



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:55 am GMT

PDB ID : 3J6G
EMDB ID: : EMD-5897
Title : Minimized average structure of microtubules stabilized by taxol
Authors : Alushin, G.M.; Lander, G.C.; Kellogg, E.H.; Zhang, R.; Baker, D.; Nogales, E.
Deposited on : 2014-02-19
Resolution : 5.50 Å(reported)
Based on PDB ID : 1JFF

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

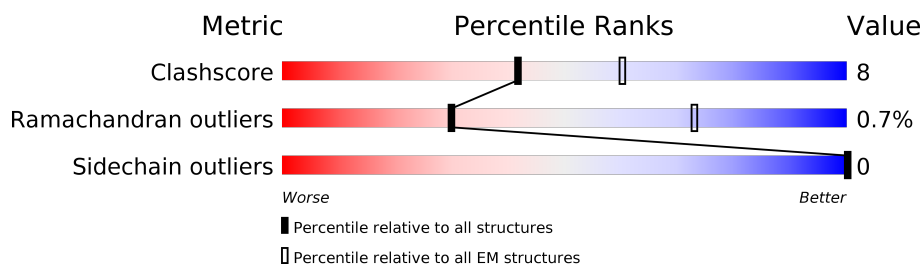
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	439	72% 19% 6% .
1	C	439	71% 20% 6% .
1	E	439	72% 19% 6% .
1	G	439	72% 19% 6% .
1	I	439	73% 18% 6% .
1	K	439	73% 18% 6% .
1	M	439	72% 20% 6% .
1	O	439	73% 19% 6% .
1	Q	439	73% 18% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	427	 75% 23% •
2	D	427	 77% 22% •
2	F	427	 77% 21% •
2	H	427	 76% 22% •
2	J	427	 76% 22% •
2	L	427	 77% 21% •
2	N	427	 76% 22% •
2	P	427	 75% 23% •
2	R	427	 76% 22% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 61461 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		

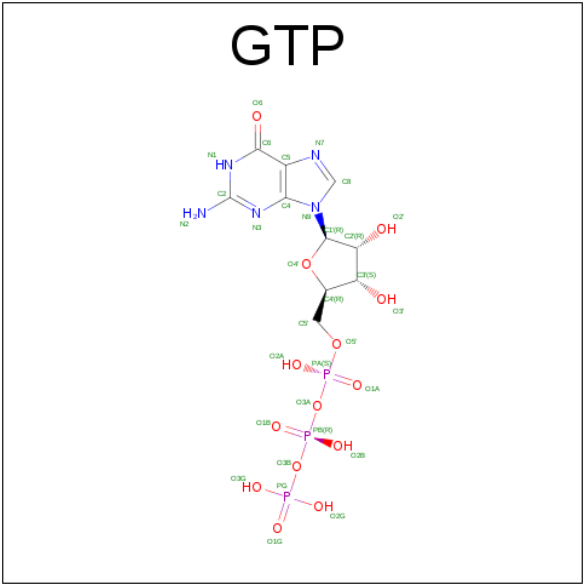
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	CONFLICT	UNP P02550
C	265	GLY	ALA	CONFLICT	UNP P02550
E	265	GLY	ALA	CONFLICT	UNP P02550
G	265	GLY	ALA	CONFLICT	UNP P02550
I	265	GLY	ALA	CONFLICT	UNP P02550
K	265	GLY	ALA	CONFLICT	UNP P02550
M	265	GLY	ALA	CONFLICT	UNP P02550
O	265	GLY	ALA	CONFLICT	UNP P02550
Q	265	GLY	ALA	CONFLICT	UNP P02550

- 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		
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 (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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	

Continued on next page...

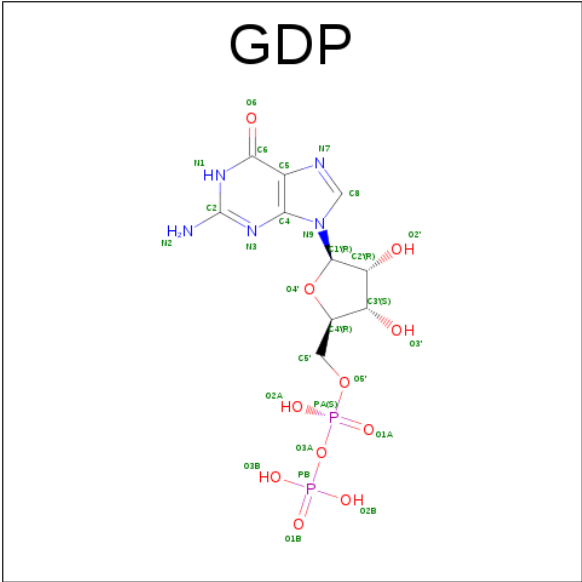
Continued from previous page...

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

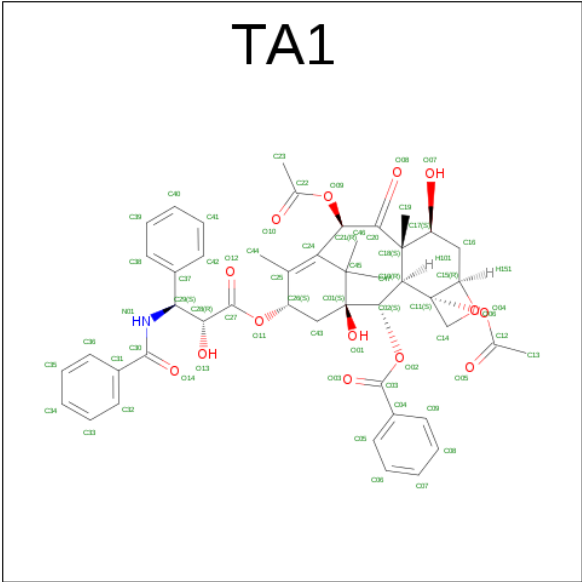
Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total	Mg	0
			1	1	
4	Q	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	O	1	Total	Mg	0
			1	1	
4	M	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: 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 TAXOL (three-letter code: TA1) (formula: C₄₇H₅₁NO₁₄).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			62	47	1	14	
6	D	1	Total	C	N	O	0
			62	47	1	14	
6	F	1	Total	C	N	O	0
			62	47	1	14	
6	H	1	Total	C	N	O	0
			62	47	1	14	
6	J	1	Total	C	N	O	0
			62	47	1	14	
6	L	1	Total	C	N	O	0
			62	47	1	14	
6	N	1	Total	C	N	O	0
			62	47	1	14	
6	P	1	Total	C	N	O	0
			62	47	1	14	
6	R	1	Total	C	N	O	0
			62	47	1	14	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	4	Total	O	0
			4	4	
7	C	4	Total	O	0
			4	4	
7	E	4	Total	O	0
			4	4	

Continued on next page...

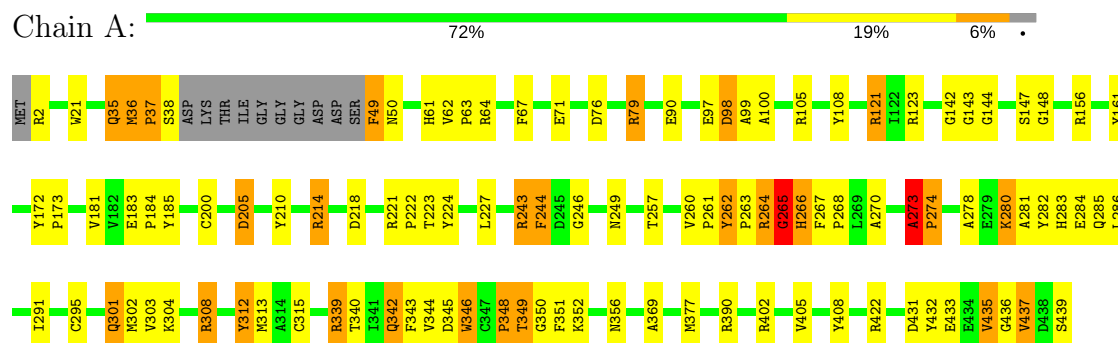
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
7	G	4	Total 4	O 4	0
7	I	4	Total 4	O 4	0
7	K	4	Total 4	O 4	0
7	M	4	Total 4	O 4	0
7	O	4	Total 4	O 4	0
7	Q	4	Total 4	O 4	0

