:114:MET:HG2	3:I:118:PHE:CZ	2.24	0.72
2:L:101:DC:H4'	3:I:152:LYS:HD3	1.71	0.72
3:I:112:ARG:O	3:I:112:ARG:HG2	1.90	0.72
2:P:111:DT:H5''	4:N:309:LYS:HD2	1.72	0.71
4:B:205:ARG:NH1	4:B:208:ARG:HE	1.88	0.71
3:I:268:LYS:NZ	3:I:308:THR:OG1	2.22	0.71
4:R:174:LEU:CD1	4:R:241:VAL:HG11	2.20	0.71
2:L:108:DT:OP1	4:J:210:THR:HG21	1.90	0.71
3:Q:290:ARG:NH2	3:Q:316:LEU:O	2.22	0.71
4:F:180:LEU:H	4:F:180:LEU:CD2	2.01	0.71
4:J:318:ARG:HG2	4:J:322:TYR:CE2	2.26	0.71
3:M:137:ARG:HE	3:M:170:GLN:HE22	1.38	0.71
3:Q:224:LEU:HD23	3:Q:228:VAL:CG1	2.20	0.71
3:A:128:ILE:HG12	3:A:183:VAL:HG11	1.73	0.71
3:M:305:LYS:N	3:M:305:LYS:HD3	2.03	0.71
4:F:180:LEU:HD23	4:F:181:LYS:HZ1	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:166:GLN:NE2	4:R:261:SER:HB3	2.06	0.71
3:A:248:ARG:CG	3:A:248:ARG:HH21	2.03	0.70
3:M:306:PHE:HD1	3:M:308:THR:O	1.75	0.70
1:G:8:DT:H2''	1:G:9:DA:H5'	1.72	0.70
4:R:186:ARG:NE	4:R:244:LEU:HG	2.05	0.70
3:M:111:ASP:C	3:M:113:ALA:H	2.00	0.70
3:M:143:LYS:HE2	3:M:147:GLU:OE2	1.92	0.70
4:R:235:ARG:HA	4:R:250:PHE:CE1	2.26	0.70
3:I:222:LEU:HD23	3:I:277:ILE:HD13	1.72	0.70
2:D:110:DA:H2''	2:D:111:DT:H5'	1.73	0.70
4:F:205:ARG:HD2	4:F:205:ARG:N	2.02	0.70
4:N:237:TYR:O	4:N:241:VAL:HG23	1.90	0.70
4:N:304:ILE:HD13	4:N:332:LEU:HD11	1.72	0.70
1:S:9:DA:H2''	1:S:10:DT:H5'	1.73	0.69
4:B:196:ARG:NH2	5:B:381:HOH:O	2.23	0.69
3:I:309:PRO:CG	3:I:312:LYS:HG2	2.13	0.69
3:M:225:PRO:O	3:M:228:VAL:HG22	1.92	0.69
3:A:111:ASP:C	3:A:113:ALA:H	2.00	0.69
4:B:298:PRO:HB2	4:B:300:ILE:HD13	1.73	0.69
3:M:112:ARG:HG3	3:M:112:ARG:HH21	1.56	0.69
3:M:304:PHE:CZ	3:M:305:LYS:HE3	2.28	0.69
3:I:270:THR:CG2	3:I:273:GLU:HG3	2.22	0.69
2:P:110:DA:H2''	2:P:111:DT:C5'	2.22	0.69
4:B:300:ILE:HD11	4:B:320:GLU:HB3	1.73	0.69
4:N:256:GLN:HA	4:N:256:GLN:NE2	2.07	0.69
4:N:279:GLN:NE2	4:N:280:PHE:CE2	2.59	0.69
4:R:235:ARG:HA	4:R:250:PHE:HE1	1.57	0.69
4:F:180:LEU:HD23	4:F:181:LYS:NZ	2.07	0.69
4:F:194:PRO:HG2	4:F:195:LYS:HE3	1.74	0.69
4:F:257:ASN:HD21	4:F:314:GLY:H	1.39	0.69
3:M:231:ALA:O	3:M:235:ILE:HG13	1.92	0.69
1:K:8:DT:H2''	1:K:9:DA:H5'	1.74	0.69
3:Q:236:ALA:O	3:Q:240:VAL:HG23	1.92	0.69
4:R:179:ASP:HB3	4:R:182:THR:CG2	2.23	0.69
3:E:224:LEU:HD21	3:E:269:ARG:HD3	1.75	0.68
4:F:203:ARG:HG2	4:F:210:THR:HG23	1.76	0.68
1:C:7:DC:H2'	1:C:8:DT:C6	2.29	0.68
1:C:9:DA:H2''	1:C:10:DT:H5'	1.73	0.68
3:Q:111:ASP:C	3:Q:113:ALA:H	2.00	0.68
3:E:137:ARG:HE	3:E:170:GLN:NE2	1.91	0.68
3:I:204:THR:HG22	3:I:205:SER:N	2.08	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:276:THR:OG1	4:J:277:HIS:CD2	2.47	0.68
2:D:105:DC:H2''	2:D:106:DT:H5'	1.75	0.68
3:I:143:LYS:O	3:I:147:GLU:HG3	1.94	0.68
4:R:271:GLU:OE2	4:R:271:GLU:N	2.26	0.68
4:B:202:MET:HE3	4:B:213:ILE:CD1	2.25	0.68
1:G:7:DC:H2''	1:G:8:DT:H5'	1.76	0.67
4:J:279:GLN:HG2	4:J:280:PHE:HD2	1.58	0.67
3:Q:224:LEU:HD23	3:Q:228:VAL:HG21	1.71	0.67
1:S:11:DA:H2''	1:S:12:DA:C5'	2.17	0.67
3:I:225:PRO:HG2	3:I:228:VAL:HG23	1.76	0.67
3:M:112:ARG:HH21	3:M:112:ARG:CG	2.06	0.67
4:R:165:LEU:O	4:R:225:LYS:CD	2.41	0.67
4:R:188:ARG:CZ	4:R:189:ASN:HD21	2.07	0.67
2:L:105:DC:H2''	2:L:106:DT:H5'	1.76	0.67
2:T:110:DA:H2''	2:T:111:DT:C5'	2.24	0.67
4:J:279:GLN:CG	4:J:280:PHE:CD2	2.77	0.67
3:M:134:ILE:HD13	3:M:171:GLU:HG3	1.77	0.67
1:O:11:DA:H2''	1:O:12:DA:C5'	2.14	0.66
1:O:9:DA:H2''	1:O:10:DT:H5'	1.78	0.66
4:J:209:THR:HG22	4:J:210:THR:N	2.09	0.66
1:K:11:DA:C2'	1:K:12:DA:H5'	2.11	0.66
3:I:221:ASN:N	3:I:221:ASN:ND2	2.44	0.66
3:M:175:ARG:HH11	3:M:175:ARG:CG	2.06	0.66
3:M:311:ASP:N	3:M:311:ASP:OD2	2.28	0.66
4:F:173:ASN:HB2	4:F:218:LYS:HE2	1.76	0.66
3:I:271:GLN:NE2	3:I:316:LEU:HD21	2.11	0.66
3:A:134:ILE:HD12	3:A:171:GLU:HG3	1.78	0.66
4:N:267:PRO:HG2	4:N:337:LYS:HB2	1.77	0.66
4:R:204:ILE:HG23	4:R:237:TYR:CE1	2.30	0.66
3:E:111:ASP:C	3:E:113:ALA:H	2.04	0.66
4:N:276:THR:HG21	4:N:335:PHE:HZ	1.60	0.66
3:Q:128:ILE:HG13	3:Q:130:LEU:HG	1.78	0.66
3:Q:270:THR:OG1	3:Q:273:GLU:HG3	1.96	0.66
3:Q:190:GLU:OE2	3:Q:193:ARG:NH1	2.30	0.66
2:T:109:DT:C5'	4:R:167:ASN:HD22	2.08	0.65
4:N:297:LYS:HE3	4:N:298:PRO:HA	1.77	0.65
3:A:271:GLN:NE2	3:A:316:LEU:HD21	2.11	0.65
4:B:268:ILE:HD13	4:B:332:LEU:HG	1.77	0.65
3:M:270:THR:HG22	3:M:273:GLU:CD	2.21	0.65
3:Q:173:VAL:HG12	3:Q:173:VAL:O	1.94	0.65
4:R:259:VAL:CG2	4:R:313:THR:HG22	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:107:DT:OP1	4:F:196:ARG:NH1	2.26	0.65
3:Q:226:LYS:H	3:Q:226:LYS:CD	2.07	0.65
3:I:225:PRO:CD	3:I:267:GLU:HG3	2.25	0.65
4:N:180:LEU:HD22	4:N:180:LEU:H	1.62	0.65
4:R:255:ILE:O	4:R:316:LYS:HD2	1.96	0.65
3:Q:217:ARG:O	3:Q:221:ASN:OD1	2.13	0.65
3:E:157:ASP:HB2	3:E:185:ARG:NH2	2.12	0.65
4:F:168:ILE:HD13	4:F:258:MET:HB3	1.78	0.65
3:M:224:LEU:HD21	3:M:269:ARG:NE	2.12	0.65
4:N:288:PHE:CD1	4:N:289:PRO:HD2	2.32	0.65
4:B:296:ILE:HG23	4:B:299:ARG:NH1	2.12	0.64
4:F:213:ILE:HG12	4:F:219:MET:CE	2.27	0.64
4:J:268:ILE:HD13	4:J:332:LEU:HG	1.79	0.64
3:A:270:THR:HG23	3:A:272:LYS:H	1.62	0.64
3:M:227:GLN:OE1	3:M:305:LYS:HE2	1.97	0.64
3:M:209:ILE:H	3:M:209:ILE:CD1	1.90	0.64
3:Q:228:VAL:HG22	3:Q:229:GLN:N	2.13	0.64
3:E:310:VAL:HG13	3:E:311:ASP:OD1	1.98	0.64
4:J:267:PRO:HG2	4:J:337:LYS:HB2	1.79	0.64
4:N:204:ILE:HG23	4:N:237:TYR:CE1	2.33	0.64
2:H:108:DT:OP1	4:F:203:ARG:NH2	2.31	0.64
3:Q:226:LYS:HD3	3:Q:226:LYS:N	2.13	0.64
3:Q:306:PHE:CZ	3:Q:310:VAL:HG23	2.33	0.64
3:M:225:PRO:HG2	3:M:228:VAL:HG13	1.78	0.63
3:Q:173:VAL:CG1	3:Q:173:VAL:O	2.46	0.63
4:J:205:ARG:O	4:J:205:ARG:CD	2.45	0.63
4:R:254:LYS:HD3	4:R:256:GLN:HE22	1.62	0.63
4:R:329:TYR:HB3	4:R:330:PRO:HD3	1.80	0.63
4:F:271:GLU:CD	4:F:271:GLU:H	2.06	0.63
4:R:179:ASP:CG	4:R:182:THR:HG22	2.23	0.63
4:R:269:ARG:HG3	4:R:335:PHE:O	1.97	0.63
4:B:219:MET:HE1	4:B:237:TYR:HB2	1.80	0.63
4:N:329:TYR:HB3	4:N:330:PRO:HD3	1.79	0.63
4:J:279:GLN:HG3	4:J:280:PHE:CD2	2.34	0.63
4:R:196:ARG:HH22	4:R:201:ILE:CD1	2.12	0.63
4:J:209:THR:CG2	4:J:210:THR:N	2.62	0.62
4:R:299:ARG:O	4:R:300:ILE:HD12	1.99	0.62
3:A:193:ARG:NH1	5:A:334:HOH:O	2.33	0.62
4:J:178:LEU:CD2	4:J:183:ILE:HD11	2.30	0.62
4:J:296:ILE:HG23	4:J:299:ARG:NH2	2.14	0.62
4:N:229:GLN:NE2	4:N:232:LEU:HD12	2.10	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:312:LYS:HG2	3:M:312:LYS:O	1.98	0.62
