



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:58 PM UTC

PDB ID : 5XXW / pdb_00005xxw
EMDB ID : EMD-6782
Title : GDP-microtubule complexed with KIF5C in ATP state
Authors : Morikawa, M.; Shigematsu, H.; Nitta, R.; Hirokawa, N.
Deposited on : 2017-07-05
Resolution : 6.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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:

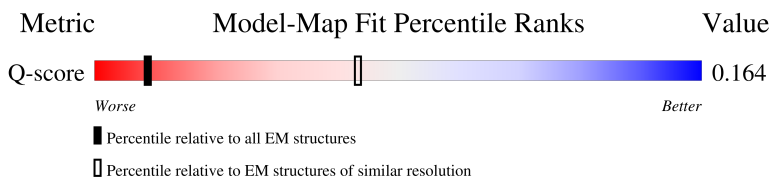
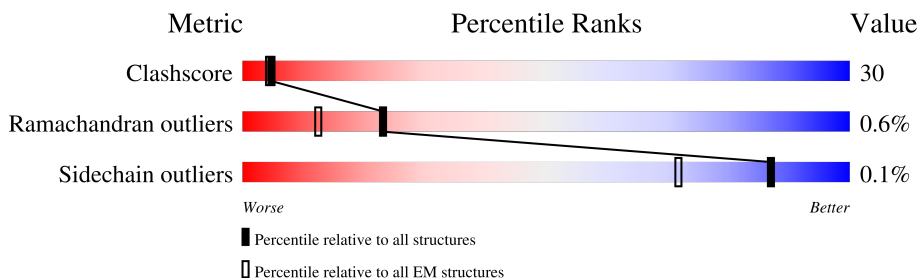
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 6.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	525 (5.50 - 6.50)

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

Mol	Chain	Length	Quality of chain
1	A	438	32% 66% 26% 5%
1	C	438	32% 67% 25% 5%
1	E	438	32% 68% 24% 5%
1	G	438	36% 68% 24% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	438	
1	K	438	
1	M	438	
1	O	438	
1	Q	438	
2	B	426	
2	D	426	
2	F	426	
2	H	426	
2	J	426	
2	L	426	
2	N	426	
2	P	426	
2	R	426	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 60903 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	C	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	E	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	G	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	I	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	K	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	M	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	O	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	Q	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		

- Molecule 2 is a protein called Tubulin beta chain.

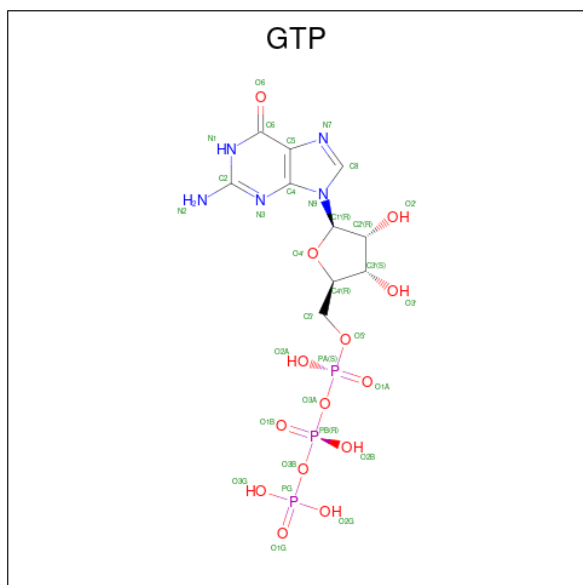
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	D	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	F	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	H	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	J	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	L	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	P	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	R	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

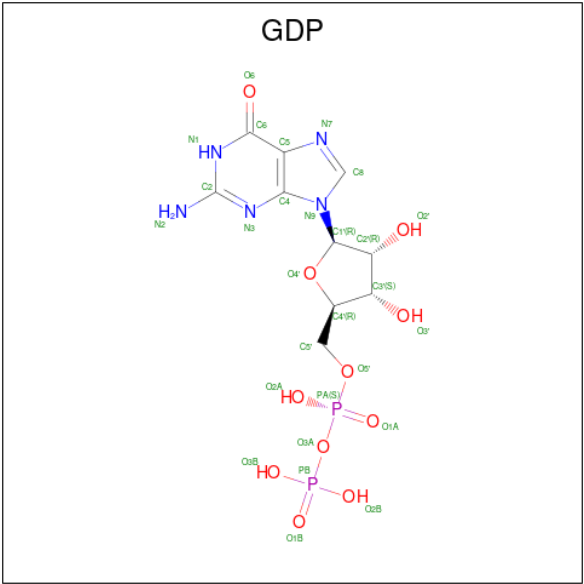
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
3	Q	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	G	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	M	1	Total	Mg	0
			1	1	
4	O	1	Total	Mg	0
			1	1	
4	Q	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	D	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	F	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	H	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	J	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	L	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	N	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	P	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	R	1	Total	C	N	O	P	0
			28	10	5	11	2	

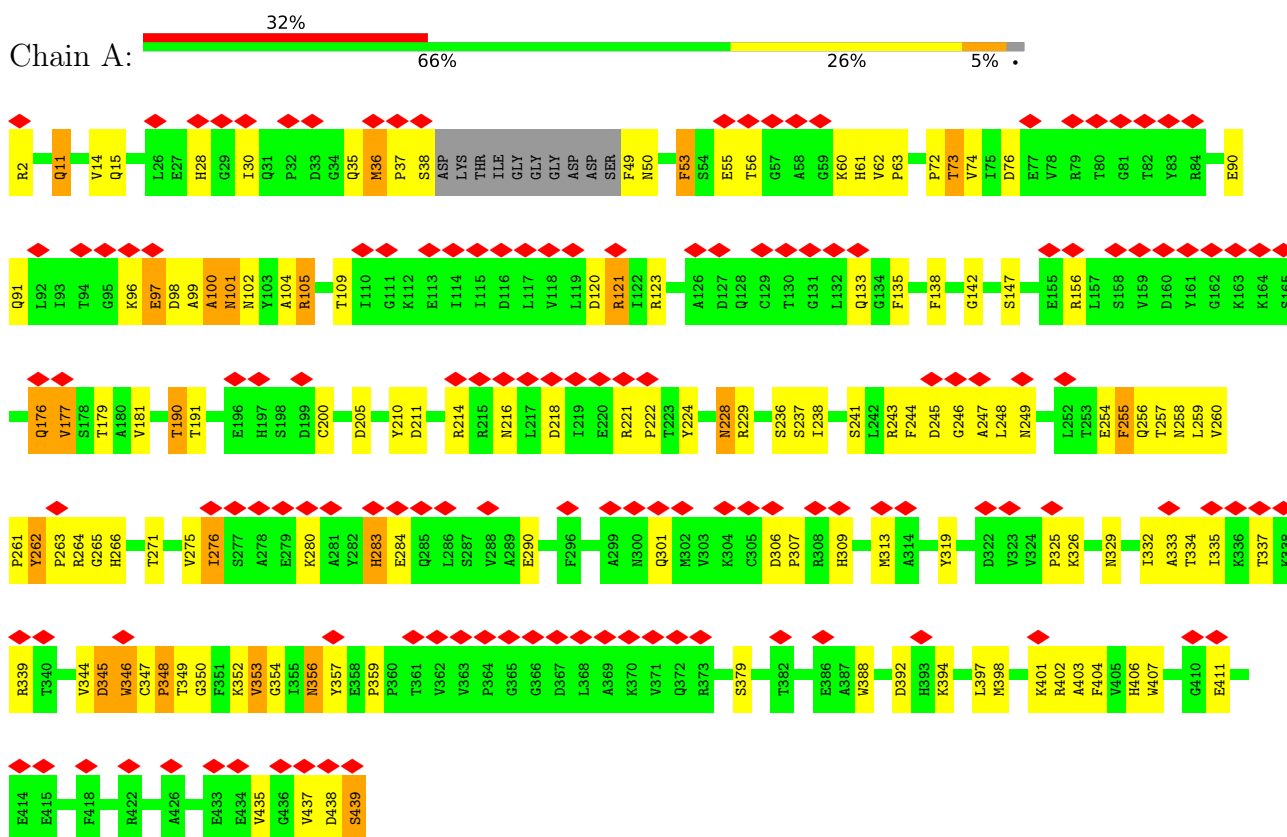
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	4	Total	O	0
			4	4	
6	C	4	Total	O	0
			4	4	
6	E	4	Total	O	0
			4	4	
6	G	4	Total	O	0
			4	4	
6	I	4	Total	O	0
			4	4	
6	K	4	Total	O	0
			4	4	
6	M	4	Total	O	0
			4	4	
6	O	4	Total	O	0
			4	4	
6	Q	4	Total	O	0
			4	4	

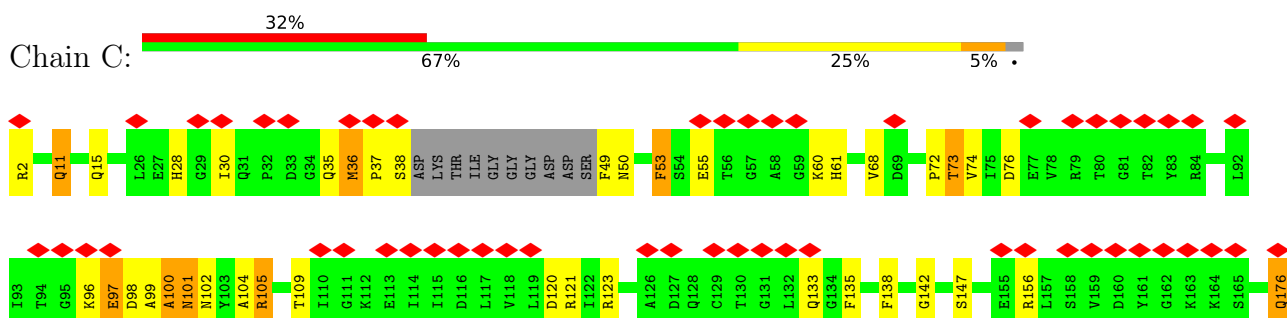
3 Residue-property plots

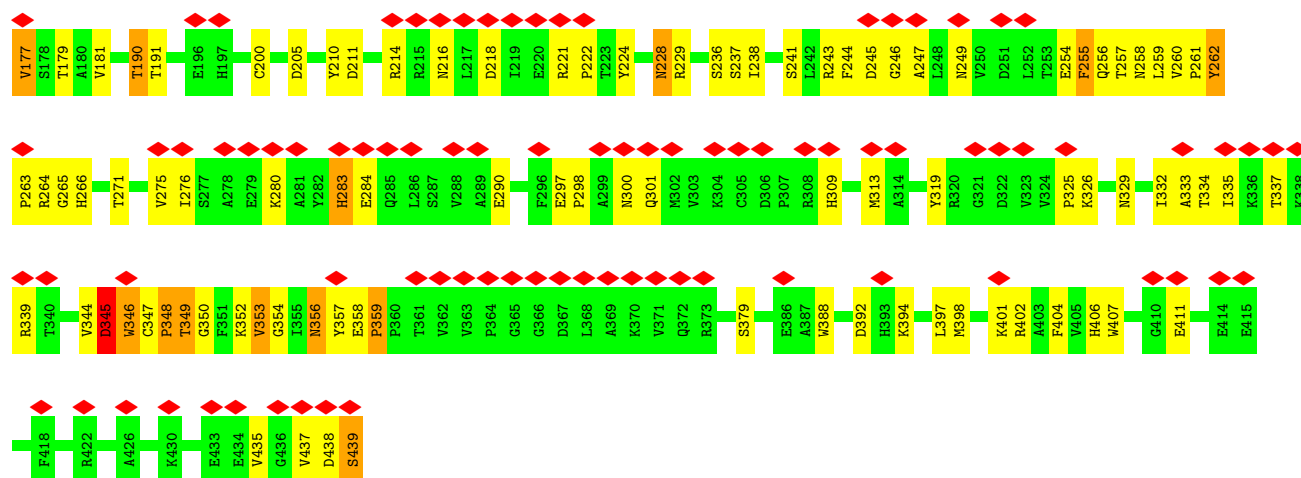
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Tubulin alpha-1A chain

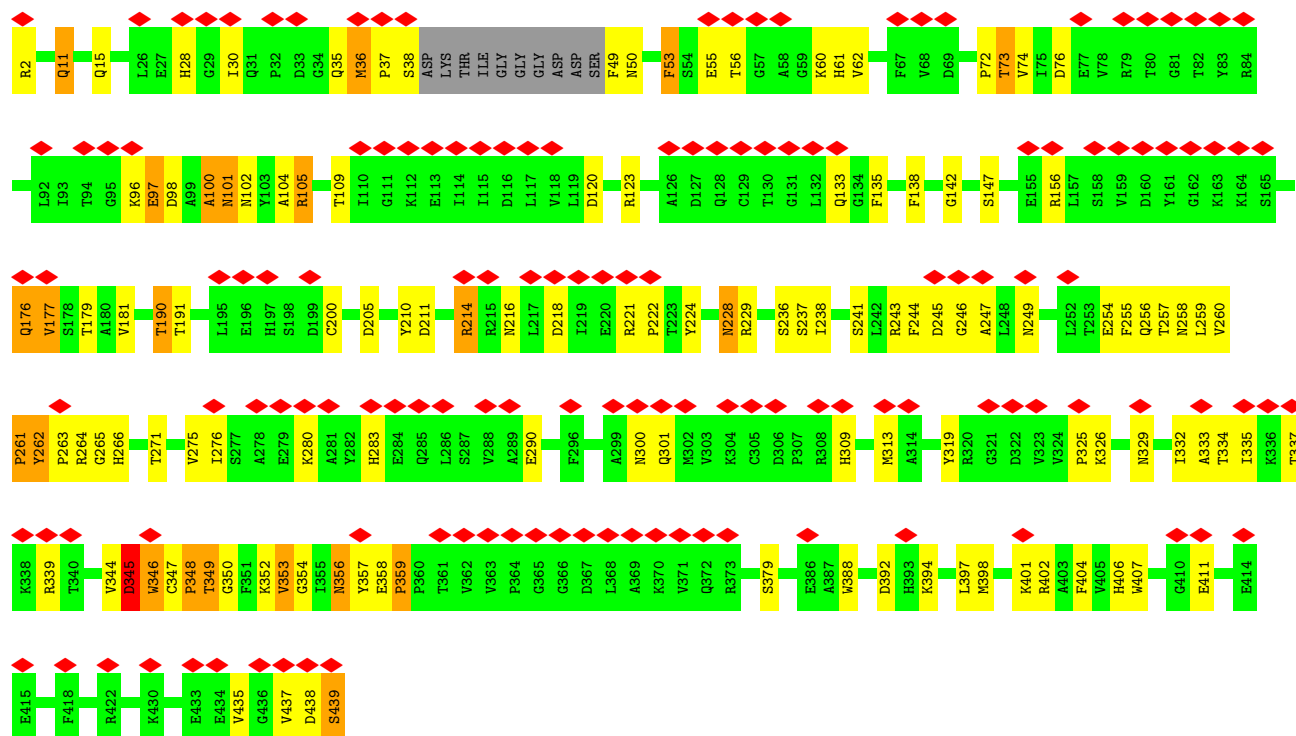


- Molecule 1: Tubulin alpha-1A chain

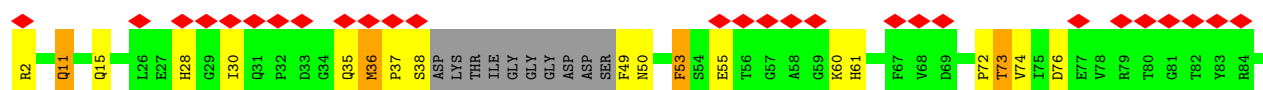


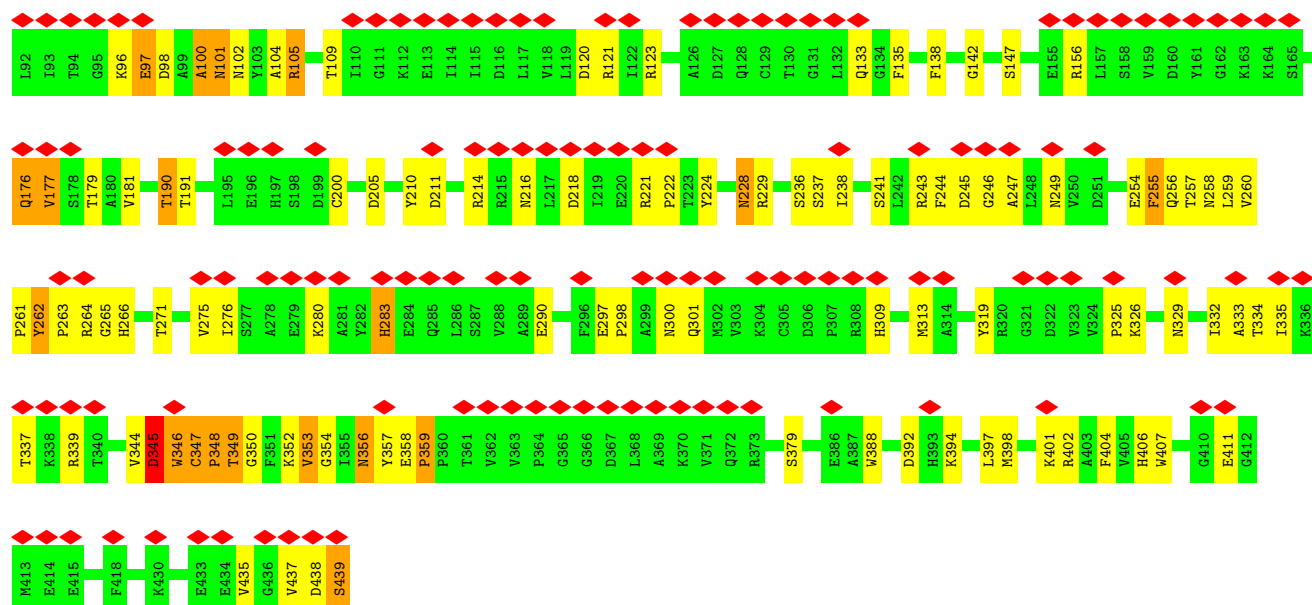


• Molecule 1: Tubulin alpha-1A chain

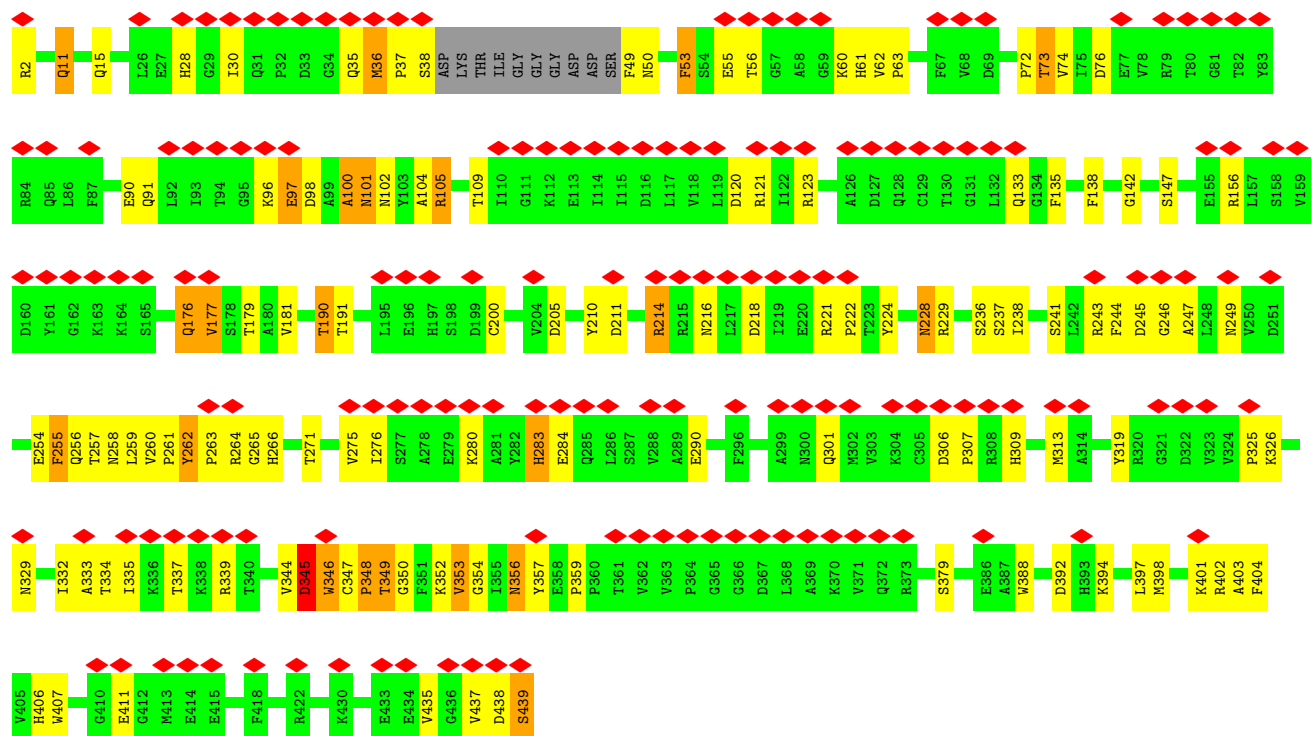


• Molecule 1: Tubulin alpha-1A chain



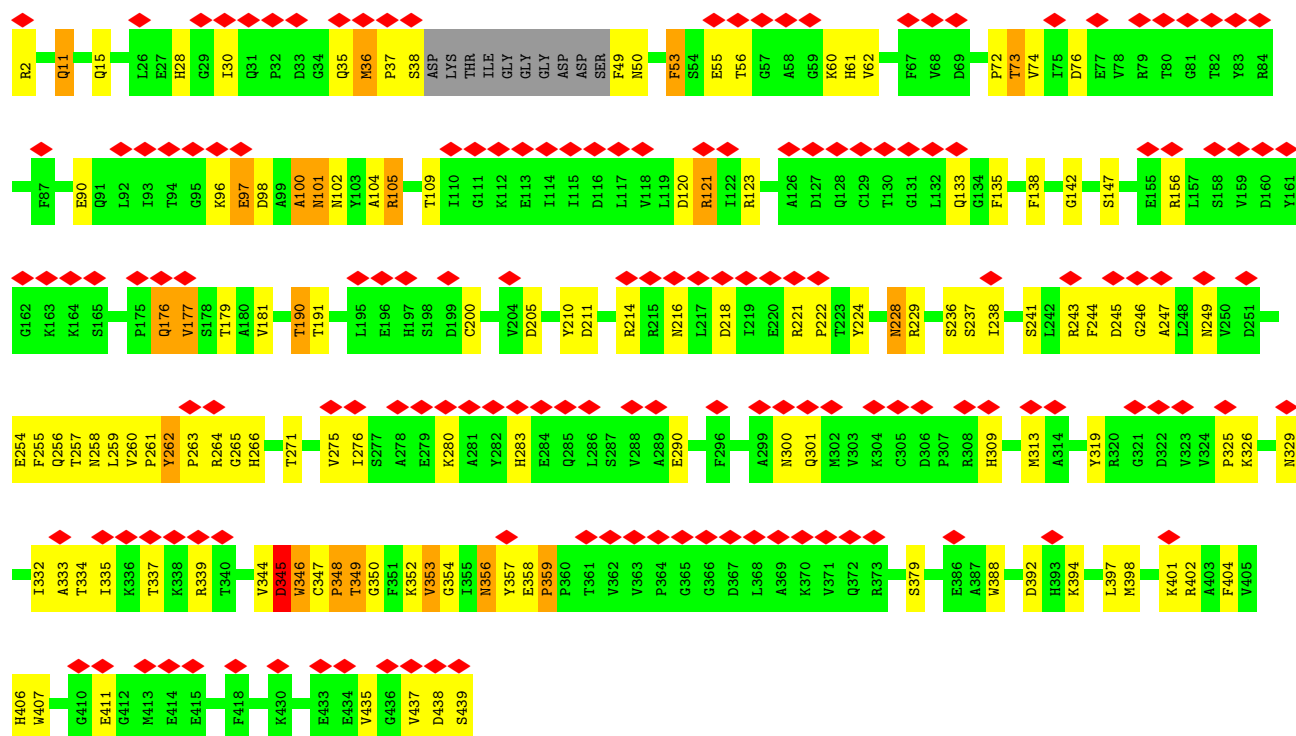


• Molecule 1: Tubulin alpha-1A chain

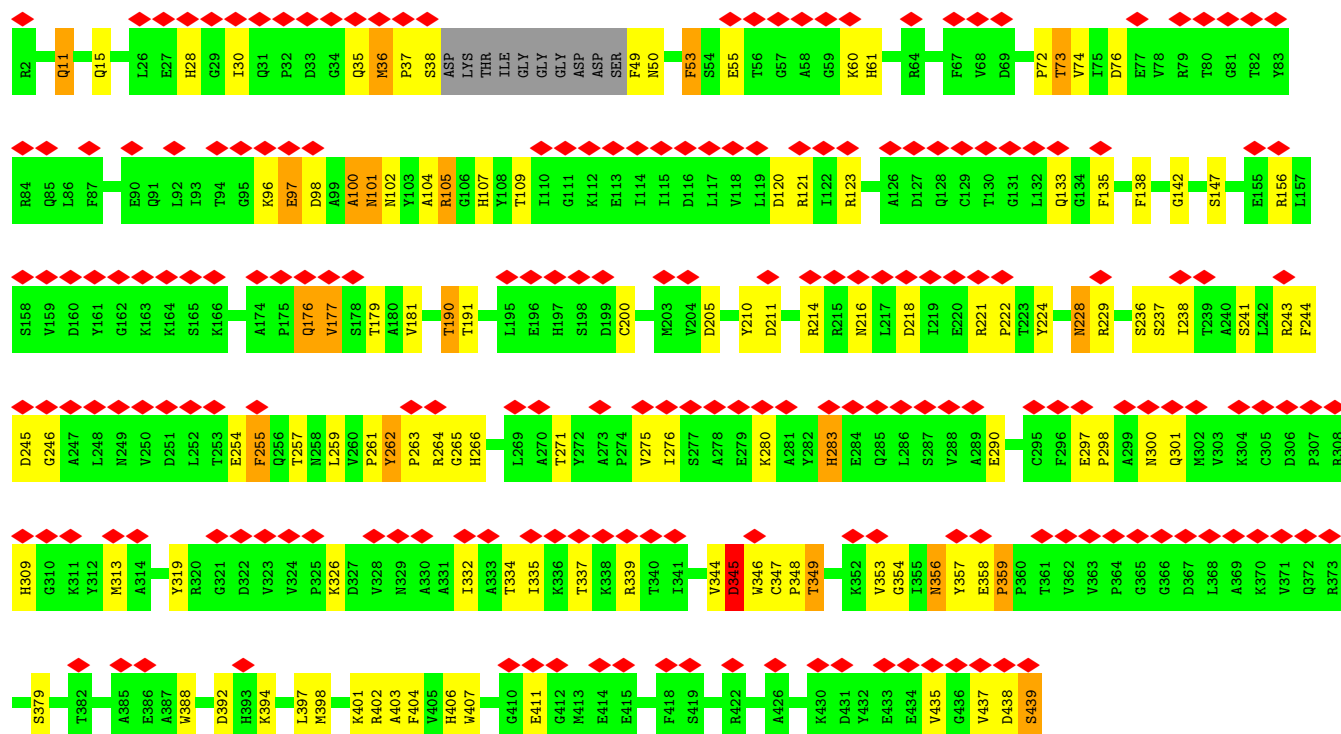
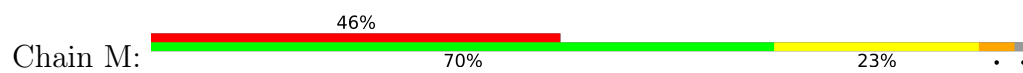


• Molecule 1: Tubulin alpha-1A chain

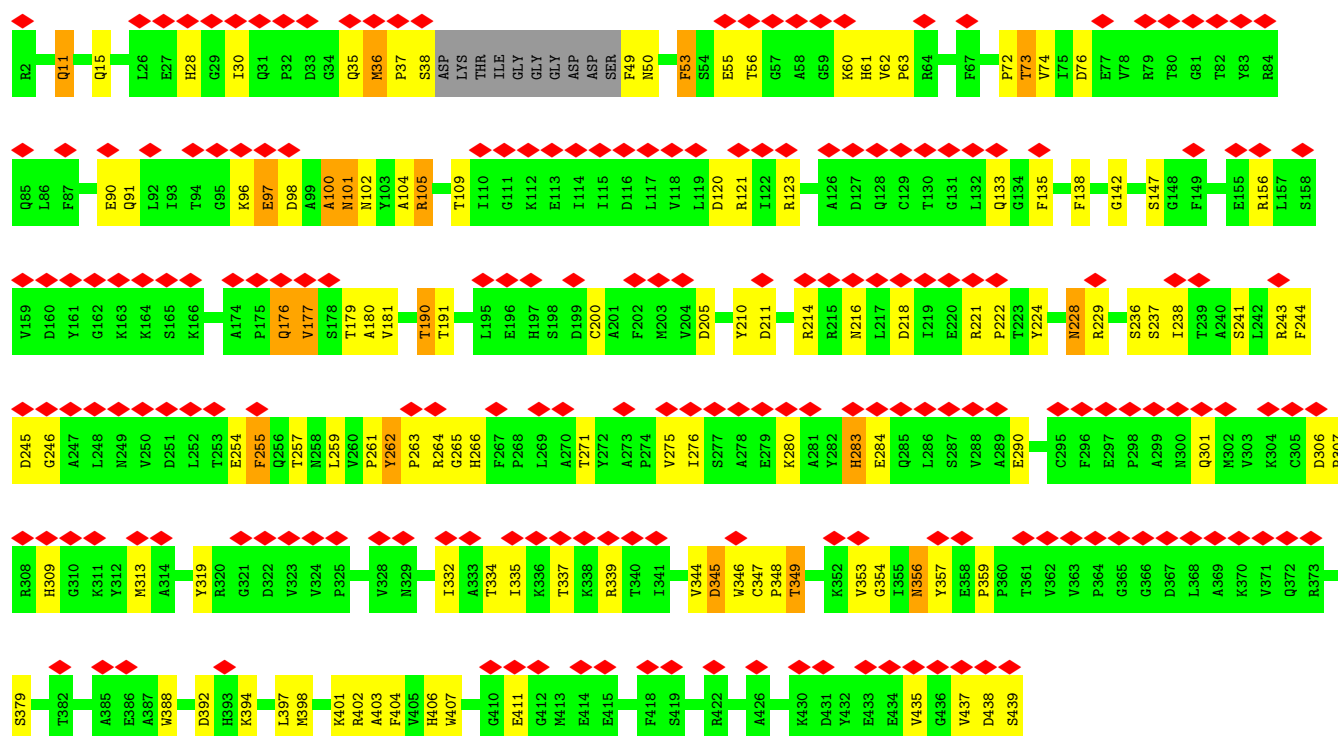




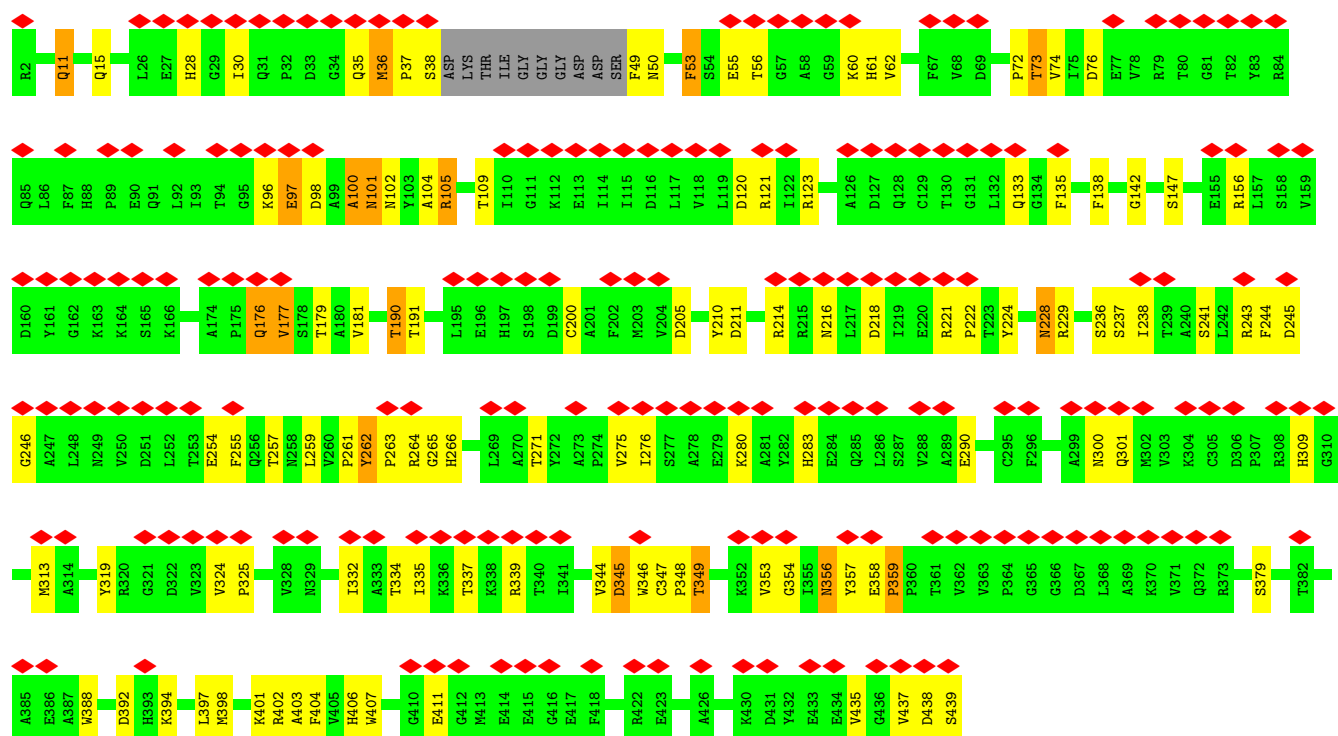
• Molecule 1: Tubulin alpha-1A chain



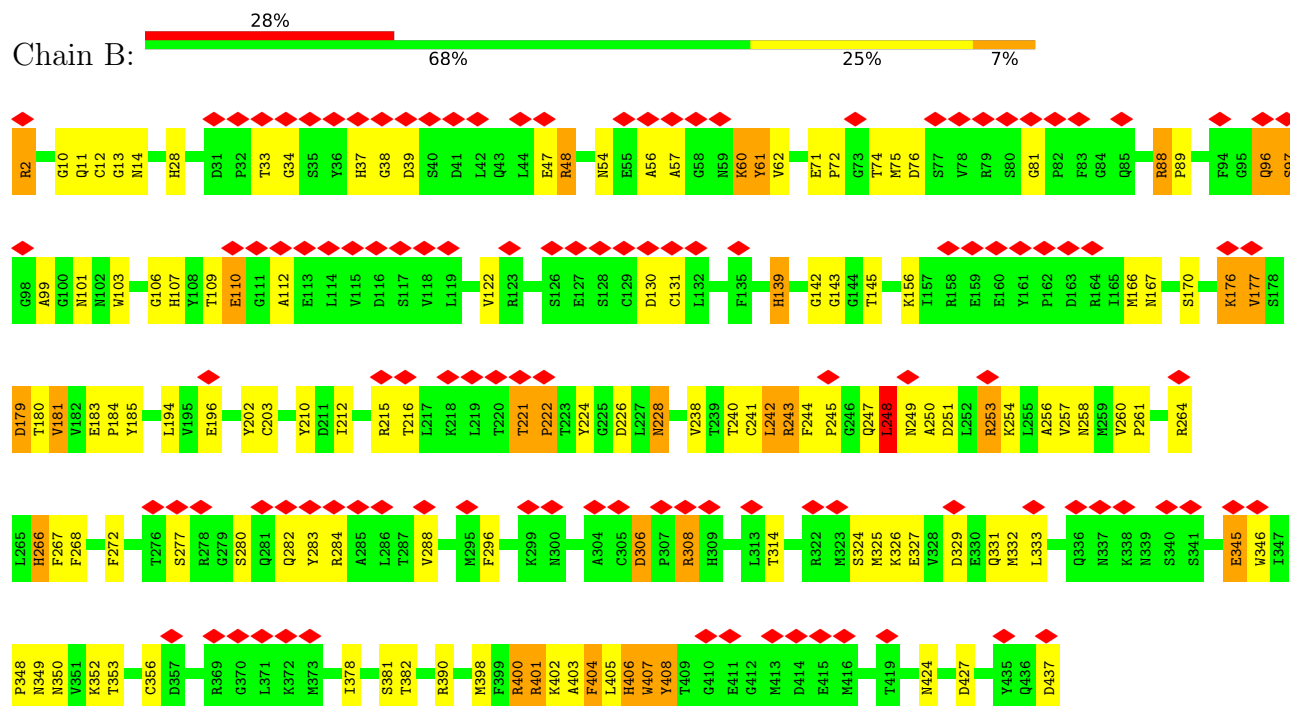
• Molecule 1: Tubulin alpha-1A chain



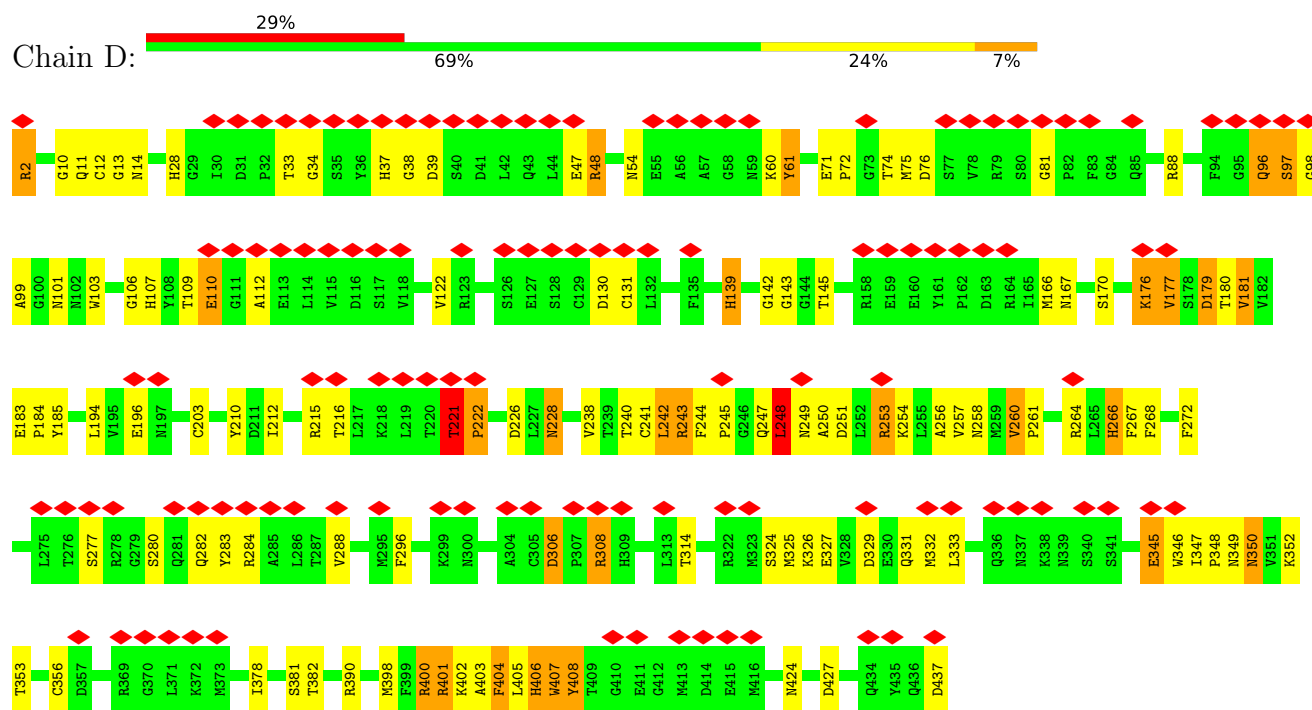
• Molecule 1: Tubulin alpha-1A chain



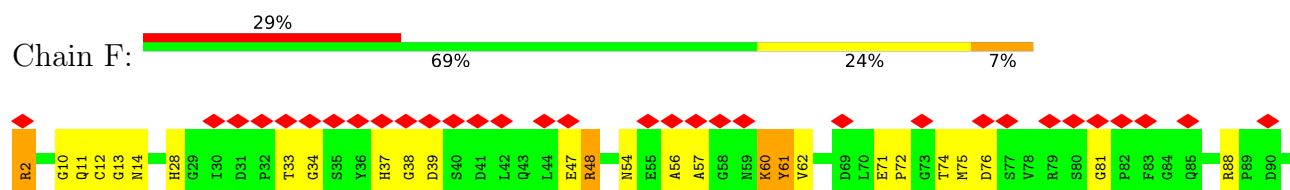
- Molecule 2: Tubulin beta chain

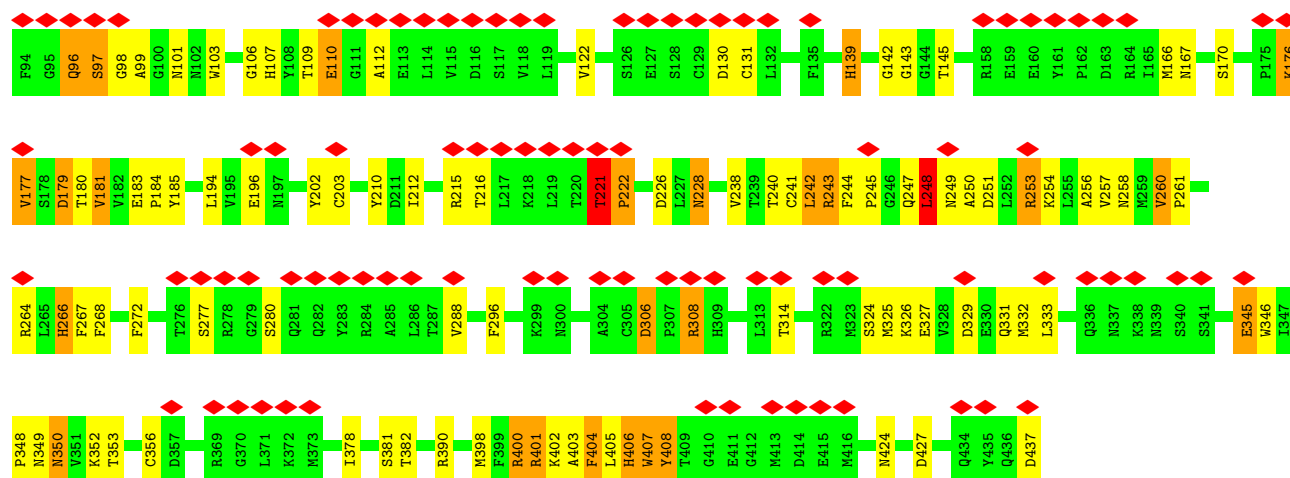


- Molecule 2: Tubulin beta chain

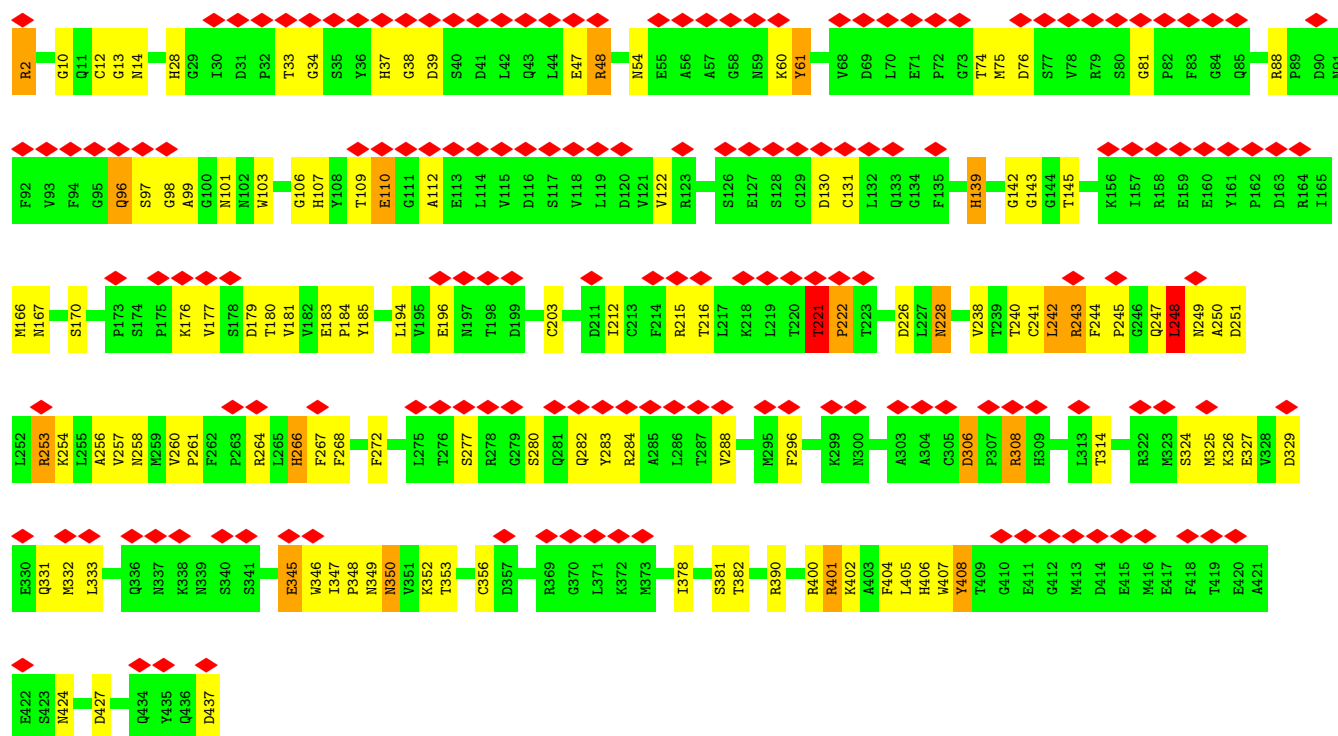
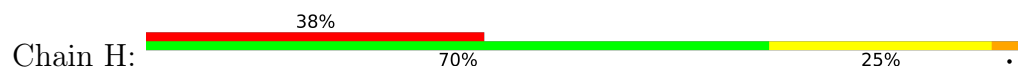


- Molecule 2: Tubulin beta chain

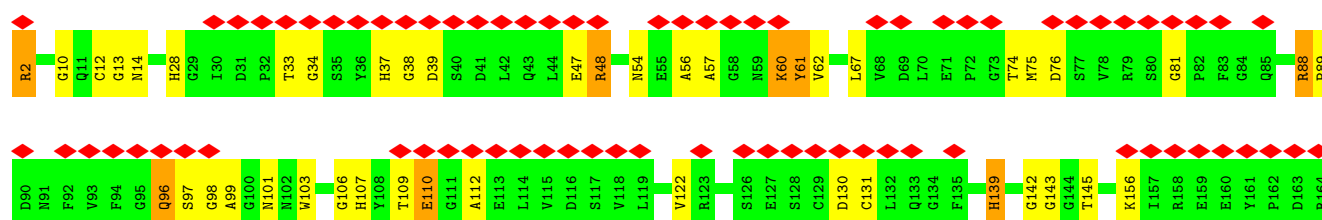


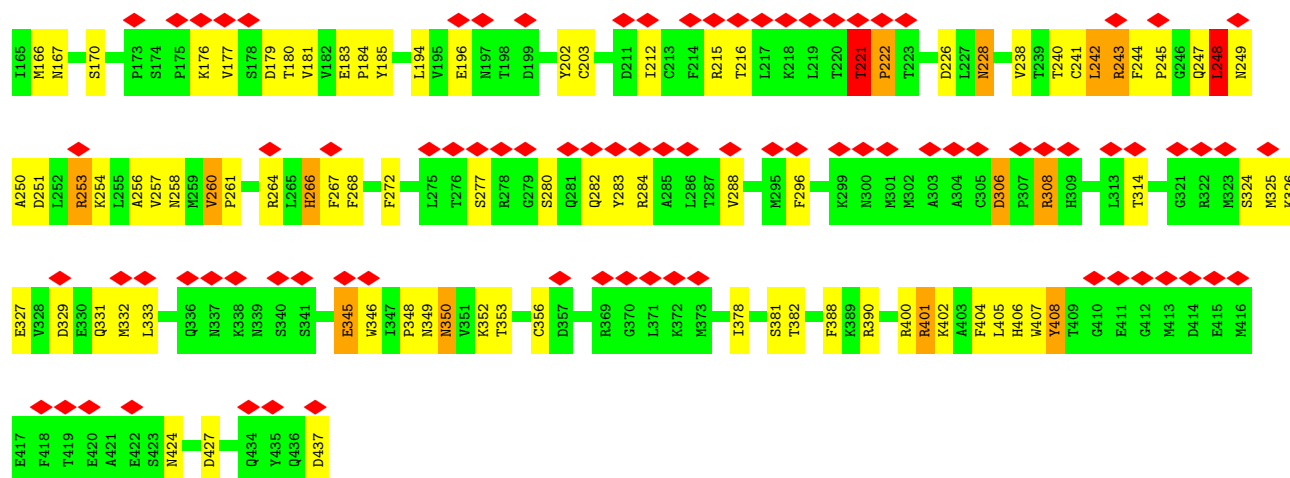


• Molecule 2: Tubulin beta chain

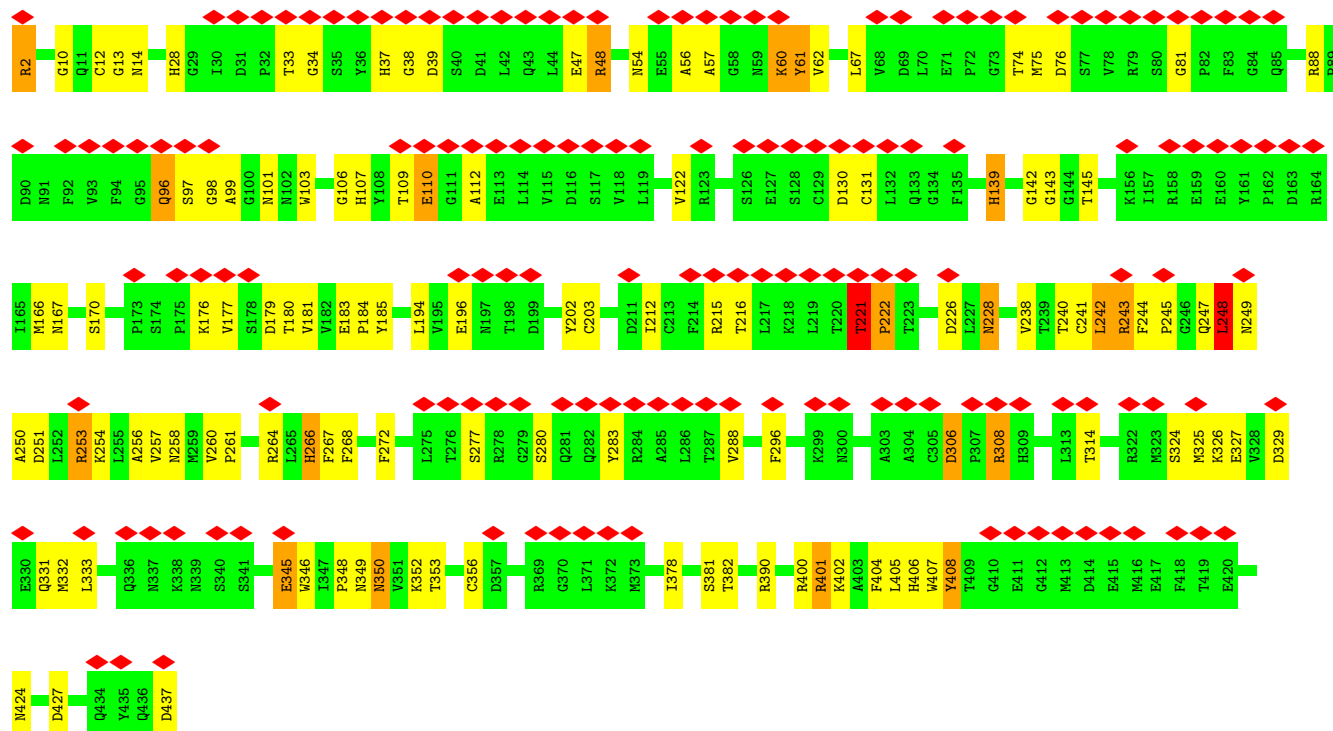


• Molecule 2: Tubulin beta chain

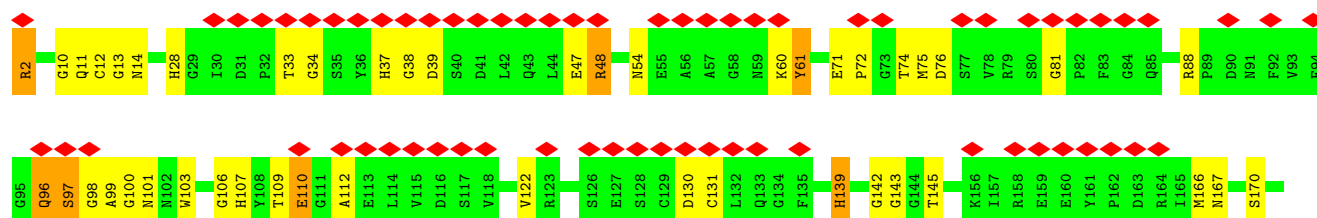


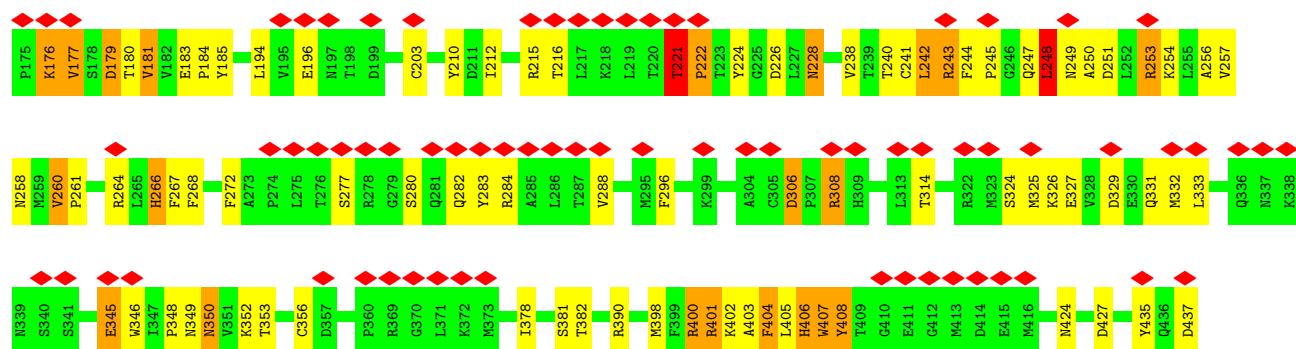


• Molecule 2: Tubulin beta chain

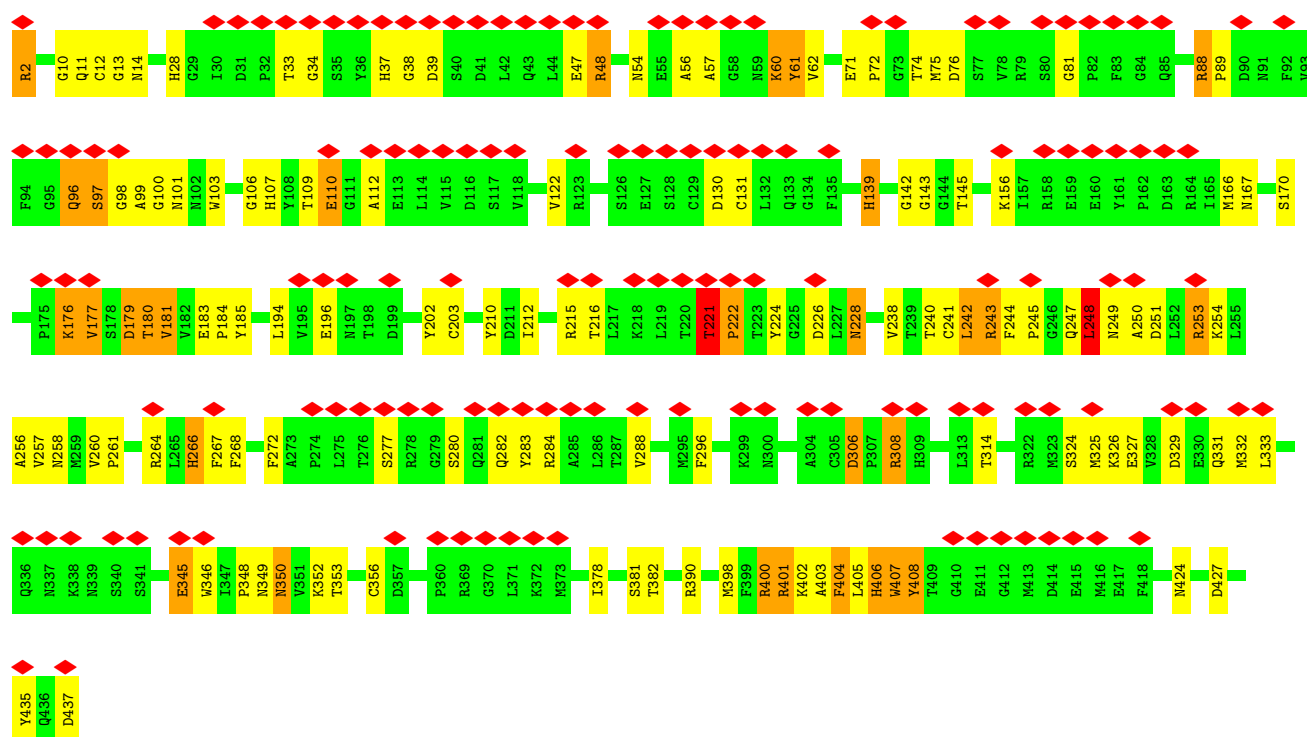


• Molecule 2: Tubulin beta chain

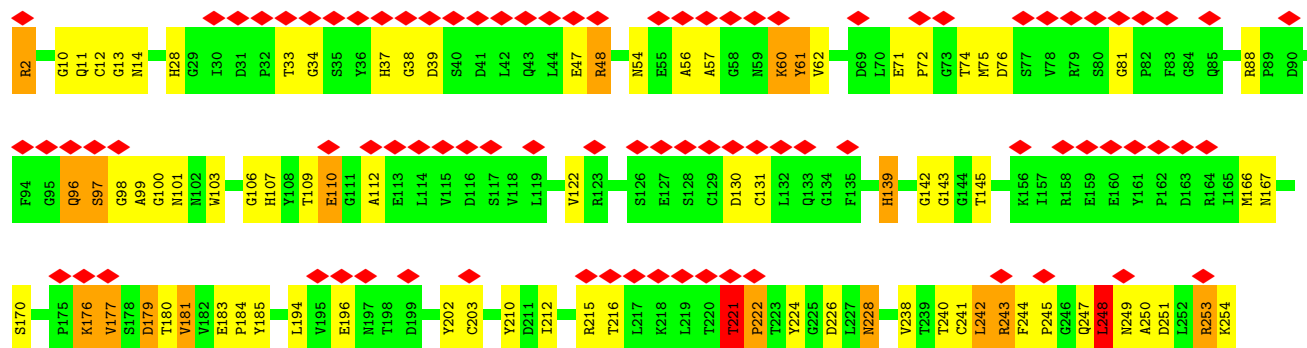


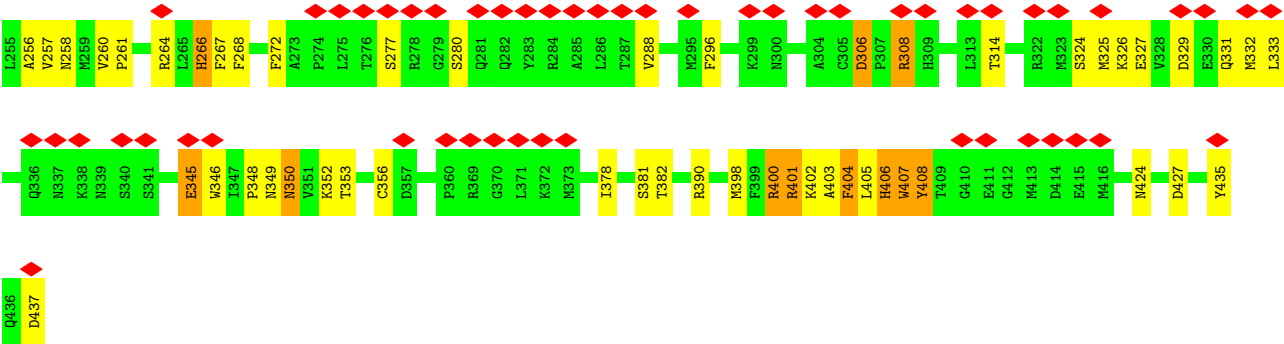


• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.7619°, rise=8.70662 Å, axial sym=C1	Depositor
Number of segments used	14302	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	11.973	Depositor
Minimum map value	-2.929	Depositor
Average map value	0.777	Depositor
Map value standard deviation	2.451	Depositor
Recommended contour level	7.4	Depositor
Map size (Å)	246.52802, 246.52802, 282.48	wwPDB
Map dimensions	192, 192, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.284, 1.284, 1.284	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.48	32/3427 (0.9%)	1.80	80/4651 (1.7%)
1	C	1.48	32/3427 (0.9%)	1.80	81/4651 (1.7%)
1	E	1.48	32/3427 (0.9%)	1.80	80/4651 (1.7%)
1	G	1.48	31/3427 (0.9%)	1.80	80/4651 (1.7%)
1	I	1.48	31/3427 (0.9%)	1.80	79/4651 (1.7%)
1	K	1.48	30/3427 (0.9%)	1.80	80/4651 (1.7%)
1	M	1.48	32/3427 (0.9%)	1.80	81/4651 (1.7%)
1	O	1.48	31/3427 (0.9%)	1.81	78/4651 (1.7%)
1	Q	1.48	30/3427 (0.9%)	1.80	80/4651 (1.7%)
2	B	1.35	26/3427 (0.8%)	1.82	96/4642 (2.1%)
2	D	1.35	26/3427 (0.8%)	1.82	98/4642 (2.1%)
2	F	1.35	26/3427 (0.8%)	1.82	98/4642 (2.1%)
2	H	1.35	26/3427 (0.8%)	1.82	96/4642 (2.1%)
2	J	1.35	26/3427 (0.8%)	1.82	101/4642 (2.2%)
2	L	1.35	26/3427 (0.8%)	1.82	97/4642 (2.1%)
2	N	1.35	26/3427 (0.8%)	1.82	97/4642 (2.1%)
2	P	1.35	26/3427 (0.8%)	1.82	95/4642 (2.0%)
2	R	1.35	26/3427 (0.8%)	1.82	95/4642 (2.0%)
All	All	1.42	515/61686 (0.8%)	1.81	1592/83637 (1.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
2	N	0	1
2	P	0	1
2	R	0	1
All	All	0	9