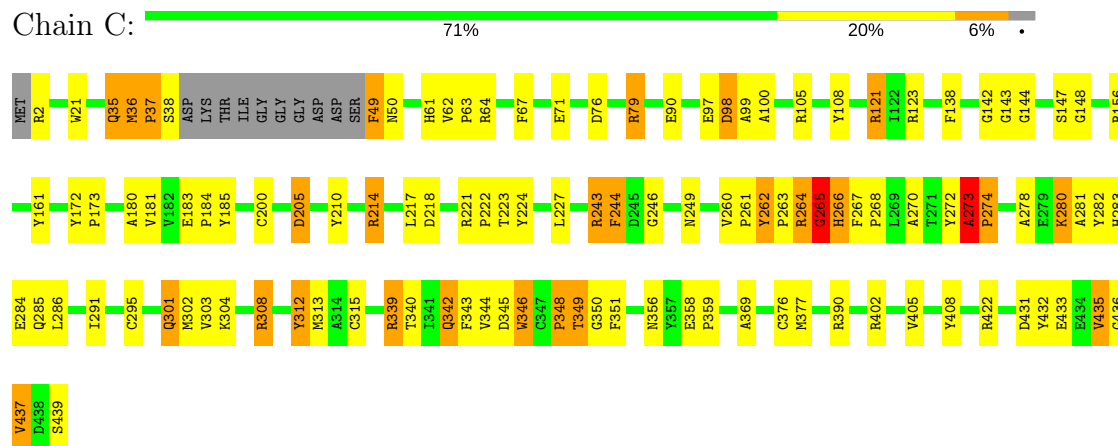
3 Residue-property plots

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

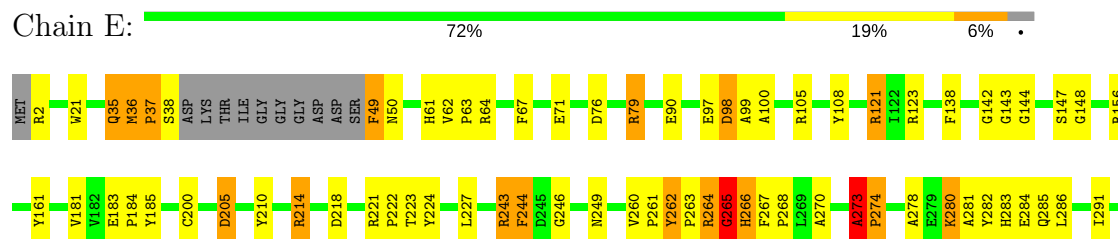
• Molecule 1: Tubulin alpha-1A chain



• Molecule 1: Tubulin alpha-1A chain



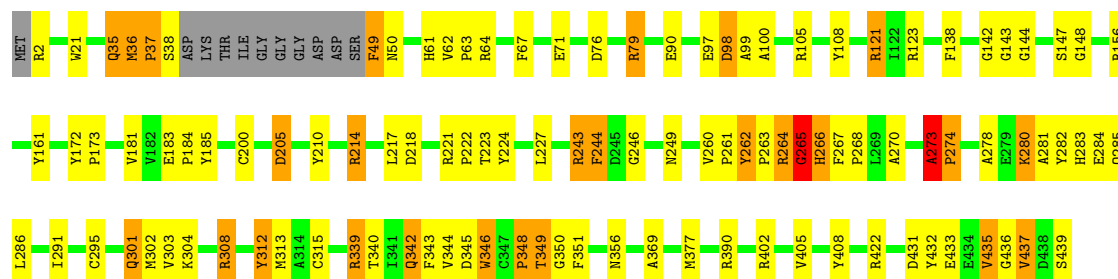
• Molecule 1: Tubulin alpha-1A chain





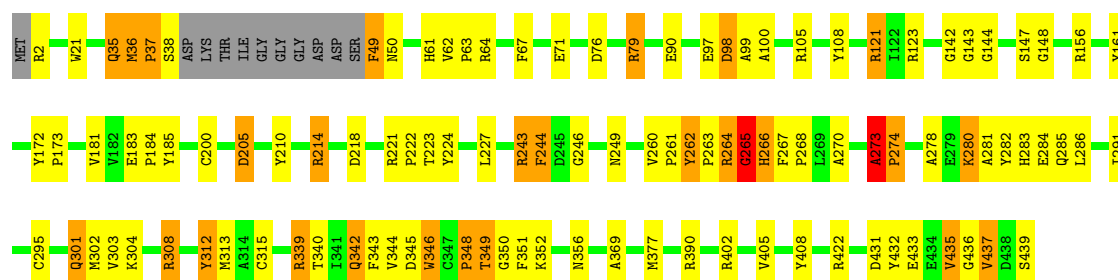
• Molecule 1: Tubulin alpha-1A chain

Chain G: 72% 19% 6%



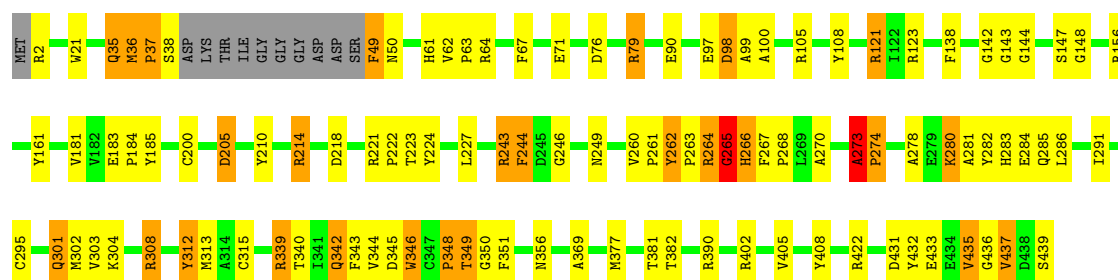
• Molecule 1: Tubulin alpha-1A chain

Chain I: 73% 18% 6%



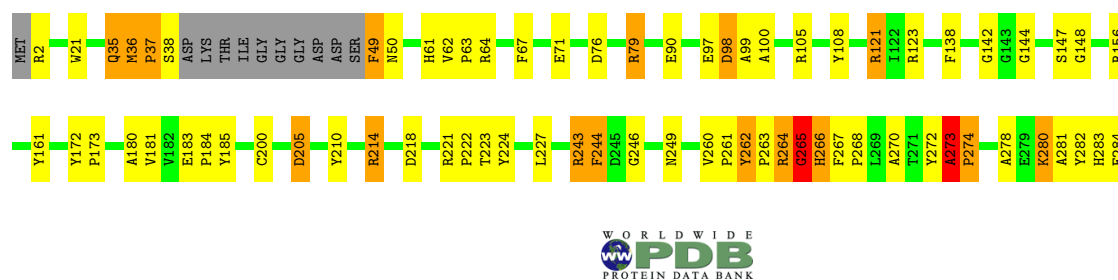
• Molecule 1: Tubulin alpha-1A chain

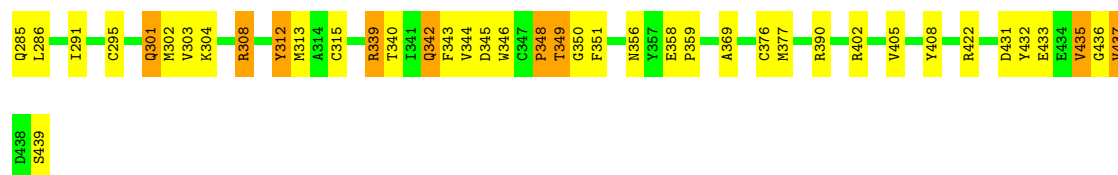
Chain K: 73% 18% 6%



• Molecule 1: Tubulin alpha-1A chain

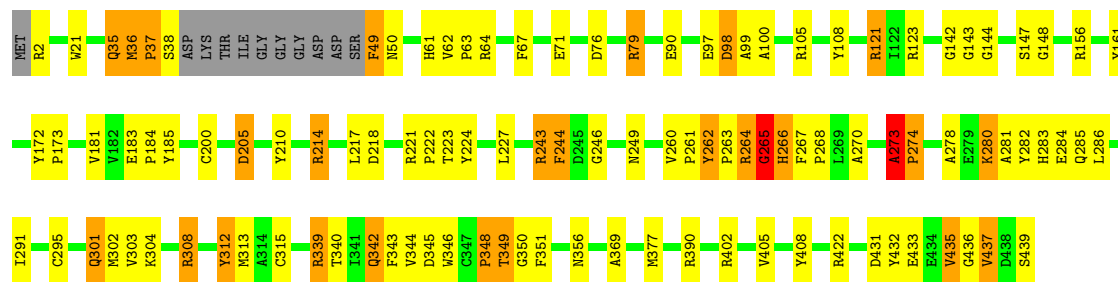
Chain M: 72% 20% 6%





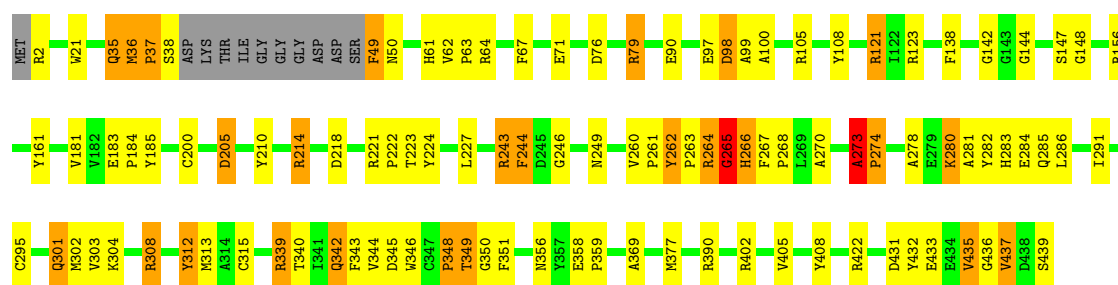
• Molecule 1: Tubulin alpha-1A chain

Chain O: 73% 19% 6%



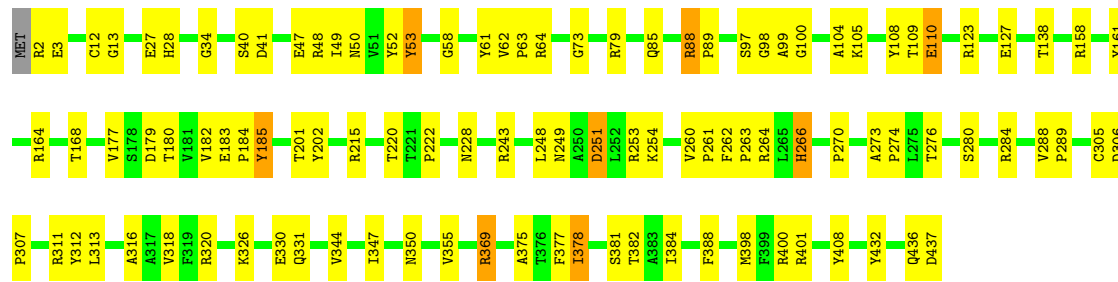
• Molecule 1: Tubulin alpha-1A chain

Chain Q: 73% 18% 6%



• Molecule 2: Tubulin beta chain

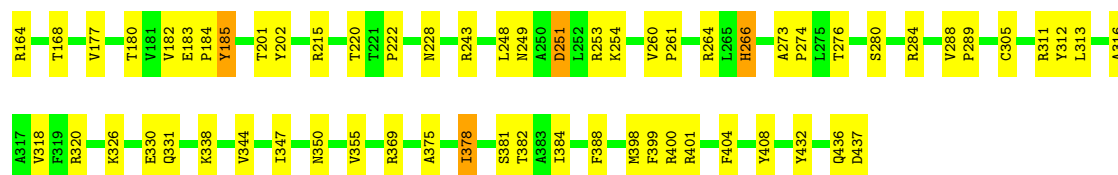
Chain B: 75% 23% 2%



• Molecule 2: Tubulin beta chain

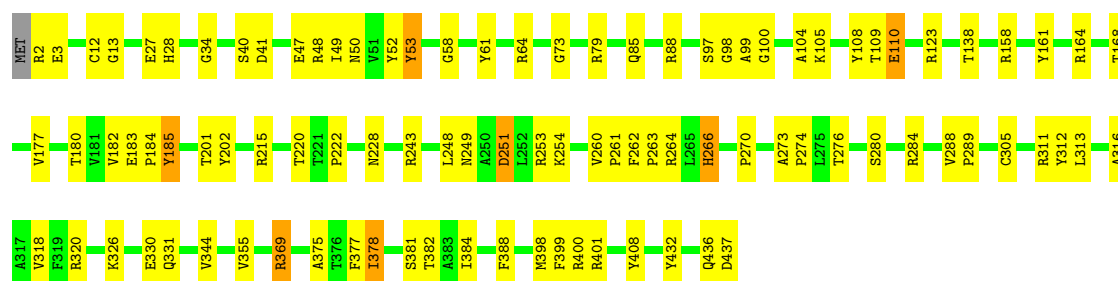
Chain D: 77% 22% 1%





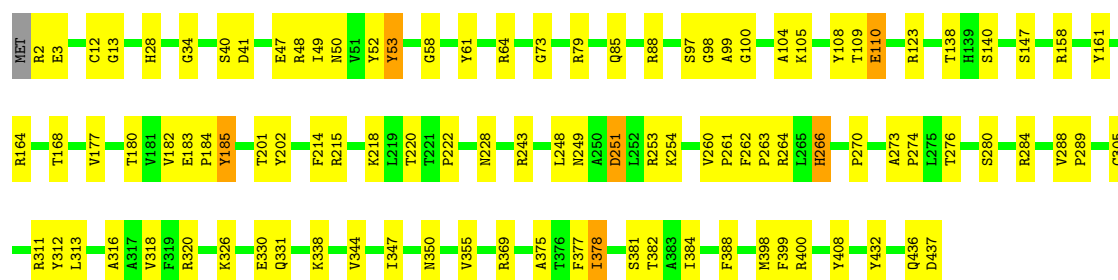
• Molecule 2: Tubulin beta chain

Chain F: 77% 21%



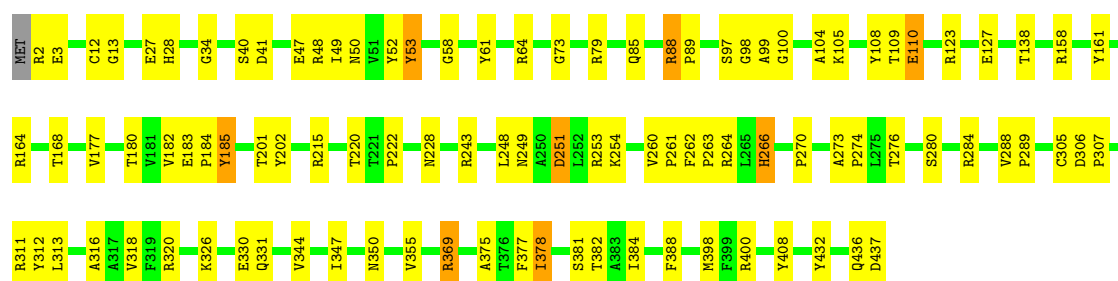
• Molecule 2: Tubulin beta chain

Chain H: 76% 22%



• Molecule 2: Tubulin beta chain

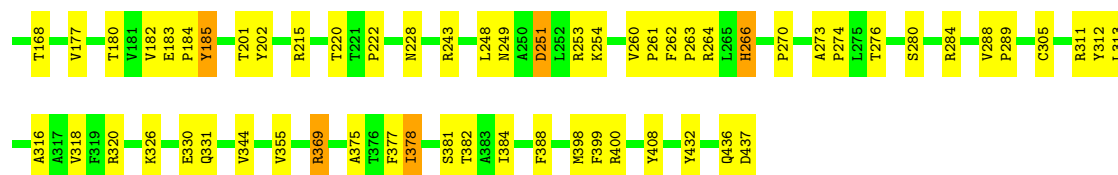
Chain J: 76% 22%



• Molecule 2: Tubulin beta chain

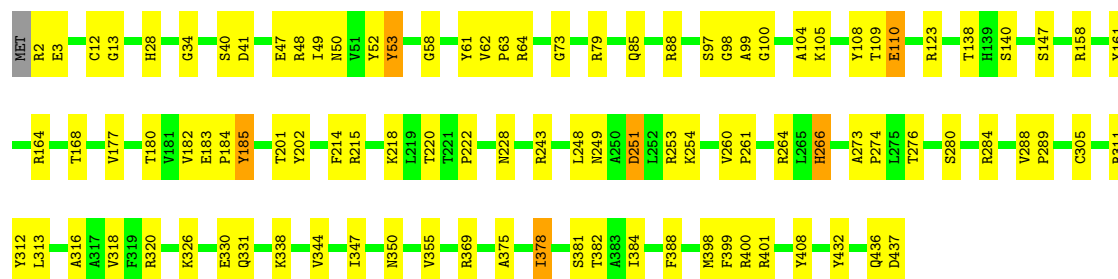
Chain L: 77% 21%





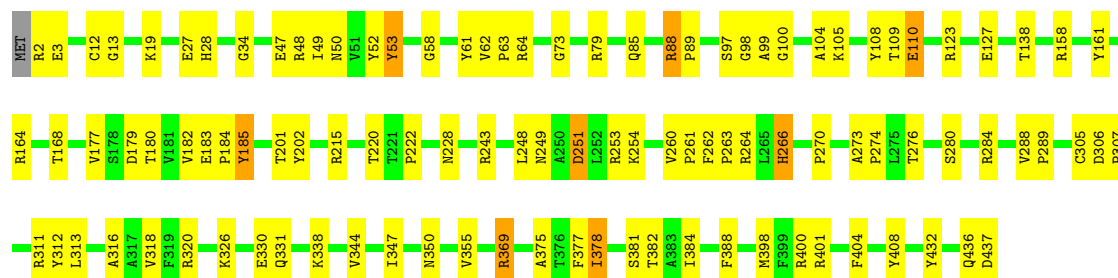
• Molecule 2: Tubulin beta chain

Chain N: 76% 22%



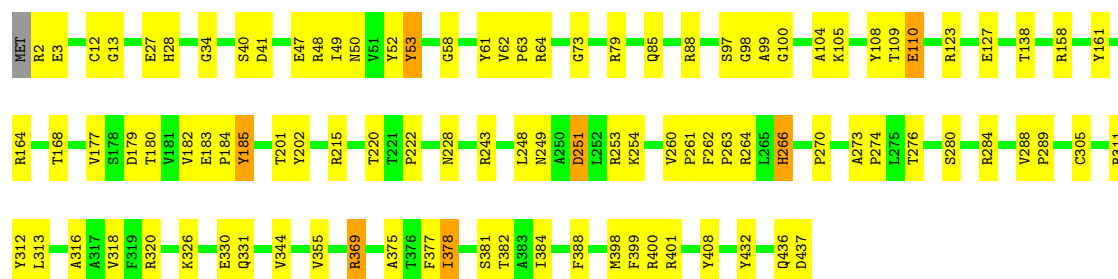
• Molecule 2: Tubulin beta chain

Chain P: 75% 23%



• Molecule 2: Tubulin beta chain

Chain R: 76% 22%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	24357	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	ctftilt	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.0	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	72000	Depositor
Image detector	KODAK SO-163 film	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG, TA1

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 >2	RMSZ	# Z >2
1	A	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	C	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	E	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	G	1.34	32/3427 (0.9%)	1.68	86/4651 (1.8%)
1	I	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	K	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	M	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	O	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	Q	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
2	B	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	D	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	F	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	H	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	J	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	L	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	N	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	P	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	R	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
All	All	1.27	388/61686 (0.6%)	1.62	1188/83637 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	C	0	6
1	E	0	6
1	G	0	6
1	I	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	6
1	M	0	6
1	O	0	6
1	Q	0	6
All	All	0	54

All (388) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	GLU	N-CA	-12.57	1.21	1.46
2	N	3	GLU	N-CA	-12.56	1.21	1.46
2	R	3	GLU	N-CA	-12.56	1.21	1.46
2	H	3	GLU	N-CA	-12.55	1.21	1.46
2	B	3	GLU	N-CA	-12.54	1.21	1.46
2	P	3	GLU	N-CA	-12.54	1.21	1.46
2	F	3	GLU	N-CA	-12.54	1.21	1.46
2	J	3	GLU	N-CA	-12.54	1.21	1.46
2	L	3	GLU	N-CA	-12.52	1.21	1.46
2	D	249	ASN	CA-C	-12.21	1.21	1.52
2	F	249	ASN	CA-C	-12.20	1.21	1.52
2	R	249	ASN	CA-C	-12.20	1.21	1.52
2	H	249	ASN	CA-C	-12.19	1.21	1.52
2	B	249	ASN	CA-C	-12.19	1.21	1.52
2	N	249	ASN	CA-C	-12.19	1.21	1.52
2	P	249	ASN	CA-C	-12.19	1.21	1.52
2	L	249	ASN	CA-C	-12.18	1.21	1.52
2	J	249	ASN	CA-C	-12.17	1.21	1.52
1	K	266	HIS	N-CA	-12.14	1.22	1.46
1	E	266	HIS	N-CA	-12.13	1.22	1.46
1	G	266	HIS	N-CA	-12.13	1.22	1.46
1	C	266	HIS	N-CA	-12.12	1.22	1.46
1	A	266	HIS	N-CA	-12.12	1.22	1.46
1	I	266	HIS	N-CA	-12.12	1.22	1.46
1	O	266	HIS	N-CA	-12.12	1.22	1.46
1	M	266	HIS	N-CA	-12.11	1.22	1.46
1	Q	266	HIS	N-CA	-12.08	1.22	1.46
1	Q	436	GLY	CA-C	-9.38	1.36	1.51
1	I	436	GLY	CA-C	-9.37	1.36	1.51
1	M	436	GLY	CA-C	-9.36	1.36	1.51
1	A	436	GLY	CA-C	-9.36	1.36	1.51
1	O	436	GLY	CA-C	-9.35	1.36	1.51
1	K	436	GLY	CA-C	-9.35	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	436	GLY	CA-C	-9.34	1.36	1.51
1	G	436	GLY	CA-C	-9.34	1.36	1.51
1	C	436	GLY	CA-C	-9.31	1.36	1.51
1	K	36	MET	CA-C	-9.25	1.28	1.52
1	E	36	MET	CA-C	-9.22	1.28	1.52
1	A	36	MET	CA-C	-9.21	1.28	1.52
1	I	36	MET	CA-C	-9.22	1.28	1.52
1	C	36	MET	CA-C	-9.21	1.28	1.52
1	M	36	MET	CA-C	-9.21	1.28	1.52
1	O	36	MET	CA-C	-9.21	1.28	1.52
1	G	36	MET	CA-C	-9.20	1.29	1.52
1	Q	36	MET	CA-C	-9.18	1.29	1.52
1	C	350	GLY	N-CA	-8.85	1.32	1.46
1	Q	350	GLY	N-CA	-8.84	1.32	1.46
1	E	350	GLY	N-CA	-8.84	1.32	1.46
1	I	350	GLY	N-CA	-8.84	1.32	1.46
1	A	350	GLY	N-CA	-8.83	1.32	1.46
1	O	350	GLY	N-CA	-8.82	1.32	1.46
1	M	350	GLY	N-CA	-8.81	1.32	1.46
1	K	350	GLY	N-CA	-8.80	1.32	1.46
1	G	350	GLY	N-CA	-8.78	1.32	1.46
1	E	348	PRO	CA-C	-8.60	1.35	1.52
1	M	348	PRO	CA-C	-8.59	1.35	1.52
1	Q	348	PRO	CA-C	-8.58	1.35	1.52
1	A	348	PRO	CA-C	-8.58	1.35	1.52
1	I	348	PRO	CA-C	-8.58	1.35	1.52
1	G	348	PRO	CA-C	-8.57	1.35	1.52
1	O	348	PRO	CA-C	-8.57	1.35	1.52
1	C	348	PRO	CA-C	-8.56	1.35	1.52
1	K	348	PRO	CA-C	-8.54	1.35	1.52
1	C	38	SER	N-CA	-8.37	1.29	1.46
1	G	38	SER	N-CA	-8.36	1.29	1.46
1	I	38	SER	N-CA	-8.36	1.29	1.46
1	A	38	SER	N-CA	-8.36	1.29	1.46
1	M	38	SER	N-CA	-8.36	1.29	1.46
1	K	38	SER	N-CA	-8.36	1.29	1.46
1	E	38	SER	N-CA	-8.36	1.29	1.46
1	O	38	SER	N-CA	-8.35	1.29	1.46
1	Q	38	SER	N-CA	-8.35	1.29	1.46
2	F	100	GLY	N-CA	-8.32	1.33	1.46
2	N	100	GLY	N-CA	-8.32	1.33	1.46
2	B	100	GLY	N-CA	-8.32	1.33	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	100	GLY	N-CA	-8.31	1.33	1.46
2	H	100	GLY	N-CA	-8.30	1.33	1.46
2	J	100	GLY	N-CA	-8.30	1.33	1.46
2	D	100	GLY	N-CA	-8.29	1.33	1.46
1	G	283	HIS	CA-C	-8.29	1.31	1.52
1	I	283	HIS	CA-C	-8.28	1.31	1.52
1	E	283	HIS	CA-C	-8.27	1.31	1.52
1	A	283	HIS	CA-C	-8.27	1.31	1.52
1	C	283	HIS	CA-C	-8.27	1.31	1.52
2	P	100	GLY	N-CA	-8.27	1.33	1.46
1	Q	283	HIS	CA-C	-8.27	1.31	1.52
1	K	283	HIS	CA-C	-8.26	1.31	1.52
1	M	283	HIS	CA-C	-8.26	1.31	1.52
2	R	100	GLY	N-CA	-8.26	1.33	1.46
1	Q	284	GLU	N-CA	-8.25	1.29	1.46
1	E	284	GLU	N-CA	-8.24	1.29	1.46
1	G	284	GLU	N-CA	-8.23	1.29	1.46
1	O	283	HIS	CA-C	-8.23	1.31	1.52
1	K	284	GLU	N-CA	-8.22	1.29	1.46
1	C	284	GLU	N-CA	-8.22	1.29	1.46
1	I	284	GLU	N-CA	-8.22	1.29	1.46
1	A	284	GLU	N-CA	-8.21	1.29	1.46
1	M	284	GLU	N-CA	-8.20	1.29	1.46
1	O	284	GLU	N-CA	-8.20	1.29	1.46
1	E	282	TYR	N-CA	-7.93	1.30	1.46
1	G	282	TYR	N-CA	-7.92	1.30	1.46
1	O	282	TYR	N-CA	-7.92	1.30	1.46
1	Q	282	TYR	N-CA	-7.92	1.30	1.46
1	K	282	TYR	N-CA	-7.92	1.30	1.46
1	A	282	TYR	N-CA	-7.91	1.30	1.46
1	M	282	TYR	N-CA	-7.91	1.30	1.46
1	I	282	TYR	N-CA	-7.90	1.30	1.46
1	C	282	TYR	N-CA	-7.87	1.30	1.46
1	O	340	THR	N-CA	-7.53	1.31	1.46
1	C	340	THR	N-CA	-7.51	1.31	1.46
1	Q	340	THR	N-CA	-7.50	1.31	1.46
1	G	340	THR	N-CA	-7.50	1.31	1.46
1	M	340	THR	N-CA	-7.50	1.31	1.46
1	I	340	THR	N-CA	-7.50	1.31	1.46
1	E	340	THR	N-CA	-7.49	1.31	1.46
1	A	340	THR	N-CA	-7.49	1.31	1.46
1	K	340	THR	N-CA	-7.48	1.31	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	281	ALA	CA-C	-7.41	1.33	1.52
1	E	281	ALA	CA-C	-7.40	1.33	1.52
1	G	281	ALA	CA-C	-7.40	1.33	1.52
1	K	281	ALA	CA-C	-7.40	1.33	1.52
1	M	281	ALA	CA-C	-7.38	1.33	1.52
1	A	281	ALA	CA-C	-7.38	1.33	1.52
1	C	281	ALA	CA-C	-7.37	1.33	1.52
1	O	281	ALA	CA-C	-7.37	1.33	1.52
1	Q	281	ALA	CA-C	-7.36	1.33	1.52
1	O	283	HIS	N-CA	-7.34	1.31	1.46
1	M	283	HIS	N-CA	-7.34	1.31	1.46
1	C	283	HIS	N-CA	-7.31	1.31	1.46
2	F	437	ASP	N-CA	-7.31	1.31	1.46
1	A	283	HIS	N-CA	-7.31	1.31	1.46
1	E	283	HIS	N-CA	-7.30	1.31	1.46
2	H	437	ASP	N-CA	-7.30	1.31	1.46
1	I	283	HIS	N-CA	-7.30	1.31	1.46
1	K	283	HIS	N-CA	-7.30	1.31	1.46
2	N	437	ASP	N-CA	-7.29	1.31	1.46
1	Q	283	HIS	N-CA	-7.29	1.31	1.46
1	G	283	HIS	N-CA	-7.28	1.31	1.46
2	P	437	ASP	N-CA	-7.26	1.31	1.46
2	R	437	ASP	N-CA	-7.25	1.31	1.46
2	B	437	ASP	N-CA	-7.25	1.31	1.46
2	D	437	ASP	N-CA	-7.23	1.31	1.46