3:Q:128:ILE:HG21	3:Q:183:VAL:HG11	1.78	0.62
4:B:173:ASN:ND2	4:B:175:GLY:H	1.96	0.62
3:A:112:ARG:HD3	3:A:112:ARG:N	2.09	0.62
4:N:171:THR:HG23	4:N:256:GLN:HG3	1.81	0.62
4:R:209:THR:HG22	4:R:210:THR:N	2.13	0.62
3:A:114:MET:HE1	3:A:143:LYS:HG3	1.81	0.62
3:A:174:PRO:O	3:A:217:ARG:NH2	2.33	0.62
3:E:305:LYS:O	3:E:305:LYS:HD3	2.00	0.62
4:N:193:ASN:CB	4:N:196:ARG:HG2	2.29	0.62
2:L:101:DC:H4'	3:I:152:LYS:CD	2.30	0.62
4:R:163:PRO:HA	4:R:262:CYS:HB3	1.82	0.61
3:E:150:SER:C	3:E:151:LEU:HD12	2.25	0.61
4:J:296:ILE:HG23	4:J:299:ARG:HH22	1.64	0.61
4:R:179:ASP:O	4:R:182:THR:HG23	2.00	0.61
4:R:171:THR:CG2	4:R:256:GLN:HG2	2.30	0.61
2:H:102:DC:H2''	2:H:103:DC:O5'	2.01	0.61
2:P:110:DA:C5'	4:N:166:GLN:HG2	2.27	0.61
3:I:133:ASN:ND2	3:I:133:ASN:N	2.44	0.61
3:I:225:PRO:HD2	3:I:267:GLU:HG3	1.82	0.61
4:J:257:ASN:HD21	4:J:314:GLY:H	1.47	0.61
3:M:254:ALA:O	3:M:258:ILE:HG13	2.00	0.61
4:N:257:ASN:HD21	4:N:314:GLY:N	1.95	0.61
4:N:300:ILE:HD11	4:N:315:ALA:HB2	1.81	0.61
4:R:174:LEU:HD12	4:R:241:VAL:HG11	1.83	0.61
2:H:106:DT:H2''	2:H:107:DT:H5'	1.81	0.61
3:M:117:ALA:O	3:M:121:ILE:HG13	2.00	0.61
3:A:269:ARG:HH11	3:A:269:ARG:CG	2.14	0.61
1:C:2:DG:OP2	5:C:172:HOH:O	2.16	0.61
3:I:295:ARG:HG3	3:I:295:ARG:NH1	2.12	0.61
4:N:173:ASN:ND2	4:N:175:GLY:H	1.98	0.61
3:Q:112:ARG:HD2	3:Q:112:ARG:N	2.15	0.61
4:F:196:ARG:NH2	5:F:361:HOH:O	2.27	0.61
3:M:224:LEU:HB3	3:M:228:VAL:CG2	2.28	0.61
1:K:14:DA:H1'	4:J:214:PHE:CZ	2.36	0.61
2:T:106:DT:H2''	2:T:107:DT:H5'	1.81	0.60
3:M:262:SER:OG	3:M:269:ARG:N	2.34	0.60
4:R:174:LEU:HD11	4:R:241:VAL:HG21	1.82	0.60
4:R:278:GLN:OE1	4:R:278:GLN:HA	2.00	0.60
2:D:108:DT:OP1	4:B:203:ARG:NH2	2.32	0.60
1:O:8:DT:H2''	1:O:9:DA:C5'	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:173:VAL:CG1	3:Q:175:ARG:HH22	2.12	0.60
2:T:105:DC:H2''	2:T:106:DT:H5'	1.82	0.60
4:N:256:GLN:HE21	4:N:256:GLN:CA	2.10	0.60
2:D:101:DC:H2''	2:D:102:DC:H5'	1.83	0.60
3:E:112:ARG:NH2	3:E:114:MET:HE3	2.14	0.60
3:I:216:SER:HA	3:I:229:GLN:NE2	2.17	0.60
3:I:231:ALA:O	3:I:235:ILE:HG13	2.02	0.60
3:M:133:ASN:H	3:M:133:ASN:ND2	1.97	0.60
4:J:172:VAL:HG21	4:J:250:PHE:CE1	2.37	0.60
2:T:108:DT:H1'	4:R:167:ASN:ND2	2.17	0.60
4:J:211:ALA:HB1	4:J:219:MET:CE	2.32	0.60
3:A:221:ASN:HD22	3:A:221:ASN:H	1.48	0.60
3:M:289:TYR:CD2	3:M:316:LEU:HD12	2.36	0.60
4:N:237:TYR:O	4:N:240:VAL:HG22	2.02	0.60
4:J:243:LYS:HZ2	4:J:243:LYS:HB3	1.66	0.59
3:M:268:LYS:NZ	3:M:308:THR:OG1	2.34	0.59
4:J:279:GLN:HG2	4:J:280:PHE:CD2	2.37	0.59
3:M:263:GLN:HG2	3:M:314:PRO:CG	2.30	0.59
4:N:249:LYS:HB3	4:N:251:LEU:CD1	2.32	0.59
3:I:282:ASP:O	3:I:286:ARG:HG3	2.02	0.59
4:J:191:GLU:HG3	4:J:201:ILE:O	2.02	0.59
3:M:114:MET:HE1	3:M:143:LYS:HD2	1.84	0.59
3:M:207:ASP:OD2	3:M:207:ASP:N	2.27	0.59
3:M:298:ASP:OD2	3:M:298:ASP:N	2.35	0.59
4:N:268:ILE:HD13	4:N:332:LEU:HG	1.84	0.59
4:R:171:THR:CG2	4:R:256:GLN:CG	2.80	0.59
3:I:112:ARG:O	3:I:112:ARG:CG	2.51	0.59
1:G:18:DG:O3'	3:M:316:LEU:CD2	2.50	0.59
3:M:169:ARG:NH2	3:M:206:VAL:HG23	2.18	0.59
2:L:110:DA:H2''	2:L:111:DT:C5'	2.31	0.59
3:Q:173:VAL:HG13	3:Q:175:ARG:NH2	2.18	0.59
3:A:158:ALA:HA	3:A:186:ILE:HG13	1.85	0.59
4:F:235:ARG:HH21	4:F:235:ARG:CG	2.12	0.59
4:F:239:ARG:HH21	4:F:242:GLN:HE22	1.50	0.59
3:M:131:PRO:HG2	3:M:134:ILE:CG1	2.32	0.59
3:M:307:ASP:OD1	3:M:307:ASP:C	2.46	0.59
1:C:14:DA:H1'	4:B:214:PHE:CE1	2.38	0.59
3:A:248:ARG:HH21	3:A:248:ARG:HG3	1.67	0.59
3:E:204:THR:HG22	3:E:205:SER:N	2.18	0.59
4:R:171:THR:HG23	4:R:256:GLN:HG2	1.84	0.58
4:R:199:ALA:HB1	4:R:213:ILE:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:219:MET:HE1	4:B:237:TYR:CB	2.33	0.58
4:F:203:ARG:CG	4:F:210:THR:HG23	2.33	0.58
3:M:110:SER:O	3:M:113:ALA:HB2	2.03	0.58
3:M:125:ALA:HA	3:M:130:LEU:CD1	2.23	0.58
3:M:238:LYS:HB3	3:M:299:LEU:HD22	1.84	0.58
4:N:239:ARG:HG2	4:N:242:GLN:NE2	2.17	0.58
4:N:306:VAL:HG22	5:N:340:HOH:O	2.02	0.58
4:R:279:GLN:HB3	4:R:280:PHE:CE2	2.38	0.58
2:P:105:DC:H2''	2:P:106:DT:H5'	1.85	0.58
1:S:7:DC:H2''	1:S:8:DT:C5'	2.34	0.58
4:R:317:VAL:HG23	4:R:319:ALA:H	1.67	0.58
4:J:209:THR:HG23	4:J:222:THR:O	2.04	0.58
3:I:225:PRO:CG	3:I:267:GLU:HG3	2.34	0.58
4:J:205:ARG:HD3	4:J:208:ARG:HG3	1.86	0.58
3:Q:176:THR:HG22	3:Q:251:ILE:CD1	2.34	0.58
4:R:205:ARG:O	4:R:205:ARG:HG3	2.03	0.58
2:P:106:DT:H2''	2:P:107:DT:H5'	1.86	0.58
2:D:104:DC:H2''	2:D:105:DC:H5'	1.85	0.57
1:G:11:DA:OP1	4:F:294:ARG:NH2	2.35	0.57
4:F:180:LEU:HD22	4:F:180:LEU:N	2.10	0.57
4:F:213:ILE:HG12	4:F:219:MET:HE2	1.86	0.57
3:A:122:THR:HG22	3:A:123:THR:N	2.17	0.57
3:A:133:ASN:N	3:A:133:ASN:ND2	2.50	0.57
3:I:226:LYS:HE2	3:I:226:LYS:H	1.70	0.57
4:R:178:LEU:HD22	4:R:246:PHE:CD2	2.39	0.57
1:O:14:DA:H1'	4:N:214:PHE:CZ	2.39	0.57
3:I:130:LEU:HD22	3:I:134:ILE:HD12	1.87	0.57
4:B:168:ILE:HD12	4:B:226:SER:C	2.29	0.57
3:Q:111:ASP:O	3:Q:114:MET:HG3	2.04	0.57
4:N:196:ARG:HG3	4:N:197:PHE:H	1.69	0.57
4:N:202:MET:CE	4:N:213:ILE:CD1	2.83	0.57
4:R:224:ALA:HA	4:R:229:GLN:NE2	2.16	0.57
4:R:325:PHE:O	4:R:328:ILE:HG22	2.04	0.57
1:C:7:DC:H2''	1:C:8:DT:H5'	1.85	0.57
2:P:111:DT:H5''	4:N:309:LYS:CD	2.34	0.57
3:A:286:ARG:HG2	3:A:316:LEU:HD23	1.86	0.57
4:F:179:ASP:OD1	4:F:182:THR:HG22	2.05	0.57
4:J:279:GLN:CG	4:J:280:PHE:HD2	2.15	0.57
2:T:102:DC:H2''	2:T:103:DC:O5'	2.04	0.57
3:A:224:LEU:CD2	3:A:269:ARG:NH1	2.67	0.57
4:F:283:TYR:HB2	4:F:291:LEU:HD22	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:173:VAL:O	3:M:173:VAL:CG2	2.53	0.57
3:A:157:ASP:HB2	3:A:185:ARG:NH2	2.20	0.56
3:I:173:VAL:HG23	3:I:173:VAL:O	2.04	0.56
3:I:222:LEU:HB2	3:I:224:LEU:HD12	1.85	0.56
3:M:175:ARG:HG2	3:M:175:ARG:NH1	2.07	0.56
3:I:137:ARG:HD2	3:I:171:GLU:HG2	1.87	0.56
3:M:270:THR:HG22	3:M:273:GLU:CG	2.36	0.56
4:R:269:ARG:CG	4:R:337:LYS:HG2	2.22	0.56
1:G:15:DG:C2'	1:G:16:DG:H5''	2.34	0.56
3:I:132:ARG:NH1	3:I:136:ASP:OD1	2.39	0.56
3:I:207:ASP:OD1	3:I:207:ASP:N	2.29	0.56
3:Q:164:LEU:HD23	3:Q:180:ILE:HD12	1.86	0.56
3:Q:262:SER:OG	3:Q:269:ARG:N	2.38	0.56
4:R:209:THR:HG21	4:R:221:CYS:SG	2.45	0.56
3:A:133:ASN:H	3:A:133:ASN:ND2	2.01	0.56
4:F:185:LEU:C	4:F:185:LEU:HD23	2.29	0.56
3:A:117:ALA:O	3:A:121:ILE:HG13	2.06	0.56
3:I:131:PRO:HB2	3:I:133:ASN:ND2	2.19	0.56
3:I:225:PRO:HG3	3:I:267:GLU:OE1	2.06	0.56
3:A:309:PRO:HG3	3:A:312:LYS:HE3	1.88	0.56