All (515) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	265	GLY	CA-C	-19.65	1.27	1.52
1	Q	265	GLY	CA-C	-19.63	1.27	1.52
1	E	265	GLY	CA-C	-19.60	1.27	1.52
1	I	265	GLY	CA-C	-19.58	1.27	1.52
1	G	265	GLY	CA-C	-19.57	1.27	1.52
1	C	265	GLY	CA-C	-19.57	1.27	1.52
1	O	265	GLY	CA-C	-19.55	1.27	1.52
1	A	265	GLY	CA-C	-19.51	1.27	1.52
1	K	265	GLY	CA-C	-19.50	1.27	1.52
1	I	266	HIS	N-CA	-17.59	1.24	1.45
1	C	266	HIS	N-CA	-17.55	1.24	1.45
1	E	266	HIS	N-CA	-17.52	1.24	1.45
1	O	266	HIS	N-CA	-17.52	1.24	1.45
1	M	266	HIS	N-CA	-17.51	1.24	1.45
1	K	266	HIS	N-CA	-17.48	1.24	1.45
1	A	266	HIS	N-CA	-17.45	1.24	1.45
1	Q	266	HIS	N-CA	-17.45	1.24	1.45
1	G	266	HIS	N-CA	-17.42	1.24	1.45
2	N	250	ALA	N-CA	-16.02	1.20	1.46
2	L	250	ALA	N-CA	-15.94	1.20	1.46
2	B	250	ALA	N-CA	-15.94	1.20	1.46
2	J	250	ALA	N-CA	-15.93	1.20	1.46
2	H	250	ALA	N-CA	-15.93	1.20	1.46
2	D	250	ALA	N-CA	-15.92	1.20	1.46
2	R	250	ALA	N-CA	-15.91	1.20	1.46
2	P	250	ALA	N-CA	-15.84	1.20	1.46
2	F	250	ALA	N-CA	-15.81	1.20	1.46
1	E	264	ARG	CA-C	-14.27	1.33	1.53
1	K	264	ARG	CA-C	-14.20	1.33	1.53
1	G	264	ARG	CA-C	-14.18	1.33	1.53
1	Q	264	ARG	CA-C	-14.17	1.33	1.53
1	O	264	ARG	CA-C	-14.17	1.33	1.53
1	C	264	ARG	CA-C	-14.16	1.33	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	264	ARG	CA-C	-14.15	1.33	1.53
1	A	264	ARG	CA-C	-14.15	1.33	1.53
1	I	264	ARG	CA-C	-14.13	1.33	1.53
1	C	438	ASP	CA-C	-14.06	1.34	1.52
1	A	438	ASP	CA-C	-13.99	1.34	1.52
1	G	438	ASP	CA-C	-13.96	1.34	1.52
1	M	438	ASP	CA-C	-13.96	1.34	1.52
1	K	438	ASP	CA-C	-13.96	1.34	1.52
1	O	438	ASP	CA-C	-13.94	1.34	1.52
1	E	438	ASP	CA-C	-13.93	1.34	1.52
1	Q	438	ASP	CA-C	-13.93	1.34	1.52
1	I	438	ASP	CA-C	-13.89	1.34	1.52
2	H	96	GLN	CA-C	-13.35	1.35	1.52
2	B	96	GLN	CA-C	-13.29	1.35	1.52
2	P	96	GLN	CA-C	-13.26	1.35	1.52
2	D	96	GLN	CA-C	-13.25	1.35	1.52
2	R	96	GLN	CA-C	-13.23	1.35	1.52
2	F	96	GLN	CA-C	-12.75	1.35	1.52
2	L	96	GLN	CA-C	-12.71	1.35	1.52
2	N	96	GLN	CA-C	-12.67	1.35	1.52
2	J	96	GLN	CA-C	-12.63	1.35	1.52
2	B	39	ASP	N-CA	-12.03	1.36	1.47
1	K	348	PRO	N-CA	-11.97	1.33	1.46
1	C	348	PRO	N-CA	-11.96	1.33	1.46
1	I	348	PRO	N-CA	-11.96	1.33	1.46
1	A	348	PRO	N-CA	-11.95	1.33	1.46
1	G	348	PRO	N-CA	-11.95	1.33	1.46
2	L	39	ASP	N-CA	-11.92	1.36	1.47
1	E	348	PRO	N-CA	-11.87	1.33	1.46
2	H	39	ASP	N-CA	-11.86	1.36	1.47
1	O	348	PRO	N-CA	-11.84	1.33	1.46
1	Q	348	PRO	CA-C	-11.84	1.38	1.52
1	Q	348	PRO	N-CA	-11.83	1.33	1.46
2	D	39	ASP	N-CA	-11.81	1.36	1.47
2	P	39	ASP	N-CA	-11.81	1.36	1.47
1	M	348	PRO	N-CA	-11.81	1.33	1.46
1	K	348	PRO	CA-C	-11.79	1.38	1.52
2	R	39	ASP	N-CA	-11.78	1.36	1.47
2	F	39	ASP	N-CA	-11.77	1.36	1.47
2	J	39	ASP	N-CA	-11.76	1.36	1.47
1	A	348	PRO	CA-C	-11.74	1.38	1.52
2	N	39	ASP	N-CA	-11.74	1.36	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	348	PRO	CA-C	-11.72	1.38	1.52
1	M	348	PRO	CA-C	-11.72	1.38	1.52
1	E	348	PRO	CA-C	-11.70	1.38	1.52
1	I	348	PRO	CA-C	-11.69	1.38	1.52
1	C	348	PRO	CA-C	-11.65	1.38	1.52
1	O	348	PRO	CA-C	-11.60	1.39	1.52
1	E	347	CYS	CA-C	-11.51	1.40	1.52
1	C	347	CYS	CA-C	-11.50	1.40	1.52
1	K	347	CYS	CA-C	-11.50	1.40	1.52
1	A	347	CYS	CA-C	-11.48	1.40	1.52
1	G	347	CYS	CA-C	-11.47	1.40	1.52
1	Q	347	CYS	CA-C	-11.47	1.40	1.52
1	M	347	CYS	CA-C	-11.46	1.40	1.52
1	I	347	CYS	CA-C	-11.42	1.40	1.52
1	O	347	CYS	CA-C	-11.36	1.40	1.52
1	Q	437	VAL	CA-C	-9.56	1.42	1.53
2	D	97	SER	N-CA	-9.55	1.34	1.46
1	O	437	VAL	CA-C	-9.50	1.42	1.53
1	A	437	VAL	CA-C	-9.50	1.42	1.53
2	F	97	SER	N-CA	-9.49	1.34	1.46
1	M	437	VAL	CA-C	-9.49	1.42	1.53
2	B	97	SER	N-CA	-9.47	1.34	1.46
1	G	437	VAL	CA-C	-9.47	1.42	1.53
1	I	437	VAL	CA-C	-9.46	1.42	1.53
1	E	437	VAL	CA-C	-9.46	1.42	1.53
2	N	97	SER	N-CA	-9.45	1.35	1.46
2	H	97	SER	N-CA	-9.45	1.35	1.46
2	P	97	SER	N-CA	-9.43	1.35	1.46
2	R	97	SER	N-CA	-9.42	1.35	1.46
1	C	437	VAL	CA-C	-9.41	1.42	1.53
2	J	97	SER	N-CA	-9.41	1.35	1.46
2	L	97	SER	N-CA	-9.40	1.35	1.46
1	K	437	VAL	CA-C	-9.39	1.42	1.53
1	K	347	CYS	N-CA	-8.76	1.33	1.46
1	M	347	CYS	N-CA	-8.76	1.33	1.46
1	E	347	CYS	N-CA	-8.75	1.33	1.46
1	O	347	CYS	N-CA	-8.74	1.33	1.46
1	I	347	CYS	N-CA	-8.73	1.33	1.46
1	C	347	CYS	N-CA	-8.72	1.34	1.46
1	Q	347	CYS	N-CA	-8.71	1.34	1.46
2	B	242	LEU	N-CA	-8.66	1.34	1.46
2	F	242	LEU	N-CA	-8.64	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	CYS	N-CA	-8.64	1.34	1.46
1	G	347	CYS	N-CA	-8.63	1.34	1.46
2	N	242	LEU	N-CA	-8.63	1.35	1.46
2	P	242	LEU	N-CA	-8.62	1.35	1.46
2	H	242	LEU	N-CA	-8.61	1.35	1.46
2	D	242	LEU	N-CA	-8.60	1.35	1.46
2	R	242	LEU	N-CA	-8.60	1.35	1.46
2	L	242	LEU	N-CA	-8.59	1.35	1.46
2	J	242	LEU	N-CA	-8.55	1.35	1.46
1	G	345	ASP	CA-C	-8.13	1.41	1.52
1	A	345	ASP	CA-C	-8.12	1.41	1.52
2	J	240	THR	CA-C	-8.10	1.41	1.52
1	O	345	ASP	CA-C	-8.07	1.42	1.52
1	K	345	ASP	CA-C	-8.06	1.42	1.52
1	Q	345	ASP	CA-C	-8.06	1.42	1.52
2	B	240	THR	CA-C	-8.06	1.41	1.52
2	F	240	THR	CA-C	-8.05	1.41	1.52
1	C	345	ASP	CA-C	-8.05	1.42	1.52
1	C	100	ALA	CA-C	-8.02	1.43	1.53
1	E	345	ASP	CA-C	-8.02	1.42	1.52
2	H	240	THR	CA-C	-8.02	1.41	1.52
2	P	240	THR	CA-C	-8.01	1.41	1.52
2	N	240	THR	CA-C	-8.01	1.41	1.52
1	I	345	ASP	CA-C	-8.00	1.42	1.52
2	D	240	THR	CA-C	-7.98	1.41	1.52
2	B	241	CYS	CA-C	-7.97	1.41	1.52
2	R	240	THR	CA-C	-7.97	1.41	1.52
1	M	345	ASP	CA-C	-7.96	1.42	1.52
1	I	100	ALA	CA-C	-7.95	1.43	1.53
2	L	241	CYS	CA-C	-7.93	1.41	1.52
2	D	241	CYS	CA-C	-7.93	1.41	1.52
2	N	241	CYS	CA-C	-7.92	1.41	1.52
2	L	240	THR	CA-C	-7.92	1.41	1.52
1	M	100	ALA	CA-C	-7.91	1.43	1.53
2	H	241	CYS	CA-C	-7.89	1.41	1.52
1	K	100	ALA	CA-C	-7.89	1.43	1.53
2	J	241	CYS	CA-C	-7.89	1.41	1.52
1	O	100	ALA	CA-C	-7.89	1.43	1.53
2	R	241	CYS	CA-C	-7.89	1.41	1.52
1	G	100	ALA	CA-C	-7.88	1.43	1.53
1	Q	100	ALA	CA-C	-7.87	1.43	1.53
2	P	241	CYS	CA-C	-7.87	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	265	GLY	N-CA	-7.86	1.32	1.45
1	E	100	ALA	CA-C	-7.86	1.43	1.53
1	C	265	GLY	N-CA	-7.85	1.33	1.45
1	I	265	GLY	N-CA	-7.84	1.33	1.45
1	G	265	GLY	N-CA	-7.84	1.33	1.45
1	A	100	ALA	CA-C	-7.83	1.43	1.53
1	M	265	GLY	N-CA	-7.82	1.33	1.45
2	F	241	CYS	CA-C	-7.80	1.41	1.52
1	Q	344	VAL	CA-C	-7.77	1.43	1.52
1	A	265	GLY	N-CA	-7.77	1.33	1.45
1	E	265	GLY	N-CA	-7.76	1.33	1.45
1	C	344	VAL	CA-C	-7.76	1.43	1.52
1	G	344	VAL	CA-C	-7.75	1.43	1.52
1	Q	265	GLY	N-CA	-7.75	1.33	1.45
1	I	344	VAL	CA-C	-7.75	1.43	1.52
1	O	265	GLY	N-CA	-7.72	1.33	1.45
1	K	439	SER	N-CA	-7.71	1.31	1.46
1	K	344	VAL	CA-C	-7.69	1.44	1.52
1	M	344	VAL	CA-C	-7.69	1.44	1.52
1	M	439	SER	N-CA	-7.67	1.31	1.46
1	C	439	SER	N-CA	-7.67	1.31	1.46
1	I	439	SER	N-CA	-7.67	1.31	1.46
1	A	439	SER	N-CA	-7.65	1.31	1.46
1	E	344	VAL	CA-C	-7.65	1.44	1.52
1	G	439	SER	N-CA	-7.63	1.31	1.46
2	H	38	GLY	CA-C	-7.63	1.41	1.51
1	E	439	SER	N-CA	-7.62	1.31	1.46
1	Q	439	SER	N-CA	-7.61	1.31	1.46
1	A	344	VAL	CA-C	-7.61	1.44	1.52
1	O	344	VAL	CA-C	-7.58	1.44	1.52
1	O	439	SER	N-CA	-7.58	1.31	1.46
2	J	38	GLY	CA-C	-7.57	1.41	1.51
2	F	38	GLY	CA-C	-7.55	1.41	1.51
2	R	38	GLY	CA-C	-7.55	1.41	1.51
2	N	38	GLY	CA-C	-7.55	1.41	1.51
2	P	38	GLY	CA-C	-7.55	1.41	1.51
2	D	38	GLY	CA-C	-7.54	1.41	1.51
2	B	38	GLY	CA-C	-7.53	1.41	1.51
2	L	38	GLY	CA-C	-7.51	1.41	1.51
1	E	346	TRP	N-CA	-7.16	1.36	1.46
1	G	346	TRP	N-CA	-7.16	1.36	1.46
1	Q	346	TRP	N-CA	-7.15	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	TRP	N-CA	-7.12	1.36	1.46
1	M	346	TRP	N-CA	-7.12	1.36	1.46
1	O	346	TRP	N-CA	-7.10	1.36	1.46
1	C	346	TRP	N-CA	-7.10	1.36	1.46
2	D	97	SER	CA-C	-7.09	1.45	1.53
2	B	97	SER	CA-C	-7.08	1.45	1.53
1	K	346	TRP	N-CA	-7.07	1.37	1.46
1	I	346	TRP	N-CA	-7.05	1.37	1.46
2	R	97	SER	CA-C	-7.03	1.45	1.53
2	J	97	SER	CA-C	-7.03	1.45	1.53
2	P	97	SER	CA-C	-7.02	1.45	1.53
2	F	97	SER	CA-C	-7.01	1.45	1.53
2	L	97	SER	CA-C	-6.99	1.45	1.53
1	I	438	ASP	N-CA	-6.92	1.37	1.45
2	N	97	SER	CA-C	-6.91	1.45	1.53
2	H	97	SER	CA-C	-6.88	1.45	1.53
1	O	438	ASP	N-CA	-6.88	1.37	1.45
1	A	438	ASP	N-CA	-6.86	1.37	1.45
1	C	438	ASP	N-CA	-6.84	1.37	1.45
1	M	438	ASP	N-CA	-6.84	1.37	1.45
1	Q	438	ASP	N-CA	-6.83	1.37	1.45
1	G	438	ASP	N-CA	-6.75	1.37	1.45
1	E	438	ASP	N-CA	-6.71	1.37	1.45
1	K	438	ASP	N-CA	-6.69	1.37	1.45
2	B	222	PRO	N-CA	-6.69	1.38	1.47
2	H	222	PRO	N-CA	-6.69	1.38	1.47
2	P	222	PRO	N-CA	-6.69	1.38	1.47
2	L	222	PRO	N-CA	-6.66	1.38	1.47
2	J	222	PRO	N-CA	-6.64	1.38	1.47
1	K	97	GLU	CA-C	-6.63	1.44	1.52
1	O	97	GLU	CA-C	-6.61	1.44	1.52
2	D	222	PRO	N-CA	-6.58	1.38	1.47
2	F	250	ALA	CA-C	-6.58	1.46	1.53
1	A	97	GLU	CA-C	-6.57	1.44	1.52
2	L	243	ARG	N-CA	-6.57	1.38	1.46
2	N	243	ARG	N-CA	-6.57	1.38	1.46
2	N	222	PRO	N-CA	-6.56	1.39	1.47
2	B	250	ALA	CA-C	-6.56	1.46	1.53
2	D	250	ALA	CA-C	-6.56	1.46	1.53
2	R	250	ALA	CA-C	-6.56	1.46	1.53
1	I	97	GLU	CA-C	-6.55	1.44	1.52
2	P	243	ARG	N-CA	-6.54	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	222	PRO	N-CA	-6.53	1.39	1.47
2	L	250	ALA	CA-C	-6.53	1.46	1.53
2	F	243	ARG	N-CA	-6.52	1.38	1.46
2	R	243	ARG	N-CA	-6.52	1.38	1.46
2	R	222	PRO	N-CA	-6.52	1.39	1.47
1	Q	97	GLU	CA-C	-6.52	1.44	1.52
1	A	37	PRO	CA-C	-6.51	1.45	1.52
1	C	97	GLU	CA-C	-6.49	1.44	1.52
2	B	243	ARG	N-CA	-6.49	1.38	1.46
1	G	37	PRO	CA-C	-6.49	1.45	1.52
2	J	250	ALA	CA-C	-6.49	1.46	1.53
2	H	250	ALA	CA-C	-6.48	1.46	1.53
1	M	97	GLU	CA-C	-6.47	1.44	1.52
2	N	250	ALA	CA-C	-6.47	1.46	1.53
2	P	250	ALA	CA-C	-6.46	1.46	1.53
1	E	97	GLU	CA-C	-6.46	1.44	1.52
2	J	243	ARG	N-CA	-6.46	1.38	1.46
1	C	37	PRO	CA-C	-6.45	1.45	1.52
1	Q	37	PRO	CA-C	-6.45	1.45	1.52
1	E	37	PRO	CA-C	-6.44	1.45	1.52
2	D	243	ARG	N-CA	-6.44	1.38	1.46
2	B	107	HIS	CA-C	-6.44	1.45	1.52
1	M	37	PRO	CA-C	-6.43	1.45	1.52
1	I	37	PRO	CA-C	-6.43	1.45	1.52
2	J	107	HIS	CA-C	-6.42	1.45	1.52
2	N	107	HIS	CA-C	-6.42	1.45	1.52
1	G	97	GLU	CA-C	-6.41	1.44	1.52
2	H	243	ARG	N-CA	-6.37	1.38	1.46
1	K	37	PRO	CA-C	-6.36	1.45	1.52
2	D	107	HIS	CA-C	-6.36	1.45	1.52
1	O	37	PRO	CA-C	-6.35	1.45	1.52
2	P	107	HIS	CA-C	-6.33	1.45	1.52
2	L	107	HIS	CA-C	-6.32	1.45	1.52
2	F	107	HIS	CA-C	-6.30	1.45	1.52
2	R	107	HIS	CA-C	-6.29	1.45	1.52
2	H	107	HIS	CA-C	-6.28	1.45	1.52
1	G	265	GLY	C-N	-6.09	1.24	1.33
1	I	262	TYR	N-CA	-6.07	1.41	1.46
1	C	265	GLY	C-N	-6.06	1.24	1.33
2	D	241	CYS	N-CA	-6.06	1.38	1.46
1	E	262	TYR	N-CA	-6.05	1.41	1.46
1	I	265	GLY	C-N	-6.05	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	241	CYS	N-CA	-6.05	1.38	1.46
1	M	265	GLY	C-N	-6.04	1.24	1.33
1	O	265	GLY	C-N	-6.03	1.24	1.33
1	E	265	GLY	C-N	-6.03	1.24	1.33
2	N	241	CYS	N-CA	-6.02	1.38	1.46
2	R	241	CYS	N-CA	-6.01	1.38	1.46
2	F	241	CYS	N-CA	-5.98	1.38	1.46
1	M	262	TYR	N-CA	-5.98	1.41	1.46
2	D	177	VAL	CA-C	-5.97	1.47	1.52
1	K	265	GLY	C-N	-5.97	1.24	1.33
2	L	241	CYS	N-CA	-5.96	1.38	1.46
1	A	265	GLY	C-N	-5.96	1.24	1.33
2	H	241	CYS	N-CA	-5.96	1.38	1.46
2	P	241	CYS	N-CA	-5.95	1.38	1.46
2	H	177	VAL	CA-C	-5.94	1.47	1.52
1	K	346	TRP	CA-C	-5.94	1.44	1.52
1	A	262	TYR	N-CA	-5.94	1.41	1.46
2	P	177	VAL	CA-C	-5.93	1.47	1.52
1	E	346	TRP	CA-C	-5.90	1.44	1.52
1	A	346	TRP	CA-C	-5.90	1.44	1.52
1	C	346	TRP	CA-C	-5.89	1.44	1.52
2	P	405	LEU	CA-C	-5.89	1.44	1.52
1	Q	265	GLY	C-N	-5.89	1.25	1.33
2	B	177	VAL	CA-C	-5.89	1.47	1.52
1	Q	346	TRP	CA-C	-5.89	1.44	1.52
1	G	346	TRP	CA-C	-5.89	1.44	1.52
1	I	346	TRP	CA-C	-5.88	1.44	1.52
1	G	262	TYR	N-CA	-5.88	1.41	1.46
2	R	177	VAL	CA-C	-5.87	1.47	1.52
1	O	262	TYR	N-CA	-5.87	1.41	1.46
2	F	177	VAL	CA-C	-5.86	1.47	1.52
2	L	405	LEU	CA-C	-5.86	1.44	1.52
1	K	262	TYR	N-CA	-5.85	1.41	1.46
2	N	405	LEU	CA-C	-5.85	1.44	1.52
2	R	180	THR	CA-C	-5.85	1.45	1.52
1	Q	262	TYR	N-CA	-5.85	1.41	1.46
2	R	405	LEU	CA-C	-5.85	1.44	1.52
2	H	405	LEU	CA-C	-5.85	1.44	1.52
2	J	241	CYS	N-CA	-5.84	1.38	1.46
1	O	346	TRP	CA-C	-5.84	1.44	1.52
2	J	177	VAL	CA-C	-5.83	1.47	1.52
2	J	405	LEU	CA-C	-5.83	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	180	THR	CA-C	-5.82	1.45	1.52
1	M	346	TRP	CA-C	-5.82	1.44	1.52
2	N	177	VAL	CA-C	-5.81	1.47	1.52
2	L	177	VAL	CA-C	-5.81	1.47	1.52
2	D	405	LEU	CA-C	-5.81	1.44	1.52
2	H	180	THR	CA-C	-5.81	1.45	1.52
1	C	262	TYR	N-CA	-5.80	1.41	1.46
2	J	180	THR	CA-C	-5.80	1.45	1.52
2	F	405	LEU	CA-C	-5.79	1.44	1.52
2	P	248	LEU	CA-C	-5.78	1.44	1.53
2	B	405	LEU	CA-C	-5.77	1.44	1.52
2	D	180	THR	CA-C	-5.77	1.45	1.52
2	H	110	GLU	CA-C	-5.75	1.45	1.52
2	P	180	THR	CA-C	-5.75	1.45	1.52
1	M	37	PRO	N-CA	-5.74	1.41	1.47
2	B	180	THR	CA-C	-5.74	1.45	1.52
2	N	248	LEU	CA-C	-5.74	1.44	1.53
2	R	248	LEU	CA-C	-5.74	1.44	1.53
2	J	110	GLU	CA-C	-5.73	1.45	1.52
2	R	110	GLU	CA-C	-5.73	1.45	1.52
2	B	242	LEU	CA-C	-5.73	1.44	1.52
2	F	180	THR	CA-C	-5.73	1.45	1.52
2	N	180	THR	CA-C	-5.73	1.45	1.52
1	M	38	SER	CA-C	-5.72	1.41	1.52
1	E	38	SER	CA-C	-5.72	1.41	1.52
1	I	38	SER	CA-C	-5.72	1.41	1.52
1	C	38	SER	CA-C	-5.72	1.41	1.52
2	B	110	GLU	CA-C	-5.72	1.45	1.52
2	L	248	LEU	CA-C	-5.72	1.44	1.53
2	D	248	LEU	CA-C	-5.71	1.44	1.53
2	F	248	LEU	CA-C	-5.71	1.44	1.53
2	J	248	LEU	CA-C	-5.71	1.44	1.53
1	K	38	SER	CA-C	-5.71	1.41	1.52
1	O	38	SER	CA-C	-5.71	1.41	1.52
2	B	248	LEU	CA-C	-5.70	1.44	1.53
2	H	248	LEU	CA-C	-5.70	1.44	1.53
1	O	37	PRO	N-CA	-5.70	1.41	1.47
1	A	38	SER	CA-C	-5.69	1.41	1.52
1	Q	38	SER	CA-C	-5.69	1.41	1.52
1	G	38	SER	CA-C	-5.68	1.41	1.52
1	Q	349	THR	N-CA	-5.68	1.38	1.46
2	D	110	GLU	CA-C	-5.67	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	242	LEU	CA-C	-5.67	1.45	1.52
1	E	37	PRO	N-CA	-5.67	1.41	1.47
1	I	37	PRO	N-CA	-5.66	1.41	1.47
2	H	242	LEU	CA-C	-5.66	1.45	1.52
2	N	110	GLU	CA-C	-5.65	1.45	1.52
1	Q	264	ARG	C-N	-5.65	1.24	1.33
2	L	242	LEU	CA-C	-5.65	1.45	1.52
2	F	110	GLU	CA-C	-5.64	1.45	1.52
2	P	110	GLU	CA-C	-5.64	1.45	1.52
1	C	37	PRO	N-CA	-5.64	1.41	1.47
2	F	242	LEU	CA-C	-5.64	1.45	1.52
1	G	37	PRO	N-CA	-5.64	1.41	1.47
2	J	242	LEU	CA-C	-5.64	1.45	1.52
1	C	264	ARG	C-N	-5.63	1.24	1.33
1	I	264	ARG	C-N	-5.63	1.24	1.33
2	R	242	LEU	CA-C	-5.63	1.45	1.52
2	N	242	LEU	CA-C	-5.62	1.45	1.52
1	A	264	ARG	C-N	-5.62	1.24	1.33
1	O	264	ARG	C-N	-5.61	1.24	1.33
1	K	37	PRO	N-CA	-5.61	1.41	1.47
1	E	349	THR	N-CA	-5.60	1.39	1.46
1	G	264	ARG	C-N	-5.60	1.24	1.33
1	E	264	ARG	C-N	-5.59	1.24	1.33
1	O	262	TYR	CA-C	-5.58	1.46	1.52
1	G	349	THR	N-CA	-5.58	1.39	1.46
1	Q	37	PRO	N-CA	-5.57	1.41	1.47
2	P	242	LEU	CA-C	-5.56	1.45	1.52
1	M	349	THR	N-CA	-5.56	1.39	1.46
2	L	110	GLU	CA-C	-5.55	1.45	1.52
1	A	349	THR	N-CA	-5.54	1.39	1.46
2	P	407	TRP	N-CA	-5.54	1.39	1.46
1	M	264	ARG	C-N	-5.53	1.24	1.33
1	A	37	PRO	N-CA	-5.53	1.41	1.47
2	N	407	TRP	N-CA	-5.52	1.39	1.46
1	I	349	THR	N-CA	-5.52	1.39	1.46
2	R	407	TRP	N-CA	-5.52	1.39	1.46
1	C	349	THR	N-CA	-5.51	1.39	1.46
1	K	349	THR	N-CA	-5.51	1.39	1.46
1	K	264	ARG	C-N	-5.51	1.24	1.33
2	J	280	SER	CA-C	-5.49	1.45	1.52
2	B	280	SER	CA-C	-5.48	1.45	1.52
1	O	349	THR	N-CA	-5.48	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	407	TRP	N-CA	-5.46	1.39	1.46
2	L	407	TRP	N-CA	-5.45	1.39	1.46
1	Q	262	TYR	CA-C	-5.44	1.46	1.52
2	J	407	TRP	N-CA	-5.44	1.39	1.46
2	D	407	TRP	N-CA	-5.43	1.39	1.46
1	A	262	TYR	CA-C	-5.43	1.46	1.52
2	D	280	SER	CA-C	-5.43	1.45	1.52
2	H	280	SER	CA-C	-5.43	1.45	1.52
2	L	280	SER	CA-C	-5.42	1.45	1.52
2	B	407	TRP	N-CA	-5.42	1.39	1.46
2	H	407	TRP	N-CA	-5.42	1.39	1.46
1	I	262	TYR	CA-C	-5.41	1.46	1.52
1	E	262	TYR	CA-C	-5.40	1.46	1.52
2	R	280	SER	CA-C	-5.40	1.45	1.52
2	D	181	VAL	CA-CB	-5.40	1.46	1.54
1	Q	49	PHE	N-CA	-5.38	1.36	1.46
2	N	280	SER	CA-C	-5.38	1.45	1.52
1	E	49	PHE	N-CA	-5.38	1.36	1.46
2	F	280	SER	CA-C	-5.37	1.45	1.52
1	M	36	MET	CA-C	-5.37	1.47	1.52
2	P	280	SER	CA-C	-5.37	1.45	1.52
1	K	262	TYR	CA-C	-5.35	1.46	1.52
1	K	49	PHE	N-CA	-5.35	1.36	1.46
2	N	37	HIS	CA-C	-5.35	1.46	1.53
1	I	36	MET	CA-C	-5.35	1.47	1.52
1	E	35	GLN	CA-C	-5.34	1.45	1.52
1	I	49	PHE	N-CA	-5.33	1.36	1.46
1	O	35	GLN	CA-C	-5.33	1.45	1.52
2	R	181	VAL	CA-CB	-5.33	1.46	1.54
1	E	60	LYS	CA-C	-5.33	1.46	1.52
2	P	181	VAL	CA-CB	-5.32	1.46	1.54
1	M	262	TYR	CA-C	-5.32	1.46	1.52
1	I	35	GLN	CA-C	-5.32	1.45	1.52
1	C	262	TYR	CA-C	-5.31	1.46	1.52
1	G	60	LYS	CA-C	-5.31	1.46	1.52
2	J	181	VAL	CA-CB	-5.31	1.47	1.54
2	N	181	VAL	CA-CB	-5.31	1.47	1.54
1	A	36	MET	CA-C	-5.31	1.47	1.52
1	M	49	PHE	N-CA	-5.31	1.36	1.46
1	C	36	MET	CA-C	-5.30	1.47	1.52
1	O	49	PHE	N-CA	-5.30	1.36	1.46
1	Q	36	MET	CA-C	-5.30	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	262	TYR	CA-C	-5.29	1.46	1.52
1	G	49	PHE	N-CA	-5.29	1.36	1.46
1	O	36	MET	CA-C	-5.29	1.47	1.52
1	O	60	LYS	CA-C	-5.29	1.46	1.52
2	R	37	HIS	CA-C	-5.29	1.46	1.53
2	L	181	VAL	CA-CB	-5.28	1.47	1.54
1	A	49	PHE	N-CA	-5.28	1.36	1.46
2	D	112	ALA	N-CA	-5.27	1.39	1.46
1	G	36	MET	CA-C	-5.27	1.47	1.52
1	Q	60	LYS	CA-C	-5.27	1.46	1.52
1	A	60	LYS	CA-C	-5.26	1.46	1.52
2	F	181	VAL	CA-CB	-5.26	1.47	1.54
2	F	112	ALA	N-CA	-5.26	1.39	1.46
1	K	36	MET	CA-C	-5.26	1.47	1.52
1	G	35	GLN	CA-C	-5.26	1.45	1.52
1	M	35	GLN	CA-C	-5.26	1.45	1.52
1	A	35	GLN	CA-C	-5.26	1.45	1.52
2	N	112	ALA	N-CA	-5.26	1.39	1.46
1	E	36	MET	CA-C	-5.26	1.47	1.52
2	F	37	HIS	CA-C	-5.25	1.46	1.53
2	H	181	VAL	CA-CB	-5.24	1.47	1.54
2	P	37	HIS	CA-C	-5.24	1.46	1.53
1	C	60	LYS	CA-C	-5.24	1.46	1.52
2	B	181	VAL	CA-CB	-5.23	1.47	1.54
2	J	112	ALA	N-CA	-5.23	1.39	1.46
1	M	60	LYS	CA-C	-5.23	1.46	1.52
1	K	35	GLN	CA-C	-5.23	1.45	1.52
1	C	49	PHE	N-CA	-5.22	1.36	1.46
1	I	60	LYS	CA-C	-5.22	1.46	1.52
2	H	112	ALA	N-CA	-5.22	1.39	1.46
2	L	112	ALA	N-CA	-5.22	1.39	1.46
2	R	112	ALA	N-CA	-5.22	1.39	1.46
2	J	37	HIS	CA-C	-5.21	1.46	1.53
2	H	37	HIS	CA-C	-5.21	1.46	1.53
2	D	37	HIS	CA-C	-5.21	1.46	1.53
1	C	35	GLN	CA-C	-5.19	1.45	1.52
2	L	37	HIS	CA-C	-5.18	1.46	1.53
2	P	112	ALA	N-CA	-5.18	1.39	1.46
1	Q	35	GLN	CA-C	-5.18	1.45	1.52
2	B	112	ALA	N-CA	-5.18	1.39	1.46
1	K	60	LYS	CA-C	-5.18	1.46	1.52
2	P	99	ALA	CA-C	-5.16	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	HIS	CA-C	-5.15	1.46	1.53
1	E	98	ASP	N-CA	-5.08	1.39	1.45
2	D	99	ALA	CA-C	-5.08	1.46	1.52
1	G	98	ASP	N-CA	-5.07	1.39	1.45
2	F	99	ALA	CA-C	-5.06	1.46	1.52
2	R	99	ALA	CA-C	-5.06	1.46	1.52
1	C	98	ASP	N-CA	-5.05	1.39	1.45
1	C	99	ALA	CA-C	-5.05	1.45	1.52
1	I	98	ASP	N-CA	-5.03	1.39	1.45
1	O	102	ASN	N-CA	-5.02	1.40	1.46
1	M	98	ASP	N-CA	-5.02	1.39	1.45
1	M	102	ASN	N-CA	-5.02	1.40	1.46
2	B	99	ALA	CA-C	-5.02	1.46	1.52
2	L	99	ALA	CA-C	-5.02	1.46	1.52
1	E	102	ASN	N-CA	-5.02	1.40	1.46
2	H	99	ALA	CA-C	-5.01	1.46	1.52
1	A	99	ALA	CA-C	-5.01	1.45	1.52
2	N	99	ALA	CA-C	-5.01	1.46	1.52
2	J	99	ALA	CA-C	-5.01	1.46	1.52
1	A	98	ASP	N-CA	-5.00	1.39	1.45

All (1592) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	264	ARG	CA-C-N	-18.86	101.46	121.45
1	G	264	ARG	C-N-CA	-18.86	101.46	121.45
1	E	264	ARG	CA-C-N	-18.84	101.48	121.45
1	E	264	ARG	C-N-CA	-18.84	101.48	121.45
1	O	264	ARG	CA-C-N	-18.81	101.51	121.45
1	O	264	ARG	C-N-CA	-18.81	101.51	121.45
1	K	264	ARG	CA-C-N	-18.80	101.52	121.45
1	K	264	ARG	C-N-CA	-18.80	101.52	121.45
1	C	264	ARG	CA-C-N	-18.79	101.53	121.45
1	C	264	ARG	C-N-CA	-18.79	101.53	121.45
1	M	264	ARG	CA-C-N	-18.79	101.53	121.45
1	M	264	ARG	C-N-CA	-18.79	101.53	121.45
1	Q	264	ARG	CA-C-N	-18.78	101.54	121.45
1	Q	264	ARG	C-N-CA	-18.78	101.54	121.45
1	A	264	ARG	CA-C-N	-18.77	101.55	121.45
1	A	264	ARG	C-N-CA	-18.77	101.55	121.45
1	I	264	ARG	CA-C-N	-18.74	101.58	121.45
1	I	264	ARG	C-N-CA	-18.74	101.58	121.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	96	GLN	CA-C-N	-13.35	102.44	122.47
2	L	96	GLN	C-N-CA	-13.35	102.44	122.47
2	J	96	GLN	CA-C-N	-13.34	102.45	122.47
2	J	96	GLN	C-N-CA	-13.34	102.45	122.47
2	N	96	GLN	CA-C-N	-13.34	102.46	122.47
2	N	96	GLN	C-N-CA	-13.34	102.46	122.47
2	H	96	GLN	CA-C-N	-13.31	102.51	122.47
2	H	96	GLN	C-N-CA	-13.31	102.51	122.47
2	D	96	GLN	CA-C-N	-13.30	102.52	122.47
2	D	96	GLN	C-N-CA	-13.30	102.52	122.47
2	P	96	GLN	CA-C-N	-13.29	102.54	122.47
2	P	96	GLN	C-N-CA	-13.29	102.54	122.47
2	B	96	GLN	CA-C-N	-13.27	102.57	122.47
2	B	96	GLN	C-N-CA	-13.27	102.57	122.47
2	R	96	GLN	CA-C-N	-13.27	102.57	122.47
2	R	96	GLN	C-N-CA	-13.27	102.57	122.47
2	F	96	GLN	CA-C-N	-13.26	102.58	122.47
2	F	96	GLN	C-N-CA	-13.26	102.58	122.47
2	B	101	ASN	CA-CB-CG	-11.54	101.06	112.60
2	J	101	ASN	CA-CB-CG	-11.54	101.06	112.60
2	D	101	ASN	CA-CB-CG	-11.53	101.07	112.60
2	P	101	ASN	CA-CB-CG	-11.52	101.08	112.60
2	L	101	ASN	CA-CB-CG	-11.52	101.08	112.60
2	N	101	ASN	CA-CB-CG	-11.51	101.09	112.60
2	R	101	ASN	CA-CB-CG	-11.50	101.10	112.60
2	F	101	ASN	CA-CB-CG	-11.49	101.11	112.60
2	H	101	ASN	CA-CB-CG	-11.43	101.17	112.60
1	O	142	GLY	CA-C-N	-10.80	109.09	121.83
1	O	142	GLY	C-N-CA	-10.80	109.09	121.83
1	Q	142	GLY	CA-C-N	-10.71	109.19	121.83
1	Q	142	GLY	C-N-CA	-10.71	109.19	121.83
1	I	142	GLY	CA-C-N	-10.71	109.20	121.83
1	I	142	GLY	C-N-CA	-10.71	109.20	121.83
1	K	142	GLY	CA-C-N	-10.70	109.21	121.83
1	K	142	GLY	C-N-CA	-10.70	109.21	121.83
1	C	142	GLY	CA-C-N	-10.69	109.21	121.83
1	C	142	GLY	C-N-CA	-10.69	109.21	121.83
1	A	142	GLY	CA-C-N	-10.65	109.26	121.83
1	A	142	GLY	C-N-CA	-10.65	109.26	121.83
1	E	142	GLY	CA-C-N	-10.64	109.27	121.83
1	E	142	GLY	C-N-CA	-10.64	109.27	121.83
1	G	142	GLY	CA-C-N	-10.64	109.27	121.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	142	GLY	C-N-CA	-10.64	109.27	121.83
1	M	142	GLY	CA-C-N	-10.64	109.27	121.83
1	M	142	GLY	C-N-CA	-10.64	109.27	121.83
1	C	11	GLN	CB-CA-C	-10.51	94.38	110.88
1	K	11	GLN	CB-CA-C	-10.44	94.49	110.88
1	O	11	GLN	CB-CA-C	-10.43	94.50	110.88
1	Q	11	GLN	CB-CA-C	-10.43	94.50	110.88
1	M	11	GLN	CB-CA-C	-10.43	94.51	110.88
1	E	11	GLN	CB-CA-C	-10.42	94.52	110.88
1	A	11	GLN	CB-CA-C	-10.41	94.53	110.88
1	I	11	GLN	CB-CA-C	-10.41	94.53	110.88
1	G	11	GLN	CB-CA-C	-10.40	94.54	110.88
1	E	244	PHE	CA-CB-CG	-10.31	103.49	113.80
1	Q	244	PHE	CA-CB-CG	-10.27	103.53	113.80
1	I	244	PHE	CA-CB-CG	-10.27	103.53	113.80
1	O	244	PHE	CA-CB-CG	-10.27	103.53	113.80
1	C	244	PHE	CA-CB-CG	-10.26	103.54	113.80
1	K	244	PHE	CA-CB-CG	-10.26	103.54	113.80
1	M	244	PHE	CA-CB-CG	-10.25	103.55	113.80
1	A	244	PHE	CA-CB-CG	-10.22	103.58	113.80
1	G	244	PHE	CA-CB-CG	-10.21	103.59	113.80
1	A	265	GLY	CA-C-N	-10.11	106.94	122.81
1	A	265	GLY	C-N-CA	-10.11	106.94	122.81
1	K	265	GLY	CA-C-N	-10.10	106.95	122.81
1	K	265	GLY	C-N-CA	-10.10	106.95	122.81
1	Q	265	GLY	CA-C-N	-10.10	106.96	122.81
1	Q	265	GLY	C-N-CA	-10.10	106.96	122.81
1	G	265	GLY	CA-C-N	-10.09	106.97	122.81
1	G	265	GLY	C-N-CA	-10.09	106.97	122.81
1	I	265	GLY	CA-C-N	-10.09	106.97	122.81
1	I	265	GLY	C-N-CA	-10.09	106.97	122.81
1	M	265	GLY	CA-C-N	-10.09	106.97	122.81
1	M	265	GLY	C-N-CA	-10.09	106.97	122.81
1	E	265	GLY	CA-C-N	-10.06	107.02	122.81
1	E	265	GLY	C-N-CA	-10.06	107.02	122.81
1	C	265	GLY	CA-C-N	-10.06	107.02	122.81
1	C	265	GLY	C-N-CA	-10.06	107.02	122.81
1	O	265	GLY	CA-C-N	-10.05	107.03	122.81
1	O	265	GLY	C-N-CA	-10.05	107.03	122.81
1	A	265	GLY	O-C-N	9.99	137.19	123.11
1	G	265	GLY	O-C-N	9.98	137.19	123.11
1	K	265	GLY	O-C-N	9.97	137.17	123.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	265	GLY	O-C-N	9.97	137.16	123.11
1	Q	265	GLY	O-C-N	9.96	137.16	123.11
1	M	265	GLY	O-C-N	9.96	137.15	123.11
1	C	265	GLY	O-C-N	9.93	137.11	123.11
1	E	265	GLY	O-C-N	9.92	137.09	123.11
1	O	265	GLY	O-C-N	9.91	137.09	123.11
1	I	73	THR	N-CA-C	9.79	122.85	111.11
1	M	73	THR	N-CA-C	9.76	122.83	111.11
1	A	73	THR	N-CA-C	9.72	122.78	111.11
1	O	73	THR	N-CA-C	9.71	122.77	111.11
1	Q	73	THR	N-CA-C	9.69	122.73	111.11
1	K	73	THR	N-CA-C	9.69	122.73	111.11
1	C	73	THR	N-CA-C	9.68	122.72	111.11
1	G	73	THR	N-CA-C	9.67	122.71	111.11
1	E	73	THR	N-CA-C	9.66	122.71	111.11
2	H	378	ILE	CA-C-N	-9.39	114.38	121.61
2	H	378	ILE	C-N-CA	-9.39	114.38	121.61
2	D	378	ILE	CA-C-N	-9.36	114.40	121.61
2	D	378	ILE	C-N-CA	-9.36	114.40	121.61
2	P	378	ILE	CA-C-N	-9.32	114.43	121.61
2	P	378	ILE	C-N-CA	-9.32	114.43	121.61
2	F	378	ILE	CA-C-N	-9.26	114.48	121.61
2	F	378	ILE	C-N-CA	-9.26	114.48	121.61
2	B	378	ILE	CA-C-N	-9.24	114.49	121.61
2	B	378	ILE	C-N-CA	-9.24	114.49	121.61
2	L	378	ILE	CA-C-N	-9.24	114.50	121.61
2	L	378	ILE	C-N-CA	-9.24	114.50	121.61
2	N	378	ILE	CA-C-N	-9.24	114.50	121.61
2	N	378	ILE	C-N-CA	-9.24	114.50	121.61
2	R	378	ILE	CA-C-N	-9.21	114.52	121.61
2	R	378	ILE	C-N-CA	-9.21	114.52	121.61
2	F	101	ASN	CB-CG-ND2	9.17	130.15	116.40
2	H	101	ASN	CB-CG-ND2	9.16	130.13	116.40
2	J	378	ILE	CA-C-N	-9.15	114.56	121.61
2	J	378	ILE	C-N-CA	-9.15	114.56	121.61
2	P	101	ASN	CB-CG-ND2	9.14	130.12	116.40
2	D	101	ASN	CB-CG-ND2	9.13	130.09	116.40
2	J	101	ASN	CB-CG-ND2	9.12	130.09	116.40
2	R	101	ASN	CB-CG-ND2	9.12	130.08	116.40
2	L	101	ASN	CB-CG-ND2	9.11	130.07	116.40
2	N	101	ASN	CB-CG-ND2	9.10	130.05	116.40
2	B	101	ASN	CB-CG-ND2	9.09	130.03	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	98	ASP	N-CA-C	9.03	123.88	110.52
1	G	98	ASP	N-CA-C	9.02	123.86	110.52
1	O	98	ASP	N-CA-C	9.01	123.86	110.52
1	I	98	ASP	N-CA-C	9.01	123.86	110.52
1	Q	98	ASP	N-CA-C	9.01	123.85	110.52
1	C	98	ASP	N-CA-C	9.00	123.84	110.52
2	H	48	ARG	NE-CZ-NH1	9.00	130.50	121.50
1	M	98	ASP	N-CA-C	8.99	123.83	110.52
1	A	98	ASP	N-CA-C	8.99	123.82	110.52
1	K	98	ASP	N-CA-C	8.98	123.82	110.52
2	R	48	ARG	NE-CZ-NH1	8.98	130.48	121.50
2	P	48	ARG	NE-CZ-NH1	8.96	130.46	121.50
2	B	48	ARG	NE-CZ-NH1	8.94	130.44	121.50
2	D	48	ARG	NE-CZ-NH1	8.89	130.39	121.50
2	N	48	ARG	NE-CZ-NH1	8.89	130.39	121.50
2	F	48	ARG	NE-CZ-NH1	8.89	130.39	121.50
2	J	48	ARG	NE-CZ-NH1	8.88	130.38	121.50
2	L	48	ARG	NE-CZ-NH1	8.87	130.37	121.50
1	M	228	ASN	CA-CB-CG	-8.77	103.83	112.60
1	O	228	ASN	CA-CB-CG	-8.70	103.90	112.60
1	A	228	ASN	CA-CB-CG	-8.69	103.91	112.60
1	C	228	ASN	CA-CB-CG	-8.69	103.91	112.60
1	I	228	ASN	CA-CB-CG	-8.69	103.92	112.60
1	G	228	ASN	CA-CB-CG	-8.68	103.92	112.60
2	L	96	GLN	N-CA-C	8.63	124.50	113.88
1	E	228	ASN	CA-CB-CG	-8.63	103.97	112.60
2	J	96	GLN	N-CA-C	8.63	124.49	113.88
1	Q	228	ASN	CA-CB-CG	-8.62	103.98	112.60
2	F	96	GLN	N-CA-C	8.61	124.47	113.88
1	K	228	ASN	CA-CB-CG	-8.60	104.00	112.60
2	H	400	ARG	NE-CZ-NH2	8.60	126.94	119.20
1	K	347	CYS	N-CA-C	8.59	125.00	108.85
1	O	347	CYS	N-CA-C	8.59	125.00	108.85
1	I	347	CYS	N-CA-C	8.58	124.98	108.85
1	C	347	CYS	N-CA-C	8.58	124.97	108.85
1	E	347	CYS	N-CA-C	8.58	124.97	108.85
2	N	96	GLN	N-CA-C	8.56	124.41	113.88
1	G	347	CYS	N-CA-C	8.56	124.94	108.85
1	Q	347	CYS	N-CA-C	8.56	124.94	108.85
1	A	347	CYS	N-CA-C	8.56	124.94	108.85
2	L	400	ARG	NE-CZ-NH2	8.55	126.90	119.20
1	M	347	CYS	N-CA-C	8.55	124.92	108.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	ARG	NE-CZ-NH2	8.54	126.88	119.20
2	R	400	ARG	NE-CZ-NH2	8.51	126.86	119.20
2	P	400	ARG	NE-CZ-NH2	8.49	126.84	119.20
2	F	400	ARG	NE-CZ-NH2	8.48	126.84	119.20
2	J	400	ARG	NE-CZ-NH2	8.48	126.83	119.20
2	N	400	ARG	NE-CZ-NH2	8.46	126.82	119.20
1	E	438	ASP	CA-C-N	-8.41	106.56	121.70
1	E	438	ASP	C-N-CA	-8.41	106.56	121.70
2	D	400	ARG	NE-CZ-NH2	8.41	126.77	119.20
1	O	438	ASP	CA-C-N	-8.41	106.57	121.70
1	O	438	ASP	C-N-CA	-8.41	106.57	121.70
1	G	438	ASP	CA-C-N	-8.39	106.60	121.70
1	G	438	ASP	C-N-CA	-8.39	106.60	121.70
1	M	438	ASP	CA-C-N	-8.39	106.60	121.70
1	M	438	ASP	C-N-CA	-8.39	106.60	121.70
2	F	308	ARG	NE-CZ-NH2	-8.38	111.66	119.20
1	Q	438	ASP	CA-C-N	-8.37	106.63	121.70
1	Q	438	ASP	C-N-CA	-8.37	106.63	121.70
2	L	308	ARG	NE-CZ-NH2	-8.37	111.67	119.20
1	C	438	ASP	CA-C-N	-8.36	106.65	121.70
1	C	438	ASP	C-N-CA	-8.36	106.65	121.70
1	K	438	ASP	CA-C-N	-8.34	106.69	121.70
1	K	438	ASP	C-N-CA	-8.34	106.69	121.70
1	I	438	ASP	CA-C-N	-8.34	106.69	121.70
1	I	438	ASP	C-N-CA	-8.34	106.69	121.70
1	A	438	ASP	CA-C-N	-8.34	106.70	121.70
1	A	438	ASP	C-N-CA	-8.34	106.70	121.70
2	J	308	ARG	NE-CZ-NH2	-8.33	111.70	119.20
2	P	308	ARG	NE-CZ-NH2	-8.30	111.73	119.20
2	B	308	ARG	NE-CZ-NH2	-8.29	111.74	119.20
2	R	308	ARG	NE-CZ-NH2	-8.28	111.75	119.20
2	D	308	ARG	NE-CZ-NH2	-8.28	111.75	119.20
1	C	266	HIS	CA-CB-CG	-8.26	105.54	113.80
1	A	266	HIS	CA-CB-CG	-8.25	105.55	113.80
1	O	266	HIS	CA-CB-CG	-8.25	105.55	113.80
2	H	308	ARG	NE-CZ-NH2	-8.24	111.79	119.20
1	I	266	HIS	CA-CB-CG	-8.24	105.56	113.80
1	G	266	HIS	CA-CB-CG	-8.23	105.57	113.80
2	R	96	GLN	N-CA-C	8.23	124.51	113.97
2	N	308	ARG	NE-CZ-NH2	-8.23	111.79	119.20
2	B	96	GLN	N-CA-C	8.23	124.50	113.97
2	D	96	GLN	N-CA-C	8.22	124.50	113.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	266	HIS	CA-CB-CG	-8.22	105.58	113.80
1	M	266	HIS	CA-CB-CG	-8.22	105.58	113.80
1	E	266	HIS	CA-CB-CG	-8.21	105.59	113.80
2	H	96	GLN	N-CA-C	8.19	124.45	113.97
2	P	96	GLN	N-CA-C	8.17	124.43	113.97
1	Q	266	HIS	CA-CB-CG	-8.15	105.65	113.80
1	K	190	THR	CB-CA-C	-8.11	95.10	110.67
1	M	190	THR	CB-CA-C	-8.09	95.13	110.67
1	O	190	THR	CB-CA-C	-8.08	95.15	110.67
1	Q	190	THR	CB-CA-C	-8.07	95.18	110.67
1	C	190	THR	CB-CA-C	-8.06	95.19	110.67
1	A	190	THR	CB-CA-C	-8.06	95.20	110.67
1	I	190	THR	CB-CA-C	-8.06	95.20	110.67
1	E	190	THR	CB-CA-C	-8.05	95.20	110.67
1	G	190	THR	CB-CA-C	-8.04	95.23	110.67
1	O	11	GLN	N-CA-CB	8.00	121.61	110.01
1	I	11	GLN	N-CA-CB	7.99	121.60	110.01
1	C	11	GLN	N-CA-CB	7.99	121.59	110.01
1	A	11	GLN	N-CA-CB	7.96	121.56	110.01
1	M	11	GLN	N-CA-CB	7.95	121.54	110.01
1	G	11	GLN	N-CA-CB	7.94	121.53	110.01
1	E	11	GLN	N-CA-CB	7.94	121.53	110.01
1	A	176	GLN	CA-C-N	-7.94	112.54	123.10
1	A	176	GLN	C-N-CA	-7.94	112.54	123.10
1	K	11	GLN	N-CA-CB	7.94	121.53	110.01
1	Q	11	GLN	N-CA-CB	7.93	121.51	110.01
1	G	176	GLN	CA-C-N	-7.92	112.56	123.10
1	G	176	GLN	C-N-CA	-7.92	112.56	123.10
1	C	176	GLN	CA-C-N	-7.91	112.59	123.10
1	C	176	GLN	C-N-CA	-7.91	112.59	123.10
1	K	176	GLN	CA-C-N	-7.90	112.59	123.10
1	K	176	GLN	C-N-CA	-7.90	112.59	123.10
1	M	176	GLN	CA-C-N	-7.90	112.60	123.10
1	M	176	GLN	C-N-CA	-7.90	112.60	123.10
1	E	176	GLN	CA-C-N	-7.89	112.60	123.10
1	E	176	GLN	C-N-CA	-7.89	112.60	123.10
1	I	176	GLN	CA-C-N	-7.88	112.62	123.10
1	I	176	GLN	C-N-CA	-7.88	112.62	123.10
1	O	176	GLN	CA-C-N	-7.87	112.63	123.10
1	O	176	GLN	C-N-CA	-7.87	112.63	123.10
1	Q	176	GLN	CA-C-N	-7.85	112.66	123.10
1	Q	176	GLN	C-N-CA	-7.85	112.66	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	76	ASP	CA-CB-CG	7.79	120.39	112.60
1	G	438	ASP	O-C-N	7.79	132.05	122.86
2	L	222	PRO	N-CA-C	7.79	123.60	111.21
2	B	222	PRO	N-CA-C	7.79	123.59	111.21
2	P	76	ASP	CA-CB-CG	7.78	120.38	112.60
2	F	76	ASP	CA-CB-CG	7.77	120.37	112.60
2	P	222	PRO	N-CA-C	7.77	123.56	111.21
2	F	222	PRO	N-CA-C	7.76	123.55	111.21
2	D	222	PRO	N-CA-C	7.76	123.55	111.21
1	Q	438	ASP	O-C-N	7.76	132.02	122.86
2	J	76	ASP	CA-CB-CG	7.75	120.35	112.60
2	R	76	ASP	CA-CB-CG	7.75	120.35	112.60
2	R	222	PRO	N-CA-C	7.74	123.52	111.21
1	E	438	ASP	O-C-N	7.74	132.00	122.86
2	D	76	ASP	CA-CB-CG	7.74	120.33	112.60
2	H	76	ASP	CA-CB-CG	7.73	120.33	112.60
2	J	222	PRO	N-CA-C	7.73	123.50	111.21
2	N	222	PRO	N-CA-C	7.73	123.50	111.21
2	H	222	PRO	N-CA-C	7.71	123.47	111.21
1	C	438	ASP	O-C-N	7.71	131.96	122.86
1	O	438	ASP	O-C-N	7.70	131.94	122.86
1	I	438	ASP	O-C-N	7.70	131.94	122.86
2	B	76	ASP	CA-CB-CG	7.69	120.29	112.60
2	F	139	HIS	N-CA-C	7.69	119.82	108.60
1	K	438	ASP	O-C-N	7.69	131.93	122.86
1	M	438	ASP	O-C-N	7.68	131.92	122.86
2	N	76	ASP	CA-CB-CG	7.68	120.28	112.60
2	N	139	HIS	N-CA-C	7.68	119.81	108.60
2	R	2	ARG	NE-CZ-NH1	7.67	129.17	121.50
2	J	139	HIS	N-CA-C	7.66	119.79	108.60
2	N	2	ARG	NE-CZ-NH1	7.66	129.16	121.50
2	P	139	HIS	N-CA-C	7.66	119.79	108.60
2	H	2	ARG	NE-CZ-NH1	7.66	129.16	121.50
2	R	139	HIS	N-CA-C	7.65	119.77	108.60
1	M	49	PHE	CA-CB-CG	7.65	121.45	113.80
1	A	438	ASP	O-C-N	7.65	131.88	122.86
2	D	139	HIS	N-CA-C	7.65	119.76	108.60
2	L	139	HIS	N-CA-C	7.64	119.75	108.60
2	F	2	ARG	NE-CZ-NH1	7.63	129.13	121.50
2	B	139	HIS	N-CA-C	7.63	119.74	108.60
2	P	2	ARG	NE-CZ-NH1	7.62	129.12	121.50
2	J	2	ARG	NE-CZ-NH1	7.61	129.11	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	139	HIS	N-CA-C	7.61	119.71	108.60
1	E	49	PHE	CA-CB-CG	7.61	121.41	113.80
1	G	49	PHE	CA-CB-CG	7.61	121.41	113.80
2	D	2	ARG	NE-CZ-NH1	7.61	129.11	121.50
1	I	49	PHE	CA-CB-CG	7.60	121.40	113.80
2	L	2	ARG	NE-CZ-NH1	7.60	129.10	121.50
2	B	2	ARG	NE-CZ-NH1	7.59	129.09	121.50
1	O	49	PHE	CA-CB-CG	7.59	121.39	113.80
1	A	49	PHE	CA-CB-CG	7.58	121.38	113.80
1	Q	49	PHE	CA-CB-CG	7.58	121.38	113.80
2	F	33	THR	CA-C-N	-7.57	114.60	123.08
2	F	33	THR	C-N-CA	-7.57	114.60	123.08
1	C	49	PHE	CA-CB-CG	7.56	121.36	113.80
1	K	120	ASP	CA-CB-CG	-7.55	105.05	112.60
2	B	33	THR	CA-C-N	-7.55	114.62	123.08
2	B	33	THR	C-N-CA	-7.55	114.62	123.08
1	O	347	CYS	CA-C-N	-7.55	112.91	120.31
1	O	347	CYS	C-N-CA	-7.55	112.91	120.31
1	I	120	ASP	CA-CB-CG	-7.54	105.06	112.60
1	K	49	PHE	CA-CB-CG	7.54	121.34	113.80
2	J	33	THR	CA-C-N	-7.53	114.64	123.08
2	J	33	THR	C-N-CA	-7.53	114.64	123.08
1	G	120	ASP	CA-CB-CG	-7.53	105.07	112.60
1	M	347	CYS	CA-C-N	-7.53	112.93	120.31
1	M	347	CYS	C-N-CA	-7.53	112.93	120.31
2	P	33	THR	CA-C-N	-7.53	114.65	123.08
2	P	33	THR	C-N-CA	-7.53	114.65	123.08
1	O	120	ASP	CA-CB-CG	-7.53	105.07	112.60
1	Q	347	CYS	CA-C-N	-7.52	112.94	120.31
1	Q	347	CYS	C-N-CA	-7.52	112.94	120.31
2	H	33	THR	CA-C-N	-7.52	114.66	123.08
2	H	33	THR	C-N-CA	-7.52	114.66	123.08
1	Q	120	ASP	CA-CB-CG	-7.52	105.08	112.60
1	E	120	ASP	CA-CB-CG	-7.51	105.09	112.60
2	N	33	THR	CA-C-N	-7.51	114.67	123.08
2	N	33	THR	C-N-CA	-7.51	114.67	123.08
1	C	120	ASP	CA-CB-CG	-7.50	105.10	112.60
1	I	347	CYS	CA-C-N	-7.50	112.96	120.31
1	I	347	CYS	C-N-CA	-7.50	112.96	120.31
2	L	33	THR	CA-C-N	-7.50	114.69	123.08
2	L	33	THR	C-N-CA	-7.50	114.69	123.08
2	R	33	THR	CA-C-N	-7.49	114.69	123.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	33	THR	C-N-CA	-7.49	114.69	123.08
1	K	347	CYS	CA-C-N	-7.49	112.97	120.31
1	K	347	CYS	C-N-CA	-7.49	112.97	120.31
2	D	33	THR	CA-C-N	-7.49	114.70	123.08
2	D	33	THR	C-N-CA	-7.49	114.70	123.08
2	H	185	TYR	CB-CA-C	-7.47	98.15	110.85
1	M	120	ASP	CA-CB-CG	-7.47	105.13	112.60
2	L	185	TYR	CB-CA-C	-7.46	98.16	110.85
2	J	185	TYR	CB-CA-C	-7.46	98.16	110.85
1	A	347	CYS	CA-C-N	-7.46	113.00	120.31
1	A	347	CYS	C-N-CA	-7.46	113.00	120.31
1	A	120	ASP	CA-CB-CG	-7.46	105.14	112.60
1	G	347	CYS	CA-C-N	-7.45	113.00	120.31
1	G	347	CYS	C-N-CA	-7.45	113.00	120.31
2	R	185	TYR	CB-CA-C	-7.45	98.18	110.85
2	D	185	TYR	CB-CA-C	-7.45	98.19	110.85
2	F	185	TYR	CB-CA-C	-7.45	98.19	110.85
1	A	50	ASN	CA-CB-CG	-7.44	105.16	112.60
2	B	185	TYR	CB-CA-C	-7.44	98.21	110.85
1	G	50	ASN	CA-CB-CG	-7.43	105.17	112.60
2	P	101	ASN	CB-CG-OD1	-7.43	105.94	120.80
2	P	185	TYR	CB-CA-C	-7.43	98.22	110.85
2	P	177	VAL	N-CA-C	7.42	117.00	106.53
1	E	347	CYS	CA-C-N	-7.42	113.04	120.31
1	E	347	CYS	C-N-CA	-7.42	113.04	120.31
2	D	177	VAL	N-CA-C	7.42	116.99	106.53
2	L	101	ASN	CB-CG-OD1	-7.42	105.97	120.80
2	N	185	TYR	CB-CA-C	-7.42	98.24	110.85
2	J	101	ASN	CB-CG-OD1	-7.41	105.97	120.80
1	O	50	ASN	CA-CB-CG	-7.41	105.19	112.60
2	D	88	ARG	NE-CZ-NH1	7.41	128.91	121.50
2	L	177	VAL	N-CA-C	7.40	116.97	106.53
2	N	101	ASN	CB-CG-OD1	-7.40	106.00	120.80
1	E	50	ASN	CA-CB-CG	-7.40	105.20	112.60
2	F	177	VAL	N-CA-C	7.40	116.96	106.53
2	H	101	ASN	CB-CG-OD1	-7.40	106.00	120.80
1	I	50	ASN	CA-CB-CG	-7.40	105.20	112.60
2	R	177	VAL	N-CA-C	7.40	116.96	106.53
2	F	101	ASN	CB-CG-OD1	-7.39	106.01	120.80
2	B	101	ASN	CB-CG-OD1	-7.39	106.02	120.80
1	C	347	CYS	CA-C-N	-7.39	113.06	120.31
1	C	347	CYS	C-N-CA	-7.39	113.06	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	88	ARG	NE-CZ-NH1	7.39	128.89	121.50
1	M	50	ASN	CA-CB-CG	-7.39	105.21	112.60
2	R	101	ASN	CB-CG-OD1	-7.39	106.02	120.80
2	H	177	VAL	N-CA-C	7.39	116.95	106.53
1	Q	50	ASN	CA-CB-CG	-7.38	105.22	112.60
2	D	101	ASN	CB-CG-OD1	-7.38	106.04	120.80
2	N	177	VAL	N-CA-C	7.38	116.93	106.53
2	J	177	VAL	N-CA-C	7.37	116.93	106.53
1	K	50	ASN	CA-CB-CG	-7.37	105.23	112.60
2	B	177	VAL	N-CA-C	7.37	116.92	106.53
1	C	50	ASN	CA-CB-CG	-7.36	105.24	112.60
2	N	88	ARG	NE-CZ-NH1	7.35	128.85	121.50
2	B	88	ARG	NE-CZ-NH1	7.34	128.84	121.50
1	Q	346	TRP	N-CA-C	7.34	121.33	112.38
2	P	88	ARG	NE-CZ-NH1	7.31	128.81	121.50
1	G	346	TRP	N-CA-C	7.30	121.28	112.38
2	H	88	ARG	NE-CZ-NH1	7.29	128.79	121.50
1	O	346	TRP	N-CA-C	7.29	121.27	112.38
2	R	88	ARG	NE-CZ-NH1	7.28	128.78	121.50
1	I	346	TRP	N-CA-C	7.28	121.26	112.38
2	F	88	ARG	NE-CZ-NH1	7.27	128.77	121.50
1	E	346	TRP	N-CA-C	7.26	121.23	112.38
1	A	346	TRP	N-CA-C	7.25	121.22	112.38
1	C	346	TRP	N-CA-C	7.25	121.22	112.38
1	K	346	TRP	N-CA-C	7.24	121.21	112.38
2	J	88	ARG	NE-CZ-NH1	7.24	128.74	121.50
1	M	346	TRP	N-CA-C	7.23	121.20	112.38
1	I	28	HIS	CA-CB-CG	-7.18	106.62	113.80
2	H	196	GLU	CB-CG-CD	7.16	124.78	112.60
2	J	196	GLU	CB-CG-CD	7.16	124.78	112.60
2	B	196	GLU	CB-CG-CD	7.16	124.77	112.60
2	P	196	GLU	CB-CG-CD	7.15	124.75	112.60
2	D	196	GLU	CB-CG-CD	7.14	124.73	112.60
2	R	196	GLU	CB-CG-CD	7.13	124.72	112.60
2	N	196	GLU	CB-CG-CD	7.12	124.71	112.60
1	C	28	HIS	CA-CB-CG	-7.12	106.69	113.80
2	L	196	GLU	CB-CG-CD	7.11	124.69	112.60
1	A	28	HIS	CA-CB-CG	-7.11	106.69	113.80
1	O	28	HIS	CA-CB-CG	-7.11	106.69	113.80
1	Q	28	HIS	CA-CB-CG	-7.10	106.70	113.80
2	F	196	GLU	CB-CG-CD	7.10	124.66	112.60
1	G	28	HIS	CA-CB-CG	-7.05	106.75	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	28	HIS	CA-CB-CG	-7.04	106.76	113.80
1	E	28	HIS	CA-CB-CG	-7.03	106.77	113.80
1	K	28	HIS	CA-CB-CG	-7.03	106.77	113.80
2	R	251	ASP	CA-CB-CG	-7.02	105.58	112.60
2	L	251	ASP	CA-CB-CG	-6.99	105.61	112.60
2	P	251	ASP	CA-CB-CG	-6.99	105.61	112.60
2	F	251	ASP	CA-CB-CG	-6.98	105.62	112.60
1	Q	36	MET	CG-SD-CE	6.98	116.25	100.90
2	J	251	ASP	CA-CB-CG	-6.97	105.63	112.60
2	N	251	ASP	CA-CB-CG	-6.96	105.64	112.60
1	A	36	MET	CG-SD-CE	6.96	116.20	100.90
1	M	36	MET	CG-SD-CE	6.95	116.19	100.90
2	D	251	ASP	CA-CB-CG	-6.95	105.65	112.60
1	C	36	MET	CG-SD-CE	6.95	116.18	100.90
1	E	36	MET	CG-SD-CE	6.94	116.17	100.90
1	I	36	MET	CG-SD-CE	6.94	116.17	100.90
1	G	36	MET	CG-SD-CE	6.93	116.15	100.90
1	K	36	MET	CG-SD-CE	6.93	116.15	100.90
2	B	251	ASP	CA-CB-CG	-6.92	105.68	112.60
1	O	36	MET	CG-SD-CE	6.92	116.12	100.90
2	H	251	ASP	CA-CB-CG	-6.91	105.69	112.60
2	R	110	GLU	N-CA-C	6.86	120.12	111.69
2	P	110	GLU	N-CA-C	6.84	120.11	111.69
2	D	110	GLU	N-CA-C	6.83	120.09	111.69
2	B	110	GLU	N-CA-C	6.82	120.08	111.69
2	F	110	GLU	N-CA-C	6.82	120.08	111.69
2	N	110	GLU	N-CA-C	6.81	120.06	111.69
2	N	266	HIS	CA-CB-CG	-6.81	106.99	113.80
2	L	110	GLU	N-CA-C	6.80	120.06	111.69
2	R	48	ARG	NE-CZ-NH2	-6.80	113.08	119.20
2	D	427	ASP	CA-CB-CG	-6.77	105.83	112.60
2	J	110	GLU	N-CA-C	6.77	120.02	111.69
2	L	194	LEU	N-CA-C	6.77	118.45	111.14
2	J	427	ASP	CA-CB-CG	-6.77	105.83	112.60
2	L	266	HIS	CA-CB-CG	-6.76	107.04	113.80
2	B	48	ARG	NE-CZ-NH2	-6.76	113.12	119.20
2	H	110	GLU	N-CA-C	6.76	120.00	111.69
2	R	427	ASP	CA-CB-CG	-6.75	105.85	112.60
2	H	266	HIS	CA-CB-CG	-6.75	107.05	113.80
2	H	194	LEU	N-CA-C	6.75	118.43	111.14
2	R	266	HIS	CA-CB-CG	-6.74	107.06	113.80
2	B	194	LEU	N-CA-C	6.74	118.42	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	194	LEU	N-CA-C	6.73	118.41	111.14
2	F	427	ASP	CA-CB-CG	-6.73	105.87	112.60
2	F	266	HIS	CA-CB-CG	-6.73	107.07	113.80
2	D	266	HIS	CA-CB-CG	-6.72	107.08	113.80
2	P	427	ASP	CA-CB-CG	-6.72	105.88	112.60
2	D	48	ARG	NE-CZ-NH2	-6.72	113.15	119.20
2	P	266	HIS	CA-CB-CG	-6.72	107.08	113.80
2	F	48	ARG	NE-CZ-NH2	-6.72	113.15	119.20
2	B	427	ASP	CA-CB-CG	-6.71	105.89	112.60
2	N	194	LEU	N-CA-C	6.71	118.38	111.14
2	P	176	LYS	CA-C-N	-6.71	114.82	122.93
2	P	176	LYS	C-N-CA	-6.71	114.82	122.93
2	H	48	ARG	NE-CZ-NH2	-6.70	113.17	119.20
2	R	194	LEU	N-CA-C	6.70	118.38	111.14
2	N	427	ASP	CA-CB-CG	-6.70	105.90	112.60
2	N	176	LYS	CA-C-N	-6.70	114.83	122.93
2	N	176	LYS	C-N-CA	-6.70	114.83	122.93
2	B	266	HIS	CA-CB-CG	-6.69	107.11	113.80
2	P	48	ARG	NE-CZ-NH2	-6.69	113.18	119.20
2	P	194	LEU	N-CA-C	6.69	118.37	111.14
2	J	48	ARG	NE-CZ-NH2	-6.69	113.18	119.20
2	L	48	ARG	NE-CZ-NH2	-6.69	113.18	119.20
2	L	427	ASP	CA-CB-CG	-6.69	105.91	112.60
2	B	176	LYS	CA-C-N	-6.67	114.86	122.93
2	B	176	LYS	C-N-CA	-6.67	114.86	122.93
2	H	427	ASP	CA-CB-CG	-6.67	105.93	112.60
2	N	48	ARG	NE-CZ-NH2	-6.67	113.20	119.20
2	H	176	LYS	CA-C-N	-6.66	114.87	122.93
2	H	176	LYS	C-N-CA	-6.66	114.87	122.93
2	J	266	HIS	CA-CB-CG	-6.64	107.16	113.80
2	J	176	LYS	CA-C-N	-6.63	114.91	122.93
2	J	176	LYS	C-N-CA	-6.63	114.91	122.93
2	D	194	LEU	N-CA-C	6.63	118.30	111.14
2	L	176	LYS	CA-C-N	-6.63	114.91	122.93
2	L	176	LYS	C-N-CA	-6.63	114.91	122.93
2	F	176	LYS	CA-C-N	-6.62	114.92	122.93
2	F	176	LYS	C-N-CA	-6.62	114.92	122.93
2	D	176	LYS	CA-C-N	-6.61	114.93	122.93
2	D	176	LYS	C-N-CA	-6.61	114.93	122.93
2	R	176	LYS	CA-C-N	-6.61	114.93	122.93
2	R	176	LYS	C-N-CA	-6.61	114.93	122.93
2	H	14	ASN	CA-CB-CG	-6.60	106.00	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	194	LEU	N-CA-C	6.60	118.27	111.14
2	B	14	ASN	CA-CB-CG	-6.59	106.01	112.60
2	R	14	ASN	CA-CB-CG	-6.57	106.03	112.60
2	F	14	ASN	CA-CB-CG	-6.57	106.03	112.60
2	J	179	ASP	CA-CB-CG	6.56	119.16	112.60
2	N	14	ASN	CA-CB-CG	-6.55	106.05	112.60
2	P	14	ASN	CA-CB-CG	-6.55	106.05	112.60
2	P	179	ASP	CA-CB-CG	6.54	119.14	112.60
2	N	179	ASP	CA-CB-CG	6.54	119.14	112.60
2	L	14	ASN	CA-CB-CG	-6.54	106.06	112.60
2	L	401	ARG	NE-CZ-NH2	6.52	125.07	119.20
2	J	14	ASN	CA-CB-CG	-6.51	106.08	112.60
2	H	401	ARG	NE-CZ-NH2	6.51	125.06	119.20
2	B	179	ASP	CA-CB-CG	6.51	119.11	112.60
2	L	179	ASP	CA-CB-CG	6.51	119.11	112.60
2	R	179	ASP	CA-CB-CG	6.51	119.11	112.60
2	F	401	ARG	NE-CZ-NH2	6.50	125.05	119.20
2	R	401	ARG	NE-CZ-NH2	6.49	125.04	119.20
2	N	401	ARG	NE-CZ-NH2	6.47	125.03	119.20
2	P	401	ARG	NE-CZ-NH2	6.46	125.01	119.20
2	D	179	ASP	CA-CB-CG	6.45	119.05	112.60
2	F	179	ASP	CA-CB-CG	6.45	119.05	112.60
2	D	14	ASN	CA-CB-CG	-6.45	106.15	112.60
2	D	401	ARG	NE-CZ-NH2	6.45	125.00	119.20
2	J	401	ARG	NE-CZ-NH2	6.45	125.00	119.20
2	H	179	ASP	CA-CB-CG	6.42	119.02	112.60
2	H	88	ARG	NE-CZ-NH2	-6.42	113.43	119.20
2	L	88	ARG	NE-CZ-NH2	-6.41	113.43	119.20
2	B	88	ARG	NE-CZ-NH2	-6.40	113.44	119.20
2	R	34	GLY	N-CA-C	6.39	122.09	114.48
2	B	401	ARG	NE-CZ-NH2	6.38	124.94	119.20
2	N	88	ARG	NE-CZ-NH2	-6.36	113.48	119.20
2	F	88	ARG	NE-CZ-NH2	-6.35	113.48	119.20
2	N	240	THR	N-CA-C	6.35	120.29	112.54
1	C	353	VAL	CA-C-N	-6.35	116.83	122.73
1	C	353	VAL	C-N-CA	-6.35	116.83	122.73
2	L	34	GLY	N-CA-C	6.35	122.03	114.48
1	O	353	VAL	CA-C-N	-6.34	116.83	122.73
1	O	353	VAL	C-N-CA	-6.34	116.83	122.73
2	H	34	GLY	N-CA-C	6.34	122.03	114.48
2	R	240	THR	N-CA-C	6.34	120.27	112.54
2	L	240	THR	N-CA-C	6.33	120.26	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	88	ARG	NE-CZ-NH2	-6.32	113.51	119.20
2	P	34	GLY	N-CA-C	6.32	122.00	114.48
2	J	34	GLY	N-CA-C	6.32	121.99	114.48
2	J	240	THR	N-CA-C	6.32	120.24	112.54
1	M	105	ARG	NE-CZ-NH2	-6.32	113.52	119.20
2	B	34	GLY	N-CA-C	6.31	121.99	114.48
2	D	240	THR	N-CA-C	6.30	120.22	112.54
2	B	240	THR	N-CA-C	6.30	120.22	112.54
1	A	353	VAL	CA-C-N	-6.29	116.88	122.73
1	A	353	VAL	C-N-CA	-6.29	116.88	122.73
2	D	88	ARG	NE-CZ-NH2	-6.29	113.54	119.20
1	C	261	PRO	CA-C-N	-6.29	114.90	123.96
1	C	261	PRO	C-N-CA	-6.29	114.90	123.96
1	K	353	VAL	CA-C-N	-6.29	116.88	122.73
1	K	353	VAL	C-N-CA	-6.29	116.88	122.73
1	A	265	GLY	CA-C-O	6.29	129.45	121.53
2	N	34	GLY	N-CA-C	6.28	121.96	114.48
2	P	240	THR	N-CA-C	6.28	120.21	112.54
2	D	34	GLY	N-CA-C	6.28	121.95	114.48
2	F	34	GLY	N-CA-C	6.28	121.95	114.48
1	K	105	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	Q	265	GLY	CA-C-O	6.28	129.44	121.53
2	H	240	THR	N-CA-C	6.27	120.19	112.54
1	M	261	PRO	CA-C-N	-6.27	114.94	123.96
1	M	261	PRO	C-N-CA	-6.27	114.94	123.96
2	P	88	ARG	NE-CZ-NH2	-6.26	113.56	119.20
1	E	353	VAL	CA-C-N	-6.26	116.91	122.73
1	E	353	VAL	C-N-CA	-6.26	116.91	122.73
1	I	261	PRO	CA-C-N	-6.26	114.95	123.96
1	I	261	PRO	C-N-CA	-6.26	114.95	123.96
1	G	353	VAL	CA-C-N	-6.26	116.91	122.73
1	G	353	VAL	C-N-CA	-6.26	116.91	122.73
1	G	261	PRO	CA-C-N	-6.25	114.96	123.96
1	G	261	PRO	C-N-CA	-6.25	114.96	123.96
1	E	265	GLY	CA-C-O	6.25	129.40	121.53
1	I	105	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	K	261	PRO	CA-C-N	-6.25	114.97	123.96
1	K	261	PRO	C-N-CA	-6.25	114.97	123.96
1	O	261	PRO	CA-C-N	-6.24	114.97	123.96
1	O	261	PRO	C-N-CA	-6.24	114.97	123.96
2	J	88	ARG	NE-CZ-NH2	-6.24	113.59	119.20
1	Q	261	PRO	CA-C-N	-6.24	114.98	123.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	261	PRO	C-N-CA	-6.24	114.98	123.96
1	Q	353	VAL	CA-C-N	-6.24	116.93	122.73
1	Q	353	VAL	C-N-CA	-6.24	116.93	122.73
1	O	265	GLY	CA-C-O	6.23	129.38	121.53
1	K	265	GLY	CA-C-O	6.23	129.38	121.53
1	E	105	ARG	NE-CZ-NH2	-6.23	113.60	119.20
1	A	261	PRO	CA-C-N	-6.22	115.00	123.96
1	A	261	PRO	C-N-CA	-6.22	115.00	123.96
1	I	353	VAL	CA-C-N	-6.22	116.95	122.73
1	I	353	VAL	C-N-CA	-6.22	116.95	122.73
1	C	265	GLY	CA-C-O	6.22	129.36	121.53
1	E	261	PRO	CA-C-N	-6.21	115.02	123.96
1	E	261	PRO	C-N-CA	-6.21	115.02	123.96
2	F	240	THR	N-CA-C	6.21	120.11	112.54
1	M	265	GLY	CA-C-O	6.21	129.35	121.53
1	M	353	VAL	CA-C-N	-6.20	116.96	122.73
1	M	353	VAL	C-N-CA	-6.20	116.96	122.73
1	A	105	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	O	105	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	G	265	GLY	CA-C-O	6.18	129.32	121.53
1	A	177	VAL	N-CA-C	6.18	116.78	107.75
1	C	105	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	K	177	VAL	N-CA-C	6.17	116.75	107.75
1	E	177	VAL	N-CA-C	6.16	116.75	107.75
1	I	265	GLY	CA-C-O	6.16	129.30	121.53
1	I	177	VAL	N-CA-C	6.16	116.74	107.75
1	Q	177	VAL	N-CA-C	6.16	116.74	107.75
1	C	177	VAL	N-CA-C	6.16	116.74	107.75
1	G	105	ARG	NE-CZ-NH2	-6.15	113.66	119.20
1	M	177	VAL	N-CA-C	6.15	116.72	107.75
1	E	236	SER	CB-CA-C	-6.14	99.26	110.63
1	I	53	PHE	N-CA-C	6.14	119.72	109.95
1	Q	105	ARG	NE-CZ-NH2	-6.14	113.67	119.20
2	B	306	ASP	CA-CB-CG	-6.14	106.46	112.60
1	O	53	PHE	N-CA-C	6.14	119.71	109.95
2	H	306	ASP	CA-CB-CG	-6.13	106.47	112.60
1	I	236	SER	CB-CA-C	-6.13	99.29	110.63
1	E	53	PHE	N-CA-C	6.12	119.69	109.95
1	G	236	SER	CB-CA-C	-6.12	99.30	110.63
1	O	177	VAL	N-CA-C	6.12	116.69	107.75
1	M	236	SER	CB-CA-C	-6.12	99.31	110.63
1	K	236	SER	CB-CA-C	-6.12	99.31	110.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	236	SER	CB-CA-C	-6.12	99.31	110.63
1	A	236	SER	CB-CA-C	-6.11	99.32	110.63
1	K	53	PHE	N-CA-C	6.11	119.66	109.95
2	N	306	ASP	CA-CB-CG	-6.10	106.50	112.60
2	D	306	ASP	CA-CB-CG	-6.10	106.50	112.60
2	J	306	ASP	CA-CB-CG	-6.10	106.50	112.60
1	O	236	SER	CB-CA-C	-6.10	99.35	110.63
1	Q	53	PHE	N-CA-C	6.10	119.65	109.95
1	G	177	VAL	N-CA-C	6.09	116.65	107.75
2	F	306	ASP	CA-CB-CG	-6.09	106.51	112.60
1	G	53	PHE	N-CA-C	6.08	119.62	109.95
1	E	392	ASP	CA-CB-CG	-6.08	106.53	112.60
1	M	53	PHE	N-CA-C	6.08	119.61	109.95
1	A	53	PHE	N-CA-C	6.07	119.60	109.95
1	C	236	SER	CB-CA-C	-6.07	99.41	110.63
1	O	276	ILE	N-CA-C	6.07	116.85	108.12
2	L	306	ASP	CA-CB-CG	-6.06	106.54	112.60
1	G	11	GLN	CA-CB-CG	6.06	126.22	114.10
2	P	306	ASP	CA-CB-CG	-6.06	106.54	112.60
2	R	306	ASP	CA-CB-CG	-6.06	106.54	112.60
1	A	276	ILE	N-CA-C	6.05	116.83	108.12
1	C	53	PHE	N-CA-C	6.05	119.57	109.95
1	M	276	ILE	N-CA-C	6.05	116.83	108.12
1	G	276	ILE	N-CA-C	6.04	116.82	108.12
1	E	11	GLN	CA-CB-CG	6.04	126.18	114.10
2	R	267	PHE	CA-CB-CG	-6.04	107.76	113.80
2	B	185	TYR	N-CA-CB	6.04	119.10	110.16
1	C	276	ILE	N-CA-C	6.03	116.81	108.12
1	E	276	ILE	N-CA-C	6.03	116.81	108.12
2	L	185	TYR	N-CA-CB	6.03	119.08	110.16
1	I	276	ILE	N-CA-C	6.02	116.80	108.12
1	A	11	GLN	CA-CB-CG	6.02	126.14	114.10
2	F	185	TYR	N-CA-CB	6.02	119.07	110.16
1	I	11	GLN	CA-CB-CG	6.02	126.14	114.10
1	Q	11	GLN	CA-CB-CG	6.02	126.14	114.10
2	D	185	TYR	N-CA-CB	6.01	119.06	110.16
1	M	11	GLN	CA-CB-CG	6.01	126.13	114.10
1	I	392	ASP	CA-CB-CG	-6.01	106.59	112.60
2	J	267	PHE	CA-CB-CG	-6.01	107.79	113.80
2	L	404	PHE	CA-CB-CG	6.01	119.81	113.80
2	N	185	TYR	N-CA-CB	6.01	119.06	110.16
2	F	404	PHE	CA-CB-CG	6.01	119.81	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	185	TYR	N-CA-CB	6.01	119.05	110.16
2	J	185	TYR	N-CA-CB	6.01	119.05	110.16
2	D	401	ARG	N-CA-C	6.00	120.60	113.28
2	H	185	TYR	N-CA-CB	6.00	119.05	110.16
1	K	11	GLN	CA-CB-CG	6.00	126.10	114.10
1	O	11	GLN	CA-CB-CG	6.00	126.10	114.10
1	Q	276	ILE	N-CA-C	5.99	116.75	108.12
1	C	11	GLN	CA-CB-CG	5.99	126.08	114.10
2	H	267	PHE	CA-CB-CG	-5.99	107.81	113.80
1	K	276	ILE	N-CA-C	5.99	116.74	108.12
2	B	244	PHE	N-CA-C	5.98	118.23	110.40
1	G	392	ASP	CA-CB-CG	-5.98	106.62	112.60
2	B	267	PHE	CA-CB-CG	-5.98	107.82	113.80
2	N	143	GLY	CA-C-N	5.98	126.62	119.98
2	N	143	GLY	C-N-CA	5.98	126.62	119.98
2	R	185	TYR	N-CA-CB	5.98	119.01	110.16
2	J	404	PHE	CA-CB-CG	5.97	119.77	113.80
2	B	404	PHE	CA-CB-CG	5.97	119.77	113.80
2	J	143	GLY	CA-C-N	5.97	126.61	119.98
2	J	143	GLY	C-N-CA	5.97	126.61	119.98
1	C	392	ASP	CA-CB-CG	-5.97	106.63	112.60
2	F	244	PHE	N-CA-C	5.97	118.22	110.40
2	L	248	LEU	O-C-N	5.97	130.65	122.59
2	N	404	PHE	CA-CB-CG	5.97	119.77	113.80
2	D	248	LEU	O-C-N	5.96	130.64	122.59
2	L	267	PHE	CA-CB-CG	-5.96	107.84	113.80
2	P	143	GLY	CA-C-N	5.96	126.60	119.98
2	P	143	GLY	C-N-CA	5.96	126.60	119.98
1	K	392	ASP	CA-CB-CG	-5.96	106.64	112.60
2	F	401	ARG	N-CA-C	5.96	120.55	113.28
2	L	143	GLY	CA-C-N	5.96	126.60	119.98
2	L	143	GLY	C-N-CA	5.96	126.60	119.98
2	L	244	PHE	N-CA-C	5.96	118.21	110.40
2	P	404	PHE	CA-CB-CG	5.96	119.76	113.80
1	Q	392	ASP	CA-CB-CG	-5.96	106.64	112.60
1	A	392	ASP	CA-CB-CG	-5.96	106.64	112.60
1	K	229	ARG	NE-CZ-NH2	5.96	124.56	119.20
2	N	244	PHE	N-CA-C	5.95	118.20	110.40
2	H	404	PHE	CA-CB-CG	5.95	119.75	113.80
2	N	401	ARG	N-CA-C	5.95	120.54	113.28
2	F	248	LEU	O-C-N	5.94	130.61	122.59
2	N	248	LEU	O-C-N	5.94	130.61	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	267	PHE	CA-CB-CG	-5.94	107.86	113.80
2	J	244	PHE	N-CA-C	5.94	118.18	110.40
2	R	248	LEU	O-C-N	5.93	130.60	122.59
2	D	267	PHE	CA-CB-CG	-5.93	107.87	113.80
2	L	401	ARG	N-CA-C	5.93	120.52	113.28
2	P	248	LEU	O-C-N	5.93	130.60	122.59
2	R	404	PHE	CA-CB-CG	5.93	119.73	113.80
2	J	248	LEU	O-C-N	5.93	130.60	122.59
2	H	244	PHE	N-CA-C	5.93	118.17	110.40
2	D	404	PHE	CA-CB-CG	5.92	119.72	113.80
2	P	401	ARG	N-CA-C	5.92	120.58	113.23
2	R	244	PHE	N-CA-C	5.92	118.16	110.40
2	B	143	GLY	CA-C-N	5.92	126.55	119.98
2	B	143	GLY	C-N-CA	5.92	126.55	119.98
2	B	248	LEU	O-C-N	5.92	130.59	122.59
2	R	216	THR	CB-CA-C	-5.92	99.44	109.03
2	D	244	PHE	N-CA-C	5.92	118.15	110.40
1	M	392	ASP	CA-CB-CG	-5.92	106.68	112.60
2	H	248	LEU	O-C-N	5.92	130.58	122.59
1	E	102	ASN	CA-CB-CG	5.92	118.52	112.60
1	I	102	ASN	CA-CB-CG	5.91	118.51	112.60
2	P	267	PHE	CA-CB-CG	-5.91	107.89	113.80
2	H	401	ARG	N-CA-C	5.91	120.49	113.28
2	N	106	GLY	N-CA-C	5.90	119.35	112.50
2	J	268	PHE	CA-CB-CG	-5.90	107.90	113.80
1	I	229	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	Q	229	ARG	NE-CZ-NH2	5.90	124.51	119.20
2	B	401	ARG	N-CA-C	5.89	120.54	113.23
1	I	348	PRO	CA-N-CD	5.89	120.25	112.00
1	O	102	ASN	CA-CB-CG	5.89	118.49	112.60
2	H	143	GLY	CA-C-N	5.89	126.52	119.98
2	H	143	GLY	C-N-CA	5.89	126.52	119.98
1	Q	102	ASN	CA-CB-CG	5.89	118.49	112.60
2	F	267	PHE	CA-CB-CG	-5.89	107.91	113.80
2	H	216	THR	CB-CA-C	-5.89	99.49	109.03
2	D	61	TYR	CA-CB-CG	-5.88	103.31	113.90
2	J	408	TYR	N-CA-C	5.88	117.78	111.36
1	O	392	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	102	ASN	CA-CB-CG	5.88	118.48	112.60
2	D	143	GLY	CA-C-N	5.88	126.51	119.98
2	D	143	GLY	C-N-CA	5.88	126.51	119.98
2	F	143	GLY	CA-C-N	5.88	126.51	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	143	GLY	C-N-CA	5.88	126.51	119.98
1	Q	348	PRO	CA-N-CD	5.88	120.23	112.00
2	H	61	TYR	CA-CB-CG	-5.88	103.32	113.90
2	R	408	TYR	N-CA-C	5.88	117.77	111.36
2	N	61	TYR	CA-CB-CG	-5.88	103.32	113.90
1	A	357	TYR	N-CA-C	-5.88	105.20	112.90
1	G	102	ASN	CA-CB-CG	5.87	118.47	112.60
2	B	216	THR	CB-CA-C	-5.87	99.53	109.03
2	B	61	TYR	CA-CB-CG	-5.87	103.34	113.90
2	F	61	TYR	CA-CB-CG	-5.87	103.34	113.90
1	C	102	ASN	CA-CB-CG	5.86	118.46	112.60
2	D	408	TYR	N-CA-C	5.86	117.75	111.36
1	C	229	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	M	102	ASN	CA-CB-CG	5.86	118.46	112.60
1	K	102	ASN	CA-CB-CG	5.86	118.46	112.60
1	Q	357	TYR	N-CA-C	-5.86	105.22	112.90
2	J	401	ARG	N-CA-C	5.86	120.43	113.28
1	K	348	PRO	CA-N-CD	5.86	120.20	112.00
1	C	348	PRO	CA-N-CD	5.86	120.20	112.00
2	J	216	THR	CB-CA-C	-5.86	99.55	109.03
2	P	106	GLY	N-CA-C	5.86	119.29	112.50
1	A	348	PRO	CA-N-CD	5.85	120.19	112.00
2	L	408	TYR	N-CA-C	5.85	117.74	111.36
2	R	61	TYR	CA-CB-CG	-5.85	103.37	113.90
2	R	401	ARG	N-CA-C	5.85	120.48	113.23
2	L	216	THR	CB-CA-C	-5.84	99.56	109.03
2	N	408	TYR	N-CA-C	5.84	117.73	111.36
1	O	357	TYR	N-CA-C	-5.84	105.25	112.90
2	B	106	GLY	N-CA-C	5.84	119.27	112.50
1	E	229	ARG	NE-CZ-NH2	5.84	124.46	119.20
2	J	61	TYR	CA-CB-CG	-5.84	103.39	113.90
1	A	229	ARG	NE-CZ-NH2	5.84	124.45	119.20
1	I	357	TYR	N-CA-C	-5.84	105.25	112.90
2	H	408	TYR	N-CA-C	5.84	117.72	111.36
2	L	61	TYR	CA-CB-CG	-5.84	103.39	113.90
2	P	216	THR	CB-CA-C	-5.84	99.57	109.03
2	R	143	GLY	CA-C-N	5.84	126.46	119.98
2	R	143	GLY	C-N-CA	5.84	126.46	119.98
1	C	357	TYR	N-CA-C	-5.83	105.26	112.90
2	P	61	TYR	CA-CB-CG	-5.83	103.41	113.90
2	D	216	THR	CB-CA-C	-5.83	99.59	109.03
2	P	244	PHE	N-CA-C	5.83	118.04	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	408	TYR	N-CA-C	5.83	117.71	111.36
2	R	268	PHE	CA-CB-CG	-5.83	107.97	113.80
2	N	268	PHE	CA-CB-CG	-5.83	107.97	113.80
2	B	408	TYR	N-CA-C	5.83	117.71	111.36
1	E	357	TYR	N-CA-C	-5.83	105.27	112.90
2	F	408	TYR	N-CA-C	5.83	117.71	111.36
2	J	106	GLY	N-CA-C	5.83	119.26	112.50
2	H	106	GLY	N-CA-C	5.82	119.26	112.50
2	F	216	THR	CB-CA-C	-5.82	99.60	109.03
1	O	348	PRO	CA-N-CD	5.82	120.15	112.00
2	R	106	GLY	N-CA-C	5.82	119.25	112.50
1	O	229	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	K	357	TYR	N-CA-C	-5.81	105.28	112.90
2	N	216	THR	CB-CA-C	-5.81	99.61	109.03
1	E	348	PRO	CA-N-CD	5.81	120.13	112.00
1	M	229	ARG	NE-CZ-NH2	5.81	124.43	119.20
2	H	268	PHE	CA-CB-CG	-5.80	108.00	113.80
2	P	268	PHE	CA-CB-CG	-5.80	108.00	113.80
1	M	348	PRO	CA-N-CD	5.80	120.12	112.00
2	F	106	GLY	N-CA-C	5.80	119.23	112.50
2	F	268	PHE	CA-CB-CG	-5.80	108.00	113.80
2	D	268	PHE	CA-CB-CG	-5.80	108.00	113.80
1	G	348	PRO	CA-N-CD	5.80	120.12	112.00
1	M	357	TYR	N-CA-C	-5.79	105.32	112.90
1	G	229	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	G	357	TYR	N-CA-C	-5.78	105.33	112.90
2	P	96	GLN	O-C-N	5.78	129.47	122.48
2	B	268	PHE	CA-CB-CG	-5.77	108.03	113.80
2	B	96	GLN	O-C-N	5.77	129.46	122.48
2	D	106	GLY	N-CA-C	5.76	119.18	112.50
2	L	268	PHE	CA-CB-CG	-5.76	108.04	113.80
2	P	268	PHE	N-CA-C	5.76	118.94	109.72
2	R	96	GLN	O-C-N	5.76	129.45	122.48
2	D	96	GLN	O-C-N	5.76	129.45	122.48
2	L	106	GLY	N-CA-C	5.75	119.17	112.50
1	M	339	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	G	339	ARG	NE-CZ-NH2	5.74	124.37	119.20
2	R	268	PHE	N-CA-C	5.74	118.91	109.72
2	F	268	PHE	N-CA-C	5.73	118.89	109.72
2	L	268	PHE	N-CA-C	5.73	118.89	109.72
2	J	215	ARG	NE-CZ-NH2	-5.73	114.05	119.20
1	E	339	ARG	NE-CZ-NH2	5.72	124.35	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	268	PHE	N-CA-C	5.72	118.87	109.72
2	B	268	PHE	N-CA-C	5.72	118.87	109.72
2	F	215	ARG	NE-CZ-NH2	-5.72	114.06	119.20
1	K	339	ARG	NE-CZ-NH2	5.72	124.34	119.20
1	E	347	CYS	CB-CA-C	-5.71	102.47	110.13
1	I	339	ARG	NE-CZ-NH2	5.71	124.34	119.20
2	L	215	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	M	347	CYS	CB-CA-C	-5.71	102.48	110.13
2	J	268	PHE	N-CA-C	5.71	118.85	109.72
2	H	96	GLN	O-C-N	5.71	129.38	122.48
2	H	268	PHE	N-CA-C	5.70	118.84	109.72
1	O	339	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	O	347	CYS	CB-CA-C	-5.70	102.49	110.13
2	B	215	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	K	347	CYS	CB-CA-C	-5.70	102.50	110.13
1	A	339	ARG	NE-CZ-NH2	5.69	124.32	119.20
2	N	268	PHE	N-CA-C	5.69	118.83	109.72
1	E	356	ASN	CA-CB-CG	-5.68	106.92	112.60
2	R	215	ARG	NE-CZ-NH2	-5.68	114.09	119.20
1	I	347	CYS	CB-CA-C	-5.68	102.52	110.13
1	Q	339	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	C	337	THR	N-CA-C	5.67	120.33	113.41
2	L	177	VAL	CB-CA-C	-5.67	105.02	111.59
1	K	337	THR	N-CA-C	5.66	120.32	113.41
2	P	177	VAL	CB-CA-C	-5.66	105.02	111.59
1	Q	359	PRO	CA-C-N	5.66	125.57	119.85
1	Q	359	PRO	C-N-CA	5.66	125.57	119.85
2	N	177	VAL	CB-CA-C	-5.66	105.02	111.59
1	A	347	CYS	CB-CA-C	-5.66	102.55	110.13
2	L	406	HIS	CA-C-N	-5.66	112.26	120.29
2	L	406	HIS	C-N-CA	-5.66	112.26	120.29
1	A	337	THR	N-CA-C	5.65	120.31	113.41
1	C	339	ARG	NE-CZ-NH2	5.65	124.29	119.20
2	D	215	ARG	NE-CZ-NH2	-5.65	114.11	119.20
1	E	337	THR	N-CA-C	5.65	120.31	113.41
1	I	337	THR	N-CA-C	5.65	120.31	113.41
2	N	215	ARG	NE-CZ-NH2	-5.65	114.11	119.20
1	G	347	CYS	CB-CA-C	-5.64	102.56	110.13
2	B	177	VAL	CB-CA-C	-5.64	105.04	111.59
1	Q	356	ASN	CA-CB-CG	-5.64	106.96	112.60
1	G	356	ASN	CA-CB-CG	-5.64	106.96	112.60
2	J	424	ASN	CA-CB-CG	-5.64	106.96	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	215	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	Q	337	THR	N-CA-C	5.64	120.29	113.41
2	F	406	HIS	CA-C-N	-5.64	112.28	120.29
2	F	406	HIS	C-N-CA	-5.64	112.28	120.29
1	I	356	ASN	CA-CB-CG	-5.63	106.97	112.60
2	J	406	HIS	CA-C-N	-5.63	112.29	120.29
2	J	406	HIS	C-N-CA	-5.63	112.29	120.29
1	O	337	THR	N-CA-C	5.63	120.28	113.41
2	D	264	ARG	CA-C-N	-5.63	114.39	123.23
2	D	264	ARG	C-N-CA	-5.63	114.39	123.23
1	O	349	THR	N-CA-C	5.63	122.79	110.80
1	C	347	CYS	CB-CA-C	-5.63	102.59	110.13
1	G	337	THR	N-CA-C	5.62	120.27	113.41
2	J	177	VAL	CB-CA-C	-5.62	105.07	111.59
1	M	337	THR	N-CA-C	5.62	120.27	113.41
1	M	356	ASN	CA-CB-CG	-5.62	106.98	112.60
1	A	356	ASN	CA-CB-CG	-5.62	106.98	112.60
1	Q	347	CYS	CB-CA-C	-5.62	102.60	110.13
1	Q	349	THR	N-CA-C	5.62	122.77	110.80
2	B	406	HIS	CA-C-N	-5.62	112.31	120.29
2	B	406	HIS	C-N-CA	-5.62	112.31	120.29
2	F	264	ARG	CA-C-N	-5.62	114.41	123.23
2	F	264	ARG	C-N-CA	-5.62	114.41	123.23
1	G	359	PRO	CA-C-N	5.62	125.53	119.85
1	G	359	PRO	C-N-CA	5.62	125.53	119.85
2	L	176	LYS	N-CA-C	5.62	120.26	112.90
2	P	243	ARG	N-CA-C	5.61	118.59	111.69
2	R	264	ARG	CA-C-N	-5.61	114.42	123.23
2	R	264	ARG	C-N-CA	-5.61	114.42	123.23
2	D	177	VAL	CB-CA-C	-5.61	105.08	111.59
2	D	406	HIS	CA-C-N	-5.61	112.32	120.29
2	D	406	HIS	C-N-CA	-5.61	112.32	120.29
2	J	264	ARG	CA-C-N	-5.61	114.42	123.23
2	J	264	ARG	C-N-CA	-5.61	114.42	123.23
1	K	349	THR	N-CA-C	5.61	122.75	110.80
2	L	264	ARG	CA-C-N	-5.61	114.42	123.23
2	L	264	ARG	C-N-CA	-5.61	114.42	123.23
1	O	356	ASN	CA-CB-CG	-5.61	106.99	112.60
1	K	356	ASN	CA-CB-CG	-5.60	107.00	112.60
2	H	264	ARG	CA-C-N	-5.60	114.43	123.23
2	H	264	ARG	C-N-CA	-5.60	114.43	123.23
1	C	359	PRO	CA-C-N	5.60	125.51	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	359	PRO	C-N-CA	5.60	125.51	119.85
2	P	176	LYS	N-CA-C	5.60	120.24	112.90
2	R	177	VAL	CB-CA-C	-5.60	105.09	111.59
1	A	349	THR	N-CA-C	5.60	122.72	110.80
1	G	349	THR	N-CA-C	5.60	122.72	110.80
2	H	406	HIS	CA-C-N	-5.60	112.34	120.29
2	H	406	HIS	C-N-CA	-5.60	112.34	120.29
2	N	406	HIS	CA-C-N	-5.60	112.34	120.29
2	N	406	HIS	C-N-CA	-5.60	112.34	120.29
2	D	424	ASN	CA-CB-CG	-5.59	107.01	112.60
2	L	424	ASN	CA-CB-CG	-5.59	107.01	112.60
2	N	243	ARG	N-CA-C	5.59	118.57	111.69
1	M	359	PRO	CA-C-N	5.59	125.50	119.85
1	M	359	PRO	C-N-CA	5.59	125.50	119.85
1	G	200	CYS	CA-C-N	-5.59	115.11	122.99
1	G	200	CYS	C-N-CA	-5.59	115.11	122.99
1	M	349	THR	N-CA-C	5.59	122.71	110.80
2	B	424	ASN	CA-CB-CG	-5.59	107.01	112.60
2	F	243	ARG	N-CA-C	5.59	118.56	111.69
2	F	176	LYS	N-CA-C	5.58	120.22	112.90
2	P	221	THR	N-CA-C	5.58	122.15	109.81
1	C	356	ASN	CA-CB-CG	-5.58	107.02	112.60
2	J	176	LYS	N-CA-C	5.58	120.21	112.90
2	R	221	THR	N-CA-C	5.58	122.15	109.81
2	H	215	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	I	349	THR	N-CA-C	5.58	122.68	110.80
2	L	221	THR	N-CA-C	5.58	122.13	109.81
2	F	177	VAL	CB-CA-C	-5.57	105.12	111.59
2	H	176	LYS	N-CA-C	5.57	120.20	112.90
1	K	200	CYS	CA-C-N	-5.57	115.13	122.99
1	K	200	CYS	C-N-CA	-5.57	115.13	122.99
2	B	243	ARG	N-CA-C	5.57	118.54	111.69
1	C	200	CYS	CA-C-N	-5.57	115.14	122.99
1	C	200	CYS	C-N-CA	-5.57	115.14	122.99
2	J	243	ARG	N-CA-C	5.57	118.54	111.69
2	B	264	ARG	CA-C-N	-5.57	114.49	123.23
2	B	264	ARG	C-N-CA	-5.57	114.49	123.23
1	C	349	THR	N-CA-C	5.57	122.66	110.80
1	E	349	THR	N-CA-C	5.57	122.66	110.80
2	N	221	THR	N-CA-C	5.57	122.12	109.81
2	R	176	LYS	N-CA-C	5.57	120.19	112.90
2	F	88	ARG	CA-C-N	5.56	125.92	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	88	ARG	C-N-CA	5.56	125.92	119.47
2	P	264	ARG	CA-C-N	-5.56	114.49	123.23
2	P	264	ARG	C-N-CA	-5.56	114.49	123.23
1	A	200	CYS	CA-C-N	-5.56	115.15	122.99
1	A	200	CYS	C-N-CA	-5.56	115.15	122.99
2	D	176	LYS	N-CA-C	5.56	120.19	112.90
2	H	177	VAL	CB-CA-C	-5.56	105.14	111.59
2	P	54	ASN	CA-C-N	-5.56	114.79	122.30
2	P	54	ASN	C-N-CA	-5.56	114.79	122.30
2	D	221	THR	N-CA-C	5.56	122.10	109.81
1	E	283	HIS	CA-CB-CG	-5.56	108.24	113.80
2	B	176	LYS	N-CA-C	5.56	120.18	112.90
1	M	200	CYS	CA-C-N	-5.56	115.15	122.99
1	M	200	CYS	C-N-CA	-5.56	115.15	122.99
1	A	359	PRO	CA-C-N	5.56	125.46	119.85
1	A	359	PRO	C-N-CA	5.56	125.46	119.85
2	J	60	LYS	CA-C-N	-5.55	115.16	122.99
2	J	60	LYS	C-N-CA	-5.55	115.16	122.99
2	L	243	ARG	N-CA-C	5.55	118.52	111.69
2	N	264	ARG	CA-C-N	-5.55	114.51	123.23
2	N	264	ARG	C-N-CA	-5.55	114.51	123.23
2	P	424	ASN	CA-CB-CG	-5.55	107.05	112.60
2	R	243	ARG	N-CA-C	5.55	118.52	111.69
2	H	60	LYS	CA-C-N	-5.55	115.16	122.99
2	H	60	LYS	C-N-CA	-5.55	115.16	122.99
2	H	221	THR	N-CA-C	5.55	122.08	109.81
2	N	176	LYS	N-CA-C	5.55	120.17	112.90
1	O	200	CYS	CA-C-N	-5.55	115.16	122.99
1	O	200	CYS	C-N-CA	-5.55	115.16	122.99
1	A	309	HIS	CA-C-N	-5.55	116.78	122.27
1	A	309	HIS	C-N-CA	-5.55	116.78	122.27
2	J	221	THR	N-CA-C	5.55	122.07	109.81
2	B	221	THR	N-CA-C	5.55	122.07	109.81
2	F	424	ASN	CA-CB-CG	-5.55	107.05	112.60
1	G	354	GLY	CA-C-N	-5.55	115.46	123.11
1	G	354	GLY	C-N-CA	-5.55	115.46	123.11
2	N	424	ASN	CA-CB-CG	-5.54	107.06	112.60
1	O	283	HIS	CA-CB-CG	-5.54	108.26	113.80
1	I	283	HIS	CA-CB-CG	-5.54	108.26	113.80
1	E	319	TYR	N-CA-C	5.54	118.51	109.59
1	I	309	HIS	CA-C-N	-5.54	116.79	122.27
1	I	309	HIS	C-N-CA	-5.54	116.79	122.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	283	HIS	CA-CB-CG	-5.54	108.26	113.80
2	P	406	HIS	CA-C-N	-5.54	112.43	120.29
2	P	406	HIS	C-N-CA	-5.54	112.43	120.29
2	R	60	LYS	CA-C-N	-5.54	115.18	122.99
2	R	60	LYS	C-N-CA	-5.54	115.18	122.99
2	R	424	ASN	CA-CB-CG	-5.54	107.06	112.60
1	O	359	PRO	CA-C-N	5.54	125.44	119.85
1	O	359	PRO	C-N-CA	5.54	125.44	119.85
1	Q	283	HIS	CA-CB-CG	-5.54	108.27	113.80
1	E	200	CYS	CA-C-N	-5.53	115.19	122.99
1	E	200	CYS	C-N-CA	-5.53	115.19	122.99
1	K	359	PRO	CA-C-N	5.53	125.44	119.85
1	K	359	PRO	C-N-CA	5.53	125.44	119.85
1	E	359	PRO	CA-C-N	5.53	125.43	119.85
1	E	359	PRO	C-N-CA	5.53	125.43	119.85
1	O	354	GLY	CA-C-N	-5.53	115.48	123.11
1	O	354	GLY	C-N-CA	-5.53	115.48	123.11
2	F	221	THR	N-CA-C	5.53	122.02	109.81
2	H	424	ASN	CA-CB-CG	-5.52	107.08	112.60
2	R	406	HIS	CA-C-N	-5.52	112.45	120.29
2	R	406	HIS	C-N-CA	-5.52	112.45	120.29
1	Q	345	ASP	N-CA-C	5.52	122.56	110.80
1	A	345	ASP	N-CA-C	5.52	122.56	110.80
1	E	309	HIS	CA-C-N	-5.52	116.81	122.27
1	E	309	HIS	C-N-CA	-5.52	116.81	122.27
2	F	60	LYS	CA-C-N	-5.52	115.21	122.99
2	F	60	LYS	C-N-CA	-5.52	115.21	122.99
1	I	359	PRO	CA-C-N	5.52	125.42	119.85
1	I	359	PRO	C-N-CA	5.52	125.42	119.85
1	Q	200	CYS	CA-C-N	-5.52	115.21	122.99
1	Q	200	CYS	C-N-CA	-5.52	115.21	122.99
2	B	60	LYS	CA-C-N	-5.51	115.21	122.99
2	B	60	LYS	C-N-CA	-5.51	115.21	122.99
2	H	243	ARG	N-CA-C	5.51	118.47	111.69
2	N	253	ARG	NE-CZ-NH2	5.51	124.16	119.20
2	R	88	ARG	CA-C-N	5.51	125.86	119.47
2	R	88	ARG	C-N-CA	5.51	125.86	119.47
2	H	345	GLU	N-CA-C	5.51	119.48	112.87
2	L	60	LYS	CA-C-N	-5.51	115.22	122.99
2	L	60	LYS	C-N-CA	-5.51	115.22	122.99
2	D	60	LYS	CA-C-N	-5.51	115.22	122.99
2	D	60	LYS	C-N-CA	-5.51	115.22	122.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	345	ASP	N-CA-C	5.51	122.53	110.80
2	F	345	GLU	N-CA-C	5.51	119.48	112.87
1	M	309	HIS	CA-C-N	-5.51	116.81	122.27
1	M	309	HIS	C-N-CA	-5.51	116.81	122.27
2	J	88	ARG	CA-C-N	5.51	125.86	119.47
2	J	88	ARG	C-N-CA	5.51	125.86	119.47
2	R	253	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	G	283	HIS	CA-CB-CG	-5.50	108.30	113.80
2	N	54	ASN	CA-C-N	-5.50	114.87	122.30
2	N	54	ASN	C-N-CA	-5.50	114.87	122.30
2	P	60	LYS	CA-C-N	-5.50	115.23	122.99
2	P	60	LYS	C-N-CA	-5.50	115.23	122.99
1	C	345	ASP	N-CA-C	5.50	122.51	110.80
2	N	345	GLU	N-CA-C	5.50	119.47	112.87
1	A	354	GLY	CA-C-N	-5.50	115.53	123.11
1	A	354	GLY	C-N-CA	-5.50	115.53	123.11
1	C	354	GLY	CA-C-N	-5.50	115.53	123.11
1	C	354	GLY	C-N-CA	-5.50	115.53	123.11
1	E	354	GLY	CA-C-N	-5.50	115.53	123.11
1	E	354	GLY	C-N-CA	-5.50	115.53	123.11
1	G	309	HIS	CA-C-N	-5.49	116.83	122.27
1	G	309	HIS	C-N-CA	-5.49	116.83	122.27
1	G	319	TYR	N-CA-C	5.49	118.43	109.59
2	N	60	LYS	CA-C-N	-5.49	115.24	122.99
2	N	60	LYS	C-N-CA	-5.49	115.24	122.99
2	D	253	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	J	345	GLU	N-CA-C	5.49	119.46	112.87
1	O	319	TYR	N-CA-C	5.49	118.43	109.59
2	J	54	ASN	CA-C-N	-5.49	114.89	122.30
2	J	54	ASN	C-N-CA	-5.49	114.89	122.30
1	M	354	GLY	CA-C-N	-5.49	115.53	123.11
1	M	354	GLY	C-N-CA	-5.49	115.53	123.11
2	F	54	ASN	CA-C-N	-5.49	114.90	122.30
2	F	54	ASN	C-N-CA	-5.49	114.90	122.30
1	A	319	TYR	N-CA-C	5.48	118.42	109.59
2	L	253	ARG	NE-CZ-NH2	5.48	124.14	119.20
2	P	88	ARG	CA-C-N	5.48	125.83	119.47
2	P	88	ARG	C-N-CA	5.48	125.83	119.47
1	K	354	GLY	CA-C-N	-5.48	115.54	123.11
1	K	354	GLY	C-N-CA	-5.48	115.54	123.11
2	N	88	ARG	CA-C-N	5.48	125.83	119.47
2	N	88	ARG	C-N-CA	5.48	125.83	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	253	ARG	NE-CZ-NH2	5.48	124.14	119.20
1	C	283	HIS	CA-CB-CG	-5.48	108.32	113.80
1	M	345	ASP	N-CA-C	5.48	122.47	110.80
1	O	345	ASP	N-CA-C	5.48	122.47	110.80
1	A	283	HIS	CA-CB-CG	-5.48	108.32	113.80
1	I	319	TYR	N-CA-C	5.48	118.41	109.59
2	L	88	ARG	CA-C-N	5.48	125.82	119.47
2	L	88	ARG	C-N-CA	5.48	125.82	119.47
1	K	319	TYR	N-CA-C	5.48	118.41	109.59
2	H	54	ASN	CA-C-N	-5.47	114.91	122.30
2	H	54	ASN	C-N-CA	-5.47	114.91	122.30
1	O	309	HIS	CA-C-N	-5.47	116.85	122.27
1	O	309	HIS	C-N-CA	-5.47	116.85	122.27
1	Q	354	GLY	CA-C-N	-5.47	115.56	123.11
1	Q	354	GLY	C-N-CA	-5.47	115.56	123.11
1	C	309	HIS	CA-C-N	-5.47	116.85	122.27
1	C	309	HIS	C-N-CA	-5.47	116.85	122.27
2	F	253	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	I	200	CYS	CA-C-N	-5.47	115.28	122.99
1	I	200	CYS	C-N-CA	-5.47	115.28	122.99
1	G	345	ASP	N-CA-C	5.47	122.44	110.80
1	I	354	GLY	CA-C-N	-5.47	115.57	123.11
1	I	354	GLY	C-N-CA	-5.47	115.57	123.11
2	R	54	ASN	CA-C-N	-5.47	114.92	122.30
2	R	54	ASN	C-N-CA	-5.47	114.92	122.30
2	B	54	ASN	CA-C-N	-5.46	114.92	122.30
2	B	54	ASN	C-N-CA	-5.46	114.92	122.30
1	I	345	ASP	N-CA-C	5.46	122.44	110.80
1	K	283	HIS	CA-CB-CG	-5.46	108.34	113.80
2	B	253	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	K	345	ASP	N-CA-C	5.46	122.44	110.80
1	A	101	ASN	CA-C-N	-5.46	113.52	121.76
1	A	101	ASN	C-N-CA	-5.46	113.52	121.76
2	D	243	ARG	N-CA-C	5.46	118.41	111.69
1	E	101	ASN	CA-C-N	-5.46	113.52	121.76
1	E	101	ASN	C-N-CA	-5.46	113.52	121.76
2	L	345	GLU	N-CA-C	5.46	119.42	112.87
2	B	88	ARG	CA-C-N	5.46	125.80	119.47
2	B	88	ARG	C-N-CA	5.46	125.80	119.47
1	O	101	ASN	CA-C-N	-5.46	113.52	121.76
1	O	101	ASN	C-N-CA	-5.46	113.52	121.76
2	R	81	GLY	CA-C-N	5.46	125.38	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	81	GLY	C-N-CA	5.46	125.38	119.76
1	I	101	ASN	CA-C-N	-5.45	113.53	121.76
1	I	101	ASN	C-N-CA	-5.45	113.53	121.76
1	K	309	HIS	CA-C-N	-5.45	116.88	122.27
1	K	309	HIS	C-N-CA	-5.45	116.88	122.27
2	B	345	GLU	N-CA-C	5.45	119.41	112.87
2	H	308	ARG	CD-NE-CZ	5.45	132.02	124.40
2	P	345	GLU	N-CA-C	5.45	119.40	112.87
2	D	345	GLU	N-CA-C	5.44	119.40	112.87
2	L	356	CYS	CA-C-N	-5.44	113.56	122.54
2	L	356	CYS	C-N-CA	-5.44	113.56	122.54
2	N	308	ARG	CD-NE-CZ	5.44	132.02	124.40
1	C	101	ASN	CA-C-N	-5.44	113.54	121.76
1	C	101	ASN	C-N-CA	-5.44	113.54	121.76
1	C	319	TYR	N-CA-C	5.44	118.34	109.59
1	M	319	TYR	N-CA-C	5.44	118.34	109.59
2	D	88	ARG	CA-C-N	5.43	125.77	119.47
2	D	88	ARG	C-N-CA	5.43	125.77	119.47
2	L	54	ASN	CA-C-N	-5.43	114.97	122.30
2	L	54	ASN	C-N-CA	-5.43	114.97	122.30
2	D	54	ASN	CA-C-N	-5.43	114.97	122.30
2	D	54	ASN	C-N-CA	-5.43	114.97	122.30
1	Q	101	ASN	CA-C-N	-5.43	113.56	121.76
1	Q	101	ASN	C-N-CA	-5.43	113.56	121.76
1	Q	319	TYR	N-CA-C	5.43	118.33	109.59
1	G	101	ASN	CA-C-N	-5.43	113.56	121.76
1	G	101	ASN	C-N-CA	-5.43	113.56	121.76
2	D	356	CYS	CA-C-N	-5.43	113.59	122.54
2	D	356	CYS	C-N-CA	-5.43	113.59	122.54
2	H	277	SER	CA-C-N	5.43	128.30	120.38
2	H	277	SER	C-N-CA	5.43	128.30	120.38
2	R	308	ARG	CD-NE-CZ	5.43	132.00	124.40
2	F	356	CYS	CA-C-N	-5.42	113.59	122.54
2	F	356	CYS	C-N-CA	-5.42	113.59	122.54
1	Q	309	HIS	CA-C-N	-5.42	116.91	122.27
1	Q	309	HIS	C-N-CA	-5.42	116.91	122.27
2	D	308	ARG	CD-NE-CZ	5.42	131.98	124.40
2	P	356	CYS	CA-C-N	-5.42	113.60	122.54
2	P	356	CYS	C-N-CA	-5.42	113.60	122.54
1	M	101	ASN	CA-C-N	-5.41	113.58	121.76
1	M	101	ASN	C-N-CA	-5.41	113.58	121.76
2	L	81	GLY	CA-C-N	5.41	125.33	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	81	GLY	C-N-CA	5.41	125.33	119.76
2	N	356	CYS	CA-C-N	-5.41	113.61	122.54
2	N	356	CYS	C-N-CA	-5.41	113.61	122.54
2	P	81	GLY	CA-C-N	5.41	125.33	119.76
2	P	81	GLY	C-N-CA	5.41	125.33	119.76
2	B	81	GLY	CA-C-N	5.40	125.33	119.76
2	B	81	GLY	C-N-CA	5.40	125.33	119.76
2	B	308	ARG	CD-NE-CZ	5.40	131.97	124.40
2	H	88	ARG	CA-C-N	5.40	125.74	119.47
2	H	88	ARG	C-N-CA	5.40	125.74	119.47
2	J	272	PHE	N-CA-C	5.40	117.99	108.75
2	R	356	CYS	CA-C-N	-5.40	113.63	122.54
2	R	356	CYS	C-N-CA	-5.40	113.63	122.54
2	P	272	PHE	N-CA-C	5.40	117.98	108.75
2	J	253	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	P	308	ARG	CD-NE-CZ	5.40	131.96	124.40
2	D	296	PHE	CA-CB-CG	-5.39	108.41	113.80
2	H	253	ARG	NE-CZ-NH2	5.39	124.06	119.20
2	J	308	ARG	CD-NE-CZ	5.39	131.95	124.40
2	B	356	CYS	CA-C-N	-5.39	113.64	122.54
2	B	356	CYS	C-N-CA	-5.39	113.64	122.54
1	E	123	ARG	NE-CZ-NH2	-5.39	114.35	119.20
2	J	277	SER	CA-C-N	5.39	128.25	120.38
2	J	277	SER	C-N-CA	5.39	128.25	120.38
2	D	81	GLY	CA-C-N	5.39	125.31	119.76
2	D	81	GLY	C-N-CA	5.39	125.31	119.76
2	D	277	SER	CA-C-N	5.39	128.24	120.38
2	D	277	SER	C-N-CA	5.39	128.24	120.38
2	J	81	GLY	CA-C-N	5.38	125.31	119.76
2	J	81	GLY	C-N-CA	5.38	125.31	119.76
2	R	345	GLU	N-CA-C	5.38	119.33	112.87
2	J	264	ARG	N-CA-C	5.38	120.00	113.38
2	N	272	PHE	N-CA-C	5.38	117.95	108.75
2	B	272	PHE	N-CA-C	5.38	117.95	108.75
2	B	185	TYR	CA-CB-CG	5.38	123.58	113.90
2	F	264	ARG	N-CA-C	5.37	119.99	113.38
2	H	356	CYS	CA-C-N	-5.37	113.67	122.54
2	H	356	CYS	C-N-CA	-5.37	113.67	122.54
1	M	123	ARG	NE-CZ-NH2	-5.37	114.36	119.20
2	R	277	SER	CA-C-N	5.37	128.22	120.38
2	R	277	SER	C-N-CA	5.37	128.22	120.38
1	K	101	ASN	CA-C-N	-5.37	113.65	121.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	101	ASN	C-N-CA	-5.37	113.65	121.76
2	B	277	SER	CA-C-N	5.37	128.22	120.38
2	B	277	SER	C-N-CA	5.37	128.22	120.38
2	J	185	TYR	CA-CB-CG	5.37	123.56	113.90
2	F	81	GLY	CA-C-N	5.37	125.29	119.76
2	F	81	GLY	C-N-CA	5.37	125.29	119.76
2	L	277	SER	CA-C-N	5.37	128.22	120.38
2	L	277	SER	C-N-CA	5.37	128.22	120.38
2	L	308	ARG	CD-NE-CZ	5.37	131.91	124.40
2	H	81	GLY	CA-C-N	5.36	125.28	119.76
2	H	81	GLY	C-N-CA	5.36	125.28	119.76
2	H	296	PHE	CA-CB-CG	-5.36	108.44	113.80
2	P	185	TYR	CA-CB-CG	5.36	123.56	113.90
2	F	272	PHE	N-CA-C	5.36	117.92	108.75
2	N	185	TYR	CA-CB-CG	5.36	123.55	113.90
2	N	264	ARG	N-CA-C	5.36	119.97	113.38
2	R	264	ARG	N-CA-C	5.36	119.97	113.38
2	F	277	SER	CA-C-N	5.36	128.20	120.38
2	F	277	SER	C-N-CA	5.36	128.20	120.38
1	C	55	GLU	N-CA-C	5.36	118.96	109.96
2	J	356	CYS	CA-C-N	-5.36	113.70	122.54
2	J	356	CYS	C-N-CA	-5.36	113.70	122.54
1	O	123	ARG	NE-CZ-NH2	-5.36	114.38	119.20
2	P	277	SER	CA-C-N	5.36	128.20	120.38
2	P	277	SER	C-N-CA	5.36	128.20	120.38
1	Q	156	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	D	272	PHE	N-CA-C	5.35	117.91	108.75
2	R	272	PHE	N-CA-C	5.35	117.91	108.75
2	H	272	PHE	N-CA-C	5.35	117.90	108.75
1	O	205	ASP	CA-CB-CG	5.35	117.95	112.60
2	L	212	ILE	CB-CA-C	-5.35	104.92	112.14
2	P	264	ARG	N-CA-C	5.35	119.96	113.38
2	B	296	PHE	CA-CB-CG	-5.35	108.45	113.80
2	N	81	GLY	CA-C-N	5.35	125.27	119.76
2	N	81	GLY	C-N-CA	5.35	125.27	119.76
2	L	264	ARG	N-CA-C	5.34	119.95	113.38
2	B	264	ARG	N-CA-C	5.34	119.95	113.38
1	Q	123	ARG	NE-CZ-NH2	-5.34	114.39	119.20
2	D	185	TYR	CA-CB-CG	5.34	123.51	113.90
2	F	308	ARG	CD-NE-CZ	5.34	131.87	124.40
2	L	272	PHE	N-CA-C	5.33	117.87	108.75
1	I	156	ARG	NE-CZ-NH2	5.33	124.00	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	296	PHE	CA-CB-CG	-5.33	108.47	113.80
1	G	55	GLU	N-CA-C	5.33	118.91	109.96
1	K	55	GLU	N-CA-C	5.33	118.91	109.96
2	N	277	SER	CA-C-N	5.33	128.16	120.38
2	N	277	SER	C-N-CA	5.33	128.16	120.38
2	J	96	GLN	O-C-N	5.33	129.50	122.36
1	M	55	GLU	N-CA-C	5.33	118.91	109.96
1	I	109	THR	N-CA-C	5.33	122.15	110.80
1	A	55	GLU	N-CA-C	5.33	118.91	109.96
1	K	123	ARG	NE-CZ-NH2	-5.33	114.41	119.20
2	R	185	TYR	CA-CB-CG	5.32	123.48	113.90
1	I	55	GLU	N-CA-C	5.32	118.90	109.96
1	O	135	PHE	N-CA-C	5.32	116.37	108.60
1	A	135	PHE	N-CA-C	5.32	116.36	108.60
1	G	109	THR	N-CA-C	5.32	122.12	110.80
2	H	264	ARG	N-CA-C	5.32	119.92	113.38
1	K	245	ASP	N-CA-C	5.32	118.15	110.28
2	R	405	LEU	N-CA-CB	5.32	119.34	110.41
1	A	205	ASP	CA-CB-CG	5.32	117.92	112.60
2	F	185	TYR	CA-CB-CG	5.32	123.47	113.90
1	E	245	ASP	N-CA-C	5.31	118.14	110.28
2	F	405	LEU	N-CA-CB	5.31	119.34	110.41
1	M	245	ASP	N-CA-C	5.31	118.14	110.28
1	O	245	ASP	N-CA-C	5.31	118.14	110.28
2	B	405	LEU	N-CA-CB	5.31	119.33	110.41
1	C	205	ASP	CA-CB-CG	5.31	117.91	112.60
1	M	205	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	109	THR	N-CA-C	5.31	122.11	110.80
1	C	123	ARG	NE-CZ-NH2	-5.31	114.42	119.20
2	R	296	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	156	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	I	379	SER	N-CA-C	5.31	117.83	108.75
2	N	296	PHE	CA-CB-CG	-5.31	108.49	113.80
1	M	109	THR	N-CA-C	5.31	122.10	110.80
1	A	109	THR	N-CA-C	5.30	122.10	110.80
1	O	109	THR	N-CA-C	5.30	122.10	110.80
2	B	166	MET	CA-C-N	-5.30	113.92	122.82
2	B	166	MET	C-N-CA	-5.30	113.92	122.82
1	K	109	THR	N-CA-C	5.30	122.09	110.80
1	A	123	ARG	NE-CZ-NH2	-5.30	114.43	119.20
2	H	405	LEU	N-CA-CB	5.30	119.31	110.41
1	I	135	PHE	N-CA-C	5.30	116.34	108.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	296	PHE	CA-CB-CG	-5.30	108.50	113.80
1	Q	135	PHE	N-CA-C	5.30	116.34	108.60
1	M	156	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	G	135	PHE	N-CA-C	5.30	116.33	108.60
2	L	405	LEU	N-CA-CB	5.30	119.31	110.41
2	J	350	ASN	N-CA-C	5.29	122.08	110.80
1	Q	205	ASP	CA-CB-CG	5.29	117.89	112.60
2	D	405	LEU	N-CA-CB	5.29	119.30	110.41
1	E	109	THR	N-CA-C	5.29	122.08	110.80
2	L	350	ASN	N-CA-C	5.29	122.07	110.80
1	O	379	SER	N-CA-C	5.29	117.80	108.75
2	P	350	ASN	N-CA-C	5.29	122.07	110.80
2	D	264	ARG	N-CA-C	5.29	119.89	113.38
2	H	185	TYR	CA-CB-CG	5.29	123.43	113.90
1	E	379	SER	N-CA-C	5.29	117.80	108.75
2	F	212	ILE	CB-CA-C	-5.29	105.00	112.14
2	B	212	ILE	CB-CA-C	-5.29	105.00	112.14
2	D	203	CYS	N-CA-C	5.29	117.58	107.75
1	Q	109	THR	N-CA-C	5.29	122.06	110.80
1	C	156	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	379	SER	N-CA-C	5.29	117.79	108.75
2	N	405	LEU	N-CA-CB	5.29	119.29	110.41
1	O	55	GLU	N-CA-C	5.29	118.84	109.96
1	C	135	PHE	N-CA-C	5.28	116.31	108.60
1	I	123	ARG	NE-CZ-NH2	-5.28	114.44	119.20
1	K	205	ASP	CA-CB-CG	5.28	117.88	112.60
2	N	96	GLN	O-C-N	5.28	129.44	122.36
2	N	122	VAL	CB-CA-C	-5.28	105.21	111.97
1	Q	55	GLU	N-CA-C	5.28	118.84	109.96
1	C	334	THR	CA-C-N	-5.28	111.87	120.64
1	C	334	THR	C-N-CA	-5.28	111.87	120.64
1	I	205	ASP	CA-CB-CG	5.28	117.88	112.60
2	L	185	TYR	CA-CB-CG	5.28	123.41	113.90
1	G	156	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	E	205	ASP	CA-CB-CG	5.28	117.88	112.60
2	H	350	ASN	N-CA-C	5.28	122.05	110.80
1	M	135	PHE	N-CA-C	5.28	116.31	108.60
2	J	405	LEU	N-CA-CB	5.28	119.28	110.41
1	M	379	SER	N-CA-C	5.27	117.77	108.75
2	L	203	CYS	N-CA-C	5.27	117.56	107.75
1	Q	245	ASP	N-CA-C	5.27	118.08	110.28
2	B	350	ASN	N-CA-C	5.27	122.03	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	212	ILE	CB-CA-C	-5.27	105.02	112.14
2	L	96	GLN	O-C-N	5.27	129.42	122.36
2	D	212	ILE	CB-CA-C	-5.27	105.03	112.14
1	O	259	LEU	N-CA-C	5.27	120.71	113.97
2	F	296	PHE	CA-CB-CG	-5.26	108.54	113.80
1	G	259	LEU	N-CA-C	5.26	120.71	113.97
2	R	166	MET	CA-C-N	-5.26	113.97	122.82
2	R	166	MET	C-N-CA	-5.26	113.97	122.82
2	R	228	ASN	CA-CB-CG	-5.26	107.33	112.60
2	B	228	ASN	CA-CB-CG	-5.26	107.34	112.60
1	E	55	GLU	N-CA-C	5.26	118.80	109.96
2	H	166	MET	CA-C-N	-5.26	113.98	122.82
2	H	166	MET	C-N-CA	-5.26	113.98	122.82
2	J	166	MET	CA-C-N	-5.26	113.98	122.82
2	J	166	MET	C-N-CA	-5.26	113.98	122.82
2	N	350	ASN	N-CA-C	5.26	122.00	110.80
2	P	405	LEU	N-CA-CB	5.26	119.25	110.41
2	D	122	VAL	CB-CA-C	-5.26	105.24	111.97
2	D	350	ASN	N-CA-C	5.26	122.00	110.80
2	H	203	CYS	N-CA-C	5.26	117.53	107.75
2	H	212	ILE	CB-CA-C	-5.26	105.04	112.14
1	K	135	PHE	N-CA-C	5.26	116.28	108.60
1	Q	259	LEU	N-CA-C	5.26	120.70	113.97
2	F	350	ASN	N-CA-C	5.26	122.00	110.80
1	G	379	SER	N-CA-C	5.26	117.74	108.75
2	N	212	ILE	CB-CA-C	-5.26	105.04	112.14
1	E	334	THR	CA-C-N	-5.26	111.91	120.64
1	E	334	THR	C-N-CA	-5.26	111.91	120.64
1	G	245	ASP	N-CA-C	5.26	118.06	110.28
2	N	166	MET	CA-C-N	-5.26	113.99	122.82
2	N	166	MET	C-N-CA	-5.26	113.99	122.82
2	D	166	MET	CA-C-N	-5.25	113.99	122.82
2	D	166	MET	C-N-CA	-5.25	113.99	122.82
1	G	123	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	C	245	ASP	N-CA-C	5.25	118.06	110.28
2	F	203	CYS	N-CA-C	5.25	117.52	107.75
2	J	203	CYS	N-CA-C	5.25	117.52	107.75
1	E	135	PHE	N-CA-C	5.25	116.27	108.60
2	D	228	ASN	CA-CB-CG	-5.25	107.35	112.60
1	Q	379	SER	N-CA-C	5.25	117.73	108.75
1	C	379	SER	N-CA-C	5.25	117.72	108.75
2	H	228	ASN	CA-CB-CG	-5.25	107.35	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	245	ASP	N-CA-C	5.25	118.05	110.28
2	P	212	ILE	CB-CA-C	-5.25	105.05	112.14
2	J	296	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	245	ASP	N-CA-C	5.25	118.04	110.28
1	I	259	LEU	N-CA-C	5.24	120.68	113.97
2	R	203	CYS	N-CA-C	5.24	117.50	107.75
2	J	212	ILE	CB-CA-C	-5.24	105.06	112.14
1	G	264	ARG	O-C-N	5.24	128.81	122.68
2	P	166	MET	CA-C-N	-5.24	114.02	122.82
2	P	166	MET	C-N-CA	-5.24	114.02	122.82
2	B	203	CYS	N-CA-C	5.24	117.50	107.75
1	G	205	ASP	CA-CB-CG	5.24	117.84	112.60
1	O	264	ARG	O-C-N	5.24	128.81	122.68
2	R	350	ASN	N-CA-C	5.24	121.96	110.80
2	P	203	CYS	N-CA-C	5.24	117.49	107.75
2	F	96	GLN	O-C-N	5.23	129.37	122.36
2	H	122	VAL	CB-CA-C	-5.23	105.27	111.97
1	K	259	LEU	N-CA-C	5.23	120.67	113.97
2	L	166	MET	CA-C-N	-5.23	114.03	122.82
2	L	166	MET	C-N-CA	-5.23	114.03	122.82
2	N	203	CYS	N-CA-C	5.23	117.48	107.75
1	A	259	LEU	N-CA-C	5.23	120.66	113.97
2	F	228	ASN	CA-CB-CG	-5.23	107.37	112.60
1	C	259	LEU	N-CA-C	5.22	120.66	113.97
1	O	156	ARG	NE-CZ-NH2	5.22	123.90	119.20
2	P	228	ASN	CA-CB-CG	-5.22	107.38	112.60
1	M	334	THR	CA-C-N	-5.22	111.97	120.64
1	M	334	THR	C-N-CA	-5.22	111.97	120.64
2	J	122	VAL	CB-CA-C	-5.22	105.29	111.97
2	B	122	VAL	CB-CA-C	-5.22	105.29	111.97
2	J	228	ASN	CA-CB-CG	-5.22	107.38	112.60
1	K	379	SER	N-CA-C	5.22	117.67	108.75
1	K	156	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	D	238	VAL	CA-C-N	-5.21	112.49	121.66
2	D	238	VAL	C-N-CA	-5.21	112.49	121.66
1	E	264	ARG	O-C-N	5.21	128.78	122.68
1	E	156	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	N	238	VAL	CA-C-N	-5.21	112.49	121.66
2	N	238	VAL	C-N-CA	-5.21	112.49	121.66
1	Q	264	ARG	O-C-N	5.21	128.77	122.68
2	F	166	MET	CA-C-N	-5.21	114.07	122.82
2	F	166	MET	C-N-CA	-5.21	114.07	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	334	THR	CA-C-N	-5.21	112.00	120.64
1	G	334	THR	C-N-CA	-5.21	112.00	120.64
2	L	238	VAL	CA-C-N	-5.21	112.50	121.66
2	L	238	VAL	C-N-CA	-5.21	112.50	121.66
1	E	259	LEU	N-CA-C	5.20	120.63	113.97
1	M	259	LEU	N-CA-C	5.20	120.63	113.97
1	A	264	ARG	O-C-N	5.20	128.76	122.68
2	B	238	VAL	CA-C-N	-5.20	112.51	121.66
2	B	238	VAL	C-N-CA	-5.20	112.51	121.66
1	A	334	THR	CA-C-N	-5.20	112.02	120.64
1	A	334	THR	C-N-CA	-5.20	112.02	120.64
2	H	238	VAL	CA-C-N	-5.20	112.52	121.66
2	H	238	VAL	C-N-CA	-5.20	112.52	121.66
2	L	228	ASN	CA-CB-CG	-5.20	107.40	112.60
1	M	138	PHE	CA-CB-CG	-5.20	108.61	113.80
1	O	334	THR	CA-C-N	-5.20	112.01	120.64
1	O	334	THR	C-N-CA	-5.20	112.01	120.64
1	Q	334	THR	CA-C-N	-5.20	112.02	120.64
1	Q	334	THR	C-N-CA	-5.20	112.02	120.64
2	P	122	VAL	CB-CA-C	-5.19	105.32	111.97
2	B	47	GLU	N-CA-C	5.19	119.94	111.37
1	I	334	THR	CA-C-N	-5.19	112.02	120.64
1	I	334	THR	C-N-CA	-5.19	112.02	120.64
2	F	122	VAL	CB-CA-C	-5.19	105.33	111.97
2	N	228	ASN	CA-CB-CG	-5.19	107.41	112.60
1	C	138	PHE	CA-CB-CG	-5.18	108.62	113.80
1	C	264	ARG	O-C-N	5.18	128.74	122.68
2	R	122	VAL	CB-CA-C	-5.18	105.34	111.97
1	K	334	THR	CA-C-N	-5.18	112.04	120.64
1	K	334	THR	C-N-CA	-5.18	112.04	120.64
2	P	226	ASP	N-CA-C	-5.18	106.12	112.90
2	N	226	ASP	N-CA-C	-5.17	106.12	112.90
2	J	238	VAL	CA-C-N	-5.17	112.56	121.66
2	J	238	VAL	C-N-CA	-5.17	112.56	121.66
2	F	226	ASP	N-CA-C	-5.17	106.13	112.90
1	I	138	PHE	CA-CB-CG	-5.17	108.63	113.80
1	M	98	ASP	O-C-N	5.17	128.73	122.94
1	O	138	PHE	CA-CB-CG	-5.17	108.63	113.80
2	R	238	VAL	CA-C-N	-5.17	112.56	121.66
2	R	238	VAL	C-N-CA	-5.17	112.56	121.66
2	P	238	VAL	CA-C-N	-5.17	112.57	121.66
2	P	238	VAL	C-N-CA	-5.17	112.57	121.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	47	GLU	N-CA-C	5.16	119.88	111.37
2	D	226	ASP	N-CA-C	-5.16	106.14	112.90
2	J	47	GLU	N-CA-C	5.16	119.88	111.37
2	B	226	ASP	N-CA-C	-5.16	106.14	112.90
2	H	226	ASP	N-CA-C	-5.15	106.15	112.90
2	H	47	GLU	N-CA-C	5.15	119.87	111.37
2	L	226	ASP	N-CA-C	-5.15	106.15	112.90
1	Q	138	PHE	CA-CB-CG	-5.15	108.65	113.80
1	K	264	ARG	O-C-N	5.15	128.71	122.68
2	F	238	VAL	CA-C-N	-5.15	112.60	121.66
2	F	238	VAL	C-N-CA	-5.15	112.60	121.66
2	N	47	GLU	N-CA-C	5.15	119.86	111.37
2	J	226	ASP	N-CA-C	-5.14	106.16	112.90
1	K	98	ASP	O-C-N	5.14	128.70	122.94
1	A	98	ASP	O-C-N	5.14	128.70	122.94
1	O	98	ASP	O-C-N	5.14	128.70	122.94
2	F	47	GLU	N-CA-C	5.14	119.85	111.37
1	M	264	ARG	O-C-N	5.14	128.69	122.68
2	P	47	GLU	N-CA-C	5.13	119.84	111.37
1	I	264	ARG	O-C-N	5.13	128.68	122.68
1	G	138	PHE	CA-CB-CG	-5.13	108.67	113.80
2	R	226	ASP	N-CA-C	-5.13	106.18	112.90
1	A	121	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	E	339	ARG	NH1-CZ-NH2	-5.13	112.64	119.30
1	I	98	ASP	O-C-N	5.12	128.68	122.94
1	G	98	ASP	O-C-N	5.12	128.67	122.94
2	L	122	VAL	CB-CA-C	-5.11	105.43	111.97
2	D	47	GLU	N-CA-C	5.11	119.80	111.37
1	E	138	PHE	CA-CB-CG	-5.11	108.69	113.80
1	E	98	ASP	O-C-N	5.10	128.66	122.94
1	K	138	PHE	CA-CB-CG	-5.10	108.70	113.80
1	G	339	ARG	NH1-CZ-NH2	-5.10	112.67	119.30
2	L	47	GLU	N-CA-C	5.10	119.78	111.37
1	C	98	ASP	O-C-N	5.10	128.65	122.94
1	A	138	PHE	CA-CB-CG	-5.09	108.70	113.80
1	Q	98	ASP	O-C-N	5.09	128.65	122.94
1	Q	339	ARG	NH1-CZ-NH2	-5.09	112.69	119.30
2	N	139	HIS	CA-CB-CG	-5.08	108.72	113.80
1	Q	300	ASN	CA-CB-CG	-5.08	107.52	112.60
1	M	121	ARG	NE-CZ-NH1	-5.08	116.42	121.50
2	J	139	HIS	CA-CB-CG	-5.07	108.73	113.80
2	H	97	SER	O-C-N	5.07	129.63	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	HIS	CA-CB-CG	-5.07	108.73	113.80
2	P	139	HIS	CA-CB-CG	-5.07	108.73	113.80
1	E	300	ASN	CA-CB-CG	-5.06	107.54	112.60
2	P	97	SER	O-C-N	5.06	129.62	123.14
2	R	97	SER	O-C-N	5.06	129.62	123.14
1	C	339	ARG	NH1-CZ-NH2	-5.05	112.73	119.30
2	R	139	HIS	CA-CB-CG	-5.05	108.75	113.80
2	H	139	HIS	CA-CB-CG	-5.05	108.75	113.80
1	M	300	ASN	CA-CB-CG	-5.05	107.55	112.60
2	F	260	VAL	CA-C-N	5.04	124.74	119.64
2	F	260	VAL	C-N-CA	5.04	124.74	119.64
1	C	68	VAL	N-CA-C	5.04	115.11	107.75
2	F	400	ARG	NE-CZ-NH1	-5.04	116.46	121.50
2	J	97	SER	O-C-N	5.04	129.60	123.14
1	K	300	ASN	CA-CB-CG	-5.04	107.56	112.60
2	B	139	HIS	CA-CB-CG	-5.04	108.76	113.80
2	F	97	SER	O-C-N	5.04	129.59	123.14
2	J	400	ARG	NE-CZ-NH1	-5.04	116.46	121.50
2	N	97	SER	O-C-N	5.04	129.59	123.14
1	O	339	ARG	NH1-CZ-NH2	-5.03	112.76	119.30
1	Q	121	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	M	339	ARG	NH1-CZ-NH2	-5.03	112.76	119.30
1	A	339	ARG	NH1-CZ-NH2	-5.03	112.77	119.30
1	I	214	ARG	NE-CZ-NH2	-5.03	114.67	119.20
2	N	260	VAL	CA-C-N	5.03	124.72	119.64
2	N	260	VAL	C-N-CA	5.03	124.72	119.64
2	B	97	SER	O-C-N	5.03	129.57	123.14
1	I	339	ARG	NH1-CZ-NH2	-5.02	112.77	119.30
2	L	97	SER	O-C-N	5.02	129.57	123.14
2	F	356	CYS	N-CA-CB	-5.02	102.09	110.83
2	J	260	VAL	CA-C-N	5.02	124.71	119.64
2	J	260	VAL	C-N-CA	5.02	124.71	119.64
1	K	339	ARG	NH1-CZ-NH2	-5.02	112.77	119.30
2	P	400	ARG	NE-CZ-NH1	-5.02	116.48	121.50
2	D	356	CYS	N-CA-CB	-5.02	102.09	110.83
2	J	356	CYS	N-CA-CB	-5.02	102.09	110.83
1	K	121	ARG	NE-CZ-NH1	-5.02	116.48	121.50
2	L	400	ARG	NE-CZ-NH1	-5.02	116.48	121.50
2	B	215	ARG	N-CA-C	5.02	116.44	111.07
2	D	260	VAL	CA-C-N	5.02	124.71	119.64
2	D	260	VAL	C-N-CA	5.02	124.71	119.64
1	E	214	ARG	NE-CZ-NH2	-5.02	114.68	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	67	LEU	CA-C-N	-5.02	116.14	123.06
2	L	67	LEU	C-N-CA	-5.02	116.14	123.06
2	H	400	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	F	139	HIS	CA-CB-CG	-5.01	108.79	113.80
2	L	139	HIS	CA-CB-CG	-5.01	108.79	113.80
1	G	121	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	N	400	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	D	97	SER	O-C-N	5.01	129.55	123.14
1	G	300	ASN	CA-CB-CG	-5.01	107.59	112.60
1	C	300	ASN	CA-CB-CG	-5.01	107.59	112.60
2	J	215	ARG	N-CA-C	5.01	116.43	111.07
1	A	14	VAL	N-CA-C	5.00	115.23	110.53
2	B	356	CYS	N-CA-CB	-5.00	102.12	110.83
1	M	107	HIS	CA-CB-CG	5.00	118.80	113.80
2	R	356	CYS	N-CA-CB	-5.00	102.12	110.83
1	C	121	ARG	NE-CZ-NH1	-5.00	116.50	121.50
2	D	215	ARG	N-CA-C	5.00	116.42	111.07
2	H	215	ARG	N-CA-C	5.00	116.42	111.07
2	J	67	LEU	CA-C-N	-5.00	116.16	123.06
2	J	67	LEU	C-N-CA	-5.00	116.16	123.06