2	L	437	ASP	N-CA	-7.22	1.31	1.46
2	J	437	ASP	N-CA	-7.22	1.31	1.46
1	E	285	GLN	N-CA	-7.06	1.32	1.46
1	M	285	GLN	N-CA	-7.05	1.32	1.46
1	I	285	GLN	N-CA	-7.04	1.32	1.46
1	G	285	GLN	N-CA	-7.03	1.32	1.46
1	O	285	GLN	N-CA	-7.03	1.32	1.46
1	A	285	GLN	N-CA	-7.03	1.32	1.46
1	Q	285	GLN	N-CA	-7.03	1.32	1.46
1	C	285	GLN	N-CA	-7.02	1.32	1.46
1	K	285	GLN	N-CA	-7.00	1.32	1.46
2	N	436	GLN	CA-C	-6.84	1.35	1.52
2	B	436	GLN	CA-C	-6.84	1.35	1.52
2	H	436	GLN	CA-C	-6.84	1.35	1.52
2	R	436	GLN	CA-C	-6.83	1.35	1.52
2	P	436	GLN	CA-C	-6.83	1.35	1.52
2	F	436	GLN	CA-C	-6.82	1.35	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	436	GLN	CA-C	-6.82	1.35	1.52
2	J	436	GLN	CA-C	-6.82	1.35	1.52
2	L	436	GLN	CA-C	-6.81	1.35	1.52
1	E	282	TYR	CA-C	-6.80	1.35	1.52
1	I	282	TYR	CA-C	-6.79	1.35	1.52
1	C	282	TYR	CA-C	-6.79	1.35	1.52
1	O	282	TYR	CA-C	-6.79	1.35	1.52
1	A	282	TYR	CA-C	-6.79	1.35	1.52
1	G	282	TYR	CA-C	-6.79	1.35	1.52
1	K	282	TYR	CA-C	-6.79	1.35	1.52
1	M	282	TYR	CA-C	-6.79	1.35	1.52
1	Q	264	ARG	CA-C	-6.78	1.35	1.52
1	K	264	ARG	CA-C	-6.78	1.35	1.52
1	C	264	ARG	CA-C	-6.77	1.35	1.52
1	A	264	ARG	CA-C	-6.76	1.35	1.52
1	Q	282	TYR	CA-C	-6.76	1.35	1.52
1	I	264	ARG	CA-C	-6.76	1.35	1.52
1	M	264	ARG	CA-C	-6.76	1.35	1.52
1	O	264	ARG	CA-C	-6.75	1.35	1.52
2	J	99	ALA	CA-C	-6.75	1.35	1.52
2	L	99	ALA	CA-C	-6.75	1.35	1.52
2	D	99	ALA	CA-C	-6.75	1.35	1.52
1	E	264	ARG	CA-C	-6.75	1.35	1.52
2	B	99	ALA	CA-C	-6.75	1.35	1.52
2	H	99	ALA	CA-C	-6.74	1.35	1.52
2	P	99	ALA	CA-C	-6.74	1.35	1.52
2	F	58	GLY	CA-C	-6.74	1.41	1.51
2	N	99	ALA	CA-C	-6.74	1.35	1.52
1	G	264	ARG	CA-C	-6.74	1.35	1.52
2	H	58	GLY	CA-C	-6.73	1.41	1.51
2	R	99	ALA	CA-C	-6.73	1.35	1.52
2	F	99	ALA	CA-C	-6.72	1.35	1.52
2	P	58	GLY	CA-C	-6.72	1.41	1.51
2	N	58	GLY	CA-C	-6.72	1.41	1.51
2	B	58	GLY	CA-C	-6.71	1.41	1.51
2	D	58	GLY	CA-C	-6.71	1.41	1.51
2	R	58	GLY	CA-C	-6.70	1.41	1.51
2	J	58	GLY	CA-C	-6.70	1.41	1.51
2	L	58	GLY	CA-C	-6.66	1.41	1.51
1	G	284	GLU	CA-C	-6.46	1.36	1.52
1	K	284	GLU	CA-C	-6.45	1.36	1.52
1	M	284	GLU	CA-C	-6.45	1.36	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	284	GLU	CA-C	-6.44	1.36	1.52
1	A	284	GLU	CA-C	-6.43	1.36	1.52
1	C	284	GLU	CA-C	-6.43	1.36	1.52
1	E	284	GLU	CA-C	-6.41	1.36	1.52
1	I	284	GLU	CA-C	-6.41	1.36	1.52
1	Q	284	GLU	CA-C	-6.41	1.36	1.52
1	O	349	THR	CA-C	-6.40	1.36	1.52
1	K	349	THR	CA-C	-6.39	1.36	1.52
1	G	349	THR	CA-C	-6.38	1.36	1.52
1	A	349	THR	CA-C	-6.37	1.36	1.52
1	M	349	THR	CA-C	-6.37	1.36	1.52
1	Q	349	THR	CA-C	-6.37	1.36	1.52
1	C	349	THR	CA-C	-6.37	1.36	1.52
1	I	349	THR	CA-C	-6.37	1.36	1.52
1	E	349	THR	CA-C	-6.36	1.36	1.52
1	C	281	ALA	N-CA	-6.31	1.33	1.46
1	Q	281	ALA	N-CA	-6.30	1.33	1.46
1	A	281	ALA	N-CA	-6.30	1.33	1.46
1	E	281	ALA	N-CA	-6.29	1.33	1.46
1	M	281	ALA	N-CA	-6.29	1.33	1.46
1	O	281	ALA	N-CA	-6.29	1.33	1.46
1	K	281	ALA	N-CA	-6.27	1.33	1.46
1	G	281	ALA	N-CA	-6.27	1.33	1.46
1	I	281	ALA	N-CA	-6.26	1.33	1.46
2	N	34	GLY	CA-C	-6.20	1.42	1.51
2	H	34	GLY	CA-C	-6.18	1.42	1.51
2	L	34	GLY	CA-C	-6.18	1.42	1.51
2	J	34	GLY	CA-C	-6.17	1.42	1.51
2	B	34	GLY	CA-C	-6.17	1.42	1.51
2	R	34	GLY	CA-C	-6.16	1.42	1.51
2	P	34	GLY	CA-C	-6.15	1.42	1.51
2	D	34	GLY	CA-C	-6.15	1.42	1.51
2	F	34	GLY	CA-C	-6.14	1.42	1.51
1	C	437	VAL	N-CA	-6.10	1.34	1.46
1	G	437	VAL	N-CA	-6.10	1.34	1.46
1	E	437	VAL	N-CA	-6.10	1.34	1.46
1	A	437	VAL	N-CA	-6.08	1.34	1.46
1	Q	437	VAL	N-CA	-6.08	1.34	1.46
1	I	437	VAL	N-CA	-6.07	1.34	1.46
1	K	437	VAL	N-CA	-6.06	1.34	1.46
1	M	348	PRO	N-CA	-6.06	1.36	1.47
1	M	349	THR	N-CA	-6.06	1.34	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	THR	N-CA	-6.06	1.34	1.46
1	E	349	THR	N-CA	-6.06	1.34	1.46
1	C	349	THR	N-CA	-6.06	1.34	1.46
1	O	437	VAL	N-CA	-6.05	1.34	1.46
1	M	437	VAL	N-CA	-6.05	1.34	1.46
1	Q	348	PRO	N-CA	-6.05	1.36	1.47
1	G	349	THR	N-CA	-6.05	1.34	1.46
1	O	349	THR	N-CA	-6.04	1.34	1.46
1	I	349	THR	N-CA	-6.04	1.34	1.46
1	C	348	PRO	N-CA	-6.04	1.36	1.47
1	Q	349	THR	N-CA	-6.04	1.34	1.46
1	A	348	PRO	N-CA	-6.04	1.36	1.47
1	G	339	ARG	CA-C	-6.04	1.37	1.52
1	E	348	PRO	N-CA	-6.03	1.36	1.47
1	K	349	THR	N-CA	-6.03	1.34	1.46
1	K	339	ARG	CA-C	-6.02	1.37	1.52
1	E	339	ARG	CA-C	-6.02	1.37	1.52
1	K	348	PRO	N-CA	-6.02	1.37	1.47
1	G	348	PRO	N-CA	-6.02	1.37	1.47
1	A	339	ARG	CA-C	-6.01	1.37	1.52
1	O	339	ARG	CA-C	-6.01	1.37	1.52
1	O	348	PRO	N-CA	-6.01	1.37	1.47
1	I	339	ARG	CA-C	-6.01	1.37	1.52
1	C	339	ARG	CA-C	-6.01	1.37	1.52
1	I	348	PRO	N-CA	-6.00	1.37	1.47
1	M	339	ARG	CA-C	-5.99	1.37	1.52
1	Q	339	ARG	CA-C	-5.98	1.37	1.52
1	Q	280	LYS	CA-C	-5.94	1.37	1.52
1	A	280	LYS	CA-C	-5.93	1.37	1.52
1	E	280	LYS	CA-C	-5.93	1.37	1.52
1	K	280	LYS	CA-C	-5.93	1.37	1.52
1	M	280	LYS	CA-C	-5.93	1.37	1.52
1	G	280	LYS	CA-C	-5.93	1.37	1.52
1	O	280	LYS	CA-C	-5.93	1.37	1.52
1	C	280	LYS	CA-C	-5.92	1.37	1.52
2	P	100	GLY	CA-C	-5.92	1.42	1.51
2	R	100	GLY	CA-C	-5.90	1.42	1.51
1	I	280	LYS	CA-C	-5.90	1.37	1.52
2	H	100	GLY	CA-C	-5.90	1.42	1.51
2	L	100	GLY	CA-C	-5.86	1.42	1.51
2	B	100	GLY	CA-C	-5.86	1.42	1.51
2	N	100	GLY	CA-C	-5.86	1.42	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	100	GLY	CA-C	-5.85	1.42	1.51
2	D	100	GLY	CA-C	-5.84	1.42	1.51
2	J	100	GLY	CA-C	-5.84	1.42	1.51
1	O	98	ASP	CA-C	-5.66	1.38	1.52
1	K	98	ASP	CA-C	-5.65	1.38	1.52
1	C	98	ASP	CA-C	-5.65	1.38	1.52
1	M	98	ASP	CA-C	-5.65	1.38	1.52
1	G	98	ASP	CA-C	-5.64	1.38	1.52
1	E	98	ASP	CA-C	-5.64	1.38	1.52
1	A	98	ASP	CA-C	-5.64	1.38	1.52
2	N	222	PRO	N-CA	-5.64	1.37	1.47
1	Q	98	ASP	CA-C	-5.64	1.38	1.52
1	I	98	ASP	CA-C	-5.63	1.38	1.52
2	B	222	PRO	N-CA	-5.61	1.37	1.47
2	F	222	PRO	N-CA	-5.61	1.37	1.47
2	P	222	PRO	N-CA	-5.61	1.37	1.47
2	L	222	PRO	N-CA	-5.61	1.37	1.47
2	D	222	PRO	N-CA	-5.60	1.37	1.47
2	J	222	PRO	N-CA	-5.60	1.37	1.47
2	R	222	PRO	N-CA	-5.60	1.37	1.47
2	H	222	PRO	N-CA	-5.58	1.37	1.47
1	Q	339	ARG	N-CA	-5.55	1.35	1.46
1	I	339	ARG	N-CA	-5.54	1.35	1.46
1	G	339	ARG	N-CA	-5.54	1.35	1.46
1	K	339	ARG	N-CA	-5.53	1.35	1.46
1	M	339	ARG	N-CA	-5.53	1.35	1.46
1	O	99	ALA	N-CA	-5.53	1.35	1.46
1	C	339	ARG	N-CA	-5.53	1.35	1.46
1	A	339	ARG	N-CA	-5.52	1.35	1.46
1	O	339	ARG	N-CA	-5.52	1.35	1.46
1	M	99	ALA	N-CA	-5.52	1.35	1.46
1	E	339	ARG	N-CA	-5.52	1.35	1.46
1	E	99	ALA	N-CA	-5.51	1.35	1.46
1	A	99	ALA	N-CA	-5.51	1.35	1.46
1	K	99	ALA	N-CA	-5.50	1.35	1.46
1	C	49	PHE	CA-C	-5.50	1.38	1.52
1	I	49	PHE	CA-C	-5.49	1.38	1.52
1	C	99	ALA	N-CA	-5.49	1.35	1.46
1	I	99	ALA	N-CA	-5.49	1.35	1.46
1	Q	99	ALA	N-CA	-5.49	1.35	1.46
1	O	49	PHE	CA-C	-5.49	1.38	1.52
1	G	49	PHE	CA-C	-5.48	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	99	ALA	N-CA	-5.48	1.35	1.46
1	E	49	PHE	CA-C	-5.48	1.38	1.52
1	A	49	PHE	CA-C	-5.47	1.38	1.52
1	K	49	PHE	CA-C	-5.47	1.38	1.52
1	Q	49	PHE	CA-C	-5.47	1.38	1.52
1	M	49	PHE	CA-C	-5.46	1.38	1.52
1	G	436	GLY	N-CA	-5.34	1.38	1.46
1	M	436	GLY	N-CA	-5.34	1.38	1.46
1	Q	436	GLY	N-CA	-5.34	1.38	1.46
1	K	436	GLY	N-CA	-5.33	1.38	1.46
1	C	436	GLY	N-CA	-5.32	1.38	1.46
1	I	436	GLY	N-CA	-5.31	1.38	1.46
1	E	436	GLY	N-CA	-5.30	1.38	1.46
1	A	436	GLY	N-CA	-5.29	1.38	1.46
1	Q	437	VAL	CA-C	-5.29	1.39	1.52
1	I	437	VAL	CA-C	-5.29	1.39	1.52
1	M	437	VAL	CA-C	-5.28	1.39	1.52
1	A	437	VAL	CA-C	-5.28	1.39	1.52
1	C	437	VAL	CA-C	-5.28	1.39	1.52
1	O	436	GLY	N-CA	-5.28	1.38	1.46
1	K	437	VAL	CA-C	-5.27	1.39	1.52
1	O	437	VAL	CA-C	-5.27	1.39	1.52
1	E	437	VAL	CA-C	-5.26	1.39	1.52
1	G	437	VAL	CA-C	-5.26	1.39	1.52
1	M	49	PHE	N-CA	-5.19	1.35	1.46
1	O	49	PHE	N-CA	-5.19	1.35	1.46
1	K	49	PHE	N-CA	-5.17	1.36	1.46
1	Q	50	ASN	N-CA	-5.16	1.36	1.46
1	K	50	ASN	N-CA	-5.16	1.36	1.46
1	E	50	ASN	N-CA	-5.16	1.36	1.46
2	J	58	GLY	N-CA	-5.15	1.38	1.46
1	G	50	ASN	N-CA	-5.15	1.36	1.46
1	C	49	PHE	N-CA	-5.15	1.36	1.46
1	I	50	ASN	N-CA	-5.15	1.36	1.46
1	G	49	PHE	N-CA	-5.14	1.36	1.46
1	A	50	ASN	N-CA	-5.14	1.36	1.46
1	M	50	ASN	N-CA	-5.14	1.36	1.46
1	A	49	PHE	N-CA	-5.14	1.36	1.46
1	Q	49	PHE	N-CA	-5.14	1.36	1.46
1	C	50	ASN	N-CA	-5.14	1.36	1.46
1	O	50	ASN	N-CA	-5.13	1.36	1.46
1	E	49	PHE	N-CA	-5.12	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	58	GLY	N-CA	-5.11	1.38	1.46
1	I	49	PHE	N-CA	-5.11	1.36	1.46
2	P	58	GLY	N-CA	-5.11	1.38	1.46
2	N	58	GLY	N-CA	-5.11	1.38	1.46
2	D	58	GLY	N-CA	-5.10	1.38	1.46
2	H	58	GLY	N-CA	-5.10	1.38	1.46
2	B	58	GLY	N-CA	-5.10	1.38	1.46
2	F	58	GLY	N-CA	-5.10	1.38	1.46
2	J	274	PRO	N-CA	-5.08	1.38	1.47
2	R	58	GLY	N-CA	-5.08	1.38	1.46
2	D	274	PRO	N-CA	-5.07	1.38	1.47
2	L	274	PRO	N-CA	-5.07	1.38	1.47
2	B	274	PRO	N-CA	-5.07	1.38	1.47
2	F	274	PRO	N-CA	-5.06	1.38	1.47
2	H	274	PRO	N-CA	-5.06	1.38	1.47
2	R	274	PRO	N-CA	-5.04	1.38	1.47
2	N	274	PRO	N-CA	-5.04	1.38	1.47
1	G	142	GLY	CA-C	-5.03	1.43	1.51
2	P	274	PRO	N-CA	-5.03	1.38	1.47