4:B:205:ARG:HH12	4:B:208:ARG:HE	1.54	0.56
3:Q:117:ALA:O	3:Q:121:ILE:HG13	2.06	0.56
3:I:157:ASP:CB	3:I:185:ARG:NH2	2.69	0.56
4:F:163:PRO:HA	4:F:262:CYS:HB3	1.88	0.56
3:E:133:ASN:ND2	3:E:133:ASN:N	2.54	0.56
3:M:121:ILE:HD13	3:M:138:THR:HG22	1.88	0.56
3:M:308:THR:HG23	3:M:312:LYS:HD2	1.87	0.56
3:Q:176:THR:HG22	3:Q:251:ILE:HD13	1.88	0.56
1:O:7:DC:H2'	1:O:8:DT:C6	2.41	0.56
4:N:286:GLU:HG3	5:N:338:HOH:O	2.05	0.56
4:R:280:PHE:N	4:R:280:PHE:CD2	2.74	0.56
3:A:204:THR:HG22	3:A:205:SER:H	1.70	0.55
3:I:221:ASN:HD22	3:I:221:ASN:H	1.50	0.55
3:M:186:ILE:HG22	3:M:187:SER:N	2.21	0.55
3:A:148:GLN:NE2	3:A:150:SER:OG	2.35	0.55
3:I:295:ARG:CG	3:I:295:ARG:NH1	2.62	0.55
3:Q:262:SER:OG	3:Q:268:LYS:HA	2.07	0.55
4:J:279:GLN:H	4:J:279:GLN:HE21	1.53	0.55
4:N:294:ARG:HG2	4:N:301:VAL:HG22	1.87	0.55
3:Q:154:ARG:NH2	3:Q:190:GLU:OE1	2.37	0.55
2:P:101:DC:H2''	2:P:102:DC:O5'	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:317:VAL:HG23	4:J:320:GLU:HG3	1.87	0.55
4:N:246:PHE:C	4:N:248:ALA:H	2.14	0.55
3:E:196:LYS:HE2	5:E:371:HOH:O	2.06	0.55
3:I:221:ASN:ND2	3:I:221:ASN:H	2.04	0.55
3:I:270:THR:HG22	3:I:273:GLU:CB	2.36	0.55
4:J:246:PHE:C	4:J:248:ALA:H	2.15	0.55
4:R:278:GLN:OE1	4:R:278:GLN:CA	2.55	0.55
3:I:311:ASP:C	3:I:313:LEU:H	2.15	0.55
4:B:204:ILE:HG23	4:B:237:TYR:CE1	2.42	0.55
3:E:131:PRO:HB2	3:E:133:ASN:HD21	1.72	0.55
4:J:174:LEU:HD12	4:J:248:ALA:HB1	1.89	0.55
4:J:239:ARG:NH1	4:J:242:GLN:HE22	2.05	0.54
4:J:329:TYR:HB3	4:J:330:PRO:HD3	1.90	0.54
3:M:209:ILE:N	3:M:209:ILE:CD1	2.58	0.54
2:L:101:DC:H2''	2:L:102:DC:H5'	1.89	0.54
3:A:186:ILE:HG22	3:A:187:SER:N	2.22	0.54
3:A:289:TYR:CD2	3:A:316:LEU:HD22	2.41	0.54
4:F:259:VAL:HG13	4:F:313:THR:CG2	2.36	0.54
3:I:309:PRO:CG	3:I:312:LYS:HE2	2.37	0.54
4:F:179:ASP:O	4:F:182:THR:CG2	2.54	0.54
4:R:231:ARG:HB3	4:R:231:ARG:NH1	2.22	0.54
4:F:264:VAL:HG11	4:F:332:LEU:HD23	1.88	0.54
3:Q:193:ARG:O	3:Q:197:LEU:CD2	2.55	0.54
3:Q:193:ARG:O	3:Q:197:LEU:HD22	2.08	0.54
4:R:196:ARG:HH22	4:R:201:ILE:HD11	1.72	0.54
3:E:110:SER:O	3:E:113:ALA:HB2	2.08	0.54
3:I:267:GLU:CD	3:I:267:GLU:H	2.16	0.54
3:A:189:LYS:CE	3:A:193:ARG:NH2	2.66	0.54
4:R:209:THR:CG2	4:R:210:THR:N	2.70	0.54
3:E:311:ASP:C	3:E:313:LEU:H	2.16	0.54
4:J:237:TYR:O	4:J:240:VAL:HG22	2.08	0.54
3:Q:128:ILE:CG2	3:Q:183:VAL:CG1	2.77	0.54
3:E:296:ALA:N	3:E:297:PRO:HD2	2.24	0.54
4:F:299:ARG:C	4:F:300:ILE:HD13	2.32	0.54
4:N:273:LEU:O	4:N:273:LEU:HD23	2.07	0.54
1:O:11:DA:C2'	1:O:12:DA:H5'	2.15	0.53
3:A:311:ASP:C	3:A:313:LEU:H	2.17	0.53
3:I:293:TYR:HB3	3:I:294:PRO:HD3	1.91	0.53
3:I:141:LEU:O	3:I:145:VAL:CG2	2.56	0.53
4:J:259:VAL:HG13	4:J:313:THR:CG2	2.39	0.53
3:A:296:ALA:N	3:A:297:PRO:HD2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:205:ARG:CD	4:F:205:ARG:N	2.56	0.53
3:M:228:VAL:HG23	3:M:229:GLN:N	2.24	0.53
1:S:7:DC:H2'	1:S:8:DT:C6	2.43	0.53
4:F:219:MET:HE1	4:F:237:TYR:HB3	1.89	0.53
1:C:7:DC:H2''	1:C:8:DT:C5'	2.37	0.53
3:Q:128:ILE:HD11	3:Q:130:LEU:HD11	1.89	0.53
2:D:101:DC:H2''	2:D:102:DC:C5'	2.39	0.53
4:R:170:SER:OG	4:R:221:CYS:HB3	2.08	0.53
3:A:134:ILE:HG22	3:A:135:VAL:N	2.24	0.53
4:J:251:LEU:N	4:J:251:LEU:HD23	2.23	0.53
4:N:173:ASN:HB2	4:N:218:LYS:HD3	1.91	0.53
4:R:213:ILE:HD11	4:R:219:MET:HB3	1.87	0.53
4:R:246:PHE:C	4:R:248:ALA:H	2.15	0.53
3:E:154:ARG:NH1	3:E:190:GLU:OE1	2.42	0.53
3:A:310:VAL:O	3:A:313:LEU:HB2	2.10	0.52
4:F:207:PRO:HD3	4:F:236:LYS:HE3	1.91	0.52
4:F:259:VAL:CG2	4:F:313:THR:HG22	2.32	0.52
4:J:277:HIS:CE1	4:J:331:ILE:HD13	2.44	0.52
3:Q:234:HIS:CG	3:Q:301:PRO:HG3	2.44	0.52
3:A:226:LYS:CG	3:A:230:MET:HE2	2.37	0.52
3:I:133:ASN:HD22	3:I:133:ASN:N	1.91	0.52
3:I:141:LEU:O	3:I:145:VAL:HG23	2.09	0.52
4:J:178:LEU:HD23	4:J:183:ILE:HD11	1.90	0.52
3:A:215:MET:HG3	3:A:233:THR:OG1	2.09	0.52
4:F:180:LEU:CD2	4:F:215:SER:HB3	2.25	0.52
4:N:163:PRO:HA	4:N:262:CYS:HB3	1.89	0.52
1:O:3:DG:N3	5:O:225:HOH:O	2.33	0.52
3:A:270:THR:HG23	3:A:272:LYS:N	2.25	0.52
4:B:288:PHE:CD1	4:B:289:PRO:HD2	2.44	0.52
3:E:137:ARG:HE	3:E:170:GLN:HE22	1.54	0.52
3:Q:133:ASN:ND2	3:Q:171:GLU:CD	2.67	0.52
2:L:106:DT:H2''	2:L:107:DT:H5'	1.91	0.52
3:A:176:THR:OG1	3:A:179:GLU:HG3	2.09	0.52
3:I:312:LYS:N	3:I:312:LYS:CD	2.56	0.52
4:J:203:ARG:HG2	4:J:210:THR:HB	1.90	0.52
4:N:229:GLN:HE22	4:N:232:LEU:CD1	2.15	0.52
3:A:310:VAL:HA	3:A:313:LEU:HD22	1.91	0.52
3:E:224:LEU:HD21	3:E:269:ARG:CD	2.40	0.52
3:M:112:ARG:CG	3:M:112:ARG:NH2	2.70	0.52
3:I:181:CYS:SG	3:I:188:LYS:N	2.82	0.52
4:N:228:GLU:OE2	4:N:228:GLU:HA	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:254:ALA:O	3:Q:258:ILE:HG13	2.09	0.52
1:O:14:DA:H1'	4:N:214:PHE:CE1	2.45	0.52
2:P:102:DC:H2''	2:P:103:DC:O5'	2.09	0.52
3:A:259:TYR:CE2	3:A:271:GLN:HG3	2.44	0.52
3:I:310:VAL:O	3:I:313:LEU:HB2	2.09	0.52
1:C:18:DG:H3'	3:E:271:GLN:NE2	2.24	0.52
2:H:108:DT:H2''	2:H:109:DT:C5'	2.31	0.52
4:N:288:PHE:CG	4:N:289:PRO:HD2	2.45	0.52
4:F:180:LEU:HB3	4:F:200:VAL:CG2	2.40	0.51
4:J:174:LEU:HD23	4:J:217:GLY:O	2.09	0.51
1:G:7:DC:H2'	1:G:8:DT:C6	2.45	0.51
4:J:231:ARG:HA	4:J:253:PHE:CE2	2.45	0.51
3:Q:169:ARG:NH1	4:R:284:GLU:OE1	2.31	0.51
3:I:111:ASP:C	3:I:113:ALA:N	2.64	0.51
4:N:243:LYS:HD3	4:N:243:LYS:C	2.32	0.51
3:A:131:PRO:HB2	3:A:133:ASN:ND2	2.25	0.51
3:A:157:ASP:HB2	3:A:185:ARG:HH21	1.74	0.51
4:F:179:ASP:HB3	4:F:182:THR:CG2	2.41	0.51
4:F:182:THR:HG23	4:F:183:ILE:N	2.25	0.51
4:N:193:ASN:ND2	4:N:196:ARG:HG2	2.25	0.51
3:A:157:ASP:CG	3:A:185:ARG:HH21	2.18	0.51
3:M:174:PRO:O	3:M:217:ARG:NH1	2.32	0.51
3:M:311:ASP:C	3:M:313:LEU:H	2.17	0.51
1:C:18:DG:O3'	3:E:316:LEU:CD1	2.59	0.51
4:N:295:MET:HE3	4:N:298:PRO:HD2	1.92	0.51
4:R:207:PRO:CB	4:R:229:GLN:OE1	2.50	0.51
4:J:246:PHE:O	4:J:248:ALA:N	2.36	0.51
3:M:148:GLN:HB3	3:M:150:SER:OG	2.11	0.51
4:R:249:LYS:HB2	4:R:251:LEU:CD1	2.40	0.51
4:R:317:VAL:HG22	4:R:320:GLU:HG3	1.91	0.51
3:A:248:ARG:CG	3:A:248:ARG:NH2	2.71	0.51
4:F:180:LEU:HB3	4:F:200:VAL:HG23	1.92	0.51
4:J:259:VAL:HG13	4:J:313:THR:HG22	1.93	0.51
4:R:271:GLU:CD	4:R:271:GLU:N	2.55	0.51
3:M:231:ALA:HB2	3:M:304:PHE:CE2	2.46	0.51
3:Q:176:THR:CG2	3:Q:251:ILE:HD13	2.40	0.51
4:R:327:ASN:O	4:R:331:ILE:HD12	2.11	0.51
1:S:8:DT:H2''	1:S:9:DA:H5'	1.93	0.50
3:A:248:ARG:HG3	3:A:248:ARG:NH2	2.25	0.50