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	248	LEU	Peptide
2	D	248	LEU	Peptide
2	F	248	LEU	Peptide
2	H	248	LEU	Peptide
2	J	248	LEU	Peptide
2	L	248	LEU	Peptide
2	N	248	LEU	Peptide
2	P	248	LEU	Peptide
2	R	248	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3350	0	3254	405	0
1	C	3350	0	3254	366	0
1	E	3350	0	3254	373	0
1	G	3350	0	3254	372	0
1	I	3350	0	3254	391	0
1	K	3350	0	3254	366	0
1	M	3350	0	3254	305	0
1	O	3350	0	3254	336	0
1	Q	3350	0	3254	301	0
2	B	3352	0	3227	393	0
2	D	3352	0	3227	362	0
2	F	3352	0	3227	364	0
2	H	3352	0	3227	302	0
2	J	3352	0	3227	329	0
2	L	3352	0	3227	302	0
2	N	3352	0	3227	412	0
2	P	3352	0	3227	474	0
2	R	3352	0	3227	411	0
3	A	32	0	12	3	0
3	C	32	0	12	3	0
3	E	32	0	12	3	0
3	G	32	0	12	3	0
3	I	32	0	12	3	0
3	K	32	0	12	3	0
3	M	32	0	12	3	0
3	O	32	0	12	3	0
3	Q	32	0	12	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
5	B	28	0	12	2	0
5	D	28	0	12	2	0
5	F	28	0	12	2	0
5	H	28	0	12	2	0
5	J	28	0	12	2	0
5	L	28	0	12	2	0
5	N	28	0	12	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	28	0	12	3	0
5	R	28	0	12	2	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
6	E	4	0	0	0	0
6	G	4	0	0	0	0
6	I	4	0	0	0	0
6	K	4	0	0	0	0
6	M	4	0	0	0	0
6	O	4	0	0	0	0
6	Q	4	0	0	0	0
All	All	60903	0	58545	3602	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 (3602) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:CA	2:H:352:LYS:HE3	1.19	1.64
1:E:181:VAL:CA	2:F:352:LYS:HE3	1.25	1.62
1:I:181:VAL:CA	2:J:352:LYS:HE3	1.17	1.61
1:C:181:VAL:CA	2:D:352:LYS:HE3	1.28	1.58
1:M:181:VAL:CA	2:N:352:LYS:HE3	1.17	1.58
1:K:181:VAL:CA	2:L:352:LYS:HE3	1.18	1.58
1:A:181:VAL:CA	2:B:352:LYS:HE3	1.28	1.57
1:O:181:VAL:CA	2:P:352:LYS:HE3	1.11	1.57
1:Q:181:VAL:CA	2:R:352:LYS:HE3	1.16	1.55
1:O:181:VAL:HA	2:P:352:LYS:CE	1.38	1.52
1:I:224:TYR:CE1	2:J:325:MET:SD	2.04	1.51
1:K:224:TYR:CE1	2:L:325:MET:SD	2.04	1.50
1:O:101:ASN:CB	2:P:254:LYS:HE3	1.33	1.50
1:O:176:GLN:CB	2:P:333:LEU:HD22	1.37	1.48
1:I:101:ASN:CB	2:J:254:LYS:HE3	1.40	1.48
1:O:176:GLN:HB3	2:P:333:LEU:CD2	1.43	1.47
1:G:224:TYR:CE1	2:H:325:MET:SD	2.08	1.47
1:Q:101:ASN:CB	2:R:254:LYS:HE3	1.43	1.47
1:M:101:ASN:CB	2:N:254:LYS:HE3	1.40	1.47
1:G:101:ASN:CB	2:H:254:LYS:HE3	1.43	1.46
1:M:176:GLN:CB	2:N:333:LEU:HD22	1.44	1.46
1:M:181:VAL:HA	2:N:352:LYS:CE	1.44	1.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:101:ASN:CB	2:L:254:LYS:HE3	1.45	1.45
1:O:210:TYR:CE2	2:P:326:LYS:HA	1.53	1.44
1:Q:181:VAL:HA	2:R:352:LYS:CE	1.44	1.44
1:I:176:GLN:HB3	2:J:333:LEU:CD2	1.48	1.44
1:A:346:TRP:CZ3	2:P:403:ALA:HB1	1.52	1.43
1:A:346:TRP:CE3	2:P:403:ALA:HB2	1.53	1.43
1:I:176:GLN:CB	2:J:333:LEU:HD22	1.45	1.43
1:Q:176:GLN:CB	2:R:333:LEU:HD22	1.44	1.42
1:G:176:GLN:CB	2:H:333:LEU:HD22	1.48	1.42
1:A:101:ASN:CB	2:B:254:LYS:HE3	1.49	1.42
1:O:179:THR:CG2	2:P:353:THR:OG1	1.68	1.42
1:M:176:GLN:HB3	2:N:333:LEU:CD2	1.49	1.42
1:Q:176:GLN:HB3	2:R:333:LEU:CD2	1.47	1.42
1:I:181:VAL:HA	2:J:352:LYS:CE	1.48	1.42
1:A:2:ARG:CG	2:P:96:GLN:HE22	1.30	1.41
1:G:176:GLN:HB3	2:H:333:LEU:CD2	1.50	1.41
1:O:101:ASN:HB2	2:P:254:LYS:CE	1.46	1.41
1:E:224:TYR:CE1	2:F:325:MET:SD	2.14	1.41
1:K:176:GLN:CB	2:L:333:LEU:HD22	1.49	1.41
1:E:346:TRP:CZ3	2:R:403:ALA:HB1	1.55	1.40
1:I:101:ASN:HB2	2:J:254:LYS:CE	1.49	1.40
1:K:176:GLN:HB3	2:L:333:LEU:CD2	1.48	1.40
1:A:224:TYR:CE1	2:B:325:MET:SD	2.13	1.40
1:C:101:ASN:CB	2:D:254:LYS:HE3	1.51	1.40
1:M:210:TYR:CE2	2:N:326:LYS:HA	1.57	1.40
1:A:329:ASN:OD1	2:P:177:VAL:CG2	1.67	1.39
1:A:346:TRP:HB3	2:P:401:ARG:CG	1.50	1.39
1:C:224:TYR:CE1	2:D:325:MET:SD	2.16	1.39
1:C:346:TRP:CZ3	2:N:403:ALA:HB1	1.57	1.38
1:G:181:VAL:HA	2:H:352:LYS:CE	1.51	1.38
1:I:210:TYR:CE2	2:J:326:LYS:HA	1.59	1.38
1:C:2:ARG:CG	2:N:96:GLN:HE22	1.36	1.37
1:G:101:ASN:HB2	2:H:254:LYS:CE	1.52	1.37
1:K:181:VAL:HA	2:L:352:LYS:CE	1.51	1.37
1:Q:210:TYR:CZ	2:R:326:LYS:HA	1.60	1.37
1:Q:210:TYR:CE2	2:R:326:LYS:HA	1.59	1.37
1:E:346:TRP:CE3	2:R:403:ALA:HB2	1.59	1.36
1:A:2:ARG:HG3	2:P:96:GLN:NE2	1.36	1.36
1:K:101:ASN:HB2	2:L:254:LYS:CE	1.55	1.36
1:E:101:ASN:CB	2:F:254:LYS:HE3	1.54	1.36
1:C:346:TRP:CE3	2:N:403:ALA:HB2	1.59	1.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:101:ASN:HB2	2:N:254:LYS:CE	1.52	1.36
1:O:210:TYR:CE1	2:P:326:LYS:HB2	1.58	1.36
1:Q:101:ASN:HB2	2:R:254:LYS:CE	1.55	1.36
1:Q:97:GLU:CD	2:R:2:ARG:HH21	1.34	1.35
1:M:179:THR:HG22	2:N:353:THR:OG1	1.18	1.35
1:O:97:GLU:CD	2:P:2:ARG:HH21	1.35	1.35
1:C:2:ARG:HG3	2:N:96:GLN:NE2	1.41	1.35
1:M:179:THR:CG2	2:N:353:THR:OG1	1.73	1.35
1:Q:210:TYR:CE1	2:R:326:LYS:HB2	1.60	1.35
1:C:346:TRP:HB3	2:N:401:ARG:CG	1.56	1.34
1:E:329:ASN:OD1	2:R:177:VAL:CG2	1.72	1.34
1:Q:179:THR:CG2	2:R:353:THR:OG1	1.74	1.34
1:C:329:ASN:OD1	2:N:177:VAL:CG2	1.72	1.34
1:O:210:TYR:CZ	2:P:326:LYS:HA	1.61	1.34
2:B:403:ALA:HB1	1:I:346:TRP:CZ3	1.61	1.34
1:G:210:TYR:CE2	2:H:326:LYS:HA	1.62	1.34
1:A:346:TRP:CB	2:P:401:ARG:HG3	1.56	1.34
1:A:350:GLY:O	2:P:181:VAL:CG2	1.77	1.33
1:E:2:ARG:CG	2:R:96:GLN:HE22	1.39	1.33
1:M:210:TYR:CZ	2:N:326:LYS:HA	1.62	1.33
1:A:346:TRP:CZ3	2:P:403:ALA:CB	2.11	1.33
1:A:101:ASN:HB2	2:B:254:LYS:CE	1.57	1.33
1:A:181:VAL:HA	2:B:352:LYS:CE	1.58	1.32
1:M:97:GLU:CD	2:N:2:ARG:HH21	1.36	1.32
1:M:210:TYR:CE1	2:N:326:LYS:HB2	1.62	1.32
2:D:177:VAL:HG23	1:G:329:ASN:OD1	1.14	1.32
1:E:181:VAL:HA	2:F:352:LYS:CE	1.58	1.32
2:F:177:VAL:HG23	1:K:329:ASN:OD1	1.16	1.31
1:K:210:TYR:CE2	2:L:326:LYS:HA	1.65	1.31
1:O:210:TYR:CZ	2:P:326:LYS:CA	2.13	1.31
1:I:179:THR:CG2	2:J:353:THR:OG1	1.79	1.31
1:K:210:TYR:CZ	2:L:326:LYS:HA	1.66	1.31
1:C:181:VAL:HA	2:D:352:LYS:CE	1.59	1.31
1:I:210:TYR:CE1	2:J:326:LYS:HB2	1.62	1.31
2:J:283:TYR:HA	2:L:56:ALA:CB	1.57	1.31
1:C:350:GLY:O	2:N:181:VAL:HG22	1.23	1.31
1:G:179:THR:HG22	2:H:353:THR:OG1	1.25	1.31
2:D:403:ALA:HB1	1:G:346:TRP:CZ3	1.66	1.30
1:K:97:GLU:CD	2:L:2:ARG:HH21	1.39	1.30
1:O:97:GLU:OE2	2:P:2:ARG:NE	1.61	1.30
1:C:101:ASN:HB2	2:D:254:LYS:CE	1.60	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:101:ASN:N	2:P:254:LYS:HD2	1.45	1.30
1:O:177:VAL:HG21	2:P:329:ASP:C	1.53	1.30
2:B:403:ALA:HB2	1:I:346:TRP:CE3	1.65	1.30
1:C:346:TRP:CB	2:N:401:ARG:HG3	1.59	1.30
1:C:176:GLN:CB	2:D:333:LEU:HD22	1.61	1.29
1:E:176:GLN:HB3	2:F:333:LEU:CD2	1.59	1.29
1:I:210:TYR:CZ	2:J:326:LYS:HA	1.66	1.29
1:K:210:TYR:CE1	2:L:326:LYS:HB2	1.64	1.29
1:O:97:GLU:OE1	2:P:2:ARG:NH2	1.63	1.29
2:P:283:TYR:HA	2:R:56:ALA:CB	1.61	1.29
1:E:97:GLU:CD	2:F:2:ARG:HH21	1.39	1.29
1:G:210:TYR:CE1	2:H:326:LYS:HB2	1.66	1.29
2:B:177:VAL:CG2	1:I:329:ASN:OD1	1.78	1.29
1:O:179:THR:HG22	2:P:353:THR:OG1	1.12	1.29
1:E:346:TRP:HB3	2:R:401:ARG:CG	1.62	1.29
1:I:97:GLU:CD	2:J:2:ARG:HH21	1.41	1.29
1:Q:210:TYR:CZ	2:R:326:LYS:CA	2.16	1.28
1:A:176:GLN:CB	2:B:333:LEU:HD22	1.61	1.28
1:A:179:THR:HG22	2:B:353:THR:OG1	1.28	1.28
1:E:176:GLN:CB	2:F:333:LEU:HD22	1.62	1.28
1:I:97:GLU:OE2	2:J:2:ARG:NE	1.66	1.28
1:C:176:GLN:HB3	2:D:333:LEU:CD2	1.62	1.28
1:C:346:TRP:CZ3	2:N:403:ALA:CB	2.16	1.28
2:F:403:ALA:HB1	1:K:346:TRP:CZ3	1.67	1.28
1:I:179:THR:HG22	2:J:353:THR:OG1	1.22	1.28
1:M:210:TYR:CZ	2:N:326:LYS:CA	2.17	1.28
1:A:176:GLN:HB3	2:B:333:LEU:CD2	1.63	1.27
1:O:210:TYR:CD1	2:P:326:LYS:HB2	1.69	1.27
2:B:177:VAL:HG23	1:I:329:ASN:OD1	1.09	1.27
1:E:101:ASN:HB2	2:F:254:LYS:CE	1.64	1.27
1:E:2:ARG:HG3	2:R:96:GLN:NE2	1.47	1.27
1:A:97:GLU:CD	2:B:2:ARG:HH21	1.42	1.27
1:A:350:GLY:O	2:P:181:VAL:HG22	1.18	1.26
2:B:401:ARG:CG	1:I:346:TRP:HB3	1.65	1.26
1:E:346:TRP:CZ3	2:R:403:ALA:CB	2.17	1.26
2:B:181:VAL:HG22	1:I:350:GLY:O	1.31	1.26
1:C:350:GLY:O	2:N:181:VAL:CG2	1.83	1.26
1:E:350:GLY:O	2:R:181:VAL:HG22	1.30	1.26
1:G:179:THR:CG2	2:H:353:THR:OG1	1.83	1.26
2:D:177:VAL:CG2	1:G:329:ASN:OD1	1.82	1.26
1:K:179:THR:CG2	2:L:353:THR:OG1	1.83	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE2	2:B:326:LYS:HA	1.71	1.26
2:D:96:GLN:HE22	1:G:2:ARG:CG	1.49	1.26
1:C:97:GLU:CD	2:D:2:ARG:HH21	1.44	1.25
1:M:97:GLU:OE2	2:N:2:ARG:NE	1.67	1.25
1:M:210:TYR:CD1	2:N:326:LYS:HB2	1.72	1.25
1:Q:177:VAL:HG21	2:R:329:ASP:O	1.36	1.25
1:Q:179:THR:HG22	2:R:353:THR:OG1	1.22	1.25
2:B:96:GLN:HE22	1:I:2:ARG:CG	1.49	1.25
1:C:179:THR:HG22	2:D:353:THR:OG1	1.30	1.25
1:G:97:GLU:CD	2:H:2:ARG:HH21	1.43	1.25
1:I:210:TYR:CZ	2:J:326:LYS:CA	2.20	1.25
1:A:260:VAL:O	2:P:406:HIS:CE1	1.87	1.25
2:D:96:GLN:NE2	1:G:2:ARG:HG3	1.52	1.24
1:G:210:TYR:CZ	2:H:326:LYS:HA	1.70	1.24
2:H:283:TYR:HA	2:J:56:ALA:CB	1.66	1.24
1:M:177:VAL:HG21	2:N:329:ASP:C	1.60	1.24
1:Q:210:TYR:CD1	2:R:326:LYS:HB2	1.72	1.24
1:O:105:ARG:NH2	2:P:253:ARG:NH2	1.84	1.24
2:D:403:ALA:HB2	1:G:346:TRP:CE3	1.70	1.24
2:F:177:VAL:CG2	1:K:329:ASN:OD1	1.83	1.24
1:K:179:THR:HG22	2:L:353:THR:OG1	1.29	1.24
1:O:177:VAL:HG21	2:P:329:ASP:O	1.34	1.24
1:G:97:GLU:OE2	2:H:2:ARG:NE	1.70	1.24
1:M:97:GLU:OE1	2:N:2:ARG:NH2	1.69	1.24
1:M:101:ASN:N	2:N:254:LYS:HD2	1.50	1.24
1:Q:97:GLU:OE2	2:R:2:ARG:NE	1.69	1.24
2:F:403:ALA:HB2	1:K:346:TRP:CE3	1.72	1.23
1:O:97:GLU:CD	2:P:2:ARG:NH2	1.96	1.23
1:A:179:THR:CG2	2:B:353:THR:OG1	1.86	1.23
2:B:401:ARG:HG3	1:I:346:TRP:CB	1.67	1.23
1:C:210:TYR:CE2	2:D:326:LYS:HA	1.72	1.23
1:E:346:TRP:CB	2:R:401:ARG:HG3	1.67	1.23
1:K:210:TYR:CZ	2:L:326:LYS:CA	2.22	1.23
1:E:179:THR:HG22	2:F:353:THR:OG1	1.36	1.23
1:K:97:GLU:OE2	2:L:2:ARG:NE	1.69	1.23
1:Q:97:GLU:CD	2:R:2:ARG:NH2	1.97	1.23
2:B:96:GLN:NE2	1:I:2:ARG:HG3	1.53	1.22
1:Q:177:VAL:HG21	2:R:329:ASP:C	1.62	1.22
2:B:403:ALA:CB	1:I:346:TRP:CZ3	2.23	1.22
1:M:76:ASP:OD2	2:N:48:ARG:NH2	1.71	1.22
1:I:210:TYR:CD1	2:J:326:LYS:HB2	1.74	1.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:101:ASN:N	2:R:254:LYS:HD2	1.53	1.22
1:A:97:GLU:OE2	2:B:2:ARG:NE	1.73	1.21
1:E:350:GLY:O	2:R:181:VAL:CG2	1.88	1.21
2:F:96:GLN:HE22	1:K:2:ARG:CG	1.52	1.21
2:N:283:TYR:HA	2:P:56:ALA:CB	1.68	1.21
2:D:401:ARG:CG	1:G:346:TRP:HB3	1.70	1.21
1:E:210:TYR:CE2	2:F:326:LYS:HA	1.76	1.21
1:E:329:ASN:OD1	2:R:177:VAL:HG23	1.05	1.21
1:I:177:VAL:HG21	2:J:329:ASP:C	1.61	1.21
1:M:97:GLU:CD	2:N:2:ARG:NH2	1.99	1.21
1:Q:97:GLU:OE1	2:R:2:ARG:NH2	1.71	1.21
1:O:177:VAL:CG2	2:P:329:ASP:O	1.88	1.21
2:D:181:VAL:HG22	1:G:350:GLY:O	1.34	1.21
1:G:177:VAL:HG21	2:H:329:ASP:C	1.64	1.21
1:G:210:TYR:CZ	2:H:326:LYS:CA	2.24	1.21
1:M:177:VAL:HG21	2:N:329:ASP:O	1.38	1.21
1:A:210:TYR:CZ	2:B:326:LYS:HA	1.76	1.20
1:M:222:PRO:O	2:N:324:SER:HB2	1.41	1.20
1:C:179:THR:CG2	2:D:353:THR:OG1	1.89	1.20
1:M:105:ARG:NH2	2:N:253:ARG:NH2	1.90	1.20
2:D:401:ARG:HG3	1:G:346:TRP:CB	1.69	1.20
1:E:76:ASP:OD2	2:F:48:ARG:NH2	1.75	1.20
1:Q:76:ASP:OD2	2:R:48:ARG:NH2	1.71	1.20
1:Q:222:PRO:O	2:R:324:SER:HB2	1.40	1.20
1:C:260:VAL:O	2:N:406:HIS:CE1	1.94	1.20
2:F:181:VAL:HG22	1:K:350:GLY:O	1.38	1.20
1:I:101:ASN:N	2:J:254:LYS:HD2	1.57	1.20
1:A:76:ASP:OD2	2:B:48:ARG:NH2	1.75	1.19
1:C:329:ASN:OD1	2:N:177:VAL:HG23	1.02	1.19
1:E:210:TYR:CZ	2:F:326:LYS:HA	1.77	1.19
1:O:222:PRO:O	2:P:324:SER:HB2	1.39	1.19
1:I:97:GLU:OE1	2:J:2:ARG:NH2	1.74	1.19
1:G:210:TYR:CD1	2:H:326:LYS:HB2	1.78	1.19
2:F:96:GLN:NE2	1:K:2:ARG:HG3	1.57	1.19
1:O:76:ASP:OD2	2:P:48:ARG:NH2	1.72	1.19
1:K:181:VAL:CA	2:L:352:LYS:CE	2.13	1.19
1:K:97:GLU:CD	2:L:2:ARG:NH2	2.00	1.18
1:C:210:TYR:CZ	2:D:326:LYS:HA	1.78	1.18
1:O:406:HIS:CE1	2:P:260:VAL:HG12	1.76	1.18
2:F:401:ARG:CG	1:K:346:TRP:HB3	1.74	1.18
1:E:179:THR:CG2	2:F:353:THR:OG1	1.91	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:97:GLU:CD	2:J:2:ARG:NH2	2.01	1.18
1:A:210:TYR:CE1	2:B:326:LYS:HB2	1.78	1.17
2:B:181:VAL:CG2	1:I:350:GLY:O	1.92	1.17
1:K:210:TYR:CD1	2:L:326:LYS:HB2	1.78	1.17
1:I:76:ASP:OD2	2:J:48:ARG:NH2	1.76	1.17
1:K:177:VAL:HG21	2:L:329:ASP:C	1.67	1.17
1:A:353:VAL:HB	2:P:179:ASP:OD1	1.42	1.17
2:D:403:ALA:CB	1:G:346:TRP:CZ3	2.27	1.17
1:O:404:PHE:N	2:P:261:PRO:HA	1.58	1.17
1:A:260:VAL:O	2:P:406:HIS:HE1	1.19	1.17
1:E:210:TYR:CE1	2:F:326:LYS:HB2	1.78	1.17
2:F:401:ARG:HG3	1:K:346:TRP:CB	1.74	1.17
1:G:181:VAL:CA	2:H:352:LYS:CE	2.15	1.17
1:I:181:VAL:CA	2:J:352:LYS:CE	2.13	1.17
1:I:222:PRO:O	2:J:324:SER:HB2	1.43	1.17
1:C:97:GLU:OE2	2:D:2:ARG:NE	1.78	1.16
1:E:100:ALA:HA	2:F:254:LYS:HB2	1.27	1.16
1:K:177:VAL:HG21	2:L:329:ASP:O	1.45	1.16
1:C:260:VAL:O	2:N:406:HIS:HE1	1.23	1.16
2:P:283:TYR:C	2:R:56:ALA:HB1	1.70	1.16
1:C:210:TYR:CE1	2:D:326:LYS:HB2	1.80	1.16
1:K:97:GLU:OE1	2:L:2:ARG:NH2	1.77	1.16
1:E:181:VAL:CA	2:F:352:LYS:CE	2.20	1.16
1:E:346:TRP:CE3	2:R:403:ALA:CB	2.28	1.16
1:G:101:ASN:N	2:H:254:LYS:HD2	1.61	1.16
1:K:76:ASP:OD2	2:L:48:ARG:NH2	1.75	1.16
1:Q:105:ARG:NH2	2:R:253:ARG:NH2	1.93	1.16
1:C:76:ASP:OD2	2:D:48:ARG:NH2	1.77	1.15
1:E:260:VAL:O	2:R:406:HIS:CE1	1.98	1.15
1:M:406:HIS:CE1	2:N:260:VAL:HG12	1.80	1.15
1:A:97:GLU:OE1	2:B:2:ARG:NH2	1.78	1.15
1:A:100:ALA:HA	2:B:254:LYS:HB2	1.25	1.15
1:A:346:TRP:CE3	2:P:403:ALA:CB	2.27	1.15
1:A:133:GLN:NE2	2:P:97:SER:OG	1.80	1.15
1:E:260:VAL:O	2:R:406:HIS:HE1	1.28	1.15
1:I:177:VAL:HG21	2:J:329:ASP:O	1.43	1.15
1:O:105:ARG:HH21	2:P:253:ARG:NH2	1.42	1.15
1:O:176:GLN:OE1	2:P:333:LEU:HD11	1.44	1.15
1:Q:100:ALA:HA	2:R:254:LYS:HB2	1.16	1.15
1:G:76:ASP:OD2	2:H:48:ARG:NH2	1.78	1.15
1:G:222:PRO:O	2:H:324:SER:HB2	1.46	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:ALA:HA	2:N:254:LYS:HB2	1.15	1.15
1:G:97:GLU:OE1	2:H:2:ARG:NH2	1.79	1.14
2:J:283:TYR:CA	2:L:56:ALA:CB	2.24	1.14
1:K:101:ASN:N	2:L:254:LYS:HD2	1.62	1.14
1:I:100:ALA:HA	2:J:254:LYS:HB2	1.26	1.14
1:K:222:PRO:O	2:L:324:SER:HB2	1.46	1.14
1:M:177:VAL:CG2	2:N:329:ASP:O	1.94	1.14
1:C:100:ALA:HA	2:D:254:LYS:HB2	1.27	1.14
1:M:404:PHE:N	2:N:261:PRO:HA	1.63	1.14
1:Q:177:VAL:CG2	2:R:329:ASP:O	1.94	1.14
1:A:97:GLU:CD	2:B:2:ARG:NH2	2.06	1.14
2:F:403:ALA:CB	1:K:346:TRP:CZ3	2.30	1.14
1:G:97:GLU:CD	2:H:2:ARG:NH2	2.04	1.14
1:E:97:GLU:CD	2:F:2:ARG:NH2	2.04	1.14
1:A:101:ASN:N	2:B:254:LYS:HD2	1.61	1.13
1:I:404:PHE:H	2:J:261:PRO:HA	1.10	1.13
1:Q:406:HIS:CE1	2:R:260:VAL:HG12	1.82	1.13
1:A:329:ASN:OD1	2:P:177:VAL:HG23	0.96	1.13
2:P:283:TYR:CA	2:R:56:ALA:CB	2.25	1.13
1:G:177:VAL:HG21	2:H:329:ASP:O	1.47	1.13
1:O:100:ALA:HA	2:P:254:LYS:HB2	1.14	1.13
3:Q:501:GTP:O3G	2:R:254:LYS:NZ	1.80	1.13
2:D:181:VAL:CG2	1:G:350:GLY:O	1.97	1.12
1:K:100:ALA:HA	2:L:254:LYS:HB2	1.26	1.12
1:M:176:GLN:OE1	2:N:333:LEU:HD11	1.48	1.12
1:M:105:ARG:HH21	2:N:253:ARG:NH2	1.46	1.12
1:C:353:VAL:HB	2:N:179:ASP:OD1	1.46	1.12
1:G:100:ALA:HA	2:H:254:LYS:HB2	1.28	1.12
2:H:283:TYR:HD2	2:J:62:VAL:HG22	1.11	1.12
1:O:210:TYR:CD2	2:P:326:LYS:HG3	1.84	1.12
1:Q:11:GLN:NE2	2:R:247:GLN:O	1.83	1.12
1:A:346:TRP:HB2	2:P:401:ARG:CB	1.79	1.12
1:I:177:VAL:CG2	2:J:329:ASP:O	1.97	1.12
1:A:210:TYR:CZ	2:B:326:LYS:CA	2.33	1.12
2:J:283:TYR:CD2	2:L:62:VAL:HG22	1.84	1.12
1:C:101:ASN:N	2:D:254:LYS:HD2	1.65	1.11
1:C:133:GLN:NE2	2:N:97:SER:OG	1.83	1.11
1:E:97:GLU:OE2	2:F:2:ARG:NE	1.81	1.11
1:G:401:LYS:HG3	2:H:346:TRP:CB	1.81	1.11
1:O:181:VAL:CA	2:P:352:LYS:CE	2.08	1.11
1:A:404:PHE:H	2:B:261:PRO:HA	1.11	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:96:LYS:O	2:P:2:ARG:HD2	1.47	1.11
1:Q:176:GLN:OE1	2:R:333:LEU:HD11	1.50	1.11
2:B:179:ASP:OD1	1:I:353:VAL:HB	1.51	1.10
1:C:97:GLU:CD	2:D:2:ARG:NH2	2.08	1.10
1:E:353:VAL:HB	2:R:179:ASP:OD1	1.49	1.10
1:I:105:ARG:NH2	2:J:253:ARG:NH2	1.97	1.10
3:O:501:GTP:O3G	2:P:254:LYS:NZ	1.83	1.10
1:C:97:GLU:OE1	2:D:2:ARG:NH2	1.83	1.10
1:A:177:VAL:HG21	2:B:329:ASP:C	1.75	1.10
2:B:406:HIS:HE1	1:I:260:VAL:O	1.33	1.10
1:O:176:GLN:CB	2:P:333:LEU:CD2	2.13	1.10
1:Q:404:PHE:N	2:R:261:PRO:HA	1.65	1.10
1:A:210:TYR:CD1	2:B:326:LYS:HB2	1.86	1.10
2:B:403:ALA:CB	1:I:346:TRP:CE3	2.34	1.10
1:C:210:TYR:CZ	2:D:326:LYS:CA	2.35	1.10
2:J:283:TYR:HD2	2:L:62:VAL:HG22	1.06	1.10
1:M:181:VAL:CA	2:N:352:LYS:CE	2.13	1.10
1:Q:181:VAL:CA	2:R:352:LYS:CE	2.11	1.10
1:E:210:TYR:CZ	2:F:326:LYS:CA	2.36	1.09
3:M:501:GTP:O3G	2:N:254:LYS:NZ	1.83	1.09
1:O:177:VAL:HG11	2:P:329:ASP:HA	1.23	1.09
1:A:105:ARG:NH2	2:B:253:ARG:NH2	1.99	1.09
2:B:283:TYR:HA	2:F:56:ALA:CB	1.82	1.09
1:C:404:PHE:H	2:D:261:PRO:HA	1.14	1.09
1:C:177:VAL:HG21	2:D:329:ASP:C	1.75	1.09
1:E:133:GLN:NE2	2:R:97:SER:OG	1.85	1.09
2:F:181:VAL:CG2	1:K:350:GLY:O	2.00	1.09
2:J:283:TYR:C	2:L:56:ALA:HB1	1.78	1.09
1:A:181:VAL:CA	2:B:352:LYS:CE	2.24	1.09
1:C:210:TYR:CD1	2:D:326:LYS:HB2	1.87	1.09
1:Q:177:VAL:HG11	2:R:329:ASP:HA	1.29	1.09
2:B:406:HIS:CE1	1:I:260:VAL:O	2.05	1.08
3:K:501:GTP:O3G	2:L:254:LYS:NZ	1.85	1.08
1:O:283:HIS:HA	1:Q:56:THR:HG21	1.33	1.08
1:Q:404:PHE:H	2:R:261:PRO:HA	1.00	1.08
1:A:222:PRO:O	2:B:324:SER:HB2	1.54	1.08
1:E:97:GLU:OE1	2:F:2:ARG:NH2	1.85	1.08
1:E:177:VAL:HG21	2:F:329:ASP:C	1.78	1.08
1:K:224:TYR:CE1	2:L:325:MET:CG	2.35	1.08
1:O:404:PHE:H	2:P:261:PRO:CA	1.64	1.08
1:M:11:GLN:NE2	2:N:247:GLN:O	1.87	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:404:PHE:H	2:N:261:PRO:HA	0.97	1.08
2:D:179:ASP:OD1	1:G:353:VAL:HB	1.53	1.08
1:G:105:ARG:NH2	2:H:253:ARG:NH2	2.02	1.08
1:G:177:VAL:CG2	2:H:329:ASP:O	2.01	1.08
1:I:177:VAL:HG11	2:J:329:ASP:HA	1.31	1.08
1:K:177:VAL:CG2	2:L:329:ASP:O	2.01	1.08
1:M:96:LYS:O	2:N:2:ARG:HD2	1.50	1.08
1:Q:105:ARG:HH21	2:R:253:ARG:NH2	1.50	1.08
1:C:181:VAL:CA	2:D:352:LYS:CE	2.23	1.07
1:K:11:GLN:NE2	2:L:247:GLN:O	1.87	1.07
2:N:283:TYR:C	2:P:56:ALA:HB1	1.76	1.07
2:D:406:HIS:HE1	1:G:260:VAL:O	1.36	1.07
1:E:101:ASN:N	2:F:254:LYS:HD2	1.68	1.07
1:I:401:LYS:HG3	2:J:346:TRP:CB	1.83	1.07
1:O:404:PHE:H	2:P:261:PRO:HA	0.91	1.07
2:P:283:TYR:HA	2:R:56:ALA:HB3	1.37	1.07
1:Q:176:GLN:CB	2:R:333:LEU:CD2	2.17	1.07
1:Q:210:TYR:CD2	2:R:326:LYS:HG3	1.89	1.07
1:A:283:HIS:HA	1:E:56:THR:HG21	1.33	1.07
1:G:404:PHE:H	2:H:261:PRO:HA	1.14	1.07
1:I:210:TYR:CD2	2:J:326:LYS:HG3	1.89	1.07
1:O:11:GLN:NE2	2:P:247:GLN:O	1.88	1.07
1:K:177:VAL:HG11	2:L:329:ASP:HA	1.34	1.07
1:O:406:HIS:CE1	2:P:260:VAL:O	2.08	1.07
1:Q:181:VAL:N	2:R:352:LYS:HE3	1.70	1.07
2:F:179:ASP:OD1	1:K:353:VAL:HB	1.55	1.06
1:K:105:ARG:NH2	2:L:253:ARG:NH2	2.02	1.06
1:M:210:TYR:CD2	2:N:326:LYS:HG3	1.90	1.06
1:O:105:ARG:NH2	2:P:253:ARG:CZ	2.17	1.06
1:A:177:VAL:HG21	2:B:329:ASP:O	1.54	1.06
1:C:222:PRO:O	2:D:324:SER:HB2	1.56	1.06
2:H:283:TYR:CA	2:J:56:ALA:CB	2.33	1.06
1:I:224:TYR:CE1	2:J:325:MET:CG	2.36	1.06
1:K:401:LYS:HG3	2:L:346:TRP:CB	1.84	1.06
2:N:283:TYR:CA	2:P:56:ALA:CB	2.32	1.06
1:E:177:VAL:HG21	2:F:329:ASP:O	1.56	1.06
3:E:501:GTP:O3G	2:F:254:LYS:NZ	1.87	1.06
1:G:401:LYS:HD3	2:H:346:TRP:CE2	1.90	1.06
1:K:404:PHE:H	2:L:261:PRO:HA	1.14	1.06
2:P:283:TYR:C	2:R:56:ALA:CB	2.28	1.06
1:C:105:ARG:NH2	2:D:253:ARG:NH2	2.04	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:TRP:CE3	2:N:403:ALA:CB	2.32	1.06
1:G:177:VAL:HG11	2:H:329:ASP:HA	1.34	1.06
1:M:177:VAL:HG11	2:N:329:ASP:HA	1.30	1.06
2:P:283:TYR:HD2	2:R:62:VAL:HG22	1.18	1.06
1:Q:96:LYS:O	2:R:2:ARG:HD2	1.54	1.06
1:E:401:LYS:HD3	2:F:346:TRP:CE2	1.89	1.05
3:I:501:GTP:O3G	2:J:254:LYS:NZ	1.88	1.05
1:O:394:LYS:HA	2:P:348:PRO:HG3	1.36	1.05
1:E:210:TYR:CD1	2:F:326:LYS:HB2	1.90	1.05
2:H:283:TYR:CD2	2:J:62:VAL:HG22	1.91	1.05
1:M:176:GLN:CB	2:N:333:LEU:CD2	2.19	1.05
1:O:404:PHE:CE2	2:P:258:ASN:O	2.10	1.05
2:F:403:ALA:CB	1:K:346:TRP:CE3	2.40	1.05
1:M:105:ARG:NH2	2:N:253:ARG:CZ	2.20	1.05
1:M:404:PHE:H	2:N:261:PRO:CA	1.68	1.05
2:D:406:HIS:CE1	1:G:260:VAL:O	2.09	1.05
1:A:56:THR:HG21	1:C:283:HIS:HA	1.39	1.05
1:A:346:TRP:HB2	2:P:401:ARG:HB2	1.33	1.05
1:E:222:PRO:O	2:F:324:SER:HB2	1.57	1.05
1:I:181:VAL:CB	2:J:352:LYS:HE3	1.86	1.05
1:M:394:LYS:HZ1	2:N:349:ASN:ND2	1.55	1.05
1:C:346:TRP:HB2	2:N:401:ARG:CB	1.86	1.04
1:E:11:GLN:NE2	2:F:247:GLN:O	1.89	1.04
2:F:406:HIS:HE1	1:K:260:VAL:O	1.39	1.04
3:G:501:GTP:O3G	2:H:254:LYS:NZ	1.90	1.04
1:I:11:GLN:NE2	2:J:247:GLN:O	1.91	1.04
1:A:105:ARG:HH21	2:B:253:ARG:NH2	1.54	1.04
1:G:181:VAL:CB	2:H:352:LYS:HE3	1.85	1.04
1:K:401:LYS:HD3	2:L:346:TRP:CE2	1.90	1.04
1:O:401:LYS:HG3	2:P:346:TRP:CB	1.87	1.04
1:A:96:LYS:O	2:B:2:ARG:HD2	1.57	1.04
2:B:97:SER:OG	1:I:133:GLN:NE2	1.90	1.04
1:E:401:LYS:HG3	2:F:346:TRP:CB	1.87	1.04
1:G:224:TYR:CE1	2:H:325:MET:CG	2.39	1.04
1:I:283:HIS:HA	1:K:56:THR:HG21	1.39	1.04
1:K:210:TYR:CD2	2:L:326:LYS:HG3	1.93	1.04
1:A:2:ARG:NH1	2:P:72:PRO:HB2	1.73	1.04
2:B:56:ALA:CB	2:D:283:TYR:HA	1.88	1.04
1:G:210:TYR:CD2	2:H:326:LYS:HG3	1.93	1.04
1:I:176:GLN:OE1	2:J:333:LEU:HD11	1.56	1.04
1:K:224:TYR:CD1	2:L:325:MET:HG3	1.92	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:401:LYS:HG3	2:L:346:TRP:CG	1.92	1.03
1:O:100:ALA:CA	2:P:254:LYS:HB2	1.87	1.03
1:A:258:ASN:C	2:P:404:PHE:HE2	1.65	1.03
1:C:177:VAL:HG21	2:D:329:ASP:O	1.56	1.03
1:E:401:LYS:HG3	2:F:346:TRP:CG	1.92	1.03
1:I:406:HIS:CE1	2:J:260:VAL:O	2.11	1.03
1:K:181:VAL:N	2:L:352:LYS:HE3	1.71	1.03
1:E:404:PHE:H	2:F:261:PRO:HA	1.19	1.03
2:D:97:SER:OG	1:G:133:GLN:NE2	1.89	1.03
1:G:283:HIS:HA	1:I:56:THR:HG21	1.41	1.03
1:K:181:VAL:CB	2:L:352:LYS:HE3	1.87	1.03
1:O:101:ASN:HB2	2:P:254:LYS:CD	1.88	1.03
1:O:394:LYS:CA	2:P:348:PRO:HG3	1.87	1.03
1:O:394:LYS:NZ	2:P:349:ASN:HD21	1.57	1.03
1:G:406:HIS:CE1	2:H:260:VAL:O	2.12	1.02
1:K:224:TYR:CE1	2:L:325:MET:HG3	1.93	1.02
1:M:283:HIS:HA	1:O:56:THR:HG21	1.42	1.02
1:O:101:ASN:CG	2:P:254:LYS:HE3	1.82	1.02
2:N:283:TYR:HD2	2:P:62:VAL:HG22	1.20	1.02
1:Q:105:ARG:NH2	2:R:253:ARG:CZ	2.22	1.02
1:E:260:VAL:HB	2:R:407:TRP:CZ2	1.94	1.02
2:F:97:SER:OG	1:K:133:GLN:NE2	1.92	1.02
1:G:401:LYS:HG3	2:H:346:TRP:CG	1.94	1.02
1:E:181:VAL:N	2:F:352:LYS:HE3	1.72	1.02
2:J:283:TYR:HA	2:L:56:ALA:HB3	1.40	1.02
1:K:176:GLN:CB	2:L:333:LEU:CD2	2.22	1.02
1:K:406:HIS:CE1	2:L:260:VAL:O	2.13	1.02
1:Q:404:PHE:H	2:R:261:PRO:CA	1.69	1.02
1:I:401:LYS:HD3	2:J:346:TRP:CE2	1.93	1.02
1:O:210:TYR:CE1	2:P:326:LYS:CB	2.43	1.02
1:C:401:LYS:HG3	2:D:346:TRP:CB	1.90	1.01
1:G:11:GLN:NE2	2:H:247:GLN:O	1.93	1.01
1:G:176:GLN:OE1	2:H:333:LEU:HD11	1.59	1.01
1:I:224:TYR:CE1	2:J:325:MET:HG3	1.94	1.01
1:O:210:TYR:OH	2:P:326:LYS:N	1.92	1.01
1:C:346:TRP:HB2	2:N:401:ARG:HB2	1.39	1.01
2:H:283:TYR:C	2:J:56:ALA:HB1	1.84	1.01
2:P:283:TYR:CD2	2:R:62:VAL:HG22	1.95	1.01
1:A:406:HIS:CE1	2:B:260:VAL:HG12	1.94	1.01
1:E:105:ARG:NH2	2:F:253:ARG:NH2	2.08	1.01
1:A:350:GLY:HA3	2:P:181:VAL:HA	1.41	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:283:TYR:C	2:L:56:ALA:CB	2.34	1.01
1:M:181:VAL:N	2:N:352:LYS:HE3	1.75	1.01
1:Q:406:HIS:CE1	2:R:260:VAL:O	2.14	1.01
3:A:501:GTP:O3G	2:B:254:LYS:NZ	1.92	1.01
1:C:105:ARG:HH21	2:D:253:ARG:HH21	1.04	1.01
1:C:105:ARG:HH21	2:D:253:ARG:NH2	1.59	1.01
2:D:403:ALA:CB	1:G:346:TRP:CE3	2.40	1.01
1:M:406:HIS:CE1	2:N:260:VAL:O	2.13	1.01
1:A:11:GLN:NE2	2:B:247:GLN:O	1.93	1.00
1:A:260:VAL:HB	2:P:407:TRP:CZ2	1.95	1.00
1:A:346:TRP:CB	2:P:401:ARG:CB	2.39	1.00
2:F:406:HIS:CE1	1:K:260:VAL:O	2.13	1.00
1:G:224:TYR:CE1	2:H:325:MET:HG3	1.96	1.00
1:I:96:LYS:O	2:J:2:ARG:HD2	1.59	1.00
1:M:394:LYS:HA	2:N:348:PRO:HG3	1.39	1.00
1:M:394:LYS:CA	2:N:348:PRO:HG3	1.91	1.00
1:O:181:VAL:N	2:P:352:LYS:HE3	1.75	1.00
1:I:105:ARG:HH21	2:J:253:ARG:NH2	1.57	1.00
1:M:101:ASN:HB2	2:N:254:LYS:CD	1.91	1.00
1:Q:210:TYR:CE1	2:R:326:LYS:CB	2.44	1.00
1:C:406:HIS:CE1	2:D:260:VAL:HG12	1.96	1.00
3:C:501:GTP:O3G	2:D:254:LYS:NZ	1.92	1.00
1:E:346:TRP:HB2	2:R:401:ARG:CB	1.92	1.00
1:Q:394:LYS:HZ1	2:R:349:ASN:ND2	1.60	1.00
1:A:404:PHE:N	2:B:261:PRO:HA	1.77	1.00
1:C:2:ARG:NH1	2:N:72:PRO:HB2	1.77	1.00
1:G:401:LYS:CG	2:H:346:TRP:CG	2.45	1.00
1:O:210:TYR:CE2	2:P:326:LYS:CA	2.37	1.00
1:O:181:VAL:CB	2:P:352:LYS:HE3	1.92	0.99
1:I:401:LYS:HG3	2:J:346:TRP:CG	1.96	0.99
1:M:401:LYS:HG3	2:N:346:TRP:CB	1.91	0.99
1:C:11:GLN:NE2	2:D:247:GLN:O	1.94	0.99
1:M:100:ALA:CA	2:N:254:LYS:HB2	1.91	0.99
1:O:210:TYR:HB3	2:P:326:LYS:HD2	1.44	0.99
1:Q:401:LYS:HG3	2:R:346:TRP:CB	1.91	0.99
1:E:346:TRP:HB2	2:R:401:ARG:HB2	1.42	0.99
1:E:406:HIS:CE1	2:F:260:VAL:HG12	1.98	0.99
1:O:394:LYS:HG2	2:P:348:PRO:HB2	1.42	0.99
1:I:224:TYR:CD1	2:J:325:MET:HG3	1.97	0.99
2:N:283:TYR:C	2:P:56:ALA:CB	2.35	0.99
1:C:401:LYS:HD3	2:D:346:TRP:CE2	1.97	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:401:LYS:HG3	2:R:346:TRP:CG	1.98	0.99
2:D:403:ALA:HB1	1:G:346:TRP:HZ3	1.19	0.99
1:G:181:VAL:N	2:H:352:LYS:HE3	1.76	0.99
1:O:401:LYS:CG	2:P:346:TRP:CG	2.45	0.99
1:A:177:VAL:CG2	2:B:329:ASP:O	2.11	0.99
1:I:406:HIS:CE1	2:J:260:VAL:HG12	1.95	0.99
1:K:401:LYS:CG	2:L:346:TRP:CG	2.45	0.99
2:N:283:TYR:HA	2:P:56:ALA:HB3	1.44	0.99
1:I:176:GLN:CB	2:J:333:LEU:CD2	2.21	0.99
2:J:283:TYR:CA	2:L:56:ALA:HB1	1.93	0.99
1:M:101:ASN:CG	2:N:254:LYS:HE3	1.87	0.99
1:Q:394:LYS:CA	2:R:348:PRO:HG3	1.92	0.99
1:C:258:ASN:C	2:N:404:PHE:HE2	1.70	0.98
1:E:181:VAL:CB	2:F:352:LYS:HE3	1.91	0.98
1:E:224:TYR:CE1	2:F:325:MET:CG	2.46	0.98
1:I:181:VAL:N	2:J:352:LYS:HE3	1.76	0.98
1:I:407:TRP:CE2	2:J:257:VAL:HA	1.98	0.98
2:B:283:TYR:HD2	2:F:62:VAL:HG22	1.28	0.98
1:E:224:TYR:CD1	2:F:325:MET:HG3	1.99	0.98
1:K:176:GLN:OE1	2:L:333:LEU:HD11	1.61	0.98
1:A:176:GLN:OE1	2:B:333:LEU:HD11	1.62	0.98
1:I:406:HIS:HE1	2:J:260:VAL:O	1.45	0.98
1:M:210:TYR:CE1	2:N:326:LYS:CB	2.46	0.98
1:K:406:HIS:CE1	2:L:260:VAL:HG12	1.97	0.98
1:Q:394:LYS:HA	2:R:348:PRO:HG3	1.42	0.98
2:N:283:TYR:CD2	2:P:62:VAL:HG22	1.99	0.98
1:C:96:LYS:O	2:D:2:ARG:HD2	1.63	0.98
1:Q:401:LYS:CG	2:R:346:TRP:CG	2.47	0.98
2:B:283:TYR:C	2:F:56:ALA:HB1	1.87	0.98
1:A:105:ARG:HH21	2:B:253:ARG:HH21	0.99	0.98
1:A:283:HIS:CA	1:E:56:THR:HG21	1.94	0.98
1:A:348:PRO:HD3	2:P:398:MET:CG	1.94	0.98
1:I:401:LYS:CG	2:J:346:TRP:CG	2.46	0.98
1:K:97:GLU:OE2	2:L:2:ARG:NH2	1.95	0.98
1:M:394:LYS:HG2	2:N:348:PRO:HB2	1.46	0.98
1:O:210:TYR:HB3	2:P:326:LYS:CD	1.92	0.98
1:Q:224:TYR:CG	2:R:325:MET:HG3	1.97	0.98
1:M:210:TYR:CE2	2:N:326:LYS:CA	2.43	0.98
1:A:348:PRO:CD	2:P:398:MET:CG	2.42	0.97
1:Q:100:ALA:CA	2:R:254:LYS:HB2	1.92	0.97
1:A:352:LYS:HA	2:P:179:ASP:O	1.63	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ARG:NH1	2:R:72:PRO:HB2	1.80	0.97
1:E:177:VAL:HG11	2:F:329:ASP:HA	1.45	0.97
1:G:406:HIS:HE1	2:H:260:VAL:O	1.46	0.97
1:G:407:TRP:CE2	2:H:257:VAL:HA	1.99	0.97
1:I:404:PHE:N	2:J:261:PRO:HA	1.79	0.97
1:E:105:ARG:HH21	2:F:253:ARG:HH21	1.08	0.97
1:M:404:PHE:CE2	2:N:258:ASN:O	2.17	0.97
2:P:284:ARG:O	2:R:57:ALA:N	1.95	0.97
1:C:404:PHE:N	2:D:261:PRO:HA	1.80	0.97
1:G:224:TYR:CD1	2:H:325:MET:HG3	1.99	0.97
1:I:210:TYR:CE1	2:J:326:LYS:CB	2.48	0.97
1:A:401:LYS:HG3	2:B:346:TRP:CB	1.93	0.97
1:C:177:VAL:CG2	2:D:329:ASP:O	2.12	0.97
1:A:224:TYR:CE1	2:B:325:MET:CG	2.47	0.97
1:C:181:VAL:CB	2:D:352:LYS:HE3	1.94	0.97
1:G:105:ARG:HH21	2:H:253:ARG:NH2	1.61	0.97
1:A:177:VAL:HG11	2:B:329:ASP:HA	1.44	0.96
1:E:406:HIS:CE1	2:F:260:VAL:O	2.18	0.96
1:Q:401:LYS:HD3	2:R:346:TRP:CE2	1.99	0.96
1:A:346:TRP:HE3	2:P:403:ALA:HB2	1.26	0.96
1:C:260:VAL:HB	2:N:407:TRP:CZ2	1.99	0.96
1:O:97:GLU:OE2	2:P:2:ARG:CZ	2.12	0.96
1:E:401:LYS:CG	2:F:346:TRP:CG	2.47	0.96
1:M:210:TYR:OH	2:N:326:LYS:N	1.98	0.96
2:B:401:ARG:CB	1:I:346:TRP:HB2	1.95	0.96
1:C:176:GLN:OE1	2:D:333:LEU:HD11	1.64	0.96
1:I:210:TYR:HB3	2:J:326:LYS:HD2	1.47	0.96
2:B:401:ARG:HB2	1:I:346:TRP:HB2	1.46	0.96
1:G:406:HIS:CE1	2:H:260:VAL:HG12	1.99	0.96
1:M:394:LYS:NZ	2:N:349:ASN:HD21	1.63	0.96
1:O:407:TRP:CE2	2:P:257:VAL:HA	2.01	0.96
1:K:96:LYS:O	2:L:2:ARG:HD2	1.64	0.96
1:K:97:GLU:OE2	2:L:2:ARG:CZ	2.12	0.96
1:O:397:LEU:HB3	2:P:346:TRP:O	1.66	0.96
1:A:176:GLN:HB3	2:B:333:LEU:HD22	0.96	0.96
1:K:105:ARG:HH21	2:L:253:ARG:NH2	1.62	0.96
1:O:283:HIS:CA	1:Q:56:THR:HG21	1.95	0.96
1:A:105:ARG:NH2	2:B:253:ARG:CZ	2.29	0.96
1:C:350:GLY:HA3	2:N:181:VAL:HA	1.47	0.96
1:E:96:LYS:O	2:F:2:ARG:HD2	1.66	0.96
1:G:96:LYS:O	2:H:2:ARG:HD2	1.63	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:ASN:CG	2:J:254:LYS:HE3	1.91	0.96
1:I:210:TYR:CE2	2:J:326:LYS:CA	2.44	0.96
1:Q:181:VAL:CB	2:R:352:LYS:HE3	1.95	0.96
1:A:406:HIS:CE1	2:B:260:VAL:O	2.19	0.95
1:E:105:ARG:HH21	2:F:253:ARG:NH2	1.63	0.95
1:E:177:VAL:CG2	2:F:329:ASP:O	2.13	0.95
2:H:283:TYR:HA	2:J:56:ALA:HB3	1.48	0.95
1:O:101:ASN:N	2:P:254:LYS:CD	2.29	0.95
1:C:406:HIS:CE1	2:D:260:VAL:O	2.19	0.95
1:M:401:LYS:CG	2:N:346:TRP:CG	2.49	0.95
1:G:176:GLN:CB	2:H:333:LEU:CD2	2.24	0.95
1:Q:394:LYS:HG2	2:R:348:PRO:HB2	1.47	0.95
1:Q:394:LYS:NZ	2:R:349:ASN:HD21	1.64	0.95
2:B:62:VAL:HG22	2:D:283:TYR:HD2	1.31	0.95
1:G:210:TYR:CE2	2:H:326:LYS:CA	2.46	0.95
1:G:210:TYR:HB3	2:H:326:LYS:HD2	1.48	0.95
1:I:224:TYR:CZ	2:J:325:MET:HG3	1.99	0.95
1:I:404:PHE:CE2	2:J:258:ASN:O	2.20	0.95
1:M:406:HIS:HE1	2:N:260:VAL:O	1.48	0.95
1:O:97:GLU:CD	2:P:2:ARG:HE	1.73	0.95
1:A:181:VAL:CB	2:B:352:LYS:HE3	1.95	0.95
1:C:401:LYS:HG3	2:D:346:TRP:CG	2.00	0.95
1:M:181:VAL:CB	2:N:352:LYS:HE3	1.96	0.95
1:O:394:LYS:NZ	2:P:349:ASN:ND2	2.15	0.95
1:O:401:LYS:HG3	2:P:346:TRP:CG	2.01	0.95
1:A:101:ASN:CG	2:B:254:LYS:HE3	1.91	0.95
1:C:177:VAL:HG11	2:D:329:ASP:HA	1.45	0.95
1:I:210:TYR:OH	2:J:326:LYS:N	1.99	0.95
2:N:284:ARG:O	2:P:57:ALA:N	1.99	0.95
1:O:210:TYR:CZ	2:P:326:LYS:N	2.33	0.95
1:Q:97:GLU:OE2	2:R:2:ARG:CZ	2.14	0.95
1:A:348:PRO:CD	2:P:398:MET:HG2	1.96	0.95
1:I:97:GLU:OE2	2:J:2:ARG:NH2	2.00	0.95
1:K:210:TYR:CE1	2:L:326:LYS:CB	2.49	0.95
1:K:407:TRP:CE2	2:L:257:VAL:HA	2.01	0.95
2:B:407:TRP:CZ2	1:I:260:VAL:HB	2.02	0.95
1:E:97:GLU:OE2	2:F:2:ARG:NH2	1.97	0.95
2:B:56:ALA:HB1	2:D:283:TYR:C	1.90	0.95
1:E:224:TYR:CE1	2:F:325:MET:HG3	2.01	0.95
1:E:401:LYS:HE2	2:F:346:TRP:CD1	2.02	0.95
1:O:179:THR:HG21	2:P:353:THR:OG1	1.67	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:VAL:N	2:D:352:LYS:HE3	1.80	0.95
1:C:224:TYR:CE1	2:D:325:MET:CG	2.50	0.95
1:I:97:GLU:OE2	2:J:2:ARG:CZ	2.13	0.95
1:Q:210:TYR:OH	2:R:326:LYS:N	1.99	0.95
1:A:101:ASN:HB2	2:B:254:LYS:CD	1.95	0.94
1:A:181:VAL:N	2:B:352:LYS:HE3	1.81	0.94
1:K:406:HIS:HE1	2:L:260:VAL:O	1.48	0.94
1:M:224:TYR:CG	2:N:325:MET:HG3	2.01	0.94
1:M:401:LYS:HG3	2:N:346:TRP:CG	2.02	0.94
1:O:401:LYS:HD3	2:P:346:TRP:CE2	2.02	0.94
1:C:176:GLN:HB3	2:D:333:LEU:HD22	0.95	0.94
1:M:210:TYR:HB3	2:N:326:LYS:HD2	1.49	0.94
1:Q:404:PHE:CE2	2:R:258:ASN:O	2.20	0.94
1:C:352:LYS:HA	2:N:179:ASP:O	1.66	0.94
1:K:105:ARG:HH21	2:L:253:ARG:HH21	1.01	0.94
1:O:404:PHE:HZ	2:P:314:THR:CG2	1.79	0.94
2:H:283:TYR:C	2:J:56:ALA:CB	2.40	0.94
1:K:224:TYR:CG	2:L:325:MET:HG3	2.02	0.94
1:Q:97:GLU:OE2	2:R:2:ARG:NH2	1.99	0.94
1:A:394:LYS:HA	2:B:348:PRO:HG3	1.50	0.94
1:G:401:LYS:HE2	2:H:346:TRP:CD1	2.03	0.94
1:G:404:PHE:N	2:H:261:PRO:HA	1.82	0.94
1:G:224:TYR:CZ	2:H:325:MET:HG3	2.01	0.94
1:G:401:LYS:HG3	2:H:346:TRP:HB3	1.46	0.94
1:K:404:PHE:N	2:L:261:PRO:HA	1.81	0.94
1:M:397:LEU:HB3	2:N:346:TRP:O	1.68	0.94
1:O:176:GLN:CG	2:P:333:LEU:HD21	1.97	0.94
1:I:101:ASN:HB2	2:J:254:LYS:CD	1.96	0.94
1:O:407:TRP:CD2	2:P:257:VAL:HA	2.03	0.94
1:Q:101:ASN:CG	2:R:254:LYS:HE3	1.92	0.94
1:A:348:PRO:HD3	2:P:398:MET:HG2	1.49	0.94
1:E:346:TRP:HE3	2:R:403:ALA:HB2	1.31	0.94
2:F:403:ALA:HB1	1:K:346:TRP:HZ3	1.22	0.94
1:O:101:ASN:CB	2:P:254:LYS:CE	2.20	0.94
2:B:403:ALA:HB1	1:I:346:TRP:HZ3	1.13	0.93
1:C:346:TRP:CB	2:N:401:ARG:CB	2.46	0.93
1:E:176:GLN:HB3	2:F:333:LEU:HD22	0.96	0.93
1:G:401:LYS:HD3	2:H:346:TRP:CD2	2.03	0.93
1:M:401:LYS:HD3	2:N:346:TRP:CE2	2.03	0.93
1:I:210:TYR:HB3	2:J:326:LYS:CD	1.97	0.93
1:M:179:THR:HG22	2:N:353:THR:HG1	1.20	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:101:ASN:HB2	2:R:254:LYS:CD	1.97	0.93
1:E:258:ASN:C	2:R:404:PHE:HE2	1.76	0.93
1:O:224:TYR:CD2	2:P:325:MET:HG3	2.03	0.93
1:A:224:TYR:CD1	2:B:325:MET:HG3	2.03	0.93
1:A:346:TRP:CB	2:P:401:ARG:CG	2.25	0.93
1:O:224:TYR:CG	2:P:325:MET:HG3	2.01	0.93
1:O:406:HIS:HE1	2:P:260:VAL:O	1.42	0.93
1:A:224:TYR:CE1	2:B:325:MET:HG3	2.03	0.93
2:B:283:TYR:CA	2:F:56:ALA:CB	2.46	0.93
1:C:105:ARG:NH2	2:D:253:ARG:CZ	2.32	0.93
1:E:350:GLY:HA3	2:R:181:VAL:HA	1.50	0.93
1:M:210:TYR:HB3	2:N:326:LYS:CD	1.97	0.93
1:G:101:ASN:CG	2:H:254:LYS:HE3	1.94	0.93
1:I:394:LYS:HA	2:J:348:PRO:HG3	1.51	0.93
1:I:401:LYS:HG3	2:J:346:TRP:HB3	1.49	0.93
1:M:97:GLU:OE2	2:N:2:ARG:CZ	2.16	0.93
1:M:179:THR:HG21	2:N:353:THR:OG1	1.69	0.93
1:E:224:TYR:HE1	2:F:325:MET:SD	1.87	0.93
1:O:177:VAL:HG11	2:P:329:ASP:CA	1.99	0.93
2:B:72:PRO:HB2	1:I:2:ARG:NH1	1.83	0.93
1:G:404:PHE:CE2	2:H:258:ASN:O	2.22	0.93
1:K:224:TYR:CZ	2:L:325:MET:HG3	2.03	0.93
1:E:404:PHE:N	2:F:261:PRO:HA	1.83	0.93
2:P:283:TYR:CA	2:R:56:ALA:HB1	1.94	0.93
1:A:401:LYS:HD3	2:B:346:TRP:CE2	2.03	0.93
1:E:348:PRO:HD3	2:R:398:MET:CG	1.98	0.93
1:G:210:TYR:CE1	2:H:326:LYS:CB	2.52	0.93
1:I:105:ARG:NH2	2:J:253:ARG:CZ	2.31	0.93
1:K:401:LYS:HE2	2:L:346:TRP:CD1	2.04	0.93
1:A:258:ASN:C	2:P:404:PHE:CE2	2.46	0.92
2:D:72:PRO:HB2	1:G:2:ARG:NH1	1.83	0.92
1:G:105:ARG:HH21	2:H:253:ARG:HH21	1.01	0.92
1:G:97:GLU:OE2	2:H:2:ARG:NH2	2.00	0.92
1:I:105:ARG:HH21	2:J:253:ARG:HH21	0.96	0.92
1:O:210:TYR:HB3	2:P:326:LYS:CE	1.98	0.92
1:G:97:GLU:OE2	2:H:2:ARG:CZ	2.16	0.92
1:I:283:HIS:CA	1:K:56:THR:HG21	1.99	0.92
1:O:100:ALA:C	2:P:254:LYS:HD2	1.95	0.92
1:Q:404:PHE:HZ	2:R:314:THR:CG2	1.82	0.92
1:A:249:ASN:H	2:P:11:GLN:HE22	1.17	0.92
1:E:105:ARG:NH2	2:F:253:ARG:CZ	2.33	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:179:THR:HG21	2:R:353:THR:OG1	1.68	0.92
1:C:348:PRO:HD3	2:N:398:MET:CG	1.99	0.92
1:I:224:TYR:CG	2:J:325:MET:HG3	2.05	0.92
1:K:401:LYS:HG3	2:L:346:TRP:HB3	1.51	0.92
1:Q:210:TYR:HB3	2:R:326:LYS:CD	1.99	0.92
1:C:224:TYR:CE1	2:D:325:MET:HG3	2.05	0.92
2:D:401:ARG:HB2	1:G:346:TRP:HB2	1.52	0.92
1:M:404:PHE:HZ	2:N:314:THR:CG2	1.82	0.92
2:F:72:PRO:HB2	1:K:2:ARG:NH1	1.85	0.92
1:O:394:LYS:HZ1	2:P:349:ASN:ND2	1.67	0.92
1:G:210:TYR:HB3	2:H:326:LYS:CD	2.00	0.92
1:C:348:PRO:CD	2:N:398:MET:CG	2.48	0.91
1:I:100:ALA:CA	2:J:254:LYS:HB2	2.00	0.91
1:K:210:TYR:OH	2:L:326:LYS:N	2.03	0.91
1:O:96:LYS:O	2:P:2:ARG:CD	2.18	0.91
1:Q:210:TYR:HB3	2:R:326:LYS:HD2	1.52	0.91
2:B:283:TYR:C	2:F:56:ALA:CB	2.43	0.91
1:G:101:ASN:HB2	2:H:254:LYS:CD	1.98	0.91
1:G:210:TYR:OH	2:H:326:LYS:N	2.02	0.91
1:G:224:TYR:HE1	2:H:325:MET:SD	1.81	0.91
1:M:210:TYR:CZ	2:N:326:LYS:N	2.37	0.91
1:O:179:THR:HA	2:P:353:THR:H	1.35	0.91
1:C:101:ASN:CG	2:D:254:LYS:HE3	1.95	0.91
1:C:224:TYR:CD1	2:D:325:MET:HG3	2.05	0.91
1:O:210:TYR:CZ	2:P:326:LYS:CB	2.53	0.91
1:A:401:LYS:HG3	2:B:346:TRP:CG	2.05	0.91
1:C:101:ASN:HB2	2:D:254:LYS:CD	1.99	0.91
1:Q:210:TYR:CE2	2:R:326:LYS:CA	2.45	0.91
1:C:346:TRP:CB	2:N:401:ARG:CG	2.30	0.91
1:A:404:PHE:H	2:B:261:PRO:CA	1.83	0.91
1:I:224:TYR:HE1	2:J:325:MET:SD	1.77	0.91
1:Q:105:ARG:HH21	2:R:253:ARG:HH21	0.93	0.91
1:G:401:LYS:CE	2:H:346:TRP:CD1	2.53	0.91
1:O:100:ALA:HA	2:P:254:LYS:CB	2.01	0.91
1:C:101:ASN:HB2	2:D:254:LYS:HE3	0.91	0.91
1:C:401:LYS:CG	2:D:346:TRP:CG	2.53	0.91
2:P:284:ARG:N	2:R:56:ALA:HB1	1.86	0.91
1:Q:406:HIS:HE1	2:R:260:VAL:O	1.49	0.91
1:C:394:LYS:HA	2:D:348:PRO:HG3	1.53	0.91
2:D:401:ARG:CB	1:G:346:TRP:HB2	2.01	0.91
2:F:407:TRP:CZ2	1:K:260:VAL:HB	2.06	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:TYR:CZ	2:J:325:MET:SD	2.63	0.91
1:K:105:ARG:NH2	2:L:253:ARG:CZ	2.33	0.91
1:M:224:TYR:CD2	2:N:325:MET:HG3	2.06	0.91
1:M:407:TRP:CE2	2:N:257:VAL:HA	2.06	0.91
1:O:97:GLU:CD	2:P:2:ARG:CZ	2.43	0.91
1:C:346:TRP:HE3	2:N:403:ALA:HB2	1.33	0.90
1:M:96:LYS:O	2:N:2:ARG:CD	2.19	0.90
1:O:406:HIS:NE2	2:P:260:VAL:CG1	2.34	0.90
1:Q:224:TYR:CD2	2:R:325:MET:HG3	2.05	0.90
1:A:210:TYR:CD2	2:B:326:LYS:HG3	2.06	0.90
1:E:176:GLN:OE1	2:F:333:LEU:HD11	1.70	0.90
2:F:228:ASN:HD21	5:F:901:GDP:HN1	1.17	0.90
1:K:224:TYR:CD1	2:L:325:MET:CG	2.52	0.90
2:L:228:ASN:HD21	5:L:901:GDP:HN1	1.17	0.90
1:O:224:TYR:CE2	2:P:325:MET:HG3	2.01	0.90
1:A:56:THR:HG21	1:C:283:HIS:CA	2.00	0.90
1:A:101:ASN:HB2	2:B:254:LYS:HE3	0.91	0.90
2:B:284:ARG:O	2:F:57:ALA:N	2.04	0.90
2:N:228:ASN:HD21	5:N:901:GDP:HN1	1.17	0.90
1:A:407:TRP:CE2	2:B:257:VAL:HA	2.06	0.90
1:M:101:ASN:CB	2:N:254:LYS:CE	2.27	0.90
1:Q:406:HIS:NE2	2:R:260:VAL:HG12	1.85	0.90
2:B:404:PHE:HE2	1:I:258:ASN:C	1.79	0.90
2:D:228:ASN:HD21	5:D:901:GDP:HN1	1.17	0.90
1:E:346:TRP:CB	2:R:401:ARG:CB	2.50	0.90
2:H:228:ASN:HD21	5:H:901:GDP:HN1	1.17	0.90
2:J:283:TYR:HB3	2:L:62:VAL:HG21	1.51	0.90
1:A:406:HIS:HE1	2:B:260:VAL:O	1.52	0.90
2:B:179:ASP:O	1:I:352:LYS:HA	1.70	0.90
2:D:407:TRP:CZ2	1:G:260:VAL:HB	2.07	0.90
1:G:105:ARG:NH2	2:H:253:ARG:CZ	2.35	0.90
1:I:224:TYR:CZ	2:J:325:MET:CG	2.55	0.90
1:I:401:LYS:HD3	2:J:346:TRP:CD2	2.07	0.90
1:M:105:ARG:HH21	2:N:253:ARG:HH21	0.90	0.90
1:O:97:GLU:OE2	2:P:2:ARG:NH2	2.03	0.90
1:Q:176:GLN:HB2	2:R:333:LEU:HD22	1.51	0.90
2:R:228:ASN:HD21	5:R:901:GDP:HN1	1.17	0.90
1:I:394:LYS:NZ	2:J:349:ASN:HD21	1.70	0.90
1:M:97:GLU:CD	2:N:2:ARG:HE	1.79	0.90
1:A:404:PHE:CE2	2:B:258:ASN:O	2.25	0.90
2:B:181:VAL:HA	1:I:350:GLY:HA3	1.54	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:401:LYS:HE2	2:J:346:TRP:CD1	2.07	0.90
1:I:404:PHE:H	2:J:261:PRO:CA	1.84	0.90
1:O:404:PHE:HZ	2:P:314:THR:HG22	1.36	0.90
1:O:406:HIS:NE2	2:P:260:VAL:HG12	1.85	0.90
1:Q:210:TYR:CZ	2:R:326:LYS:N	2.39	0.90
1:Q:210:TYR:HB3	2:R:326:LYS:CE	2.01	0.90
2:B:283:TYR:CD2	2:F:62:VAL:HG22	2.07	0.89
1:K:404:PHE:CE2	2:L:258:ASN:O	2.25	0.89
1:O:97:GLU:CD	2:P:2:ARG:NE	2.29	0.89
1:E:352:LYS:HA	2:R:179:ASP:O	1.70	0.89
1:Q:176:GLN:CG	2:R:333:LEU:HD21	2.02	0.89
1:E:101:ASN:HB2	2:F:254:LYS:HE3	0.91	0.89
1:O:210:TYR:CB	2:P:326:LYS:HD2	2.02	0.89
1:K:210:TYR:CE2	2:L:326:LYS:CA	2.50	0.89
1:C:210:TYR:CD2	2:D:326:LYS:HG3	2.08	0.89
1:E:210:TYR:CD2	2:F:326:LYS:HG3	2.08	0.89
1:Q:397:LEU:HB3	2:R:346:TRP:O	1.73	0.89
1:E:401:LYS:HG3	2:F:346:TRP:HB3	1.54	0.89
1:I:210:TYR:CZ	2:J:326:LYS:N	2.39	0.89
1:K:210:TYR:HB3	2:L:326:LYS:HD2	1.55	0.89
1:M:101:ASN:N	2:N:254:LYS:CD	2.34	0.89
1:O:176:GLN:HB2	2:P:333:LEU:HD22	1.50	0.89
1:C:406:HIS:HE1	2:D:260:VAL:O	1.54	0.89
1:E:348:PRO:CD	2:R:398:MET:CG	2.50	0.89
1:I:394:LYS:HZ1	2:J:349:ASN:HD21	1.17	0.89
1:K:100:ALA:CA	2:L:254:LYS:HB2	2.02	0.89
1:K:101:ASN:CG	2:L:254:LYS:HE3	1.98	0.89
2:D:179:ASP:O	1:G:352:LYS:HA	1.72	0.89
2:F:401:ARG:HB2	1:K:346:TRP:HB2	1.55	0.89
1:I:407:TRP:CD2	2:J:257:VAL:HA	2.08	0.89
1:M:97:GLU:OE2	2:N:2:ARG:NH2	2.03	0.89
1:Q:394:LYS:NZ	2:R:349:ASN:ND2	2.21	0.89
1:C:404:PHE:H	2:D:261:PRO:CA	1.85	0.89
1:G:224:TYR:CG	2:H:325:MET:HG3	2.08	0.89
1:G:394:LYS:HA	2:H:348:PRO:HG3	1.55	0.89
1:K:401:LYS:CE	2:L:346:TRP:CD1	2.55	0.89
2:P:228:ASN:HD21	5:P:901:GDP:HN1	1.17	0.89
1:C:97:GLU:OE2	2:D:2:ARG:NH2	2.05	0.88
1:C:258:ASN:C	2:N:404:PHE:CE2	2.50	0.88
1:C:346:TRP:HZ3	2:N:403:ALA:HB1	1.05	0.88
1:C:407:TRP:CE2	2:D:257:VAL:HA	2.07	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:177:VAL:HG11	2:J:329:ASP:CA	2.03	0.88
1:I:401:LYS:CE	2:J:346:TRP:CD1	2.56	0.88
1:M:176:GLN:CG	2:N:333:LEU:HD21	2.03	0.88
1:M:176:GLN:HB2	2:N:333:LEU:HD22	1.54	0.88
1:Q:407:TRP:CE2	2:R:257:VAL:HA	2.07	0.88
1:A:394:LYS:HZ1	2:B:349:ASN:HD21	1.22	0.88
1:K:401:LYS:HD3	2:L:346:TRP:CD2	2.08	0.88
1:I:224:TYR:CE2	2:J:325:MET:HG3	2.08	0.88
2:J:284:ARG:O	2:L:57:ALA:N	2.05	0.88
1:O:176:GLN:CG	2:P:333:LEU:CD2	2.51	0.88
2:B:228:ASN:HD21	5:B:901:GDP:HN1	1.17	0.88
1:E:401:LYS:HD3	2:F:346:TRP:CD2	2.08	0.88
1:M:406:HIS:NE2	2:N:260:VAL:HG12	1.87	0.88
1:A:97:GLU:OE2	2:B:2:ARG:NH2	2.05	0.88
2:B:57:ALA:N	2:D:284:ARG:O	2.05	0.88
2:B:398:MET:CG	1:I:348:PRO:HD3	2.03	0.88
2:D:404:PHE:HE2	1:G:258:ASN:C	1.82	0.88
1:A:176:GLN:CB	2:B:333:LEU:CD2	2.36	0.88
1:C:176:GLN:CB	2:D:333:LEU:CD2	2.36	0.88
1:E:181:VAL:HA	2:F:352:LYS:HE3	0.91	0.88
1:Q:404:PHE:HZ	2:R:314:THR:HG22	1.38	0.88
1:E:97:GLU:OE2	2:F:2:ARG:CZ	2.21	0.88
1:A:100:ALA:CA	2:B:254:LYS:HB2	2.02	0.88
1:C:348:PRO:CD	2:N:398:MET:HG2	2.03	0.88
1:K:394:LYS:HA	2:L:348:PRO:HG3	1.56	0.88
1:E:224:TYR:CG	2:F:325:MET:HG3	2.09	0.88
1:M:407:TRP:CD2	2:N:257:VAL:HA	2.09	0.88
1:Q:101:ASN:N	2:R:254:LYS:CD	2.36	0.88
2:B:56:ALA:CB	2:D:283:TYR:CA	2.51	0.88
1:A:401:LYS:CG	2:B:346:TRP:CG	2.56	0.87
1:E:401:LYS:CE	2:F:346:TRP:CD1	2.55	0.87
1:G:283:HIS:CA	1:I:56:THR:HG21	2.03	0.87
2:J:228:ASN:HD21	5:J:901:GDP:HN1	1.17	0.87
1:M:210:TYR:HB3	2:N:326:LYS:CE	2.03	0.87
1:A:97:GLU:OE2	2:B:2:ARG:CZ	2.21	0.87
1:C:348:PRO:HD3	2:N:398:MET:HG2	1.56	0.87
1:G:210:TYR:CZ	2:H:326:LYS:N	2.42	0.87
1:K:101:ASN:HB2	2:L:254:LYS:CD	2.03	0.87
1:M:100:ALA:HA	2:N:254:LYS:CB	2.03	0.87
1:A:329:ASN:CG	2:P:177:VAL:CG2	2.46	0.87
2:B:56:ALA:CB	2:D:283:TYR:C	2.48	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:PHE:CE2	2:D:258:ASN:O	2.28	0.87
1:G:224:TYR:CZ	2:H:325:MET:SD	2.66	0.87
1:I:210:TYR:CZ	2:J:326:LYS:CB	2.58	0.87
1:I:224:TYR:CD2	2:J:325:MET:HG3	2.09	0.87
1:K:210:TYR:HB3	2:L:326:LYS:CD	2.03	0.87
1:A:346:TRP:HZ3	2:P:403:ALA:HB1	0.98	0.87
1:M:101:ASN:HB2	2:N:254:LYS:HE3	0.88	0.87
1:M:394:LYS:NZ	2:N:349:ASN:ND2	2.19	0.87
1:O:394:LYS:HZ1	2:P:349:ASN:HD21	0.88	0.87
2:B:403:ALA:HB2	1:I:346:TRP:HE3	1.37	0.87
1:C:401:LYS:HG3	2:D:346:TRP:HB3	1.55	0.87
1:E:407:TRP:CE2	2:F:257:VAL:HA	2.10	0.87
1:G:100:ALA:CA	2:H:254:LYS:HB2	2.03	0.87
1:I:224:TYR:CD1	2:J:325:MET:CG	2.55	0.87
1:M:406:HIS:NE2	2:N:260:VAL:CG1	2.38	0.87
1:Q:176:GLN:HB3	2:R:333:LEU:HD22	0.88	0.87
1:C:401:LYS:HE2	2:D:346:TRP:CD1	2.10	0.87
1:G:404:PHE:H	2:H:261:PRO:CA	1.87	0.87
1:I:210:TYR:HB3	2:J:326:LYS:CE	2.04	0.87
1:K:404:PHE:H	2:L:261:PRO:CA	1.86	0.87
1:Q:100:ALA:HA	2:R:254:LYS:CB	2.02	0.87
1:Q:177:VAL:HG11	2:R:329:ASP:CA	2.05	0.87
1:E:406:HIS:NE2	2:F:260:VAL:HG12	1.90	0.86
2:F:401:ARG:CB	1:K:346:TRP:HB2	2.04	0.86
1:M:177:VAL:HG11	2:N:329:ASP:CA	2.05	0.86
1:Q:101:ASN:HB2	2:R:254:LYS:HE3	0.88	0.86
1:C:210:TYR:HB3	2:D:326:LYS:HD2	1.57	0.86
2:H:284:ARG:O	2:J:57:ALA:N	2.07	0.86
1:M:179:THR:HA	2:N:353:THR:H	1.40	0.86
1:O:176:GLN:HG3	2:P:333:LEU:HD21	1.56	0.86
1:Q:96:LYS:O	2:R:2:ARG:CD	2.23	0.86
1:O:105:ARG:NH2	2:P:253:ARG:HH21	1.58	0.86
1:Q:407:TRP:CD2	2:R:257:VAL:HA	2.10	0.86
1:E:406:HIS:HE1	2:F:260:VAL:O	1.55	0.86
2:F:179:ASP:O	1:K:352:LYS:HA	1.75	0.86
1:G:224:TYR:CZ	2:H:325:MET:CG	2.58	0.86
1:G:407:TRP:CD2	2:H:257:VAL:HA	2.10	0.86
1:K:177:VAL:HG11	2:L:329:ASP:CA	2.06	0.86
1:O:210:TYR:CD1	2:P:326:LYS:CB	2.58	0.86
1:A:2:ARG:CG	2:P:96:GLN:NE2	2.11	0.86
2:B:283:TYR:HA	2:F:56:ALA:HB3	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:TYR:HE1	2:L:325:MET:SD	1.77	0.86
1:M:283:HIS:CA	1:O:56:THR:HG21	2.05	0.86
1:G:177:VAL:HG11	2:H:329:ASP:CA	2.05	0.86
1:I:179:THR:HG21	2:J:353:THR:OG1	1.75	0.86
1:E:346:TRP:HZ3	2:R:403:ALA:HB1	1.08	0.86
1:E:348:PRO:HD3	2:R:398:MET:HG2	1.56	0.86
1:K:176:GLN:HB3	2:L:333:LEU:HD22	0.86	0.86
1:A:326:LYS:HB2	2:P:210:TYR:CE2	2.09	0.86
1:K:224:TYR:CZ	2:L:325:MET:SD	2.67	0.86
1:O:210:TYR:OH	2:P:325:MET:C	2.17	0.86
1:M:100:ALA:C	2:N:254:LYS:HD2	2.01	0.86
1:M:224:TYR:CE2	2:N:325:MET:HG3	2.07	0.86
1:M:404:PHE:HZ	2:N:314:THR:HG22	1.40	0.86
1:A:224:TYR:HE1	2:B:325:MET:SD	1.88	0.86
1:I:394:LYS:CA	2:J:348:PRO:HG3	2.05	0.86
1:K:224:TYR:CZ	2:L:325:MET:CG	2.58	0.86
1:Q:210:TYR:CZ	2:R:326:LYS:CB	2.58	0.86
2:B:401:ARG:CB	1:I:346:TRP:CB	2.54	0.85
1:C:210:TYR:CE2	2:D:326:LYS:CA	2.58	0.85
1:G:224:TYR:CE2	2:H:325:MET:HG3	2.11	0.85
1:G:394:LYS:NZ	2:H:349:ASN:HD21	1.74	0.85
1:K:394:LYS:NZ	2:L:349:ASN:HD21	1.74	0.85
1:A:210:TYR:HB3	2:B:326:LYS:HD2	1.58	0.85
1:C:100:ALA:CA	2:D:254:LYS:HB2	2.05	0.85
1:K:407:TRP:CD2	2:L:257:VAL:HA	2.11	0.85
1:A:224:TYR:CG	2:B:325:MET:HG3	2.11	0.85
1:I:100:ALA:C	2:J:254:LYS:HD2	2.00	0.85
1:M:176:GLN:HB3	2:N:333:LEU:HD22	0.86	0.85
1:Q:11:GLN:CD	2:R:247:GLN:O	2.18	0.85
1:Q:406:HIS:NE2	2:R:260:VAL:CG1	2.38	0.85
1:E:96:LYS:NZ	2:F:130:ASP:OD2	2.08	0.85
2:B:398:MET:CG	1:I:348:PRO:CD	2.54	0.85
2:B:401:ARG:CG	1:I:346:TRP:CB	2.39	0.85
1:E:176:GLN:CB	2:F:333:LEU:CD2	2.35	0.85
1:E:404:PHE:H	2:F:261:PRO:CA	1.87	0.85
1:K:210:TYR:HB3	2:L:326:LYS:CE	2.06	0.85
1:K:224:TYR:CD2	2:L:325:MET:HG3	2.12	0.85
1:M:97:GLU:CD	2:N:2:ARG:CZ	2.49	0.85
1:O:210:TYR:CG	2:P:326:LYS:CG	2.59	0.85
1:A:394:LYS:CA	2:B:348:PRO:HG3	2.07	0.85
1:E:249:ASN:H	2:R:11:GLN:HE22	1.25	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:177:VAL:HG22	2:P:329:ASP:O	1.75	0.85
1:A:401:LYS:HG3	2:B:346:TRP:HB3	1.57	0.85
2:B:62:VAL:HG22	2:D:283:TYR:CD2	2.11	0.85
1:E:346:TRP:CB	2:R:401:ARG:CG	2.38	0.85
2:P:283:TYR:HB3	2:R:62:VAL:HG21	1.56	0.85
1:Q:97:GLU:CD	2:R:2:ARG:CZ	2.50	0.85
1:C:97:GLU:OE2	2:D:2:ARG:CZ	2.24	0.85
1:A:96:LYS:O	2:B:2:ARG:CD	2.24	0.84
1:K:179:THR:HG21	2:L:353:THR:OG1	1.76	0.84
1:K:210:TYR:CZ	2:L:326:LYS:N	2.45	0.84
2:N:284:ARG:N	2:P:56:ALA:HB1	1.91	0.84
1:C:181:VAL:HA	2:D:352:LYS:HE3	0.87	0.84
2:J:284:ARG:N	2:L:56:ALA:HB1	1.91	0.84
1:K:210:TYR:CZ	2:L:326:LYS:CB	2.60	0.84
1:M:210:TYR:CZ	2:N:326:LYS:CB	2.59	0.84
2:F:96:GLN:HE22	1:K:2:ARG:HG3	0.71	0.84
1:I:238:ILE:O	1:I:238:ILE:HG22	1.77	0.84
1:O:11:GLN:CD	2:P:247:GLN:O	2.20	0.84
1:O:394:LYS:HG2	2:P:348:PRO:CB	2.07	0.84
1:Q:394:LYS:HG2	2:R:348:PRO:CB	2.07	0.84
1:E:101:ASN:CG	2:F:254:LYS:HE3	2.03	0.84
1:E:348:PRO:CD	2:R:398:MET:HG2	2.07	0.84
2:H:283:TYR:HB3	2:J:62:VAL:HG21	1.57	0.84
1:M:394:LYS:HG2	2:N:348:PRO:CB	2.08	0.84
1:Q:97:GLU:CD	2:R:2:ARG:HE	1.83	0.84
1:A:238:ILE:O	1:A:238:ILE:HG22	1.78	0.84
1:C:401:LYS:HD3	2:D:346:TRP:CD2	2.12	0.84
1:G:394:LYS:HZ1	2:H:349:ASN:HD21	1.23	0.84
1:M:210:TYR:OH	2:N:325:MET:C	2.21	0.84
1:O:238:ILE:O	1:O:238:ILE:HG22	1.77	0.84
1:A:397:LEU:HB3	2:B:346:TRP:O	1.76	0.84
2:D:181:VAL:HA	1:G:350:GLY:HA3	1.59	0.84
1:E:394:LYS:HA	2:F:348:PRO:HG3	1.60	0.84
1:I:97:GLU:CD	2:J:2:ARG:CZ	2.51	0.84
1:I:210:TYR:CB	2:J:326:LYS:HD2	2.06	0.84
1:O:210:TYR:CZ	2:P:326:LYS:HB2	2.11	0.84
1:A:210:TYR:CE2	2:B:326:LYS:CA	2.57	0.84
1:A:224:TYR:CZ	2:B:325:MET:HG3	2.11	0.84
1:C:394:LYS:HZ1	2:D:349:ASN:HD21	1.25	0.84
1:E:100:ALA:CA	2:F:254:LYS:HB2	2.06	0.84
1:I:97:GLU:CD	2:J:2:ARG:HE	1.85	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:210:TYR:CB	2:N:326:LYS:HD2	2.08	0.84
1:O:404:PHE:CZ	2:P:314:THR:CG2	2.60	0.84
2:B:96:GLN:HE22	1:I:2:ARG:HG3	0.68	0.84
1:C:224:TYR:HE1	2:D:325:MET:SD	1.90	0.84
1:C:238:ILE:HG22	1:C:238:ILE:O	1.77	0.84
2:J:283:TYR:HA	2:L:56:ALA:HB2	1.60	0.84
1:K:238:ILE:HG22	1:K:238:ILE:O	1.77	0.84
1:M:238:ILE:HG22	1:M:238:ILE:O	1.78	0.84
1:O:404:PHE:HE2	2:P:258:ASN:O	1.57	0.84
1:A:96:LYS:NZ	2:B:130:ASP:OD2	2.11	0.84
1:G:210:TYR:CZ	2:H:326:LYS:CB	2.61	0.84
1:G:224:TYR:CD2	2:H:325:MET:HG3	2.13	0.84
1:C:96:LYS:NZ	2:D:130:ASP:OD2	2.10	0.83
1:E:258:ASN:C	2:R:404:PHE:CE2	2.56	0.83
1:G:238:ILE:O	1:G:238:ILE:HG22	1.78	0.83
1:I:101:ASN:N	2:J:254:LYS:CD	2.41	0.83
1:O:101:ASN:HB2	2:P:254:LYS:CG	2.07	0.83
1:Q:176:GLN:HG3	2:R:333:LEU:HD21	1.60	0.83
1:A:181:VAL:HA	2:B:352:LYS:HE3	0.84	0.83
1:K:394:LYS:CA	2:L:348:PRO:HG3	2.08	0.83
1:C:249:ASN:H	2:N:11:GLN:HE22	1.23	0.83
1:E:101:ASN:HB2	2:F:254:LYS:CD	2.07	0.83
1:G:224:TYR:CD1	2:H:325:MET:CG	2.59	0.83
1:I:176:GLN:CG	2:J:333:LEU:HD21	2.07	0.83
1:K:406:HIS:NE2	2:L:260:VAL:HG12	1.93	0.83
1:A:350:GLY:O	2:P:181:VAL:HG23	1.77	0.83
1:E:238:ILE:HG22	1:E:238:ILE:O	1.78	0.83
2:F:404:PHE:HE2	1:K:258:ASN:C	1.86	0.83
1:G:179:THR:HG21	2:H:353:THR:OG1	1.79	0.83
1:K:11:GLN:CD	2:L:247:GLN:O	2.21	0.83
1:M:97:GLU:CD	2:N:2:ARG:NE	2.35	0.83
1:O:105:ARG:HH21	2:P:253:ARG:HH21	0.84	0.83
1:Q:100:ALA:C	2:R:254:LYS:HD2	2.03	0.83
1:Q:238:ILE:O	1:Q:238:ILE:HG22	1.77	0.83
1:M:101:ASN:HB2	2:N:254:LYS:CG	2.09	0.83
1:O:401:LYS:CD	2:P:346:TRP:CD1	2.61	0.83
1:C:326:LYS:HB2	2:N:210:TYR:CE2	2.13	0.83
2:F:403:ALA:HB2	1:K:346:TRP:HE3	1.44	0.83
1:I:394:LYS:HG2	2:J:348:PRO:HB2	1.59	0.83
1:O:101:ASN:HB2	2:P:254:LYS:HE3	0.84	0.83
1:O:401:LYS:HG3	2:P:346:TRP:HB3	1.61	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:VAL:HA	1:K:350:GLY:HA3	1.61	0.83
1:K:181:VAL:HA	2:L:352:LYS:HE3	0.84	0.83
1:Q:210:TYR:CD1	2:R:326:LYS:CB	2.60	0.83
1:M:11:GLN:CD	2:N:247:GLN:O	2.22	0.83
1:Q:179:THR:HA	2:R:353:THR:H	1.43	0.83
2:B:398:MET:HG2	1:I:348:PRO:HD3	1.61	0.83
1:G:210:TYR:CB	2:H:326:LYS:HD2	2.08	0.83
2:H:283:TYR:CA	2:J:56:ALA:HB1	2.01	0.83
1:O:181:VAL:HB	2:P:352:LYS:HG3	1.60	0.83
1:C:224:TYR:CZ	2:D:325:MET:HG3	2.13	0.82
1:E:224:TYR:CD1	2:F:325:MET:CG	2.61	0.82
1:O:176:GLN:HB3	2:P:333:LEU:CG	2.08	0.82
1:C:401:LYS:CE	2:D:346:TRP:CD1	2.61	0.82
1:G:176:GLN:HB3	2:H:333:LEU:HD22	0.83	0.82
1:C:224:TYR:CG	2:D:325:MET:HG3	2.13	0.82
2:D:401:ARG:CG	1:G:346:TRP:CB	2.43	0.82
1:G:394:LYS:CA	2:H:348:PRO:HG3	2.09	0.82
1:M:101:ASN:H	2:N:254:LYS:HD2	1.42	0.82
2:N:283:TYR:CA	2:P:56:ALA:HB1	2.00	0.82
1:O:210:TYR:CD2	2:P:326:LYS:CG	2.62	0.82
2:D:96:GLN:HE22	1:G:2:ARG:HG3	0.66	0.82
1:E:404:PHE:CE2	2:F:258:ASN:O	2.32	0.82
1:G:210:TYR:HB3	2:H:326:LYS:CE	2.08	0.82
1:K:224:TYR:CE2	2:L:325:MET:HG3	2.13	0.82
2:P:282:GLN:O	2:R:60:LYS:HB2	1.78	0.82
1:C:2:ARG:CG	2:N:96:GLN:NE2	2.17	0.82
2:D:398:MET:CG	1:G:348:PRO:HD3	2.09	0.82
1:E:401:LYS:NZ	2:F:437:ASP:OD2	2.11	0.82
1:I:406:HIS:NE2	2:J:260:VAL:HG12	1.94	0.82
1:K:176:GLN:CG	2:L:333:LEU:HD21	2.10	0.82
1:Q:101:ASN:CB	2:R:254:LYS:CE	2.31	0.82
1:Q:210:TYR:CG	2:R:326:LYS:CG	2.62	0.82
1:A:210:TYR:CE1	2:B:326:LYS:CB	2.62	0.82
1:E:224:TYR:CZ	2:F:325:MET:HG3	2.14	0.82
1:G:100:ALA:C	2:H:254:LYS:HD2	2.03	0.82
1:I:176:GLN:HB3	2:J:333:LEU:HD22	0.82	0.82
1:I:210:TYR:CZ	2:J:326:LYS:HB2	2.14	0.82
1:K:97:GLU:CD	2:L:2:ARG:CZ	2.53	0.82
1:Q:394:LYS:HZ1	2:R:349:ASN:HD21	0.85	0.82
2:B:210:TYR:CE2	1:I:326:LYS:HB2	2.14	0.82
1:O:101:ASN:H	2:P:254:LYS:HD2	1.39	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:177:VAL:CG1	2:P:329:ASP:HA	2.08	0.82
1:O:401:LYS:CE	2:P:346:TRP:CD1	2.63	0.82
1:K:101:ASN:HB2	2:L:254:LYS:HE3	0.82	0.82
1:A:97:GLU:CD	2:B:2:ARG:HE	1.86	0.81
2:F:398:MET:CG	1:K:348:PRO:HD3	2.09	0.81
1:I:11:GLN:CD	2:J:247:GLN:O	2.23	0.81
1:Q:210:TYR:OH	2:R:325:MET:C	2.22	0.81
1:A:256:GLN:HG2	2:P:407:TRP:CH2	2.15	0.81
1:G:406:HIS:NE2	2:H:260:VAL:HG12	1.95	0.81
1:K:404:PHE:HZ	2:L:314:THR:HG22	1.45	0.81
1:O:210:TYR:CG	2:P:326:LYS:HG3	2.15	0.81
2:B:404:PHE:CE2	1:I:258:ASN:C	2.58	0.81
1:G:101:ASN:HB2	2:H:254:LYS:HE3	0.81	0.81
1:I:397:LEU:HB3	2:J:346:TRP:O	1.80	0.81
1:K:100:ALA:C	2:L:254:LYS:HD2	2.04	0.81
1:Q:101:ASN:H	2:R:254:LYS:HD2	1.42	0.81
1:C:394:LYS:CA	2:D:348:PRO:HG3	2.09	0.81
1:C:397:LEU:HB3	2:D:346:TRP:O	1.81	0.81
1:I:394:LYS:NZ	2:J:349:ASN:ND2	2.29	0.81
1:M:210:TYR:CG	2:N:326:LYS:CG	2.63	0.81
1:M:404:PHE:HE2	2:N:258:ASN:O	1.63	0.81
1:A:329:ASN:CG	2:P:177:VAL:HG23	2.04	0.81
2:B:398:MET:HG2	1:I:348:PRO:CD	2.10	0.81
1:C:406:HIS:NE2	2:D:260:VAL:HG12	1.95	0.81
1:K:176:GLN:HB2	2:L:333:LEU:HD22	1.59	0.81
1:A:210:TYR:OH	2:B:326:LYS:N	2.13	0.81
1:G:176:GLN:CG	2:H:333:LEU:HD21	2.11	0.81
1:I:176:GLN:HB2	2:J:333:LEU:HD22	1.59	0.81
1:M:176:GLN:CG	2:N:333:LEU:CD2	2.57	0.81
1:M:176:GLN:HG3	2:N:333:LEU:HD21	1.61	0.81
1:Q:210:TYR:CG	2:R:326:LYS:HG3	2.15	0.81
1:A:401:LYS:HE2	2:B:346:TRP:CD1	2.15	0.81
2:B:284:ARG:N	2:F:56:ALA:HB1	1.95	0.81
1:A:407:TRP:CD2	2:B:257:VAL:HA	2.16	0.81
1:I:97:GLU:CD	2:J:2:ARG:NE	2.39	0.81
1:Q:176:GLN:CG	2:R:333:LEU:CD2	2.58	0.81
1:C:329:ASN:CG	2:N:177:VAL:CG2	2.52	0.81
2:N:283:TYR:HB3	2:P:62:VAL:HG21	1.60	0.81
1:A:133:GLN:HE22	2:P:97:SER:CB	1.93	0.81
1:A:394:LYS:HG2	2:B:348:PRO:HB2	1.61	0.81
1:C:210:TYR:CE1	2:D:326:LYS:CB	2.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:HA	2:H:352:LYS:HE3	0.82	0.80
1:E:2:ARG:CG	2:R:96:GLN:NE2	2.20	0.80
1:G:394:LYS:HG2	2:H:348:PRO:HB2	1.63	0.80
1:G:401:LYS:CD	2:H:346:TRP:CG	2.65	0.80
1:I:404:PHE:HE2	2:J:258:ASN:O	1.61	0.80
1:K:394:LYS:HG2	2:L:348:PRO:HB2	1.62	0.80
1:Q:97:GLU:CD	2:R:2:ARG:NE	2.38	0.80
1:Q:210:TYR:CB	2:R:326:LYS:HD2	2.10	0.80
1:Q:401:LYS:CE	2:R:346:TRP:CD1	2.65	0.80
1:C:96:LYS:O	2:D:2:ARG:CD	2.28	0.80
2:D:210:TYR:CE2	1:G:326:LYS:HB2	2.17	0.80
1:A:224:TYR:CZ	2:B:325:MET:SD	2.73	0.80
1:G:210:TYR:CZ	2:H:326:LYS:HB2	2.16	0.80
1:M:96:LYS:NZ	2:N:130:ASP:OD2	2.13	0.80
1:G:404:PHE:HE2	2:H:258:ASN:O	1.63	0.80
1:I:96:LYS:O	2:J:2:ARG:CD	2.29	0.80
1:I:404:PHE:HZ	2:J:314:THR:HG22	1.46	0.80
2:J:282:GLN:O	2:L:60:LYS:HB2	1.80	0.80
1:I:101:ASN:CB	2:J:254:LYS:CE	2.28	0.80
1:I:179:THR:HA	2:J:353:THR:H	1.47	0.80
1:Q:401:LYS:HE2	2:R:346:TRP:CD1	2.17	0.80
1:A:247:ALA:O	2:P:11:GLN:OE1	1.98	0.80
1:I:101:ASN:HB2	2:J:254:LYS:HE3	0.81	0.80
1:A:401:LYS:HD3	2:B:346:TRP:CD2	2.17	0.80
1:A:406:HIS:NE2	2:B:260:VAL:HG12	1.96	0.80
1:I:210:TYR:OH	2:J:325:MET:C	2.24	0.80
1:K:401:LYS:NZ	2:L:437:ASP:OD2	2.14	0.80
1:K:404:PHE:HZ	2:L:314:THR:CG2	1.94	0.80
1:M:401:LYS:HG3	2:N:346:TRP:HB3	1.63	0.80
2:D:398:MET:CG	1:G:348:PRO:CD	2.60	0.80
1:G:97:GLU:CD	2:H:2:ARG:CZ	2.55	0.80
1:G:97:GLU:CD	2:H:2:ARG:HE	1.90	0.80
1:Q:401:LYS:NZ	2:R:437:ASP:OD2	2.15	0.80
1:A:210:TYR:HB3	2:B:326:LYS:CD	2.12	0.80
2:D:404:PHE:CE2	1:G:258:ASN:C	2.59	0.80
1:E:210:TYR:HB3	2:F:326:LYS:HD2	1.63	0.80
1:M:404:PHE:CZ	2:N:314:THR:CG2	2.64	0.80
1:O:105:ARG:CZ	2:P:253:ARG:NE	2.45	0.80
1:O:406:HIS:CE1	2:P:260:VAL:CG1	2.65	0.80
1:Q:176:GLN:HB3	2:R:333:LEU:CG	2.10	0.80
1:A:210:TYR:CZ	2:B:326:LYS:N	2.50	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:LYS:HB2	2:R:210:TYR:CE2	2.16	0.79
1:E:329:ASN:OD1	2:R:177:VAL:HG21	1.82	0.79
1:G:401:LYS:CG	2:H:346:TRP:HB3	2.12	0.79
1:A:394:LYS:NZ	2:B:349:ASN:HD21	1.80	0.79
2:B:56:ALA:HB3	2:D:283:TYR:HA	1.62	0.79
1:E:133:GLN:HE22	2:R:97:SER:CB	1.95	0.79
1:O:179:THR:CA	2:P:353:THR:H	1.96	0.79
1:Q:179:THR:O	2:R:352:LYS:HB3	1.82	0.79
1:A:224:TYR:CD1	2:B:325:MET:CG	2.64	0.79
1:C:210:TYR:OH	2:D:326:LYS:N	2.15	0.79
1:K:210:TYR:CZ	2:L:326:LYS:HB2	2.17	0.79
1:O:404:PHE:CZ	2:P:314:THR:HG21	2.17	0.79
1:O:407:TRP:CZ2	2:P:256:ALA:O	2.35	0.79
1:Q:404:PHE:CZ	2:R:314:THR:CG2	2.64	0.79
1:A:258:ASN:O	2:P:404:PHE:CZ	2.35	0.79
1:C:394:LYS:HG2	2:D:348:PRO:HB2	1.64	0.79
1:E:179:THR:HG21	2:F:353:THR:OG1	1.82	0.79