All (1188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	262	TYR	CB-CG-CD1	-17.46	110.53	121.00
1	G	262	TYR	CB-CG-CD1	-17.44	110.53	121.00
1	A	262	TYR	CB-CG-CD1	-17.43	110.54	121.00
1	E	262	TYR	CB-CG-CD1	-17.42	110.55	121.00
1	I	262	TYR	CB-CG-CD1	-17.41	110.55	121.00
1	O	262	TYR	CB-CG-CD1	-17.41	110.55	121.00
1	C	262	TYR	CB-CG-CD1	-17.41	110.56	121.00
1	Q	262	TYR	CB-CG-CD1	-17.39	110.57	121.00
1	M	262	TYR	CB-CG-CD1	-17.38	110.57	121.00
2	D	320	ARG	NE-CZ-NH1	16.36	128.48	120.30
2	N	320	ARG	NE-CZ-NH1	16.32	128.46	120.30
2	J	320	ARG	NE-CZ-NH1	16.29	128.45	120.30
2	B	320	ARG	NE-CZ-NH1	16.28	128.44	120.30
2	H	320	ARG	NE-CZ-NH1	16.28	128.44	120.30
2	P	320	ARG	NE-CZ-NH1	16.28	128.44	120.30
2	L	320	ARG	NE-CZ-NH1	16.26	128.43	120.30
2	R	320	ARG	NE-CZ-NH1	16.21	128.41	120.30
2	F	320	ARG	NE-CZ-NH1	16.19	128.40	120.30
1	Q	221	ARG	NE-CZ-NH2	-14.71	112.94	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	ARG	NE-CZ-NH2	-14.71	112.95	120.30
1	G	221	ARG	NE-CZ-NH2	-14.70	112.95	120.30
1	I	221	ARG	NE-CZ-NH2	-14.70	112.95	120.30
1	K	221	ARG	NE-CZ-NH2	-14.70	112.95	120.30
1	A	221	ARG	NE-CZ-NH2	-14.66	112.97	120.30
1	M	221	ARG	NE-CZ-NH2	-14.65	112.97	120.30
1	O	221	ARG	NE-CZ-NH2	-14.63	112.99	120.30
1	C	221	ARG	NE-CZ-NH2	-14.59	113.00	120.30
1	E	105	ARG	NE-CZ-NH2	-13.60	113.50	120.30
1	M	105	ARG	NE-CZ-NH2	-13.60	113.50	120.30
1	O	105	ARG	NE-CZ-NH2	-13.58	113.51	120.30
1	A	105	ARG	NE-CZ-NH2	-13.57	113.51	120.30
1	Q	105	ARG	NE-CZ-NH2	-13.57	113.52	120.30
1	I	105	ARG	NE-CZ-NH2	-13.56	113.52	120.30
1	K	105	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	C	105	ARG	NE-CZ-NH2	-13.52	113.54	120.30
1	G	105	ARG	NE-CZ-NH2	-13.49	113.55	120.30
2	R	369	ARG	NE-CZ-NH2	-12.85	113.88	120.30
2	J	369	ARG	NE-CZ-NH2	-12.84	113.88	120.30
2	D	369	ARG	NE-CZ-NH2	-12.83	113.89	120.30
2	N	369	ARG	NE-CZ-NH2	-12.81	113.90	120.30
2	F	369	ARG	NE-CZ-NH2	-12.81	113.90	120.30
2	L	369	ARG	NE-CZ-NH2	-12.79	113.90	120.30
2	B	369	ARG	NE-CZ-NH2	-12.78	113.91	120.30
2	H	369	ARG	NE-CZ-NH2	-12.78	113.91	120.30
2	P	369	ARG	NE-CZ-NH2	-12.77	113.92	120.30
2	N	164	ARG	NE-CZ-NH2	12.22	126.41	120.30
2	P	164	ARG	NE-CZ-NH2	12.19	126.39	120.30
2	F	164	ARG	NE-CZ-NH2	12.16	126.38	120.30
2	B	164	ARG	NE-CZ-NH2	12.14	126.37	120.30
2	J	164	ARG	NE-CZ-NH2	12.13	126.37	120.30
2	L	164	ARG	NE-CZ-NH2	12.11	126.36	120.30
2	D	164	ARG	NE-CZ-NH2	12.11	126.35	120.30
2	R	164	ARG	NE-CZ-NH2	12.11	126.35	120.30
2	H	164	ARG	NE-CZ-NH2	12.06	126.33	120.30
2	R	264	ARG	NE-CZ-NH2	-11.75	114.42	120.30
2	P	264	ARG	NE-CZ-NH2	-11.71	114.44	120.30
2	B	264	ARG	NE-CZ-NH2	-11.65	114.47	120.30
2	N	185	TYR	CB-CG-CD2	-11.65	114.01	121.00
2	L	264	ARG	NE-CZ-NH2	-11.64	114.48	120.30
2	N	264	ARG	NE-CZ-NH2	-11.64	114.48	120.30
2	F	264	ARG	NE-CZ-NH2	-11.63	114.49	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	185	TYR	CB-CG-CD2	-11.63	114.02	121.00
2	F	185	TYR	CB-CG-CD2	-11.62	114.03	121.00
2	J	264	ARG	NE-CZ-NH2	-11.61	114.49	120.30
2	H	264	ARG	NE-CZ-NH2	-11.60	114.50	120.30
2	P	185	TYR	CB-CG-CD2	-11.59	114.05	121.00
2	B	185	TYR	CB-CG-CD2	-11.59	114.05	121.00
2	D	264	ARG	NE-CZ-NH2	-11.59	114.51	120.30
2	D	185	TYR	CB-CG-CD2	-11.57	114.06	121.00
2	N	243	ARG	NE-CZ-NH1	11.57	126.08	120.30
2	H	243	ARG	NE-CZ-NH1	11.56	126.08	120.30
2	L	185	TYR	CB-CG-CD2	-11.55	114.07	121.00
2	J	185	TYR	CB-CG-CD2	-11.54	114.07	121.00
2	R	243	ARG	NE-CZ-NH1	11.54	126.07	120.30
2	F	243	ARG	NE-CZ-NH1	11.53	126.07	120.30
2	P	243	ARG	NE-CZ-NH1	11.51	126.05	120.30
1	C	262	TYR	CB-CG-CD2	11.50	127.90	121.00
2	H	185	TYR	CB-CG-CD2	-11.50	114.10	121.00
2	B	243	ARG	NE-CZ-NH1	11.49	126.04	120.30
2	L	243	ARG	NE-CZ-NH1	11.47	126.03	120.30
2	D	243	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	A	262	TYR	CB-CG-CD2	11.44	127.86	121.00
1	G	262	TYR	CB-CG-CD2	11.43	127.86	121.00
2	J	243	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	M	262	TYR	CB-CG-CD2	11.42	127.85	121.00
1	I	262	TYR	CB-CG-CD2	11.41	127.85	121.00
1	O	262	TYR	CB-CG-CD2	11.41	127.84	121.00
1	E	262	TYR	CB-CG-CD2	11.40	127.84	121.00
1	K	262	TYR	CB-CG-CD2	11.40	127.84	121.00
1	Q	262	TYR	CB-CG-CD2	11.38	127.83	121.00
2	R	311	ARG	NE-CZ-NH1	11.02	125.81	120.30
2	J	311	ARG	NE-CZ-NH1	11.00	125.80	120.30
2	F	311	ARG	NE-CZ-NH1	11.00	125.80	120.30
2	B	311	ARG	NE-CZ-NH1	10.96	125.78	120.30
2	H	311	ARG	NE-CZ-NH1	10.95	125.78	120.30
2	D	311	ARG	NE-CZ-NH1	10.94	125.77	120.30
2	P	311	ARG	NE-CZ-NH1	10.93	125.77	120.30
2	N	311	ARG	NE-CZ-NH1	10.92	125.76	120.30
2	L	311	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	I	274	PRO	CA-N-CD	-10.77	96.42	111.50
1	G	274	PRO	CA-N-CD	-10.76	96.43	111.50
1	E	274	PRO	CA-N-CD	-10.76	96.44	111.50
1	A	274	PRO	CA-N-CD	-10.76	96.44	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	274	PRO	CA-N-CD	-10.76	96.44	111.50
1	K	274	PRO	CA-N-CD	-10.76	96.44	111.50
1	Q	274	PRO	CA-N-CD	-10.76	96.44	111.50
1	M	274	PRO	CA-N-CD	-10.75	96.45	111.50
1	C	274	PRO	CA-N-CD	-10.74	96.46	111.50
2	D	320	ARG	NH1-CZ-NH2	-10.59	107.75	119.40
2	B	320	ARG	NH1-CZ-NH2	-10.55	107.80	119.40
2	N	320	ARG	NH1-CZ-NH2	-10.55	107.80	119.40
2	H	320	ARG	NH1-CZ-NH2	-10.54	107.80	119.40
2	J	320	ARG	NH1-CZ-NH2	-10.54	107.80	119.40
2	R	320	ARG	NH1-CZ-NH2	-10.54	107.80	119.40
2	P	320	ARG	NH1-CZ-NH2	-10.54	107.81	119.40
2	F	320	ARG	NH1-CZ-NH2	-10.53	107.82	119.40
2	L	320	ARG	NH1-CZ-NH2	-10.52	107.83	119.40
2	D	64	ARG	NE-CZ-NH2	10.51	125.56	120.30
2	J	64	ARG	NE-CZ-NH2	10.50	125.55	120.30
2	P	64	ARG	NE-CZ-NH2	10.49	125.54	120.30
2	B	64	ARG	NE-CZ-NH2	10.46	125.53	120.30
2	F	64	ARG	NE-CZ-NH2	10.44	125.52	120.30
2	H	64	ARG	NE-CZ-NH2	10.44	125.52	120.30
2	N	64	ARG	NE-CZ-NH2	10.43	125.51	120.30
2	R	64	ARG	NE-CZ-NH2	10.42	125.51	120.30
2	L	64	ARG	NE-CZ-NH2	10.39	125.50	120.30
2	F	48	ARG	NE-CZ-NH2	10.26	125.43	120.30
2	N	48	ARG	NE-CZ-NH2	10.21	125.41	120.30
2	B	48	ARG	NE-CZ-NH2	10.21	125.40	120.30
2	P	48	ARG	NE-CZ-NH2	10.20	125.40	120.30
2	D	48	ARG	NE-CZ-NH2	10.19	125.40	120.30
2	J	48	ARG	NE-CZ-NH2	10.19	125.39	120.30
1	Q	67	PHE	CE1-CZ-CE2	10.18	138.33	120.00
1	A	67	PHE	CE1-CZ-CE2	10.17	138.31	120.00
1	C	67	PHE	CE1-CZ-CE2	10.17	138.31	120.00
2	R	48	ARG	NE-CZ-NH2	10.17	125.39	120.30
1	M	67	PHE	CE1-CZ-CE2	10.17	138.30	120.00
2	P	123	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	E	67	PHE	CE1-CZ-CE2	10.16	138.29	120.00
1	G	67	PHE	CE1-CZ-CE2	10.16	138.29	120.00
2	L	48	ARG	NE-CZ-NH2	10.16	125.38	120.30
2	H	48	ARG	NE-CZ-NH2	10.15	125.38	120.30
1	O	67	PHE	CE1-CZ-CE2	10.14	138.26	120.00
1	K	67	PHE	CE1-CZ-CE2	10.13	138.24	120.00
1	I	67	PHE	CE1-CZ-CE2	10.12	138.23	120.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	123	ARG	NE-CZ-NH2	-10.08	115.26	120.30
2	L	123	ARG	NE-CZ-NH2	-10.06	115.27	120.30
2	D	123	ARG	NE-CZ-NH2	-10.06	115.27	120.30
2	B	123	ARG	NE-CZ-NH2	-10.04	115.28	120.30
2	N	123	ARG	NE-CZ-NH2	-10.04	115.28	120.30
2	J	123	ARG	NE-CZ-NH2	-9.99	115.31	120.30
2	R	123	ARG	NE-CZ-NH2	-9.97	115.31	120.30
2	H	123	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	K	346	TRP	CD2-CE3-CZ3	-9.88	105.96	118.80
1	M	346	TRP	CD2-CE3-CZ3	-9.87	105.96	118.80
1	C	346	TRP	CD2-CE3-CZ3	-9.86	105.98	118.80
1	I	346	TRP	CD2-CE3-CZ3	-9.86	105.98	118.80
1	E	346	TRP	CD2-CE3-CZ3	-9.86	105.99	118.80
1	A	346	TRP	CD2-CE3-CZ3	-9.84	106.01	118.80
1	Q	346	TRP	CD2-CE3-CZ3	-9.84	106.01	118.80
1	G	346	TRP	CD2-CE3-CZ3	-9.83	106.03	118.80
1	O	346	TRP	CD2-CE3-CZ3	-9.82	106.03	118.80
1	M	244	PHE	CB-CG-CD2	-9.44	114.19	120.80
2	N	253	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	O	244	PHE	CB-CG-CD2	-9.38	114.23	120.80
1	C	244	PHE	CB-CG-CD2	-9.38	114.23	120.80
1	G	244	PHE	CB-CG-CD2	-9.37	114.24	120.80
1	K	244	PHE	CB-CG-CD2	-9.35	114.25	120.80
1	Q	244	PHE	CB-CG-CD2	-9.35	114.25	120.80
1	A	244	PHE	CB-CG-CD2	-9.35	114.26	120.80
1	I	244	PHE	CB-CG-CD2	-9.34	114.26	120.80
1	K	343	PHE	CB-CG-CD1	-9.34	114.26	120.80
1	Q	343	PHE	CB-CG-CD1	-9.33	114.27	120.80
1	C	343	PHE	CB-CG-CD1	-9.33	114.27	120.80
1	M	343	PHE	CB-CG-CD1	-9.32	114.28	120.80
2	R	253	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	A	343	PHE	CB-CG-CD1	-9.30	114.29	120.80
1	E	343	PHE	CB-CG-CD1	-9.30	114.29	120.80
1	E	244	PHE	CB-CG-CD2	-9.30	114.29	120.80
1	G	343	PHE	CB-CG-CD1	-9.30	114.29	120.80
1	O	343	PHE	CB-CG-CD1	-9.29	114.30	120.80
1	I	343	PHE	CB-CG-CD1	-9.29	114.30	120.80
2	F	253	ARG	NE-CZ-NH2	9.29	124.94	120.30
2	P	253	ARG	NE-CZ-NH2	9.28	124.94	120.30
2	H	253	ARG	NE-CZ-NH2	9.27	124.93	120.30
2	J	253	ARG	NE-CZ-NH2	9.24	124.92	120.30
1	I	346	TRP	CE3-CZ3-CH2	9.24	131.36	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	253	ARG	NE-CZ-NH2	9.23	124.92	120.30
2	L	253	ARG	NE-CZ-NH2	9.23	124.92	120.30
2	D	253	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	C	346	TRP	CE3-CZ3-CH2	9.21	131.33	121.20
1	K	346	TRP	CE3-CZ3-CH2	9.20	131.32	121.20
1	M	346	TRP	CE3-CZ3-CH2	9.20	131.32	121.20
1	E	67	PHE	CD1-CE1-CZ	-9.18	109.08	120.10
1	E	346	TRP	CE3-CZ3-CH2	9.18	131.30	121.20
1	A	67	PHE	CD1-CE1-CZ	-9.17	109.09	120.10
1	A	346	TRP	CE3-CZ3-CH2	9.17	131.29	121.20
1	O	67	PHE	CD1-CE1-CZ	-9.17	109.10	120.10
1	Q	346	TRP	CE3-CZ3-CH2	9.16	131.28	121.20
1	M	67	PHE	CD1-CE1-CZ	-9.16	109.11	120.10
1	O	346	TRP	CE3-CZ3-CH2	9.15	131.27	121.20
1	K	67	PHE	CD1-CE1-CZ	-9.15	109.12	120.10
1	C	67	PHE	CD1-CE1-CZ	-9.15	109.12	120.10
1	G	346	TRP	CE3-CZ3-CH2	9.14	131.25	121.20
1	Q	67	PHE	CD1-CE1-CZ	-9.14	109.13	120.10
1	G	67	PHE	CD1-CE1-CZ	-9.13	109.14	120.10
1	I	67	PHE	CD1-CE1-CZ	-9.13	109.14	120.10
1	G	205	ASP	CB-CG-OD2	-9.06	110.15	118.30
1	K	205	ASP	CB-CG-OD2	-9.05	110.15	118.30
1	E	205	ASP	CB-CG-OD2	-9.04	110.16	118.30
1	I	205	ASP	CB-CG-OD2	-9.04	110.16	118.30
1	O	205	ASP	CB-CG-OD2	-9.04	110.16	118.30
1	A	205	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	Q	205	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	K	339	ARG	CA-C-N	-9.00	97.41	117.20
1	C	339	ARG	CA-C-N	-8.99	97.41	117.20
1	Q	339	ARG	CA-C-N	-8.99	97.42	117.20
1	M	205	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	A	339	ARG	CA-C-N	-8.99	97.43	117.20
1	M	339	ARG	CA-C-N	-8.99	97.43	117.20
1	E	339	ARG	CA-C-N	-8.97	97.45	117.20
1	I	339	ARG	CA-C-N	-8.97	97.46	117.20
1	K	343	PHE	CB-CG-CD2	8.97	127.08	120.80
1	O	339	ARG	CA-C-N	-8.97	97.46	117.20
1	G	339	ARG	CA-C-N	-8.97	97.47	117.20
1	C	205	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	C	343	PHE	CB-CG-CD2	8.95	127.06	120.80
1	M	343	PHE	CB-CG-CD2	8.93	127.05	120.80
1	O	343	PHE	CB-CG-CD2	8.92	127.05	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	343	PHE	CB-CG-CD2	8.91	127.04	120.80
1	G	343	PHE	CB-CG-CD2	8.91	127.04	120.80
1	A	343	PHE	CB-CG-CD2	8.90	127.03	120.80
1	G	98	ASP	N-CA-CB	-8.90	94.58	110.60
1	C	98	ASP	N-CA-CB	-8.89	94.59	110.60
1	I	343	PHE	CB-CG-CD2	8.89	127.03	120.80
1	Q	98	ASP	N-CA-CB	-8.89	94.59	110.60
1	M	98	ASP	N-CA-CB	-8.89	94.59	110.60
1	K	98	ASP	N-CA-CB	-8.89	94.60	110.60
1	Q	343	PHE	CB-CG-CD2	8.89	127.02	120.80
1	A	98	ASP	N-CA-CB	-8.89	94.61	110.60
1	O	98	ASP	N-CA-CB	-8.88	94.62	110.60
1	E	98	ASP	N-CA-CB	-8.87	94.63	110.60
1	I	98	ASP	N-CA-CB	-8.87	94.63	110.60
1	O	431	ASP	CB-CG-OD2	8.81	126.23	118.30
1	M	67	PHE	CZ-CE2-CD2	-8.81	109.53	120.10
1	Q	67	PHE	CZ-CE2-CD2	-8.80	109.54	120.10
1	C	67	PHE	CZ-CE2-CD2	-8.79	109.55	120.10
1	A	67	PHE	CZ-CE2-CD2	-8.78	109.56	120.10
1	K	431	ASP	CB-CG-OD2	8.78	126.20	118.30
1	G	67	PHE	CZ-CE2-CD2	-8.78	109.57	120.10
1	M	431	ASP	CB-CG-OD2	8.78	126.20	118.30
1	A	431	ASP	CB-CG-OD2	8.76	126.19	118.30
1	K	67	PHE	CZ-CE2-CD2	-8.74	109.61	120.10
1	E	67	PHE	CZ-CE2-CD2	-8.74	109.61	120.10
1	I	67	PHE	CZ-CE2-CD2	-8.74	109.61	120.10
1	Q	431	ASP	CB-CG-OD2	8.74	126.17	118.30
1	E	431	ASP	CB-CG-OD2	8.73	126.16	118.30
1	O	67	PHE	CZ-CE2-CD2	-8.73	109.62	120.10
1	I	431	ASP	CB-CG-OD2	8.72	126.15	118.30
1	C	431	ASP	CB-CG-OD2	8.71	126.14	118.30
1	G	431	ASP	CB-CG-OD2	8.71	126.14	118.30
1	G	64	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	O	64	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	Q	64	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	I	64	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	K	64	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	M	64	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	A	64	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	E	64	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	C	64	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	I	348	PRO	CA-N-CD	8.29	123.30	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	348	PRO	CA-N-CD	8.28	123.29	111.70
1	A	348	PRO	CA-N-CD	8.28	123.28	111.70
1	M	348	PRO	CA-N-CD	8.28	123.29	111.70
1	G	348	PRO	CA-N-CD	8.27	123.28	111.70
1	C	348	PRO	CA-N-CD	8.27	123.28	111.70
1	K	348	PRO	CA-N-CD	8.27	123.28	111.70
1	O	348	PRO	CA-N-CD	8.27	123.27	111.70
1	E	348	PRO	CA-N-CD	8.25	123.25	111.70
1	E	308	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	I	308	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	C	308	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	A	308	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	O	308	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	Q	308	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	G	308	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	K	308	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	M	308	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	J	436	GLN	O-C-N	8.02	135.53	122.70
2	N	436	GLN	O-C-N	8.01	135.52	122.70
2	L	436	GLN	O-C-N	8.01	135.51	122.70
2	R	436	GLN	O-C-N	8.00	135.50	122.70
2	D	436	GLN	O-C-N	8.00	135.50	122.70
2	B	436	GLN	O-C-N	8.00	135.50	122.70
2	F	436	GLN	O-C-N	8.00	135.50	122.70
2	P	436	GLN	O-C-N	8.00	135.50	122.70
2	H	436	GLN	O-C-N	7.98	135.47	122.70
2	L	408	TYR	CB-CG-CD1	-7.98	116.21	121.00
2	N	408	TYR	CB-CG-CD1	-7.98	116.21	121.00
2	D	408	TYR	CB-CG-CD1	-7.97	116.22	121.00
1	E	390	ARG	NE-CZ-NH2	7.96	124.28	120.30
2	P	408	TYR	CB-CG-CD1	-7.96	116.22	121.00
1	K	390	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	M	390	ARG	NE-CZ-NH2	7.95	124.27	120.30
1	A	390	ARG	NE-CZ-NH2	7.93	124.27	120.30
2	R	408	TYR	CB-CG-CD1	-7.93	116.25	121.00
2	B	408	TYR	CB-CG-CD1	-7.92	116.25	121.00
2	F	408	TYR	CB-CG-CD1	-7.91	116.25	121.00
1	I	390	ARG	NE-CZ-NH2	7.91	124.25	120.30
2	J	408	TYR	CB-CG-CD1	-7.91	116.26	121.00
1	Q	390	ARG	NE-CZ-NH2	7.90	124.25	120.30
2	H	408	TYR	CB-CG-CD1	-7.89	116.27	121.00
1	C	390	ARG	NE-CZ-NH2	7.89	124.24	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	390	ARG	NE-CZ-NH2	7.87	124.23	120.30
1	O	390	ARG	NE-CZ-NH2	7.85	124.23	120.30
1	C	281	ALA	C-N-CA	-7.85	102.08	121.70
1	A	281	ALA	C-N-CA	-7.83	102.11	121.70
1	G	281	ALA	C-N-CA	-7.83	102.11	121.70
1	I	281	ALA	C-N-CA	-7.83	102.12	121.70
1	M	281	ALA	C-N-CA	-7.83	102.12	121.70
1	O	281	ALA	C-N-CA	-7.83	102.13	121.70
1	Q	281	ALA	C-N-CA	-7.83	102.13	121.70
1	K	281	ALA	C-N-CA	-7.82	102.14	121.70
1	E	281	ALA	C-N-CA	-7.81	102.17	121.70
1	I	274	PRO	N-CD-CG	7.80	114.90	103.20
1	E	274	PRO	N-CD-CG	7.79	114.89	103.20
1	K	274	PRO	N-CD-CG	7.79	114.88	103.20
1	G	274	PRO	N-CD-CG	7.78	114.88	103.20
1	I	97	GLU	C-N-CA	7.77	141.13	121.70
1	A	274	PRO	N-CD-CG	7.77	114.86	103.20
1	C	274	PRO	N-CD-CG	7.77	114.85	103.20
1	O	274	PRO	N-CD-CG	7.77	114.85	103.20
1	M	274	PRO	N-CD-CG	7.77	114.85	103.20
1	C	97	GLU	C-N-CA	7.76	141.11	121.70
1	E	97	GLU	C-N-CA	7.76	141.11	121.70
1	M	97	GLU	C-N-CA	7.76	141.11	121.70
1	Q	274	PRO	N-CD-CG	7.76	114.84	103.20
1	Q	97	GLU	C-N-CA	7.75	141.09	121.70
1	A	97	GLU	C-N-CA	7.75	141.08	121.70
1	G	97	GLU	C-N-CA	7.75	141.08	121.70
1	O	97	GLU	C-N-CA	7.75	141.06	121.70
1	K	97	GLU	C-N-CA	7.74	141.05	121.70
2	J	284	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	L	164	ARG	NH1-CZ-NH2	-7.72	110.91	119.40
2	J	436	GLN	CA-C-N	-7.71	100.25	117.20
2	R	164	ARG	NH1-CZ-NH2	-7.70	110.93	119.40
2	H	215	ARG	NE-CZ-NH2	-7.70	116.45	120.30
2	J	164	ARG	NH1-CZ-NH2	-7.69	110.94	119.40
2	P	436	GLN	CA-C-N	-7.68	100.30	117.20
2	H	436	GLN	CA-C-N	-7.68	100.31	117.20
2	L	215	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	B	436	GLN	CA-C-N	-7.68	100.31	117.20
2	F	215	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	R	436	GLN	CA-C-N	-7.67	100.32	117.20
2	L	436	GLN	CA-C-N	-7.67	100.32	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	164	ARG	NH1-CZ-NH2	-7.67	110.97	119.40
2	D	436	GLN	CA-C-N	-7.67	100.33	117.20
2	D	164	ARG	NH1-CZ-NH2	-7.66	110.97	119.40
1	I	79	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	N	436	GLN	CA-C-N	-7.66	100.35	117.20
2	F	436	GLN	CA-C-N	-7.66	100.36	117.20
2	L	284	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	F	164	ARG	NH1-CZ-NH2	-7.64	111.00	119.40
2	N	164	ARG	NH1-CZ-NH2	-7.64	111.00	119.40
2	P	164	ARG	NH1-CZ-NH2	-7.63	111.01	119.40
2	R	215	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	C	79	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	F	284	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	D	284	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	H	164	ARG	NH1-CZ-NH2	-7.61	111.03	119.40
2	D	215	ARG	NE-CZ-NH2	-7.61	116.50	120.30
2	B	284	ARG	NE-CZ-NH2	-7.60	116.50	120.30
2	P	215	ARG	NE-CZ-NH2	-7.60	116.50	120.30
2	P	284	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	G	214	ARG	NE-CZ-NH2	-7.59	116.51	120.30
2	B	215	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	N	215	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	J	215	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	R	284	ARG	NE-CZ-NH2	-7.57	116.51	120.30
2	H	284	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	I	214	ARG	NE-CZ-NH2	-7.55	116.52	120.30
2	N	284	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	G	79	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	M	79	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	O	79	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	79	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	Q	214	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	Q	79	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	214	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	K	214	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	K	79	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	E	79	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	O	214	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	Q	123	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	G	98	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	M	98	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	C	98	ASP	CB-CG-OD2	-7.42	111.62	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	E	214	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	E	98	ASP	CB-CG-OD2	-7.42	111.63	118.30