4:B:173:ASN:HD22	4:B:174:LEU:N	2.08	0.50
3:M:154:ARG:HD3	3:M:194:CYS:SG	2.52	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:251:LEU:HD12	4:R:251:LEU:H	1.76	0.50
2:D:102:DC:H2''	2:D:103:DC:O5'	2.10	0.50
3:A:179:GLU:OE2	3:A:217:ARG:NH1	2.44	0.50
4:B:173:ASN:HD22	4:B:173:ASN:C	2.20	0.50
3:E:224:LEU:HD23	3:E:269:ARG:HH11	1.77	0.50
4:F:249:LYS:HB2	4:F:251:LEU:HD22	1.94	0.50
4:R:192:TYR:CD1	4:R:194:PRO:HD3	2.46	0.50
3:A:224:LEU:HD21	3:A:269:ARG:HH11	1.74	0.50
3:M:224:LEU:CD2	3:M:269:ARG:HE	2.19	0.50
2:T:104:DC:OP1	3:Q:193:ARG:NH2	2.44	0.50
3:E:204:THR:CG2	3:E:205:SER:N	2.75	0.50
4:J:178:LEU:HD22	4:J:183:ILE:HD11	1.92	0.50
3:Q:169:ARG:NH2	3:Q:206:VAL:HG23	2.26	0.50
2:D:115:DC:OP2	3:A:284:THR:OG1	2.26	0.50
3:A:307:ASP:OD1	3:A:307:ASP:C	2.55	0.50
4:B:257:ASN:HD21	4:B:314:GLY:N	2.03	0.50
4:J:180:LEU:HB3	4:J:200:VAL:HG23	1.94	0.50
4:J:204:ILE:HG23	4:J:237:TYR:CE1	2.46	0.50
3:M:215:MET:HE3	3:M:233:THR:HA	1.94	0.50
4:F:257:ASN:HD21	4:F:314:GLY:N	2.07	0.50
4:J:167:ASN:HD21	4:J:223:GLY:N	2.00	0.50
4:J:167:ASN:ND2	4:J:168:ILE:H	2.09	0.50
3:M:116:ASN:OD1	3:M:116:ASN:N	2.44	0.50
4:R:236:LYS:O	4:R:239:ARG:HB2	2.12	0.50
4:F:274:VAL:O	4:F:278:GLN:HG2	2.11	0.50
1:S:15:DG:H2''	1:S:16:DG:H5''	1.93	0.49
3:A:131:PRO:HB2	3:A:133:ASN:HD21	1.77	0.49
3:A:137:ARG:HD2	3:A:171:GLU:OE1	2.11	0.49
3:A:179:GLU:CD	3:A:217:ARG:HH12	2.20	0.49
4:F:246:PHE:C	4:F:248:ALA:H	2.20	0.49
4:J:202:MET:HE3	4:J:213:ILE:CD1	2.42	0.49
3:M:304:PHE:CE2	3:M:305:LYS:HE3	2.45	0.49
2:H:105:DC:H2''	2:H:106:DT:H5'	1.95	0.49
2:T:104:DC:P	3:Q:193:ARG:NH2	2.86	0.49
3:E:289:TYR:CE2	3:E:316:LEU:HD23	2.47	0.49
4:R:266:PHE:HB2	4:R:336:ARG:HD2	1.94	0.49
3:A:245:VAL:HG21	3:A:253:VAL:HG21	1.93	0.49
2:H:109:DT:OP1	4:F:208:ARG:NH2	2.45	0.49
3:A:270:THR:CG2	3:A:272:LYS:HB3	2.42	0.49
4:B:227:GLU:OE1	4:B:318:ARG:NH1	2.37	0.49
4:F:179:ASP:HB3	4:F:182:THR:HG22	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:193:ARG:O	3:I:197:LEU:HD23	2.12	0.49
4:N:162:VAL:O	4:N:162:VAL:HG13	2.11	0.49
4:R:171:THR:HG23	4:R:256:GLN:HE21	1.76	0.49
4:F:317:VAL:HG22	4:F:320:GLU:OE2	2.11	0.49
3:I:204:THR:CG2	3:I:205:SER:H	2.16	0.49
4:J:280:PHE:CD2	4:J:280:PHE:N	2.80	0.49
3:Q:128:ILE:CD1	3:Q:130:LEU:HD11	2.42	0.49
4:B:173:ASN:ND2	4:B:173:ASN:C	2.70	0.49
3:M:306:PHE:CD1	3:M:308:THR:O	2.60	0.49
4:N:203:ARG:HD3	4:N:208:ARG:HH21	1.77	0.49
3:Q:185:ARG:O	3:Q:185:ARG:HG3	2.13	0.49
3:Q:293:TYR:CE2	3:Q:314:PRO:O	2.66	0.49
3:A:286:ARG:HD2	5:A:324:HOH:O	2.12	0.49
3:M:259:TYR:CE2	3:M:271:GLN:HG3	2.48	0.49
4:R:205:ARG:HB3	4:R:206:GLU:OE1	2.12	0.49
4:F:273:LEU:HD12	4:F:273:LEU:O	2.13	0.49
3:Q:177:PHE:CE2	4:R:287:LEU:HD13	2.48	0.49
3:A:120:GLU:OE2	3:A:120:GLU:HA	2.13	0.48
4:B:205:ARG:HA	4:B:205:ARG:HD2	1.60	0.48
4:F:229:GLN:CA	4:F:229:GLN:NE2	2.65	0.48
4:J:243:LYS:HB3	4:J:243:LYS:NZ	2.25	0.48
4:R:278:GLN:OE1	4:R:278:GLN:O	2.30	0.48
4:B:326:GLU:O	4:B:330:PRO:HD3	2.12	0.48
3:E:176:THR:HG22	3:E:251:ILE:CD1	2.43	0.48
3:E:177:PHE:HB3	3:E:188:LYS:HG3	1.95	0.48
3:I:235:ILE:HG23	3:I:299:LEU:HB3	1.94	0.48
3:M:221:ASN:N	3:M:221:ASN:HD22	2.10	0.48
3:Q:177:PHE:HB3	3:Q:188:LYS:HG3	1.95	0.48
3:A:113:ALA:HA	3:A:116:ASN:ND2	2.27	0.48
4:B:205:ARG:NH2	4:B:208:ARG:HD2	2.28	0.48
3:E:311:ASP:OD1	3:E:311:ASP:N	2.46	0.48
3:I:179:GLU:OE1	3:I:217:ARG:NH2	2.46	0.48
2:L:101:DC:H2''	2:L:102:DC:C5'	2.42	0.48
3:I:266:ALA:HB2	3:I:307:ASP:OD2	2.13	0.48
4:N:202:MET:CE	4:N:213:ILE:HD12	2.43	0.48
3:Q:306:PHE:CZ	3:Q:310:VAL:CG2	2.96	0.48
3:M:237:ARG:HH21	3:M:237:ARG:HG3	1.79	0.48
4:N:229:GLN:HE21	4:N:229:GLN:N	2.10	0.48
3:Q:214:PHE:HB3	3:Q:218:PHE:CE1	2.49	0.48
4:N:277:HIS:NE2	4:N:331:ILE:HD13	2.28	0.48
3:Q:248:ARG:HH22	3:Q:287:GLN:NE2	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:225:LYS:H	4:R:229:GLN:NE2	2.11	0.48
1:C:18:DG:H3'	3:E:271:GLN:HE22	1.78	0.48
4:F:205:ARG:HH11	4:F:205:ARG:CG	2.26	0.48
3:I:226:LYS:H	3:I:226:LYS:CE	2.26	0.48
3:Q:311:ASP:C	3:Q:313:LEU:H	2.22	0.48
3:A:113:ALA:HA	3:A:116:ASN:HD22	1.78	0.48
3:E:313:LEU:HD12	3:E:314:PRO:CD	2.43	0.48
3:M:128:ILE:HG13	3:M:130:LEU:HG	1.96	0.48
4:N:196:ARG:HG3	4:N:197:PHE:N	2.29	0.48
4:N:266:PHE:CD1	4:N:336:ARG:HB2	2.49	0.48
3:E:151:LEU:HD12	3:E:151:LEU:N	2.28	0.48
3:E:176:THR:HG22	3:E:251:ILE:HD11	1.95	0.48
3:E:193:ARG:O	3:E:197:LEU:HD22	2.14	0.48
4:J:168:ILE:HD13	4:J:258:MET:HB3	1.95	0.48
4:R:188:ARG:NH2	4:R:189:ASN:ND2	2.49	0.48
4:N:231:ARG:HA	4:N:253:PHE:HE2	1.74	0.48
4:R:315:ALA:HA	4:R:320:GLU:OE1	2.14	0.48
4:J:178:LEU:HD12	4:J:217:GLY:HA2	1.96	0.47
4:N:174:LEU:HD21	4:N:219:MET:HE3	1.96	0.47
3:I:157:ASP:CB	3:I:185:ARG:HH21	2.27	0.47
3:A:295:ARG:C	3:A:297:PRO:HD2	2.39	0.47
3:Q:303:ASP:CG	3:Q:303:ASP:O	2.57	0.47
2:T:101:DC:H2''	2:T:102:DC:C5'	2.45	0.47
3:I:222:LEU:CB	3:I:224:LEU:HD12	2.45	0.47
4:J:253:PHE:CD1	4:J:253:PHE:C	2.92	0.47
4:J:317:VAL:CG2	4:J:320:GLU:HG3	2.44	0.47
3:M:259:TYR:CE2	3:M:271:GLN:CG	2.97	0.47
4:F:267:PRO:HG2	4:F:337:LYS:HB2	1.97	0.47
3:I:174:PRO:O	3:I:217:ARG:NH1	2.48	0.47
3:I:293:TYR:OH	3:I:315:GLN:HG2	2.14	0.47
1:C:1:DG:H2''	5:C:172:HOH:O	2.14	0.47
4:J:235:ARG:CG	4:J:250:PHE:CZ	2.98	0.47
4:J:259:VAL:HG22	4:J:313:THR:CG2	2.39	0.47
4:N:279:GLN:NE2	4:N:280:PHE:HE2	2.10	0.47
1:K:13:DA:C4'	4:J:256:GLN:HG3	2.45	0.47
2:T:101:DC:H2''	2:T:102:DC:H5'	1.97	0.47
4:B:209:THR:CG2	4:B:210:THR:N	2.78	0.47
3:I:110:SER:O	3:I:113:ALA:HB2	2.15	0.47
3:M:208:LEU:HD12	3:M:208:LEU:HA	1.68	0.47
3:M:296:ALA:N	3:M:297:PRO:HD2	2.30	0.47
4:N:239:ARG:O	4:N:240:VAL:C	2.56	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:295:MET:SD	4:R:298:PRO:HD2	2.55	0.47
3:I:128:ILE:HG23	3:I:183:VAL:HG11	1.96	0.47
3:A:224:LEU:HD23	3:A:269:ARG:NH1	2.30	0.47
3:I:281:ALA:O	3:I:284:THR:HB	2.15	0.47
4:J:163:PRO:HA	4:J:262:CYS:HB3	1.97	0.47
4:N:267:PRO:HB2	4:N:337:LYS:HD2	1.96	0.47
4:R:209:THR:CG2	4:R:210:THR:H	2.28	0.47
3:M:271:GLN:HE22	3:M:316:LEU:CD2	2.28	0.47
3:M:305:LYS:HD3	3:M:305:LYS:C	2.40	0.47
3:M:308:THR:HG23	3:M:309:PRO:HD2	1.96	0.47
4:R:228:GLU:OE2	4:R:231:ARG:NH1	2.32	0.47
4:B:167:ASN:HD21	4:B:223:GLY:H	1.63	0.46
4:B:205:ARG:CZ	4:B:208:ARG:HG3	2.45	0.46
3:E:154:ARG:NH1	3:E:190:GLU:OE2	2.48	0.46
3:E:169:ARG:HH22	4:F:284:GLU:CD	2.23	0.46