1:I:210:TYR:CG	2:J:326:LYS:CG	2.65	0.79
1:K:101:ASN:N	2:L:254:LYS:CD	2.44	0.79
1:M:210:TYR:CG	2:N:326:LYS:HG3	2.18	0.79
1:O:176:GLN:HB3	2:P:333:LEU:HD22	0.80	0.79
1:C:210:TYR:HB3	2:D:326:LYS:CD	2.12	0.79
1:C:407:TRP:CD2	2:D:257:VAL:HA	2.18	0.79
1:G:176:GLN:HB2	2:H:333:LEU:HD22	1.63	0.79
1:O:179:THR:HB	2:P:353:THR:O	1.82	0.79
2:D:401:ARG:CB	1:G:346:TRP:CB	2.61	0.79
2:H:284:ARG:N	2:J:56:ALA:HB1	1.96	0.79
1:M:401:LYS:CE	2:N:346:TRP:CD1	2.66	0.79
1:O:177:VAL:HG21	2:P:329:ASP:CA	2.12	0.79
1:Q:96:LYS:NZ	2:R:130:ASP:OD2	2.15	0.79
1:E:210:TYR:CE1	2:F:326:LYS:CB	2.63	0.79
2:F:210:TYR:CE2	1:K:326:LYS:HB2	2.17	0.79
1:O:101:ASN:CA	2:P:254:LYS:HE3	2.13	0.79
1:O:398:MET:HG3	2:P:348:PRO:HD2	1.65	0.79
1:Q:210:TYR:CZ	2:R:326:LYS:HB2	2.18	0.79
2:B:283:TYR:HB3	2:F:62:VAL:HG21	1.65	0.79
2:N:345:GLU:OE1	2:N:345:GLU:N	2.16	0.79
1:O:397:LEU:HB3	2:P:346:TRP:C	2.07	0.79
1:Q:404:PHE:HE2	2:R:258:ASN:O	1.66	0.79
1:C:224:TYR:CZ	2:D:325:MET:SD	2.75	0.79
1:G:11:GLN:CD	2:H:247:GLN:O	2.26	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:401:LYS:CD	2:J:346:TRP:CG	2.66	0.79
1:I:404:PHE:HZ	2:J:314:THR:CG2	1.94	0.79
2:F:401:ARG:HG3	1:K:346:TRP:HB3	0.86	0.79
1:I:181:VAL:HA	2:J:352:LYS:HE3	0.79	0.79
1:M:176:GLN:HB3	2:N:333:LEU:CG	2.12	0.79
1:E:394:LYS:CA	2:F:348:PRO:HG3	2.13	0.78
1:A:401:LYS:CE	2:B:346:TRP:CD1	2.66	0.78
2:B:11:GLN:HE22	1:I:249:ASN:H	1.30	0.78
1:G:101:ASN:N	2:H:254:LYS:CD	2.44	0.78
2:J:345:GLU:OE1	2:J:345:GLU:N	2.16	0.78
1:M:177:VAL:HG22	2:N:329:ASP:O	1.83	0.78
1:A:179:THR:HG21	2:B:353:THR:OG1	1.81	0.78
2:B:345:GLU:OE1	2:B:345:GLU:N	2.16	0.78
1:E:210:TYR:OH	2:F:326:LYS:N	2.16	0.78
1:I:176:GLN:CG	2:J:333:LEU:CD2	2.62	0.78
1:Q:401:LYS:CD	2:R:346:TRP:CD1	2.66	0.78
1:K:100:ALA:HA	2:L:254:LYS:CB	2.11	0.78
1:Q:101:ASN:HB2	2:R:254:LYS:CG	2.13	0.78
1:C:179:THR:HG21	2:D:353:THR:OG1	1.83	0.78
1:E:404:PHE:HZ	2:F:314:THR:HG22	1.47	0.78
1:G:404:PHE:HZ	2:H:314:THR:CG2	1.97	0.78
1:O:401:LYS:HD3	2:P:346:TRP:CD1	2.17	0.78
2:P:345:GLU:OE1	2:P:345:GLU:N	2.16	0.78
1:C:224:TYR:CD1	2:D:325:MET:CG	2.66	0.78
1:C:256:GLN:HG2	2:N:407:TRP:CH2	2.17	0.78
1:G:101:ASN:CB	2:H:254:LYS:CE	2.31	0.78
1:I:401:LYS:CD	2:J:346:TRP:CD1	2.67	0.78
1:K:181:VAL:HA	2:L:352:LYS:NZ	1.98	0.78
1:M:394:LYS:HZ1	2:N:349:ASN:HD21	0.81	0.78
1:O:210:TYR:CG	2:P:326:LYS:HD2	2.19	0.78
1:A:404:PHE:HZ	2:B:314:THR:CG2	1.96	0.78
1:E:247:ALA:O	2:R:11:GLN:OE1	2.00	0.78
1:E:329:ASN:CG	2:R:177:VAL:CG2	2.56	0.78
1:G:401:LYS:CD	2:H:346:TRP:CD1	2.66	0.78
1:K:97:GLU:CD	2:L:2:ARG:HE	1.91	0.78
1:Q:401:LYS:HG3	2:R:346:TRP:HB3	1.64	0.78
1:E:407:TRP:CD2	2:F:257:VAL:HA	2.18	0.78
1:G:397:LEU:HB3	2:H:346:TRP:O	1.84	0.78
1:I:401:LYS:CG	2:J:346:TRP:HB3	2.13	0.78
1:O:401:LYS:HE2	2:P:346:TRP:CD1	2.19	0.78
2:P:283:TYR:HB3	2:R:62:VAL:CG2	2.14	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:398:MET:CG	1:K:348:PRO:CD	2.61	0.78
1:G:181:VAL:HA	2:H:352:LYS:NZ	1.98	0.78
1:G:210:TYR:OH	2:H:325:MET:C	2.27	0.78
1:K:210:TYR:CB	2:L:326:LYS:HD2	2.13	0.78
1:C:404:PHE:HZ	2:D:314:THR:CG2	1.97	0.77
1:M:401:LYS:CD	2:N:346:TRP:CD1	2.67	0.77
1:K:394:LYS:HZ1	2:L:349:ASN:HD21	1.31	0.77
1:A:97:GLU:CD	2:B:2:ARG:CZ	2.57	0.77
2:D:403:ALA:HB2	1:G:346:TRP:HE3	1.44	0.77
1:E:96:LYS:O	2:F:2:ARG:CD	2.31	0.77
2:L:345:GLU:OE1	2:L:345:GLU:N	2.16	0.77
1:O:401:LYS:HD3	2:P:346:TRP:CD2	2.19	0.77
1:G:96:LYS:O	2:H:2:ARG:CD	2.32	0.77
1:G:394:LYS:NZ	2:H:349:ASN:ND2	2.32	0.77
1:I:181:VAL:HA	2:J:352:LYS:NZ	1.98	0.77
2:J:283:TYR:HB3	2:L:62:VAL:CG2	2.13	0.77
1:M:210:TYR:CZ	2:N:326:LYS:HB2	2.18	0.77
2:B:56:ALA:HB1	2:D:284:ARG:N	1.99	0.77
1:C:394:LYS:NZ	2:D:349:ASN:HD21	1.82	0.77
1:K:401:LYS:CD	2:L:346:TRP:CD1	2.68	0.77
1:A:101:ASN:CB	2:B:254:LYS:CE	2.35	0.77
1:C:133:GLN:HE22	2:N:97:SER:CB	1.96	0.77
1:C:210:TYR:CZ	2:D:326:LYS:N	2.51	0.77
2:F:345:GLU:OE1	2:F:345:GLU:N	2.16	0.77
1:G:181:VAL:CB	2:H:352:LYS:CE	2.55	0.77
1:K:394:LYS:NZ	2:L:349:ASN:ND2	2.33	0.77
1:M:210:TYR:CD1	2:N:326:LYS:CB	2.61	0.77
1:O:96:LYS:NZ	2:P:130:ASP:OD2	2.18	0.77
1:A:100:ALA:C	2:B:254:LYS:HD2	2.09	0.77
1:A:224:TYR:CD2	2:B:325:MET:HG3	2.19	0.77
1:A:224:TYR:CZ	2:B:325:MET:CG	2.68	0.77
1:E:11:GLN:CD	2:F:247:GLN:O	2.28	0.77
1:K:210:TYR:CD1	2:L:326:LYS:CB	2.66	0.77
2:R:345:GLU:OE1	2:R:345:GLU:N	2.16	0.77
1:O:181:VAL:HA	2:P:352:LYS:NZ	2.00	0.77
1:A:101:ASN:HB2	2:B:254:LYS:CG	2.16	0.76
1:I:401:LYS:NZ	2:J:437:ASP:OD2	2.18	0.76
1:M:105:ARG:CZ	2:N:253:ARG:NE	2.48	0.76
1:C:247:ALA:O	2:N:11:GLN:OE1	2.03	0.76
1:E:404:PHE:HZ	2:F:314:THR:CG2	1.97	0.76
1:G:179:THR:HA	2:H:353:THR:H	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:210:TYR:CD2	2:J:326:LYS:CG	2.67	0.76
1:K:397:LEU:HB3	2:L:346:TRP:O	1.85	0.76
1:C:97:GLU:CD	2:D:2:ARG:HE	1.92	0.76
2:D:398:MET:HG2	1:G:348:PRO:HD3	1.67	0.76
1:I:177:VAL:HG22	2:J:329:ASP:O	1.83	0.76
1:M:401:LYS:HE2	2:N:346:TRP:CD1	2.20	0.76
1:K:96:LYS:O	2:L:2:ARG:CD	2.33	0.76
1:A:249:ASN:H	2:P:11:GLN:NE2	1.83	0.76
1:E:177:VAL:HG11	2:F:329:ASP:CA	2.15	0.76
2:F:401:ARG:CB	1:K:346:TRP:CB	2.64	0.76
1:G:404:PHE:HZ	2:H:314:THR:HG22	1.48	0.76
1:K:210:TYR:CG	2:L:326:LYS:CG	2.68	0.76
1:M:179:THR:HB	2:N:353:THR:O	1.84	0.76
1:O:401:LYS:NZ	2:P:437:ASP:OD2	2.18	0.76
1:G:100:ALA:HA	2:H:254:LYS:CB	2.14	0.76
1:G:177:VAL:HG22	2:H:329:ASP:O	1.85	0.76
1:G:401:LYS:NZ	2:H:437:ASP:OD2	2.17	0.76
1:M:210:TYR:CD2	2:N:326:LYS:CG	2.69	0.76
1:O:101:ASN:HD22	2:P:258:ASN:HD21	1.34	0.76
1:A:97:GLU:CD	2:B:2:ARG:NE	2.43	0.76
1:A:177:VAL:HG11	2:B:329:ASP:CA	2.16	0.76
1:C:258:ASN:O	2:N:404:PHE:CZ	2.38	0.76
1:E:224:TYR:CZ	2:F:325:MET:SD	2.77	0.76
1:K:401:LYS:CD	2:L:346:TRP:CG	2.68	0.76
1:M:181:VAL:HB	2:N:352:LYS:HG3	1.67	0.76
2:N:282:GLN:O	2:P:60:LYS:HB2	1.85	0.76
1:O:11:GLN:OE1	2:P:247:GLN:O	2.04	0.76
1:Q:177:VAL:HG22	2:R:329:ASP:O	1.84	0.76
1:E:350:GLY:O	2:R:181:VAL:HG23	1.83	0.76
1:A:179:THR:HA	2:B:353:THR:H	1.51	0.76
1:C:350:GLY:O	2:N:181:VAL:HG23	1.82	0.76
1:K:404:PHE:HE2	2:L:258:ASN:O	1.65	0.76
2:P:283:TYR:C	2:R:56:ALA:HB2	2.11	0.76
1:E:100:ALA:HA	2:F:254:LYS:CB	2.11	0.76
1:E:394:LYS:NZ	2:F:349:ASN:HD21	1.84	0.76
2:F:404:PHE:CE2	1:K:258:ASN:C	2.63	0.76
1:K:97:GLU:CD	2:L:2:ARG:NE	2.44	0.76
1:M:401:LYS:HD3	2:N:346:TRP:CD2	2.21	0.76
1:C:101:ASN:CB	2:D:254:LYS:CE	2.38	0.75
2:F:11:GLN:HE22	1:K:249:ASN:H	1.34	0.75
1:K:181:VAL:CB	2:L:352:LYS:CE	2.55	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:401:LYS:CG	2:P:346:TRP:CB	2.62	0.75
1:Q:210:TYR:CD2	2:R:326:LYS:CG	2.69	0.75
1:A:224:TYR:CE2	2:B:325:MET:HG3	2.20	0.75
1:I:210:TYR:CG	2:J:326:LYS:HG3	2.21	0.75
1:A:329:ASN:CG	2:P:177:VAL:HG21	2.11	0.75
1:G:97:GLU:CD	2:H:2:ARG:NE	2.44	0.75
1:O:397:LEU:HD22	2:P:345:GLU:O	1.85	0.75
1:C:224:TYR:CD2	2:D:325:MET:HG3	2.22	0.75
1:G:210:TYR:CG	2:H:326:LYS:CG	2.69	0.75
1:I:176:GLN:HG3	2:J:333:LEU:HD21	1.68	0.75
1:A:329:ASN:CB	2:P:177:VAL:HG21	2.17	0.75
1:A:394:LYS:NZ	2:B:349:ASN:ND2	2.34	0.75
1:G:176:GLN:CG	2:H:333:LEU:CD2	2.65	0.75
1:K:11:GLN:OE1	2:L:247:GLN:O	2.05	0.75
1:Q:105:ARG:CZ	2:R:253:ARG:NE	2.50	0.75
1:Q:401:LYS:HD3	2:R:346:TRP:CD2	2.21	0.75
1:A:404:PHE:HE2	2:B:258:ASN:O	1.68	0.75
1:K:210:TYR:OH	2:L:325:MET:C	2.29	0.75
1:M:397:LEU:HB3	2:N:346:TRP:C	2.11	0.75
1:M:401:LYS:NZ	2:N:437:ASP:OD2	2.19	0.75
1:M:404:PHE:CZ	2:N:314:THR:HG21	2.21	0.75
1:O:179:THR:O	2:P:352:LYS:HB3	1.87	0.75
1:M:177:VAL:CG1	2:N:329:ASP:HA	2.15	0.75
1:M:179:THR:O	2:N:352:LYS:HB3	1.86	0.75
1:O:401:LYS:HD3	2:P:346:TRP:NE1	2.00	0.75
1:A:101:ASN:N	2:B:254:LYS:CD	2.46	0.75
2:D:398:MET:HG2	1:G:348:PRO:CD	2.17	0.75
1:E:243:ARG:NH2	2:R:71:GLU:OE2	2.20	0.75
1:I:210:TYR:CG	2:J:326:LYS:HD2	2.22	0.75
1:M:179:THR:CG2	2:N:353:THR:HG1	1.80	0.75
1:M:179:THR:CA	2:N:353:THR:H	1.99	0.75
1:A:406:HIS:NE2	2:B:260:VAL:CG1	2.50	0.75
1:C:177:VAL:HG11	2:D:329:ASP:CA	2.17	0.75
1:E:210:TYR:CZ	2:F:326:LYS:N	2.55	0.75
2:H:283:TYR:HA	2:J:56:ALA:HB2	1.68	0.75
1:K:401:LYS:CG	2:L:346:TRP:HB3	2.17	0.75
1:E:406:HIS:NE2	2:F:260:VAL:CG1	2.49	0.74
2:B:283:TYR:CA	2:F:56:ALA:HB1	2.15	0.74
2:D:11:GLN:HE22	1:G:249:ASN:H	1.32	0.74
2:D:401:ARG:HG3	1:G:346:TRP:HB3	0.81	0.74
1:E:224:TYR:CD2	2:F:325:MET:HG3	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:398:MET:HG2	1:K:348:PRO:HD3	1.68	0.74
1:K:210:TYR:CG	2:L:326:LYS:HG3	2.22	0.74
1:Q:179:THR:CG2	2:R:353:THR:HG1	2.00	0.74
1:Q:181:VAL:HA	2:R:352:LYS:NZ	2.02	0.74
1:I:181:VAL:CB	2:J:352:LYS:CE	2.55	0.74
1:Q:11:GLN:OE1	2:R:247:GLN:O	2.05	0.74
1:Q:404:PHE:CZ	2:R:314:THR:HG21	2.22	0.74
1:E:2:ARG:HG3	2:R:96:GLN:HE22	0.62	0.74
2:F:401:ARG:CG	1:K:346:TRP:CB	2.48	0.74
1:I:11:GLN:OE1	2:J:247:GLN:O	2.06	0.74
1:I:177:VAL:HG21	2:J:329:ASP:CA	2.18	0.74
1:O:401:LYS:CG	2:P:346:TRP:HB3	2.17	0.74
1:Q:398:MET:HG3	2:R:348:PRO:HD2	1.69	0.74
1:A:100:ALA:HA	2:B:254:LYS:CB	2.13	0.74
1:C:224:TYR:CZ	2:D:325:MET:CG	2.70	0.74
1:M:177:VAL:HG21	2:N:329:ASP:CA	2.17	0.74
1:O:105:ARG:CZ	2:P:253:ARG:HE	1.99	0.74
1:Q:401:LYS:HD3	2:R:346:TRP:NE1	2.03	0.74
1:C:101:ASN:N	2:D:254:LYS:CD	2.49	0.74
1:C:224:TYR:CE2	2:D:325:MET:HG3	2.22	0.74
1:C:404:PHE:HE2	2:D:258:ASN:O	1.70	0.74
1:E:210:TYR:CE2	2:F:326:LYS:CA	2.61	0.74
1:E:394:LYS:HG2	2:F:348:PRO:HB2	1.68	0.74
1:I:100:ALA:HA	2:J:254:LYS:CB	2.11	0.74
1:I:181:VAL:HB	2:J:352:LYS:HG3	1.69	0.74
1:C:401:LYS:NZ	2:D:437:ASP:OD2	2.20	0.74
1:E:210:TYR:HB3	2:F:326:LYS:CD	2.16	0.74
1:G:177:VAL:HG21	2:H:329:ASP:CA	2.18	0.74
1:I:210:TYR:CD1	2:J:326:LYS:CB	2.64	0.74
1:I:406:HIS:NE2	2:J:260:VAL:CG1	2.50	0.74
1:I:407:TRP:CZ2	2:J:256:ALA:O	2.41	0.74
1:Q:179:THR:CA	2:R:353:THR:H	2.01	0.74
1:A:348:PRO:CG	2:P:398:MET:SD	2.75	0.74
1:K:179:THR:HA	2:L:353:THR:H	1.53	0.74
1:M:407:TRP:CZ2	2:N:256:ALA:O	2.41	0.74
1:A:348:PRO:HD3	2:P:398:MET:HG3	1.68	0.74
1:C:100:ALA:C	2:D:254:LYS:HD2	2.12	0.74
1:C:404:PHE:HZ	2:D:314:THR:HG22	1.51	0.74
1:I:177:VAL:CG1	2:J:329:ASP:HA	2.15	0.74
1:K:176:GLN:CG	2:L:333:LEU:CD2	2.66	0.74
1:O:401:LYS:CD	2:P:346:TRP:CG	2.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:179:THR:HB	2:R:353:THR:O	1.88	0.74
1:M:101:ASN:CA	2:N:254:LYS:HE3	2.18	0.73
1:Q:101:ASN:CA	2:R:254:LYS:HE3	2.18	0.73
2:H:282:GLN:O	2:J:60:LYS:HB2	1.88	0.73
1:O:397:LEU:CB	2:P:346:TRP:O	2.36	0.73
1:C:101:ASN:HB2	2:D:254:LYS:CG	2.19	0.73
1:E:224:TYR:CZ	2:F:325:MET:CG	2.71	0.73
1:I:398:MET:HG3	2:J:348:PRO:HD2	1.69	0.73
1:Q:407:TRP:CZ2	2:R:256:ALA:O	2.41	0.73
1:C:406:HIS:NE2	2:D:260:VAL:CG1	2.51	0.73
1:E:401:LYS:CD	2:F:346:TRP:CG	2.71	0.73
1:G:210:TYR:CD2	2:H:326:LYS:CG	2.70	0.73
2:J:266:HIS:ND1	2:J:266:HIS:O	2.22	0.73
1:G:398:MET:HG3	2:H:348:PRO:HD2	1.70	0.73
1:K:406:HIS:NE2	2:L:260:VAL:CG1	2.50	0.73
1:O:176:GLN:OE1	2:P:333:LEU:CD1	2.31	0.73
1:O:181:VAL:HG23	2:P:352:LYS:HE2	1.70	0.73
1:A:404:PHE:HZ	2:B:314:THR:HG22	1.51	0.73
2:B:177:VAL:CG2	1:I:329:ASN:CG	2.61	0.73
2:B:266:HIS:ND1	2:B:266:HIS:O	2.22	0.73
1:E:101:ASN:N	2:F:254:LYS:CD	2.50	0.73
1:E:401:LYS:CD	2:F:346:TRP:CD1	2.71	0.73
1:I:176:GLN:HB3	2:J:333:LEU:CG	2.18	0.73
1:A:350:GLY:CA	2:P:181:VAL:HA	2.15	0.73
2:B:62:VAL:HG21	2:D:283:TYR:HB3	1.70	0.73
1:E:181:VAL:HA	2:F:352:LYS:NZ	2.03	0.73
2:J:283:TYR:CA	2:L:56:ALA:HB2	2.15	0.73
1:O:100:ALA:HB1	2:P:254:LYS:HA	1.69	0.73
2:P:266:HIS:ND1	2:P:266:HIS:O	2.22	0.73
1:A:11:GLN:CD	2:B:247:GLN:O	2.31	0.73
1:E:97:GLU:CD	2:F:2:ARG:CZ	2.62	0.73
2:H:345:GLU:OE1	2:H:345:GLU:N	2.16	0.73
1:K:179:THR:HG22	2:L:353:THR:HG1	1.52	0.73
2:P:282:GLN:O	2:R:60:LYS:CB	2.35	0.73
2:B:97:SER:CB	1:I:133:GLN:HE22	2.01	0.73
1:C:97:GLU:CD	2:D:2:ARG:CZ	2.62	0.73
1:K:398:MET:HG3	2:L:348:PRO:HD2	1.71	0.73
1:O:181:VAL:CB	2:P:352:LYS:CE	2.58	0.73
1:C:100:ALA:HA	2:D:254:LYS:CB	2.14	0.73
1:K:176:GLN:HG3	2:L:333:LEU:HD21	1.70	0.73
1:K:407:TRP:CZ2	2:L:256:ALA:O	2.42	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:224:TYR:CE2	2:R:325:MET:HG3	2.09	0.73
1:E:397:LEU:HB3	2:F:346:TRP:O	1.89	0.72
2:F:398:MET:HG2	1:K:348:PRO:CD	2.19	0.72
1:K:177:VAL:HG22	2:L:329:ASP:O	1.88	0.72
1:M:398:MET:HG3	2:N:348:PRO:HD2	1.70	0.72
1:Q:181:VAL:HA	2:R:352:LYS:HE3	0.73	0.72
1:A:329:ASN:OD1	2:P:177:VAL:HG21	1.84	0.72
2:D:345:GLU:OE1	2:D:345:GLU:N	2.16	0.72
2:N:266:HIS:ND1	2:N:266:HIS:O	2.22	0.72
1:Q:176:GLN:HB3	2:R:333:LEU:CD1	2.18	0.72
2:D:266:HIS:ND1	2:D:266:HIS:O	2.22	0.72
1:G:210:TYR:CD1	2:H:326:LYS:CB	2.68	0.72
2:H:266:HIS:ND1	2:H:266:HIS:O	2.22	0.72
1:I:96:LYS:NZ	2:J:130:ASP:OD2	2.22	0.72
1:I:101:ASN:H	2:J:254:LYS:HD2	1.51	0.72
1:I:105:ARG:NH2	2:J:253:ARG:HH21	1.66	0.72
1:K:101:ASN:H	2:L:254:LYS:HD2	1.53	0.72
2:N:283:TYR:HB3	2:P:62:VAL:CG2	2.18	0.72
1:C:179:THR:HA	2:D:353:THR:H	1.53	0.72
1:G:407:TRP:CZ2	2:H:256:ALA:O	2.43	0.72
1:I:101:ASN:HB2	2:J:254:LYS:CG	2.19	0.72
1:M:11:GLN:OE1	2:N:247:GLN:O	2.08	0.72
1:M:101:ASN:HD22	2:N:258:ASN:HD21	1.37	0.72
1:O:101:ASN:CA	2:P:254:LYS:CE	2.68	0.72
1:C:394:LYS:NZ	2:D:349:ASN:ND2	2.36	0.72
1:E:348:PRO:HD3	2:R:398:MET:HG3	1.71	0.72
2:F:96:GLN:NE2	1:K:2:ARG:CG	2.33	0.72
1:G:406:HIS:NE2	2:H:260:VAL:CG1	2.52	0.72
2:L:266:HIS:ND1	2:L:266:HIS:O	2.22	0.72
1:C:11:GLN:CD	2:D:247:GLN:O	2.33	0.72
1:G:96:LYS:NZ	2:H:130:ASP:OD2	2.21	0.72
2:H:283:TYR:HB3	2:J:62:VAL:CG2	2.19	0.72
1:M:407:TRP:NE1	2:N:260:VAL:HB	2.05	0.72
1:Q:105:ARG:NH2	2:R:253:ARG:NE	2.37	0.72
1:Q:181:VAL:CB	2:R:352:LYS:CE	2.61	0.72
1:A:256:GLN:O	2:P:407:TRP:CZ2	2.42	0.72
1:Q:397:LEU:HB3	2:R:346:TRP:C	2.14	0.72
2:F:71:GLU:OE2	1:K:243:ARG:NH2	2.23	0.72
1:G:181:VAL:HB	2:H:352:LYS:HG3	1.72	0.72
1:G:210:TYR:CG	2:H:326:LYS:HD2	2.24	0.72
2:J:283:TYR:C	2:L:56:ALA:HB2	2.13	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:101:ASN:CB	2:L:254:LYS:CE	2.34	0.72
1:Q:11:GLN:HE22	2:R:247:GLN:C	1.98	0.72
2:D:97:SER:CB	1:G:133:GLN:HE22	2.02	0.72
1:M:105:ARG:CZ	2:N:253:ARG:HE	2.03	0.72
1:O:105:ARG:NH2	2:P:253:ARG:NE	2.38	0.71
1:O:210:TYR:CG	2:P:326:LYS:HB2	2.26	0.71
1:Q:181:VAL:HB	2:R:352:LYS:HG3	1.70	0.71
1:Q:210:TYR:CG	2:R:326:LYS:HD2	2.25	0.71
1:E:181:VAL:CB	2:F:352:LYS:CE	2.61	0.71
1:E:256:GLN:HG2	2:R:407:TRP:CH2	2.25	0.71
1:K:210:TYR:CG	2:L:326:LYS:HD2	2.25	0.71
1:M:181:VAL:HA	2:N:352:LYS:NZ	2.04	0.71
1:M:210:TYR:CG	2:N:326:LYS:HD2	2.25	0.71
2:R:266:HIS:ND1	2:R:266:HIS:O	2.22	0.71
1:A:243:ARG:NH2	2:P:71:GLU:OE2	2.24	0.71
2:B:181:VAL:HG23	1:I:350:GLY:O	1.89	0.71
2:B:401:ARG:HG3	1:I:346:TRP:HB3	0.78	0.71
1:E:100:ALA:C	2:F:254:LYS:HD2	2.14	0.71
1:A:249:ASN:N	2:P:11:GLN:HE22	1.86	0.71
2:B:96:GLN:NE2	1:I:2:ARG:CG	2.29	0.71
1:E:394:LYS:HZ1	2:F:349:ASN:HD21	1.39	0.71
1:K:179:THR:O	2:L:352:LYS:HB3	1.90	0.71
1:E:179:THR:O	2:F:352:LYS:HB3	1.90	0.71
2:F:97:SER:CB	1:K:133:GLN:HE22	2.03	0.71
1:K:176:GLN:HB3	2:L:333:LEU:CG	2.19	0.71
1:K:210:TYR:CD2	2:L:326:LYS:CG	2.72	0.71
1:O:394:LYS:C	2:P:348:PRO:HG3	2.16	0.71
1:A:101:ASN:H	2:B:254:LYS:HD2	1.53	0.71
1:A:210:TYR:CZ	2:B:326:LYS:CB	2.74	0.71
1:C:329:ASN:CG	2:N:177:VAL:HG21	2.16	0.71
2:D:96:GLN:NE2	1:G:2:ARG:CG	2.29	0.71
2:F:266:HIS:ND1	2:F:266:HIS:O	2.22	0.71
1:K:224:TYR:CD1	2:L:325:MET:SD	2.81	0.71
1:A:210:TYR:OH	2:B:325:MET:C	2.34	0.71
1:A:353:VAL:CB	2:P:179:ASP:OD1	2.31	0.71
1:G:11:GLN:OE1	2:H:247:GLN:O	2.09	0.71
1:G:210:TYR:CG	2:H:326:LYS:HG3	2.26	0.71
1:M:401:LYS:HD3	2:N:346:TRP:NE1	2.05	0.71
1:A:401:LYS:NZ	2:B:437:ASP:OD2	2.24	0.71
2:B:71:GLU:OE2	1:I:243:ARG:NH2	2.24	0.71
1:E:224:TYR:CE2	2:F:325:MET:HG3	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:LYS:NZ	2:L:130:ASP:OD2	2.22	0.71
1:Q:100:ALA:HB1	2:R:254:LYS:HA	1.70	0.71
1:C:401:LYS:CD	2:D:346:TRP:CG	2.74	0.71
1:M:176:GLN:HB3	2:N:333:LEU:CD1	2.21	0.71
1:A:394:LYS:HG2	2:B:348:PRO:CB	2.21	0.71
1:C:249:ASN:H	2:N:11:GLN:NE2	1.87	0.71
1:E:329:ASN:CG	2:R:177:VAL:HG21	2.16	0.71
1:I:181:VAL:HG23	2:J:352:LYS:HE2	1.72	0.70
1:M:176:GLN:OE1	2:N:333:LEU:CD1	2.35	0.70
1:M:401:LYS:HD3	2:N:346:TRP:CD1	2.24	0.70
1:A:348:PRO:HG3	2:P:398:MET:SD	2.32	0.70
1:C:329:ASN:OD1	2:N:177:VAL:HG21	1.86	0.70
1:E:249:ASN:H	2:R:11:GLN:NE2	1.88	0.70
1:Q:407:TRP:NE1	2:R:260:VAL:HB	2.05	0.70
1:A:283:HIS:C	1:E:56:THR:CG2	2.63	0.70
2:F:177:VAL:HG21	1:K:329:ASN:OD1	1.90	0.70
1:G:177:VAL:CG1	2:H:329:ASP:HA	2.18	0.70
1:M:181:VAL:HA	2:N:352:LYS:HE3	0.70	0.70
1:M:105:ARG:NH2	2:N:253:ARG:NE	2.38	0.70
1:O:404:PHE:CA	2:P:261:PRO:HA	2.21	0.70
1:C:401:LYS:CG	2:D:346:TRP:HB3	2.22	0.70
1:E:210:TYR:CZ	2:F:326:LYS:CB	2.74	0.70
1:E:401:LYS:CG	2:F:346:TRP:HB3	2.22	0.70
1:G:176:GLN:HG3	2:H:333:LEU:HD21	1.72	0.70
1:Q:404:PHE:CA	2:R:261:PRO:HA	2.21	0.70
1:G:101:ASN:HB2	2:H:254:LYS:CG	2.22	0.70
2:N:283:TYR:C	2:P:56:ALA:HB2	2.17	0.70
1:Q:177:VAL:HG21	2:R:329:ASP:CA	2.21	0.70
2:D:407:TRP:CH2	1:G:256:GLN:HG2	2.27	0.70
1:G:181:VAL:HG23	2:H:352:LYS:HE2	1.73	0.70
1:K:401:LYS:HD3	2:L:346:TRP:NE1	2.06	0.70
1:O:407:TRP:NE1	2:P:260:VAL:HB	2.05	0.70
1:C:210:TYR:OH	2:D:325:MET:C	2.35	0.70
1:C:238:ILE:O	1:C:238:ILE:CG2	2.40	0.70
1:C:401:LYS:CD	2:D:346:TRP:CD1	2.75	0.70
1:M:100:ALA:HB1	2:N:254:LYS:HA	1.72	0.70
1:Q:105:ARG:CZ	2:R:253:ARG:HE	2.03	0.70
2:B:11:GLN:OE1	1:I:247:ALA:O	2.09	0.70
1:G:176:GLN:HB3	2:H:333:LEU:CG	2.22	0.70
1:G:238:ILE:O	1:G:238:ILE:CG2	2.40	0.70
1:O:11:GLN:HE22	2:P:247:GLN:C	2.00	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ARG:HG3	2:N:96:GLN:HE22	0.55	0.69
1:M:401:LYS:CD	2:N:346:TRP:CG	2.75	0.69
2:P:283:TYR:CA	2:R:56:ALA:HB2	2.20	0.69
1:A:210:TYR:HB3	2:B:326:LYS:CE	2.21	0.69
1:C:97:GLU:CD	2:D:2:ARG:NE	2.49	0.69
1:E:97:GLU:CD	2:F:2:ARG:HE	1.99	0.69
1:E:101:ASN:H	2:F:254:LYS:HD2	1.55	0.69
1:I:394:LYS:HG2	2:J:348:PRO:CB	2.22	0.69
1:M:238:ILE:O	1:M:238:ILE:CG2	2.40	0.69
1:M:397:LEU:CB	2:N:346:TRP:O	2.39	0.69
1:O:404:PHE:CZ	2:P:314:THR:HG22	2.24	0.69
1:A:176:GLN:CG	2:B:333:LEU:HD21	2.22	0.69
2:B:283:TYR:HB3	2:F:62:VAL:CG2	2.21	0.69
1:E:394:LYS:NZ	2:F:349:ASN:ND2	2.41	0.69
1:O:179:THR:HG22	2:P:353:THR:CB	2.21	0.69
1:Q:238:ILE:O	1:Q:238:ILE:CG2	2.40	0.69
2:B:398:MET:HG3	1:I:348:PRO:HD3	1.74	0.69
2:D:11:GLN:OE1	1:G:247:ALA:O	2.10	0.69
1:E:404:PHE:HE2	2:F:258:ASN:O	1.72	0.69
1:I:404:PHE:CZ	2:J:314:THR:CG2	2.75	0.69
1:A:210:TYR:CB	2:B:326:LYS:HD2	2.21	0.69
1:C:179:THR:HG22	2:D:353:THR:HG1	1.57	0.69
1:C:348:PRO:HD3	2:N:398:MET:HG3	1.71	0.69
2:D:332:MET:HA	2:D:332:MET:HE2	1.75	0.69
2:F:332:MET:HE2	2:F:332:MET:HA	1.75	0.69
2:H:332:MET:HE2	2:H:332:MET:HA	1.75	0.69
1:K:394:LYS:HG2	2:L:348:PRO:CB	2.23	0.69
1:A:179:THR:HB	2:B:353:THR:O	1.92	0.69
1:C:210:TYR:CZ	2:D:326:LYS:CB	2.75	0.69
1:K:238:ILE:O	1:K:238:ILE:CG2	2.40	0.69
1:M:11:GLN:HE22	2:N:247:GLN:C	1.99	0.69
1:M:401:LYS:CG	2:N:346:TRP:HB3	2.22	0.69
2:N:332:MET:HE2	2:N:332:MET:HA	1.75	0.69
1:A:258:ASN:O	2:P:404:PHE:CE2	2.44	0.69
1:E:238:ILE:O	1:E:238:ILE:CG2	2.40	0.69
1:K:181:VAL:HB	2:L:352:LYS:HG3	1.75	0.69
2:L:332:MET:HA	2:L:332:MET:HE2	1.75	0.69
1:M:404:PHE:CA	2:N:261:PRO:HA	2.22	0.69
1:O:179:THR:CG2	2:P:353:THR:HG1	2.03	0.69
1:Q:401:LYS:CD	2:R:346:TRP:CG	2.75	0.69
2:R:332:MET:HE2	2:R:332:MET:HA	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLN:CG	2:D:333:LEU:HD21	2.23	0.69
1:C:181:VAL:CB	2:D:352:LYS:CE	2.64	0.69
1:C:243:ARG:NH2	2:N:71:GLU:OE2	2.25	0.69
2:D:71:GLU:OE2	1:G:243:ARG:NH2	2.25	0.69
1:E:260:VAL:HB	2:R:407:TRP:HZ2	1.57	0.69
1:O:283:HIS:HA	1:Q:56:THR:CG2	2.17	0.69
1:A:177:VAL:HG21	2:B:329:ASP:CA	2.23	0.69
1:C:210:TYR:CB	2:D:326:LYS:HD2	2.22	0.69
1:E:176:GLN:HB2	2:F:333:LEU:HD22	1.71	0.69
1:E:210:TYR:HB3	2:F:326:LYS:CE	2.22	0.69
2:B:176:LYS:HD3	1:I:333:ALA:HB2	1.74	0.69
2:B:282:GLN:O	2:F:60:LYS:HB2	1.92	0.69
1:E:348:PRO:CG	2:R:398:MET:SD	2.81	0.69
1:E:353:VAL:CB	2:R:179:ASP:OD1	2.36	0.69
2:F:176:LYS:HD3	1:K:333:ALA:HB2	1.74	0.69
1:K:179:THR:CG2	2:L:353:THR:HG1	2.03	0.69
1:O:176:GLN:HB3	2:P:333:LEU:CD1	2.22	0.69
2:B:407:TRP:CH2	1:I:256:GLN:HG2	2.27	0.68
1:C:181:VAL:HA	2:D:352:LYS:NZ	2.08	0.68
2:D:177:VAL:CG2	1:G:329:ASN:CG	2.65	0.68
1:I:179:THR:O	2:J:352:LYS:HB3	1.93	0.68
1:K:394:LYS:HZ3	2:L:349:ASN:ND2	1.90	0.68
1:Q:101:ASN:HD22	2:R:258:ASN:HD21	1.41	0.68
1:Q:401:LYS:HD3	2:R:346:TRP:CD1	2.25	0.68
1:C:177:VAL:HG21	2:D:329:ASP:CA	2.23	0.68
1:C:394:LYS:HG2	2:D:348:PRO:CB	2.24	0.68
1:I:238:ILE:O	1:I:238:ILE:CG2	2.40	0.68
1:K:404:PHE:CZ	2:L:314:THR:CG2	2.75	0.68
1:O:394:LYS:HA	2:P:348:PRO:CG	2.19	0.68
2:B:404:PHE:CZ	1:I:258:ASN:O	2.46	0.68
1:C:249:ASN:N	2:N:11:GLN:HE22	1.90	0.68
1:C:329:ASN:CB	2:N:177:VAL:HG21	2.23	0.68
1:E:249:ASN:N	2:R:11:GLN:HE22	1.90	0.68
1:E:407:TRP:CZ2	2:F:256:ALA:O	2.47	0.68
1:I:179:THR:HB	2:J:353:THR:O	1.92	0.68
1:O:210:TYR:CG	2:P:326:LYS:CD	2.76	0.68
1:A:283:HIS:HA	1:E:56:THR:CG2	2.17	0.68
1:E:179:THR:HA	2:F:353:THR:H	1.59	0.68
1:E:407:TRP:CZ2	2:F:260:VAL:HB	2.28	0.68
1:M:397:LEU:HD22	2:N:345:GLU:O	1.93	0.68
1:O:283:HIS:C	1:Q:56:THR:CG2	2.66	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:O	1:A:238:ILE:CG2	2.40	0.68
1:E:176:GLN:CG	2:F:333:LEU:HD21	2.24	0.68
1:O:407:TRP:CB	2:P:257:VAL:HG13	2.24	0.68
1:A:401:LYS:CG	2:B:346:TRP:HB3	2.23	0.68
2:F:11:GLN:OE1	1:K:247:ALA:O	2.10	0.68
1:I:401:LYS:HD3	2:J:346:TRP:NE1	2.07	0.68
2:P:283:TYR:HA	2:R:56:ALA:HB2	1.69	0.68
1:A:249:ASN:ND2	2:P:11:GLN:OE1	2.27	0.68
1:C:348:PRO:CG	2:N:398:MET:SD	2.82	0.68
1:E:258:ASN:O	2:R:404:PHE:CZ	2.45	0.68
1:O:238:ILE:O	1:O:238:ILE:CG2	2.40	0.68
1:O:401:LYS:HD3	2:P:346:TRP:CG	2.29	0.68
1:A:401:LYS:CD	2:B:346:TRP:CG	2.77	0.68
1:C:210:TYR:HB3	2:D:326:LYS:CE	2.23	0.68
1:E:401:LYS:HD3	2:F:346:TRP:NE1	2.08	0.68
1:Q:401:LYS:CG	2:R:346:TRP:HB3	2.23	0.68
1:A:401:LYS:CD	2:B:346:TRP:CD1	2.77	0.68
2:B:332:MET:HE2	2:B:332:MET:HA	1.75	0.68
1:C:179:THR:HB	2:D:353:THR:O	1.94	0.68
1:O:100:ALA:C	2:P:254:LYS:CD	2.66	0.68
2:P:332:MET:HE2	2:P:332:MET:HA	1.75	0.68
1:C:176:GLN:HB2	2:D:333:LEU:HD22	1.72	0.67
1:M:407:TRP:HE1	2:N:260:VAL:HB	1.58	0.67
2:B:11:GLN:NE2	1:I:249:ASN:H	1.92	0.67
1:G:179:THR:HB	2:H:353:THR:O	1.94	0.67
2:N:282:GLN:O	2:P:60:LYS:CB	2.41	0.67
1:A:407:TRP:CZ2	2:B:256:ALA:O	2.48	0.67
2:D:404:PHE:CZ	1:G:258:ASN:O	2.47	0.67
1:E:224:TYR:CD1	2:F:325:MET:SD	2.86	0.67
1:G:401:LYS:HD3	2:H:346:TRP:NE1	2.07	0.67
2:J:282:GLN:O	2:L:60:LYS:CB	2.41	0.67
1:K:177:VAL:HG21	2:L:329:ASP:CA	2.25	0.67
1:G:179:THR:O	2:H:352:LYS:HB3	1.94	0.67
1:I:179:THR:CA	2:J:353:THR:H	2.08	0.67
2:J:332:MET:HE2	2:J:332:MET:HA	1.75	0.67
1:M:181:VAL:HG23	2:N:352:LYS:HE2	1.76	0.67
1:Q:397:LEU:HD22	2:R:345:GLU:O	1.94	0.67
2:B:177:VAL:HG21	1:I:329:ASN:OD1	1.90	0.67
1:C:179:THR:O	2:D:352:LYS:HB3	1.94	0.67
1:I:210:TYR:CG	2:J:326:LYS:HB2	2.30	0.67
1:M:181:VAL:CB	2:N:352:LYS:CE	2.62	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:HG21	2:B:248:LEU:HD13	1.76	0.67
1:A:181:VAL:HB	2:B:352:LYS:HG3	1.76	0.67
1:C:350:GLY:CA	2:N:181:VAL:HA	2.22	0.67
2:D:176:LYS:HD3	1:G:333:ALA:HB2	1.75	0.67
1:E:210:TYR:CZ	2:F:326:LYS:HB2	2.29	0.67
1:I:401:LYS:HD3	2:J:346:TRP:CD1	2.28	0.67
1:A:105:ARG:CZ	2:B:253:ARG:NE	2.57	0.67
1:E:101:ASN:HB2	2:F:254:LYS:CG	2.24	0.67
1:C:256:GLN:O	2:N:407:TRP:CZ2	2.48	0.67
1:Q:243:ARG:NE	1:Q:243:ARG:HA	2.10	0.67
1:E:401:LYS:CG	2:F:346:TRP:CD2	2.78	0.67
1:G:101:ASN:H	2:H:254:LYS:HD2	1.54	0.67
1:K:101:ASN:HB2	2:L:254:LYS:CG	2.24	0.67
1:K:181:VAL:HG23	2:L:352:LYS:HE2	1.77	0.67
1:O:177:VAL:HB	2:P:329:ASP:HB3	1.77	0.67
1:A:2:ARG:HG3	2:P:96:GLN:HE22	0.51	0.66
1:A:179:THR:O	2:B:352:LYS:HB3	1.93	0.66
2:B:11:GLN:OE1	1:I:249:ASN:ND2	2.28	0.66
1:C:243:ARG:NE	1:C:243:ARG:HA	2.10	0.66
1:E:105:ARG:NH2	2:F:253:ARG:NE	2.41	0.66
2:F:177:VAL:CG2	1:K:329:ASN:CG	2.68	0.66
1:G:243:ARG:HA	1:G:243:ARG:NE	2.10	0.66
1:K:401:LYS:CD	2:L:346:TRP:CD2	2.78	0.66
1:O:179:THR:HG21	2:P:248:LEU:HD13	1.76	0.66
1:O:397:LEU:HB2	2:P:348:PRO:HD3	1.76	0.66
1:Q:407:TRP:HE1	2:R:260:VAL:HB	1.60	0.66
1:A:181:VAL:CB	2:B:352:LYS:CE	2.65	0.66
1:A:210:TYR:CZ	2:B:326:LYS:HB2	2.29	0.66
1:A:283:HIS:C	1:E:56:THR:HG21	2.18	0.66
1:E:101:ASN:CB	2:F:254:LYS:CE	2.42	0.66
1:E:243:ARG:HA	1:E:243:ARG:NE	2.10	0.66
1:E:401:LYS:CD	2:F:346:TRP:CD2	2.78	0.66
1:K:243:ARG:NE	1:K:243:ARG:HA	2.10	0.66
1:A:352:LYS:CA	2:P:179:ASP:O	2.41	0.66
1:C:249:ASN:ND2	2:N:11:GLN:OE1	2.28	0.66
1:C:407:TRP:CZ2	2:D:256:ALA:O	2.49	0.66
2:D:179:ASP:OD1	1:G:353:VAL:CB	2.40	0.66
2:H:283:TYR:C	2:J:56:ALA:HB2	2.19	0.66
1:I:224:TYR:CD1	2:J:325:MET:SD	2.83	0.66
1:A:345:ASP:CG	2:P:400:ARG:HH22	2.02	0.66
1:C:210:TYR:CZ	2:D:326:LYS:HB2	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:394:LYS:HG2	2:H:348:PRO:CB	2.26	0.66
1:O:407:TRP:HE1	2:P:260:VAL:HB	1.59	0.66
1:Q:397:LEU:CB	2:R:346:TRP:O	2.43	0.66
1:A:176:GLN:HB2	2:B:333:LEU:HD22	1.71	0.66
2:D:11:GLN:OE1	1:G:249:ASN:ND2	2.28	0.66
1:G:404:PHE:CZ	2:H:314:THR:CG2	2.78	0.66
1:I:243:ARG:NE	1:I:243:ARG:HA	2.10	0.66
1:K:100:ALA:HB1	2:L:254:LYS:HA	1.77	0.66
1:Q:176:GLN:OE1	2:R:333:LEU:CD1	2.38	0.66
1:A:348:PRO:HD2	2:P:398:MET:HG2	1.78	0.66
1:C:179:THR:HG21	2:D:248:LEU:HD13	1.77	0.66
1:E:11:GLN:OE1	2:F:247:GLN:O	2.14	0.66
1:E:394:LYS:HG2	2:F:348:PRO:CB	2.26	0.66
1:E:398:MET:HG3	2:F:348:PRO:HD2	1.77	0.66
1:A:243:ARG:NE	1:A:243:ARG:HA	2.10	0.66
1:E:404:PHE:CZ	2:F:314:THR:CG2	2.78	0.66
1:G:401:LYS:HD3	2:H:346:TRP:CD1	2.29	0.66
1:M:101:ASN:CA	2:N:254:LYS:CE	2.74	0.66
1:O:101:ASN:HD22	2:P:258:ASN:ND2	1.94	0.66
1:O:177:VAL:CG2	2:P:329:ASP:C	2.45	0.66
2:B:62:VAL:CG2	2:D:283:TYR:HB3	2.26	0.66
1:E:97:GLU:CD	2:F:2:ARG:NE	2.53	0.66
1:G:401:LYS:HD3	2:H:346:TRP:CG	2.29	0.66
1:I:105:ARG:CZ	2:J:253:ARG:NE	2.59	0.66
1:I:401:LYS:CD	2:J:346:TRP:CD2	2.79	0.66
1:O:243:ARG:HA	1:O:243:ARG:NE	2.10	0.66
1:M:179:THR:HG21	2:N:248:LEU:HD13	1.77	0.65
1:A:176:GLN:HG3	2:B:333:LEU:HD21	1.78	0.65
1:O:394:LYS:O	2:P:348:PRO:HG3	1.96	0.65
1:C:333:ALA:HB2	2:N:176:LYS:HD3	1.78	0.65
1:G:401:LYS:CD	2:H:346:TRP:CD2	2.76	0.65
1:Q:177:VAL:CG1	2:R:329:ASP:HA	2.16	0.65
1:Q:210:TYR:HB3	2:R:326:LYS:HE2	1.77	0.65
2:B:56:ALA:HB1	2:D:283:TYR:CA	2.19	0.65
1:M:101:ASN:HB2	2:N:254:LYS:HG3	1.78	0.65
1:M:243:ARG:HA	1:M:243:ARG:NE	2.10	0.65
1:O:176:GLN:HG3	2:P:333:LEU:CD2	2.22	0.65
2:B:282:GLN:O	2:F:60:LYS:CB	2.44	0.65
1:E:179:THR:HG22	2:F:353:THR:HG1	1.59	0.65
1:I:283:HIS:C	1:K:56:THR:CG2	2.69	0.65
2:J:283:TYR:HD2	2:L:62:VAL:CG2	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:394:LYS:C	2:R:348:PRO:HG3	2.22	0.65
1:A:210:TYR:CG	2:B:326:LYS:CG	2.79	0.65
1:G:179:THR:HG21	2:H:248:LEU:HD13	1.78	0.65
1:I:401:LYS:HD3	2:J:346:TRP:CG	2.29	0.65
1:O:406:HIS:HE1	2:P:260:VAL:C	2.04	0.65
1:A:56:THR:CG2	1:C:283:HIS:C	2.69	0.65
2:B:381:SER:OG	2:B:382:THR:N	2.29	0.65
1:C:181:VAL:HB	2:D:352:LYS:HG3	1.78	0.65
1:E:210:TYR:OH	2:F:325:MET:C	2.38	0.65
1:E:210:TYR:CB	2:F:326:LYS:HD2	2.26	0.65
1:E:348:PRO:HG3	2:R:398:MET:SD	2.37	0.65
1:E:350:GLY:CA	2:R:181:VAL:HA	2.24	0.65
1:I:100:ALA:HB1	2:J:254:LYS:HA	1.78	0.65
1:M:210:TYR:CG	2:N:326:LYS:HB2	2.30	0.65
1:O:181:VAL:HG12	2:P:258:ASN:OD1	1.96	0.65
1:O:210:TYR:CE2	2:P:326:LYS:CB	2.77	0.65
1:O:210:TYR:CG	2:P:326:LYS:CB	2.80	0.65
2:P:381:SER:OG	2:P:382:THR:N	2.29	0.65
1:A:404:PHE:CZ	2:B:314:THR:CG2	2.78	0.65
1:I:179:THR:HG21	2:J:248:LEU:HD13	1.78	0.65
1:O:283:HIS:C	1:Q:56:THR:HG21	2.20	0.65
1:A:56:THR:CG2	1:C:283:HIS:HA	2.23	0.65
1:A:181:VAL:HA	2:B:352:LYS:NZ	2.09	0.65
1:A:333:ALA:HB2	2:P:176:LYS:HD3	1.78	0.65
1:C:345:ASP:CG	2:N:400:ARG:HH22	2.04	0.65
2:D:11:GLN:NE2	1:G:249:ASN:H	1.93	0.65
2:F:407:TRP:CH2	1:K:256:GLN:HG2	2.32	0.65
2:J:381:SER:OG	2:J:382:THR:N	2.29	0.65
1:K:105:ARG:NH2	2:L:253:ARG:NE	2.45	0.65
1:O:406:HIS:HE1	2:P:260:VAL:HG12	1.54	0.65
2:B:11:GLN:HE22	1:I:249:ASN:N	1.95	0.65
2:B:407:TRP:HZ2	1:I:260:VAL:HB	1.61	0.65
2:D:177:VAL:HG21	1:G:329:ASN:OD1	1.90	0.65
2:D:398:MET:HG3	1:G:348:PRO:HD3	1.78	0.65
2:F:398:MET:HG3	1:K:348:PRO:HD3	1.79	0.65
1:G:224:TYR:CD1	2:H:325:MET:SD	2.86	0.65
1:G:401:LYS:CG	2:H:346:TRP:CD2	2.80	0.64
1:O:15:GLN:OE1	1:O:15:GLN:HA	1.98	0.64
1:A:15:GLN:OE1	1:A:15:GLN:HA	1.98	0.64
2:B:60:LYS:HB2	2:D:282:GLN:O	1.97	0.64
1:C:348:PRO:HG3	2:N:398:MET:SD	2.38	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:GLN:OE1	1:G:15:GLN:HA	1.98	0.64
1:I:181:VAL:HG12	2:J:258:ASN:OD1	1.96	0.64
1:I:210:TYR:CG	2:J:326:LYS:CD	2.80	0.64
1:K:179:THR:HB	2:L:353:THR:O	1.97	0.64
1:O:73:THR:HG21	2:P:245:PRO:HA	1.79	0.64
1:A:11:GLN:OE1	2:B:247:GLN:O	2.16	0.64
1:A:56:THR:HG21	1:C:283:HIS:C	2.22	0.64
1:C:15:GLN:OE1	1:C:15:GLN:HA	1.98	0.64
2:F:11:GLN:NE2	1:K:249:ASN:H	1.94	0.64
1:I:407:TRP:CE3	2:J:257:VAL:HG22	2.31	0.64
1:M:15:GLN:HA	1:M:15:GLN:OE1	1.98	0.64
1:I:15:GLN:OE1	1:I:15:GLN:HA	1.98	0.64
1:K:401:LYS:CG	2:L:346:TRP:CD2	2.80	0.64
1:O:101:ASN:HB2	2:P:254:LYS:HG3	1.79	0.64
3:O:501:GTP:O1A	2:P:249:ASN:HB3	1.96	0.64
1:Q:15:GLN:OE1	1:Q:15:GLN:HA	1.98	0.64
1:Q:101:ASN:CA	2:R:254:LYS:CE	2.75	0.64
1:C:352:LYS:CA	2:N:179:ASP:O	2.44	0.64
1:E:15:GLN:HA	1:E:15:GLN:OE1	1.98	0.64
2:F:11:GLN:OE1	1:K:249:ASN:ND2	2.30	0.64
2:F:181:VAL:HG23	1:K:350:GLY:O	1.95	0.64
1:G:407:TRP:CE3	2:H:257:VAL:HG22	2.31	0.64
1:Q:179:THR:HG22	2:R:353:THR:CB	2.26	0.64
1:A:176:GLN:CG	2:B:333:LEU:CD2	2.75	0.64
1:E:346:TRP:HB3	2:R:401:ARG:HG3	0.78	0.64
1:K:15:GLN:OE1	1:K:15:GLN:HA	1.98	0.64
1:K:105:ARG:CZ	2:L:253:ARG:NE	2.61	0.64
1:M:394:LYS:C	2:N:348:PRO:HG3	2.22	0.64
1:O:404:PHE:HE2	2:P:258:ASN:C	2.05	0.64
1:E:105:ARG:CZ	2:F:253:ARG:NE	2.61	0.64
1:M:179:THR:HG22	2:N:353:THR:CB	2.25	0.64
1:O:179:THR:HA	2:P:353:THR:N	2.10	0.64
1:O:404:PHE:CE2	2:P:258:ASN:C	2.75	0.64
1:E:329:ASN:CB	2:R:177:VAL:HG21	2.28	0.64
1:E:333:ALA:HB2	2:R:176:LYS:HD3	1.79	0.64
1:G:181:VAL:HG12	2:H:258:ASN:OD1	1.97	0.64
1:I:101:ASN:CA	2:J:254:LYS:HE3	2.23	0.64
3:M:501:GTP:O1A	2:N:249:ASN:HB3	1.97	0.64
1:O:397:LEU:C	2:P:346:TRP:O	2.40	0.64
1:A:181:VAL:HG12	2:B:258:ASN:OD1	1.98	0.64
1:C:404:PHE:CZ	2:D:314:THR:CG2	2.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:ARG:HH22	2:R:71:GLU:CD	2.06	0.64
1:Q:210:TYR:CB	2:R:326:LYS:CD	2.74	0.64
1:A:210:TYR:CG	2:B:326:LYS:HG3	2.33	0.64
1:C:105:ARG:CZ	2:D:253:ARG:NE	2.61	0.64
1:O:181:VAL:HA	2:P:352:LYS:HE3	0.64	0.64
2:D:181:VAL:HG23	1:G:350:GLY:O	1.94	0.63
1:G:100:ALA:HB1	2:H:254:LYS:HA	1.80	0.63
1:G:179:THR:CA	2:H:353:THR:H	2.11	0.63
1:Q:179:THR:HG22	2:R:353:THR:HG1	1.54	0.63
1:K:179:THR:CA	2:L:353:THR:H	2.11	0.63
1:A:177:VAL:HG22	2:B:329:ASP:O	1.96	0.63
2:B:398:MET:SD	1:I:348:PRO:CG	2.86	0.63
1:C:258:ASN:O	2:N:404:PHE:CE2	2.50	0.63
1:O:210:TYR:HB3	2:P:326:LYS:HE2	1.79	0.63
1:C:179:THR:CG2	2:D:353:THR:HG1	2.11	0.63
1:E:100:ALA:HB1	2:F:254:LYS:HA	1.79	0.63
1:E:345:ASP:CG	2:R:400:ARG:HH22	2.05	0.63
2:F:179:ASP:OD1	1:K:353:VAL:CB	2.41	0.63
2:J:283:TYR:CD2	2:L:62:VAL:CG2	2.74	0.63
1:Q:181:VAL:HG23	2:R:352:LYS:HE2	1.79	0.63
1:C:176:GLN:CG	2:D:333:LEU:CD2	2.76	0.63
1:C:353:VAL:CB	2:N:179:ASP:OD1	2.35	0.63
1:K:176:GLN:HB3	2:L:333:LEU:CD1	2.28	0.63
1:O:181:VAL:HB	2:P:352:LYS:CG	2.28	0.63
1:A:105:ARG:NH2	2:B:253:ARG:NE	2.45	0.63
1:M:101:ASN:HD22	2:N:258:ASN:ND2	1.96	0.63
1:Q:210:TYR:CG	2:R:326:LYS:CD	2.81	0.63
1:C:210:TYR:CG	2:D:326:LYS:CG	2.81	0.63
1:E:177:VAL:HG22	2:F:329:ASP:O	1.98	0.63
1:G:210:TYR:CG	2:H:326:LYS:HB2	2.31	0.63
1:I:407:TRP:CB	2:J:257:VAL:HG13	2.28	0.63
2:N:283:TYR:CA	2:P:56:ALA:HB2	2.26	0.63
1:K:407:TRP:CE3	2:L:257:VAL:HG22	2.33	0.63
1:O:105:ARG:HH22	2:P:253:ARG:NH2	1.95	0.63
1:A:256:GLN:CG	2:P:407:TRP:CH2	2.82	0.63
1:C:105:ARG:NH2	2:D:253:ARG:NE	2.46	0.63
2:F:404:PHE:CZ	1:K:258:ASN:O	2.52	0.63
1:I:283:HIS:HA	1:K:56:THR:CG2	2.21	0.63
1:M:176:GLN:HG3	2:N:333:LEU:CD2	2.27	0.63
1:O:101:ASN:CB	2:P:254:LYS:CD	2.69	0.63
2:B:177:VAL:HG21	1:I:329:ASN:CG	2.23	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:ASP:OD1	1:I:353:VAL:CB	2.38	0.62
1:I:105:ARG:NH2	2:J:253:ARG:NE	2.47	0.62
1:K:401:LYS:HD3	2:L:346:TRP:CD1	2.31	0.62
1:C:176:GLN:HG3	2:D:333:LEU:HD21	1.80	0.62
1:G:105:ARG:CZ	2:H:253:ARG:NE	2.63	0.62
1:G:407:TRP:CG	2:H:257:VAL:HG13	2.34	0.62
1:I:105:ARG:CZ	2:J:253:ARG:HE	2.11	0.62
1:A:407:TRP:NE1	2:B:260:VAL:HB	2.15	0.62
2:D:11:GLN:HE22	1:G:249:ASN:N	1.97	0.62
2:H:282:GLN:O	2:J:60:LYS:CB	2.46	0.62
2:H:283:TYR:CA	2:J:56:ALA:HB2	2.24	0.62
1:M:283:HIS:HA	1:O:56:THR:CG2	2.26	0.62
1:Q:73:THR:HG21	2:R:245:PRO:HA	1.82	0.62
1:K:407:TRP:CZ2	2:L:260:VAL:HB	2.34	0.62
1:M:181:VAL:HG12	2:N:258:ASN:OD1	2.00	0.62
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.48	0.62
1:C:398:MET:HG3	2:D:348:PRO:HD2	1.81	0.62
1:E:249:ASN:ND2	2:R:11:GLN:OE1	2.32	0.62
1:G:283:HIS:HA	1:I:56:THR:CG2	2.26	0.62
1:I:404:PHE:CZ	2:J:314:THR:HG21	2.34	0.62
2:N:381:SER:OG	2:N:382:THR:N	2.29	0.62
1:C:11:GLN:OE1	2:D:247:GLN:O	2.18	0.62
1:E:256:GLN:O	2:R:407:TRP:CZ2	2.53	0.62
2:F:11:GLN:HE22	1:K:249:ASN:N	1.97	0.62
1:M:404:PHE:H	2:N:261:PRO:C	2.07	0.62
1:Q:101:ASN:HB2	2:R:254:LYS:HG3	1.80	0.62
1:C:401:LYS:HD3	2:D:346:TRP:NE1	2.14	0.62
1:E:407:TRP:NE1	2:F:260:VAL:HB	2.15	0.62
1:G:177:VAL:HG11	2:H:329:ASP:OD1	1.99	0.62
1:G:283:HIS:C	1:I:56:THR:CG2	2.72	0.62
1:I:11:GLN:HE22	2:J:247:GLN:C	2.05	0.62
1:I:101:ASN:HD22	2:J:258:ASN:HD21	1.48	0.62
1:I:283:HIS:HB3	1:K:62:VAL:HG22	1.81	0.62
1:K:177:VAL:CG1	2:L:329:ASP:HA	2.20	0.62
1:E:210:TYR:CG	2:F:326:LYS:CG	2.82	0.62
1:G:283:HIS:C	1:I:56:THR:HG21	2.25	0.62
1:K:11:GLN:HE22	2:L:247:GLN:C	2.04	0.62
1:M:406:HIS:HE1	2:N:260:VAL:HG12	1.57	0.62
1:A:179:THR:CA	2:B:353:THR:H	2.13	0.62
2:D:381:SER:OG	2:D:382:THR:N	2.29	0.62
1:E:352:LYS:CA	2:R:179:ASP:O	2.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:210:TYR:CE2	2:J:326:LYS:CB	2.82	0.62
1:Q:101:ASN:HD22	2:R:258:ASN:ND2	1.98	0.62
1:A:105:ARG:CZ	2:B:253:ARG:HE	2.13	0.61
2:B:60:LYS:CB	2:D:282:GLN:O	2.48	0.61
2:B:400:ARG:HH22	1:I:345:ASP:CG	2.07	0.61
1:E:177:VAL:HG21	2:F:329:ASP:CA	2.30	0.61
1:I:176:GLN:HB3	2:J:333:LEU:CD1	2.30	0.61
1:I:397:LEU:HD22	2:J:345:GLU:O	2.00	0.61
1:M:100:ALA:C	2:N:254:LYS:CD	2.72	0.61
1:Q:404:PHE:H	2:R:261:PRO:C	2.07	0.61
1:A:243:ARG:HH22	2:P:71:GLU:CD	2.08	0.61
1:A:404:PHE:CZ	2:B:314:THR:HG21	2.36	0.61
1:A:435:VAL:HG22	2:P:401:ARG:NH2	2.14	0.61
1:C:177:VAL:HG22	2:D:329:ASP:O	1.96	0.61
1:C:210:TYR:CG	2:D:326:LYS:HG3	2.36	0.61
1:I:177:VAL:HB	2:J:329:ASP:HB3	1.81	0.61
1:K:105:ARG:CZ	2:L:253:ARG:HE	2.12	0.61
1:O:72:PRO:HB2	2:P:48:ARG:NH1	2.15	0.61
1:A:181:VAL:HG23	2:B:352:LYS:HE2	1.81	0.61
2:B:177:VAL:HG21	1:I:329:ASN:CB	2.31	0.61
1:G:177:VAL:HG11	2:H:329:ASP:CB	2.31	0.61
2:H:381:SER:OG	2:H:382:THR:N	2.29	0.61
1:I:407:TRP:CG	2:J:257:VAL:HG13	2.34	0.61
1:K:101:ASN:CA	2:L:254:LYS:HE3	2.24	0.61
1:M:210:TYR:CG	2:N:326:LYS:CD	2.82	0.61
1:M:407:TRP:CB	2:N:257:VAL:HG13	2.30	0.61
1:O:100:ALA:C	2:P:254:LYS:CG	2.73	0.61
1:O:404:PHE:H	2:P:261:PRO:C	2.09	0.61
1:C:181:VAL:HG12	2:D:258:ASN:OD1	2.00	0.61
1:G:11:GLN:HE22	2:H:247:GLN:C	2.07	0.61
1:K:210:TYR:CG	2:L:326:LYS:CD	2.84	0.61
1:M:179:THR:HA	2:N:353:THR:N	2.14	0.61
1:A:210:TYR:CD1	2:B:326:LYS:CB	2.75	0.61
2:B:283:TYR:C	2:F:56:ALA:HB2	2.23	0.61
1:C:177:VAL:HG11	2:D:329:ASP:OD1	2.00	0.61
1:C:181:VAL:HG23	2:D:352:LYS:HE2	1.82	0.61
1:E:181:VAL:HB	2:F:352:LYS:HG3	1.83	0.61
1:E:210:TYR:CG	2:F:326:LYS:HG3	2.35	0.61
1:I:100:ALA:C	2:J:254:LYS:CD	2.74	0.61
1:I:101:ASN:CA	2:J:254:LYS:CE	2.78	0.61
1:O:100:ALA:HB1	2:P:254:LYS:CA	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:381:SER:OG	2:R:382:THR:N	2.29	0.61
1:E:176:GLN:HG3	2:F:333:LEU:HD21	1.83	0.61
1:I:176:GLN:OE1	2:J:333:LEU:CD1	2.42	0.61
1:M:394:LYS:HA	2:N:348:PRO:CG	2.24	0.61
1:C:101:ASN:H	2:D:254:LYS:HD2	1.56	0.61
1:C:407:TRP:NE1	2:D:260:VAL:HB	2.16	0.61
1:I:283:HIS:C	1:K:56:THR:HG21	2.24	0.61
1:M:210:TYR:CG	2:N:326:LYS:CB	2.84	0.61
1:A:256:GLN:O	2:P:407:TRP:CE2	2.54	0.61
2:B:210:TYR:OH	1:I:325:PRO:HB2	2.01	0.61
2:F:71:GLU:CD	1:K:243:ARG:HH22	2.09	0.61
1:A:177:VAL:HG11	2:B:329:ASP:OD1	2.01	0.61
1:E:11:GLN:HE22	2:F:247:GLN:C	2.07	0.61
2:F:381:SER:OG	2:F:382:THR:N	2.29	0.61
1:G:407:TRP:CB	2:H:257:VAL:HG13	2.30	0.61
1:M:401:LYS:HD3	2:N:346:TRP:CG	2.35	0.61
1:Q:100:ALA:C	2:R:254:LYS:CD	2.74	0.61
2:B:71:GLU:CD	1:I:243:ARG:HH22	2.09	0.61
2:D:177:VAL:HG21	1:G:329:ASN:CG	2.26	0.61
2:D:210:TYR:OH	1:G:325:PRO:HB2	2.01	0.61
1:G:210:TYR:CG	2:H:326:LYS:CD	2.84	0.61
1:Q:407:TRP:CE2	2:R:260:VAL:HB	2.35	0.61
1:A:11:GLN:HE22	2:B:247:GLN:C	2.08	0.60
1:E:176:GLN:CG	2:F:333:LEU:CD2	2.79	0.60
2:F:210:TYR:OH	1:K:325:PRO:HB2	2.01	0.60
1:I:401:LYS:CG	2:J:346:TRP:CD2	2.84	0.60
1:K:401:LYS:HD3	2:L:346:TRP:CG	2.34	0.60
1:M:73:THR:HG21	2:N:245:PRO:HA	1.83	0.60
1:O:100:ALA:CA	2:P:254:LYS:CB	2.70	0.60
1:Q:181:VAL:N	2:R:352:LYS:CE	2.50	0.60
1:E:181:VAL:HG23	2:F:352:LYS:HE2	1.84	0.60
1:G:105:ARG:NH2	2:H:253:ARG:NE	2.48	0.60
1:I:394:LYS:O	2:J:348:PRO:HG3	2.01	0.60
1:M:210:TYR:HB3	2:N:326:LYS:HE2	1.81	0.60
1:A:101:ASN:HB2	2:B:254:LYS:HG3	1.82	0.60
1:A:398:MET:HG3	2:B:348:PRO:HD2	1.82	0.60
1:A:407:TRP:HE1	2:B:260:VAL:HB	1.66	0.60
2:B:398:MET:SD	1:I:348:PRO:HG3	2.41	0.60
1:E:179:THR:CG2	2:F:353:THR:HG1	2.11	0.60
2:L:381:SER:OG	2:L:382:THR:N	2.29	0.60
2:D:407:TRP:HZ2	1:G:260:VAL:HB	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ARG:CZ	2:F:253:ARG:HE	2.14	0.60
1:E:407:TRP:CE2	2:F:260:VAL:HB	2.37	0.60
2:F:407:TRP:HZ2	1:K:260:VAL:HB	1.62	0.60
2:H:221:THR:N	2:H:222:PRO:HD3	2.17	0.60
1:M:397:LEU:HB2	2:N:348:PRO:HD3	1.83	0.60
1:O:97:GLU:OE2	2:P:2:ARG:N	2.35	0.60
1:Q:407:TRP:CZ2	2:R:260:VAL:HB	2.37	0.60
1:Q:407:TRP:CB	2:R:257:VAL:HG13	2.32	0.60
2:D:221:THR:N	2:D:222:PRO:HD3	2.17	0.60
1:I:177:VAL:HG11	2:J:329:ASP:OD1	2.01	0.60
1:A:176:GLN:HB3	2:B:333:LEU:CG	2.30	0.60
1:C:348:PRO:HD2	2:N:398:MET:HG2	1.84	0.60
1:O:407:TRP:CG	2:P:257:VAL:HA	2.36	0.60
1:C:243:ARG:HH22	2:N:71:GLU:CD	2.10	0.60
1:E:394:LYS:HZ3	2:F:349:ASN:ND2	1.98	0.60
2:F:221:THR:N	2:F:222:PRO:HD3	2.16	0.60
1:G:394:LYS:O	2:H:348:PRO:HG3	2.02	0.60
2:L:221:THR:N	2:L:222:PRO:HD3	2.17	0.60
2:N:221:THR:N	2:N:222:PRO:HD3	2.17	0.60
1:O:181:VAL:N	2:P:352:LYS:CE	2.52	0.60
1:O:403:ALA:HB1	2:P:261:PRO:HB3	1.83	0.60
1:A:100:ALA:HB1	2:B:254:LYS:HA	1.82	0.60
1:A:210:TYR:CD2	2:B:326:LYS:CG	2.84	0.60
3:A:501:GTP:O1A	2:B:249:ASN:HB3	2.02	0.60
1:C:256:GLN:CG	2:N:407:TRP:CH2	2.85	0.60
1:G:101:ASN:CA	2:H:254:LYS:HE3	2.26	0.60
1:I:283:HIS:HB3	1:K:62:VAL:CG2	2.32	0.60
1:K:100:ALA:HA	2:L:254:LYS:HD2	1.84	0.60
1:K:404:PHE:CZ	2:L:314:THR:HG21	2.37	0.60
1:K:407:TRP:CB	2:L:257:VAL:HG13	2.32	0.60
1:A:401:LYS:HD3	2:B:346:TRP:NE1	2.17	0.60
1:E:179:THR:HB	2:F:353:THR:O	2.01	0.60
1:G:105:ARG:CZ	2:H:253:ARG:HE	2.14	0.60
2:P:306:ASP:C	2:P:306:ASP:OD1	2.40	0.60
1:Q:210:TYR:OH	2:R:326:LYS:HA	2.01	0.60
1:A:283:HIS:HB3	1:E:62:VAL:HG22	1.83	0.60
1:A:283:HIS:HB3	1:E:62:VAL:CG2	2.32	0.60
1:G:394:LYS:HZ3	2:H:349:ASN:ND2	1.98	0.60
1:M:283:HIS:C	1:O:56:THR:CG2	2.74	0.60
1:Q:397:LEU:HD13	2:R:345:GLU:O	2.02	0.60
2:B:179:ASP:O	1:I:352:LYS:CA	2.47	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASP:C	2:B:306:ASP:OD1	2.40	0.59
1:C:100:ALA:HB1	2:D:254:LYS:HA	1.82	0.59
1:C:176:GLN:HB3	2:D:333:LEU:CG	2.32	0.59
1:E:76:ASP:CG	2:F:48:ARG:HH22	1.95	0.59
1:I:100:ALA:CA	2:J:254:LYS:HD2	2.32	0.59
1:K:407:TRP:CG	2:L:257:VAL:HG13	2.37	0.59
1:Q:394:LYS:O	2:R:348:PRO:HG3	2.01	0.59
2:R:221:THR:N	2:R:222:PRO:HD3	2.17	0.59
2:D:400:ARG:HH22	1:G:345:ASP:CG	2.10	0.59
1:I:397:LEU:HB3	2:J:346:TRP:C	2.26	0.59
1:K:100:ALA:CA	2:L:254:LYS:HD2	2.32	0.59
1:M:404:PHE:CZ	2:N:314:THR:HG22	2.29	0.59
1:M:406:HIS:HE1	2:N:260:VAL:C	2.10	0.59
1:A:176:GLN:HB3	2:B:333:LEU:CD1	2.32	0.59
1:E:404:PHE:CA	2:F:261:PRO:HA	2.31	0.59
1:G:210:TYR:CE2	2:H:326:LYS:CB	2.84	0.59
1:I:394:LYS:HZ3	2:J:349:ASN:ND2	1.98	0.59
1:K:179:THR:HG21	2:L:248:LEU:HD13	1.84	0.59
1:M:177:VAL:HB	2:N:329:ASP:HB3	1.84	0.59
1:O:100:ALA:CA	2:P:254:LYS:HD2	2.33	0.59
2:P:221:THR:N	2:P:222:PRO:HD3	2.17	0.59
1:Q:179:THR:HG21	2:R:248:LEU:HD13	1.83	0.59
1:A:258:ASN:CA	2:P:404:PHE:HE2	2.16	0.59
2:B:181:VAL:HA	1:I:350:GLY:CA	2.29	0.59
2:B:221:THR:N	2:B:222:PRO:HD3	2.17	0.59
1:G:177:VAL:HB	2:H:329:ASP:HB3	1.83	0.59
1:I:177:VAL:HG11	2:J:329:ASP:CB	2.31	0.59
1:K:210:TYR:HB3	2:L:326:LYS:HE2	1.83	0.59
1:O:407:TRP:CD1	2:P:257:VAL:O	2.55	0.59
1:C:101:ASN:HB2	2:D:254:LYS:HG3	1.84	0.59
1:C:105:ARG:CZ	2:D:253:ARG:HE	2.15	0.59
1:C:179:THR:CA	2:D:353:THR:H	2.15	0.59
2:F:177:VAL:HG21	1:K:329:ASN:CG	2.28	0.59
1:K:181:VAL:HG12	2:L:258:ASN:OD1	2.02	0.59
1:M:407:TRP:CE2	2:N:260:VAL:HB	2.38	0.59
3:Q:501:GTP:O1A	2:R:249:ASN:HB3	2.01	0.59
1:A:258:ASN:O	2:P:404:PHE:HZ	1.84	0.59
1:A:346:TRP:HB3	2:P:401:ARG:HG3	0.67	0.59
2:D:71:GLU:CD	1:G:243:ARG:HH22	2.11	0.59
1:E:179:THR:HG21	2:F:248:LEU:HD13	1.85	0.59
1:E:181:VAL:N	2:F:352:LYS:CE	2.54	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:GLN:OE1	2:H:333:LEU:CD1	2.44	0.59
2:J:221:THR:N	2:J:222:PRO:HD3	2.17	0.59
2:J:345:GLU:H	2:J:345:GLU:CD	2.10	0.59
1:K:394:LYS:O	2:L:348:PRO:HG3	2.03	0.59
2:B:345:GLU:H	2:B:345:GLU:CD	2.10	0.59
1:C:11:GLN:HG2	1:C:74:VAL:HG21	1.84	0.59
1:C:224:TYR:CD1	2:D:325:MET:SD	2.90	0.59
2:J:306:ASP:C	2:J:306:ASP:OD1	2.40	0.59
1:M:11:GLN:HG2	1:M:74:VAL:HG21	1.84	0.59
1:G:176:GLN:HB3	2:H:333:LEU:CD1	2.33	0.59
1:I:210:TYR:CG	2:J:326:LYS:CB	2.86	0.59
1:K:11:GLN:HG2	1:K:74:VAL:HG21	1.84	0.59
1:E:11:GLN:HG2	1:E:74:VAL:HG21	1.84	0.59
1:O:100:ALA:CB	2:P:254:LYS:HB2	2.33	0.59
1:O:407:TRP:CE3	2:P:257:VAL:HG22	2.38	0.59
1:Q:11:GLN:HG2	1:Q:74:VAL:HG21	1.84	0.59
1:Q:210:TYR:CG	2:R:326:LYS:CB	2.86	0.59
1:Q:401:LYS:HD3	2:R:346:TRP:CG	2.37	0.59
1:A:258:ASN:HA	2:P:404:PHE:CE2	2.37	0.59
1:C:407:TRP:CZ2	2:D:260:VAL:HB	2.38	0.59
1:G:11:GLN:HG2	1:G:74:VAL:HG21	1.84	0.59
1:I:177:VAL:CB	2:J:329:ASP:HB3	2.33	0.59
1:K:177:VAL:HG11	2:L:329:ASP:CB	2.33	0.59
1:Q:176:GLN:HB3	2:R:333:LEU:HD13	1.84	0.59
1:A:345:ASP:OD1	2:P:400:ARG:NH2	2.34	0.58
1:A:397:LEU:HB3	2:B:346:TRP:C	2.27	0.58
1:G:177:VAL:CB	2:H:329:ASP:HB3	2.33	0.58
1:M:394:LYS:O	2:N:348:PRO:HG3	2.02	0.58
1:M:404:PHE:HE2	2:N:258:ASN:C	2.11	0.58
1:O:101:ASN:CB	2:P:254:LYS:HG3	2.33	0.58
1:O:177:VAL:HG11	2:P:329:ASP:OD1	2.01	0.58
2:P:345:GLU:H	2:P:345:GLU:CD	2.10	0.58
1:C:401:LYS:HD3	2:D:346:TRP:CD1	2.37	0.58
1:I:11:GLN:HG2	1:I:74:VAL:HG21	1.84	0.58
1:M:97:GLU:OE2	2:N:2:ARG:N	2.35	0.58
1:M:283:HIS:C	1:O:56:THR:HG21	2.28	0.58
1:O:177:VAL:CB	2:P:329:ASP:HB3	2.32	0.58
1:A:11:GLN:HG2	1:A:74:VAL:HG21	1.84	0.58
1:C:101:ASN:HD22	2:D:258:ASN:HD21	1.51	0.58
1:E:176:GLN:HB3	2:F:333:LEU:CG	2.31	0.58
2:F:179:ASP:O	1:K:352:LYS:CA	2.49	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:ASN:HD22	2:H:258:ASN:HD21	1.51	0.58
1:G:397:LEU:HD22	2:H:345:GLU:O	2.03	0.58
1:I:73:THR:HG21	2:J:245:PRO:HA	1.85	0.58
1:I:181:VAL:N	2:J:352:LYS:CE	2.55	0.58
1:K:404:PHE:CA	2:L:261:PRO:HA	2.33	0.58
1:M:101:ASN:CB	2:N:254:LYS:CD	2.74	0.58
1:O:11:GLN:HG2	1:O:74:VAL:HG21	1.84	0.58
1:A:97:GLU:OE2	2:B:2:ARG:N	2.36	0.58
2:D:179:ASP:O	1:G:352:LYS:CA	2.48	0.58
1:K:181:VAL:N	2:L:352:LYS:CE	2.51	0.58
1:M:210:TYR:CE1	2:N:326:LYS:CA	2.78	0.58
1:A:290:GLU:OE1	1:A:290:GLU:HA	2.03	0.58
1:K:73:THR:HG21	2:L:245:PRO:HA	1.86	0.58
1:K:100:ALA:C	2:L:254:LYS:CD	2.77	0.58
1:M:72:PRO:HB2	2:N:48:ARG:NH1	2.19	0.58
1:M:176:GLN:HB3	2:N:333:LEU:HD13	1.85	0.58
1:M:283:HIS:HB3	1:O:62:VAL:HG22	1.85	0.58
1:O:290:GLU:OE1	1:O:290:GLU:HA	2.04	0.58
1:O:407:TRP:CE2	2:P:260:VAL:HB	2.39	0.58
1:A:210:TYR:CG	2:B:326:LYS:HD2	2.38	0.58
1:A:224:TYR:CD1	2:B:325:MET:SD	2.88	0.58
1:A:401:LYS:HD3	2:B:346:TRP:CD1	2.38	0.58
1:C:210:TYR:CD1	2:D:326:LYS:CB	2.77	0.58
1:C:404:PHE:CZ	2:D:314:THR:HG21	2.38	0.58
1:E:176:GLN:HB3	2:F:333:LEU:CD1	2.34	0.58
1:K:407:TRP:NE1	2:L:260:VAL:HB	2.18	0.58
1:M:404:PHE:CE2	2:N:258:ASN:C	2.81	0.58
1:E:258:ASN:O	2:R:404:PHE:CE2	2.55	0.58
1:G:407:TRP:CZ2	2:H:260:VAL:HB	2.38	0.58
1:I:290:GLU:OE1	1:I:290:GLU:HA	2.04	0.58
1:I:407:TRP:NE1	2:J:260:VAL:HB	2.19	0.58
1:O:394:LYS:CG	2:P:348:PRO:HB2	2.26	0.58
1:O:210:TYR:CB	2:P:326:LYS:CD	2.68	0.58
1:C:401:LYS:CG	2:D:346:TRP:CD2	2.87	0.58
1:C:404:PHE:CA	2:D:261:PRO:HA	2.34	0.58
1:K:176:GLN:O	2:L:333:LEU:HD13	2.04	0.58
2:N:283:TYR:HA	2:P:56:ALA:HB2	1.74	0.58
1:G:404:PHE:CZ	2:H:314:THR:HG21	2.38	0.58
2:H:345:GLU:H	2:H:345:GLU:CD	2.10	0.58
1:K:290:GLU:OE1	1:K:290:GLU:HA	2.03	0.58
1:C:258:ASN:CA	2:N:404:PHE:HE2	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:TRP:HE1	2:D:260:VAL:HB	1.68	0.57
3:C:501:GTP:O1A	2:D:249:ASN:HB3	2.04	0.57
1:G:100:ALA:HA	2:H:254:LYS:HD2	1.86	0.57
2:D:345:GLU:H	2:D:345:GLU:CD	2.10	0.57
1:G:100:ALA:CA	2:H:254:LYS:HD2	2.34	0.57
1:I:404:PHE:HE2	2:J:258:ASN:C	2.12	0.57
1:K:397:LEU:HD22	2:L:345:GLU:O	2.04	0.57
1:Q:290:GLU:HA	1:Q:290:GLU:OE1	2.03	0.57
2:R:306:ASP:C	2:R:306:ASP:OD1	2.40	0.57
1:A:404:PHE:CA	2:B:261:PRO:HA	2.34	0.57
1:E:290:GLU:OE1	1:E:290:GLU:HA	2.04	0.57
1:K:101:ASN:CA	2:L:254:LYS:CE	2.82	0.57
1:A:260:VAL:HB	2:P:407:TRP:HZ2	1.62	0.57
1:C:176:GLN:HB3	2:D:333:LEU:CD1	2.34	0.57
1:C:258:ASN:HA	2:N:404:PHE:CE2	2.38	0.57
2:H:306:ASP:C	2:H:306:ASP:OD1	2.40	0.57
1:I:404:PHE:CA	2:J:261:PRO:HA	2.35	0.57
1:K:401:LYS:HG2	2:L:346:TRP:CD2	2.40	0.57
1:M:181:VAL:N	2:N:352:LYS:CE	2.54	0.57
1:M:290:GLU:OE1	1:M:290:GLU:HA	2.03	0.57
2:N:345:GLU:H	2:N:345:GLU:CD	2.10	0.57
1:E:210:TYR:CG	2:F:326:LYS:HD2	2.40	0.57
1:E:401:LYS:HG2	2:F:346:TRP:CD2	2.40	0.57
1:G:101:ASN:CA	2:H:254:LYS:CE	2.81	0.57
1:M:177:VAL:HG11	2:N:329:ASP:OD1	2.05	0.57
2:N:306:ASP:C	2:N:306:ASP:OD1	2.40	0.57
1:O:177:VAL:HG11	2:P:329:ASP:CB	2.33	0.57
1:Q:176:GLN:O	2:R:333:LEU:HD13	2.03	0.57
1:C:401:LYS:HD3	2:D:346:TRP:CG	2.38	0.57
2:F:398:MET:SD	1:K:348:PRO:CG	2.93	0.57
1:I:394:LYS:C	2:J:348:PRO:HG3	2.29	0.57
2:L:306:ASP:OD1	2:L:306:ASP:C	2.40	0.57
1:M:406:HIS:CE1	2:N:260:VAL:CG1	2.69	0.57
1:O:283:HIS:HB3	1:Q:62:VAL:CG2	2.35	0.57
1:A:62:VAL:HG22	1:C:283:HIS:HB3	1.86	0.57
1:C:290:GLU:OE1	1:C:290:GLU:HA	2.03	0.57
2:D:306:ASP:C	2:D:306:ASP:OD1	2.39	0.57
2:D:398:MET:SD	1:G:348:PRO:CG	2.92	0.57
1:E:404:PHE:CZ	2:F:314:THR:HG21	2.40	0.57
1:G:210:TYR:CG	2:H:326:LYS:CB	2.88	0.57
1:I:100:ALA:HA	2:J:254:LYS:HD2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:ALA:HB1	2:N:254:LYS:CA	2.34	0.57
1:M:210:TYR:CE2	2:N:326:LYS:CB	2.84	0.57
1:O:179:THR:HG21	2:P:248:LEU:CD1	2.34	0.57
1:O:394:LYS:CA	2:P:348:PRO:CG	2.74	0.57
1:A:326:LYS:CB	2:P:210:TYR:CE2	2.85	0.57
1:C:401:LYS:CD	2:D:346:TRP:CD2	2.84	0.57
1:I:397:LEU:HB2	2:J:348:PRO:HD3	1.87	0.57
1:K:101:ASN:HD22	2:L:258:ASN:HD21	1.53	0.57
1:Q:101:ASN:ND2	2:R:258:ASN:OD1	2.38	0.57
1:Q:177:VAL:HB	2:R:329:ASP:HB3	1.87	0.57
1:C:210:TYR:CG	2:D:326:LYS:HD2	2.39	0.57
1:E:179:THR:CA	2:F:353:THR:H	2.18	0.57
2:F:306:ASP:C	2:F:306:ASP:OD1	2.40	0.57
2:F:400:ARG:HH22	1:K:345:ASP:CG	2.12	0.57
1:G:290:GLU:OE1	1:G:290:GLU:HA	2.03	0.57
1:O:401:LYS:HG2	2:P:346:TRP:CG	2.37	0.57
1:A:348:PRO:CG	2:P:398:MET:CG	2.82	0.57
2:B:56:ALA:HB2	2:D:283:TYR:C	2.28	0.57
1:C:346:TRP:HB3	2:N:401:ARG:HG3	0.70	0.57
1:M:101:ASN:CB	2:N:254:LYS:HG3	2.35	0.57
1:O:181:VAL:HG11	2:P:258:ASN:O	2.04	0.57
1:O:283:HIS:HB3	1:Q:62:VAL:HG22	1.86	0.57
1:O:406:HIS:NE2	2:P:260:VAL:HG11	2.18	0.57
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.86	0.56
1:C:435:VAL:HG22	2:N:401:ARG:NH2	2.19	0.56
2:D:177:VAL:HG21	1:G:329:ASN:CB	2.35	0.56
1:E:262:TYR:HB3	1:E:263:PRO:HD2	1.86	0.56
1:E:435:VAL:HG22	2:R:401:ARG:NH2	2.19	0.56
1:K:210:TYR:OH	2:L:326:LYS:HA	2.03	0.56
1:M:397:LEU:C	2:N:346:TRP:O	2.48	0.56
1:O:262:TYR:HB3	1:O:263:PRO:HD2	1.86	0.56
1:Q:210:TYR:CG	2:R:326:LYS:HB2	2.33	0.56
1:A:346:TRP:HZ3	2:P:403:ALA:CB	1.79	0.56
1:G:283:HIS:HB3	1:I:62:VAL:HG22	1.87	0.56
1:M:100:ALA:CA	2:N:254:LYS:CB	2.73	0.56
1:Q:100:ALA:CA	2:R:254:LYS:HD2	2.36	0.56
1:C:325:PRO:HB2	2:N:210:TYR:OH	2.05	0.56
1:E:210:TYR:CD2	2:F:326:LYS:CG	2.87	0.56
1:G:181:VAL:HB	2:H:352:LYS:CE	2.35	0.56
1:I:262:TYR:HB3	1:I:263:PRO:HD2	1.86	0.56
1:I:407:TRP:CZ2	2:J:260:VAL:HB	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:181:VAL:HB	2:N:352:LYS:CG	2.35	0.56
1:M:397:LEU:HD13	2:N:345:GLU:O	2.05	0.56
1:Q:179:THR:HA	2:R:353:THR:N	2.16	0.56
1:Q:262:TYR:HB3	1:Q:263:PRO:HD2	1.86	0.56
1:C:256:GLN:HG2	2:N:407:TRP:CZ2	2.41	0.56
1:E:326:LYS:CB	2:R:210:TYR:CE2	2.88	0.56
1:E:401:LYS:HD3	2:F:346:TRP:CD1	2.36	0.56
1:Q:100:ALA:HB1	2:R:254:LYS:CA	2.34	0.56
1:Q:210:TYR:CE2	2:R:326:LYS:CB	2.86	0.56
1:C:97:GLU:OE2	2:D:2:ARG:N	2.39	0.56
1:C:262:TYR:HB3	1:C:263:PRO:HD2	1.86	0.56
1:G:262:TYR:HB3	1:G:263:PRO:HD2	1.86	0.56
3:I:501:GTP:O1A	2:J:249:ASN:HB3	2.05	0.56
1:K:210:TYR:CE2	2:L:326:LYS:CB	2.87	0.56
1:K:262:TYR:HB3	1:K:263:PRO:HD2	1.86	0.56
1:M:262:TYR:HB3	1:M:263:PRO:HD2	1.86	0.56
1:Q:100:ALA:C	2:R:254:LYS:CG	2.78	0.56
1:E:101:ASN:HB2	2:F:254:LYS:HG3	1.88	0.56
1:I:283:HIS:O	1:K:62:VAL:HG21	2.05	0.56
1:Q:181:VAL:HG12	2:R:258:ASN:OD1	2.04	0.56
1:Q:401:LYS:CG	2:R:346:TRP:CD2	2.88	0.56
1:A:101:ASN:CA	2:B:254:LYS:HE3	2.31	0.56
1:M:100:ALA:C	2:N:254:LYS:CG	2.78	0.56
1:Q:394:LYS:HA	2:R:348:PRO:CG	2.27	0.56
1:C:258:ASN:O	2:N:404:PHE:HZ	1.85	0.56
1:E:401:LYS:HD3	2:F:346:TRP:CG	2.38	0.56
1:G:404:PHE:CA	2:H:261:PRO:HA	2.36	0.56
1:I:210:TYR:HB3	2:J:326:LYS:HE2	1.84	0.56
1:M:407:TRP:CZ2	2:N:260:VAL:HB	2.41	0.56
1:O:210:TYR:CD2	2:P:326:LYS:CB	2.89	0.56
1:O:407:TRP:CG	2:P:257:VAL:HG13	2.40	0.56
1:Q:406:HIS:HE1	2:R:260:VAL:C	2.11	0.56
1:A:401:LYS:HD3	2:B:346:TRP:CG	2.39	0.56
1:K:181:VAL:HB	2:L:352:LYS:CE	2.35	0.56
1:A:260:VAL:HB	2:P:407:TRP:CE2	2.40	0.55
1:A:350:GLY:C	2:P:181:VAL:HG22	2.19	0.55
1:A:397:LEU:CB	2:B:346:TRP:O	2.51	0.55
1:C:210:TYR:CD2	2:D:326:LYS:CG	2.85	0.55
1:E:177:VAL:HG11	2:F:329:ASP:CB	2.36	0.55
1:I:179:THR:CG2	2:J:353:THR:HG1	2.13	0.55
1:K:397:LEU:HB3	2:L:346:TRP:C	2.30	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:179:THR:HG21	2:P:353:THR:HG1	1.66	0.55
1:O:397:LEU:HD13	2:P:345:GLU:O	2.05	0.55
1:A:407:TRP:CZ2	2:B:260:VAL:HB	2.41	0.55
1:E:177:VAL:HG11	2:F:329:ASP:OD1	2.07	0.55
1:G:407:TRP:NE1	2:H:260:VAL:HB	2.21	0.55
1:M:210:TYR:CB	2:N:326:LYS:CD	2.73	0.55
1:O:407:TRP:CZ2	2:P:256:ALA:C	2.83	0.55
2:B:407:TRP:CZ2	1:I:256:GLN:O	2.59	0.55
1:C:326:LYS:CB	2:N:210:TYR:CE2	2.88	0.55
1:C:397:LEU:HB3	2:D:346:TRP:C	2.31	0.55
2:F:210:TYR:CE2	1:K:326:LYS:CB	2.89	0.55
1:K:177:VAL:HG11	2:L:329:ASP:OD1	2.07	0.55
1:M:407:TRP:CE3	2:N:257:VAL:HG22	2.42	0.55
1:Q:397:LEU:HB2	2:R:348:PRO:HD3	1.86	0.55
1:A:407:TRP:CE3	2:B:257:VAL:HG22	2.41	0.55
1:E:348:PRO:HD2	2:R:398:MET:HG2	1.89	0.55
1:G:397:LEU:HB3	2:H:346:TRP:C	2.30	0.55
1:G:401:LYS:HG2	2:H:346:TRP:CD2	2.41	0.55
1:M:181:VAL:HG11	2:N:258:ASN:O	2.06	0.55
1:Q:394:LYS:CG	2:R:348:PRO:HB2	2.29	0.55
1:A:260:VAL:CB	2:P:407:TRP:CZ2	2.80	0.55
1:O:394:LYS:HZ3	2:P:349:ASN:ND2	2.02	0.55
1:Q:101:ASN:CB	2:R:254:LYS:CD	2.79	0.55
1:A:256:GLN:HG2	2:P:407:TRP:CZ2	2.42	0.55
1:E:181:VAL:HG12	2:F:258:ASN:OD1	2.07	0.55
3:G:501:GTP:O1A	2:H:249:ASN:HB3	2.07	0.55
1:K:177:VAL:HB	2:L:329:ASP:HB3	1.87	0.55
1:A:181:VAL:N	2:B:352:LYS:CE	2.62	0.55
1:C:177:VAL:HG21	2:D:329:ASP:HB3	1.89	0.55
1:I:401:LYS:CG	2:J:346:TRP:CB	2.63	0.55
1:K:176:GLN:OE1	2:L:333:LEU:CD1	2.48	0.55
1:K:407:TRP:CE2	2:L:260:VAL:HB	2.42	0.55
1:M:283:HIS:HB3	1:O:62:VAL:CG2	2.36	0.55
1:Q:97:GLU:OE2	2:R:2:ARG:N	2.40	0.55
1:C:394:LYS:HZ3	2:D:349:ASN:ND2	2.05	0.55
1:I:176:GLN:HG3	2:J:333:LEU:CD2	2.33	0.55
1:M:100:ALA:CA	2:N:254:LYS:HD2	2.37	0.55
1:Q:397:LEU:C	2:R:346:TRP:O	2.49	0.55
1:Q:404:PHE:CZ	2:R:314:THR:HG22	2.28	0.55
1:Q:406:HIS:HE1	2:R:260:VAL:HG12	1.60	0.55
1:A:176:GLN:OE1	2:B:333:LEU:CD1	2.48	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LYS:HB2	2:P:210:TYR:HE2	1.69	0.55
1:E:210:TYR:CD1	2:F:326:LYS:CB	2.79	0.55
1:E:260:VAL:HB	2:R:407:TRP:CE2	2.40	0.55
1:K:394:LYS:C	2:L:348:PRO:HG3	2.31	0.55
1:M:403:ALA:HB1	2:N:261:PRO:HB3	1.87	0.55
1:E:407:TRP:HE1	2:F:260:VAL:HB	1.71	0.55
1:G:401:LYS:CG	2:H:346:TRP:CB	2.62	0.55
1:I:181:VAL:HB	2:J:352:LYS:CG	2.37	0.55
1:M:101:ASN:ND2	2:N:258:ASN:OD1	2.40	0.55
2:D:398:MET:SD	1:G:348:PRO:HG3	2.47	0.54
1:E:407:TRP:CE3	2:F:257:VAL:HG22	2.42	0.54
1:G:397:LEU:HB2	2:H:348:PRO:HD3	1.89	0.54
1:O:176:GLN:HB3	2:P:333:LEU:HD13	1.88	0.54
1:A:101:ASN:CA	2:B:254:LYS:CE	2.85	0.54
1:A:329:ASN:HA	2:P:177:VAL:CG2	2.37	0.54
1:C:256:GLN:O	2:N:407:TRP:CE2	2.60	0.54
1:C:407:TRP:CE3	2:D:257:VAL:HG22	2.41	0.54
2:F:177:VAL:HG21	1:K:329:ASN:CB	2.38	0.54
1:G:404:PHE:HE2	2:H:258:ASN:C	2.14	0.54
2:F:398:MET:SD	1:K:348:PRO:HG3	2.48	0.54
1:G:179:THR:HG21	2:H:248:LEU:CD1	2.38	0.54
1:I:179:THR:HG21	2:J:248:LEU:CD1	2.38	0.54
1:I:406:HIS:HE1	2:J:260:VAL:C	2.14	0.54
1:A:325:PRO:HB2	2:P:210:TYR:OH	2.06	0.54
1:A:348:PRO:CD	2:P:398:MET:HG3	2.28	0.54
1:A:407:TRP:CB	2:B:257:VAL:HG13	2.37	0.54
1:C:177:VAL:HG11	2:D:329:ASP:CB	2.38	0.54
1:C:407:TRP:CE2	2:D:260:VAL:HB	2.43	0.54
2:D:181:VAL:HA	1:G:350:GLY:CA	2.35	0.54
1:O:100:ALA:C	2:P:254:LYS:HG3	2.33	0.54
1:Q:401:LYS:HG2	2:R:346:TRP:CD2	2.43	0.54
1:A:346:TRP:CB	2:P:401:ARG:HB2	2.15	0.54
1:A:404:PHE:HE2	2:B:258:ASN:C	2.15	0.54
1:C:260:VAL:HB	2:N:407:TRP:HZ2	1.64	0.54
2:D:404:PHE:HZ	1:G:258:ASN:O	1.90	0.54
1:I:176:GLN:O	2:J:333:LEU:HD13	2.08	0.54
1:I:407:TRP:CD1	2:J:257:VAL:O	2.61	0.54
1:M:177:VAL:HG11	2:N:329:ASP:CB	2.38	0.54
1:A:283:HIS:CA	1:E:56:THR:CG2	2.78	0.54
2:D:407:TRP:CZ2	1:G:256:GLN:HG2	2.42	0.54
1:G:100:ALA:C	2:H:254:LYS:CD	2.77	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:401:LYS:HG2	2:J:346:TRP:CD2	2.43	0.54
1:Q:401:LYS:CG	2:R:346:TRP:CB	2.68	0.54
1:Q:407:TRP:CE3	2:R:257:VAL:HG22	2.42	0.54
1:A:62:VAL:CG2	1:C:283:HIS:HB3	2.37	0.54
1:C:176:GLN:OE1	2:D:333:LEU:CD1	2.49	0.54