1	M	123	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	M	214	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	E	408	TYR	CB-CG-CD1	-7.41	116.55	121.00
2	F	99	ALA	C-N-CA	-7.41	106.75	122.30
1	A	408	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	G	123	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	M	408	TYR	CB-CG-CD1	-7.40	116.56	121.00
2	N	99	ALA	C-N-CA	-7.40	106.76	122.30
1	K	408	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	Q	98	ASP	CB-CG-OD2	-7.40	111.64	118.30
2	J	99	ALA	C-N-CA	-7.40	106.77	122.30
2	P	99	ALA	C-N-CA	-7.40	106.76	122.30
1	E	123	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	C	408	TYR	CB-CG-CD1	-7.39	116.56	121.00
1	I	123	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	98	ASP	CB-CG-OD2	-7.39	111.65	118.30
2	L	99	ALA	C-N-CA	-7.39	106.78	122.30
2	D	99	ALA	C-N-CA	-7.39	106.79	122.30
2	B	99	ALA	C-N-CA	-7.39	106.79	122.30
2	R	99	ALA	C-N-CA	-7.39	106.79	122.30
2	H	99	ALA	C-N-CA	-7.38	106.80	122.30
1	C	123	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	Q	408	TYR	CB-CG-CD1	-7.38	116.57	121.00
1	K	123	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	I	98	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	I	408	TYR	CB-CG-CD1	-7.37	116.58	121.00
1	A	123	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	K	98	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	G	408	TYR	CB-CG-CD1	-7.36	116.59	121.00
1	O	408	TYR	CB-CG-CD1	-7.35	116.59	121.00
1	O	98	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	K	349	THR	C-N-CA	-7.33	106.90	122.30
1	O	123	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	Q	349	THR	C-N-CA	-7.33	106.90	122.30
1	A	349	THR	C-N-CA	-7.32	106.93	122.30
1	G	349	THR	C-N-CA	-7.32	106.93	122.30
1	M	349	THR	C-N-CA	-7.32	106.94	122.30
1	C	349	THR	C-N-CA	-7.31	106.94	122.30
1	I	349	THR	C-N-CA	-7.31	106.94	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	349	THR	C-N-CA	-7.31	106.94	122.30
1	E	349	THR	C-N-CA	-7.29	106.98	122.30
1	O	283	HIS	C-N-CA	-7.27	103.52	121.70
1	C	283	HIS	C-N-CA	-7.27	103.53	121.70
1	M	283	HIS	C-N-CA	-7.27	103.53	121.70
1	Q	283	HIS	C-N-CA	-7.26	103.54	121.70
1	A	283	HIS	C-N-CA	-7.25	103.56	121.70
1	E	283	HIS	C-N-CA	-7.25	103.56	121.70
1	K	283	HIS	C-N-CA	-7.25	103.57	121.70
1	I	283	HIS	C-N-CA	-7.24	103.60	121.70
1	G	283	HIS	C-N-CA	-7.22	103.64	121.70
1	M	283	HIS	CA-C-N	-7.17	101.42	117.20
1	O	283	HIS	CA-C-N	-7.17	101.42	117.20
1	C	283	HIS	CA-C-N	-7.16	101.46	117.20
1	Q	283	HIS	CA-C-N	-7.15	101.47	117.20
1	A	283	HIS	CA-C-N	-7.15	101.48	117.20
1	K	283	HIS	CA-C-N	-7.14	101.48	117.20
1	I	283	HIS	CA-C-N	-7.14	101.50	117.20
1	E	283	HIS	CA-C-N	-7.13	101.52	117.20
1	G	283	HIS	CA-C-N	-7.13	101.52	117.20
2	R	88	ARG	NE-CZ-NH1	7.05	123.82	120.30
2	H	88	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	I	349	THR	CA-C-N	-7.00	102.21	116.20
1	K	349	THR	CA-C-N	-6.99	102.21	116.20
2	H	312	TYR	CB-CG-CD2	-6.99	116.81	121.00
2	D	312	TYR	CB-CG-CD2	-6.99	116.81	121.00
2	L	88	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	M	349	THR	CA-C-N	-6.99	102.23	116.20
1	Q	349	THR	CA-C-N	-6.98	102.23	116.20
1	A	349	THR	CA-C-N	-6.98	102.24	116.20
1	E	349	THR	CA-C-N	-6.98	102.23	116.20
2	P	312	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	G	349	THR	CA-C-N	-6.98	102.24	116.20
2	P	88	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	C	349	THR	CA-C-N	-6.97	102.25	116.20
2	R	312	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	O	349	THR	CA-C-N	-6.97	102.26	116.20
2	N	312	TYR	CB-CG-CD2	-6.96	116.82	121.00
2	R	320	ARG	NE-CZ-NH2	6.96	123.78	120.30
2	N	88	ARG	NE-CZ-NH1	6.95	123.77	120.30
2	B	312	TYR	CB-CG-CD2	-6.94	116.83	121.00
2	F	320	ARG	NE-CZ-NH2	6.94	123.77	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	88	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	K	205	ASP	CB-CG-OD1	6.93	124.54	118.30
1	K	308	ARG	NE-CZ-NH2	-6.93	116.83	120.30
2	F	312	TYR	CB-CG-CD2	-6.93	116.84	121.00
2	P	48	ARG	NE-CZ-NH1	-6.93	116.84	120.30
2	J	312	TYR	CB-CG-CD2	-6.92	116.84	121.00
2	B	88	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	D	88	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	I	308	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	F	48	ARG	NE-CZ-NH1	-6.91	116.84	120.30
2	L	312	TYR	CB-CG-CD2	-6.91	116.85	121.00
1	E	21	TRP	CA-CB-CG	-6.91	100.58	113.70
2	D	320	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	I	205	ASP	CB-CG-OD1	6.90	124.51	118.30
1	Q	21	TRP	CA-CB-CG	-6.90	100.59	113.70
2	B	320	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	I	21	TRP	CA-CB-CG	-6.90	100.59	113.70
1	A	21	TRP	CA-CB-CG	-6.89	100.60	113.70
1	G	205	ASP	CB-CG-OD1	6.89	124.50	118.30
1	K	21	TRP	CA-CB-CG	-6.89	100.60	113.70
1	O	21	TRP	CA-CB-CG	-6.89	100.60	113.70
1	Q	205	ASP	CB-CG-OD1	6.89	124.50	118.30
1	M	205	ASP	CB-CG-OD1	6.89	124.50	118.30
1	C	21	TRP	CA-CB-CG	-6.89	100.61	113.70
1	E	205	ASP	CB-CG-OD1	6.89	124.50	118.30
2	H	320	ARG	NE-CZ-NH2	6.89	123.74	120.30
1	M	21	TRP	CA-CB-CG	-6.89	100.62	113.70
1	C	308	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	205	ASP	CB-CG-OD1	6.88	124.49	118.30
1	G	21	TRP	CA-CB-CG	-6.88	100.63	113.70
1	O	205	ASP	CB-CG-OD1	6.88	124.49	118.30
2	P	320	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	E	308	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	J	320	ARG	NE-CZ-NH2	6.88	123.74	120.30
2	L	48	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	C	205	ASP	CB-CG-OD1	6.87	124.48	118.30
2	H	48	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	308	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	Q	308	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	N	320	ARG	NE-CZ-NH2	6.86	123.73	120.30
2	L	320	ARG	NE-CZ-NH2	6.85	123.73	120.30
2	B	48	ARG	NE-CZ-NH1	-6.85	116.87	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	88	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	J	64	ARG	NH1-CZ-NH2	-6.85	111.86	119.40
2	P	64	ARG	NH1-CZ-NH2	-6.85	111.87	119.40
1	O	308	ARG	NE-CZ-NH2	-6.85	116.88	120.30
2	J	48	ARG	NE-CZ-NH1	-6.84	116.88	120.30
2	R	64	ARG	NH1-CZ-NH2	-6.84	111.88	119.40
2	D	64	ARG	NH1-CZ-NH2	-6.84	111.88	119.40
2	F	64	ARG	NH1-CZ-NH2	-6.83	111.88	119.40
1	G	308	ARG	NE-CZ-NH2	-6.83	116.89	120.30
2	D	48	ARG	NE-CZ-NH1	-6.82	116.89	120.30
2	B	64	ARG	NH1-CZ-NH2	-6.82	111.90	119.40
2	N	48	ARG	NE-CZ-NH1	-6.81	116.89	120.30
2	L	64	ARG	NH1-CZ-NH2	-6.81	111.91	119.40
2	H	64	ARG	NH1-CZ-NH2	-6.80	111.92	119.40
2	N	64	ARG	NH1-CZ-NH2	-6.80	111.92	119.40
1	M	308	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	K	436	GLY	C-N-CA	-6.74	104.85	121.70
2	R	48	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	C	436	GLY	C-N-CA	-6.73	104.86	121.70
1	I	436	GLY	C-N-CA	-6.73	104.88	121.70
1	M	436	GLY	C-N-CA	-6.73	104.88	121.70
1	A	436	GLY	C-N-CA	-6.73	104.88	121.70
1	O	436	GLY	C-N-CA	-6.72	104.90	121.70
1	Q	436	GLY	C-N-CA	-6.72	104.90	121.70
1	E	436	GLY	C-N-CA	-6.72	104.90	121.70
1	O	284	GLU	CA-C-N	-6.72	102.42	117.20
1	I	161	TYR	CB-CG-CD2	-6.71	116.97	121.00
1	Q	284	GLU	CA-C-N	-6.71	102.44	117.20
1	G	161	TYR	CB-CG-CD2	-6.71	116.98	121.00
1	G	284	GLU	CA-C-N	-6.71	102.45	117.20
1	G	436	GLY	C-N-CA	-6.71	104.94	121.70
1	A	284	GLU	CA-C-N	-6.70	102.45	117.20
1	C	284	GLU	CA-C-N	-6.70	102.46	117.20
1	I	284	GLU	CA-C-N	-6.70	102.46	117.20
1	E	284	GLU	CA-C-N	-6.70	102.47	117.20
1	M	284	GLU	CA-C-N	-6.69	102.48	117.20
1	K	284	GLU	CA-C-N	-6.68	102.50	117.20
1	K	161	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	A	161	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	C	161	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	M	161	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	E	161	TYR	CB-CG-CD2	-6.61	117.03	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	210	TYR	CB-CG-CD2	-6.61	117.04	121.00
1	O	98	ASP	CA-CB-CG	6.60	127.91	113.40
1	I	98	ASP	CA-CB-CG	6.59	127.91	113.40
1	E	98	ASP	CA-CB-CG	6.59	127.90	113.40
2	J	400	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	98	ASP	CA-CB-CG	6.58	127.88	113.40
1	O	161	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	Q	161	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	Q	98	ASP	CA-CB-CG	6.58	127.87	113.40
1	K	98	ASP	CA-CB-CG	6.58	127.87	113.40
1	M	98	ASP	CA-CB-CG	6.57	127.86	113.40
1	O	210	TYR	CB-CG-CD2	-6.57	117.06	121.00
2	R	400	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	C	121	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	G	98	ASP	CA-CB-CG	6.57	127.84	113.40
1	C	98	ASP	CA-CB-CG	6.56	127.82	113.40
2	N	400	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	I	121	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	K	121	ARG	NE-CZ-NH1	6.55	123.57	120.30
2	P	400	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	E	210	TYR	CB-CG-CD2	-6.54	117.08	121.00
2	B	400	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	210	TYR	CB-CG-CD2	-6.51	117.09	121.00
2	D	400	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	121	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	H	400	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	L	400	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	C	210	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	M	210	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	M	121	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	O	121	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	K	210	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	G	97	GLU	CA-C-N	-6.45	103.01	117.20
1	G	210	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	Q	121	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	F	400	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	I	210	TYR	CB-CG-CD2	-6.44	117.13	121.00
1	O	97	GLU	CA-C-N	-6.44	103.03	117.20
1	A	97	GLU	CA-C-N	-6.44	103.04	117.20
1	K	97	GLU	CA-C-N	-6.43	103.04	117.20
1	E	121	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	E	97	GLU	CA-C-N	-6.43	103.05	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	97	GLU	CA-C-N	-6.43	103.05	117.20
1	C	97	GLU	CA-C-N	-6.43	103.05	117.20
1	Q	97	GLU	CA-C-N	-6.43	103.06	117.20
1	I	97	GLU	CA-C-N	-6.42	103.08	117.20
1	G	121	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	K	301	GLN	N-CA-C	6.37	128.20	111.00
1	O	301	GLN	N-CA-C	6.37	128.19	111.00
1	A	301	GLN	N-CA-C	6.36	128.17	111.00
1	I	301	GLN	N-CA-C	6.36	128.18	111.00
1	G	301	GLN	N-CA-C	6.36	128.16	111.00
1	C	301	GLN	N-CA-C	6.35	128.15	111.00
1	Q	301	GLN	N-CA-C	6.35	128.14	111.00
1	M	301	GLN	N-CA-C	6.34	128.13	111.00
1	E	301	GLN	N-CA-C	6.34	128.12	111.00
1	M	98	ASP	CA-C-N	-6.33	103.28	117.20
1	C	98	ASP	CA-C-N	-6.32	103.31	117.20
1	G	98	ASP	CA-C-N	-6.32	103.30	117.20
1	I	282	TYR	C-N-CA	-6.32	105.91	121.70
1	K	282	TYR	C-N-CA	-6.31	105.92	121.70
1	Q	282	TYR	C-N-CA	-6.31	105.92	121.70
1	A	98	ASP	CA-C-N	-6.31	103.32	117.20
1	C	282	TYR	C-N-CA	-6.31	105.93	121.70
1	I	98	ASP	CA-C-N	-6.31	103.32	117.20
1	A	282	TYR	C-N-CA	-6.30	105.94	121.70
1	O	282	TYR	C-N-CA	-6.30	105.95	121.70
1	Q	98	ASP	CA-C-N	-6.30	103.34	117.20
1	E	98	ASP	CA-C-N	-6.30	103.35	117.20
1	M	282	TYR	C-N-CA	-6.30	105.96	121.70
1	G	282	TYR	C-N-CA	-6.29	105.96	121.70
1	E	282	TYR	C-N-CA	-6.29	105.97	121.70
1	K	98	ASP	CA-C-N	-6.29	103.37	117.20
1	O	98	ASP	CA-C-N	-6.29	103.36	117.20
1	I	243	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	O	283	HIS	O-C-N	6.25	132.70	122.70
1	E	243	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	Q	283	HIS	O-C-N	6.22	132.66	122.70
1	C	283	HIS	O-C-N	6.22	132.65	122.70
1	K	243	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	M	283	HIS	O-C-N	6.21	132.63	122.70
2	D	110	GLU	C-N-CA	-6.20	109.28	122.30
1	A	283	HIS	O-C-N	6.20	132.62	122.70
1	K	283	HIS	O-C-N	6.20	132.62	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH1	-6.20	117.20	120.30
2	F	110	GLU	C-N-CA	-6.20	109.29	122.30
2	N	110	GLU	C-N-CA	-6.20	109.29	122.30
1	E	283	HIS	O-C-N	6.19	132.60	122.70
1	K	98	ASP	N-CA-C	6.19	127.71	111.00
2	P	110	GLU	C-N-CA	-6.19	109.30	122.30
1	Q	98	ASP	N-CA-C	6.19	127.71	111.00
2	H	110	GLU	C-N-CA	-6.18	109.31	122.30
1	O	98	ASP	N-CA-C	6.18	127.70	111.00
2	J	110	GLU	C-N-CA	-6.18	109.32	122.30
2	L	266	HIS	CA-CB-CG	-6.18	103.09	113.60
2	B	110	GLU	C-N-CA	-6.18	109.32	122.30
2	N	266	HIS	CA-CB-CG	-6.18	103.09	113.60
1	Q	243	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	A	98	ASP	N-CA-C	6.17	127.67	111.00
1	E	98	ASP	N-CA-C	6.17	127.66	111.00
2	H	266	HIS	CA-CB-CG	-6.17	103.11	113.60
1	M	274	PRO	N-CA-CB	6.17	110.71	103.30
2	R	110	GLU	C-N-CA	-6.17	109.34	122.30
1	I	283	HIS	O-C-N	6.17	132.57	122.70
2	B	266	HIS	CA-CB-CG	-6.17	103.11	113.60
1	C	98	ASP	N-CA-C	6.17	127.66	111.00
1	G	98	ASP	N-CA-C	6.17	127.65	111.00
2	P	53	TYR	CB-CG-CD1	-6.17	117.30	121.00
2	R	266	HIS	CA-CB-CG	-6.17	103.11	113.60
1	C	274	PRO	N-CA-CB	6.17	110.70	103.30
2	P	266	HIS	CA-CB-CG	-6.17	103.12	113.60
2	D	266	HIS	CA-CB-CG	-6.16	103.12	113.60
1	M	98	ASP	N-CA-C	6.16	127.64	111.00
2	R	53	TYR	CB-CG-CD1	-6.16	117.30	121.00
2	F	266	HIS	CA-CB-CG	-6.16	103.13	113.60
2	J	266	HIS	CA-CB-CG	-6.16	103.13	113.60
1	G	283	HIS	O-C-N	6.16	132.55	122.70
1	I	98	ASP	N-CA-C	6.16	127.62	111.00
2	L	110	GLU	C-N-CA	-6.16	109.37	122.30
1	O	274	PRO	N-CA-CB	6.16	110.69	103.30
1	A	274	PRO	N-CA-CB	6.15	110.68	103.30
1	E	274	PRO	N-CA-CB	6.15	110.68	103.30
1	G	243	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	G	274	PRO	N-CA-CB	6.15	110.68	103.30
1	Q	274	PRO	N-CA-CB	6.15	110.68	103.30
1	C	243	ARG	NE-CZ-NH1	-6.14	117.23	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	251	ASP	CB-CG-OD1	6.14	123.83	118.30
1	K	274	PRO	N-CA-CB	6.14	110.67	103.30
2	L	53	TYR	CB-CG-CD1	-6.14	117.32	121.00
1	M	243	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	I	274	PRO	N-CA-CB	6.12	110.65	103.30
2	D	251	ASP	CB-CG-OD1	6.12	123.81	118.30
2	H	53	TYR	CB-CG-CD1	-6.12	117.33	121.00
2	F	53	TYR	CB-CG-CD1	-6.12	117.33	121.00
2	P	251	ASP	CB-CG-OD1	6.11	123.80	118.30
2	B	53	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	O	432	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	O	390	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
1	I	390	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
1	K	390	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	G	432	TYR	CB-CG-CD1	-6.09	117.35	121.00
1	O	243	ARG	NE-CZ-NH1	-6.09	117.25	120.30
2	B	251	ASP	CB-CG-OD1	6.09	123.78	118.30
2	D	79	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	390	ARG	NH1-CZ-NH2	-6.08	112.71	119.40
2	R	251	ASP	CB-CG-OD1	6.08	123.77	118.30
2	J	53	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	A	390	ARG	NH1-CZ-NH2	-6.08	112.72	119.40
2	H	251	ASP	CB-CG-OD1	6.08	123.77	118.30
1	M	432	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	E	390	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
2	L	251	ASP	CB-CG-OD1	6.07	123.77	118.30
2	R	79	ARG	NE-CZ-NH1	6.07	123.34	120.30
2	D	53	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	C	142	GLY	C-N-CA	-6.07	109.56	122.30
1	I	142	GLY	C-N-CA	-6.06	109.57	122.30
1	M	142	GLY	C-N-CA	-6.06	109.57	122.30
1	Q	390	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
2	R	158	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	G	142	GLY	C-N-CA	-6.06	109.58	122.30
1	K	142	GLY	C-N-CA	-6.06	109.58	122.30
1	A	142	GLY	C-N-CA	-6.05	109.59	122.30
2	N	53	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	E	142	GLY	C-N-CA	-6.05	109.60	122.30
2	N	158	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	O	142	GLY	C-N-CA	-6.05	109.60	122.30
2	J	79	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	M	390	ARG	NH1-CZ-NH2	-6.04	112.75	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	79	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	G	390	ARG	NH1-CZ-NH2	-6.04	112.76	119.40
2	L	34	GLY	N-CA-C	6.04	128.19	113.10
1	C	432	TYR	CB-CG-CD1	-6.03	117.38	121.00
2	N	251	ASP	CB-CG-OD1	6.03	123.73	118.30
1	Q	142	GLY	C-N-CA	-6.03	109.63	122.30
2	B	79	ARG	NE-CZ-NH1	6.03	123.32	120.30
2	P	158	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	A	432	TYR	CB-CG-CD1	-6.03	117.38	121.00
2	J	34	GLY	N-CA-C	6.02	128.16	113.10
2	D	158	ARG	NE-CZ-NH2	6.02	123.31	120.30
2	F	34	GLY	N-CA-C	6.02	128.15	113.10
2	J	251	ASP	CB-CG-OD1	6.02	123.72	118.30
2	P	34	GLY	N-CA-C	6.02	128.14	113.10
2	H	34	GLY	N-CA-C	6.02	128.14	113.10
2	B	34	GLY	N-CA-C	6.01	128.13	113.10
2	D	34	GLY	N-CA-C	6.01	128.13	113.10
2	B	158	ARG	NE-CZ-NH2	6.01	123.30	120.30
2	F	79	ARG	NE-CZ-NH1	6.01	123.30	120.30
2	N	34	GLY	N-CA-C	6.00	128.11	113.10
1	K	348	PRO	C-N-CA	-6.00	106.70	121.70
1	E	432	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	G	348	PRO	C-N-CA	-6.00	106.71	121.70
1	I	432	TYR	CB-CG-CD1	-6.00	117.40	121.00
2	J	158	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	E	348	PRO	C-N-CA	-5.99	106.72	121.70
1	Q	348	PRO	C-N-CA	-5.99	106.72	121.70
2	R	34	GLY	N-CA-C	5.99	128.08	113.10
1	A	348	PRO	C-N-CA	-5.99	106.73	121.70
1	Q	432	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	M	348	PRO	C-N-CA	-5.99	106.73	121.70
1	C	348	PRO	C-N-CA	-5.98	106.75	121.70
1	O	348	PRO	C-N-CA	-5.98	106.75	121.70
1	I	348	PRO	C-N-CA	-5.98	106.76	121.70
1	K	432	TYR	CB-CG-CD1	-5.96	117.42	121.00
2	P	79	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	I	273	ALA	C-N-CA	-5.96	96.98	122.00
2	H	158	ARG	NE-CZ-NH2	5.96	123.28	120.30
2	L	79	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	G	273	ALA	C-N-CA	-5.95	97.00	122.00
1	K	437	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	C	273	ALA	C-N-CA	-5.95	97.01	122.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	437	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	O	273	ALA	C-N-CA	-5.95	97.01	122.00
1	A	273	ALA	C-N-CA	-5.95	97.02	122.00
1	E	273	ALA	C-N-CA	-5.95	97.02	122.00
2	L	158	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	Q	273	ALA	C-N-CA	-5.95	97.03	122.00
1	K	273	ALA	C-N-CA	-5.94	97.04	122.00
1	A	437	VAL	CG1-CB-CG2	-5.94	101.39	110.90
1	M	273	ALA	C-N-CA	-5.94	97.05	122.00
1	I	437	VAL	CG1-CB-CG2	-5.94	101.40	110.90
2	F	158	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	Q	437	VAL	CG1-CB-CG2	-5.93	101.41	110.90
1	O	437	VAL	CG1-CB-CG2	-5.93	101.41	110.90
1	E	437	VAL	CG1-CB-CG2	-5.93	101.42	110.90
1	C	437	VAL	CG1-CB-CG2	-5.92	101.42	110.90
1	M	437	VAL	CG1-CB-CG2	-5.92	101.43	110.90
2	N	253	ARG	NH1-CZ-NH2	-5.91	112.89	119.40
2	N	378	ILE	C-N-CA	-5.90	109.90	122.30
2	D	378	ILE	C-N-CA	-5.90	109.91	122.30
2	J	52	TYR	CB-CG-CD1	-5.90	117.46	121.00
2	B	378	ILE	C-N-CA	-5.90	109.92	122.30
2	P	253	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