4:F:235:ARG:CG	4:F:235:ARG:NH2	2.73	0.46
4:J:172:VAL:HG21	4:J:250:PHE:CD1	2.50	0.46
2:D:106:DT:H2''	2:D:107:DT:H5'	1.97	0.46
1:O:7:DC:H2''	1:O:8:DT:H5'	1.96	0.46
3:E:310:VAL:O	3:E:313:LEU:HB2	2.14	0.46
2:L:109:DT:H6	2:L:109:DT:H2'	1.43	0.46
3:I:145:VAL:HG11	3:I:198:ILE:HG12	1.97	0.46
3:M:120:GLU:OE2	3:M:120:GLU:HA	2.15	0.46
3:M:176:THR:HG22	3:M:251:ILE:HD13	1.97	0.46
4:N:166:GLN:NE2	4:N:261:SER:OG	2.49	0.46
4:R:224:ALA:CA	4:R:229:GLN:HE22	2.22	0.46
4:R:249:LYS:CB	4:R:251:LEU:HD11	2.46	0.46
1:G:12:DA:C2	4:F:169:VAL:HG21	2.50	0.46
2:H:109:DT:H2''	2:H:110:DA:C8	2.51	0.46
3:A:200:LYS:HD3	3:A:200:LYS:HA	1.88	0.46
3:I:186:ILE:HG22	3:I:187:SER:N	2.31	0.46
1:G:18:DG:HO3'	3:M:316:LEU:HD23	1.79	0.46
4:N:300:ILE:CD1	4:N:315:ALA:HB2	2.46	0.46
3:Q:224:LEU:HD23	3:Q:228:VAL:CG2	2.37	0.46
4:R:213:ILE:O	4:R:213:ILE:HG22	2.16	0.46
3:E:189:LYS:O	3:E:193:ARG:HG3	2.16	0.46
4:N:253:PHE:CD1	4:N:253:PHE:C	2.93	0.46
4:N:298:PRO:HG3	4:N:323:GLU:HB3	1.98	0.46
3:Q:271:GLN:HB3	3:Q:282:ASP:HB3	1.97	0.46
4:R:168:ILE:HD12	4:R:226:SER:CA	2.46	0.46
4:R:325:PHE:HA	4:R:328:ILE:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:110:SER:O	3:A:113:ALA:HB2	2.15	0.46
4:N:172:VAL:HG21	4:N:250:PHE:CD1	2.51	0.46
4:N:279:GLN:NE2	4:N:280:PHE:CD2	2.84	0.46
4:R:186:ARG:NH1	4:R:244:LEU:HG	2.31	0.46
1:G:14:DA:H1'	4:F:214:PHE:CZ	2.51	0.46
4:J:167:ASN:ND2	4:J:168:ILE:N	2.64	0.46
4:J:193:ASN:C	4:J:193:ASN:HD22	2.22	0.46
3:Q:265:SER:O	3:Q:268:LYS:NZ	2.38	0.46
4:B:165:LEU:HA	4:B:165:LEU:HD12	1.75	0.46
4:B:176:CYS:SG	4:B:247:PRO:HD2	2.56	0.46
4:R:177:LYS:HB3	4:R:177:LYS:HE3	1.79	0.46
3:I:311:ASP:HB2	3:I:312:LYS:NZ	2.31	0.45
4:R:178:LEU:HD13	4:R:183:ILE:HD11	1.96	0.45
3:E:310:VAL:HA	3:E:313:LEU:HD22	1.97	0.45
4:N:246:PHE:O	4:N:248:ALA:N	2.37	0.45
4:F:182:THR:HG23	4:F:183:ILE:H	1.82	0.45
3:I:262:SER:O	3:I:268:LYS:HA	2.16	0.45
3:M:289:TYR:CD2	3:M:316:LEU:CD1	2.99	0.45
1:O:15:DG:H2''	1:O:16:DG:H5''	1.98	0.45
2:P:101:DC:H2''	2:P:102:DC:C5'	2.46	0.45
4:F:239:ARG:NH2	4:F:242:GLN:HE22	2.12	0.45
3:I:114:MET:CE	3:I:146:TYR:CD1	3.00	0.45
3:M:154:ARG:HH21	3:M:154:ARG:HG3	1.82	0.45
4:R:192:TYR:CE1	4:R:194:PRO:HD3	2.51	0.45
3:E:176:THR:OG1	3:E:179:GLU:HG3	2.16	0.45
1:C:1:DG:H5''	5:K:176:HOH:O	2.16	0.45
3:A:267:GLU:OE2	3:A:267:GLU:CA	2.51	0.45
4:J:235:ARG:HG3	4:J:250:PHE:CZ	2.51	0.45
4:N:256:GLN:NE2	4:N:256:GLN:CA	2.76	0.45
3:Q:124:MET:HE1	3:Q:161:SER:HA	1.98	0.45
1:C:14:DA:H1'	4:B:214:PHE:CZ	2.52	0.45
3:E:237:ARG:HA	3:E:237:ARG:HD2	1.72	0.45
3:I:193:ARG:O	3:I:197:LEU:CD2	2.65	0.45
4:J:167:ASN:ND2	4:J:223:GLY:H	2.03	0.45
3:Q:111:ASP:C	3:Q:113:ALA:N	2.68	0.45
3:A:221:ASN:N	3:A:221:ASN:ND2	2.56	0.45
3:E:111:ASP:O	3:E:114:MET:HG3	2.16	0.45
3:E:131:PRO:HB2	3:E:133:ASN:ND2	2.32	0.45
3:Q:306:PHE:CE2	3:Q:310:VAL:HG23	2.51	0.45
1:C:7:DC:H2'	1:C:8:DT:H71	1.99	0.45
2:D:104:DC:H2''	2:D:105:DC:C5'	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:103:DC:OP1	3:Q:154:ARG:NH1	2.49	0.45
3:A:234:HIS:CD2	3:A:237:ARG:HH22	2.35	0.45
2:H:103:DC:H2''	2:H:104:DC:O5'	2.17	0.44
4:F:189:ASN:ND2	4:F:205:ARG:HH21	2.15	0.44
3:I:117:ALA:O	3:I:121:ILE:HG13	2.16	0.44
3:I:164:LEU:HD23	3:I:180:ILE:HD12	1.98	0.44
3:I:267:GLU:N	3:I:267:GLU:CD	2.72	0.44
4:N:188:ARG:HD2	4:N:189:ASN:OD1	2.17	0.44
1:G:9:DA:H2''	1:G:10:DT:C5'	2.39	0.44
2:T:101:DC:H2''	2:T:102:DC:O5'	2.18	0.44
3:A:309:PRO:HG3	3:A:312:LYS:CE	2.47	0.44
4:J:214:PHE:CD1	4:J:214:PHE:N	2.85	0.44
4:N:219:MET:HE1	4:N:237:TYR:HB3	1.99	0.44
4:R:273:LEU:O	4:R:273:LEU:HD23	2.17	0.44
1:G:12:DA:H8	1:G:12:DA:H2'	1.67	0.44
3:M:122:THR:HG22	3:M:123:THR:N	2.32	0.44
1:G:8:DT:H2''	1:G:9:DA:C5'	2.43	0.44
3:I:217:ARG:O	3:I:221:ASN:ND2	2.50	0.44
3:M:137:ARG:HH22	3:M:144:GLN:HE22	1.65	0.44
4:N:181:LYS:O	4:N:185:LEU:HD23	2.18	0.44
4:N:318:ARG:CG	4:N:322:TYR:CE2	2.96	0.44
3:Q:188:LYS:NZ	4:R:286:GLU:O	2.45	0.44
4:R:249:LYS:HB2	4:R:251:LEU:HD12	1.99	0.44
3:M:266:ALA:HA	3:M:307:ASP:OD2	2.17	0.44
4:N:246:PHE:C	4:N:248:ALA:N	2.75	0.44
2:L:102:DC:H2''	2:L:103:DC:O5'	2.17	0.44
2:T:109:DT:H6	2:T:109:DT:H2'	1.55	0.44
3:A:165:TYR:O	5:A:319:HOH:O	2.21	0.44
3:A:169:ARG:HH22	4:B:284:GLU:CD	2.25	0.44
4:B:296:ILE:HG23	4:B:299:ARG:HH12	1.82	0.44
4:J:209:THR:CG2	4:J:210:THR:H	2.29	0.44
4:R:259:VAL:HG13	4:R:313:THR:HG23	2.00	0.44
3:A:224:LEU:CD2	3:A:269:ARG:HH11	2.30	0.44
4:B:264:VAL:HG11	4:B:332:LEU:HD23	2.00	0.44
3:I:267:GLU:HB2	3:I:269:ARG:NH1	2.26	0.44
4:J:280:PHE:HD2	4:J:280:PHE:N	2.16	0.44
4:R:229:GLN:HE21	4:R:229:GLN:HB3	1.43	0.44
2:H:110:DA:H2''	2:H:111:DT:C5'	2.43	0.44
3:A:157:ASP:CB	3:A:185:ARG:HH21	2.30	0.44
3:A:173:VAL:HG23	3:A:173:VAL:O	2.18	0.44
4:B:235:ARG:HG2	4:B:250:PHE:CZ	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:238:LYS:HB3	3:E:299:LEU:CD2	2.48	0.44
4:F:329:TYR:HB3	4:F:330:PRO:HD3	2.00	0.44
4:J:246:PHE:C	4:J:248:ALA:N	2.75	0.44
3:Q:141:LEU:HD12	3:Q:141:LEU:HA	1.83	0.44
3:Q:181:CYS:SG	3:Q:188:LYS:HA	2.57	0.44
4:R:276:THR:HG21	4:R:335:PHE:HZ	1.82	0.44
2:D:110:DA:H2''	2:D:111:DT:C5'	2.46	0.44
2:L:107:DT:H6	2:L:107:DT:H2'	1.70	0.44
3:A:196:LYS:HE2	5:A:335:HOH:O	2.18	0.44
3:I:157:ASP:OD2	3:I:185:ARG:NH2	2.50	0.44
3:M:145:VAL:HG22	3:M:202:LEU:HD11	1.99	0.44
1:C:18:DG:O3'	3:E:316:LEU:HD11	2.18	0.43
3:A:148:GLN:HB3	3:A:150:SER:OG	2.17	0.43
3:I:295:ARG:O	3:I:299:LEU:HG	2.18	0.43
3:Q:224:LEU:HA	3:Q:225:PRO:HD2	1.93	0.43
4:R:203:ARG:HG2	4:R:210:THR:OG1	2.18	0.43
4:F:166:GLN:NE2	4:F:225:LYS:NZ	2.66	0.43
4:F:189:ASN:N	4:F:189:ASN:OD1	2.50	0.43
4:F:235:ARG:HG3	4:F:235:ARG:NH2	2.17	0.43
3:I:266:ALA:HB3	3:I:267:GLU:OE2	2.18	0.43
4:J:249:LYS:HB3	4:J:251:LEU:HD21	2.00	0.43
4:R:231:ARG:HA	4:R:253:PHE:CE1	2.53	0.43
3:I:173:VAL:HG23	3:I:175:ARG:NH2	2.33	0.43
4:J:189:ASN:N	4:J:189:ASN:OD1	2.51	0.43
3:A:202:LEU:O	3:A:203:GLU:C	2.60	0.43
4:F:205:ARG:CG	4:F:205:ARG:NH1	2.81	0.43
3:M:169:ARG:HG2	3:M:174:PRO:HG3	2.00	0.43
3:M:238:LYS:HB3	3:M:299:LEU:CD2	2.48	0.43
4:R:179:ASP:O	4:R:182:THR:CG2	2.67	0.43
4:R:193:ASN:HB3	4:R:196:ARG:HB3	2.01	0.43
3:A:139:ASN:N	3:A:139:ASN:HD22	2.16	0.43
3:E:154:ARG:NH1	3:E:190:GLU:CD	2.77	0.43
3:E:174:PRO:O	5:E:359:HOH:O	2.22	0.43
4:F:271:GLU:O	4:F:274:VAL:HG12	2.19	0.43