1:I:407:TRP:HE1	2:J:260:VAL:HB	1.73	0.54
1:G:73:THR:HG21	2:H:245:PRO:HA	1.90	0.54
1:K:177:VAL:CB	2:L:329:ASP:HB3	2.38	0.54
1:M:179:THR:HG21	2:N:248:LEU:CD1	2.38	0.54
1:M:401:LYS:CG	2:N:346:TRP:CB	2.68	0.54
1:A:404:PHE:H	2:B:261:PRO:C	2.15	0.54
1:O:176:GLN:O	2:P:333:LEU:HD13	2.07	0.54
2:R:228:ASN:ND2	5:R:901:GDP:HN1	1.98	0.54
1:C:76:ASP:CG	2:D:48:ARG:HH22	1.99	0.53
2:F:228:ASN:ND2	5:F:901:GDP:HN1	1.98	0.53
1:K:210:TYR:CE1	2:L:326:LYS:CA	2.83	0.53
2:L:228:ASN:ND2	5:L:901:GDP:HN1	1.98	0.53
1:O:105:ARG:NE	2:P:253:ARG:HE	2.05	0.53
1:I:404:PHE:CE2	2:J:258:ASN:C	2.85	0.53
1:Q:404:PHE:HE2	2:R:258:ASN:C	2.15	0.53
1:E:260:VAL:CB	2:R:407:TRP:CZ2	2.80	0.53
1:G:177:VAL:HG21	2:H:329:ASP:HB3	1.90	0.53
1:G:394:LYS:C	2:H:348:PRO:HG3	2.32	0.53
1:G:404:PHE:CZ	2:H:314:THR:HG22	2.37	0.53
1:K:210:TYR:CG	2:L:326:LYS:CB	2.91	0.53
1:M:407:TRP:CG	2:N:257:VAL:HA	2.43	0.53
1:Q:72:PRO:HB2	2:R:48:ARG:NH1	2.24	0.53
1:Q:101:ASN:CB	2:R:254:LYS:HG3	2.38	0.53
2:D:210:TYR:CE2	1:G:326:LYS:CB	2.89	0.53
1:G:406:HIS:HE1	2:H:260:VAL:C	2.16	0.53
1:O:101:ASN:ND2	2:P:258:ASN:OD1	2.41	0.53
1:A:72:PRO:HB2	2:B:48:ARG:NH1	2.24	0.53
1:M:176:GLN:O	2:N:333:LEU:HD13	2.08	0.53
1:O:407:TRP:HB3	2:P:257:VAL:HG13	1.89	0.53
2:B:210:TYR:CE2	1:I:326:LYS:CB	2.88	0.53
2:D:407:TRP:CZ2	1:G:256:GLN:O	2.62	0.53
1:I:101:ASN:HB2	2:J:254:LYS:HG3	1.89	0.53
1:M:105:ARG:HH22	2:N:253:ARG:NH2	2.01	0.53
1:M:283:HIS:O	1:O:62:VAL:HG21	2.08	0.53
1:O:72:PRO:HB2	2:P:48:ARG:HH12	1.72	0.53
1:O:407:TRP:CZ2	2:P:260:VAL:HB	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:181:VAL:HB	2:R:352:LYS:CG	2.37	0.53
2:B:398:MET:HG2	1:I:348:PRO:HD2	1.91	0.53
2:B:404:PHE:CE2	1:I:258:ASN:O	2.60	0.53
1:C:101:ASN:CA	2:D:254:LYS:HE3	2.33	0.53
1:E:325:PRO:HB2	2:R:210:TYR:OH	2.08	0.53
1:G:210:TYR:HB3	2:H:326:LYS:HE2	1.89	0.53
1:K:216:ASN:HB3	1:K:275:VAL:O	2.09	0.53
1:M:388:TRP:HA	1:M:388:TRP:CE3	2.44	0.53
1:Q:216:ASN:HB3	1:Q:275:VAL:O	2.09	0.53
1:Q:401:LYS:CD	2:R:346:TRP:CD2	2.91	0.53
1:A:101:ASN:HD22	2:B:258:ASN:ND2	2.07	0.53
1:A:179:THR:HG21	2:B:248:LEU:CD1	2.39	0.53
1:C:210:TYR:CG	2:D:326:LYS:HB2	2.40	0.53
1:C:388:TRP:CE3	1:C:388:TRP:HA	2.44	0.53
1:E:101:ASN:HD22	2:F:258:ASN:HD21	1.56	0.53
1:E:181:VAL:HB	2:F:352:LYS:CE	2.37	0.53
1:E:216:ASN:HB3	1:E:275:VAL:O	2.09	0.53
2:F:181:VAL:HA	1:K:350:GLY:CA	2.37	0.53
1:G:176:GLN:HG3	2:H:333:LEU:CD2	2.36	0.53
1:G:388:TRP:HA	1:G:388:TRP:CE3	2.44	0.53
2:H:228:ASN:ND2	5:H:901:GDP:HN1	1.98	0.53
1:K:407:TRP:HE1	2:L:260:VAL:HB	1.74	0.53
1:M:271:THR:OG1	1:M:301:GLN:NE2	2.42	0.53
1:O:210:TYR:CD1	2:P:326:LYS:HD2	2.44	0.53
1:Q:100:ALA:C	2:R:254:LYS:HG3	2.34	0.53
1:Q:179:THR:CB	2:R:353:THR:H	2.22	0.53
1:A:216:ASN:HB3	1:A:275:VAL:O	2.09	0.53
1:A:407:TRP:CG	2:B:257:VAL:HG13	2.43	0.53
1:C:397:LEU:CB	2:D:346:TRP:O	2.55	0.53
1:E:101:ASN:CA	2:F:254:LYS:HE3	2.31	0.53
1:G:176:GLN:O	2:H:333:LEU:HD13	2.09	0.53
1:G:181:VAL:HB	2:H:352:LYS:CG	2.39	0.53
1:G:271:THR:OG1	1:G:301:GLN:NE2	2.42	0.53
2:H:221:THR:H	2:H:222:PRO:HD3	1.73	0.53
1:M:100:ALA:CB	2:N:254:LYS:HB2	2.39	0.53
1:M:407:TRP:CG	2:N:257:VAL:HG13	2.44	0.53
1:O:216:ASN:HB3	1:O:275:VAL:O	2.09	0.53
1:Q:404:PHE:CE2	2:R:258:ASN:C	2.86	0.53
1:A:401:LYS:CG	2:B:346:TRP:CD2	2.92	0.53
1:C:345:ASP:OD1	2:N:400:ARG:NH2	2.39	0.53
2:D:221:THR:H	2:D:222:PRO:HD3	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:404:PHE:CE2	1:G:258:ASN:HA	2.44	0.53
1:E:326:LYS:HB2	2:R:210:TYR:HE2	1.71	0.53
1:G:283:HIS:O	1:I:62:VAL:HG21	2.08	0.53
1:I:210:TYR:OH	2:J:326:LYS:HA	2.06	0.53
2:N:221:THR:H	2:N:222:PRO:HD3	1.73	0.53
1:O:401:LYS:HE3	2:P:435:TYR:HD2	1.74	0.53
1:Q:100:ALA:HA	2:R:254:LYS:HD2	1.91	0.53
1:Q:176:GLN:HG3	2:R:333:LEU:CD2	2.28	0.53
1:Q:177:VAL:HG11	2:R:329:ASP:CB	2.38	0.53
1:Q:394:LYS:CB	2:R:348:PRO:HG3	2.38	0.53
1:Q:401:LYS:HG2	2:R:346:TRP:CG	2.41	0.53
1:C:271:THR:OG1	1:C:301:GLN:NE2	2.42	0.52
1:C:407:TRP:CG	2:D:257:VAL:HG13	2.44	0.52
1:E:100:ALA:HA	2:F:254:LYS:HD2	1.90	0.52
1:E:271:THR:OG1	1:E:301:GLN:NE2	2.42	0.52
1:E:388:TRP:HA	1:E:388:TRP:CE3	2.44	0.52
1:G:283:HIS:HB3	1:I:62:VAL:CG2	2.38	0.52
1:I:216:ASN:HB3	1:I:275:VAL:O	2.09	0.52
1:K:271:THR:OG1	1:K:301:GLN:NE2	2.42	0.52
1:K:406:HIS:HE1	2:L:260:VAL:C	2.15	0.52
1:M:177:VAL:CB	2:N:329:ASP:HB3	2.38	0.52
1:O:388:TRP:HA	1:O:388:TRP:CE3	2.44	0.52
1:A:177:VAL:HG11	2:B:329:ASP:CB	2.38	0.52
2:B:221:THR:H	2:B:222:PRO:HD3	1.73	0.52
2:D:228:ASN:ND2	5:D:901:GDP:HN1	1.98	0.52
1:I:72:PRO:HB2	2:J:48:ARG:NH1	2.25	0.52
2:J:221:THR:H	2:J:222:PRO:HD3	1.73	0.52
1:M:407:TRP:CD1	2:N:257:VAL:O	2.62	0.52
1:O:394:LYS:CB	2:P:348:PRO:CG	2.88	0.52
2:P:221:THR:H	2:P:222:PRO:HD3	1.73	0.52
1:Q:271:THR:OG1	1:Q:301:GLN:NE2	2.42	0.52
1:Q:388:TRP:HA	1:Q:388:TRP:CE3	2.44	0.52
1:A:283:HIS:O	1:E:62:VAL:HG21	2.08	0.52
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.44	0.52
1:C:216:ASN:HB3	1:C:275:VAL:O	2.09	0.52
2:F:306:ASP:OD1	2:F:308:ARG:HG2	2.09	0.52
1:I:210:TYR:CB	2:J:326:LYS:CD	2.73	0.52
2:L:306:ASP:OD1	2:L:308:ARG:HG2	2.10	0.52
1:M:101:ASN:ND2	2:N:258:ASN:HD21	2.07	0.52
1:M:216:ASN:HB3	1:M:275:VAL:O	2.09	0.52
1:O:407:TRP:CH2	2:P:256:ALA:HB1	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:283:TYR:HD2	2:R:62:VAL:CG2	2.07	0.52
1:Q:100:ALA:CA	2:R:254:LYS:CB	2.73	0.52
2:R:306:ASP:OD1	2:R:308:ARG:HG2	2.09	0.52
1:A:73:THR:HG21	2:B:245:PRO:HA	1.92	0.52
1:A:394:LYS:HZ3	2:B:349:ASN:ND2	2.05	0.52
1:G:216:ASN:HB3	1:G:275:VAL:O	2.09	0.52
1:G:407:TRP:CD1	2:H:257:VAL:O	2.63	0.52
1:I:388:TRP:HA	1:I:388:TRP:CE3	2.44	0.52
1:K:388:TRP:CE3	1:K:388:TRP:HA	2.44	0.52
1:M:406:HIS:NE2	2:N:260:VAL:HG11	2.21	0.52
1:Q:407:TRP:CG	2:R:257:VAL:HG13	2.45	0.52
2:B:306:ASP:OD1	2:B:308:ARG:HG2	2.09	0.52
2:B:404:PHE:CE2	1:I:258:ASN:HA	2.44	0.52
1:C:260:VAL:CB	2:N:407:TRP:CZ2	2.84	0.52
1:G:177:VAL:HG11	2:H:329:ASP:CG	2.33	0.52
1:I:97:GLU:OE2	2:J:2:ARG:N	2.43	0.52
2:N:228:ASN:ND2	5:N:901:GDP:HN1	1.98	0.52
2:P:306:ASP:OD1	2:P:308:ARG:HG2	2.09	0.52
1:Q:181:VAL:HG11	2:R:258:ASN:O	2.08	0.52
1:A:348:PRO:HG3	2:P:398:MET:CG	2.40	0.52
1:A:407:TRP:CE2	2:B:260:VAL:HB	2.44	0.52
1:E:176:GLN:O	2:F:333:LEU:HD13	2.10	0.52
2:F:221:THR:H	2:F:222:PRO:HD3	1.73	0.52
1:I:179:THR:HA	2:J:353:THR:N	2.22	0.52
1:I:271:THR:OG1	1:I:301:GLN:NE2	2.42	0.52
2:P:10:GLY:HA2	2:P:145:THR:OG1	2.10	0.52
1:A:62:VAL:HG21	1:C:283:HIS:O	2.09	0.52
1:A:177:VAL:CG1	2:B:329:ASP:HA	2.28	0.52
1:A:256:GLN:O	2:P:407:TRP:NE1	2.43	0.52
1:C:11:GLN:HE22	2:D:247:GLN:C	2.09	0.52
1:C:346:TRP:HZ3	2:N:403:ALA:CB	1.85	0.52
1:E:407:TRP:CB	2:F:257:VAL:HG13	2.40	0.52
2:J:221:THR:N	2:J:222:PRO:CD	2.73	0.52
1:K:101:ASN:HB2	2:L:254:LYS:HG3	1.91	0.52
1:M:105:ARG:NE	2:N:253:ARG:HE	2.07	0.52
1:Q:177:VAL:HG11	2:R:329:ASP:OD1	2.09	0.52
1:A:271:THR:OG1	1:A:301:GLN:NE2	2.42	0.52
1:A:401:LYS:CD	2:B:346:TRP:CD2	2.89	0.52
2:B:221:THR:N	2:B:222:PRO:CD	2.73	0.52
1:C:407:TRP:CB	2:D:257:VAL:HG13	2.39	0.52
2:D:10:GLY:HA2	2:D:145:THR:OG1	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:306:ASP:OD1	2:J:308:ARG:HG2	2.10	0.52
2:L:221:THR:H	2:L:222:PRO:HD3	1.73	0.52
1:O:100:ALA:HA	2:P:254:LYS:HD2	1.92	0.52
1:O:271:THR:OG1	1:O:301:GLN:NE2	2.42	0.52
1:O:401:LYS:HG2	2:P:346:TRP:CD2	2.45	0.52
2:P:221:THR:N	2:P:222:PRO:CD	2.73	0.52
1:Q:100:ALA:CB	2:R:254:LYS:HB2	2.40	0.52
2:R:10:GLY:HA2	2:R:145:THR:OG1	2.10	0.52
1:A:176:GLN:HB3	2:B:333:LEU:HD13	1.92	0.52
1:C:179:THR:HG21	2:D:248:LEU:CD1	2.40	0.52
1:E:407:TRP:NE1	2:F:260:VAL:O	2.42	0.52
1:K:210:TYR:CG	2:L:326:LYS:HB2	2.37	0.52
1:K:397:LEU:CB	2:L:346:TRP:O	2.58	0.52
1:M:394:LYS:CB	2:N:348:PRO:HG3	2.39	0.52
1:M:401:LYS:CG	2:N:346:TRP:CD2	2.93	0.52
2:N:10:GLY:HA2	2:N:145:THR:OG1	2.10	0.52
1:O:401:LYS:CG	2:P:346:TRP:CD2	2.92	0.52
2:B:10:GLY:HA2	2:B:145:THR:OG1	2.10	0.52
2:B:401:ARG:NH2	1:I:435:VAL:HG22	2.25	0.52
2:F:10:GLY:HA2	2:F:145:THR:OG1	2.10	0.52
2:F:210:TYR:HE2	1:K:326:LYS:HB2	1.73	0.52
1:G:101:ASN:HB2	2:H:254:LYS:HG3	1.91	0.52
2:H:10:GLY:HA2	2:H:145:THR:OG1	2.10	0.52
1:I:101:ASN:HD22	2:J:258:ASN:ND2	2.08	0.52
2:J:10:GLY:HA2	2:J:145:THR:OG1	2.10	0.52
2:L:10:GLY:HA2	2:L:145:THR:OG1	2.10	0.52
1:Q:403:ALA:HB1	2:R:261:PRO:HB3	1.91	0.52
1:A:177:VAL:HG21	2:B:329:ASP:HB3	1.90	0.51
1:A:325:PRO:HG2	2:P:224:TYR:CE1	2.45	0.51
1:A:346:TRP:CA	2:P:401:ARG:HG3	2.32	0.51
2:H:306:ASP:OD1	2:H:308:ARG:HG2	2.09	0.51
1:K:404:PHE:HE2	2:L:258:ASN:C	2.18	0.51
2:R:221:THR:H	2:R:222:PRO:HD3	1.73	0.51
1:A:397:LEU:HD22	2:B:345:GLU:O	2.10	0.51
2:D:221:THR:N	2:D:222:PRO:CD	2.73	0.51
1:I:407:TRP:CE2	2:J:260:VAL:HB	2.45	0.51
1:K:407:TRP:CD1	2:L:257:VAL:O	2.63	0.51
2:N:221:THR:N	2:N:222:PRO:CD	2.73	0.51
1:Q:407:TRP:CD1	2:R:257:VAL:O	2.62	0.51
2:B:210:TYR:HE2	1:I:326:LYS:HB2	1.72	0.51
1:C:388:TRP:HA	1:C:388:TRP:HE3	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:TRP:CG	2:F:257:VAL:HG13	2.45	0.51
2:H:390:ARG:HA	2:H:390:ARG:NE	2.26	0.51
2:L:345:GLU:H	2:L:345:GLU:CD	2.10	0.51
1:M:388:TRP:HA	1:M:388:TRP:HE3	1.74	0.51
1:C:260:VAL:HB	2:N:407:TRP:CE2	2.44	0.51
1:G:388:TRP:HA	1:G:388:TRP:HE3	1.74	0.51
2:H:221:THR:N	2:H:222:PRO:CD	2.73	0.51
1:M:401:LYS:HG2	2:N:346:TRP:CG	2.43	0.51
1:O:394:LYS:CB	2:P:348:PRO:HG3	2.39	0.51
1:A:258:ASN:CA	2:P:404:PHE:CE2	2.93	0.51
1:A:329:ASN:HB2	2:P:177:VAL:HG21	1.92	0.51
1:C:101:ASN:CA	2:D:254:LYS:CE	2.88	0.51
1:C:404:PHE:H	2:D:261:PRO:C	2.17	0.51
2:D:390:ARG:NE	2:D:390:ARG:HA	2.26	0.51
2:J:390:ARG:NE	2:J:390:ARG:HA	2.26	0.51
1:M:394:LYS:CG	2:N:348:PRO:HB2	2.30	0.51
2:B:407:TRP:CZ2	1:I:256:GLN:HG2	2.46	0.51
1:C:177:VAL:CG1	2:D:329:ASP:HA	2.29	0.51
2:D:306:ASP:OD1	2:D:308:ARG:HG2	2.10	0.51
1:E:100:ALA:CA	2:F:254:LYS:HD2	2.41	0.51
3:E:501:GTP:O1A	2:F:249:ASN:HB3	2.10	0.51
2:F:345:GLU:H	2:F:345:GLU:CD	2.10	0.51
1:G:181:VAL:N	2:H:352:LYS:CE	2.55	0.51
1:I:210:TYR:CD2	2:J:326:LYS:CB	2.94	0.51
1:I:397:LEU:CB	2:J:346:TRP:O	2.54	0.51
1:I:404:PHE:CZ	2:J:314:THR:HG22	2.35	0.51
1:K:100:ALA:HA	2:L:254:LYS:CD	2.40	0.51
2:L:221:THR:N	2:L:222:PRO:CD	2.73	0.51
2:N:390:ARG:NE	2:N:390:ARG:HA	2.26	0.51
1:O:388:TRP:HA	1:O:388:TRP:HE3	1.74	0.51
1:Q:210:TYR:CD1	2:R:326:LYS:HD2	2.46	0.51
1:A:348:PRO:HG3	2:P:398:MET:HG3	1.93	0.51
2:B:404:PHE:HZ	1:I:258:ASN:O	1.91	0.51
1:G:407:TRP:CE2	2:H:260:VAL:HB	2.46	0.51
1:I:181:VAL:HB	2:J:352:LYS:CE	2.37	0.51
2:N:306:ASP:OD1	2:N:308:ARG:HG2	2.10	0.51
1:C:397:LEU:HD22	2:D:345:GLU:O	2.11	0.51
1:G:237:SER:O	1:G:241:SER:OG	2.29	0.51
1:I:100:ALA:C	2:J:254:LYS:CG	2.84	0.51
1:I:105:ARG:HH22	2:J:253:ARG:NH2	2.04	0.51
2:L:390:ARG:NE	2:L:390:ARG:HA	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:401:LYS:HE3	2:N:435:TYR:HD2	1.76	0.51
2:B:390:ARG:NE	2:B:390:ARG:HA	2.26	0.51
1:C:237:SER:O	1:C:241:SER:OG	2.29	0.51
2:F:221:THR:N	2:F:222:PRO:CD	2.73	0.51
2:F:390:ARG:NE	2:F:390:ARG:HA	2.26	0.51
2:P:390:ARG:HA	2:P:390:ARG:NE	2.26	0.51
1:I:177:VAL:HG11	2:J:329:ASP:CG	2.35	0.51
1:K:397:LEU:HB2	2:L:348:PRO:HD3	1.93	0.51
1:M:179:THR:CB	2:N:353:THR:H	2.24	0.51
1:Q:177:VAL:CB	2:R:329:ASP:HB3	2.41	0.51
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.74	0.50
1:C:177:VAL:HG11	2:D:329:ASP:CG	2.36	0.50
1:G:407:TRP:HE1	2:H:260:VAL:HB	1.76	0.50
2:H:283:TYR:HD2	2:J:62:VAL:CG2	2.03	0.50
1:K:210:TYR:CD1	2:L:326:LYS:HD2	2.46	0.50
1:M:237:SER:O	1:M:241:SER:OG	2.29	0.50
1:O:179:THR:CB	2:P:353:THR:H	2.24	0.50
1:Q:406:HIS:NE2	2:R:260:VAL:HG11	2.23	0.50
1:C:404:PHE:HE2	2:D:258:ASN:C	2.18	0.50
1:E:256:GLN:CG	2:R:407:TRP:CH2	2.92	0.50
1:G:97:GLU:OE2	2:H:2:ARG:N	2.44	0.50
3:K:501:GTP:O1A	2:L:249:ASN:HB3	2.10	0.50
1:M:100:ALA:C	2:N:254:LYS:HG3	2.36	0.50
2:R:221:THR:N	2:R:222:PRO:CD	2.73	0.50
2:R:345:GLU:H	2:R:345:GLU:CD	2.10	0.50
1:E:388:TRP:HA	1:E:388:TRP:HE3	1.74	0.50
1:E:394:LYS:O	2:F:348:PRO:HG3	2.11	0.50
1:I:237:SER:O	1:I:241:SER:OG	2.29	0.50
1:I:388:TRP:HA	1:I:388:TRP:HE3	1.74	0.50
1:M:394:LYS:CB	2:N:348:PRO:CG	2.89	0.50
2:R:390:ARG:NE	2:R:390:ARG:HA	2.26	0.50
1:A:237:SER:O	1:A:241:SER:OG	2.29	0.50
1:E:73:THR:HG21	2:F:245:PRO:HA	1.94	0.50
1:I:397:LEU:C	2:J:346:TRP:O	2.55	0.50
1:M:401:LYS:HG2	2:N:346:TRP:CD2	2.47	0.50
1:Q:237:SER:O	1:Q:241:SER:OG	2.29	0.50
1:Q:388:TRP:HA	1:Q:388:TRP:HE3	1.74	0.50
1:Q:394:LYS:CB	2:R:348:PRO:CG	2.89	0.50
1:A:210:TYR:CG	2:B:326:LYS:HB2	2.39	0.50
1:C:329:ASN:HA	2:N:177:VAL:CG2	2.42	0.50
1:I:177:VAL:HG21	2:J:329:ASP:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:407:TRP:CG	2:R:257:VAL:HA	2.46	0.50
1:C:348:PRO:CG	2:N:398:MET:CG	2.89	0.50
1:E:258:ASN:O	2:R:404:PHE:HZ	1.92	0.50
1:E:397:LEU:HB3	2:F:346:TRP:C	2.36	0.50
1:G:177:VAL:CG2	2:H:329:ASP:HB3	2.42	0.50
1:I:100:ALA:CB	2:J:254:LYS:HB2	2.41	0.50
1:I:210:TYR:CD1	2:J:326:LYS:HD2	2.47	0.50
1:K:388:TRP:HA	1:K:388:TRP:HE3	1.74	0.50
1:O:237:SER:O	1:O:241:SER:OG	2.29	0.50
1:A:397:LEU:HB2	2:B:348:PRO:HD3	1.94	0.50
1:C:346:TRP:CB	2:N:401:ARG:HB2	2.22	0.50
2:D:404:PHE:HE2	1:G:258:ASN:CA	2.25	0.50
1:E:237:SER:O	1:E:241:SER:OG	2.29	0.50
1:O:101:ASN:ND2	2:P:258:ASN:HD21	2.05	0.50
1:C:258:ASN:CA	2:N:404:PHE:CE2	2.94	0.50
2:F:407:TRP:CZ2	1:K:256:GLN:HG2	2.46	0.50
1:I:100:ALA:HA	2:J:254:LYS:CD	2.42	0.50
1:A:2:ARG:N	2:P:96:GLN:NE2	2.60	0.50
2:B:167:ASN:C	2:B:167:ASN:OD1	2.55	0.50
1:C:181:VAL:HB	2:D:352:LYS:CE	2.42	0.50
1:E:101:ASN:CA	2:F:254:LYS:CE	2.90	0.50
1:E:258:ASN:HA	2:R:404:PHE:CE2	2.46	0.50
1:G:177:VAL:HG21	2:H:329:ASP:CB	2.42	0.50
1:I:407:TRP:CZ2	2:J:256:ALA:C	2.90	0.50
2:N:12:CYS:SG	2:N:13:GLY:N	2.85	0.50
2:D:404:PHE:CE2	1:G:258:ASN:O	2.64	0.49
1:E:345:ASP:OD1	2:R:400:ARG:NH2	2.42	0.49
1:G:210:TYR:OH	2:H:326:LYS:CA	2.53	0.49
1:G:210:TYR:CB	2:H:326:LYS:CD	2.76	0.49
2:H:12:CYS:SG	2:H:13:GLY:N	2.85	0.49
1:I:407:TRP:HB3	2:J:257:VAL:HG13	1.93	0.49
2:J:167:ASN:C	2:J:167:ASN:OD1	2.56	0.49
1:K:176:GLN:HB3	2:L:333:LEU:HD13	1.94	0.49
1:C:101:ASN:HD22	2:D:258:ASN:ND2	2.10	0.49
2:D:12:CYS:SG	2:D:13:GLY:N	2.86	0.49
2:D:167:ASN:C	2:D:167:ASN:OD1	2.56	0.49
2:F:167:ASN:C	2:F:167:ASN:OD1	2.56	0.49
1:K:181:VAL:HB	2:L:352:LYS:CG	2.41	0.49
1:K:237:SER:O	1:K:241:SER:OG	2.29	0.49
1:K:404:PHE:CZ	2:L:314:THR:HG22	2.35	0.49
1:K:407:TRP:HB3	2:L:257:VAL:HG13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:ARG:N	2:L:131:CYS:O	2.45	0.49
2:L:167:ASN:C	2:L:167:ASN:OD1	2.56	0.49
1:M:100:ALA:HA	2:N:254:LYS:HD2	1.94	0.49
1:O:181:VAL:N	2:P:352:LYS:CD	2.75	0.49
2:R:167:ASN:C	2:R:167:ASN:OD1	2.56	0.49
2:B:404:PHE:HE2	1:I:258:ASN:CA	2.25	0.49
1:E:177:VAL:HG21	2:F:329:ASP:HB3	1.93	0.49
1:E:256:GLN:HG2	2:R:407:TRP:CZ2	2.47	0.49
2:H:167:ASN:C	2:H:167:ASN:OD1	2.56	0.49
2:J:2:ARG:N	2:J:131:CYS:O	2.45	0.49
1:M:210:TYR:CD2	2:N:326:LYS:CB	2.95	0.49
1:M:210:TYR:HH	2:N:325:MET:C	2.18	0.49
2:N:167:ASN:C	2:N:167:ASN:OD1	2.56	0.49
1:O:105:ARG:HH22	2:P:253:ARG:CZ	2.20	0.49
2:P:167:ASN:C	2:P:167:ASN:OD1	2.56	0.49
1:C:176:GLN:HB3	2:D:333:LEU:HD13	1.94	0.49
1:C:177:VAL:CB	2:D:329:ASP:HB3	2.43	0.49
1:E:100:ALA:C	2:F:254:LYS:CD	2.86	0.49
1:E:404:PHE:H	2:F:261:PRO:C	2.19	0.49
2:F:2:ARG:N	2:F:131:CYS:O	2.45	0.49
1:O:210:TYR:HH	2:P:325:MET:C	2.17	0.49
1:O:283:HIS:O	1:Q:62:VAL:HG21	2.11	0.49
1:A:177:VAL:HG11	2:B:329:ASP:CG	2.37	0.49
2:B:2:ARG:N	2:B:131:CYS:O	2.45	0.49
2:B:283:TYR:CA	2:F:56:ALA:HB2	2.38	0.49
1:C:181:VAL:N	2:D:352:LYS:CE	2.61	0.49
1:E:397:LEU:HD22	2:F:345:GLU:O	2.13	0.49
1:I:181:VAL:CG2	2:J:352:LYS:HE2	2.41	0.49
2:J:12:CYS:SG	2:J:13:GLY:N	2.85	0.49
1:M:407:TRP:CZ2	2:N:256:ALA:C	2.90	0.49
2:N:2:ARG:N	2:N:131:CYS:O	2.45	0.49
2:P:282:GLN:O	2:R:60:LYS:CG	2.61	0.49
1:Q:407:TRP:HB3	2:R:257:VAL:HG13	1.93	0.49
2:R:96:GLN:NE2	2:R:96:GLN:O	2.46	0.49
1:E:256:GLN:O	2:R:407:TRP:CE2	2.65	0.49
2:F:96:GLN:NE2	2:F:96:GLN:O	2.46	0.49
2:F:404:PHE:CE2	1:K:258:ASN:HA	2.47	0.49
1:G:181:VAL:CG2	2:H:352:LYS:HE2	2.42	0.49
2:J:228:ASN:ND2	5:J:901:GDP:HN1	1.98	0.49
2:R:2:ARG:N	2:R:131:CYS:O	2.45	0.49
2:R:12:CYS:SG	2:R:13:GLY:N	2.85	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:CYS:SG	2:B:13:GLY:N	2.85	0.49
2:B:228:ASN:ND2	5:B:901:GDP:HN1	1.98	0.49
1:C:2:ARG:N	2:N:96:GLN:NE2	2.61	0.49
2:D:2:ARG:N	2:D:131:CYS:O	2.45	0.49
1:E:101:ASN:ND2	2:F:258:ASN:OD1	2.45	0.49
1:E:177:VAL:CG1	2:F:329:ASP:HA	2.30	0.49
1:E:404:PHE:CZ	2:F:314:THR:HG22	2.38	0.49
2:F:12:CYS:SG	2:F:13:GLY:N	2.85	0.49
1:G:210:TYR:CD2	2:H:326:LYS:CB	2.96	0.49
1:G:397:LEU:CB	2:H:346:TRP:O	2.58	0.49
2:H:2:ARG:N	2:H:131:CYS:O	2.45	0.49
1:I:176:GLN:HB3	2:J:333:LEU:HD13	1.94	0.49
1:I:179:THR:HG22	2:J:353:THR:CB	2.32	0.49
1:K:101:ASN:HD22	2:L:258:ASN:ND2	2.11	0.49
1:K:101:ASN:ND2	2:L:258:ASN:OD1	2.46	0.49
1:K:401:LYS:CG	2:L:346:TRP:CB	2.65	0.49
2:P:2:ARG:N	2:P:131:CYS:O	2.45	0.49
1:A:404:PHE:CE2	2:B:258:ASN:C	2.88	0.49
2:D:96:GLN:NE2	2:D:96:GLN:O	2.46	0.49
2:H:96:GLN:NE2	2:H:96:GLN:O	2.46	0.49
2:L:12:CYS:SG	2:L:13:GLY:N	2.85	0.49
1:O:101:ASN:CA	2:P:254:LYS:CD	2.90	0.49
2:P:12:CYS:SG	2:P:13:GLY:N	2.85	0.49
1:A:100:ALA:C	2:B:254:LYS:CD	2.83	0.49
1:E:210:TYR:CG	2:F:326:LYS:HB2	2.45	0.49
1:E:406:HIS:HE1	2:F:260:VAL:C	2.19	0.49
2:L:96:GLN:O	2:L:96:GLN:NE2	2.46	0.49
2:N:96:GLN:NE2	2:N:96:GLN:O	2.46	0.49
1:A:2:ARG:HG2	2:P:96:GLN:NE2	2.20	0.49
1:A:100:ALA:CA	2:B:254:LYS:HD2	2.43	0.49
1:C:401:LYS:HG2	2:D:346:TRP:CD2	2.48	0.49
2:F:407:TRP:CZ2	1:K:256:GLN:O	2.66	0.49
1:G:100:ALA:HA	2:H:254:LYS:CD	2.43	0.49
2:P:228:ASN:ND2	5:P:901:GDP:HN1	1.98	0.49
1:E:346:TRP:CB	2:R:401:ARG:HB2	2.22	0.48
1:G:404:PHE:CE2	2:H:258:ASN:C	2.88	0.48
1:K:100:ALA:C	2:L:254:LYS:CG	2.86	0.48
1:O:73:THR:HG23	2:P:245:PRO:HG3	1.95	0.48
1:A:101:ASN:CB	2:B:254:LYS:HG3	2.42	0.48
1:A:177:VAL:CB	2:B:329:ASP:HB3	2.43	0.48
1:A:346:TRP:HB2	2:P:401:ARG:HB3	1.85	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:GLN:NE2	2:B:96:GLN:O	2.46	0.48
1:C:100:ALA:HA	2:D:254:LYS:HD2	1.95	0.48
1:I:100:ALA:CA	2:J:254:LYS:CB	2.81	0.48
1:I:100:ALA:HB1	2:J:254:LYS:CA	2.41	0.48
2:J:96:GLN:O	2:J:96:GLN:NE2	2.46	0.48
1:M:72:PRO:HB2	2:N:48:ARG:HH12	1.76	0.48
1:G:72:PRO:HB2	2:H:48:ARG:NH1	2.28	0.48
1:I:177:VAL:CG2	2:J:329:ASP:HB3	2.44	0.48
1:M:210:TYR:CD1	2:N:326:LYS:HD2	2.49	0.48
2:P:96:GLN:NE2	2:P:96:GLN:O	2.46	0.48
2:P:282:GLN:HB3	2:R:60:LYS:HG3	1.95	0.48
1:Q:105:ARG:NE	2:R:253:ARG:HE	2.10	0.48
1:Q:394:LYS:HB3	2:R:348:PRO:CG	2.43	0.48
1:C:177:VAL:HG21	2:D:329:ASP:CB	2.44	0.48
1:C:326:LYS:HB2	2:N:210:TYR:HE2	1.72	0.48
2:F:404:PHE:HZ	1:K:258:ASN:O	1.95	0.48
1:O:181:VAL:CG2	2:P:352:LYS:HE2	2.40	0.48
1:A:260:VAL:O	2:P:406:HIS:NE2	2.38	0.48
1:C:72:PRO:HB2	2:D:48:ARG:NH1	2.29	0.48
1:C:256:GLN:O	2:N:407:TRP:NE1	2.46	0.48
1:G:210:TYR:OH	2:H:326:LYS:HA	2.09	0.48
1:I:283:HIS:CA	1:K:56:THR:CG2	2.83	0.48
1:O:100:ALA:HA	2:P:254:LYS:CD	2.43	0.48
1:Q:179:THR:HG21	2:R:248:LEU:CD1	2.43	0.48
1:A:2:ARG:HD3	2:P:72:PRO:HD2	1.96	0.48
1:C:397:LEU:HB2	2:D:348:PRO:HD3	1.96	0.48
2:D:176:LYS:HD3	1:G:333:ALA:CB	2.43	0.48
1:E:2:ARG:N	2:R:96:GLN:NE2	2.62	0.48
1:Q:401:LYS:HE3	2:R:435:TYR:HD2	1.78	0.48
1:A:210:TYR:CG	2:B:326:LYS:CB	2.97	0.48
2:D:407:TRP:CH2	1:G:256:GLN:CG	2.95	0.48
1:E:439:SER:OG	2:R:400:ARG:NH1	2.44	0.48
1:G:101:ASN:HD22	2:H:258:ASN:ND2	2.11	0.48
1:C:73:THR:HG21	2:D:245:PRO:HA	1.96	0.48
1:E:258:ASN:CA	2:R:404:PHE:HE2	2.26	0.48
1:I:177:VAL:HG21	2:J:329:ASP:CB	2.44	0.48
2:J:288:VAL:HB	2:J:327:GLU:HG2	1.96	0.48
1:M:407:TRP:HB3	2:N:257:VAL:HG13	1.94	0.48
2:P:288:VAL:HB	2:P:327:GLU:HG2	1.96	0.48
1:A:177:VAL:HB	2:B:329:ASP:HB3	1.95	0.48
2:B:288:VAL:HB	2:B:327:GLU:HG2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:PRO:CD	2:N:398:MET:HG3	2.33	0.48
1:E:97:GLU:OE2	2:F:2:ARG:N	2.47	0.48
1:G:407:TRP:HB3	2:H:257:VAL:HG13	1.95	0.48
1:A:254:GLU:HB2	2:P:100:GLY:HA2	1.95	0.47
2:B:407:TRP:CE2	1:I:260:VAL:HB	2.47	0.47
1:C:394:LYS:O	2:D:348:PRO:HG3	2.14	0.47
2:D:398:MET:HG2	1:G:348:PRO:HD2	1.96	0.47
1:E:176:GLN:HB3	2:F:333:LEU:HD13	1.96	0.47
1:E:177:VAL:HG11	2:F:329:ASP:CG	2.39	0.47
1:O:177:VAL:HG11	2:P:329:ASP:CG	2.38	0.47
1:O:403:ALA:HB1	2:P:261:PRO:CB	2.43	0.47
2:P:282:GLN:O	2:R:60:LYS:HG3	2.13	0.47
1:Q:224:TYR:CG	2:R:325:MET:CG	2.84	0.47
1:A:181:VAL:HB	2:B:352:LYS:CE	2.44	0.47
1:G:397:LEU:C	2:H:346:TRP:O	2.58	0.47
1:K:179:THR:HG21	2:L:248:LEU:CD1	2.44	0.47
2:B:96:GLN:NE2	1:I:2:ARG:N	2.63	0.47
1:C:177:VAL:HB	2:D:329:ASP:HB3	1.95	0.47
1:E:177:VAL:CB	2:F:329:ASP:HB3	2.45	0.47
1:E:329:ASN:HA	2:R:177:VAL:CG2	2.45	0.47
1:K:177:VAL:HG11	2:L:329:ASP:CG	2.39	0.47
1:K:397:LEU:HD13	2:L:345:GLU:O	2.14	0.47
2:L:288:VAL:HB	2:L:327:GLU:HG2	1.96	0.47
1:O:224:TYR:CG	2:P:325:MET:CG	2.86	0.47
1:A:177:VAL:HG21	2:B:329:ASP:CB	2.45	0.47
1:A:406:HIS:HE1	2:B:260:VAL:C	2.20	0.47
2:B:283:TYR:HA	2:F:56:ALA:HB2	1.85	0.47
1:C:177:VAL:CG2	2:D:329:ASP:HB3	2.45	0.47
2:D:96:GLN:NE2	1:G:2:ARG:N	2.63	0.47
1:G:53:PHE:HB3	1:G:61:HIS:HB3	1.96	0.47
1:K:100:ALA:CB	2:L:254:LYS:HB2	2.44	0.47
1:K:210:TYR:CB	2:L:326:LYS:CD	2.78	0.47
1:O:394:LYS:HB3	2:P:348:PRO:CG	2.44	0.47
1:Q:101:ASN:ND2	2:R:258:ASN:HD21	2.10	0.47
1:Q:407:TRP:CZ2	2:R:256:ALA:C	2.92	0.47
1:A:284:GLU:N	1:E:56:THR:HG22	2.29	0.47
1:A:394:LYS:C	2:B:348:PRO:HG3	2.40	0.47
1:A:402:ARG:HD3	1:A:402:ARG:HA	1.69	0.47
1:C:53:PHE:HB3	1:C:61:HIS:HB3	1.97	0.47
1:C:100:ALA:CA	2:D:254:LYS:HD2	2.44	0.47
1:C:210:TYR:CG	2:D:326:LYS:CB	2.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:288:VAL:HB	2:F:327:GLU:HG2	1.96	0.47
1:K:404:PHE:CE2	2:L:258:ASN:C	2.92	0.47
1:M:53:PHE:HB3	1:M:61:HIS:HB3	1.97	0.47
1:M:96:LYS:O	2:N:2:ARG:NE	2.48	0.47
1:O:402:ARG:HD3	1:O:402:ARG:HA	1.69	0.47
2:R:288:VAL:HB	2:R:327:GLU:HG2	1.96	0.47
1:A:210:TYR:CE2	2:B:326:LYS:CB	2.97	0.47
1:A:283:HIS:C	1:E:56:THR:HG22	2.39	0.47
2:B:400:ARG:NH2	1:I:345:ASP:OD1	2.44	0.47
1:E:101:ASN:HD22	2:F:258:ASN:ND2	2.13	0.47
1:Q:210:TYR:HH	2:R:325:MET:C	2.18	0.47
1:A:210:TYR:CG	2:B:326:LYS:CD	2.98	0.47
1:C:406:HIS:HE1	2:D:260:VAL:C	2.21	0.47
1:E:246:GLY:HA3	1:E:356:ASN:HA	1.97	0.47
2:F:176:LYS:HD3	1:K:333:ALA:CB	2.42	0.47
1:I:404:PHE:H	2:J:261:PRO:C	2.23	0.47
2:J:282:GLN:HB3	2:L:60:LYS:HG3	1.96	0.47
1:K:105:ARG:NH2	2:L:253:ARG:HH21	1.71	0.47
1:K:246:GLY:HA3	1:K:356:ASN:HA	1.97	0.47
1:K:332:ILE:HA	1:K:335:ILE:HG12	1.97	0.47
1:O:53:PHE:HB3	1:O:61:HIS:HB3	1.97	0.47
1:O:72:PRO:CB	2:P:48:ARG:HH12	2.27	0.47
1:Q:100:ALA:HA	2:R:254:LYS:CD	2.43	0.47
1:Q:246:GLY:HA3	1:Q:356:ASN:HA	1.96	0.47
1:A:2:ARG:HG3	2:P:96:GLN:CD	2.27	0.47
1:G:100:ALA:CA	2:H:254:LYS:CB	2.84	0.47
1:G:407:TRP:CZ2	2:H:256:ALA:C	2.92	0.47
1:I:53:PHE:HB3	1:I:61:HIS:HB3	1.97	0.47
1:K:100:ALA:HB1	2:L:254:LYS:CA	2.43	0.47
1:K:179:THR:HG22	2:L:353:THR:CB	2.36	0.47
1:M:394:LYS:HB3	2:N:348:PRO:CG	2.45	0.47
1:O:177:VAL:CG2	2:P:329:ASP:HB3	2.45	0.47
1:A:53:PHE:HB3	1:A:61:HIS:HB3	1.97	0.47
1:C:228:ASN:HD21	3:C:501:GTP:HN1	1.63	0.47
1:K:97:GLU:OE2	2:L:2:ARG:N	2.48	0.47
1:M:228:ASN:HD21	3:M:501:GTP:HN1	1.63	0.47
1:M:246:GLY:HA3	1:M:356:ASN:HA	1.96	0.47
2:N:282:GLN:O	2:P:60:LYS:HG3	2.15	0.47
2:B:177:VAL:CG2	1:I:329:ASN:HA	2.45	0.47
1:C:246:GLY:HA3	1:C:356:ASN:HA	1.96	0.47
1:G:100:ALA:C	2:H:254:LYS:CG	2.87	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:GLN:HB3	2:H:333:LEU:HD13	1.97	0.47
1:G:228:ASN:HD21	3:G:501:GTP:HN1	1.63	0.47
1:G:246:GLY:HA3	1:G:356:ASN:HA	1.96	0.47
1:O:404:PHE:HA	2:P:260:VAL:O	2.14	0.47
1:Q:181:VAL:N	2:R:352:LYS:CD	2.78	0.47
1:Q:332:ILE:HA	1:Q:335:ILE:HG12	1.97	0.47
2:B:176:LYS:HD3	1:I:333:ALA:CB	2.42	0.46
1:C:325:PRO:HG2	2:N:224:TYR:CE1	2.50	0.46
2:D:401:ARG:NH2	1:G:435:VAL:HG22	2.30	0.46
1:E:53:PHE:HB3	1:E:61:HIS:HB3	1.96	0.46
1:E:332:ILE:HA	1:E:335:ILE:HG12	1.97	0.46
1:G:100:ALA:CB	2:H:254:LYS:HB2	2.44	0.46
1:K:181:VAL:CG2	2:L:352:LYS:HE2	2.44	0.46
1:K:397:LEU:C	2:L:346:TRP:O	2.59	0.46
1:K:404:PHE:H	2:L:261:PRO:C	2.22	0.46
1:O:176:GLN:CD	2:P:333:LEU:HD21	2.38	0.46
1:O:177:VAL:HG21	2:P:329:ASP:CB	2.45	0.46
1:O:210:TYR:OH	2:P:326:LYS:HA	2.03	0.46
1:Q:53:PHE:HB3	1:Q:61:HIS:HB3	1.97	0.46
1:Q:210:TYR:CD2	2:R:326:LYS:CB	2.98	0.46
1:K:53:PHE:HB3	1:K:61:HIS:HB3	1.97	0.46
1:O:177:VAL:HG21	2:P:329:ASP:HB3	1.98	0.46
1:A:100:ALA:HA	2:B:254:LYS:HD2	1.96	0.46
2:B:282:GLN:O	2:F:60:LYS:HG3	2.15	0.46
2:B:407:TRP:CZ2	1:I:260:VAL:CB	2.87	0.46
2:B:407:TRP:CH2	1:I:256:GLN:CG	2.96	0.46
1:G:100:ALA:HB1	2:H:254:LYS:CA	2.44	0.46
1:G:181:VAL:HG23	2:H:352:LYS:CE	2.43	0.46
1:G:210:TYR:CD1	2:H:326:LYS:HD2	2.51	0.46
1:I:179:THR:HG21	2:J:353:THR:HG1	1.76	0.46
1:A:394:LYS:O	2:B:348:PRO:HG3	2.15	0.46
2:B:103:TRP:CD1	2:B:103:TRP:C	2.94	0.46
1:E:394:LYS:C	2:F:348:PRO:HG3	2.40	0.46
2:F:404:PHE:CE2	1:K:258:ASN:O	2.67	0.46
2:J:103:TRP:CD1	2:J:103:TRP:C	2.94	0.46
2:P:103:TRP:CD1	2:P:103:TRP:C	2.94	0.46
1:Q:96:LYS:O	2:R:2:ARG:NE	2.48	0.46
1:A:177:VAL:CG2	2:B:329:ASP:HB3	2.46	0.46
1:C:176:GLN:HG3	2:D:333:LEU:CD2	2.44	0.46
1:C:210:TYR:CE2	2:D:326:LYS:CB	2.98	0.46
1:C:332:ILE:HA	1:C:335:ILE:HG12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:TYR:HB3	2:F:326:LYS:HE2	1.96	0.46
1:G:401:LYS:NZ	2:H:346:TRP:NE1	2.64	0.46
1:I:181:VAL:HG23	2:J:352:LYS:CE	2.43	0.46
1:Q:105:ARG:HH22	2:R:253:ARG:CZ	2.23	0.46
1:A:181:VAL:HB	2:B:352:LYS:CG	2.45	0.46
1:A:348:PRO:CD	2:P:398:MET:SD	3.03	0.46
1:C:402:ARG:HD3	1:C:402:ARG:HA	1.69	0.46
2:F:96:GLN:NE2	1:K:2:ARG:N	2.64	0.46
1:G:332:ILE:HA	1:G:335:ILE:HG12	1.97	0.46
2:H:288:VAL:HB	2:H:327:GLU:HG2	1.96	0.46
1:I:72:PRO:HB2	2:J:48:ARG:HH12	1.80	0.46
1:O:407:TRP:CD1	2:P:257:VAL:HA	2.50	0.46
1:A:210:TYR:HB3	2:B:326:LYS:HE2	1.96	0.46
1:A:404:PHE:CZ	2:B:314:THR:HG22	2.41	0.46
1:C:176:GLN:O	2:D:333:LEU:HD13	2.16	0.46
1:C:394:LYS:C	2:D:348:PRO:HG3	2.40	0.46
1:C:404:PHE:CE2	2:D:258:ASN:C	2.92	0.46
2:D:103:TRP:CD1	2:D:103:TRP:C	2.94	0.46
1:E:96:LYS:O	2:F:2:ARG:NE	2.49	0.46
1:E:210:TYR:CG	2:F:326:LYS:CD	2.99	0.46
1:E:348:PRO:CD	2:R:398:MET:SD	3.04	0.46
1:E:404:PHE:HA	2:F:261:PRO:HA	1.98	0.46
1:K:407:TRP:CZ2	2:L:256:ALA:C	2.94	0.46
1:M:332:ILE:HA	1:M:335:ILE:HG12	1.97	0.46
2:N:103:TRP:CD1	2:N:103:TRP:C	2.94	0.46
1:Q:404:PHE:HA	2:R:261:PRO:HA	1.95	0.46
1:A:100:ALA:HB1	2:B:254:LYS:CA	2.45	0.46
1:A:228:ASN:HD21	3:A:501:GTP:HN1	1.62	0.46
1:A:407:TRP:CD1	2:B:257:VAL:O	2.69	0.46
2:D:288:VAL:HB	2:D:327:GLU:HG2	1.96	0.46
1:E:177:VAL:HB	2:F:329:ASP:HB3	1.97	0.46
1:G:402:ARG:HD3	1:G:402:ARG:HA	1.69	0.46
2:H:103:TRP:CD1	2:H:103:TRP:C	2.94	0.46
1:K:72:PRO:HB2	2:L:48:ARG:NH1	2.31	0.46
1:K:100:ALA:C	2:L:254:LYS:HG3	2.41	0.46
1:M:402:ARG:HD3	1:M:402:ARG:HA	1.69	0.46
2:N:288:VAL:HB	2:N:327:GLU:HG2	1.96	0.46
1:A:246:GLY:HA3	1:A:356:ASN:HA	1.96	0.46
1:A:439:SER:OG	2:P:400:ARG:NH1	2.48	0.46
2:B:60:LYS:HG3	2:D:282:GLN:O	2.16	0.46
1:C:101:ASN:ND2	2:D:258:ASN:OD1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:LEU:HD13	2:F:345:GLU:O	2.16	0.46
2:F:404:PHE:HE2	1:K:258:ASN:CA	2.29	0.46
1:K:228:ASN:HD21	3:K:501:GTP:HN1	1.62	0.46
1:O:228:ASN:HD21	3:O:501:GTP:HN1	1.63	0.46
1:O:246:GLY:HA3	1:O:356:ASN:HA	1.96	0.46
1:A:406:HIS:HE1	2:B:260:VAL:HG12	1.69	0.46
1:I:101:ASN:CB	2:J:254:LYS:HG3	2.46	0.46
1:K:407:TRP:NE1	2:L:260:VAL:O	2.49	0.46
1:M:181:VAL:N	2:N:352:LYS:CD	2.79	0.46
1:M:224:TYR:CE2	2:N:325:MET:CG	2.89	0.46
1:O:181:VAL:HB	2:P:352:LYS:CE	2.45	0.46
1:Q:11:GLN:NE2	2:R:247:GLN:C	2.67	0.46
1:Q:181:VAL:HB	2:R:352:LYS:CE	2.44	0.46
1:A:176:GLN:O	2:B:333:LEU:HD13	2.16	0.45
1:C:101:ASN:CB	2:D:254:LYS:HG3	2.44	0.45
1:E:228:ASN:HD21	3:E:501:GTP:HN1	1.62	0.45
1:M:407:TRP:CH2	2:N:256:ALA:HB1	2.51	0.45
1:Q:228:ASN:HD21	3:Q:501:GTP:HN1	1.63	0.45
1:A:100:ALA:CA	2:B:254:LYS:CB	2.84	0.45
1:A:190:THR:OG1	1:A:191:THR:N	2.49	0.45
1:G:401:LYS:HG2	2:H:346:TRP:CG	2.47	0.45
1:I:228:ASN:HD21	3:I:501:GTP:HN1	1.63	0.45
2:J:142:GLY:HA3	2:J:183:GLU:HG3	1.97	0.45
1:O:210:TYR:OH	2:P:326:LYS:CA	2.44	0.45
1:O:283:HIS:C	1:Q:56:THR:HG22	2.41	0.45
1:Q:397:LEU:HB3	2:R:346:TRP:HA	1.98	0.45
2:B:142:GLY:HA3	2:B:183:GLU:HG3	1.97	0.45
1:C:2:ARG:HD3	2:N:72:PRO:HD2	1.99	0.45
1:C:100:ALA:C	2:D:254:LYS:CD	2.85	0.45
1:C:348:PRO:HG3	2:N:398:MET:CG	2.47	0.45
2:D:210:TYR:HE2	1:G:326:LYS:HB2	1.74	0.45
1:I:101:ASN:ND2	2:J:258:ASN:OD1	2.49	0.45
2:P:142:GLY:HA3	2:P:183:GLU:HG3	1.97	0.45
2:D:28:HIS:NE2	2:D:243:ARG:NH1	2.65	0.45
1:I:246:GLY:HA3	1:I:356:ASN:HA	1.97	0.45
1:I:407:TRP:CG	2:J:257:VAL:HA	2.50	0.45
1:K:179:THR:HA	2:L:353:THR:N	2.27	0.45
2:N:28:HIS:NE2	2:N:243:ARG:NH1	2.65	0.45
1:A:72:PRO:HB2	2:B:48:ARG:HH12	1.80	0.45
1:A:101:ASN:ND2	2:B:258:ASN:OD1	2.49	0.45
2:B:401:ARG:HB2	1:I:346:TRP:CB	2.28	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASN:HB2	2:N:177:VAL:HG21	1.98	0.45
1:E:407:TRP:CD1	2:F:257:VAL:O	2.70	0.45
1:I:332:ILE:HA	1:I:335:ILE:HG12	1.97	0.45
1:M:100:ALA:HA	2:N:254:LYS:CD	2.46	0.45
1:M:403:ALA:HB1	2:N:261:PRO:CB	2.45	0.45
1:O:190:THR:OG1	1:O:191:THR:N	2.49	0.45
1:O:332:ILE:HA	1:O:335:ILE:HG12	1.97	0.45
1:A:100:ALA:C	2:B:254:LYS:CG	2.90	0.45
2:B:56:ALA:HB2	2:D:283:TYR:CA	2.44	0.45
2:B:400:ARG:NH1	1:I:439:SER:OG	2.48	0.45
1:C:210:TYR:CG	2:D:326:LYS:CD	2.99	0.45
2:D:142:GLY:HA3	2:D:183:GLU:HG3	1.97	0.45
2:H:28:HIS:NE2	2:H:243:ARG:NH1	2.65	0.45
1:I:100:ALA:C	2:J:254:LYS:HG3	2.42	0.45
1:I:181:VAL:CG2	2:J:352:LYS:CE	2.94	0.45
1:I:398:MET:CG	2:J:348:PRO:HD2	2.43	0.45
1:M:177:VAL:HG21	2:N:329:ASP:HB3	1.99	0.45
1:M:313:MET:SD	1:M:435:VAL:HG11	2.57	0.45
1:A:332:ILE:HA	1:A:335:ILE:HG12	1.97	0.45
1:C:313:MET:SD	1:C:435:VAL:HG11	2.56	0.45
2:F:398:MET:HG2	1:K:348:PRO:HD2	1.99	0.45
1:G:179:THR:HG21	2:H:353:THR:HG1	1.79	0.45
2:L:142:GLY:HA3	2:L:183:GLU:HG3	1.97	0.45
1:O:181:VAL:CG2	2:P:352:LYS:CE	2.95	0.45
1:Q:179:THR:HA	2:R:352:LYS:HA	1.97	0.45
1:A:218:ASP:OD1	1:A:280:LYS:NZ	2.50	0.45
1:A:260:VAL:HG12	2:P:406:HIS:NE2	2.30	0.45
2:B:28:HIS:NE2	2:B:243:ARG:NH1	2.65	0.45
1:C:181:VAL:HB	2:D:352:LYS:CG	2.47	0.45
1:C:260:VAL:O	2:N:406:HIS:NE2	2.45	0.45
1:E:404:PHE:HE2	2:F:258:ASN:C	2.25	0.45
2:F:142:GLY:HA3	2:F:183:GLU:HG3	1.97	0.45
1:I:218:ASP:OD1	1:I:280:LYS:NZ	2.50	0.45
1:K:398:MET:CG	2:L:348:PRO:HD2	2.43	0.45
1:M:255:PHE:HD1	1:M:255:PHE:HA	1.54	0.45
1:M:401:LYS:CD	2:N:346:TRP:CD2	2.93	0.45
2:N:142:GLY:HA3	2:N:183:GLU:HG3	1.97	0.45
2:R:331:GLN:HA	2:R:331:GLN:OE1	2.17	0.45
1:A:401:LYS:HG2	2:B:346:TRP:CD2	2.52	0.45
1:C:255:PHE:HD1	1:C:255:PHE:HA	1.54	0.45
1:E:348:PRO:CG	2:R:398:MET:CG	2.94	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:LYS:NZ	2:F:346:TRP:NE1	2.65	0.45
1:G:101:ASN:ND2	2:H:258:ASN:OD1	2.50	0.45
1:O:218:ASP:OD1	1:O:280:LYS:NZ	2.50	0.45
2:R:142:GLY:HA3	2:R:183:GLU:HG3	1.97	0.45
1:A:313:MET:SD	1:A:435:VAL:HG11	2.57	0.45
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.80	0.45
1:C:348:PRO:HG3	2:N:398:MET:HG3	1.99	0.45
2:F:401:ARG:NH2	1:K:435:VAL:HG22	2.32	0.45
1:G:190:THR:OG1	1:G:191:THR:N	2.49	0.45
2:H:142:GLY:HA3	2:H:183:GLU:HG3	1.97	0.45
1:K:177:VAL:HG21	2:L:329:ASP:HB3	1.98	0.45
2:N:282:GLN:O	2:P:60:LYS:CG	2.65	0.45
2:P:28:HIS:NE2	2:P:243:ARG:NH1	2.65	0.45
1:Q:210:TYR:CE1	2:R:326:LYS:CA	2.76	0.45
2:F:331:GLN:OE1	2:F:331:GLN:HA	2.17	0.44
1:G:313:MET:SD	1:G:435:VAL:HG11	2.57	0.44
2:L:139:HIS:O	2:L:170:SER:HA	2.16	0.44
2:L:331:GLN:OE1	2:L:331:GLN:HA	2.17	0.44
1:M:101:ASN:CA	2:N:254:LYS:CD	2.95	0.44
2:N:139:HIS:O	2:N:170:SER:HA	2.16	0.44
1:O:210:TYR:CE1	2:P:326:LYS:CA	2.77	0.44
1:O:313:MET:SD	1:O:435:VAL:HG11	2.57	0.44
2:P:248:LEU:HD23	2:P:248:LEU:HA	1.80	0.44
1:Q:313:MET:SD	1:Q:435:VAL:HG11	2.57	0.44
2:D:139:HIS:O	2:D:170:SER:HA	2.16	0.44
1:E:2:ARG:HG2	2:R:96:GLN:NE2	2.26	0.44
1:E:348:PRO:CD	2:R:398:MET:HG3	2.35	0.44
1:K:190:THR:OG1	1:K:191:THR:N	2.49	0.44
1:O:394:LYS:O	2:P:348:PRO:CG	2.64	0.44
1:C:407:TRP:CD1	2:D:257:VAL:O	2.70	0.44
1:E:313:MET:SD	1:E:435:VAL:HG11	2.57	0.44
2:F:139:HIS:O	2:F:170:SER:HA	2.16	0.44
1:I:313:MET:SD	1:I:435:VAL:HG11	2.57	0.44
1:K:179:THR:CB	2:L:353:THR:H	2.31	0.44
1:O:96:LYS:O	2:P:2:ARG:NE	2.50	0.44
2:R:103:TRP:CD1	2:R:103:TRP:C	2.94	0.44
1:A:181:VAL:HG11	2:B:258:ASN:O	2.17	0.44
1:A:397:LEU:HD13	2:B:345:GLU:O	2.18	0.44
1:C:96:LYS:O	2:D:2:ARG:NE	2.51	0.44
1:C:190:THR:OG1	1:C:191:THR:N	2.49	0.44
1:E:179:THR:HG21	2:F:248:LEU:CD1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:THR:OG1	1:E:191:THR:N	2.49	0.44
1:E:210:TYR:CE2	2:F:326:LYS:CB	3.00	0.44
1:E:325:PRO:HG2	2:R:224:TYR:CE1	2.53	0.44
1:G:181:VAL:CG2	2:H:352:LYS:CE	2.94	0.44
1:K:313:MET:SD	1:K:435:VAL:HG11	2.57	0.44
1:A:96:LYS:O	2:B:2:ARG:NE	2.50	0.44
1:A:101:ASN:CB	2:B:254:LYS:CD	2.80	0.44
2:F:103:TRP:CD1	2:F:103:TRP:C	2.94	0.44
1:G:398:MET:CG	2:H:348:PRO:HD2	2.43	0.44
2:H:139:HIS:O	2:H:170:SER:HA	2.17	0.44
1:M:190:THR:OG1	1:M:191:THR:N	2.49	0.44
1:M:218:ASP:OD1	1:M:280:LYS:NZ	2.50	0.44
1:O:397:LEU:HB3	2:P:346:TRP:CA	2.47	0.44
2:P:331:GLN:OE1	2:P:331:GLN:HA	2.17	0.44
2:R:139:HIS:O	2:R:170:SER:HA	2.17	0.44
1:A:179:THR:HA	2:B:353:THR:N	2.26	0.44
1:C:439:SER:OG	2:N:400:ARG:NH1	2.48	0.44
2:F:28:HIS:NE2	2:F:243:ARG:NH1	2.65	0.44
2:L:28:HIS:NE2	2:L:243:ARG:NH1	2.65	0.44
1:M:221:ARG:N	1:M:222:PRO:CD	2.80	0.44
1:M:404:PHE:HA	2:N:260:VAL:O	2.18	0.44
2:N:242:LEU:N	2:N:242:LEU:CD1	2.81	0.44
2:P:74:THR:OG1	2:P:75:MET:N	2.51	0.44
1:Q:398:MET:CG	2:R:348:PRO:HD2	2.45	0.44
2:R:28:HIS:NE2	2:R:243:ARG:NH1	2.65	0.44
2:B:331:GLN:HA	2:B:331:GLN:OE1	2.17	0.44
1:C:221:ARG:N	1:C:222:PRO:CD	2.80	0.44
2:D:242:LEU:N	2:D:242:LEU:CD1	2.81	0.44
1:G:221:ARG:N	1:G:222:PRO:CD	2.80	0.44
1:G:255:PHE:HD1	1:G:255:PHE:HA	1.54	0.44
2:H:331:GLN:OE1	2:H:331:GLN:HA	2.17	0.44
2:J:283:TYR:CB	2:L:62:VAL:CG2	2.92	0.44
1:M:210:TYR:OH	2:N:326:LYS:HA	2.05	0.44
2:B:139:HIS:O	2:B:170:SER:HA	2.17	0.44
1:C:218:ASP:OD1	1:C:280:LYS:NZ	2.50	0.44
1:E:100:ALA:HA	2:F:254:LYS:CD	2.47	0.44
1:E:100:ALA:C	2:F:254:LYS:CG	2.91	0.44
1:E:100:ALA:O	1:E:101:ASN:HB3	2.18	0.44
2:H:74:THR:OG1	2:H:75:MET:N	2.51	0.44
2:H:242:LEU:CD1	2:H:242:LEU:N	2.81	0.44
1:I:30:ILE:HG12	1:I:36:MET:SD	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:397:LEU:HD13	2:J:345:GLU:O	2.17	0.44
2:J:28:HIS:NE2	2:J:243:ARG:NH1	2.64	0.44
2:J:139:HIS:O	2:J:170:SER:HA	2.17	0.44
1:K:210:TYR:CD2	2:L:326:LYS:CB	3.01	0.44
2:L:103:TRP:CD1	2:L:103:TRP:C	2.94	0.44
1:M:181:VAL:HB	2:N:352:LYS:CE	2.46	0.44
2:P:139:HIS:O	2:P:170:SER:HA	2.17	0.44
1:Q:190:THR:OG1	1:Q:191:THR:N	2.49	0.44
1:A:30:ILE:HG12	1:A:36:MET:SD	2.58	0.44
1:A:105:ARG:NE	2:B:253:ARG:HE	2.16	0.44
2:B:74:THR:OG1	2:B:75:MET:N	2.51	0.44
1:C:210:TYR:CE1	2:D:326:LYS:CA	2.93	0.44
1:C:407:TRP:NE1	2:D:260:VAL:O	2.51	0.44
2:D:331:GLN:OE1	2:D:331:GLN:HA	2.17	0.44
1:E:97:GLU:HB3	2:F:253:ARG:HH22	1.82	0.44
1:I:284:GLU:N	1:K:56:THR:HG22	2.33	0.44
1:I:401:LYS:HG2	2:J:346:TRP:CG	2.46	0.44
1:K:221:ARG:N	1:K:222:PRO:CD	2.80	0.44
1:O:30:ILE:HG12	1:O:36:MET:SD	2.58	0.44
1:Q:100:ALA:O	1:Q:101:ASN:HB3	2.18	0.44
1:A:221:ARG:N	1:A:222:PRO:CD	2.80	0.43
2:D:177:VAL:CG2	1:G:329:ASN:HA	2.48	0.43
1:E:221:ARG:N	1:E:222:PRO:CD	2.80	0.43
1:I:190:THR:OG1	1:I:191:THR:N	2.49	0.43
1:I:221:ARG:N	1:I:222:PRO:CD	2.80	0.43
1:I:402:ARG:HD3	1:I:402:ARG:HA	1.69	0.43
2:J:74:THR:OG1	2:J:75:MET:N	2.51	0.43
2:J:248:LEU:HD23	2:J:248:LEU:HA	1.80	0.43
2:J:331:GLN:HA	2:J:331:GLN:OE1	2.17	0.43
1:K:218:ASP:OD1	1:K:280:LYS:NZ	2.50	0.43
2:L:242:LEU:N	2:L:242:LEU:CD1	2.81	0.43
1:M:177:VAL:HG21	2:N:329:ASP:CB	2.48	0.43
1:Q:221:ARG:N	1:Q:222:PRO:CD	2.80	0.43
2:D:74:THR:OG1	2:D:75:MET:N	2.51	0.43
2:D:407:TRP:CZ2	1:G:260:VAL:CB	2.92	0.43
2:D:407:TRP:CE2	1:G:260:VAL:HB	2.51	0.43
1:K:100:ALA:O	1:K:101:ASN:HB3	2.18	0.43
1:K:181:VAL:CB	2:L:352:LYS:HE2	2.45	0.43
1:K:404:PHE:HA	2:L:261:PRO:HA	2.01	0.43
2:N:74:THR:OG1	2:N:75:MET:N	2.51	0.43
2:N:331:GLN:OE1	2:N:331:GLN:HA	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:177:VAL:CG1	2:P:329:ASP:OD1	2.67	0.43
1:O:284:GLU:N	1:Q:56:THR:HG22	2.33	0.43
1:O:401:LYS:CD	2:P:346:TRP:CD2	2.92	0.43
1:Q:105:ARG:HH22	2:R:253:ARG:NH2	2.02	0.43
1:Q:403:ALA:HB1	2:R:261:PRO:CB	2.48	0.43
2:R:242:LEU:N	2:R:242:LEU:CD1	2.81	0.43
1:A:403:ALA:HB1	2:B:261:PRO:HB3	1.99	0.43
1:C:30:ILE:HG12	1:C:36:MET:SD	2.58	0.43
1:E:218:ASP:OD1	1:E:280:LYS:NZ	2.50	0.43
1:E:401:LYS:CE	2:F:346:TRP:NE1	2.81	0.43
2:F:242:LEU:N	2:F:242:LEU:CD1	2.81	0.43
1:G:30:ILE:HG12	1:G:36:MET:SD	2.58	0.43
1:G:404:PHE:H	2:H:261:PRO:C	2.25	0.43
1:I:407:TRP:CD2	2:J:257:VAL:HG22	2.53	0.43
1:O:221:ARG:N	1:O:222:PRO:CD	2.80	0.43
1:A:179:THR:HG22	2:B:353:THR:CB	2.38	0.43
1:A:407:TRP:CZ2	2:B:256:ALA:C	2.96	0.43
1:C:254:GLU:HB2	2:N:100:GLY:HA2	1.99	0.43
1:E:407:TRP:HB3	2:F:257:VAL:HG13	2.01	0.43
1:G:218:ASP:OD1	1:G:280:LYS:NZ	2.50	0.43
1:I:179:THR:CB	2:J:353:THR:H	2.32	0.43
1:O:407:TRP:CE2	2:P:256:ALA:O	2.69	0.43
2:P:61:TYR:CD1	2:P:61:TYR:N	2.86	0.43
1:Q:30:ILE:HG12	1:Q:36:MET:SD	2.58	0.43
1:Q:218:ASP:OD1	1:Q:280:LYS:NZ	2.50	0.43
1:Q:243:ARG:HA	1:Q:243:ARG:HE	1.81	0.43
2:B:398:MET:HG3	1:I:348:PRO:CD	2.38	0.43
2:B:407:TRP:CE2	1:I:256:GLN:O	2.72	0.43
1:C:210:TYR:HB3	2:D:326:LYS:HE2	1.99	0.43
1:E:30:ILE:HG12	1:E:36:MET:SD	2.58	0.43
2:F:183:GLU:N	2:F:184:PRO:CD	2.82	0.43
2:H:61:TYR:CD1	2:H:61:TYR:N	2.86	0.43
1:K:30:ILE:HG12	1:K:36:MET:SD	2.58	0.43
1:M:177:VAL:HG11	2:N:329:ASP:CG	2.42	0.43
1:M:181:VAL:CG2	2:N:352:LYS:HE2	2.46	0.43
1:Q:72:PRO:HB2	2:R:48:ARG:HH12	1.82	0.43
2:R:183:GLU:N	2:R:184:PRO:CD	2.82	0.43
2:D:404:PHE:CE2	1:G:258:ASN:CA	3.01	0.43
2:J:61:TYR:CD1	2:J:61:TYR:N	2.86	0.43
2:L:183:GLU:N	2:L:184:PRO:CD	2.82	0.43
1:M:30:ILE:HG12	1:M:36:MET:SD	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:61:TYR:CD1	2:N:61:TYR:N	2.86	0.43
1:O:404:PHE:HA	2:P:261:PRO:HA	1.98	0.43
1:Q:407:TRP:NE1	2:R:260:VAL:O	2.51	0.43
2:B:61:TYR:CD1	2:B:61:TYR:N	2.86	0.43
2:D:61:TYR:CD1	2:D:61:TYR:N	2.86	0.43
1:E:72:PRO:HB2	2:F:48:ARG:NH1	2.34	0.43
1:E:210:TYR:CE1	2:F:326:LYS:CA	2.93	0.43
1:E:210:TYR:CG	2:F:326:LYS:CB	3.02	0.43
1:E:397:LEU:HB2	2:F:348:PRO:HD3	2.01	0.43
2:F:407:TRP:CH2	1:K:256:GLN:CG	3.00	0.43
1:G:407:TRP:CD2	2:H:257:VAL:HG22	2.54	0.43
1:M:72:PRO:CB	2:N:48:ARG:HH12	2.30	0.43
1:M:73:THR:HG23	2:N:245:PRO:HG3	2.01	0.43
1:M:105:ARG:HH22	2:N:253:ARG:CZ	2.23	0.43
1:O:306:ASP:HA	1:O:307:PRO:HD3	1.91	0.43
1:O:397:LEU:HB3	2:P:346:TRP:HA	2.01	0.43
1:A:346:TRP:CB	2:P:401:ARG:HB3	2.40	0.43
1:I:181:VAL:CB	2:J:352:LYS:HE2	2.47	0.43
1:I:394:LYS:HA	2:J:348:PRO:CG	2.35	0.43
2:J:242:LEU:N	2:J:242:LEU:CD1	2.81	0.43
2:J:332:MET:HA	2:J:332:MET:CE	2.46	0.43
1:O:101:ASN:N	2:P:254:LYS:CE	2.79	0.43
2:P:242:LEU:CD1	2:P:242:LEU:N	2.81	0.43
1:A:100:ALA:CB	2:B:254:LYS:HB2	2.49	0.43
2:B:242:LEU:N	2:B:242:LEU:CD1	2.81	0.43
1:G:179:THR:HA	2:H:353:THR:N	2.25	0.43
1:I:326:LYS:HB3	1:I:326:LYS:HE3	1.84	0.43
2:P:183:GLU:N	2:P:184:PRO:CD	2.82	0.43
1:A:2:ARG:CA	2:P:96:GLN:NE2	2.82	0.43
2:B:183:GLU:N	2:B:184:PRO:CD	2.82	0.43
1:E:100:ALA:C	2:F:254:LYS:HG3	2.44	0.43
1:E:243:ARG:HA	1:E:243:ARG:HE	1.81	0.43
1:G:101:ASN:CB	2:H:254:LYS:HG3	2.49	0.43
2:H:109:THR:OG1	2:H:110:GLU:N	2.51	0.43
2:L:74:THR:OG1	2:L:75:MET:N	2.51	0.43
1:O:224:TYR:CE2	2:P:325:MET:CG	2.84	0.43
1:Q:101:ASN:HD22	2:R:258:ASN:CG	2.26	0.43
1:Q:402:ARG:HD3	1:Q:402:ARG:HA	1.69	0.43
1:A:100:ALA:O	1:A:101:ASN:HB3	2.18	0.42
1:C:100:ALA:CA	2:D:254:LYS:CB	2.86	0.42
1:C:100:ALA:HB1	2:D:254:LYS:CA	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:LYS:HB3	1:C:326:LYS:HE3	1.83	0.42
2:D:109:THR:OG1	2:D:110:GLU:N	2.51	0.42
1:E:256:GLN:O	2:R:407:TRP:NE1	2.52	0.42
2:F:407:TRP:CE2	1:K:260:VAL:HB	2.51	0.42
1:G:100:ALA:O	1:G:101:ASN:HB3	2.18	0.42
1:G:179:THR:HG22	2:H:353:THR:CB	2.35	0.42
1:K:147:SER:HB2	1:K:190:THR:HG21	2.01	0.42
2:L:61:TYR:CD1	2:L:61:TYR:N	2.86	0.42
2:N:109:THR:OG1	2:N:110:GLU:N	2.51	0.42
1:O:100:ALA:O	1:O:101:ASN:HB3	2.18	0.42
1:Q:147:SER:HB2	1:Q:190:THR:HG21	2.01	0.42
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.91	0.42
1:E:147:SER:HB2	1:E:190:THR:HG21	2.01	0.42
1:E:333:ALA:CB	2:R:176:LYS:HD3	2.45	0.42
2:F:74:THR:OG1	2:F:75:MET:N	2.51	0.42
1:G:72:PRO:HB2	2:H:48:ARG:HH12	1.84	0.42
1:I:254:GLU:HA	1:I:257:THR:OG1	2.20	0.42
2:J:109:THR:OG1	2:J:110:GLU:N	2.51	0.42
1:K:177:VAL:CG2	2:L:329:ASP:HB3	2.49	0.42
1:M:326:LYS:HB3	1:M:326:LYS:HE3	1.83	0.42
1:O:254:GLU:HA	1:O:257:THR:OG1	2.20	0.42
1:O:401:LYS:HG2	2:P:346:TRP:HB3	1.98	0.42
1:Q:397:LEU:HB3	2:R:346:TRP:CA	2.48	0.42
2:R:61:TYR:CD1	2:R:61:TYR:N	2.86	0.42
1:A:254:GLU:HA	1:A:257:THR:OG1	2.20	0.42
2:B:109:THR:OG1	2:B:110:GLU:N	2.51	0.42
1:C:100:ALA:O	1:C:101:ASN:HB3	2.18	0.42
1:E:177:VAL:HG21	2:F:329:ASP:CB	2.50	0.42
1:E:402:ARG:HD3	1:E:402:ARG:HA	1.69	0.42
1:G:254:GLU:HA	1:G:257:THR:OG1	2.20	0.42
1:G:326:LYS:HE3	1:G:326:LYS:HB3	1.84	0.42
2:J:183:GLU:N	2:J:184:PRO:CD	2.82	0.42
1:K:254:GLU:HA	1:K:257:THR:OG1	2.20	0.42
1:M:177:VAL:CG2	2:N:329:ASP:HB3	2.49	0.42
1:Q:407:TRP:CH2	2:R:256:ALA:HB1	2.54	0.42
2:R:109:THR:OG1	2:R:110:GLU:N	2.51	0.42
2:B:282:GLN:O	2:F:60:LYS:CG	2.68	0.42
2:B:398:MET:CG	1:I:348:PRO:CG	2.96	0.42
1:C:254:GLU:HA	1:C:257:THR:OG1	2.20	0.42
1:E:346:TRP:HZ3	2:R:403:ALA:CB	1.89	0.42
2:F:61:TYR:CD1	2:F:61:TYR:N	2.86	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:ARG:HH22	2:H:253:ARG:NH2	2.09	0.42
1:K:243:ARG:HA	1:K:243:ARG:HE	1.81	0.42
1:K:402:ARG:HD3	1:K:402:ARG:HA	1.70	0.42
2:L:109:THR:OG1	2:L:110:GLU:N	2.51	0.42
1:M:100:ALA:O	1:M:101:ASN:HB3	2.18	0.42
1:M:254:GLU:HA	1:M:257:THR:OG1	2.20	0.42
1:M:397:LEU:HB3	2:N:346:TRP:HA	2.01	0.42
2:P:156:LYS:HA	2:P:156:LYS:HD2	1.89	0.42
2:B:156:LYS:HA	2:B:156:LYS:HD2	1.89	0.42
1:E:254:GLU:HA	1:E:257:THR:OG1	2.20	0.42
1:E:260:VAL:CB	2:R:407:TRP:HZ2	2.27	0.42
2:F:109:THR:OG1	2:F:110:GLU:N	2.51	0.42
1:G:181:VAL:CB	2:H:352:LYS:HE2	2.47	0.42
1:I:100:ALA:O	1:I:101:ASN:HB3	2.18	0.42
1:K:181:VAL:N	2:L:352:LYS:CD	2.82	0.42
1:K:401:LYS:NZ	2:L:346:TRP:NE1	2.67	0.42
1:M:404:PHE:HA	2:N:261:PRO:HA	1.98	0.42
1:O:11:GLN:NE2	2:P:247:GLN:C	2.69	0.42
2:P:109:THR:OG1	2:P:110:GLU:N	2.51	0.42
1:Q:181:VAL:CG2	2:R:352:LYS:HE2	2.47	0.42
1:Q:254:GLU:HA	1:Q:257:THR:OG1	2.20	0.42
1:A:348:PRO:CG	2:P:398:MET:HG3	2.47	0.42
1:A:407:TRP:CG	2:B:257:VAL:HA	2.54	0.42
2:B:404:PHE:CE2	1:I:258:ASN:CA	3.01	0.42
1:C:100:ALA:C	2:D:254:LYS:CG	2.92	0.42
2:D:400:ARG:NH1	1:G:439:SER:OG	2.48	0.42
2:F:408:TYR:N	2:F:408:TYR:CD1	2.88	0.42
1:G:100:ALA:C	2:H:254:LYS:HG3	2.44	0.42
1:G:407:TRP:NE1	2:H:260:VAL:O	2.53	0.42
1:M:101:ASN:HD22	2:N:258:ASN:CG	2.27	0.42
1:O:177:VAL:CB	2:P:329:ASP:CB	2.96	0.42
2:R:74:THR:OG1	2:R:75:MET:N	2.51	0.42
1:A:333:ALA:CB	2:P:176:LYS:HD3	2.46	0.42
1:A:346:TRP:O	2:P:398:MET:HA	2.20	0.42
1:C:397:LEU:HD13	2:D:345:GLU:O	2.18	0.42
2:D:248:LEU:HD23	2:D:248:LEU:HA	1.80	0.42
1:E:2:ARG:HD3	2:R:72:PRO:HD2	2.02	0.42
2:F:177:VAL:CG2	1:K:329:ASN:HA	2.49	0.42
1:G:177:VAL:CG1	2:H:329:ASP:OD1	2.68	0.42
1:G:397:LEU:HD13	2:H:345:GLU:O	2.20	0.42
2:H:283:TYR:CD2	2:J:62:VAL:CG2	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:VAL:N	2:J:352:LYS:CD	2.82	0.42
1:I:306:ASP:HA	1:I:307:PRO:HD3	1.91	0.42
1:K:177:VAL:HG21	2:L:329:ASP:CB	2.50	0.42
1:K:210:TYR:OH	2:L:326:LYS:CA	2.49	0.42
2:N:183:GLU:N	2:N:184:PRO:CD	2.82	0.42
2:N:248:LEU:HD23	2:N:248:LEU:HA	1.80	0.42
2:R:408:TYR:N	2:R:408:TYR:CD1	2.87	0.42
1:A:147:SER:HB2	1:A:190:THR:HG21	2.01	0.42
2:B:224:TYR:CE1	1:I:325:PRO:HG2	2.55	0.42
2:D:183:GLU:N	2:D:184:PRO:CD	2.82	0.42
2:D:408:TYR:N	2:D:408:TYR:CD1	2.87	0.42
2:F:407:TRP:CZ2	1:K:260:VAL:CB	2.91	0.42
1:G:358:GLU:HA	1:G:359:PRO:HD2	1.90	0.42
1:I:147:SER:HB2	1:I:190:THR:HG21	2.01	0.42
2:J:156:LYS:HA	2:J:156:LYS:HD2	1.89	0.42
1:O:11:GLN:OE1	2:P:247:GLN:C	2.61	0.42
1:O:243:ARG:HA	1:O:243:ARG:HE	1.81	0.42
1:O:404:PHE:CZ	2:P:258:ASN:O	2.65	0.42
1:A:56:THR:HG22	1:C:283:HIS:C	2.45	0.42
1:A:284:GLU:N	1:E:56:THR:CG2	2.83	0.42
2:B:403:ALA:CB	1:I:346:TRP:HZ3	1.93	0.42
2:B:408:TYR:N	2:B:408:TYR:CD1	2.87	0.42
1:C:147:SER:HB2	1:C:190:THR:HG21	2.01	0.42
1:E:177:VAL:CG2	2:F:329:ASP:HB3	2.49	0.42
1:E:401:LYS:CG	2:F:346:TRP:CB	2.70	0.42
1:G:147:SER:HB2	1:G:190:THR:HG21	2.01	0.42
2:L:408:TYR:N	2:L:408:TYR:CD1	2.87	0.42
2:N:408:TYR:N	2:N:408:TYR:CD1	2.88	0.42
1:O:180:ALA:C	2:P:352:LYS:HD2	2.45	0.42
2:P:408:TYR:N	2:P:408:TYR:CD1	2.88	0.42
1:A:249:ASN:HD22	2:P:11:GLN:CD	2.25	0.42
1:A:258:ASN:OD1	2:P:180:THR:HG23	2.19	0.42
1:E:179:THR:CB	2:F:353:THR:H	2.33	0.42
1:E:211:ASP:HA	1:E:214:ARG:HG2	2.02	0.42
1:I:101:ASN:CB	2:J:254:LYS:CD	2.79	0.42
1:I:403:ALA:HB1	2:J:261:PRO:HB3	2.02	0.42
1:K:176:GLN:HG3	2:L:333:LEU:CD2	2.38	0.42
1:M:147:SER:HB2	1:M:190:THR:HG21	2.01	0.42
1:M:179:THR:HA	2:N:352:LYS:HA	2.00	0.42
1:O:147:SER:HB2	1:O:190:THR:HG21	2.01	0.42
1:Q:177:VAL:HG11	2:R:329:ASP:CG	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:211:ASP:HA	1:Q:214:ARG:HG2	2.02	0.42
1:A:56:THR:HG22	1:C:284:GLU:N	2.35	0.41
2:D:332:MET:HA	2:D:332:MET:CE	2.46	0.41
2:H:183:GLU:N	2:H:184:PRO:CD	2.82	0.41
2:H:408:TYR:N	2:H:408:TYR:CD1	2.87	0.41
1:K:147:SER:HB2	1:K:190:THR:CG2	2.50	0.41
1:K:181:VAL:CG2	2:L:352:LYS:CE	2.98	0.41
1:K:358:GLU:HA	1:K:359:PRO:HD2	1.90	0.41
1:Q:147:SER:HB2	1:Q:190:THR:CG2	2.50	0.41
1:A:176:GLN:HG3	2:B:333:LEU:CD2	2.43	0.41
1:A:243:ARG:HA	1:A:243:ARG:HE	1.81	0.41
1:A:248:LEU:HD21	5:P:901:GDP:C8	2.54	0.41
1:A:326:LYS:CG	2:P:210:TYR:CD2	3.03	0.41
1:C:358:GLU:HA	1:C:359:PRO:HD2	1.90	0.41
1:E:100:ALA:HB1	2:F:254:LYS:CA	2.47	0.41
1:G:407:TRP:CG	2:H:257:VAL:HA	2.54	0.41
1:I:401:LYS:NZ	2:J:346:TRP:NE1	2.68	0.41
2:J:408:TYR:N	2:J:408:TYR:CD1	2.88	0.41
1:K:211:ASP:HA	1:K:214:ARG:HG2	2.02	0.41
2:N:332:MET:HA	2:N:332:MET:CE	2.46	0.41
1:O:101:ASN:HD22	2:P:258:ASN:CG	2.26	0.41
1:O:211:ASP:HA	1:O:214:ARG:HG2	2.02	0.41
1:Q:210:TYR:OH	2:R:326:LYS:CA	2.46	0.41
1:A:211:ASP:HA	1:A:214:ARG:HG2	2.02	0.41
1:E:147:SER:HB2	1:E:190:THR:CG2	2.51	0.41
1:E:254:GLU:HB2	2:R:100:GLY:HA2	2.01	0.41
1:E:260:VAL:HG12	2:R:406:HIS:NE2	2.35	0.41
2:H:248:LEU:HD23	2:H:248:LEU:HA	1.80	0.41
1:I:211:ASP:HA	1:I:214:ARG:HG2	2.02	0.41
1:A:147:SER:HB2	1:A:190:THR:CG2	2.50	0.41
1:C:147:SER:HB2	1:C:190:THR:CG2	2.50	0.41
1:C:211:ASP:HA	1:C:214:ARG:HG2	2.02	0.41
1:E:181:VAL:HB	2:F:352:LYS:CG	2.48	0.41
1:G:211:ASP:HA	1:G:214:ARG:HG2	2.02	0.41
1:I:147:SER:HB2	1:I:190:THR:CG2	2.50	0.41
1:I:283:HIS:C	1:K:56:THR:HG22	2.44	0.41
1:K:401:LYS:CE	2:L:346:TRP:NE1	2.83	0.41
1:M:211:ASP:HA	1:M:214:ARG:HG2	2.02	0.41
1:O:147:SER:HB2	1:O:190:THR:CG2	2.50	0.41
1:C:333:ALA:CB	2:N:176:LYS:HD3	2.47	0.41
1:C:348:PRO:CD	2:N:398:MET:SD	3.07	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:LYS:CG	2:D:346:TRP:CB	2.72	0.41
1:E:358:GLU:HA	1:E:359:PRO:HD2	1.90	0.41
1:G:147:SER:HB2	1:G:190:THR:CG2	2.50	0.41
1:G:297:GLU:HA	1:G:298:PRO:HD3	1.89	0.41
1:I:243:ARG:HA	1:I:243:ARG:HE	1.81	0.41
1:O:388:TRP:CE3	1:O:388:TRP:CA	3.04	0.41
1:O:404:PHE:HD2	2:P:257:VAL:O	2.04	0.41
2:P:88:ARG:HA	2:P:89:PRO:HD3	1.86	0.41
1:A:388:TRP:CE3	1:A:388:TRP:CA	3.04	0.41
1:A:397:LEU:C	2:B:346:TRP:O	2.64	0.41
2:B:88:ARG:HA	2:B:89:PRO:HD3	1.86	0.41
1:E:261:PRO:C	2:R:406:HIS:CE1	2.99	0.41
2:F:401:ARG:O	2:F:402:LYS:HB2	2.21	0.41
1:K:407:TRP:CG	2:L:257:VAL:HA	2.55	0.41
1:M:243:ARG:HA	1:M:243:ARG:HE	1.81	0.41
1:O:210:TYR:CE1	2:P:326:LYS:N	2.86	0.41
1:O:255:PHE:HD1	1:O:255:PHE:HA	1.54	0.41
2:R:401:ARG:O	2:R:402:LYS:HB2	2.21	0.41
1:C:388:TRP:CE3	1:C:388:TRP:CA	3.04	0.41
2:D:401:ARG:O	2:D:402:LYS:HB2	2.21	0.41
1:E:249:ASN:H	2:R:11:GLN:CD	2.28	0.41
1:G:388:TRP:CE3	1:G:388:TRP:CA	3.04	0.41
2:L:401:ARG:O	2:L:402:LYS:HB2	2.21	0.41
1:M:147:SER:HB2	1:M:190:THR:CG2	2.50	0.41
1:M:388:TRP:CE3	1:M:388:TRP:CA	3.04	0.41
1:Q:388:TRP:CE3	1:Q:388:TRP:CA	3.04	0.41
1:A:255:PHE:HD1	1:A:255:PHE:HA	1.54	0.41
1:A:260:VAL:CG2	2:P:407:TRP:HZ2	2.34	0.41
1:A:329:ASN:HA	2:P:177:VAL:HG22	2.02	0.41
1:C:297:GLU:HA	1:C:298:PRO:HD3	1.89	0.41
1:E:346:TRP:CA	2:R:401:ARG:HG3	2.45	0.41
1:E:388:TRP:CE3	1:E:388:TRP:CA	3.04	0.41
1:K:100:ALA:CA	2:L:254:LYS:CB	2.82	0.41
1:M:297:GLU:HA	1:M:298:PRO:HD3	1.89	0.41
1:Q:100:ALA:HA	2:R:254:LYS:CG	2.51	0.41
1:A:101:ASN:ND2	2:B:258:ASN:HD21	2.16	0.41
1:A:350:GLY:O	2:P:181:VAL:CA	2.69	0.41
2:B:401:ARG:O	2:B:402:LYS:HB2	2.21	0.41
1:C:133:GLN:NE2	1:C:133:GLN:HA	2.36	0.41
1:C:181:VAL:HG11	2:D:258:ASN:O	2.20	0.41
2:D:398:MET:HG3	1:G:348:PRO:CD	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:400:ARG:NH2	1:G:345:ASP:OD1	2.50	0.41
1:G:133:GLN:NE2	1:G:133:GLN:HA	2.36	0.41
2:H:401:ARG:O	2:H:402:LYS:HB2	2.21	0.41
1:I:388:TRP:CE3	1:I:388:TRP:CA	3.04	0.41
1:K:388:TRP:CE3	1:K:388:TRP:CA	3.04	0.41
1:M:133:GLN:NE2	1:M:133:GLN:HA	2.36	0.41
1:M:358:GLU:HA	1:M:359:PRO:HD2	1.90	0.41
1:M:404:PHE:CZ	2:N:258:ASN:O	2.71	0.41
2:N:401:ARG:O	2:N:402:LYS:HB2	2.21	0.41
1:O:407:TRP:NE1	2:P:257:VAL:HA	2.31	0.41
2:P:401:ARG:O	2:P:402:LYS:HB2	2.21	0.41
1:Q:224:TYR:CE2	2:R:325:MET:CG	2.90	0.41
1:Q:404:PHE:HA	2:R:260:VAL:O	2.21	0.41
1:A:100:ALA:C	2:B:254:LYS:HG3	2.46	0.41
1:C:260:VAL:HG12	2:N:406:HIS:NE2	2.35	0.41
1:C:397:LEU:C	2:D:346:TRP:O	2.64	0.41
2:D:266:HIS:ND1	2:D:266:HIS:C	2.79	0.41
2:D:407:TRP:CE2	1:G:256:GLN:O	2.74	0.41
1:E:100:ALA:CA	2:F:254:LYS:CB	2.85	0.41
1:E:401:LYS:HZ3	2:F:346:TRP:NE1	2.19	0.41
1:G:181:VAL:N	2:H:352:LYS:CD	2.84	0.41
1:I:181:VAL:HG11	2:J:258:ASN:O	2.20	0.41
1:I:398:MET:HG3	2:J:348:PRO:CD	2.47	0.41
2:J:401:ARG:O	2:J:402:LYS:HB2	2.21	0.41
2:L:266:HIS:ND1	2:L:266:HIS:C	2.79	0.41
1:M:397:LEU:HB3	2:N:346:TRP:CA	2.49	0.41
1:O:90:GLU:OE2	1:O:121:ARG:NH1	2.54	0.41
1:A:90:GLU:OE2	1:A:121:ARG:NH1	2.55	0.40
1:C:243:ARG:HA	1:C:243:ARG:HE	1.81	0.40
1:E:133:GLN:NE2	1:E:133:GLN:HA	2.36	0.40
1:E:181:VAL:CG2	2:F:352:LYS:HE2	2.50	0.40
2:F:202:TYR:CD1	2:F:202:TYR:N	2.90	0.40
2:H:266:HIS:ND1	2:H:266:HIS:C	2.80	0.40
1:I:90:GLU:OE2	1:I:121:ARG:NH1	2.54	0.40
1:I:133:GLN:NE2	1:I:133:GLN:HA	2.35	0.40
2:L:202:TYR:CD1	2:L:202:TYR:N	2.90	0.40
1:M:224:TYR:CG	2:N:325:MET:CG	2.87	0.40
2:N:266:HIS:ND1	2:N:266:HIS:C	2.80	0.40
1:O:133:GLN:NE2	1:O:133:GLN:HA	2.36	0.40
1:O:179:THR:HA	2:P:352:LYS:HA	2.03	0.40
1:O:394:LYS:HB3	2:P:348:PRO:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:324:VAL:HA	1:Q:325:PRO:HD3	1.87	0.40
2:R:202:TYR:CD1	2:R:202:TYR:N	2.89	0.40
1:A:133:GLN:NE2	1:A:133:GLN:HA	2.36	0.40
1:A:179:THR:CB	2:B:353:THR:H	2.34	0.40
1:C:407:TRP:CZ2	2:D:256:ALA:C	2.99	0.40
1:E:397:LEU:CB	2:F:346:TRP:O	2.62	0.40
1:E:401:LYS:HG2	2:F:346:TRP:CE3	2.55	0.40
1:E:404:PHE:CE2	2:F:258:ASN:C	2.99	0.40
2:F:266:HIS:ND1	2:F:266:HIS:C	2.80	0.40
2:H:347:ILE:HA	2:H:348:PRO:HD2	1.95	0.40
1:I:255:PHE:HD1	1:I:255:PHE:HA	1.54	0.40
1:K:133:GLN:NE2	1:K:133:GLN:HA	2.36	0.40
2:N:283:TYR:HD2	2:P:62:VAL:CG2	2.11	0.40
1:O:407:TRP:CD2	2:P:257:VAL:HG22	2.56	0.40
1:Q:133:GLN:NE2	1:Q:133:GLN:HA	2.36	0.40
1:Q:358:GLU:HA	1:Q:359:PRO:HD2	1.90	0.40
2:R:266:HIS:ND1	2:R:266:HIS:C	2.80	0.40
1:A:2:ARG:CB	2:P:96:GLN:NE2	2.82	0.40
1:A:104:ALA:HB1	1:A:411:GLU:HB2	2.04	0.40
1:A:394:LYS:CB	2:B:348:PRO:HG3	2.50	0.40
1:A:407:TRP:HB3	2:B:257:VAL:HG13	2.02	0.40
2:B:202:TYR:CD1	2:B:202:TYR:N	2.89	0.40
1:C:104:ALA:HB1	1:C:411:GLU:HB2	2.04	0.40
1:C:105:ARG:NE	2:D:253:ARG:HE	2.19	0.40
2:D:347:ILE:HA	2:D:348:PRO:HD2	1.95	0.40
1:E:101:ASN:CB	2:F:254:LYS:HG3	2.49	0.40
1:E:260:VAL:CG2	2:R:407:TRP:HZ2	2.35	0.40
1:G:179:THR:CB	2:H:353:THR:H	2.34	0.40
1:G:347:CYS:HA	1:G:348:PRO:HD2	1.87	0.40
1:I:63:PRO:O	1:I:91:GLN:NE2	2.50	0.40
1:I:104:ALA:HB1	1:I:411:GLU:HB2	2.04	0.40
1:O:181:VAL:CB	2:P:352:LYS:HE2	2.47	0.40
2:P:202:TYR:CD1	2:P:202:TYR:N	2.89	0.40
2:P:283:TYR:CD2	2:R:62:VAL:CG2	2.84	0.40
1:Q:104:ALA:HB1	1:Q:411:GLU:HB2	2.04	0.40
1:E:179:THR:HA	2:F:352:LYS:HA	2.03	0.40
2:J:88:ARG:HA	2:J:89:PRO:HD3	1.86	0.40
2:J:202:TYR:CD1	2:J:202:TYR:N	2.90	0.40
1:K:90:GLU:OE2	1:K:121:ARG:NH1	2.54	0.40
1:K:398:MET:HG3	2:L:348:PRO:CD	2.46	0.40
1:M:101:ASN:CB	2:N:254:LYS:CG	2.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:104:ALA:HB1	1:M:411:GLU:HB2	2.04	0.40
1:O:104:ALA:HB1	1:O:411:GLU:HB2	2.04	0.40
1:Q:73:THR:HG23	2:R:245:PRO:HG3	2.04	0.40
1:A:63:PRO:O	1:A:91:GLN:NE2	2.50	0.40
1:A:276:ILE:HD13	1:A:276:ILE:HG21	1.91	0.40
1:E:104:ALA:HB1	1:E:411:GLU:HB2	2.04	0.40
1:G:104:ALA:HB1	1:G:411:GLU:HB2	2.04	0.40
1:G:179:THR:CG2	2:H:353:THR:HG1	2.17	0.40
2:J:388:PHE:N	2:J:388:PHE:CD1	2.89	0.40
1:K:104:ALA:HB1	1:K:411:GLU:HB2	2.04	0.40
2:L:283:TYR:CD1	2:L:283:TYR:N	2.90	0.40
1:M:345:ASP:OD2	1:M:439:SER:OG	2.35	0.40
1:O:63:PRO:O	1:O:91:GLN:NE2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/438 (17%)	72 (99%)	1 (1%)	0	100	100
1	C	287/438 (66%)	277 (96%)	8 (3%)	2 (1%)	18	56
1	E	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	G	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	I	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	K	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	M	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	O	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	Q	424/438 (97%)	408 (96%)	14 (3%)	2 (0%)	24	63
2	D	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	18	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	18	56
2	H	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	18	56
2	J	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	18	56
2	L	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	18	56
2	N	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	18	56
2	P	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	18	56
2	R	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	18	56
All	All	6720/7350 (91%)	6475 (96%)	205 (3%)	40 (1%)	23	59