2	R	378	ILE	C-N-CA	-5.89	109.92	122.30
2	H	79	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	P	378	ILE	C-N-CA	-5.89	109.93	122.30
2	F	253	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
2	J	378	ILE	C-N-CA	-5.89	109.94	122.30
2	L	378	ILE	C-N-CA	-5.88	109.94	122.30
2	H	52	TYR	CB-CG-CD1	-5.88	117.47	121.00
2	H	378	ILE	C-N-CA	-5.88	109.95	122.30
2	F	378	ILE	C-N-CA	-5.88	109.96	122.30
2	D	253	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
2	H	253	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
2	J	253	ARG	NH1-CZ-NH2	-5.87	112.95	119.40
2	R	253	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
1	M	282	TYR	CA-CB-CG	-5.86	102.27	113.40
1	G	214	ARG	NH1-CZ-NH2	5.86	125.84	119.40
1	I	214	ARG	NH1-CZ-NH2	5.85	125.84	119.40
1	O	214	ARG	NH1-CZ-NH2	5.85	125.84	119.40
2	L	253	ARG	NH1-CZ-NH2	-5.85	112.96	119.40
2	F	52	TYR	CB-CG-CD1	-5.85	117.49	121.00
2	P	52	TYR	CB-CG-CD1	-5.85	117.49	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	253	ARG	NH1-CZ-NH2	-5.84	112.97	119.40
1	G	282	TYR	CA-CB-CG	-5.84	102.30	113.40
1	E	282	TYR	CA-CB-CG	-5.84	102.30	113.40
1	A	282	TYR	CA-CB-CG	-5.84	102.31	113.40
1	A	214	ARG	NH1-CZ-NH2	5.83	125.82	119.40
1	E	214	ARG	NH1-CZ-NH2	5.83	125.82	119.40
1	K	282	TYR	CA-CB-CG	-5.83	102.32	113.40
1	Q	262	TYR	CB-CA-C	-5.83	98.74	110.40
1	Q	282	TYR	CA-CB-CG	-5.83	102.32	113.40
1	O	262	TYR	CB-CA-C	-5.83	98.74	110.40
1	C	282	TYR	CA-CB-CG	-5.83	102.33	113.40
1	K	262	TYR	CB-CA-C	-5.83	98.75	110.40
1	O	282	TYR	CA-CB-CG	-5.83	102.33	113.40
2	N	28	HIS	CA-CB-CG	-5.82	103.70	113.60
1	M	422	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	L	52	TYR	CB-CG-CD1	-5.82	117.51	121.00
2	D	28	HIS	CA-CB-CG	-5.82	103.71	113.60
1	G	262	TYR	CB-CA-C	-5.82	98.77	110.40
1	A	262	TYR	CB-CA-C	-5.82	98.77	110.40
2	B	52	TYR	CB-CG-CD1	-5.82	117.51	121.00
2	F	28	HIS	CA-CB-CG	-5.82	103.71	113.60
2	J	28	HIS	CA-CB-CG	-5.82	103.71	113.60
1	C	214	ARG	NH1-CZ-NH2	5.81	125.80	119.40
1	M	262	TYR	CB-CA-C	-5.81	98.77	110.40
1	I	262	TYR	CB-CA-C	-5.81	98.78	110.40
1	I	282	TYR	CA-CB-CG	-5.81	102.36	113.40
1	M	214	ARG	NH1-CZ-NH2	5.81	125.79	119.40
2	B	28	HIS	CA-CB-CG	-5.81	103.73	113.60
1	C	262	TYR	CB-CA-C	-5.81	98.78	110.40
1	Q	422	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	K	214	ARG	NH1-CZ-NH2	5.80	125.79	119.40
2	P	28	HIS	CA-CB-CG	-5.80	103.74	113.60
1	Q	214	ARG	NH1-CZ-NH2	5.80	125.78	119.40
2	R	28	HIS	CA-CB-CG	-5.80	103.74	113.60
1	E	422	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	E	262	TYR	CB-CA-C	-5.79	98.81	110.40
2	H	28	HIS	CA-CB-CG	-5.79	103.76	113.60
2	L	28	HIS	CA-CB-CG	-5.79	103.76	113.60
1	I	422	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	N	52	TYR	CB-CG-CD1	-5.78	117.53	121.00
2	R	52	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	O	422	ARG	NE-CZ-NH2	-5.77	117.41	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	422	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	Q	339	ARG	O-C-N	5.77	131.93	122.70
1	A	422	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	D	52	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	C	339	ARG	O-C-N	5.75	131.90	122.70
1	I	221	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	M	339	ARG	O-C-N	5.75	131.90	122.70
1	A	339	ARG	O-C-N	5.73	131.87	122.70
1	K	422	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	E	221	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	I	339	ARG	O-C-N	5.72	131.86	122.70
1	K	339	ARG	O-C-N	5.72	131.84	122.70
1	O	339	ARG	O-C-N	5.72	131.84	122.70
1	Q	221	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	E	339	ARG	O-C-N	5.71	131.84	122.70
1	C	422	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	O	273	ALA	CA-C-O	-5.70	108.13	120.10
1	G	339	ARG	O-C-N	5.70	131.82	122.70
1	M	49	PHE	C-N-CA	-5.70	107.46	121.70
1	I	273	ALA	CA-C-O	-5.69	108.16	120.10
1	O	49	PHE	C-N-CA	-5.69	107.48	121.70
1	A	273	ALA	CA-C-O	-5.68	108.17	120.10
1	I	67	PHE	CB-CG-CD1	-5.68	116.82	120.80
1	E	273	ALA	CA-C-O	-5.68	108.17	120.10
1	M	273	ALA	CA-C-O	-5.68	108.18	120.10
1	A	49	PHE	C-N-CA	-5.68	107.51	121.70
1	I	49	PHE	C-N-CA	-5.68	107.51	121.70
1	K	273	ALA	CA-C-O	-5.68	108.18	120.10
1	C	273	ALA	CA-C-O	-5.67	108.19	120.10
1	G	273	ALA	CA-C-O	-5.67	108.19	120.10
1	C	49	PHE	C-N-CA	-5.67	107.53	121.70
1	E	49	PHE	C-N-CA	-5.67	107.53	121.70
1	K	221	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	Q	273	ALA	CA-C-O	-5.67	108.20	120.10
1	G	49	PHE	C-N-CA	-5.67	107.53	121.70
1	K	49	PHE	C-N-CA	-5.67	107.54	121.70
1	Q	49	PHE	C-N-CA	-5.66	107.55	121.70
1	M	67	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	A	67	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	G	67	PHE	CB-CG-CD1	-5.65	116.84	120.80
1	E	67	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	Q	67	PHE	CB-CG-CD1	-5.64	116.85	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	67	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	K	244	PHE	CD1-CE1-CZ	-5.62	113.35	120.10
1	K	67	PHE	CB-CG-CD1	-5.61	116.87	120.80
1	M	221	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	I	244	PHE	CD1-CE1-CZ	-5.60	113.38	120.10
1	O	221	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	P	161	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	O	244	PHE	CD1-CE1-CZ	-5.58	113.40	120.10
1	I	265	GLY	C-N-CA	-5.58	107.74	121.70
1	C	244	PHE	CD1-CE1-CZ	-5.58	113.40	120.10
1	O	67	PHE	CB-CG-CD1	-5.58	116.89	120.80
1	A	244	PHE	CD1-CE1-CZ	-5.57	113.41	120.10
1	A	265	GLY	C-N-CA	-5.57	107.77	121.70
1	M	244	PHE	CD1-CE1-CZ	-5.57	113.41	120.10
1	C	265	GLY	C-N-CA	-5.57	107.77	121.70
1	G	265	GLY	C-N-CA	-5.57	107.77	121.70
1	E	244	PHE	CD1-CE1-CZ	-5.57	113.42	120.10
1	K	265	GLY	C-N-CA	-5.57	107.77	121.70
1	M	265	GLY	C-N-CA	-5.57	107.77	121.70
1	Q	265	GLY	C-N-CA	-5.57	107.77	121.70
1	C	221	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	E	265	GLY	C-N-CA	-5.57	107.78	121.70
1	O	390	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	O	265	GLY	C-N-CA	-5.56	107.79	121.70
1	G	244	PHE	CD1-CE1-CZ	-5.56	113.43	120.10
1	G	221	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	N	161	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	Q	244	PHE	CD1-CE1-CZ	-5.54	113.45	120.10
2	R	161	TYR	CB-CG-CD2	-5.53	117.68	121.00
2	D	161	TYR	CB-CG-CD2	-5.53	117.68	121.00
2	B	161	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	K	21	TRP	CZ3-CH2-CZ2	-5.51	114.98	121.60
2	H	273	ALA	N-CA-C	5.51	125.88	111.00
2	J	273	ALA	N-CA-C	5.51	125.88	111.00
2	L	273	ALA	N-CA-C	5.51	125.87	111.00
2	F	273	ALA	N-CA-C	5.51	125.87	111.00
1	I	390	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	G	21	TRP	CZ3-CH2-CZ2	-5.50	114.99	121.60
2	H	161	TYR	CB-CG-CD2	-5.50	117.70	121.00
2	B	273	ALA	N-CA-C	5.50	125.85	111.00
1	C	390	ARG	NE-CZ-NH1	5.50	123.05	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	273	ALA	N-CA-C	5.50	125.84	111.00
2	P	273	ALA	N-CA-C	5.50	125.84	111.00
1	C	21	TRP	CZ3-CH2-CZ2	-5.49	115.01	121.60
2	L	161	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	I	21	TRP	CZ3-CH2-CZ2	-5.49	115.01	121.60
2	N	273	ALA	N-CA-C	5.49	125.82	111.00
1	O	214	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	E	214	ARG	NE-CZ-NH1	-5.49	117.56	120.30
2	D	273	ALA	N-CA-C	5.49	125.81	111.00
1	A	21	TRP	CZ3-CH2-CZ2	-5.48	115.02	121.60
1	Q	21	TRP	CZ3-CH2-CZ2	-5.48	115.02	121.60
1	M	21	TRP	CZ3-CH2-CZ2	-5.48	115.03	121.60
2	F	161	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	G	35	GLN	CA-C-N	-5.47	105.16	117.20
1	O	35	GLN	CA-C-N	-5.46	105.18	117.20
1	O	21	TRP	CZ3-CH2-CZ2	-5.46	115.05	121.60
2	J	161	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	E	98	ASP	CB-CG-OD1	5.45	123.21	118.30
1	K	390	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	N	185	TYR	CD1-CG-CD2	5.45	123.90	117.90
1	E	35	GLN	CA-C-N	-5.45	105.21	117.20
1	G	435	VAL	C-N-CA	-5.45	110.86	122.30
1	C	35	GLN	CA-C-N	-5.45	105.22	117.20
1	K	98	ASP	CB-CG-OD1	5.45	123.20	118.30
1	M	35	GLN	CA-C-N	-5.45	105.22	117.20
1	C	98	ASP	CB-CG-OD1	5.44	123.20	118.30
1	E	435	VAL	C-N-CA	-5.44	110.87	122.30
1	I	435	VAL	C-N-CA	-5.44	110.88	122.30
1	A	35	GLN	CA-C-N	-5.44	105.23	117.20
1	C	214	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	390	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	435	VAL	C-N-CA	-5.44	110.88	122.30
1	E	21	TRP	CZ3-CH2-CZ2	-5.44	115.08	121.60
1	G	98	ASP	CB-CG-OD1	5.44	123.19	118.30
1	K	435	VAL	C-N-CA	-5.44	110.88	122.30
1	Q	35	GLN	CA-C-N	-5.44	105.24	117.20
1	A	435	VAL	C-N-CA	-5.43	110.89	122.30
2	F	432	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	M	214	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	I	264	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	F	185	TYR	CD1-CG-CD2	5.42	123.87	117.90
1	O	435	VAL	C-N-CA	-5.42	110.91	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	390	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	M	435	VAL	C-N-CA	-5.42	110.91	122.30
1	K	35	GLN	CA-C-N	-5.42	105.27	117.20
2	P	185	TYR	CD1-CG-CD2	5.42	123.86	117.90
1	G	390	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	214	ARG	NE-CZ-NH1	-5.42	117.59	120.30
2	B	185	TYR	CD1-CG-CD2	5.42	123.86	117.90
1	E	264	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	I	35	GLN	CA-C-N	-5.41	105.29	117.20
1	C	264	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	98	ASP	CB-CG-OD1	5.41	123.17	118.30
1	Q	98	ASP	CB-CG-OD1	5.41	123.17	118.30
1	Q	435	VAL	C-N-CA	-5.41	110.95	122.30
2	D	185	TYR	CD1-CG-CD2	5.40	123.84	117.90
2	L	61	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	E	390	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	L	185	TYR	CD1-CG-CD2	5.40	123.84	117.90
1	M	264	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	M	98	ASP	CB-CG-OD1	5.40	123.16	118.30
2	N	398	MET	CG-SD-CE	-5.39	91.57	100.20
2	R	185	TYR	CD1-CG-CD2	5.39	123.83	117.90
2	L	398	MET	CG-SD-CE	-5.39	91.57	100.20
2	D	398	MET	CG-SD-CE	-5.39	91.58	100.20
1	I	214	ARG	NE-CZ-NH1	-5.39	117.61	120.30
2	J	398	MET	CG-SD-CE	-5.39	91.58	100.20
2	H	185	TYR	CD1-CG-CD2	5.39	123.83	117.90
2	R	398	MET	CG-SD-CE	-5.39	91.58	100.20
2	N	432	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	B	398	MET	CG-SD-CE	-5.38	91.59	100.20
2	J	432	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	F	398	MET	CG-SD-CE	-5.38	91.60	100.20
2	J	185	TYR	CD1-CG-CD2	5.38	123.81	117.90
1	I	98	ASP	CB-CG-OD1	5.37	123.14	118.30
2	H	398	MET	CG-SD-CE	-5.37	91.61	100.20
2	R	432	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	B	432	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	O	98	ASP	CB-CG-OD1	5.37	123.13	118.30
2	P	398	MET	CG-SD-CE	-5.37	91.61	100.20
1	G	214	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	264	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	K	214	ARG	NE-CZ-NH1	-5.36	117.62	120.30
2	L	432	TYR	CB-CG-CD2	-5.36	117.78	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	432	TYR	CB-CG-CD2	-5.36	117.79	121.00
2	P	432	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	G	348	PRO	N-CA-C	5.35	126.02	112.10
1	K	346	TRP	CE2-CD2-CE3	5.35	125.12	118.70
1	M	346	TRP	CE2-CD2-CE3	5.35	125.12	118.70
1	C	346	TRP	CE2-CD2-CE3	5.35	125.12	118.70
1	I	346	TRP	CE2-CD2-CE3	5.35	125.12	118.70
1	E	346	TRP	CE2-CD2-CE3	5.35	125.12	118.70
1	C	348	PRO	N-CA-C	5.34	126.00	112.10
1	M	390	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	P	61	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	M	348	PRO	N-CA-C	5.34	125.99	112.10
1	A	348	PRO	N-CA-C	5.34	125.98	112.10
1	O	346	TRP	CE2-CD2-CE3	5.34	125.11	118.70
1	G	346	TRP	CE2-CD2-CE3	5.34	125.10	118.70
1	Q	348	PRO	N-CA-C	5.34	125.97	112.10
1	E	348	PRO	N-CA-C	5.33	125.97	112.10
2	N	61	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	346	TRP	CE2-CD2-CE3	5.33	125.10	118.70
1	O	264	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	O	348	PRO	N-CA-C	5.33	125.96	112.10
1	K	348	PRO	N-CA-C	5.33	125.96	112.10
2	F	61	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	I	348	PRO	N-CA-C	5.33	125.95	112.10
2	R	61	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	O	339	ARG	N-CA-C	5.33	125.38	111.00
1	M	339	ARG	N-CA-C	5.32	125.38	111.00
1	E	339	ARG	N-CA-C	5.32	125.37	111.00
1	K	339	ARG	N-CA-C	5.32	125.36	111.00
1	Q	339	ARG	N-CA-C	5.32	125.37	111.00
1	Q	346	TRP	CE2-CD2-CE3	5.32	125.08	118.70
1	G	339	ARG	N-CA-C	5.32	125.36	111.00
1	K	312	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	Q	312	TYR	CB-CG-CD1	-5.32	117.81	121.00
2	R	138	THR	CA-CB-CG2	-5.32	104.95	112.40
2	H	61	TYR	CB-CG-CD2	-5.32	117.81	121.00
2	J	138	THR	CA-CB-CG2	-5.31	104.96	112.40
1	Q	264	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	339	ARG	N-CA-C	5.31	125.34	111.00
1	I	339	ARG	N-CA-C	5.31	125.34	111.00
2	L	138	THR	CA-CB-CG2	-5.31	104.97	112.40
1	C	339	ARG	N-CA-C	5.31	125.33	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	138	THR	CA-CB-CG2	-5.31	104.97	112.40
2	N	138	THR	CA-CB-CG2	-5.31	104.97	112.40
2	N	158	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	Q	214	ARG	NE-CZ-NH1	-5.31	117.65	120.30
2	D	138	THR	CA-CB-CG2	-5.30	104.98	112.40
2	B	61	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	B	138	THR	CA-CB-CG2	-5.30	104.98	112.40
1	E	312	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	G	264	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	H	432	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	P	138	THR	CA-CB-CG2	-5.29	104.99	112.40
2	J	61	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	O	312	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	G	312	TYR	CB-CG-CD1	-5.29	117.83	121.00
2	D	61	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	K	264	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	F	138	THR	CA-CB-CG2	-5.27	105.02	112.40
1	M	244	PHE	CD1-CG-CD2	5.26	125.14	118.30
1	C	244	PHE	CD1-CG-CD2	5.26	125.13	118.30
1	A	312	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	K	244	PHE	CD1-CG-CD2	5.25	125.12	118.30
1	O	244	PHE	CD1-CG-CD2	5.25	125.12	118.30
1	O	308	ARG	C-N-CA	-5.24	108.59	121.70
1	K	308	ARG	C-N-CA	-5.24	108.59	121.70
1	C	312	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	E	308	ARG	C-N-CA	-5.24	108.61	121.70
1	G	244	PHE	CD1-CG-CD2	5.23	125.10	118.30
1	A	244	PHE	CD1-CG-CD2	5.23	125.10	118.30
1	C	308	ARG	C-N-CA	-5.23	108.63	121.70
2	P	158	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	Q	308	ARG	C-N-CA	-5.23	108.63	121.70
1	A	308	ARG	C-N-CA	-5.22	108.64	121.70
1	M	312	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	G	308	ARG	C-N-CA	-5.22	108.65	121.70
1	E	244	PHE	CD1-CG-CD2	5.22	125.08	118.30
1	I	244	PHE	CD1-CG-CD2	5.22	125.08	118.30
1	M	308	ARG	C-N-CA	-5.21	108.67	121.70
1	I	308	ARG	C-N-CA	-5.21	108.67	121.70
1	K	266	HIS	CB-CA-C	-5.21	99.98	110.40
1	Q	244	PHE	CD1-CG-CD2	5.21	125.07	118.30
1	M	266	HIS	CB-CA-C	-5.20	100.00	110.40
1	I	312	TYR	CB-CG-CD1	-5.20	117.88	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	HIS	CB-CA-C	-5.19	100.01	110.40
1	G	108	TYR	CB-CG-CD1	-5.19	117.89	121.00
2	L	158	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	266	HIS	CB-CA-C	-5.19	100.03	110.40
1	I	266	HIS	CB-CA-C	-5.19	100.03	110.40
1	E	431	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	I	263	PRO	CA-N-CD	5.18	118.96	111.70
2	D	158	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	G	156	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	K	263	PRO	CA-N-CD	5.18	118.95	111.70
1	C	263	PRO	CA-N-CD	5.18	118.95	111.70
1	G	266	HIS	CB-CA-C	-5.18	100.04	110.40
1	O	263	PRO	CA-N-CD	5.18	118.95	111.70
1	E	266	HIS	CB-CA-C	-5.18	100.05	110.40
1	A	263	PRO	CA-N-CD	5.18	118.95	111.70
1	M	263	PRO	CA-N-CD	5.17	118.94	111.70
1	M	431	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	O	108	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	Q	266	HIS	CB-CA-C	-5.17	100.06	110.40
2	F	158	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	Q	263	PRO	CA-N-CD	5.17	118.93	111.70
1	O	266	HIS	CB-CA-C	-5.16	100.08	110.40
1	C	431	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	H	158	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	Q	431	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	I	156	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	R	158	ARG	NE-CZ-NH1	-5.15	117.72	120.30
2	P	220	THR	N-CA-C	5.15	124.90	111.00
2	L	220	THR	N-CA-C	5.15	124.89	111.00
1	I	431	ASP	CB-CG-OD1	-5.14	113.67	118.30
2	B	158	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	E	263	PRO	CA-N-CD	5.14	118.90	111.70
2	H	220	THR	N-CA-C	5.14	124.89	111.00
2	B	220	THR	N-CA-C	5.14	124.88	111.00
1	G	263	PRO	CA-N-CD	5.14	118.90	111.70
2	N	220	THR	N-CA-C	5.14	124.88	111.00
2	J	220	THR	N-CA-C	5.14	124.88	111.00
1	A	431	ASP	CB-CG-OD1	-5.14	113.68	118.30
2	D	220	THR	N-CA-C	5.13	124.86	111.00
1	A	108	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	E	108	TYR	CB-CG-CD1	-5.13	117.92	121.00
2	F	220	THR	N-CA-C	5.13	124.86	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	431	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	M	108	TYR	CB-CG-CD1	-5.13	117.92	121.00
2	J	158	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	O	431	ASP	CB-CG-OD1	-5.12	113.69	118.30
2	R	220	THR	N-CA-C	5.12	124.82	111.00
1	C	108	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	Q	108	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	O	156	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	G	431	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	Q	348	PRO	N-CA-CB	-5.09	97.00	102.60
1	I	348	PRO	N-CA-CB	-5.09	97.00	102.60
1	A	156	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	348	PRO	N-CA-CB	-5.07	97.02	102.60
1	I	108	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	G	348	PRO	N-CA-CB	-5.07	97.03	102.60
1	K	108	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	K	348	PRO	N-CA-CB	-5.06	97.04	102.60
1	O	348	PRO	N-CA-CB	-5.06	97.04	102.60
1	E	348	PRO	N-CA-CB	-5.05	97.04	102.60
1	C	348	PRO	N-CA-CB	-5.05	97.04	102.60
1	M	348	PRO	N-CA-CB	-5.05	97.04	102.60
1	E	156	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	K	156	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	Q	156	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	J	180	THR	CA-C-N	-5.03	106.14	117.20
2	F	180	THR	CA-C-N	-5.03	106.14	117.20
2	D	180	THR	CA-C-N	-5.02	106.15	117.20
1	C	156	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	P	180	THR	CA-C-N	-5.02	106.16	117.20
1	M	156	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	B	180	THR	CA-C-N	-5.01	106.17	117.20
2	L	180	THR	CA-C-N	-5.01	106.17	117.20
2	R	180	THR	CA-C-N	-5.01	106.17	117.20
2	H	180	THR	CA-C-N	-5.01	106.19	117.20
2	N	180	THR	CA-C-N	-5.01	106.19	117.20