3:I:164:LEU:CD2	3:I:180:ILE:HD12	2.48	0.43
4:J:291:LEU:C	4:J:291:LEU:HD23	2.44	0.43
3:M:262:SER:O	3:M:268:LYS:HA	2.18	0.43
3:M:309:PRO:HG2	3:M:312:LYS:HB3	2.00	0.43
3:Q:310:VAL:O	3:Q:313:LEU:HB2	2.18	0.43
4:R:246:PHE:O	4:R:248:ALA:N	2.42	0.43
4:R:304:ILE:HG12	4:R:310:VAL:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:DG:H2''	1:K:16:DG:H5''	2.01	0.43
3:A:215:MET:CG	3:A:233:THR:OG1	2.66	0.43
4:N:258:MET:HG2	4:N:315:ALA:O	2.18	0.43
4:F:259:VAL:HG13	4:F:313:THR:HG23	2.00	0.43
4:F:326:GLU:O	4:F:330:PRO:HD3	2.19	0.43
4:J:235:ARG:HG2	4:J:250:PHE:CE1	2.54	0.43
2:H:101:DC:H5'	2:P:118:DC:H2''	2.01	0.43
1:K:8:DT:H2''	1:K:9:DA:C5'	2.46	0.43
1:O:12:DA:H8	1:O:12:DA:H2'	1.70	0.43
4:R:264:VAL:O	4:R:265:LYS:HB2	2.18	0.43
2:P:110:DA:N7	2:P:111:DT:C4	2.87	0.43
4:B:246:PHE:C	4:B:248:ALA:H	2.25	0.43
3:E:282:ASP:OD1	3:E:283:VAL:N	2.52	0.43
3:I:152:LYS:H	3:I:152:LYS:HG3	1.45	0.43
3:I:248:ARG:NH2	3:I:287:GLN:NE2	2.62	0.43
3:I:265:SER:O	3:I:268:LYS:HG3	2.19	0.43
4:N:193:ASN:HA	4:N:194:PRO:HD2	1.76	0.43
3:A:269:ARG:CG	3:A:269:ARG:NH1	2.80	0.42
4:J:178:LEU:HD22	4:J:183:ILE:CD1	2.49	0.42
3:M:289:TYR:OH	3:M:314:PRO:O	2.28	0.42
4:N:204:ILE:HG12	4:N:237:TYR:OH	2.19	0.42
4:N:295:MET:HE1	4:N:324:ALA:CB	2.48	0.42
1:S:12:DA:H2	4:R:169:VAL:HG21	1.84	0.42
4:B:204:ILE:HG23	4:B:237:TYR:CZ	2.54	0.42
3:I:310:VAL:HA	3:I:313:LEU:HD22	2.01	0.42
3:I:311:ASP:C	3:I:313:LEU:N	2.77	0.42
4:J:177:LYS:HB3	4:J:177:LYS:HE3	1.71	0.42
3:Q:293:TYR:N	3:Q:294:PRO:CD	2.82	0.42
4:R:302:LEU:HD23	4:R:312:LEU:HG	2.01	0.42
3:E:293:TYR:HB3	3:E:294:PRO:HD3	2.01	0.42
3:Q:110:SER:O	3:Q:113:ALA:HB2	2.20	0.42
3:Q:238:LYS:NZ	3:Q:298:ASP:O	2.53	0.42
1:G:7:DC:H2''	1:G:8:DT:C5'	2.47	0.42
1:S:12:DA:C2	4:R:169:VAL:HG21	2.55	0.42
3:A:221:ASN:H	3:A:221:ASN:ND2	2.16	0.42
3:A:224:LEU:HD23	3:A:269:ARG:HH12	1.83	0.42
3:A:245:VAL:HG21	3:A:253:VAL:CG2	2.50	0.42
3:E:151:LEU:N	3:E:151:LEU:CD1	2.82	0.42
4:F:240:VAL:O	4:F:244:LEU:HG	2.20	0.42
3:I:156:ASN:ND2	5:I:325:HOH:O	2.51	0.42
3:I:271:GLN:HE22	3:I:316:LEU:HD21	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:182:THR:HG22	4:J:183:ILE:N	2.34	0.42
4:J:202:MET:HE3	4:J:213:ILE:HD11	2.02	0.42
4:N:257:ASN:ND2	4:N:314:GLY:CA	2.82	0.42
4:B:286:GLU:HG3	5:B:338:HOH:O	2.19	0.42
3:E:186:ILE:HG22	3:E:187:SER:N	2.34	0.42
3:M:121:ILE:CG2	3:M:138:THR:HG21	2.49	0.42
3:M:311:ASP:C	3:M:313:LEU:N	2.78	0.42
3:M:313:LEU:HD22	3:M:314:PRO:HD2	2.02	0.42
4:N:326:GLU:O	4:N:330:PRO:HD3	2.19	0.42
3:Q:186:ILE:CG2	3:Q:190:GLU:HB3	2.49	0.42
4:R:231:ARG:HB3	4:R:231:ARG:HH11	1.83	0.42
1:O:16:DG:H2''	1:O:17:DG:O5'	2.20	0.42
4:F:164:GLN:HE21	4:F:164:GLN:HB2	1.65	0.42
3:I:143:LYS:HE2	3:I:147:GLU:OE1	2.18	0.42
3:I:270:THR:HG23	3:I:273:GLU:N	2.12	0.42
4:N:193:ASN:O	4:N:196:ARG:HG2	2.18	0.42
4:N:263:ASP:CG	5:N:350:HOH:O	2.61	0.42
4:R:239:ARG:O	4:R:240:VAL:C	2.63	0.42
3:A:141:LEU:HD23	3:A:141:LEU:HA	1.86	0.42
3:E:157:ASP:HB2	3:E:185:ARG:HH21	1.84	0.42
3:I:131:PRO:HG2	3:I:134:ILE:HG13	2.02	0.42
4:R:244:LEU:HD12	4:R:244:LEU:HA	1.74	0.42
4:R:246:PHE:HA	4:R:247:PRO:HD3	1.77	0.42
4:R:249:LYS:CB	4:R:251:LEU:CD1	2.98	0.42
2:P:108:DT:H6	2:P:108:DT:H2'	1.67	0.42
1:S:16:DG:H2''	1:S:17:DG:O5'	2.20	0.42
4:J:271:GLU:O	4:J:274:VAL:HG12	2.20	0.42
4:N:183:ILE:O	4:N:187:ALA:HB3	2.18	0.42
4:R:178:LEU:HD13	4:R:183:ILE:CD1	2.50	0.42
4:R:317:VAL:HG23	4:R:319:ALA:N	2.34	0.42
1:S:15:DG:C2'	1:S:16:DG:H5''	2.50	0.42
2:T:110:DA:H5'	4:R:166:GLN:CG	2.35	0.42
4:B:256:GLN:HE21	4:B:256:GLN:HA	1.84	0.42
3:E:169:ARG:HB3	3:E:206:VAL:HG11	2.01	0.42
3:E:225:PRO:HG2	3:E:228:VAL:HG23	2.02	0.42
4:F:180:LEU:CD2	4:F:180:LEU:N	2.78	0.42
4:R:186:ARG:NH1	4:R:244:LEU:HB3	2.34	0.42
3:A:114:MET:CE	3:A:143:LYS:HG3	2.49	0.41
4:B:167:ASN:ND2	4:B:223:GLY:H	2.18	0.41
4:F:239:ARG:O	4:F:240:VAL:C	2.62	0.41
4:F:328:ILE:HG13	4:F:332:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:236:ALA:O	3:I:239:ALA:HB3	2.20	0.41
3:M:228:VAL:O	3:M:231:ALA:HB3	2.20	0.41
3:M:235:ILE:HG23	3:M:299:LEU:HB3	2.02	0.41
3:I:114:MET:HE2	3:I:146:TYR:CD1	2.54	0.41
4:J:184:ALA:HB2	4:J:192:TYR:HB2	2.02	0.41
4:J:202:MET:SD	4:J:240:VAL:HG21	2.60	0.41
1:C:12:DA:H8	1:C:12:DA:H2'	1.70	0.41
3:A:189:LYS:CE	3:A:193:ARG:HH21	2.32	0.41
4:F:185:LEU:HD23	4:F:186:ARG:N	2.35	0.41
4:F:279:GLN:H	4:F:279:GLN:HG3	1.11	0.41
4:J:211:ALA:HB1	4:J:219:MET:HE2	2.01	0.41
3:M:111:ASP:C	3:M:113:ALA:N	2.68	0.41
3:M:186:ILE:CG2	3:M:187:SER:N	2.83	0.41
3:E:112:ARG:HA	3:E:112:ARG:HD3	1.85	0.41
3:E:293:TYR:CZ	3:E:315:GLN:HG3	2.55	0.41
4:R:179:ASP:CB	4:R:182:THR:HG22	2.50	0.41
4:R:180:LEU:HD22	4:R:215:SER:OG	2.21	0.41
2:P:107:DT:H6	2:P:107:DT:H2'	1.76	0.41
2:T:102:DC:O3'	3:Q:154:ARG:NH1	2.53	0.41
3:A:311:ASP:C	3:A:313:LEU:N	2.77	0.41
4:B:180:LEU:HD22	4:B:215:SER:HB3	2.02	0.41
4:B:298:PRO:HG3	4:B:323:GLU:CD	2.45	0.41
4:F:303:LEU:HB2	4:F:311:VAL:HB	2.02	0.41
3:M:216:SER:HA	3:M:229:GLN:NE2	2.34	0.41
3:M:234:HIS:HD2	3:M:299:LEU:O	2.04	0.41
4:R:219:MET:HE1	4:R:237:TYR:HB2	2.01	0.41
3:A:262:SER:O	3:A:268:LYS:HA	2.21	0.41
4:B:299:ARG:C	4:B:300:ILE:HD12	2.46	0.41
3:E:218:PHE:CZ	3:E:278:ALA:HA	2.56	0.41
4:J:190:ALA:O	4:J:191:GLU:HG2	2.21	0.41
3:M:172:GLY:C	3:M:174:PRO:HD3	2.45	0.41
3:Q:158:ALA:HA	3:Q:186:ILE:HG13	2.02	0.41
3:Q:176:THR:HG22	3:Q:251:ILE:HD11	2.02	0.41
3:Q:222:LEU:HB3	3:Q:224:LEU:HD12	2.02	0.41
3:A:293:TYR:N	3:A:294:PRO:CD	2.82	0.41
3:E:313:LEU:HD12	3:E:313:LEU:HA	1.90	0.41
3:E:313:LEU:O	3:E:314:PRO:C	2.64	0.41
4:F:251:LEU:N	4:F:251:LEU:HD13	2.35	0.41
4:F:294:ARG:HG2	4:F:299:ARG:HH12	1.85	0.41
3:I:225:PRO:HG2	3:I:228:VAL:CG2	2.47	0.41
4:J:178:LEU:HD21	4:J:241:VAL:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:189:LYS:CE	3:M:193:ARG:NH1	2.76	0.41
4:R:177:LYS:O	4:R:178:LEU:HD23	2.20	0.41
4:R:271:GLU:O	4:R:274:VAL:HG12	2.21	0.41
2:D:118:DC:H2''	2:L:101:DC:H5'	2.02	0.41
3:A:111:ASP:C	3:A:113:ALA:N	2.70	0.41
3:E:137:ARG:NE	3:E:170:GLN:HE22	2.19	0.41
3:E:265:SER:O	3:E:268:LYS:HG2	2.21	0.41
3:M:286:ARG:HD2	5:M:322:HOH:O	2.19	0.41
2:T:111:DT:H6	2:T:111:DT:H2'	1.62	0.41
3:A:270:THR:HG21	3:A:272:LYS:HB3	2.03	0.41
3:A:295:ARG:NH1	3:A:298:ASP:OD1	2.54	0.41
4:B:180:LEU:CD2	4:B:215:SER:HB3	2.50	0.41