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	98	GLY
2	F	98	GLY
2	H	98	GLY
2	J	98	GLY
2	L	98	GLY
2	N	98	GLY
2	P	98	GLY
2	R	98	GLY
1	C	345	ASP
1	E	345	ASP
1	Q	345	ASP
2	D	350	ASN
2	F	350	ASN
1	G	345	ASP
2	H	350	ASN
1	I	345	ASP
2	J	350	ASN
1	K	345	ASP
2	L	350	ASN
1	M	345	ASP
2	N	350	ASN
1	O	345	ASP
2	P	350	ASN
2	R	350	ASN
1	I	349	THR
1	M	349	THR
1	O	349	THR
1	C	349	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	349	THR
1	G	349	THR
1	K	349	THR
1	Q	349	THR
2	D	221	THR
2	F	221	THR
2	H	221	THR
2	J	221	THR
2	L	221	THR
2	N	221	THR
2	P	221	THR
2	R	221	THR

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/367 (98%)	359 (100%)	1 (0%)	86	85
1	C	360/367 (98%)	359 (100%)	1 (0%)	86	85
1	E	360/367 (98%)	359 (100%)	1 (0%)	86	85
1	G	360/367 (98%)	359 (100%)	1 (0%)	86	85
1	I	360/367 (98%)	359 (100%)	1 (0%)	86	85
1	K	360/367 (98%)	359 (100%)	1 (0%)	86	85
1	M	360/367 (98%)	359 (100%)	1 (0%)	86	85
1	O	360/367 (98%)	359 (100%)	1 (0%)	86	85
1	Q	360/367 (98%)	359 (100%)	1 (0%)	86	85
2	B	367/367 (100%)	367 (100%)	0	100	100
2	D	367/367 (100%)	367 (100%)	0	100	100
2	F	367/367 (100%)	367 (100%)	0	100	100
2	H	367/367 (100%)	367 (100%)	0	100	100
2	J	367/367 (100%)	367 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	367/367 (100%)	367 (100%)	0	100	100
2	N	367/367 (100%)	367 (100%)	0	100	100
2	P	367/367 (100%)	367 (100%)	0	100	100
2	R	367/367 (100%)	367 (100%)	0	100	100
All	All	6543/6606 (99%)	6534 (100%)	9 (0%)	87	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	PHE
1	C	255	PHE
1	E	255	PHE
1	G	255	PHE
1	I	255	PHE
1	K	255	PHE
1	M	255	PHE
1	O	255	PHE
1	Q	255	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	133	GLN
1	A	216	ASN
1	A	301	GLN
1	A	406	HIS
2	B	8	GLN
2	B	96	GLN
2	B	336	GLN
2	B	339	ASN
2	B	349	ASN
2	B	385	GLN
2	B	406	HIS
2	B	436	GLN
1	C	101	ASN
1	C	133	GLN
1	C	301	GLN
1	C	406	HIS
2	D	8	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	96	GLN
2	D	336	GLN
2	D	349	ASN
2	D	385	GLN
2	D	406	HIS
2	D	436	GLN
1	E	101	ASN
1	E	133	GLN
1	E	283	HIS
1	E	301	GLN
1	E	406	HIS
2	F	8	GLN
2	F	96	GLN
2	F	336	GLN
2	F	339	ASN
2	F	349	ASN
2	F	385	GLN
2	F	406	HIS
2	F	436	GLN
1	G	101	ASN
1	G	133	GLN
1	G	301	GLN
1	G	406	HIS
2	H	8	GLN
2	H	11	GLN
2	H	96	GLN
2	H	336	GLN
2	H	349	ASN
2	H	385	GLN
2	H	436	GLN
1	I	101	ASN
1	I	133	GLN
1	I	301	GLN
1	I	406	HIS
2	J	8	GLN
2	J	11	GLN
2	J	96	GLN
2	J	336	GLN
2	J	339	ASN
2	J	349	ASN
2	J	385	GLN
2	J	436	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	101	ASN
1	K	133	GLN
1	K	283	HIS
1	K	301	GLN
1	K	406	HIS
2	L	8	GLN
2	L	11	GLN
2	L	96	GLN
2	L	336	GLN
2	L	349	ASN
2	L	385	GLN
2	L	436	GLN
1	M	101	ASN
1	M	258	ASN
1	M	301	GLN
2	N	8	GLN
2	N	96	GLN
2	N	249	ASN
2	N	336	GLN
2	N	349	ASN
2	N	385	GLN
2	N	406	HIS
2	N	436	GLN
1	O	101	ASN
1	O	216	ASN
1	O	258	ASN
1	O	301	GLN
2	P	8	GLN
2	P	96	GLN
2	P	249	ASN
2	P	336	GLN
2	P	339	ASN
2	P	349	ASN
2	P	385	GLN
2	P	406	HIS
2	P	436	GLN
1	Q	101	ASN
1	Q	258	ASN
1	Q	283	HIS
1	Q	301	GLN
1	Q	342	GLN
2	R	8	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	96	GLN
2	R	336	GLN
2	R	339	ASN
2	R	349	ASN
2	R	385	GLN
2	R	406	HIS
2	R	436	GLN