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	PHE	Sidechain
1	A	264	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	265	GLY	Peptide
1	A	273	ALA	Mainchain,Peptide
1	A	37	PRO	Peptide
1	C	244	PHE	Sidechain
1	C	264	ARG	Peptide
1	C	265	GLY	Peptide
1	C	273	ALA	Mainchain,Peptide
1	C	37	PRO	Peptide
1	E	244	PHE	Sidechain
1	E	264	ARG	Peptide
1	E	265	GLY	Peptide
1	E	273	ALA	Mainchain,Peptide
1	E	37	PRO	Peptide
1	G	244	PHE	Sidechain
1	G	264	ARG	Peptide
1	G	265	GLY	Peptide
1	G	273	ALA	Mainchain,Peptide
1	G	37	PRO	Peptide
1	I	244	PHE	Sidechain
1	I	264	ARG	Peptide
1	I	265	GLY	Peptide
1	I	273	ALA	Mainchain,Peptide
1	I	37	PRO	Peptide
1	K	244	PHE	Sidechain
1	K	264	ARG	Peptide
1	K	265	GLY	Peptide
1	K	273	ALA	Mainchain,Peptide
1	K	37	PRO	Peptide
1	M	244	PHE	Sidechain
1	M	264	ARG	Peptide
1	M	265	GLY	Peptide
1	M	273	ALA	Mainchain,Peptide
1	M	37	PRO	Peptide
1	O	244	PHE	Sidechain
1	O	264	ARG	Peptide
1	O	265	GLY	Peptide
1	O	273	ALA	Mainchain,Peptide
1	O	37	PRO	Peptide
1	Q	244	PHE	Sidechain
1	Q	264	ARG	Peptide
1	Q	265	GLY	Peptide
1	Q	273	ALA	Mainchain,Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	Q	37	PRO	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	3253	74	0
1	C	3350	0	3253	76	0
1	E	3350	0	3253	72	0
1	G	3350	0	3253	74	0
1	I	3350	0	3253	70	0
1	K	3350	0	3253	73	0
1	M	3350	0	3253	61	0
1	O	3350	0	3253	59	0
1	Q	3350	0	3253	59	0
2	B	3352	0	3229	59	0
2	D	3352	0	3229	56	0
2	F	3352	0	3229	58	0
2	H	3352	0	3229	47	0
2	J	3352	0	3229	46	0
2	L	3352	0	3229	45	0
2	N	3352	0	3229	58	0
2	P	3352	0	3229	64	0
2	R	3352	0	3229	59	0
3	A	32	0	12	0	0
3	C	32	0	12	0	0
3	E	32	0	12	0	0
3	G	32	0	12	0	0
3	I	32	0	12	0	0
3	K	32	0	12	0	0
3	M	32	0	12	0	0
3	O	32	0	12	0	0
3	Q	32	0	12	0	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
5	P	28	0	12	2	0
5	R	28	0	12	2	0
6	B	62	0	51	4	0
6	D	62	0	51	4	0
6	F	62	0	51	4	0
6	H	62	0	51	4	0
6	J	62	0	51	4	0
6	L	62	0	51	4	0
6	N	62	0	51	4	0
6	P	62	0	51	4	0
6	R	62	0	51	4	0
7	A	4	0	0	1	0
7	C	4	0	0	1	0
7	E	4	0	0	1	0
7	G	4	0	0	1	0
7	I	4	0	0	1	0
7	K	4	0	0	1	0
7	M	4	0	0	1	0
7	O	4	0	0	1	0
7	Q	4	0	0	1	0
All	All	61461	0	59013	1008	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 8.