4:F:246:PHE:HA	4:F:247:PRO:HD3	1.82	0.41
3:I:306:PHE:CZ	3:I:310:VAL:HG22	2.56	0.41
4:J:300:ILE:HD13	4:J:312:LEU:HB3	2.03	0.41
3:M:111:ASP:OD2	3:M:146:TYR:HE1	2.03	0.41
3:M:239:ALA:HA	3:M:244:LEU:HD12	2.02	0.41
3:M:262:SER:OG	3:M:268:LYS:HA	2.20	0.41
4:N:192:TYR:CE1	4:N:194:PRO:HD3	2.56	0.41
4:N:193:ASN:HB3	4:N:196:ARG:CZ	2.31	0.41
4:N:240:VAL:HG23	4:N:241:VAL:N	2.36	0.41
4:N:302:LEU:HD12	4:N:302:LEU:N	2.35	0.41
3:Q:120:GLU:O	3:Q:124:MET:HG3	2.21	0.41
3:Q:277:ILE:HG22	3:Q:278:ALA:N	2.36	0.41
4:B:205:ARG:NH1	4:B:208:ARG:NE	2.64	0.41
3:E:121:ILE:HG21	3:E:139:ASN:ND2	2.36	0.41
4:B:185:LEU:HA	4:B:185:LEU:HD12	1.79	0.40
4:B:239:ARG:HH11	4:B:239:ARG:HD3	1.77	0.40
3:E:227:GLN:HG2	3:E:305:LYS:HE3	2.03	0.40
3:E:262:SER:O	3:E:268:LYS:HA	2.22	0.40
4:F:189:ASN:ND2	4:F:203:ARG:O	2.54	0.40
4:F:205:ARG:H	4:F:205:ARG:NE	2.16	0.40
4:J:264:VAL:O	4:J:265:LYS:HB2	2.20	0.40
3:M:111:ASP:OD2	3:M:146:TYR:CE1	2.74	0.40
3:Q:296:ALA:N	3:Q:297:PRO:HD2	2.36	0.40
2:P:109:DT:H6	2:P:109:DT:H2'	1.56	0.40
2:P:111:DT:H6	2:P:111:DT:H2'	1.57	0.40
4:J:239:ARG:O	4:J:240:VAL:C	2.64	0.40
4:J:258:MET:HG2	4:J:315:ALA:O	2.21	0.40
3:M:177:PHE:HB3	3:M:188:LYS:HG3	2.04	0.40
4:N:302:LEU:HD22	4:N:328:ILE:HG12	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:120:GLU:HG2	3:I:157:ASP:OD1	2.21	0.40
3:M:158:ALA:HA	3:M:186:ILE:HG13	2.02	0.40
3:M:311:ASP:O	3:M:313:LEU:N	2.54	0.40
3:Q:181:CYS:SG	3:Q:188:LYS:CA	3.10	0.40
2:P:101:DC:H2''	2:P:102:DC:H5'	2.04	0.40
4:F:166:GLN:NE2	4:F:225:LYS:HZ2	2.18	0.40
4:F:329:TYR:N	4:F:330:PRO:CD	2.85	0.40
3:I:176:THR:HG22	3:I:251:ILE:CD1	2.46	0.40
3:M:271:GLN:NE2	3:M:316:LEU:HD21	2.37	0.40
4:R:180:LEU:HD21	4:R:215:SER:HB2	2.03	0.40
4:R:326:GLU:O	4:R:330:PRO:HD3	2.22	0.40
3:A:269:ARG:HH11	3:A:269:ARG:HG2	1.84	0.40
4:B:246:PHE:HA	4:B:247:PRO:HD3	1.89	0.40
3:I:176:THR:CG2	3:I:251:ILE:HD13	2.47	0.40
4:N:295:MET:HE3	4:N:298:PRO:CD	2.51	0.40
3:Q:144:GLN:O	3:Q:148:GLN:HB2	2.22	0.40
4:R:227:GLU:CD	4:R:227:GLU:H	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	205/207 (99%)	195 (95%)	8 (4%)	2 (1%)	12	20
3	E	205/207 (99%)	192 (94%)	11 (5%)	2 (1%)	12	20
3	I	205/207 (99%)	194 (95%)	9 (4%)	2 (1%)	12	20
3	M	205/207 (99%)	191 (93%)	13 (6%)	1 (0%)	24	39
3	Q	205/207 (99%)	191 (93%)	12 (6%)	2 (1%)	12	20
4	B	178/180 (99%)	167 (94%)	11 (6%)	0	100	100
4	F	178/180 (99%)	162 (91%)	15 (8%)	1 (1%)	21	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	J	178/180 (99%)	163 (92%)	14 (8%)	1 (1%)	21	34
4	N	178/180 (99%)	159 (89%)	17 (10%)	2 (1%)	11	19
4	R	178/180 (99%)	162 (91%)	15 (8%)	1 (1%)	21	34
All	All	1915/1935 (99%)	1776 (93%)	125 (6%)	14 (1%)	18	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	312	LYS
3	M	312	LYS
3	E	312	LYS
3	I	112	ARG
3	Q	312	LYS
3	E	226	LYS
3	I	312	LYS
3	A	226	LYS
3	Q	226	LYS
4	N	208	ARG
4	R	247	PRO
4	F	247	PRO
4	N	247	PRO
4	J	247	PRO

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	
3	A	176/176 (100%)	148 (84%)	28 (16%)	2	3
3	E	176/176 (100%)	149 (85%)	27 (15%)	3	4
3	I	176/176 (100%)	139 (79%)	37 (21%)	1	1
3	M	176/176 (100%)	147 (84%)	29 (16%)	2	3
3	Q	176/176 (100%)	151 (86%)	25 (14%)	3	5
4	B	154/154 (100%)	131 (85%)	23 (15%)	3	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	154/154 (100%)	131 (85%)	23 (15%)	3	4
4	J	154/154 (100%)	128 (83%)	26 (17%)	2	2
4	N	154/154 (100%)	125 (81%)	29 (19%)	1	2
4	R	154/154 (100%)	118 (77%)	36 (23%)	1	1
All	All	1650/1650 (100%)	1367 (83%)	283 (17%)	2	2

All (283) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	110	SER
3	A	114	MET
3	A	119	LYS
3	A	122	THR
3	A	128	ILE
3	A	133	ASN
3	A	134	ILE
3	A	145	VAL
3	A	164	LEU
3	A	169	ARG
3	A	185	ARG
3	A	197	LEU
3	A	202	LEU
3	A	204	THR
3	A	215	MET
3	A	221	ASN
3	A	248	ARG
3	A	251	ILE
3	A	267	GLU
3	A	269	ARG
3	A	270	THR
3	A	280	VAL
3	A	287	GLN
3	A	305	LYS
3	A	310	VAL
3	A	313	LEU
3	A	315	GLN
3	A	316	LEU
4	B	162	VAL
4	B	165	LEU
4	B	180	LEU
4	B	181	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	185	LEU
4	B	188	ARG
4	B	205	ARG
4	B	206	GLU
4	B	209	THR
4	B	226	SER
4	B	227	GLU
4	B	232	LEU
4	B	239	ARG
4	B	240	VAL
4	B	255	ILE
4	B	273	LEU
4	B	278	GLN
4	B	287	LEU
4	B	297	LYS
4	B	300	ILE
4	B	306	VAL
4	B	326	GLU
4	B	332	LEU
3	E	112	ARG
3	E	119	LYS
3	E	123	THR
3	E	128	ILE
3	E	132	ARG
3	E	133	ASN
3	E	150	SER
3	E	169	ARG
3	E	185	ARG
3	E	197	LEU
3	E	200	LYS
3	E	202	LEU
3	E	205	SER
3	E	216	SER
3	E	237	ARG
3	E	238	LYS
3	E	262	SER
3	E	269	ARG
3	E	270	THR
3	E	283	VAL
3	E	287	GLN
3	E	295	ARG
3	E	302	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	305	LYS
3	E	311	ASP
3	E	312	LYS
3	E	313	LEU
4	F	164	GLN
4	F	180	LEU
4	F	185	LEU
4	F	186	ARG
4	F	195	LYS
4	F	205	ARG
4	F	219	MET
4	F	227	GLU
4	F	229	GLN
4	F	232	LEU
4	F	235	ARG
4	F	239	ARG
4	F	240	VAL
4	F	251	LEU
4	F	275	LEU
4	F	279	GLN
4	F	287	LEU
4	F	291	LEU
4	F	294	ARG
4	F	299	ARG
4	F	300	ILE
4	F	312	LEU
4	F	332	LEU
3	I	112	ARG
3	I	114	MET
3	I	126	ASP
3	I	128	ILE
3	I	133	ASN
3	I	134	ILE
3	I	145	VAL
3	I	150	SER
3	I	152	LYS
3	I	169	ARG
3	I	181	CYS
3	I	190	GLU
3	I	196	LYS
3	I	197	LEU
3	I	200	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	202	LEU
3	I	203	GLU
3	I	206	VAL
3	I	207	ASP
3	I	208	LEU
3	I	215	MET
3	I	217	ARG
3	I	221	ASN
3	I	224	LEU
3	I	226	LYS
3	I	227	GLN
3	I	242	LEU
3	I	262	SER
3	I	267	GLU
3	I	277	ILE
3	I	280	VAL
3	I	283	VAL
3	I	295	ARG
3	I	305	LYS
3	I	312	LYS
3	I	313	LEU
3	I	316	LEU
4	J	162	VAL
4	J	165	LEU
4	J	168	ILE
4	J	178	LEU
4	J	182	THR
4	J	188	ARG
4	J	191	GLU
4	J	195	LYS
4	J	208	ARG
4	J	210	THR
4	J	213	ILE
4	J	242	GLN
4	J	243	LYS
4	J	251	LEU
4	J	258	MET
4	J	271	GLU
4	J	273	LEU
4	J	275	LEU
4	J	276	THR
4	J	279	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	J	280	PHE
4	J	287	LEU
4	J	300	ILE
4	J	326	GLU
4	J	332	LEU
4	J	333	LYS
3	M	110	SER
3	M	112	ARG
3	M	116	ASN
3	M	122	THR
3	M	132	ARG
3	M	133	ASN
3	M	149	LYS
3	M	150	SER
3	M	152	LYS
3	M	173	VAL
3	M	175	ARG
3	M	197	LEU
3	M	200	LYS
3	M	207	ASP
3	M	209	ILE
3	M	217	ARG
3	M	221	ASN
3	M	226	LYS
3	M	227	GLN
3	M	237	ARG
3	M	242	LEU
3	M	263	GLN
3	M	283	VAL
3	M	298	ASP
3	M	305	LYS
3	M	307	ASP
3	M	310	VAL
3	M	311	ASP
3	M	315	GLN
4	N	164	GLN
4	N	166	GLN
4	N	174	LEU