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](#)

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GDP	F	901	-	29,30,30	2.97	12 (41%)	45,47,47	3.49	17 (37%)
5	GDP	H	901	-	29,30,30	2.95	12 (41%)	45,47,47	3.49	17 (37%)
3	GTP	K	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	M	501	4	33,34,34	1.90	3 (9%)	50,54,54	0.91	3 (6%)
5	GDP	N	901	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	A	501	4	33,34,34	1.90	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	Q	501	4	33,34,34	1.90	3 (9%)	50,54,54	0.92	3 (6%)
5	GDP	B	901	-	29,30,30	2.97	12 (41%)	45,47,47	3.49	17 (37%)
3	GTP	I	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
5	GDP	D	901	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)
5	GDP	J	901	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)
3	GTP	O	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
5	GDP	L	901	-	29,30,30	2.96	11 (37%)	45,47,47	3.49	18 (40%)
5	GDP	P	901	-	29,30,30	2.96	11 (37%)	45,47,47	3.49	18 (40%)
3	GTP	E	501	4	33,34,34	1.90	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	C	501	4	33,34,34	1.91	3 (9%)	50,54,54	0.91	3 (6%)
5	GDP	R	901	-	29,30,30	2.96	11 (37%)	45,47,47	3.49	17 (37%)
3	GTP	G	501	4	33,34,34	1.91	3 (9%)	50,54,54	0.91	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	F	901	-	-	4/16/32/32	0/3/3/3
5	GDP	H	901	-	-	4/16/32/32	0/3/3/3
3	GTP	K	501	4	-	4/22/38/38	0/3/3/3
3	GTP	M	501	4	-	4/22/38/38	0/3/3/3
5	GDP	N	901	-	-	4/16/32/32	0/3/3/3
3	GTP	A	501	4	-	4/22/38/38	0/3/3/3
3	GTP	Q	501	4	-	4/22/38/38	0/3/3/3
5	GDP	B	901	-	-	4/16/32/32	0/3/3/3
3	GTP	I	501	4	-	4/22/38/38	0/3/3/3
5	GDP	D	901	-	-	4/16/32/32	0/3/3/3
5	GDP	J	901	-	-	4/16/32/32	0/3/3/3
3	GTP	O	501	4	-	4/22/38/38	0/3/3/3
5	GDP	L	901	-	-	4/16/32/32	0/3/3/3
5	GDP	P	901	-	-	4/16/32/32	0/3/3/3
3	GTP	E	501	4	-	4/22/38/38	0/3/3/3
3	GTP	C	501	4	-	4/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	R	901	-	-	4/16/32/32	0/3/3/3
3	GTP	G	501	4	-	4/22/38/38	0/3/3/3

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	901	GDP	PA-O3A	7.61	1.67	1.59
5	N	901	GDP	PA-O3A	7.60	1.67	1.59
5	B	901	GDP	PA-O3A	7.55	1.67	1.59
5	L	901	GDP	PA-O3A	7.53	1.67	1.59
5	R	901	GDP	PA-O3A	7.51	1.67	1.59
5	D	901	GDP	PA-O3A	7.51	1.67	1.59
5	P	901	GDP	PA-O3A	7.48	1.67	1.59
5	J	901	GDP	PA-O3A	7.47	1.67	1.59
5	H	901	GDP	PA-O3A	7.47	1.67	1.59
3	C	501	GTP	PA-O3A	-6.15	1.52	1.59
3	Q	501	GTP	PA-O3A	-6.12	1.52	1.59
3	O	501	GTP	PA-O3A	-6.11	1.52	1.59
5	R	901	GDP	O6-C6	6.03	1.35	1.23
3	I	501	GTP	PA-O3A	-6.03	1.53	1.59
3	A	501	GTP	PA-O3A	-6.02	1.53	1.59
3	G	501	GTP	PA-O3A	-6.01	1.53	1.59
5	P	901	GDP	O6-C6	5.99	1.34	1.23
5	B	901	GDP	O6-C6	5.98	1.34	1.23
3	K	501	GTP	PA-O3A	-5.98	1.53	1.59
5	H	901	GDP	O6-C6	5.98	1.34	1.23
5	N	901	GDP	O6-C6	5.97	1.34	1.23
5	D	901	GDP	O6-C6	5.96	1.34	1.23
3	M	501	GTP	PA-O3A	-5.95	1.53	1.59
3	E	501	GTP	PA-O3A	-5.94	1.53	1.59
5	F	901	GDP	O6-C6	5.94	1.34	1.23
3	M	501	GTP	PB-O3A	-5.94	1.53	1.59
5	J	901	GDP	O6-C6	5.93	1.34	1.23
3	G	501	GTP	PB-O3A	-5.92	1.53	1.59
5	B	901	GDP	C8-N9	5.92	1.50	1.37
5	F	901	GDP	C8-N9	5.91	1.50	1.37
5	L	901	GDP	O6-C6	5.90	1.34	1.23
5	P	901	GDP	C8-N9	5.89	1.50	1.37
5	J	901	GDP	C8-N9	5.88	1.50	1.37
5	N	901	GDP	C8-N9	5.85	1.50	1.37
5	H	901	GDP	C8-N9	5.85	1.50	1.37
3	A	501	GTP	PB-O3A	-5.84	1.53	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	GTP	PB-O3A	-5.84	1.53	1.59
5	L	901	GDP	C8-N9	5.84	1.50	1.37
5	D	901	GDP	C8-N9	5.82	1.50	1.37
3	O	501	GTP	PB-O3A	-5.81	1.53	1.59
3	K	501	GTP	PB-O3A	-5.80	1.53	1.59
5	R	901	GDP	C8-N9	5.80	1.50	1.37
3	C	501	GTP	PB-O3A	-5.77	1.53	1.59
3	I	501	GTP	PB-O3A	-5.75	1.53	1.59
3	Q	501	GTP	PB-O3A	-5.75	1.53	1.59
3	G	501	GTP	PB-O3B	5.39	1.65	1.59
3	A	501	GTP	PB-O3B	5.39	1.65	1.59
3	C	501	GTP	PB-O3B	5.37	1.65	1.59
3	E	501	GTP	PB-O3B	5.35	1.65	1.59
3	I	501	GTP	PB-O3B	5.32	1.65	1.59
3	K	501	GTP	PB-O3B	5.32	1.65	1.59
3	M	501	GTP	PB-O3B	5.31	1.65	1.59
3	Q	501	GTP	PB-O3B	5.29	1.65	1.59
3	O	501	GTP	PB-O3B	5.20	1.65	1.59
5	P	901	GDP	C2-N1	4.76	1.49	1.37
5	R	901	GDP	C2-N1	4.75	1.49	1.37
5	L	901	GDP	C2-N1	4.75	1.49	1.37
5	B	901	GDP	C2-N1	4.74	1.49	1.37
5	H	901	GDP	C2-N1	4.74	1.49	1.37
5	D	901	GDP	C2-N1	4.73	1.49	1.37
5	J	901	GDP	C2-N1	4.72	1.49	1.37
5	F	901	GDP	C2-N1	4.71	1.49	1.37
5	N	901	GDP	C2-N1	4.71	1.49	1.37
5	F	901	GDP	PB-O1B	4.35	1.64	1.50
5	J	901	GDP	PB-O1B	4.35	1.64	1.50
5	D	901	GDP	PB-O1B	4.33	1.64	1.50
5	L	901	GDP	PB-O1B	4.32	1.63	1.50
5	B	901	GDP	PB-O1B	4.32	1.63	1.50
5	H	901	GDP	PB-O1B	4.32	1.63	1.50
5	N	901	GDP	PB-O1B	4.31	1.63	1.50
5	P	901	GDP	PB-O1B	4.31	1.63	1.50
5	R	901	GDP	PB-O1B	4.30	1.63	1.50
5	L	901	GDP	PB-O2B	-3.94	1.40	1.54
5	N	901	GDP	PB-O2B	-3.93	1.40	1.54
5	H	901	GDP	PB-O2B	-3.93	1.40	1.54
5	D	901	GDP	PB-O2B	-3.92	1.40	1.54
5	P	901	GDP	PB-O2B	-3.91	1.40	1.54
5	J	901	GDP	PB-O2B	-3.90	1.40	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	901	GDP	PB-O2B	-3.90	1.40	1.54
5	B	901	GDP	PB-O2B	-3.90	1.40	1.54
5	F	901	GDP	PB-O2B	-3.90	1.40	1.54
5	D	901	GDP	O4'-C1'	3.43	1.49	1.42
5	R	901	GDP	O4'-C1'	3.42	1.49	1.42
5	H	901	GDP	O4'-C1'	3.41	1.49	1.42
5	N	901	GDP	O4'-C1'	3.39	1.49	1.42
5	L	901	GDP	O4'-C1'	3.38	1.49	1.42
5	F	901	GDP	O4'-C1'	3.38	1.49	1.42
5	B	901	GDP	O4'-C1'	3.37	1.49	1.42
5	P	901	GDP	O4'-C1'	3.37	1.49	1.42
5	J	901	GDP	O4'-C1'	3.37	1.49	1.42
5	F	901	GDP	C8-N7	3.12	1.41	1.32
5	J	901	GDP	C8-N7	3.09	1.41	1.32
5	L	901	GDP	C8-N7	3.08	1.41	1.32
5	R	901	GDP	C8-N7	3.08	1.41	1.32
5	B	901	GDP	C8-N7	3.07	1.41	1.32
5	P	901	GDP	C8-N7	3.07	1.41	1.32
5	N	901	GDP	C8-N7	3.05	1.41	1.32
5	D	901	GDP	C8-N7	3.05	1.41	1.32
5	H	901	GDP	C8-N7	3.05	1.41	1.32
5	N	901	GDP	C5-N7	-2.98	1.33	1.39
5	D	901	GDP	C5-N7	-2.98	1.33	1.39
5	J	901	GDP	C5-N7	-2.96	1.33	1.39
5	L	901	GDP	C5-N7	-2.95	1.33	1.39
5	P	901	GDP	C5-N7	-2.95	1.33	1.39
5	R	901	GDP	C5-N7	-2.93	1.33	1.39
5	F	901	GDP	C5-N7	-2.92	1.33	1.39
5	H	901	GDP	C5-N7	-2.91	1.33	1.39
5	B	901	GDP	C5-N7	-2.90	1.33	1.39
5	L	901	GDP	C5-C4	2.72	1.46	1.38
5	H	901	GDP	C5-C4	2.72	1.46	1.38
5	J	901	GDP	C5-C4	2.71	1.46	1.38
5	F	901	GDP	C5-C4	2.71	1.46	1.38
5	B	901	GDP	C5-C4	2.70	1.46	1.38
5	D	901	GDP	C5-C4	2.69	1.46	1.38
5	P	901	GDP	C5-C4	2.69	1.46	1.38
5	N	901	GDP	C5-C4	2.69	1.46	1.38
5	R	901	GDP	C5-C4	2.67	1.46	1.38
5	D	901	GDP	C2-N3	-2.44	1.27	1.33
5	R	901	GDP	C2-N3	-2.43	1.27	1.33
5	B	901	GDP	C2-N3	-2.41	1.27	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	901	GDP	C2-N3	-2.41	1.27	1.33
5	F	901	GDP	C2-N3	-2.40	1.27	1.33
5	N	901	GDP	C2-N3	-2.39	1.27	1.33
5	H	901	GDP	C2-N3	-2.38	1.27	1.33
5	J	901	GDP	C2-N3	-2.37	1.27	1.33
5	P	901	GDP	C2-N3	-2.35	1.27	1.33
5	D	901	GDP	O3'-C3'	2.06	1.48	1.43
5	F	901	GDP	O3'-C3'	2.03	1.48	1.43
5	B	901	GDP	O3'-C3'	2.02	1.48	1.43
5	J	901	GDP	O3'-C3'	2.02	1.47	1.43
5	N	901	GDP	O3'-C3'	2.01	1.47	1.43
5	H	901	GDP	O3'-C3'	2.00	1.47	1.43

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	901	GDP	N9-C8-N7	-10.81	93.36	113.40
5	F	901	GDP	N9-C8-N7	-10.80	93.37	113.40
5	L	901	GDP	N9-C8-N7	-10.80	93.38	113.40
5	B	901	GDP	N9-C8-N7	-10.80	93.38	113.40
5	P	901	GDP	N9-C8-N7	-10.78	93.40	113.40
5	R	901	GDP	N9-C8-N7	-10.78	93.41	113.40
5	N	901	GDP	N9-C8-N7	-10.77	93.42	113.40
5	H	901	GDP	N9-C8-N7	-10.76	93.45	113.40
5	D	901	GDP	N9-C8-N7	-10.76	93.45	113.40
5	D	901	GDP	C8-N7-C5	9.30	120.82	104.26
5	N	901	GDP	C8-N7-C5	9.28	120.80	104.26
5	B	901	GDP	C8-N7-C5	9.28	120.79	104.26
5	H	901	GDP	C8-N7-C5	9.28	120.79	104.26
5	P	901	GDP	C8-N7-C5	9.27	120.78	104.26
5	R	901	GDP	C8-N7-C5	9.27	120.78	104.26
5	J	901	GDP	C8-N7-C5	9.26	120.75	104.26
5	L	901	GDP	C8-N7-C5	9.25	120.74	104.26
5	F	901	GDP	C8-N7-C5	9.25	120.73	104.26
5	D	901	GDP	C6-C5-N7	8.68	146.09	130.29
5	H	901	GDP	C6-C5-N7	8.66	146.05	130.29
5	P	901	GDP	C6-C5-N7	8.66	146.04	130.29
5	R	901	GDP	C6-C5-N7	8.65	146.04	130.29
5	B	901	GDP	C6-C5-N7	8.65	146.03	130.29
5	J	901	GDP	C6-C5-N7	8.64	146.02	130.29
5	N	901	GDP	C6-C5-N7	8.64	146.02	130.29
5	L	901	GDP	C6-C5-N7	8.63	145.99	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	901	GDP	C6-C5-N7	8.60	145.94	130.29
5	D	901	GDP	N2-C2-N3	6.29	131.95	119.67
5	R	901	GDP	N2-C2-N3	6.27	131.91	119.67
5	J	901	GDP	C6-C5-C4	-6.26	109.41	118.83
5	P	901	GDP	C6-C5-C4	-6.26	109.41	118.83
5	D	901	GDP	C6-C5-C4	-6.26	109.41	118.83
5	L	901	GDP	C6-C5-C4	-6.26	109.42	118.83
5	B	901	GDP	N2-C2-N3	6.25	131.88	119.67
5	L	901	GDP	N2-C2-N3	6.25	131.87	119.67
5	H	901	GDP	N2-C2-N3	6.25	131.87	119.67
5	N	901	GDP	N2-C2-N3	6.25	131.86	119.67
5	P	901	GDP	N2-C2-N3	6.24	131.84	119.67
5	F	901	GDP	N2-C2-N3	6.23	131.83	119.67
5	J	901	GDP	N2-C2-N3	6.23	131.82	119.67
5	B	901	GDP	C6-C5-C4	-6.23	109.46	118.83
5	N	901	GDP	C6-C5-C4	-6.22	109.47	118.83
5	H	901	GDP	C6-C5-C4	-6.22	109.47	118.83
5	R	901	GDP	C6-C5-C4	-6.22	109.47	118.83
5	F	901	GDP	C6-C5-C4	-6.20	109.50	118.83
5	L	901	GDP	C8-N9-C4	5.93	117.15	106.03
5	J	901	GDP	C8-N9-C4	5.91	117.11	106.03
5	F	901	GDP	C8-N9-C4	5.89	117.06	106.03
5	B	901	GDP	C8-N9-C4	5.88	117.04	106.03
5	R	901	GDP	C8-N9-C4	5.87	117.03	106.03
5	H	901	GDP	C8-N9-C4	5.86	117.01	106.03
5	P	901	GDP	C8-N9-C4	5.85	117.00	106.03
5	N	901	GDP	C8-N9-C4	5.84	116.98	106.03
5	D	901	GDP	C8-N9-C4	5.83	116.96	106.03
5	P	901	GDP	C5-C6-N1	4.53	124.79	113.25
5	R	901	GDP	C5-C6-N1	4.52	124.76	113.25
5	H	901	GDP	C5-C6-N1	4.51	124.74	113.25
5	J	901	GDP	C5-C6-N1	4.51	124.73	113.25
5	B	901	GDP	C5-C6-N1	4.51	124.72	113.25
5	D	901	GDP	C5-C6-N1	4.49	124.68	113.25
5	N	901	GDP	C5-C6-N1	4.49	124.67	113.25
5	F	901	GDP	C5-C6-N1	4.48	124.67	113.25
5	L	901	GDP	C5-C6-N1	4.48	124.66	113.25
5	L	901	GDP	N2-C2-N1	-4.23	107.84	116.76
5	D	901	GDP	N2-C2-N1	-4.22	107.85	116.76
5	H	901	GDP	N2-C2-N1	-4.22	107.86	116.76
5	B	901	GDP	N2-C2-N1	-4.21	107.87	116.76
5	P	901	GDP	N2-C2-N1	-4.21	107.87	116.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	901	GDP	N2-C2-N1	-4.20	107.89	116.76
5	R	901	GDP	N2-C2-N1	-4.19	107.91	116.76
5	J	901	GDP	N2-C2-N1	-4.18	107.93	116.76
5	F	901	GDP	N2-C2-N1	-4.18	107.94	116.76
5	R	901	GDP	C2-N3-C4	4.10	119.36	112.30
5	F	901	GDP	C2-N3-C4	4.09	119.34	112.30
5	D	901	GDP	C2-N3-C4	4.09	119.34	112.30
5	B	901	GDP	C2-N3-C4	4.06	119.30	112.30
5	N	901	GDP	C2-N3-C4	4.06	119.30	112.30
5	J	901	GDP	C2-N3-C4	4.06	119.30	112.30
5	H	901	GDP	C2-N3-C4	4.06	119.29	112.30
5	L	901	GDP	C2-N3-C4	4.03	119.24	112.30
5	R	901	GDP	O6-C6-C5	-4.00	115.96	126.53
5	P	901	GDP	O6-C6-C5	-4.00	115.96	126.53
5	J	901	GDP	O6-C6-C5	-4.00	115.97	126.53
5	H	901	GDP	O6-C6-C5	-4.00	115.97	126.53
5	P	901	GDP	C2-N3-C4	4.00	119.18	112.30
5	B	901	GDP	O6-C6-C5	-3.99	116.00	126.53
5	F	901	GDP	O6-C6-C5	-3.99	116.01	126.53
5	D	901	GDP	O6-C6-C5	-3.98	116.02	126.53
5	N	901	GDP	O6-C6-C5	-3.98	116.02	126.53
5	L	901	GDP	O6-C6-C5	-3.97	116.04	126.53
5	H	901	GDP	C4-C5-N7	-3.90	104.48	110.67
5	R	901	GDP	C4-C5-N7	-3.90	104.49	110.67
5	D	901	GDP	C4-C5-N7	-3.89	104.50	110.67
5	B	901	GDP	C4-C5-N7	-3.89	104.51	110.67
5	N	901	GDP	C4-C5-N7	-3.88	104.52	110.67
5	P	901	GDP	C4-C5-N7	-3.87	104.55	110.67
5	F	901	GDP	C4-C5-N7	-3.86	104.56	110.67
5	J	901	GDP	C4-C5-N7	-3.85	104.57	110.67
5	L	901	GDP	C4-C5-N7	-3.84	104.59	110.67
5	P	901	GDP	C2-N1-C6	-3.77	118.27	125.11
5	H	901	GDP	C2-N1-C6	-3.76	118.30	125.11
5	B	901	GDP	C2-N1-C6	-3.74	118.32	125.11
5	R	901	GDP	C2-N1-C6	-3.74	118.33	125.11
5	L	901	GDP	C2-N1-C6	-3.74	118.33	125.11
5	N	901	GDP	C2-N1-C6	-3.73	118.35	125.11
5	J	901	GDP	C2-N1-C6	-3.72	118.36	125.11
5	F	901	GDP	C2-N1-C6	-3.72	118.36	125.11
5	D	901	GDP	C2-N1-C6	-3.71	118.37	125.11
5	L	901	GDP	C2'-C3'-C4'	3.48	109.34	102.61
5	J	901	GDP	C2'-C3'-C4'	3.48	109.34	102.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	901	GDP	C2'-C3'-C4'	3.47	109.32	102.61
5	F	901	GDP	C2'-C3'-C4'	3.47	109.31	102.61
5	H	901	GDP	C2'-C3'-C4'	3.46	109.29	102.61
5	P	901	GDP	C2'-C3'-C4'	3.46	109.29	102.61
5	N	901	GDP	C2'-C3'-C4'	3.45	109.28	102.61
5	B	901	GDP	C2'-C3'-C4'	3.44	109.25	102.61
5	R	901	GDP	C2'-C3'-C4'	3.43	109.23	102.61
5	J	901	GDP	C1'-N9-C8	-2.69	119.09	126.73
5	L	901	GDP	C1'-N9-C8	-2.68	119.11	126.73
5	P	901	GDP	C1'-N9-C8	-2.68	119.12	126.73
5	F	901	GDP	C1'-N9-C8	-2.67	119.13	126.73
5	B	901	GDP	C1'-N9-C8	-2.67	119.14	126.73
3	G	501	GTP	O2G-PG-O3B	2.66	113.57	104.64
3	Q	501	GTP	O2G-PG-O3B	2.66	113.57	104.64
3	E	501	GTP	O2G-PG-O3B	2.66	113.54	104.64
3	A	501	GTP	O2G-PG-O3B	2.65	113.53	104.64
3	M	501	GTP	O2G-PG-O3B	2.65	113.52	104.64
5	N	901	GDP	C1'-N9-C8	-2.65	119.20	126.73
5	D	901	GDP	C1'-N9-C8	-2.64	119.22	126.73
3	K	501	GTP	O2G-PG-O3B	2.64	113.50	104.64
3	C	501	GTP	O2G-PG-O3B	2.64	113.49	104.64
3	O	501	GTP	O2G-PG-O3B	2.64	113.48	104.64
5	R	901	GDP	C1'-N9-C8	-2.64	119.24	126.73
3	I	501	GTP	O2G-PG-O3B	2.63	113.45	104.64
5	H	901	GDP	C1'-N9-C8	-2.62	119.28	126.73
5	N	901	GDP	O2'-C2'-C3'	2.34	119.30	111.82
5	H	901	GDP	O2'-C2'-C3'	2.33	119.30	111.82
5	F	901	GDP	O2'-C2'-C3'	2.33	119.29	111.82
5	P	901	GDP	O2'-C2'-C3'	2.33	119.27	111.82
5	D	901	GDP	O2'-C2'-C3'	2.32	119.26	111.82
5	J	901	GDP	O2'-C2'-C3'	2.31	119.23	111.82
5	B	901	GDP	O2'-C2'-C3'	2.31	119.23	111.82
5	R	901	GDP	O2'-C2'-C3'	2.31	119.23	111.82
5	L	901	GDP	O2'-C2'-C3'	2.31	119.22	111.82
5	D	901	GDP	O3B-PB-O2B	2.22	116.13	107.80
5	N	901	GDP	O3B-PB-O2B	2.22	116.13	107.80
5	J	901	GDP	O3B-PB-O2B	2.22	116.12	107.80
5	B	901	GDP	O3B-PB-O2B	2.21	116.11	107.80
5	L	901	GDP	O3B-PB-O2B	2.21	116.10	107.80
5	P	901	GDP	O3B-PB-O2B	2.21	116.09	107.80
5	F	901	GDP	O3B-PB-O2B	2.20	116.06	107.80
5	H	901	GDP	O3B-PB-O2B	2.20	116.05	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	901	GDP	O3B-PB-O2B	2.19	116.02	107.80
3	A	501	GTP	O5'-C5'-C4'	2.10	116.14	108.99
3	E	501	GTP	O5'-C5'-C4'	2.10	116.14	108.99
3	Q	501	GTP	O5'-C5'-C4'	2.10	116.14	108.99
3	G	501	GTP	O5'-C5'-C4'	2.10	116.13	108.99
5	H	901	GDP	C4'-O4'-C1'	2.10	114.09	109.47
5	P	901	GDP	C4'-O4'-C1'	2.09	114.09	109.47
5	F	901	GDP	C4'-O4'-C1'	2.09	114.08	109.47
3	I	501	GTP	O5'-C5'-C4'	2.09	116.10	108.99
5	L	901	GDP	C4'-O4'-C1'	2.09	114.07	109.47
3	O	501	GTP	O5'-C5'-C4'	2.08	116.09	108.99
3	M	501	GTP	O5'-C5'-C4'	2.08	116.07	108.99
3	C	501	GTP	O5'-C5'-C4'	2.08	116.07	108.99
3	K	501	GTP	O5'-C5'-C4'	2.07	116.06	108.99
5	B	901	GDP	C4'-O4'-C1'	2.07	114.04	109.47
5	J	901	GDP	C4'-O4'-C1'	2.06	114.02	109.47
5	N	901	GDP	C4'-O4'-C1'	2.06	114.01	109.47
3	I	501	GTP	O3G-PG-O3B	2.05	111.52	104.64
3	C	501	GTP	O3G-PG-O3B	2.05	111.50	104.64
3	M	501	GTP	O3G-PG-O3B	2.04	111.49	104.64
3	E	501	GTP	O3G-PG-O3B	2.04	111.49	104.64
5	R	901	GDP	C4'-O4'-C1'	2.04	113.97	109.47
3	G	501	GTP	O3G-PG-O3B	2.04	111.47	104.64
3	A	501	GTP	O3G-PG-O3B	2.04	111.46	104.64
3	K	501	GTP	O3G-PG-O3B	2.03	111.45	104.64
3	Q	501	GTP	O3G-PG-O3B	2.03	111.44	104.64
5	D	901	GDP	C4'-O4'-C1'	2.02	113.94	109.47
5	L	901	GDP	O4'-C4'-C3'	-2.02	101.14	105.15
3	O	501	GTP	O3G-PG-O3B	2.02	111.41	104.64
5	P	901	GDP	O4'-C4'-C3'	-2.00	101.18	105.15

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	GDP	PA-O3A-PB-O2B
5	B	901	GDP	C5'-O5'-PA-O3A
5	B	901	GDP	C5'-O5'-PA-O2A
5	D	901	GDP	PA-O3A-PB-O2B
5	D	901	GDP	C5'-O5'-PA-O3A
5	D	901	GDP	C5'-O5'-PA-O2A
5	F	901	GDP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	F	901	GDP	C5'-O5'-PA-O3A
5	F	901	GDP	C5'-O5'-PA-O2A
5	H	901	GDP	PA-O3A-PB-O2B
5	H	901	GDP	C5'-O5'-PA-O3A
5	H	901	GDP	C5'-O5'-PA-O2A
5	J	901	GDP	PA-O3A-PB-O2B
5	J	901	GDP	C5'-O5'-PA-O3A
5	J	901	GDP	C5'-O5'-PA-O2A
5	L	901	GDP	PA-O3A-PB-O2B
5	L	901	GDP	C5'-O5'-PA-O3A
5	L	901	GDP	C5'-O5'-PA-O2A
5	N	901	GDP	PA-O3A-PB-O2B
5	N	901	GDP	C5'-O5'-PA-O3A
5	N	901	GDP	C5'-O5'-PA-O2A
5	P	901	GDP	PA-O3A-PB-O2B
5	P	901	GDP	C5'-O5'-PA-O3A
5	P	901	GDP	C5'-O5'-PA-O2A
5	R	901	GDP	PA-O3A-PB-O2B
5	R	901	GDP	C5'-O5'-PA-O3A
5	R	901	GDP	C5'-O5'-PA-O2A
3	A	501	GTP	C3'-C4'-C5'-O5'
3	C	501	GTP	C3'-C4'-C5'-O5'
3	E	501	GTP	C3'-C4'-C5'-O5'
3	G	501	GTP	C3'-C4'-C5'-O5'
3	I	501	GTP	C3'-C4'-C5'-O5'
3	M	501	GTP	C3'-C4'-C5'-O5'
3	O	501	GTP	C3'-C4'-C5'-O5'
3	Q	501	GTP	C3'-C4'-C5'-O5'
3	K	501	GTP	C3'-C4'-C5'-O5'
3	C	501	GTP	O4'-C4'-C5'-O5'
3	E	501	GTP	O4'-C4'-C5'-O5'
3	G	501	GTP	O4'-C4'-C5'-O5'
3	I	501	GTP	O4'-C4'-C5'-O5'
3	K	501	GTP	O4'-C4'-C5'-O5'
3	M	501	GTP	O4'-C4'-C5'-O5'
3	O	501	GTP	O4'-C4'-C5'-O5'
3	Q	501	GTP	O4'-C4'-C5'-O5'
3	A	501	GTP	C5'-O5'-PA-O1A
3	C	501	GTP	C5'-O5'-PA-O1A
3	E	501	GTP	C5'-O5'-PA-O1A
3	G	501	GTP	C5'-O5'-PA-O1A
3	I	501	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	501	GTP	C5'-O5'-PA-O1A
3	M	501	GTP	C5'-O5'-PA-O1A
3	O	501	GTP	C5'-O5'-PA-O1A
3	Q	501	GTP	C5'-O5'-PA-O1A
3	A	501	GTP	O4'-C4'-C5'-O5'
5	B	901	GDP	PA-O3A-PB-O3B
5	D	901	GDP	PA-O3A-PB-O3B
5	F	901	GDP	PA-O3A-PB-O3B
5	H	901	GDP	PA-O3A-PB-O3B
5	J	901	GDP	PA-O3A-PB-O3B
5	L	901	GDP	PA-O3A-PB-O3B
5	N	901	GDP	PA-O3A-PB-O3B
5	P	901	GDP	PA-O3A-PB-O3B
5	R	901	GDP	PA-O3A-PB-O3B
3	A	501	GTP	PG-O3B-PB-O2B
3	C	501	GTP	PG-O3B-PB-O2B
3	E	501	GTP	PG-O3B-PB-O2B
3	G	501	GTP	PG-O3B-PB-O2B
3	I	501	GTP	PG-O3B-PB-O2B
3	K	501	GTP	PG-O3B-PB-O2B
3	M	501	GTP	PG-O3B-PB-O2B
3	O	501	GTP	PG-O3B-PB-O2B
3	Q	501	GTP	PG-O3B-PB-O2B

There are no ring outliers.

18 monomers are involved in 46 short contacts:

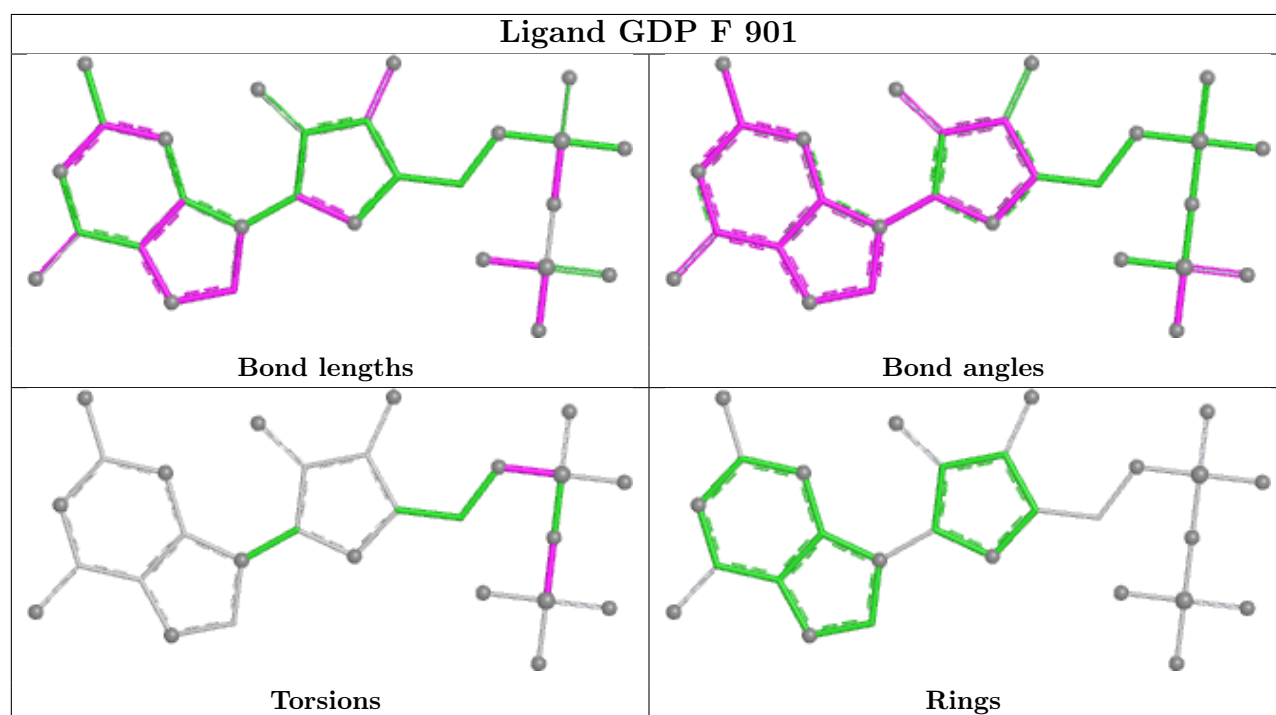
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	901	GDP	2	0
5	H	901	GDP	2	0
3	K	501	GTP	3	0
3	M	501	GTP	3	0
5	N	901	GDP	2	0
3	A	501	GTP	3	0
3	Q	501	GTP	3	0
5	B	901	GDP	2	0
3	I	501	GTP	3	0
5	D	901	GDP	2	0
5	J	901	GDP	2	0
3	O	501	GTP	3	0
5	L	901	GDP	2	0
5	P	901	GDP	3	0

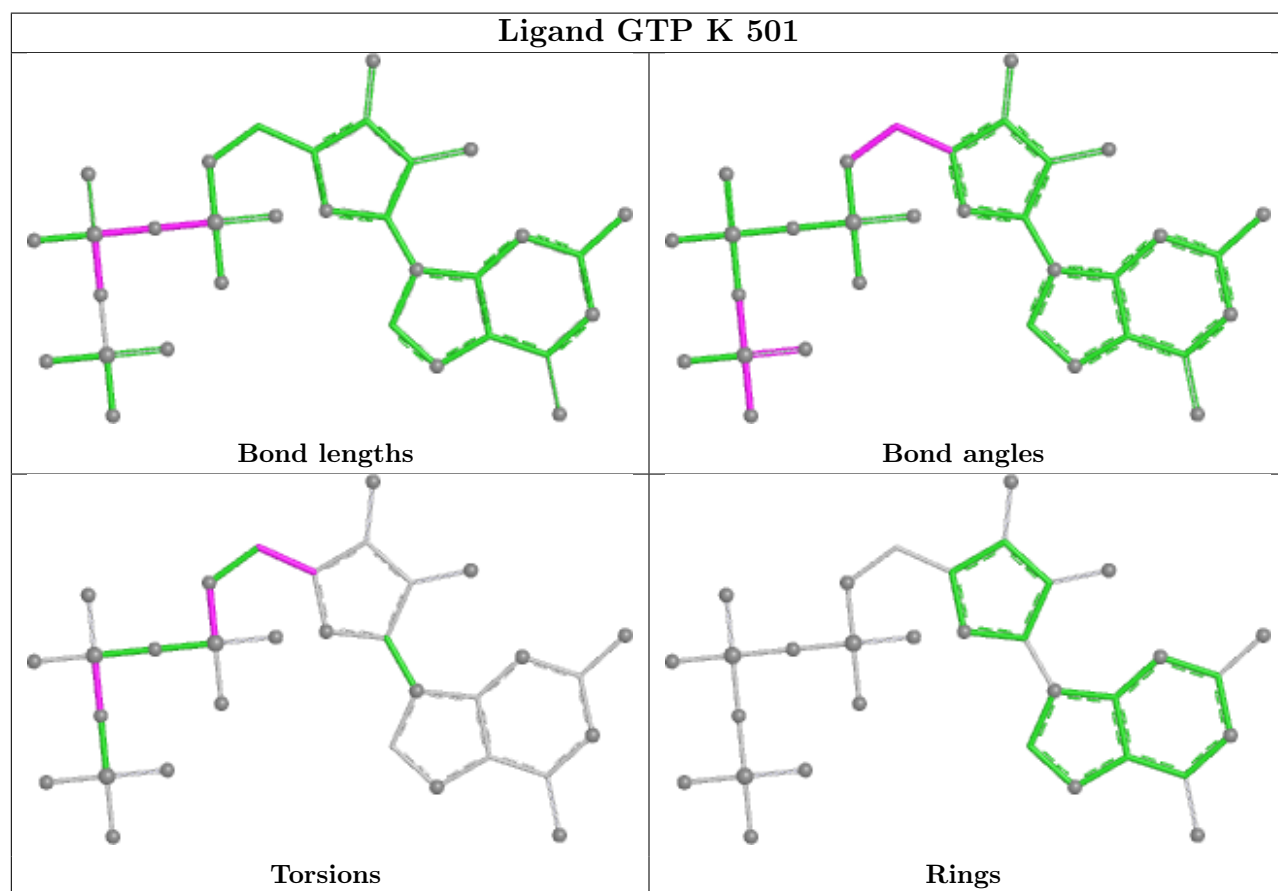
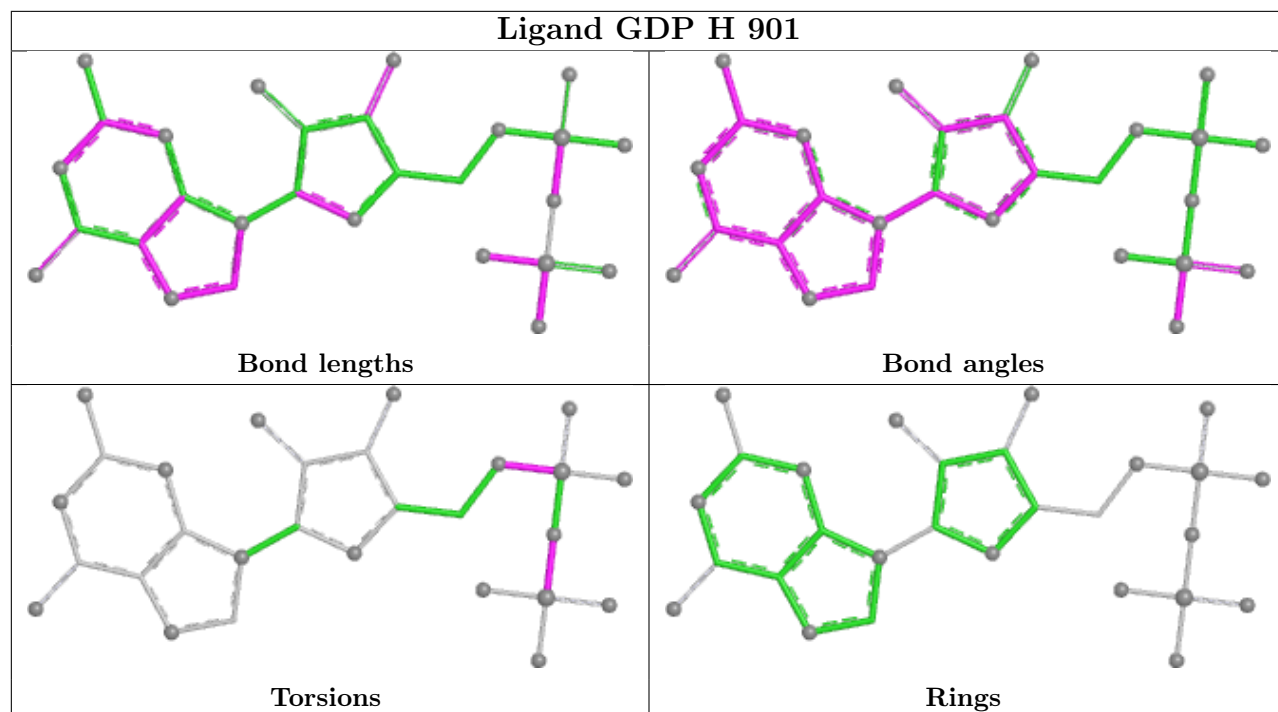
Continued on next page...

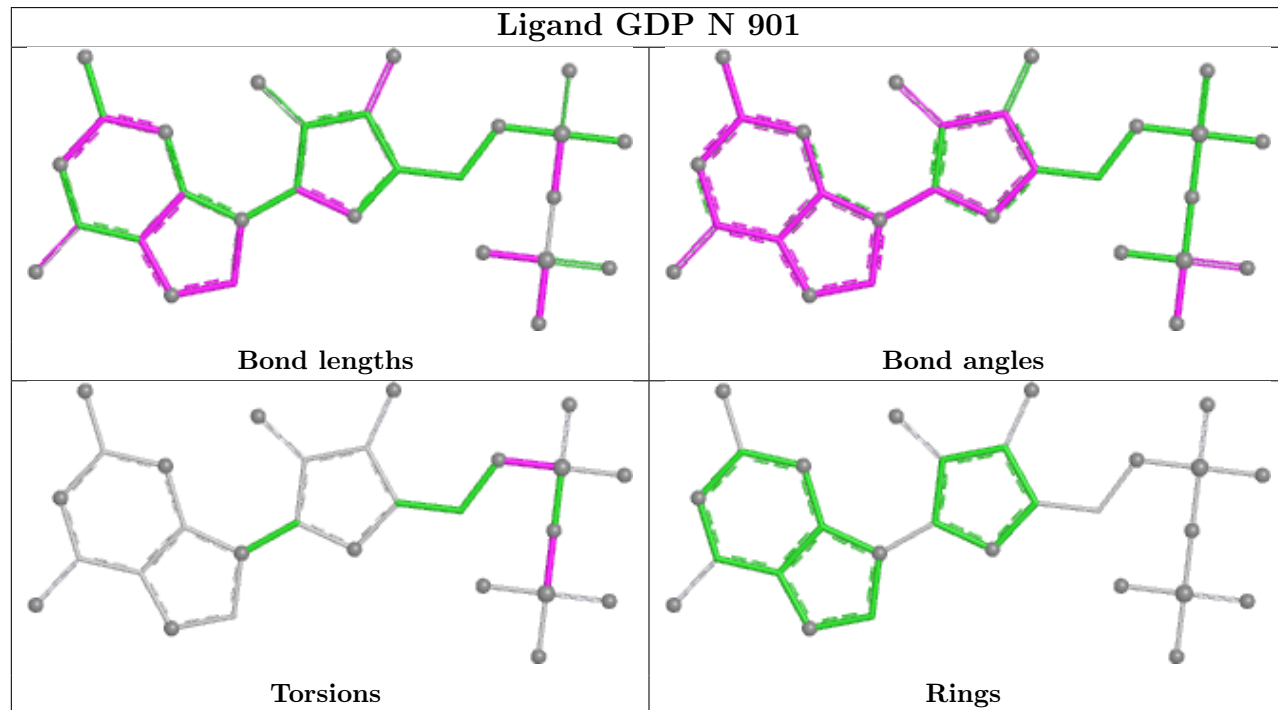
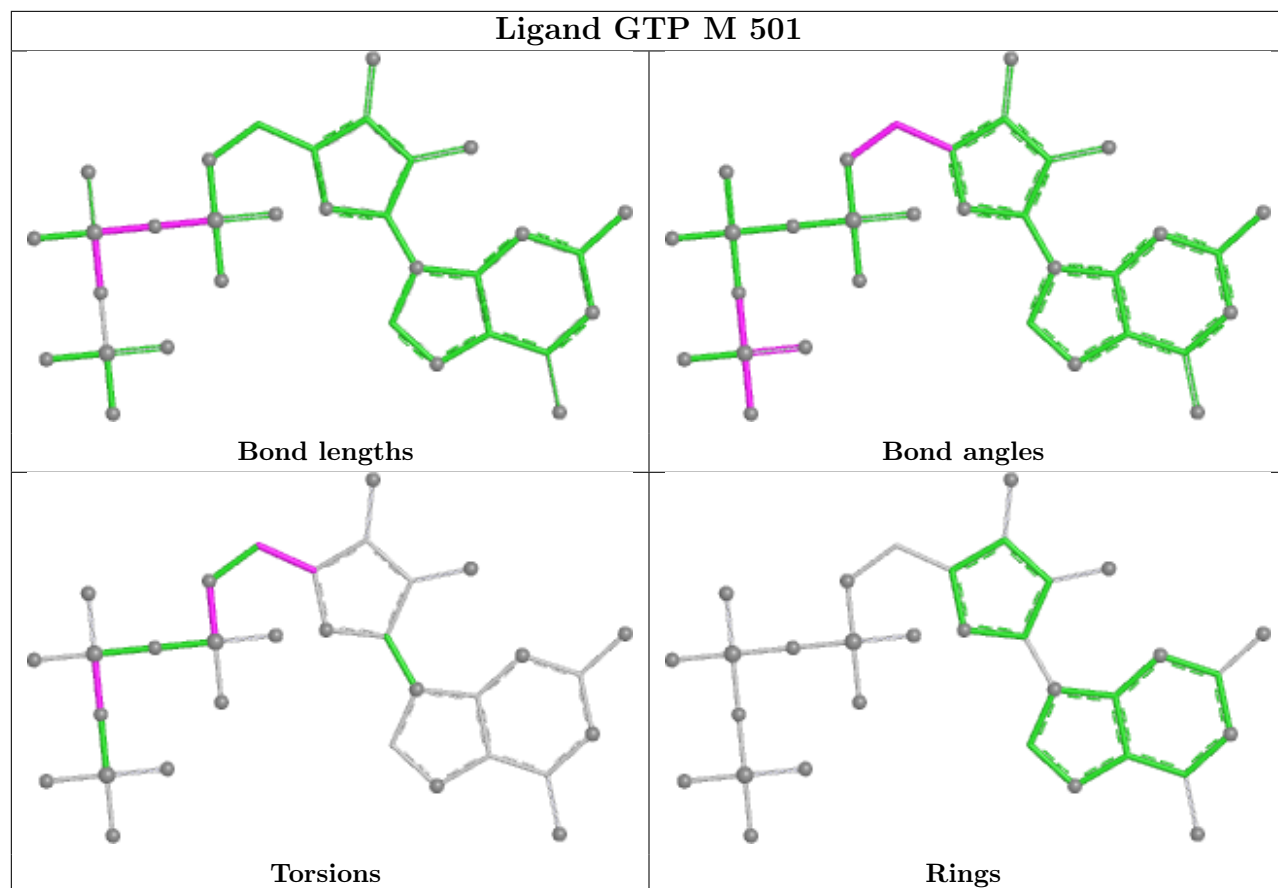
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	GTP	3	0
3	C	501	GTP	3	0
5	R	901	GDP	2	0
3	G	501	GTP	3	0

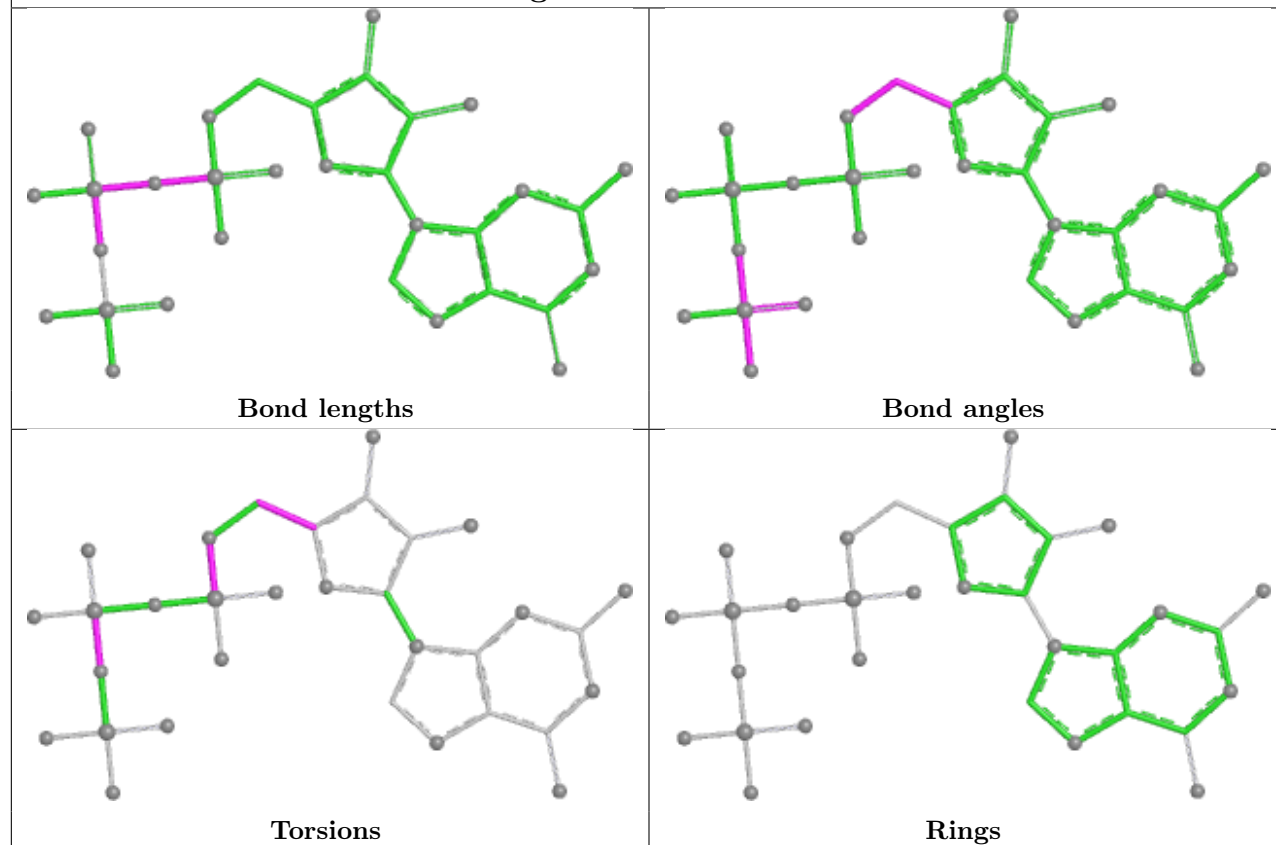
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



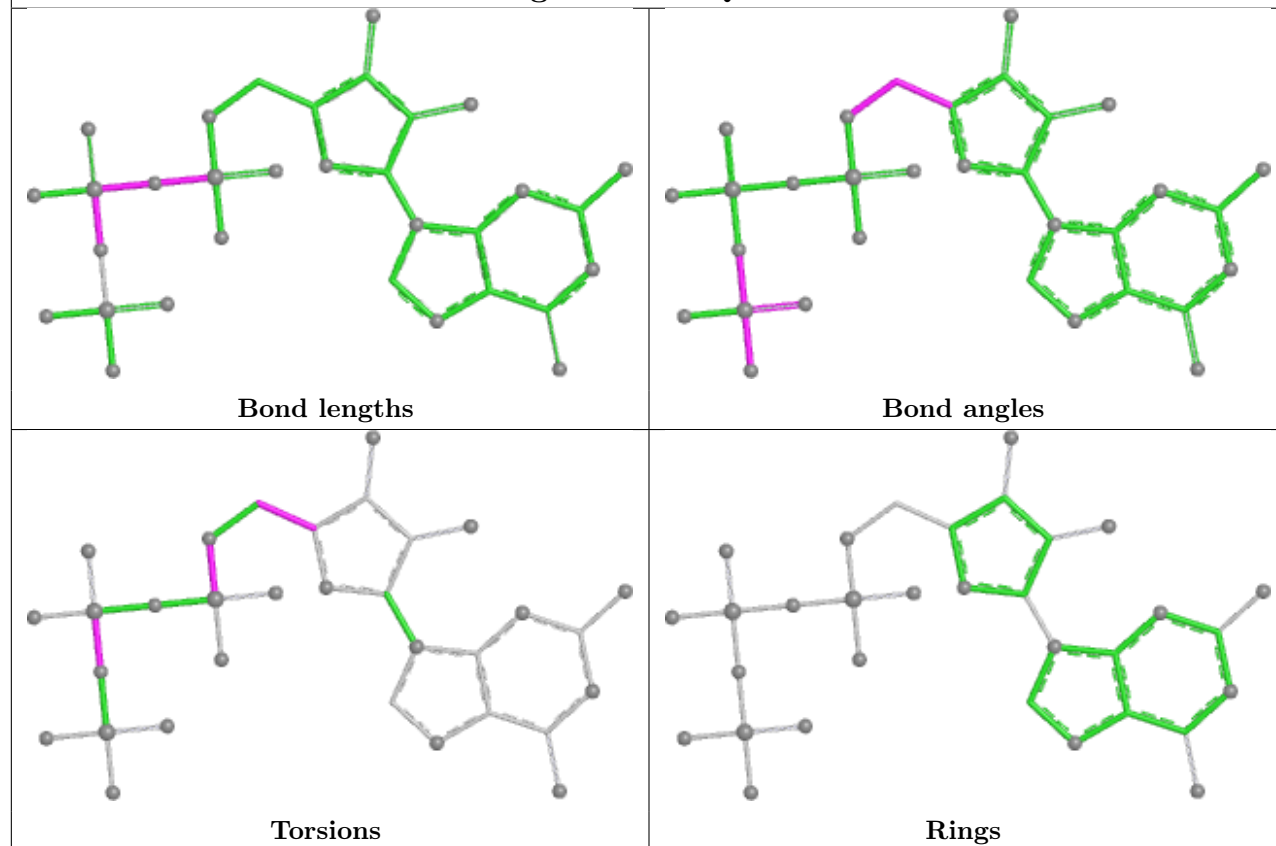


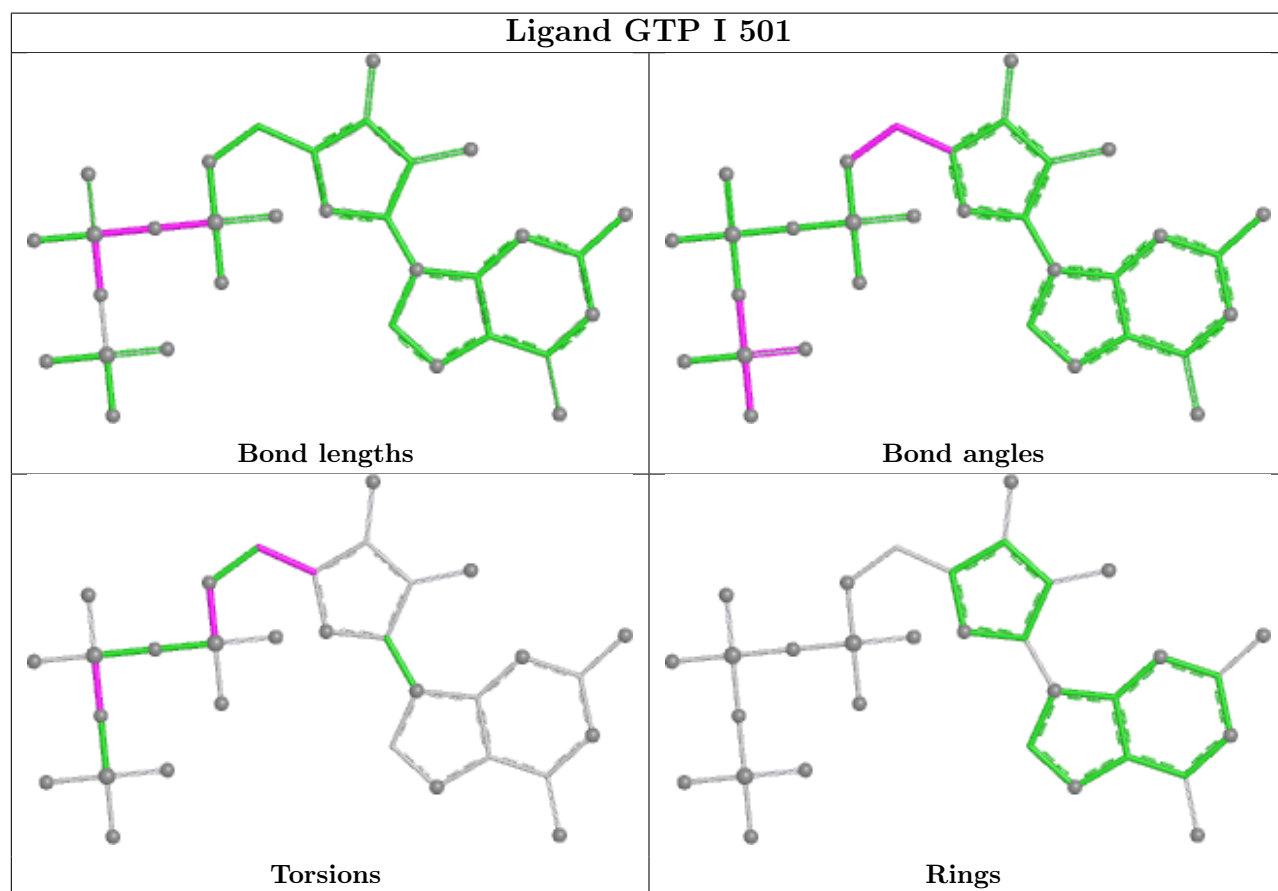
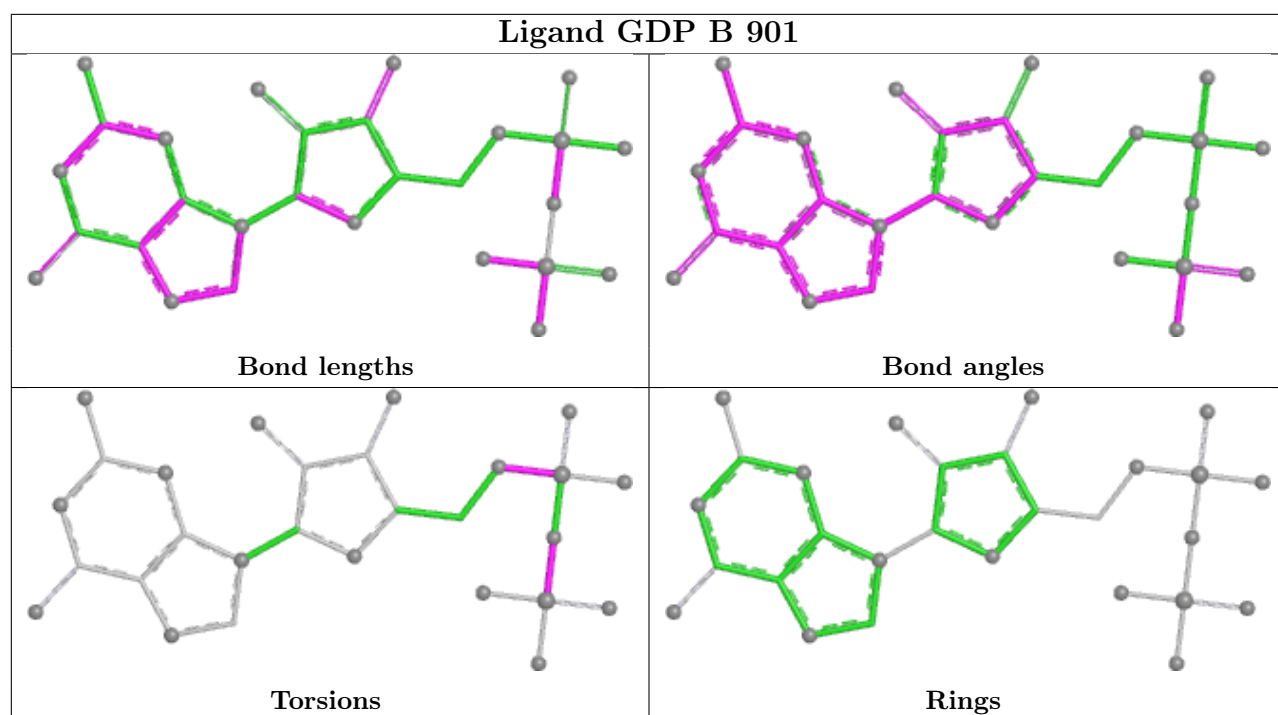


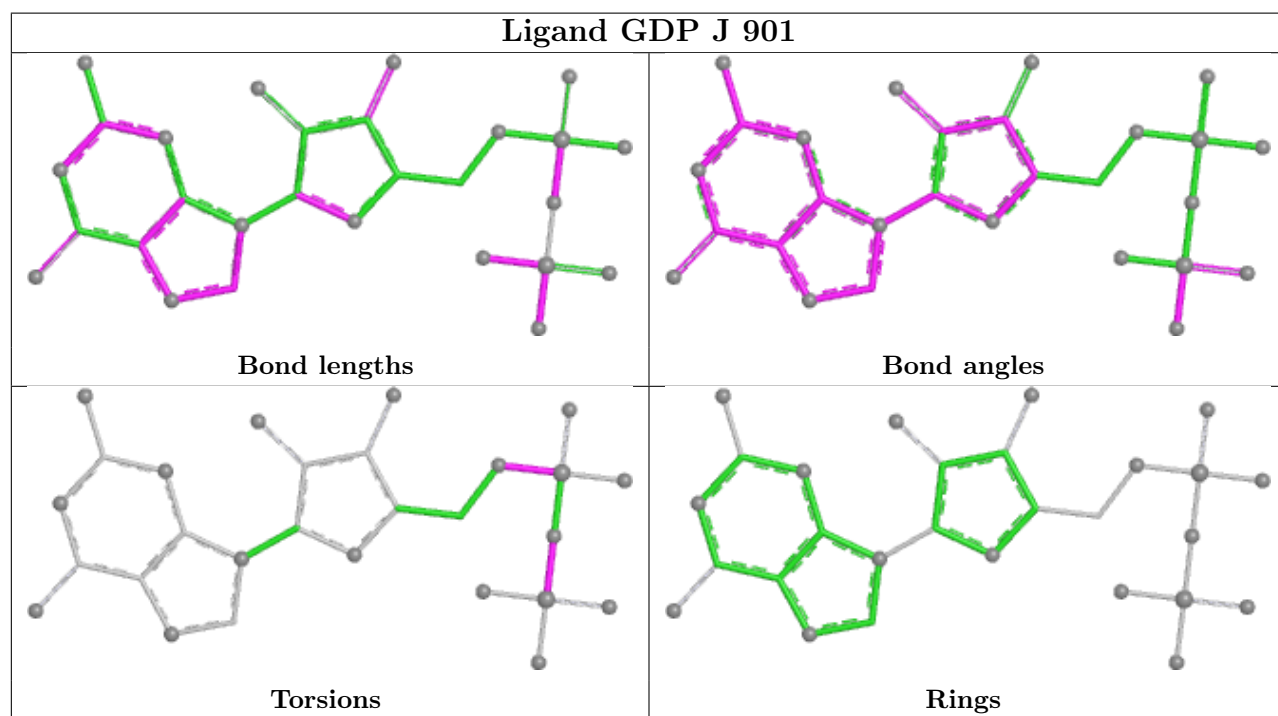
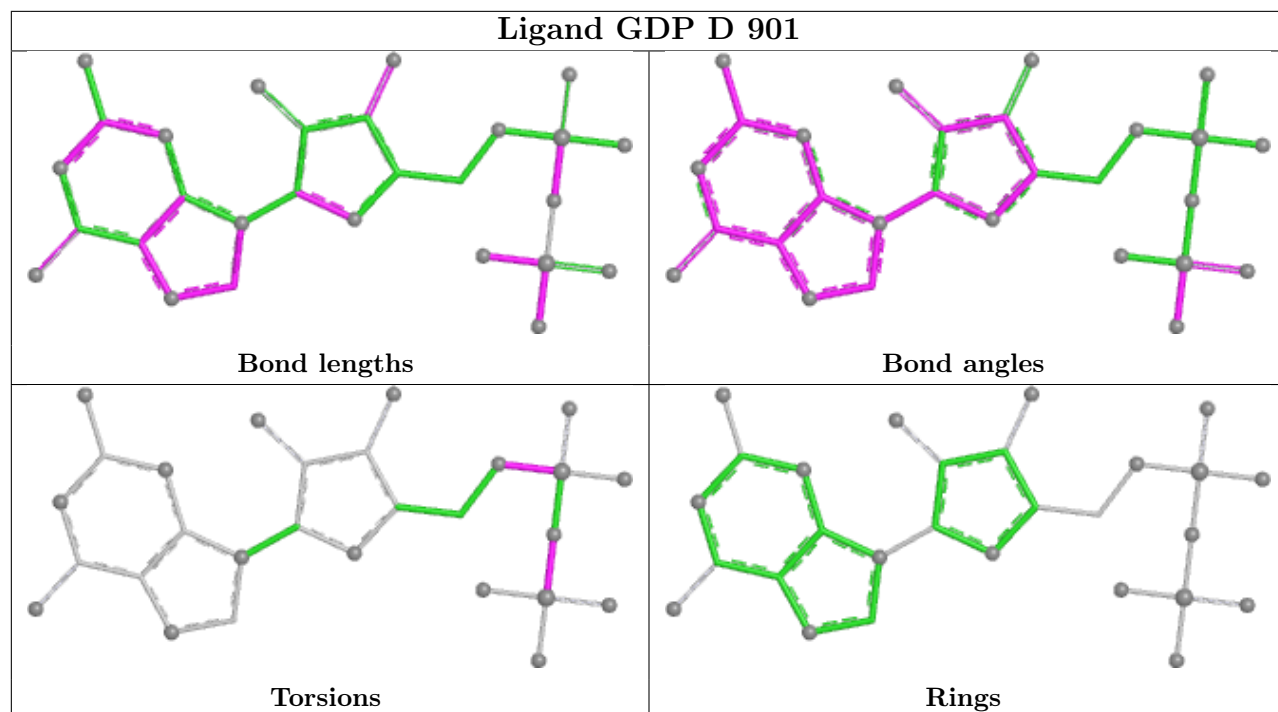
Ligand GTP A 501

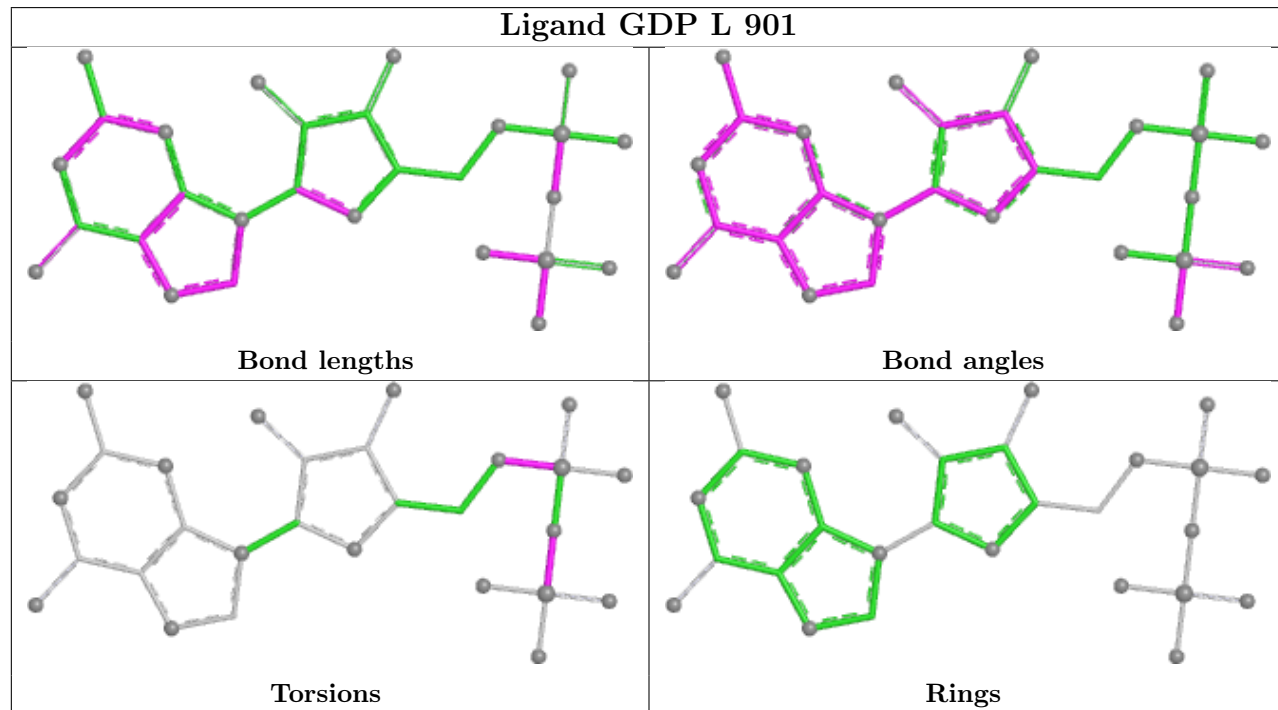
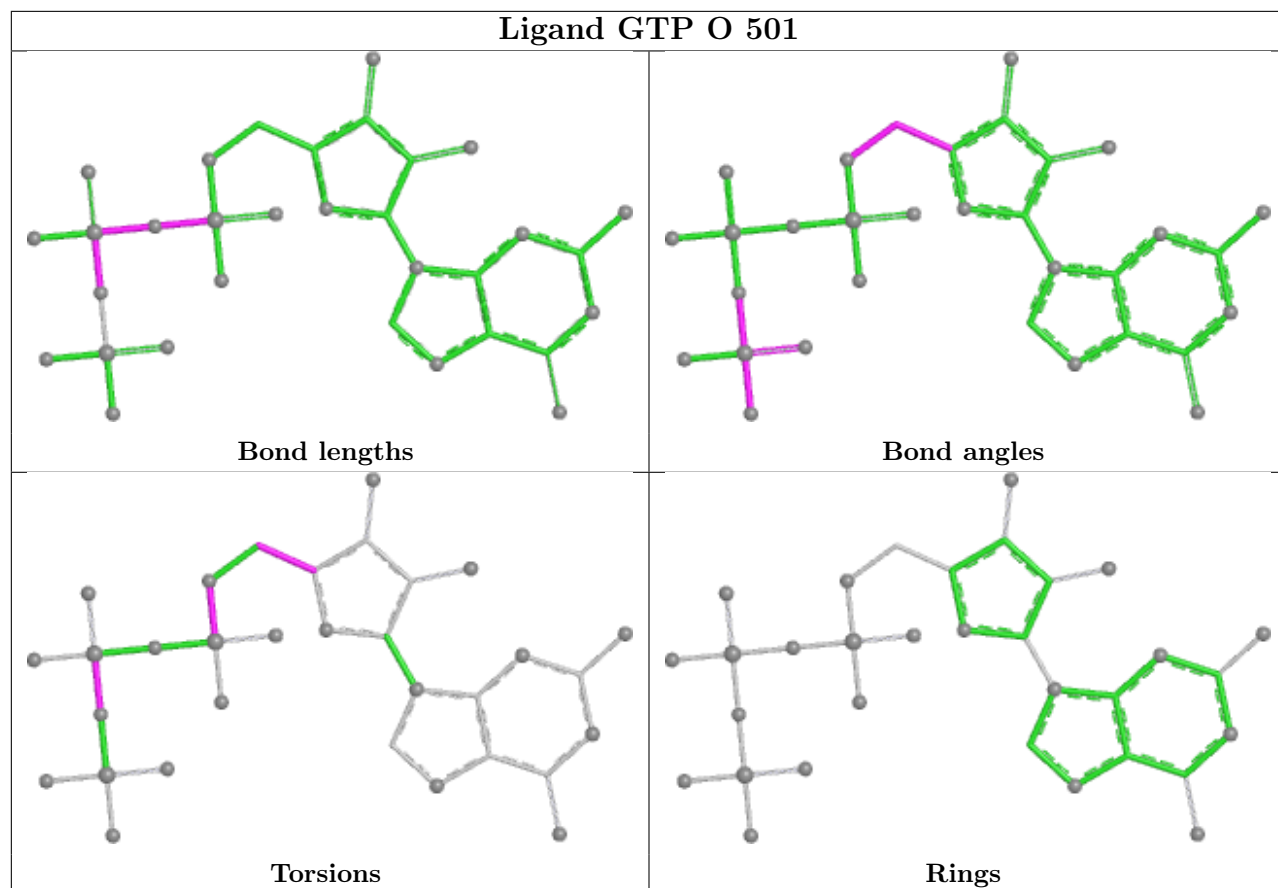


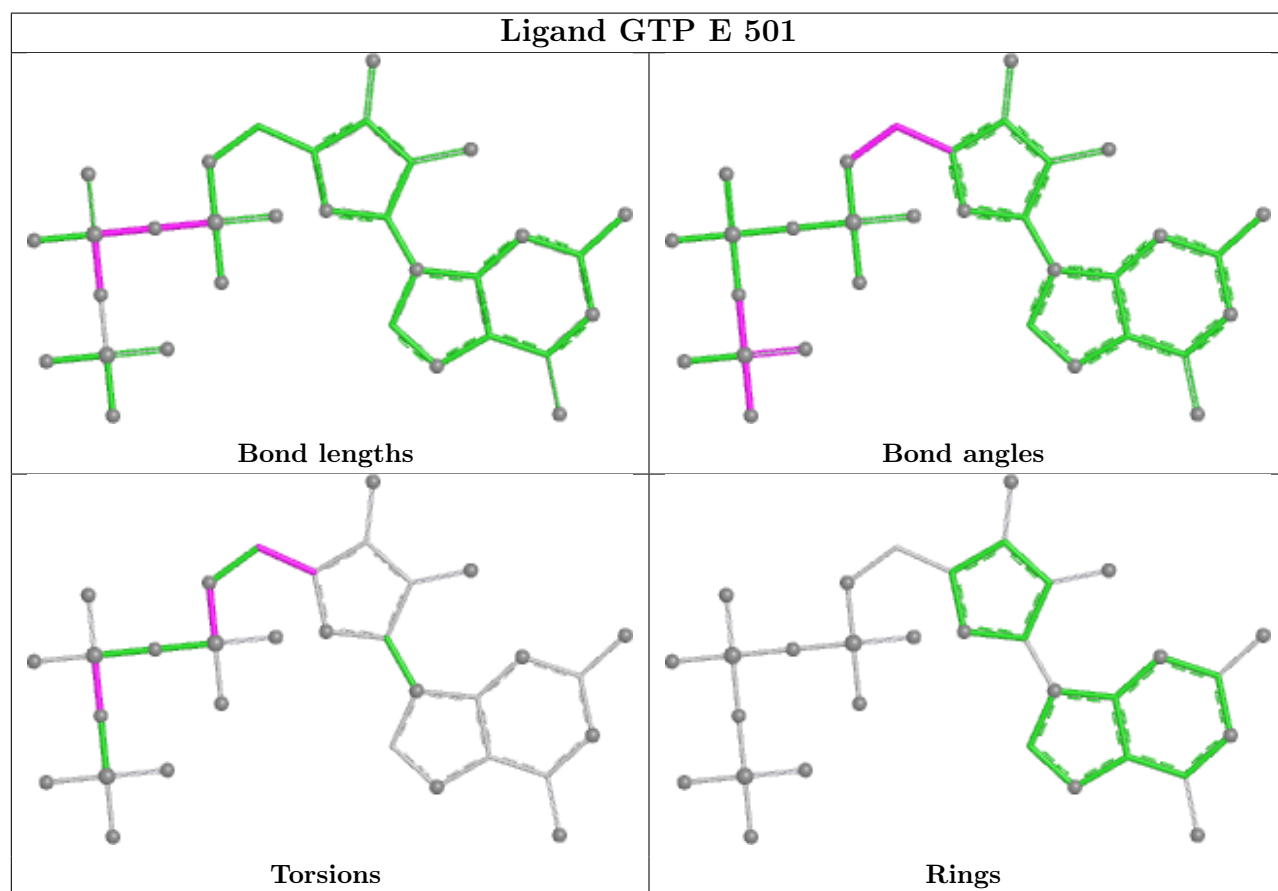
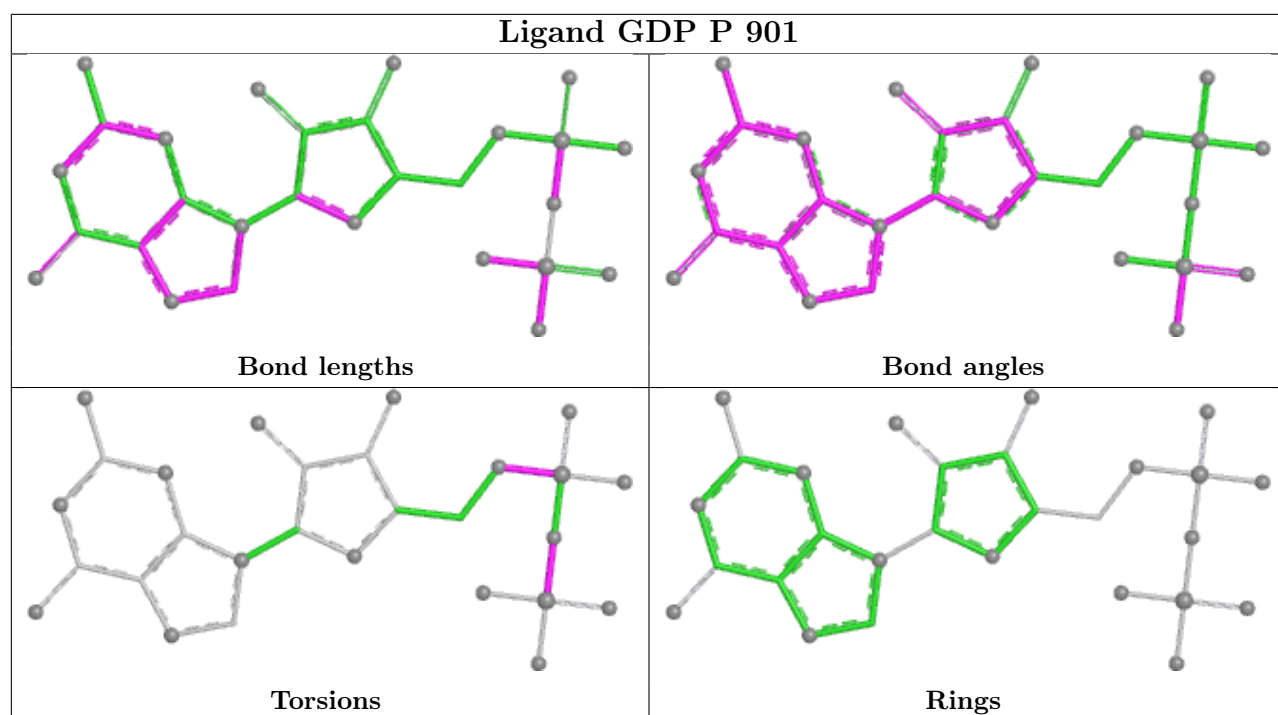
Ligand GTP Q 501

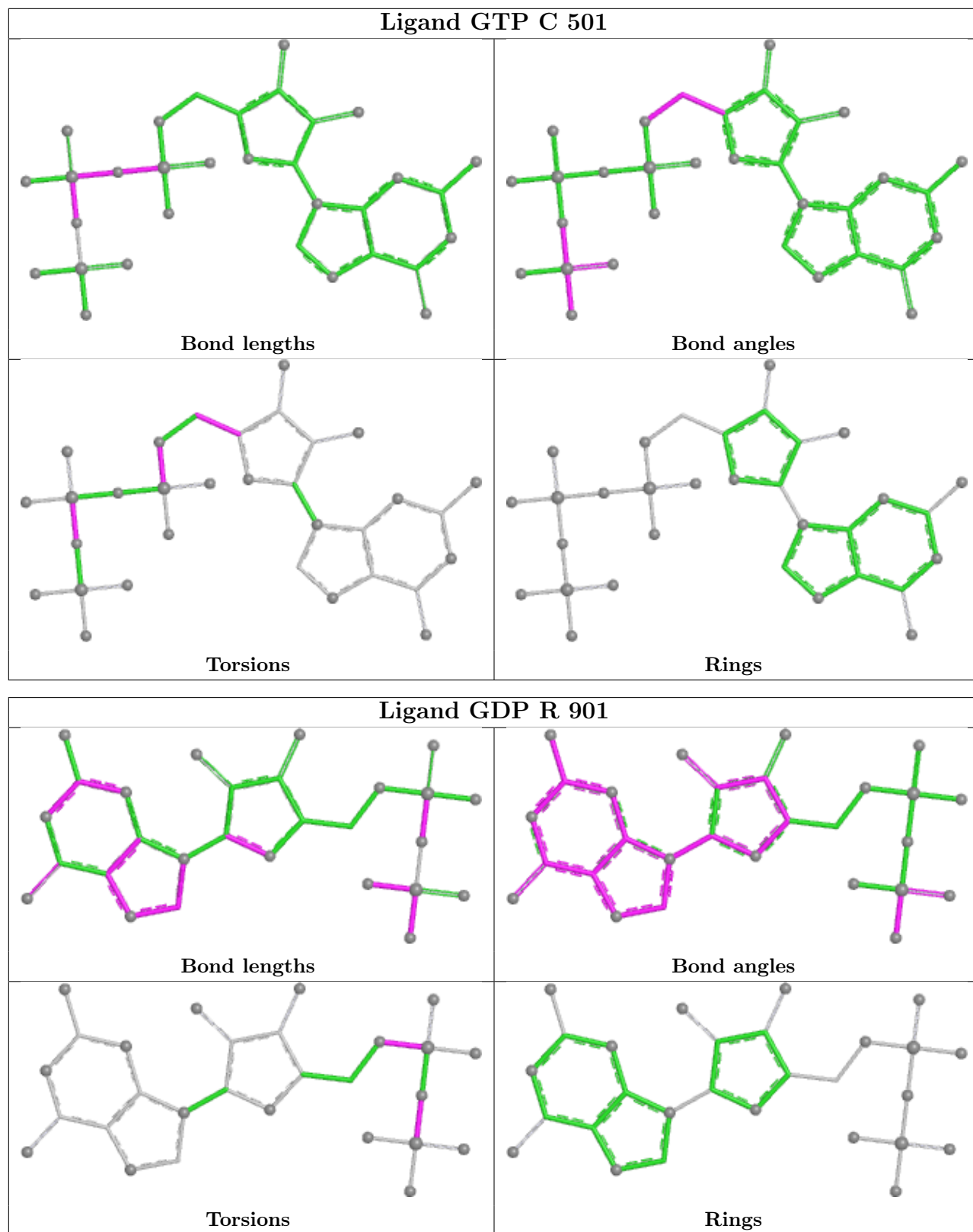


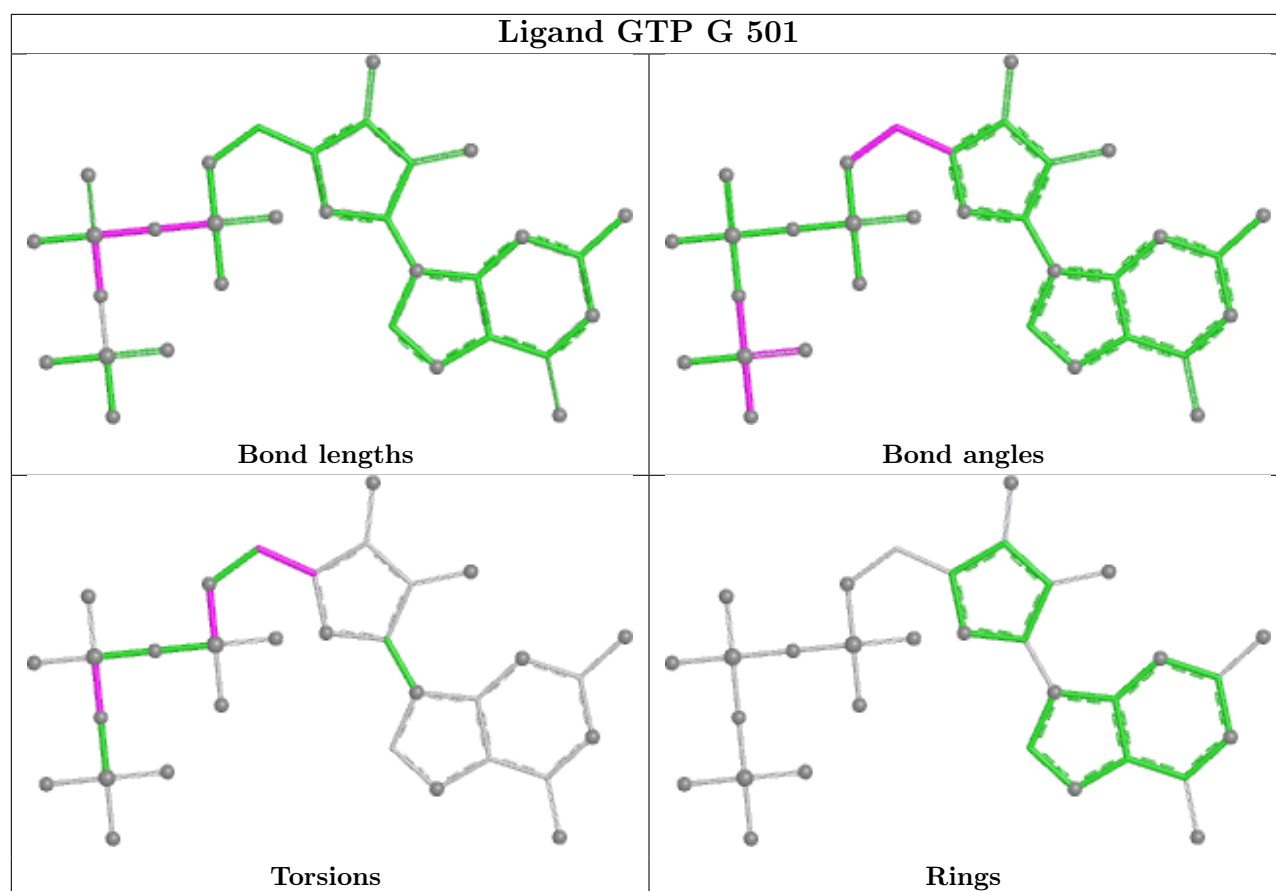












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

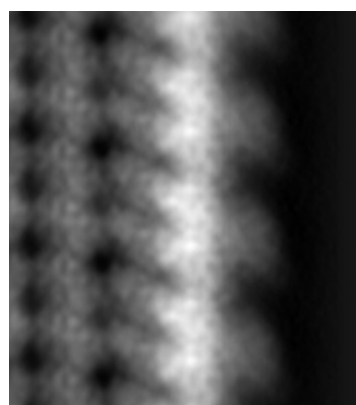
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6782. These allow visual inspection of the internal detail of the map and identification of artifacts.

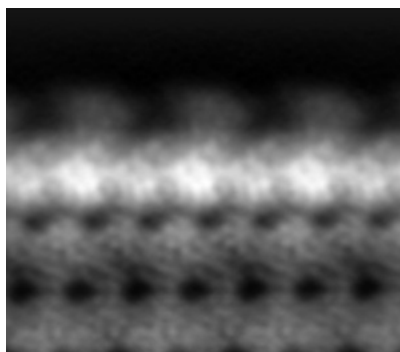
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

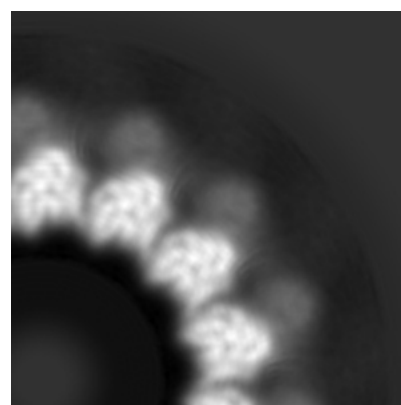
6.1.1 Primary map



X



Y

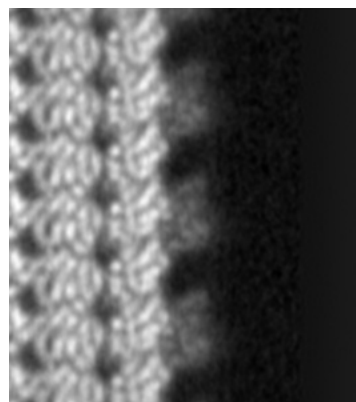


Z

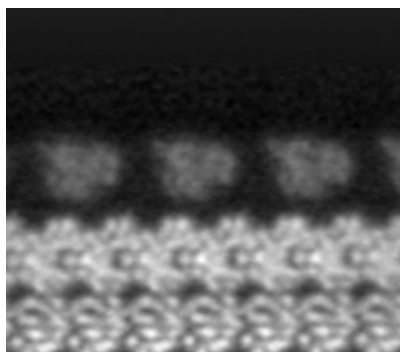
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

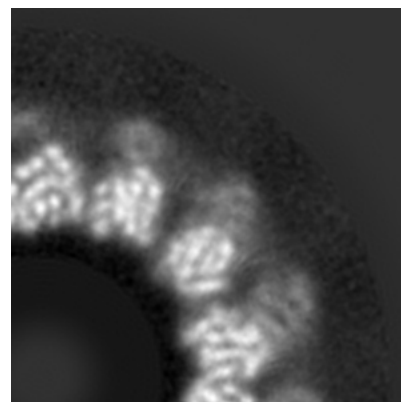
6.2.1 Primary map



X Index: 96



Y Index: 96

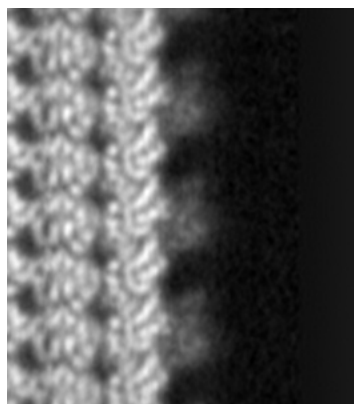


Z Index: 110

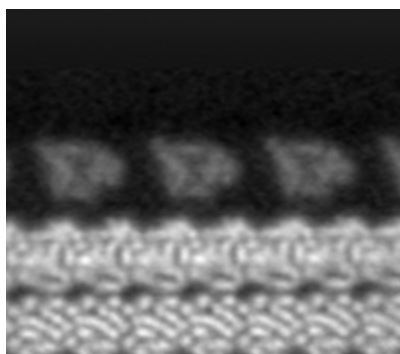
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

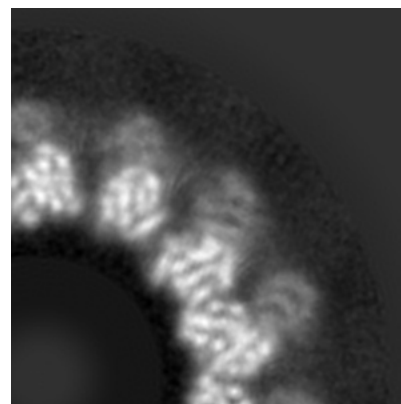
6.3.1 Primary map



X Index: 95



Y Index: 99

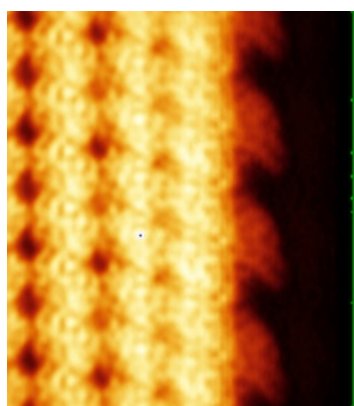


Z Index: 104

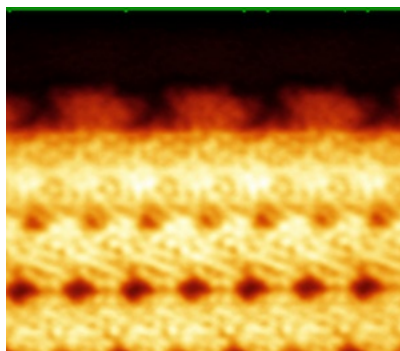
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

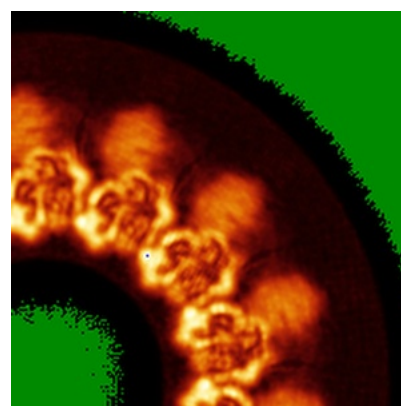
6.4.1 Primary map



X



Y

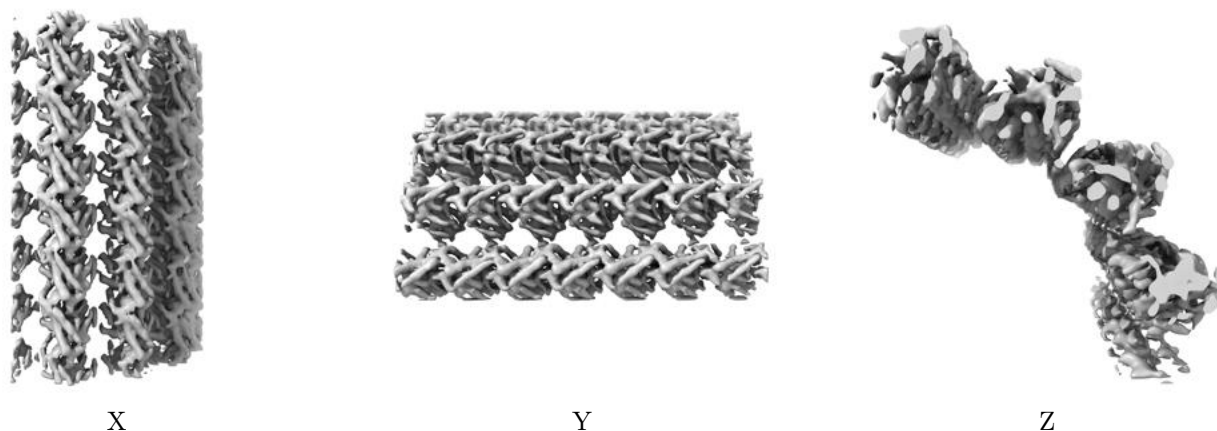


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

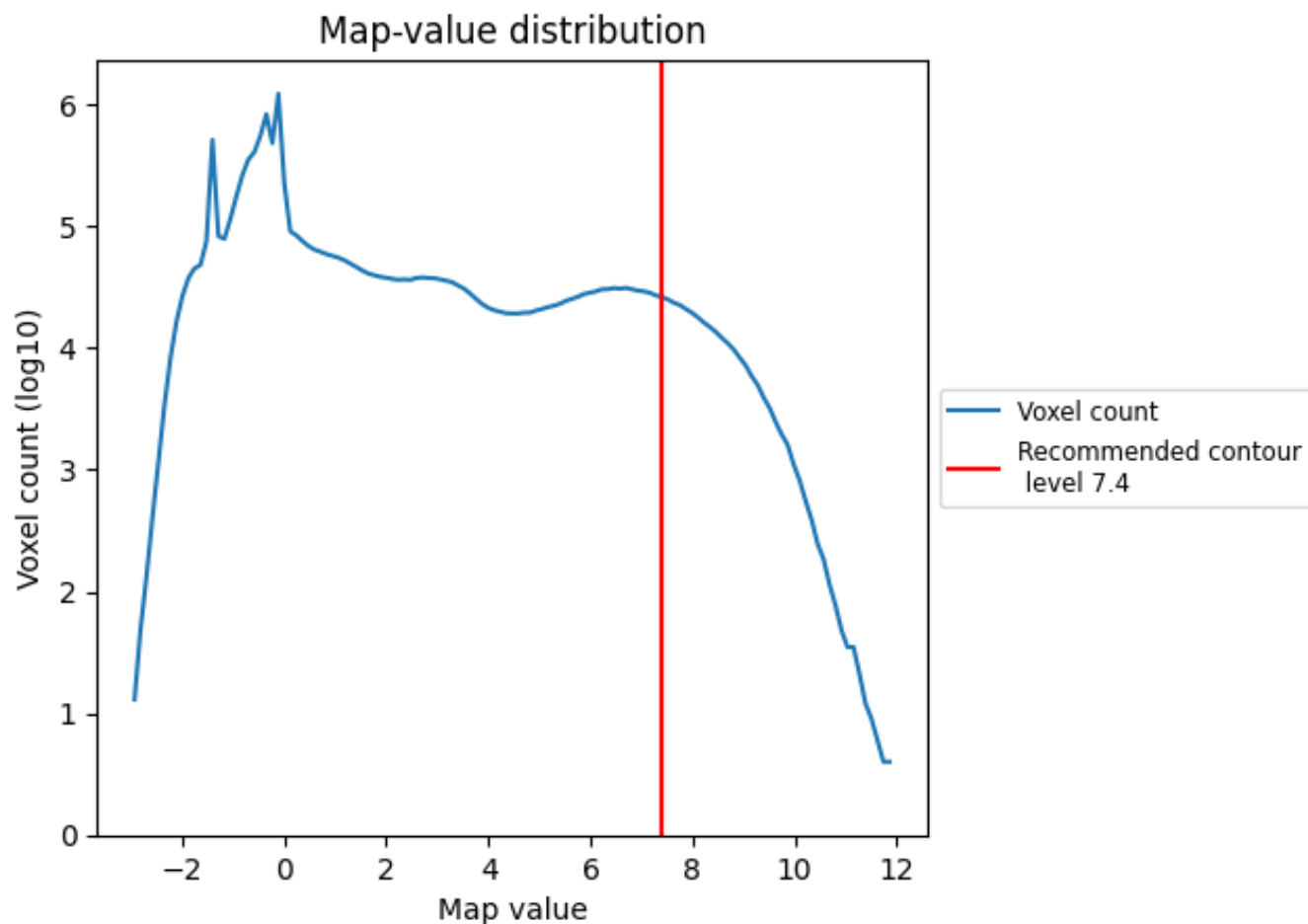
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

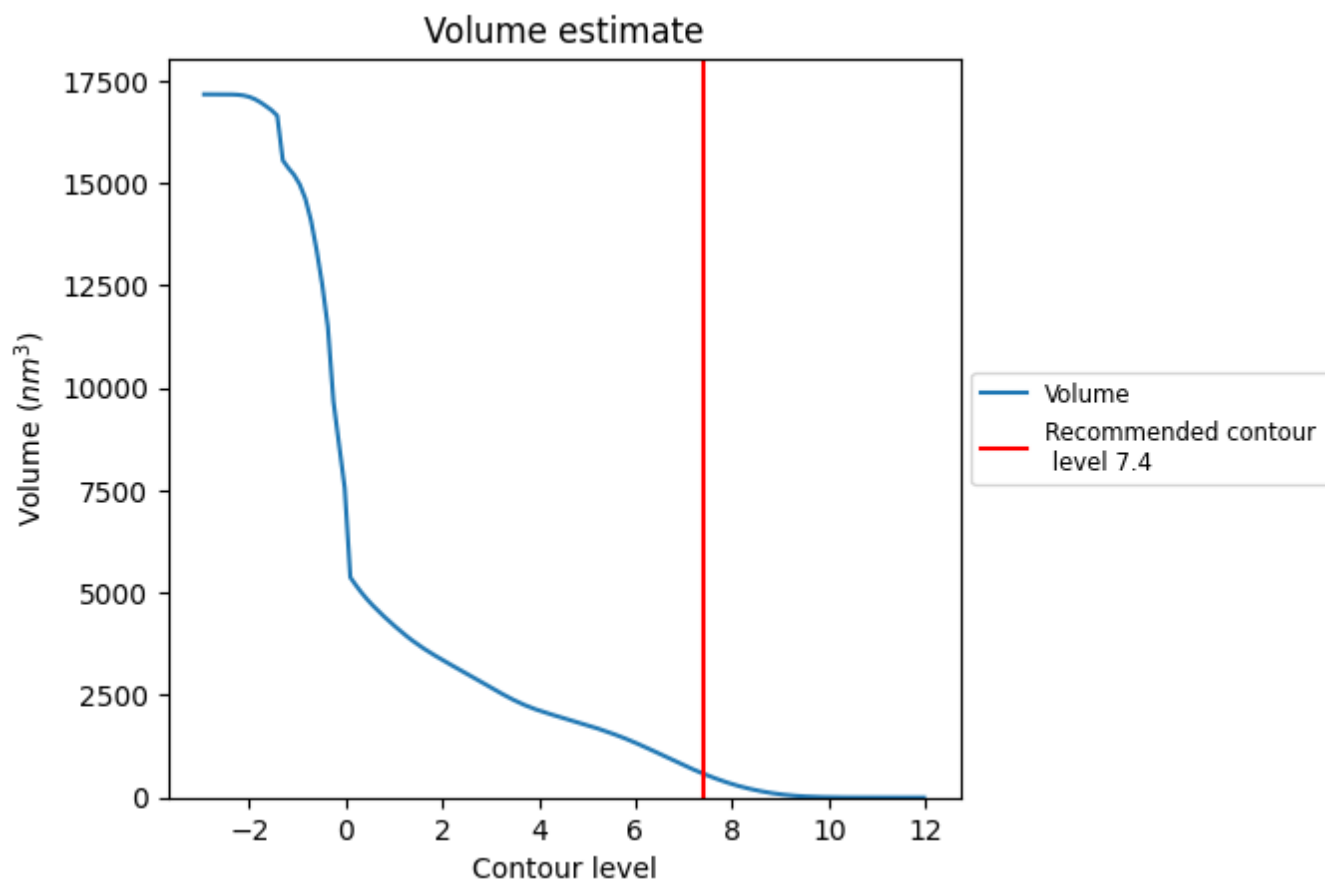
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 586 nm³; this corresponds to an approximate mass of 529 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

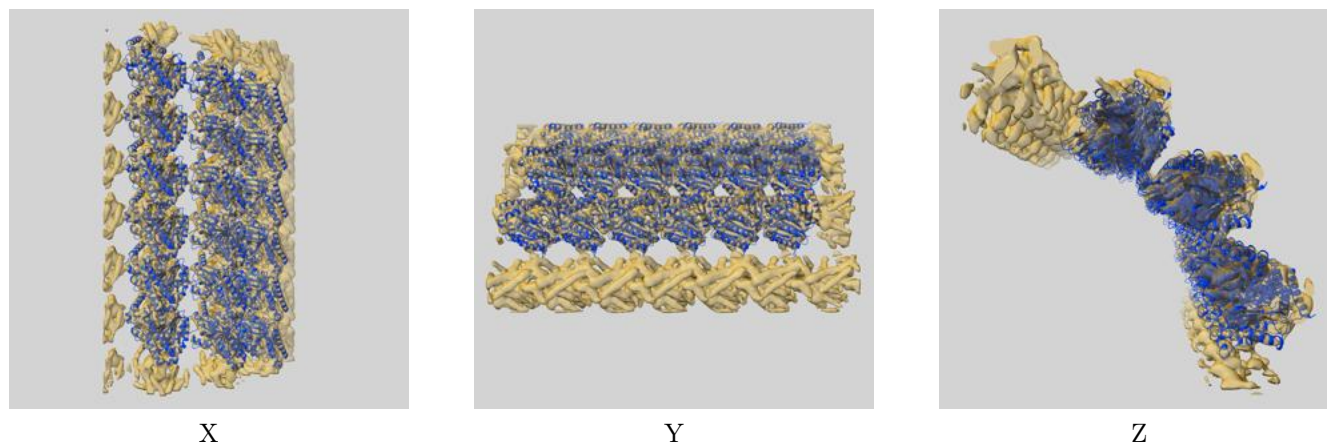
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

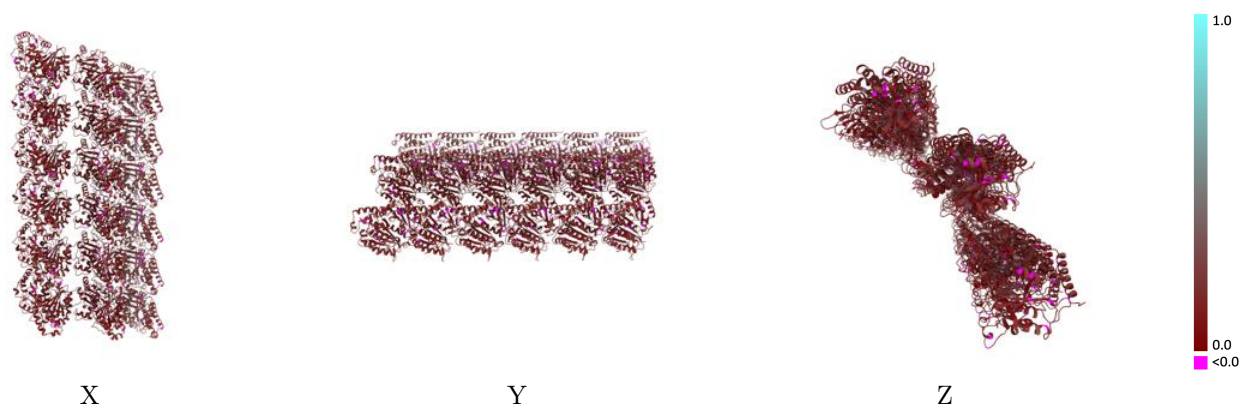
This section contains information regarding the fit between EMDB map EMD-6782 and PDB model 5XXW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



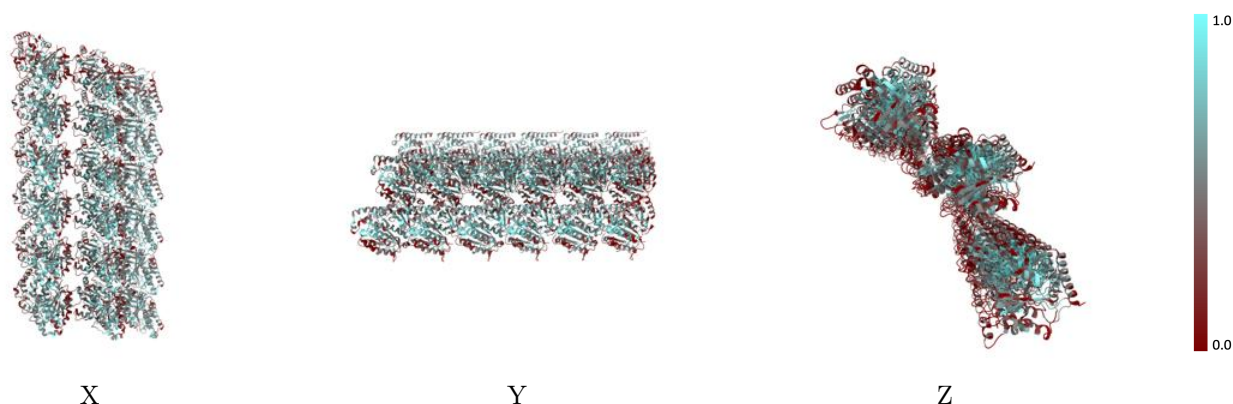
The images above show the 3D surface view of the map at the recommended contour level 7.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



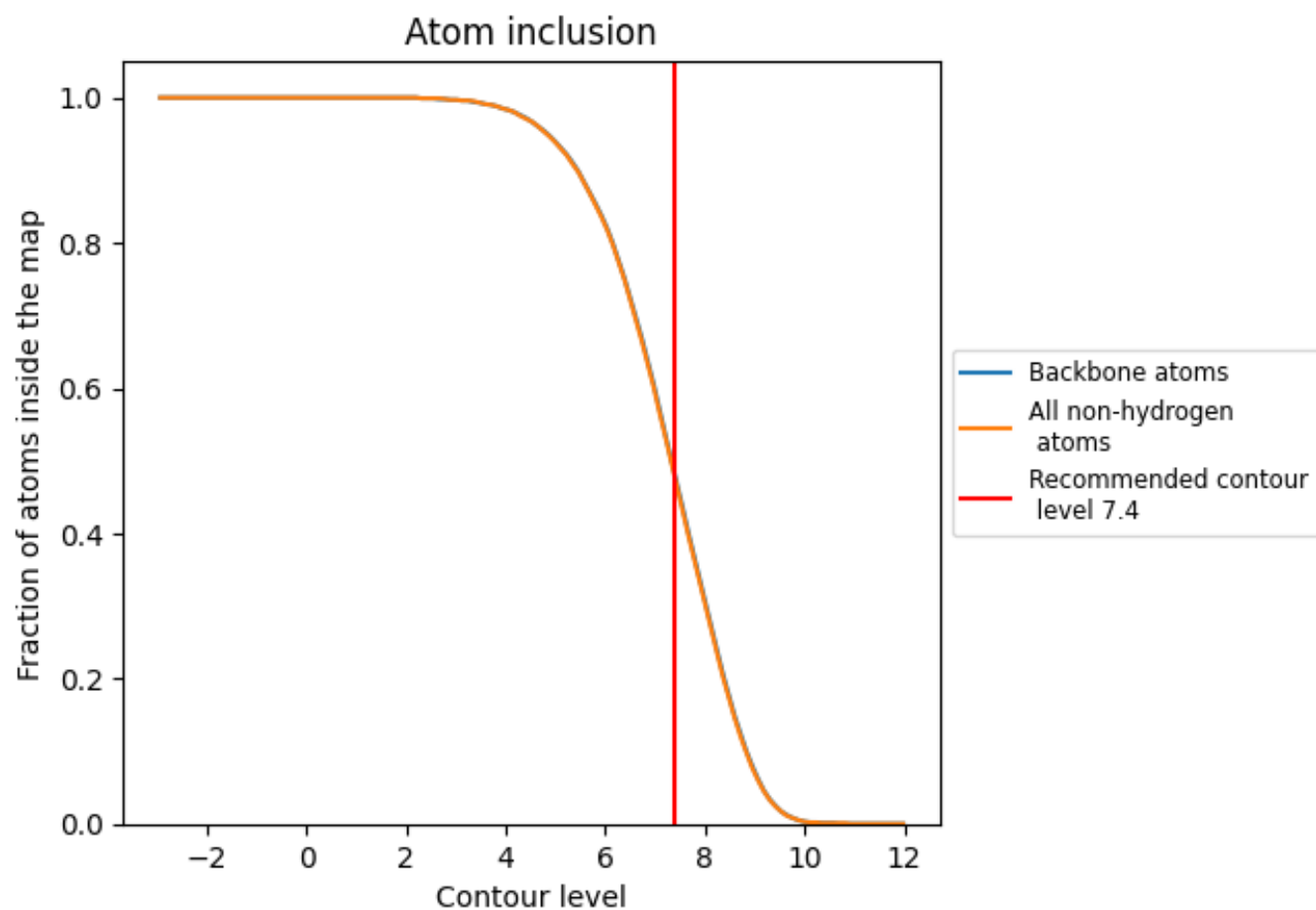
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (7.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4750	0.1640
A	0.5090	0.1690
B	0.5310	0.1630
C	0.5090	0.1690
D	0.5300	0.1660
E	0.5080	0.1670
F	0.5300	0.1610
G	0.4840	0.1680
H	0.4610	0.1630
I	0.4830	0.1640
J	0.4600	0.1590
K	0.4870	0.1650
L	0.4620	0.1600
M	0.4060	0.1640
N	0.5050	0.1670
O	0.4050	0.1640
P	0.5010	0.1670
Q	0.4100	0.1610
R	0.5010	0.1630

1.0

0.0

<0.0