4	N	181	LYS
4	N	182	THR
4	N	200	VAL
4	N	206	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	N	208	ARG
4	N	227	GLU
4	N	229	GLN
4	N	232	LEU
4	N	239	ARG
4	N	242	GLN
4	N	243	LYS
4	N	251	LEU
4	N	252	ASP
4	N	256	GLN
4	N	271	GLU
4	N	273	LEU
4	N	274	VAL
4	N	275	LEU
4	N	279	GLN
4	N	287	LEU
4	N	297	LYS
4	N	299	ARG
4	N	302	LEU
4	N	317	VAL
4	N	328	ILE
4	N	332	LEU
3	Q	119	LYS
3	Q	132	ARG
3	Q	141	LEU
3	Q	150	SER
3	Q	173	VAL
3	Q	185	ARG
3	Q	200	LYS
3	Q	202	LEU
3	Q	208	LEU
3	Q	211	THR
3	Q	216	SER
3	Q	224	LEU
3	Q	226	LYS
3	Q	227	GLN
3	Q	228	VAL
3	Q	230	MET
3	Q	241	GLU
3	Q	242	LEU
3	Q	277	ILE
3	Q	282	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	283	VAL
3	Q	295	ARG
3	Q	313	LEU
3	Q	315	GLN
3	Q	316	LEU
4	R	165	LEU
4	R	166	GLN
4	R	171	THR
4	R	174	LEU
4	R	180	LEU
4	R	182	THR
4	R	185	LEU
4	R	200	VAL
4	R	202	MET
4	R	206	GLU
4	R	212	LEU
4	R	213	ILE
4	R	215	SER
4	R	225	LYS
4	R	227	GLU
4	R	228	GLU
4	R	229	GLN
4	R	232	LEU
4	R	235	ARG
4	R	243	LYS
4	R	244	LEU
4	R	258	MET
4	R	271	GLU
4	R	273	LEU
4	R	275	LEU
4	R	276	THR
4	R	278	GLN
4	R	280	PHE
4	R	287	LEU
4	R	296	ILE
4	R	300	ILE
4	R	302	LEU
4	R	310	VAL
4	R	316	LYS
4	R	317	VAL
4	R	318	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83)

such sidechains are listed below:

Mol	Chain	Res	Type
3	A	116	ASN
3	A	133	ASN
3	A	139	ASN
3	A	144	GLN
3	A	148	GLN
3	A	170	GLN
3	A	221	ASN
3	A	229	GLN
3	A	234	HIS
3	A	263	GLN
3	A	287	GLN
4	B	166	GLN
4	B	167	ASN
4	B	173	ASN
4	B	193	ASN
4	B	256	GLN
4	B	257	ASN
4	B	278	GLN
4	B	327	ASN
3	E	133	ASN
3	E	139	ASN
3	E	148	GLN
3	E	170	GLN
3	E	221	ASN
3	E	227	GLN
3	E	263	GLN
3	E	287	GLN
4	F	164	GLN
4	F	166	GLN
4	F	167	ASN
4	F	193	ASN
4	F	229	GLN
4	F	256	GLN
4	F	257	ASN
4	F	279	GLN
4	F	327	ASN
3	I	116	ASN
3	I	133	ASN
3	I	139	ASN
3	I	156	ASN
3	I	170	GLN
3	I	221	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	229	GLN
3	I	263	GLN
3	I	287	GLN
4	J	164	GLN
4	J	166	GLN
4	J	167	ASN
4	J	193	ASN
4	J	242	GLN
4	J	256	GLN
4	J	257	ASN
4	J	277	HIS
4	J	279	GLN
4	J	327	ASN
3	M	133	ASN
3	M	144	GLN
3	M	148	GLN
3	M	170	GLN
3	M	221	ASN
3	M	234	HIS
3	M	263	GLN
4	N	166	GLN
4	N	173	ASN
4	N	229	GLN
4	N	242	GLN
4	N	256	GLN
4	N	257	ASN
4	N	279	GLN
4	N	327	ASN
3	Q	140	ASN
3	Q	156	ASN
3	Q	227	GLN
3	Q	263	GLN
3	Q	287	GLN
3	Q	315	GLN
4	R	166	GLN
4	R	167	ASN
4	R	189	ASN
4	R	193	ASN
4	R	229	GLN
4	R	256	GLN
4	R	257	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	18/18 (100%)	0.15	1 (5%) 30 24	27, 41, 52, 58	0
1	G	18/18 (100%)	-0.02	0 100 100	25, 43, 50, 57	0
1	K	18/18 (100%)	-0.02	0 100 100	32, 45, 52, 59	0
1	O	18/18 (100%)	0.02	0 100 100	29, 44, 58, 65	0
1	S	18/18 (100%)	0.23	0 100 100	33, 49, 58, 62	0
2	D	18/18 (100%)	-0.14	0 100 100	25, 37, 52, 53	0
2	H	18/18 (100%)	-0.29	0 100 100	26, 40, 50, 50	0
2	L	18/18 (100%)	-0.31	0 100 100	31, 42, 54, 55	0
2	P	18/18 (100%)	-0.18	0 100 100	31, 45, 51, 53	0
2	T	18/18 (100%)	-0.12	0 100 100	36, 47, 54, 55	0
3	A	207/207 (100%)	0.38	8 (3%) 43 35	31, 49, 66, 75	0
3	E	207/207 (100%)	0.57	13 (6%) 26 19	25, 45, 65, 71	0
3	I	207/207 (100%)	0.54	10 (4%) 35 28	33, 52, 68, 72	0
3	M	207/207 (100%)	0.63	10 (4%) 35 28	34, 54, 69, 75	0
3	Q	207/207 (100%)	0.78	20 (9%) 13 10	34, 53, 69, 75	0
4	B	180/180 (100%)	0.47	10 (5%) 30 24	23, 42, 62, 72	0
4	F	180/180 (100%)	0.43	7 (3%) 43 35	25, 46, 65, 73	0
4	J	180/180 (100%)	0.45	5 (2%) 55 48	30, 49, 66, 73	0
4	N	180/180 (100%)	0.77	14 (7%) 19 14	32, 53, 69, 74	0
4	R	180/180 (100%)	1.33	40 (22%) 2 1	35, 56, 70, 75	0
All	All	2115/2115 (100%)	0.57	138 (6%) 25 19	23, 49, 68, 75	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	110	SER	8.4
3	M	110	SER	5.7
3	Q	113	ALA	5.6
3	E	113	ALA	5.4
3	E	111	ASP	4.2
4	R	238	ALA	4.2
3	Q	301	PRO	4.1
3	E	205	SER	4.1
4	B	188	ARG	4.0
4	R	241	VAL	3.9
3	I	113	ALA	3.8
4	R	172	VAL	3.8
3	Q	110	SER	3.8
4	J	189	ASN	3.7
4	R	217	GLY	3.7
3	E	132	ARG	3.7
4	F	206	GLU	3.5
3	E	216	SER	3.5
4	R	185	LEU	3.5
4	R	237	TYR	3.5
3	Q	306	PHE	3.5
3	E	312	LYS	3.5
3	Q	264	ALA	3.4
3	E	306	PHE	3.4
3	E	112	ARG	3.4
4	F	299	ARG	3.4
3	Q	309	PRO	3.3
4	R	191	GLU	3.3
4	R	271	GLU	3.3
3	Q	310	VAL	3.2
3	E	220	SER	3.2
4	R	187	ALA	3.1
4	F	189	ASN	3.1
3	M	111	ASP	3.1
3	E	110	SER	3.1
4	F	271	GLU	2.9
4	B	196	ARG	2.9
4	R	202	MET	2.9
3	Q	266	ALA	2.9
4	N	190	ALA	2.9
4	N	241	VAL	2.9
4	R	232	LEU	2.9
3	Q	314	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	306	PHE	2.8
4	B	205	ARG	2.8
4	N	207	PRO	2.8
4	R	175	GLY	2.8
3	I	270	THR	2.8
3	Q	112	ARG	2.8
4	R	251	LEU	2.7
3	Q	302	THR	2.7
4	J	240	VAL	2.7
4	R	198	ALA	2.7
4	R	240	VAL	2.7
4	N	246	PHE	2.6
3	A	303	ASP	2.6
4	N	208	ARG	2.6
4	R	182	THR	2.6
3	Q	304	PHE	2.6
4	R	204	ILE	2.6
4	R	244	LEU	2.6
3	M	112	ARG	2.6
4	B	195	LYS	2.6
3	A	111	ASP	2.5
4	R	233	ALA	2.5
4	N	251	LEU	2.5
4	R	214	PHE	2.5
4	R	234	ALA	2.5
3	I	112	ARG	2.5
4	R	213	ILE	2.5
4	B	296	ILE	2.5
3	M	298	ASP	2.5
1	C	16	DG	2.5
4	R	192	TYR	2.5
3	A	315	GLN	2.5
3	M	140	ASN	2.4
3	I	228	VAL	2.4
4	R	170	SER	2.4
3	E	276	ASP	2.4
3	Q	181	CYS	2.4
3	I	225	PRO	2.4
3	Q	237	ARG	2.4
4	N	244	LEU	2.4
3	I	110	SER	2.4
4	R	228	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	217	ARG	2.4
3	M	227	GLN	2.3
4	R	231	ARG	2.3
3	I	302	THR	2.3
4	N	206	GLU	2.3
4	R	229	GLN	2.3
4	R	219	MET	2.3
4	R	206	GLU	2.3
3	Q	311	ASP	2.3
4	B	336	ARG	2.3
4	R	247	PRO	2.3
4	N	162	VAL	2.3
3	A	316	LEU	2.3
4	J	178	LEU	2.3
4	R	221	CYS	2.3
4	F	186	ARG	2.2
4	R	215	SER	2.2
4	R	258	MET	2.2
3	M	267	GLU	2.2
4	N	242	GLN	2.2
3	A	312	LYS	2.2
4	R	200	VAL	2.2
4	B	209	THR	2.2
4	F	195	LYS	2.2
4	N	181	LYS	2.2
4	F	251	LEU	2.2
4	R	212	LEU	2.2
3	M	115	MET	2.2
3	I	234	HIS	2.2
3	E	267	GLU	2.1
3	Q	299	LEU	2.1
3	A	311	ASP	2.1
3	M	150	SER	2.1
4	B	249	LYS	2.1
4	B	189	ASN	2.1
4	R	253	PHE	2.1
3	E	221	ASN	2.1
3	I	293	TYR	2.1
4	N	214	PHE	2.1
4	J	188	ARG	2.1
4	B	297	LYS	2.1
3	Q	227	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	173	ASN	2.1
3	A	112	ARG	2.0
4	J	203	ARG	2.0
4	R	319	ALA	2.0
4	N	249	LYS	2.0
3	Q	230	MET	2.0
4	N	185	LEU	2.0
4	R	255	ILE	2.0
4	R	246	PHE	2.0
3	I	207	ASP	2.0
3	Q	287	GLN	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 oligosaccharides 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.