All (1008) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:TRP:CD1	2:N:401:ARG:HG3	1.38	1.57
2:F:401:ARG:HG3	1:K:346:TRP:CD1	1.38	1.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ARG:HG3	1:G:346:TRP:CD1	1.36	1.54
1:E:346:TRP:CD1	2:R:401:ARG:HG3	1.43	1.53
1:A:346:TRP:CD1	2:P:401:ARG:HG3	1.49	1.48
2:B:401:ARG:HG3	1:I:346:TRP:CD1	1.64	1.31
2:D:401:ARG:CG	1:G:346:TRP:CD1	2.26	1.18
2:D:401:ARG:CD	1:G:346:TRP:NE1	2.08	1.17
2:F:401:ARG:CD	1:K:346:TRP:NE1	2.07	1.17
1:C:346:TRP:NE1	2:N:401:ARG:CD	2.09	1.15
2:F:401:ARG:CG	1:K:346:TRP:CD1	2.28	1.14
1:C:346:TRP:CD1	2:N:401:ARG:CG	2.31	1.14
1:E:346:TRP:NE1	2:R:401:ARG:CD	2.13	1.12
1:E:346:TRP:CD1	2:R:401:ARG:CG	2.35	1.09
1:A:346:TRP:NE1	2:P:401:ARG:CD	2.16	1.09
1:A:346:TRP:CD1	2:P:401:ARG:CG	2.41	1.04
2:D:401:ARG:HD2	1:G:346:TRP:HE1	1.22	1.04
1:E:346:TRP:HE1	2:R:401:ARG:HD2	1.22	1.03
1:C:346:TRP:HE1	2:N:401:ARG:HD2	1.19	1.03
2:F:401:ARG:HD2	1:K:346:TRP:HE1	1.19	1.01
1:A:346:TRP:HE1	2:P:401:ARG:HD2	1.24	1.01
1:A:346:TRP:NE1	2:P:401:ARG:HD2	1.76	0.98
2:D:401:ARG:CG	1:G:346:TRP:NE1	2.28	0.96
1:C:346:TRP:NE1	2:N:401:ARG:HG3	1.79	0.96
1:C:346:TRP:NE1	2:N:401:ARG:CG	2.29	0.96
2:D:401:ARG:CD	1:G:346:TRP:HE1	1.74	0.96
2:D:401:ARG:HG3	1:G:346:TRP:NE1	1.82	0.94
1:E:346:TRP:NE1	2:R:401:ARG:HG3	1.83	0.93
2:B:401:ARG:CD	1:I:346:TRP:NE1	2.34	0.90
2:F:401:ARG:HG3	1:K:346:TRP:NE1	1.86	0.90
1:E:346:TRP:NE1	2:R:401:ARG:HD2	1.80	0.90
2:F:401:ARG:CG	1:K:346:TRP:NE1	2.32	0.90
2:L:228:ASN:HD21	5:L:501:GDP:HN1	1.22	0.87
2:F:228:ASN:HD21	5:F:501:GDP:HN1	1.22	0.87
1:E:346:TRP:NE1	2:R:401:ARG:CG	2.34	0.87
2:R:228:ASN:HD21	5:R:501:GDP:HN1	1.22	0.87
2:B:401:ARG:CG	1:I:346:TRP:CD1	2.56	0.87
2:F:401:ARG:HD3	1:K:346:TRP:CE2	2.10	0.87
1:C:346:TRP:CE2	2:N:401:ARG:HD3	2.10	0.86
2:N:228:ASN:HD21	5:N:501:GDP:HN1	1.22	0.86
2:D:228:ASN:HD21	5:D:501:GDP:HN1	1.22	0.86
2:B:228:ASN:HD21	5:B:501:GDP:HN1	1.22	0.86
2:H:228:ASN:HD21	5:H:501:GDP:HN1	1.22	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:228:ASN:HD21	5:J:501:GDP:HN1	1.22	0.86
1:A:346:TRP:CE2	2:P:401:ARG:HD3	2.10	0.86
2:P:228:ASN:HD21	5:P:501:GDP:HN1	1.22	0.85
1:E:346:TRP:CE2	2:R:401:ARG:HD3	2.10	0.85
2:D:401:ARG:HD3	1:G:346:TRP:NE1	1.90	0.85
1:A:346:TRP:NE1	2:P:401:ARG:HG3	1.90	0.85
1:C:346:TRP:NE1	2:N:401:ARG:HD2	1.81	0.83
2:D:401:ARG:HD3	1:G:346:TRP:CE2	2.14	0.82
2:B:401:ARG:HD2	1:I:346:TRP:HE1	1.44	0.81
1:A:346:TRP:NE1	2:P:401:ARG:CG	2.41	0.81
2:B:401:ARG:HG3	1:I:346:TRP:NE1	1.96	0.80
2:F:401:ARG:HD3	1:K:346:TRP:NE1	1.94	0.80
2:F:401:ARG:HD2	1:K:346:TRP:NE1	1.82	0.80
1:Q:266:HIS:O	1:Q:266:HIS:CD2	2.35	0.80
1:E:266:HIS:O	1:E:266:HIS:CD2	2.35	0.80
1:I:266:HIS:O	1:I:266:HIS:CD2	2.35	0.79
1:K:266:HIS:O	1:K:266:HIS:CD2	2.35	0.79
1:M:266:HIS:CD2	1:M:266:HIS:O	2.35	0.79
1:C:266:HIS:CD2	1:C:266:HIS:O	2.35	0.79
1:A:266:HIS:O	1:A:266:HIS:CD2	2.35	0.79
1:G:266:HIS:CD2	1:G:266:HIS:O	2.35	0.79
1:O:266:HIS:CD2	1:O:266:HIS:O	2.35	0.79
1:G:49:PHE:O	1:G:49:PHE:CG	2.31	0.79
1:A:346:TRP:CE2	2:P:401:ARG:CD	2.65	0.79
1:K:49:PHE:CG	1:K:49:PHE:O	2.31	0.79
1:C:49:PHE:O	1:C:49:PHE:CG	2.31	0.78
1:E:49:PHE:CG	1:E:49:PHE:O	2.31	0.78
1:M:49:PHE:O	1:M:49:PHE:CG	2.31	0.78
1:Q:49:PHE:CG	1:Q:49:PHE:O	2.31	0.78
2:F:401:ARG:CD	1:K:346:TRP:HE1	1.80	0.78
1:E:346:TRP:CE2	2:R:401:ARG:CD	2.68	0.77
1:A:346:TRP:CG	2:P:401:ARG:HG3	2.15	0.76
1:C:147:SER:OG	1:C:148:GLY:N	2.18	0.76
1:M:147:SER:OG	1:M:148:GLY:N	2.18	0.76
2:B:401:ARG:HD2	1:I:346:TRP:NE1	1.99	0.76
1:G:147:SER:OG	1:G:148:GLY:N	2.18	0.76
2:D:401:ARG:HG3	1:G:346:TRP:HD1	1.39	0.75
2:F:401:ARG:HG3	1:K:346:TRP:HD1	1.46	0.75
1:E:147:SER:OG	1:E:148:GLY:N	2.18	0.74
1:K:147:SER:OG	1:K:148:GLY:N	2.18	0.74
1:Q:147:SER:OG	1:Q:148:GLY:N	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:TYR:HD1	1:E:265:GLY:HA2	1.54	0.73
1:I:49:PHE:CG	1:I:49:PHE:O	2.31	0.73
1:E:346:TRP:CG	2:R:401:ARG:HG3	2.19	0.73
1:K:262:TYR:HD1	1:K:265:GLY:HA2	1.54	0.73
1:Q:262:TYR:HD1	1:Q:265:GLY:HA2	1.54	0.73
1:C:262:TYR:HD1	1:C:265:GLY:HA2	1.54	0.73
1:M:262:TYR:HD1	1:M:265:GLY:HA2	1.54	0.73
1:G:262:TYR:HD1	1:G:265:GLY:HA2	1.54	0.73
1:A:49:PHE:O	1:A:49:PHE:CG	2.31	0.73
1:O:147:SER:OG	1:O:148:GLY:N	2.18	0.73
1:C:346:TRP:NE1	2:N:401:ARG:HD3	2.02	0.72
1:A:147:SER:OG	1:A:148:GLY:N	2.18	0.72
1:O:49:PHE:CG	1:O:49:PHE:O	2.31	0.72
2:B:401:ARG:CG	1:I:346:TRP:NE1	2.52	0.72
1:C:346:TRP:CE2	2:N:401:ARG:CD	2.70	0.72
1:I:147:SER:OG	1:I:148:GLY:N	2.18	0.72
1:A:339:ARG:O	1:A:339:ARG:HG3	1.90	0.72
1:I:339:ARG:O	1:I:339:ARG:HG3	1.90	0.72
1:O:262:TYR:HD1	1:O:265:GLY:HA2	1.54	0.72
1:O:339:ARG:HG3	1:O:339:ARG:O	1.90	0.72
1:A:262:TYR:HD1	1:A:265:GLY:HA2	1.54	0.72
1:I:262:TYR:HD1	1:I:265:GLY:HA2	1.54	0.72
1:E:339:ARG:O	1:E:339:ARG:HG3	1.89	0.71
1:K:339:ARG:O	1:K:339:ARG:HG3	1.90	0.71
1:Q:339:ARG:HG3	1:Q:339:ARG:O	1.89	0.71
1:A:342:GLN:HG3	1:A:342:GLN:O	1.90	0.71
1:O:342:GLN:HG3	1:O:342:GLN:O	1.90	0.71
1:I:342:GLN:HG3	1:I:342:GLN:O	1.90	0.70
1:C:339:ARG:O	1:C:339:ARG:HG3	1.90	0.70
1:G:339:ARG:O	1:G:339:ARG:HG3	1.90	0.70
1:K:342:GLN:O	1:K:342:GLN:HG3	1.89	0.70
1:M:342:GLN:O	1:M:342:GLN:HG3	1.90	0.70
1:M:339:ARG:HG3	1:M:339:ARG:O	1.90	0.70
1:E:342:GLN:O	1:E:342:GLN:HG3	1.90	0.70
1:C:342:GLN:O	1:C:342:GLN:HG3	1.90	0.70
1:Q:342:GLN:HG3	1:Q:342:GLN:O	1.90	0.69
1:G:342:GLN:O	1:G:342:GLN:HG3	1.90	0.69
1:C:346:TRP:CG	2:N:401:ARG:HG3	2.21	0.69
1:O:49:PHE:CD1	1:O:49:PHE:C	2.59	0.68
1:G:49:PHE:C	1:G:49:PHE:CD1	2.59	0.66
1:A:346:TRP:CZ2	2:P:401:ARG:HD3	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:49:PHE:CD1	1:K:49:PHE:C	2.59	0.66
1:C:49:PHE:CD1	1:C:49:PHE:C	2.59	0.65
1:E:49:PHE:CD1	1:E:49:PHE:C	2.59	0.65
1:I:2:ARG:HA	1:I:243:ARG:HH12	1.62	0.65
1:A:2:ARG:HA	1:A:243:ARG:HH12	1.62	0.65
1:K:185:TYR:OH	1:K:405:VAL:HG23	1.97	0.65
1:O:2:ARG:HA	1:O:243:ARG:HH12	1.62	0.65
1:Q:185:TYR:OH	1:Q:405:VAL:HG23	1.97	0.65
1:E:185:TYR:OH	1:E:405:VAL:HG23	1.97	0.65
1:Q:49:PHE:CD1	1:Q:49:PHE:C	2.59	0.65
1:A:90:GLU:HG3	1:A:121:ARG:HD2	1.79	0.65
1:M:90:GLU:HG3	1:M:121:ARG:HD2	1.79	0.65
1:Q:2:ARG:HA	1:Q:243:ARG:HH12	1.62	0.65
1:Q:90:GLU:HG3	1:Q:121:ARG:HD2	1.79	0.65
1:C:90:GLU:HG3	1:C:121:ARG:HD2	1.79	0.65
1:C:2:ARG:HA	1:C:243:ARG:HH12	1.62	0.65
1:E:90:GLU:HG3	1:E:121:ARG:HD2	1.79	0.65
1:G:2:ARG:HA	1:G:243:ARG:HH12	1.62	0.65
1:I:90:GLU:HG3	1:I:121:ARG:HD2	1.79	0.65
1:K:90:GLU:HG3	1:K:121:ARG:HD2	1.79	0.65
1:M:49:PHE:CD1	1:M:49:PHE:C	2.59	0.65
1:O:90:GLU:HG3	1:O:121:ARG:HD2	1.79	0.65
1:E:2:ARG:HA	1:E:243:ARG:HH12	1.62	0.65
1:A:185:TYR:OH	1:A:405:VAL:HG23	1.97	0.65
1:G:90:GLU:HG3	1:G:121:ARG:HD2	1.79	0.65
1:I:185:TYR:OH	1:I:405:VAL:HG23	1.97	0.65
1:M:2:ARG:HA	1:M:243:ARG:HH12	1.62	0.65
1:O:185:TYR:OH	1:O:405:VAL:HG23	1.97	0.65
1:E:346:TRP:CZ2	2:R:401:ARG:HD3	2.31	0.64
1:K:2:ARG:HA	1:K:243:ARG:HH12	1.62	0.64
2:B:401:ARG:HD3	1:I:346:TRP:CE2	2.32	0.64
1:G:185:TYR:OH	1:G:405:VAL:HG23	1.97	0.64
1:C:185:TYR:OH	1:C:405:VAL:HG23	1.97	0.64
1:M:185:TYR:OH	1:M:405:VAL:HG23	1.97	0.64
1:A:49:PHE:C	1:A:49:PHE:CD1	2.59	0.63
1:C:346:TRP:CZ2	2:N:401:ARG:HD3	2.32	0.63
6:D:502:TA1:H261	6:D:502:TA1:H463	1.80	0.63
6:H:502:TA1:H463	6:H:502:TA1:H261	1.80	0.63
6:N:502:TA1:H261	6:N:502:TA1:H463	1.80	0.63
1:I:49:PHE:C	1:I:49:PHE:CD1	2.59	0.63
6:L:502:TA1:H261	6:L:502:TA1:H463	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:502:TA1:H261	6:F:502:TA1:H463	1.80	0.63
6:R:502:TA1:H463	6:R:502:TA1:H261	1.80	0.63
2:F:2:ARG:NH1	2:F:251:ASP:OD2	2.32	0.62
2:L:2:ARG:NH1	2:L:251:ASP:OD2	2.32	0.62
2:R:2:ARG:NH1	2:R:251:ASP:OD2	2.32	0.61
2:F:276:THR:CG2	6:F:502:TA1:H162	2.30	0.61
2:L:276:THR:CG2	6:L:502:TA1:H162	2.30	0.61
2:R:276:THR:CG2	6:R:502:TA1:H162	2.30	0.61
2:H:2:ARG:NH1	2:H:251:ASP:OD2	2.32	0.61
6:J:502:TA1:H463	6:J:502:TA1:H261	1.80	0.61
6:P:502:TA1:H261	6:P:502:TA1:H463	1.80	0.61
6:B:502:TA1:H463	6:B:502:TA1:H261	1.80	0.61
2:F:401:ARG:CD	1:K:346:TRP:CE2	2.74	0.61
2:D:2:ARG:NH1	2:D:251:ASP:OD2	2.32	0.61
2:F:401:ARG:HG3	1:K:346:TRP:CG	2.23	0.61
2:N:2:ARG:NH1	2:N:251:ASP:OD2	2.32	0.61
2:B:276:THR:CG2	6:B:502:TA1:H162	2.30	0.60
2:J:276:THR:CG2	6:J:502:TA1:H162	2.30	0.60
2:N:47:GLU:HG2	2:N:47:GLU:O	2.00	0.60
2:D:47:GLU:HG2	2:D:47:GLU:O	2.00	0.60
2:H:47:GLU:O	2:H:47:GLU:HG2	2.00	0.60
2:P:276:THR:CG2	6:P:502:TA1:H162	2.30	0.60
2:H:276:THR:CG2	6:H:502:TA1:H162	2.30	0.60
2:B:47:GLU:O	2:B:47:GLU:HG2	2.00	0.60
2:D:276:THR:CG2	6:D:502:TA1:H162	2.30	0.60
2:J:47:GLU:O	2:J:47:GLU:HG2	2.00	0.60
2:L:47:GLU:O	2:L:47:GLU:HG2	2.00	0.60
2:N:276:THR:CG2	6:N:502:TA1:H162	2.30	0.60
2:P:47:GLU:HG2	2:P:47:GLU:O	2.00	0.60
2:F:47:GLU:O	2:F:47:GLU:HG2	2.00	0.60
2:R:47:GLU:O	2:R:47:GLU:HG2	2.00	0.60
1:K:49:PHE:CD1	1:K:49:PHE:O	2.54	0.59
1:G:223:THR:O	1:G:227:LEU:HG	2.03	0.59
1:E:49:PHE:CD1	1:E:49:PHE:O	2.54	0.59
1:M:223:THR:O	1:M:227:LEU:HG	2.03	0.59
1:Q:49:PHE:CD1	1:Q:49:PHE:O	2.55	0.59
1:C:223:THR:O	1:C:227:LEU:HG	2.03	0.59
1:M:49:PHE:CD1	1:M:49:PHE:O	2.54	0.59
1:A:223:THR:O	1:A:227:LEU:HG	2.03	0.59
1:C:49:PHE:CD1	1:C:49:PHE:O	2.55	0.59
1:I:223:THR:O	1:I:227:LEU:HG	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:PHE:CD1	1:I:49:PHE:O	2.54	0.59
1:O:223:THR:O	1:O:227:LEU:HG	2.03	0.59
1:A:49:PHE:O	1:A:49:PHE:CD1	2.55	0.59
1:G:49:PHE:O	1:G:49:PHE:CD1	2.55	0.59
2:R:85:GLN:H	2:R:85:GLN:CD	2.06	0.59
2:H:85:GLN:H	2:H:85:GLN:CD	2.06	0.59
1:O:49:PHE:CD1	1:O:49:PHE:O	2.55	0.59
2:F:85:GLN:CD	2:F:85:GLN:H	2.06	0.59
2:L:85:GLN:CD	2:L:85:GLN:H	2.06	0.59
2:D:85:GLN:CD	2:D:85:GLN:H	2.06	0.58
2:N:85:GLN:CD	2:N:85:GLN:H	2.06	0.58
1:Q:223:THR:O	1:Q:227:LEU:HG	2.03	0.58
1:E:223:THR:O	1:E:227:LEU:HG	2.03	0.58
2:J:2:ARG:NH1	2:J:251:ASP:OD2	2.32	0.58
1:K:223:THR:O	1:K:227:LEU:HG	2.03	0.58
2:B:2:ARG:NH1	2:B:251:ASP:OD2	2.32	0.58
1:Q:313:MET:SD	1:Q:344:VAL:HG21	2.44	0.58
2:P:2:ARG:NH1	2:P:251:ASP:OD2	2.32	0.58
1:E:313:MET:SD	1:E:344:VAL:HG21	2.44	0.58
1:K:313:MET:SD	1:K:344:VAL:HG21	2.44	0.58
2:B:85:GLN:CD	2:B:85:GLN:H	2.06	0.57
1:O:313:MET:SD	1:O:344:VAL:HG21	2.44	0.57
2:P:85:GLN:H	2:P:85:GLN:CD	2.06	0.57
1:G:313:MET:SD	1:G:344:VAL:HG21	2.44	0.57
2:J:85:GLN:H	2:J:85:GLN:CD	2.06	0.57
1:A:313:MET:SD	1:A:344:VAL:HG21	2.44	0.57
1:C:313:MET:SD	1:C:344:VAL:HG21	2.44	0.57
1:O:71:GLU:HG2	2:P:2:ARG:HH21	1.69	0.57
1:I:313:MET:SD	1:I:344:VAL:HG21	2.44	0.57
1:I:71:GLU:HG2	2:J:2:ARG:HH21	1.69	0.57
1:A:71:GLU:HG2	2:B:2:ARG:HH21	1.69	0.57
1:C:71:GLU:HG2	2:D:2:ARG:HH21	1.69	0.57
1:K:71:GLU:HG2	2:L:2:ARG:HH21	1.69	0.57
1:M:313:MET:SD	1:M:344:VAL:HG21	2.44	0.57
1:E:71:GLU:HG2	2:F:2:ARG:HH21	1.69	0.56
1:G:71:GLU:HG2	2:H:2:ARG:HH21	1.69	0.56
2:N:228:ASN:ND2	5:N:501:GDP:HN1	1.99	0.56
2:H:228:ASN:ND2	5:H:501:GDP:HN1	1.99	0.56
1:M:71:GLU:HG2	2:N:2:ARG:HH21	1.69	0.56
1:Q:71:GLU:HG2	2:R:2:ARG:HH21	1.69	0.56
2:D:228:ASN:ND2	5:D:501:GDP:HN1	1.99	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:228:ASN:ND2	5:R:501:GDP:HN1	1.99	0.56
1:C:266:HIS:HD2	1:C:266:HIS:O	1.88	0.56
2:F:228:ASN:ND2	5:F:501:GDP:HN1	1.99	0.56
1:G:266:HIS:HD2	1:G:266:HIS:O	1.88	0.56
2:B:401:ARG:CD	1:I:346:TRP:CE2	2.88	0.56
2:L:228:ASN:ND2	5:L:501:GDP:HN1	1.99	0.56
1:M:266:HIS:HD2	1:M:266:HIS:O	1.88	0.56
1:A:435:VAL:HG12	1:A:435:VAL:O	2.06	0.56
1:O:435:VAL:O	1:O:435:VAL:HG12	2.06	0.56
1:I:435:VAL:O	1:I:435:VAL:HG12	2.06	0.56
2:F:401:ARG:HD3	1:K:346:TRP:CZ2	2.40	0.55
1:K:435:VAL:O	1:K:435:VAL:HG12	2.06	0.55
2:P:228:ASN:ND2	5:P:501:GDP:HN1	1.99	0.55
2:B:228:ASN:ND2	5:B:501:GDP:HN1	1.99	0.55
1:E:435:VAL:O	1:E:435:VAL:HG12	2.06	0.55
1:Q:435:VAL:HG12	1:Q:435:VAL:O	2.06	0.55
1:M:435:VAL:HG12	1:M:435:VAL:O	2.06	0.55
2:J:228:ASN:ND2	5:J:501:GDP:HN1	1.99	0.55
1:C:435:VAL:O	1:C:435:VAL:HG12	2.06	0.55
1:I:266:HIS:HD2	1:I:266:HIS:O	1.88	0.55
1:G:435:VAL:HG12	1:G:435:VAL:O	2.06	0.54
1:A:266:HIS:O	1:A:266:HIS:HD2	1.88	0.54
1:O:266:HIS:O	1:O:266:HIS:HD2	1.88	0.54
2:D:401:ARG:HD2	1:G:346:TRP:NE1	1.91	0.53
1:A:349:THR:HG23	1:A:349:THR:O	2.09	0.53
1:C:349:THR:O	1:C:349:THR:HG23	2.09	0.53
1:I:349:THR:O	1:I:349:THR:HG23	2.09	0.53
1:M:349:THR:O	1:M:349:THR:HG23	2.09	0.53
1:O:349:THR:HG23	1:O:349:THR:O	2.09	0.53
1:G:349:THR:O	1:G:349:THR:HG23	2.09	0.53
2:B:127:GLU:OE2	2:D:338:LYS:NZ	2.42	0.53
1:K:349:THR:O	1:K:349:THR:HG23	2.09	0.53
1:E:349:THR:O	1:E:349:THR:HG23	2.09	0.52
1:Q:349:THR:HG23	1:Q:349:THR:O	2.09	0.52
2:N:12:CYS:SG	2:N:13:GLY:N	2.82	0.52
7:C:603:HOH:O	2:D:254:LYS:NZ	2.43	0.52
7:G:603:HOH:O	2:H:254:LYS:NZ	2.43	0.52
2:D:12:CYS:SG	2:D:13:GLY:N	2.83	0.52
7:M:603:HOH:O	2:N:254:LYS:NZ	2.43	0.52
2:P:183:GLU:N	2:P:184:PRO:HD2	2.25	0.52
2:P:338:LYS:NZ	2:R:127:GLU:OE2	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:GLU:N	2:B:184:PRO:HD2	2.25	0.52
2:H:12:CYS:SG	2:H:13:GLY:N	2.83	0.52
2:J:183:GLU:N	2:J:184:PRO:HD2	2.25	0.52
2:L:183:GLU:N	2:L:184:PRO:HD2	2.24	0.52
2:N:183:GLU:N	2:N:184:PRO:HD2	2.25	0.52
2:R:12:CYS:SG	2:R:13:GLY:N	2.83	0.52
2:D:183:GLU:N	2:D:184:PRO:HD2	2.25	0.51
2:F:12:CYS:SG	2:F:13:GLY:N	2.83	0.51
7:E:603:HOH:O	2:F:254:LYS:NZ	2.43	0.51
2:H:183:GLU:N	2:H:184:PRO:HD2	2.24	0.51
7:Q:603:HOH:O	2:R:254:LYS:NZ	2.43	0.51
2:J:12:CYS:SG	2:J:13:GLY:N	2.83	0.51
2:L:12:CYS:SG	2:L:13:GLY:N	2.83	0.51
2:P:266:HIS:CD2	2:P:266:HIS:N	2.79	0.51
2:D:266:HIS:N	2:D:266:HIS:CD2	2.79	0.51
2:F:183:GLU:N	2:F:184:PRO:HD2	2.25	0.51
2:D:401:ARG:HD3	1:G:346:TRP:CZ2	2.45	0.51
2:H:266:HIS:CD2	2:H:266:HIS:N	2.79	0.51
7:K:603:HOH:O	2:L:254:LYS:NZ	2.43	0.51
2:R:183:GLU:N	2:R:184:PRO:HD2	2.24	0.51
2:B:12:CYS:SG	2:B:13:GLY:N	2.83	0.51
2:F:47:GLU:CG	2:F:47:GLU:O	2.58	0.51
2:L:47:GLU:CG	2:L:47:GLU:O	2.58	0.51
2:N:266:HIS:N	2:N:266:HIS:CD2	2.79	0.51
2:R:47:GLU:O	2:R:47:GLU:CG	2.58	0.51
7:A:603:HOH:O	2:B:254:LYS:NZ	2.43	0.51
7:I:603:HOH:O	2:J:254:LYS:NZ	2.43	0.51
2:J:47:GLU:CG	2:J:47:GLU:O	2.58	0.51
2:P:12:CYS:SG	2:P:13:GLY:N	2.83	0.51
1:A:224:TYR:HD1	1:A:227:LEU:HD12	1.76	0.51
2:B:47:GLU:O	2:B:47:GLU:CG	2.58	0.51
1:I:224:TYR:HD1	1:I:227:LEU:HD12	1.76	0.51
1:E:224:TYR:HD1	1:E:227:LEU:HD12	1.76	0.51
2:J:381:SER:OG	2:J:382:THR:N	2.43	0.51
1:K:224:TYR:HD1	1:K:227:LEU:HD12	1.75	0.51
1:O:224:TYR:HD1	1:O:227:LEU:HD12	1.76	0.51
2:P:381:SER:OG	2:P:382:THR:N	2.43	0.51
2:P:47:GLU:O	2:P:47:GLU:CG	2.58	0.51
1:Q:224:TYR:HD1	1:Q:227:LEU:HD12	1.76	0.51
2:B:381:SER:OG	2:B:382:THR:N	2.43	0.51
7:O:603:HOH:O	2:P:254:LYS:NZ	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:GLU:CG	2:H:47:GLU:O	2.58	0.51
2:N:47:GLU:CG	2:N:47:GLU:O	2.58	0.50
1:C:224:TYR:HD1	1:C:227:LEU:HD12	1.75	0.50
2:D:47:GLU:CG	2:D:47:GLU:O	2.58	0.50
1:K:183:GLU:N	1:K:184:PRO:HD2	2.26	0.50
2:L:266:HIS:N	2:L:266:HIS:CD2	2.79	0.50
1:M:224:TYR:HD1	1:M:227:LEU:HD12	1.75	0.50
1:E:183:GLU:N	1:E:184:PRO:HD2	2.26	0.50
2:F:266:HIS:N	2:F:266:HIS:CD2	2.79	0.50
2:F:381:SER:OG	2:F:382:THR:N	2.43	0.50
1:I:183:GLU:N	1:I:184:PRO:HD2	2.26	0.50
1:K:266:HIS:O	1:K:266:HIS:HD2	1.88	0.50
1:Q:183:GLU:N	1:Q:184:PRO:HD2	2.26	0.50
1:C:183:GLU:N	1:C:184:PRO:HD2	2.26	0.50
2:L:381:SER:OG	2:L:382:THR:N	2.43	0.50
2:R:266:HIS:CD2	2:R:266:HIS:N	2.79	0.50
2:R:381:SER:OG	2:R:382:THR:N	2.43	0.50
1:A:183:GLU:N	1:A:184:PRO:HD2	2.26	0.50
1:G:183:GLU:N	1:G:184:PRO:HD2	2.26	0.50
1:O:183:GLU:N	1:O:184:PRO:HD2	2.26	0.50
1:A:352:LYS:NZ	2:P:179:ASP:OD2	2.44	0.50
1:G:224:TYR:HD1	1:G:227:LEU:HD12	1.76	0.50
1:M:183:GLU:N	1:M:184:PRO:HD2	2.26	0.50
2:N:381:SER:OG	2:N:382:THR:N	2.43	0.50
1:Q:2:ARG:HA	1:Q:243:ARG:NH1	2.27	0.50
2:D:381:SER:OG	2:D:382:THR:N	2.43	0.50
1:E:266:HIS:O	1:E:266:HIS:HD2	1.88	0.50
1:E:2:ARG:HA	1:E:243:ARG:NH1	2.27	0.50
1:K:2:ARG:HA	1:K:243:ARG:NH1	2.27	0.49
2:N:338:LYS:NZ	2:P:127:GLU:OE2	2.44	0.49
1:O:2:ARG:HA	1:O:243:ARG:NH1	2.27	0.49
2:H:381:SER:OG	2:H:382:THR:N	2.43	0.49
1:I:143:GLY:O	1:I:147:SER:OG	2.20	0.49
1:Q:266:HIS:HD2	1:Q:266:HIS:O	1.88	0.49
1:A:2:ARG:HA	1:A:243:ARG:NH1	2.27	0.49
1:I:2:ARG:HA	1:I:243:ARG:NH1	2.27	0.49
1:K:100:ALA:HA	2:L:254:LYS:HG2	1.95	0.49
1:Q:100:ALA:HA	2:R:254:LYS:HG2	1.95	0.49
1:A:143:GLY:O	1:A:147:SER:OG	2.20	0.49
1:E:100:ALA:HA	2:F:254:LYS:HG2	1.95	0.49
1:I:100:ALA:HA	2:J:254:LYS:HG2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2:ARG:HA	1:M:243:ARG:NH1	2.27	0.49
1:O:100:ALA:HA	2:P:254:LYS:HG2	1.95	0.49
1:Q:266:HIS:O	1:Q:266:HIS:CG	2.62	0.49
1:A:100:ALA:HA	2:B:254:LYS:HG2	1.95	0.49
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.95	0.49
1:C:2:ARG:HA	1:C:243:ARG:NH1	2.27	0.49
1:M:100:ALA:HA	2:N:254:LYS:HG2	1.95	0.49
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.95	0.49
1:C:100:ALA:HA	2:D:254:LYS:HG2	1.95	0.49
1:G:100:ALA:HA	2:H:254:LYS:HG2	1.95	0.49
1:I:278:ALA:HA	1:I:369:ALA:HB2	1.95	0.49
1:M:278:ALA:HA	1:M:369:ALA:HB2	1.95	0.49
1:O:278:ALA:HA	1:O:369:ALA:HB2	1.95	0.49
1:A:267:PHE:N	1:A:268:PRO:HD3	2.28	0.48
1:E:266:HIS:O	1:E:266:HIS:CG	2.62	0.48
1:G:278:ALA:HA	1:G:369:ALA:HB2	1.95	0.48
2:H:266:HIS:H	2:H:266:HIS:CD2	2.31	0.48
2:J:266:HIS:H	2:J:266:HIS:CD2	2.31	0.48
1:M:267:PHE:N	1:M:268:PRO:HD3	2.28	0.48
1:O:143:GLY:O	1:O:147:SER:OG	2.20	0.48
1:O:267:PHE:N	1:O:268:PRO:HD3	2.28	0.48
2:B:266:HIS:H	2:B:266:HIS:CD2	2.31	0.48
2:D:266:HIS:CD2	2:D:266:HIS:H	2.31	0.48
1:I:267:PHE:N	1:I:268:PRO:HD3	2.28	0.48
2:J:266:HIS:N	2:J:266:HIS:CD2	2.79	0.48
1:C:267:PHE:N	1:C:268:PRO:HD3	2.28	0.48
1:G:2:ARG:HA	1:G:243:ARG:NH1	2.27	0.48
1:K:266:HIS:O	1:K:266:HIS:CG	2.62	0.48
1:A:435:VAL:O	1:A:435:VAL:CG1	2.60	0.48
1:G:267:PHE:N	1:G:268:PRO:HD3	2.28	0.48
1:I:435:VAL:O	1:I:435:VAL:CG1	2.60	0.48
1:M:435:VAL:CG1	1:M:435:VAL:O	2.60	0.48
2:N:266:HIS:CD2	2:N:266:HIS:H	2.31	0.48
1:O:435:VAL:O	1:O:435:VAL:CG1	2.60	0.48
2:P:266:HIS:H	2:P:266:HIS:CD2	2.31	0.48
2:B:266:HIS:CD2	2:B:266:HIS:N	2.79	0.48
1:K:278:ALA:HA	1:K:369:ALA:HB2	1.95	0.48
1:C:435:VAL:O	1:C:435:VAL:CG1	2.60	0.48
1:E:278:ALA:HA	1:E:369:ALA:HB2	1.95	0.48
2:F:266:HIS:H	2:F:266:HIS:CD2	2.31	0.48
1:G:435:VAL:CG1	1:G:435:VAL:O	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:266:HIS:H	2:L:266:HIS:CD2	2.31	0.48
1:Q:249:ASN:C	1:Q:249:ASN:OD1	2.52	0.48
1:Q:278:ALA:HA	1:Q:369:ALA:HB2	1.95	0.48
1:E:249:ASN:C	1:E:249:ASN:OD1	2.52	0.48
1:K:249:ASN:C	1:K:249:ASN:OD1	2.52	0.48
2:R:266:HIS:CD2	2:R:266:HIS:H	2.31	0.48
2:J:388:PHE:CD1	2:J:388:PHE:N	2.81	0.48
1:O:76:ASP:HA	1:O:79:ARG:HG2	1.96	0.48
1:Q:308:ARG:CZ	1:Q:308:ARG:HB3	2.44	0.48
1:A:76:ASP:HA	1:A:79:ARG:HG2	1.96	0.48
1:E:308:ARG:HB3	1:E:308:ARG:CZ	2.44	0.48
1:K:267:PHE:N	1:K:268:PRO:HD3	2.28	0.48
2:B:388:PHE:N	2:B:388:PHE:CD1	2.81	0.47
1:E:267:PHE:N	1:E:268:PRO:HD3	2.28	0.47
1:G:249:ASN:C	1:G:249:ASN:OD1	2.52	0.47
1:I:76:ASP:HA	1:I:79:ARG:HG2	1.96	0.47
1:K:308:ARG:CZ	1:K:308:ARG:HB3	2.44	0.47
1:A:181:VAL:HG12	1:A:181:VAL:O	2.14	0.47
1:E:312:TYR:CD1	1:E:312:TYR:N	2.82	0.47
1:I:181:VAL:O	1:I:181:VAL:HG12	2.14	0.47
1:A:249:ASN:OD1	1:A:249:ASN:C	2.52	0.47
1:C:249:ASN:OD1	1:C:249:ASN:C	2.52	0.47
1:G:144:GLY:O	1:G:148:GLY:N	2.47	0.47
1:O:181:VAL:HG12	1:O:181:VAL:O	2.14	0.47
1:O:249:ASN:C	1:O:249:ASN:OD1	2.52	0.47
2:P:388:PHE:CD1	2:P:388:PHE:N	2.81	0.47
1:Q:267:PHE:N	1:Q:268:PRO:HD3	2.28	0.47
1:Q:312:TYR:CD1	1:Q:312:TYR:N	2.82	0.47
1:C:312:TYR:N	1:C:312:TYR:CD1	2.82	0.47
1:K:312:TYR:N	1:K:312:TYR:CD1	2.82	0.47
1:M:249:ASN:C	1:M:249:ASN:OD1	2.52	0.47
1:M:312:TYR:N	1:M:312:TYR:CD1	2.82	0.47
1:O:266:HIS:CG	1:O:266:HIS:O	2.62	0.47
1:G:76:ASP:HA	1:G:79:ARG:HG2	1.96	0.47
1:I:249:ASN:OD1	1:I:249:ASN:C	2.52	0.47
2:L:318:VAL:O	2:L:375:ALA:HA	2.15	0.47
2:B:401:ARG:HD3	1:I:346:TRP:CZ2	2.49	0.47
2:F:318:VAL:O	2:F:375:ALA:HA	2.15	0.47
1:G:312:TYR:CD1	1:G:312:TYR:N	2.81	0.47
1:O:144:GLY:O	1:O:148:GLY:N	2.47	0.47
1:A:144:GLY:O	1:A:148:GLY:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ASP:HA	1:C:79:ARG:HG2	1.96	0.47
1:I:308:ARG:HB3	1:I:308:ARG:CZ	2.44	0.47
2:J:318:VAL:O	2:J:375:ALA:HA	2.15	0.47
1:M:76:ASP:HA	1:M:79:ARG:HG2	1.96	0.47
1:C:144:GLY:O	1:C:148:GLY:N	2.47	0.47
1:M:144:GLY:O	1:M:148:GLY:N	2.47	0.47
1:M:36:MET:HG3	1:M:36:MET:O	2.15	0.47
2:R:318:VAL:O	2:R:375:ALA:HA	2.15	0.47
1:A:266:HIS:O	1:A:266:HIS:CG	2.62	0.47
2:B:318:VAL:O	2:B:375:ALA:HA	2.15	0.47
1:C:36:MET:O	1:C:36:MET:HG3	2.15	0.47
1:G:36:MET:HG3	1:G:36:MET:O	2.15	0.47
2:H:318:VAL:O	2:H:375:ALA:HA	2.15	0.47
1:I:312:TYR:N	1:I:312:TYR:CD1	2.82	0.47
1:Q:435:VAL:CG1	1:Q:435:VAL:O	2.60	0.47
1:A:308:ARG:HB3	1:A:308:ARG:CZ	2.44	0.47
1:A:312:TYR:N	1:A:312:TYR:CD1	2.82	0.47
1:E:435:VAL:CG1	1:E:435:VAL:O	2.60	0.47
1:O:312:TYR:N	1:O:312:TYR:CD1	2.81	0.47
2:P:318:VAL:O	2:P:375:ALA:HA	2.15	0.47
1:I:266:HIS:O	1:I:266:HIS:CG	2.62	0.47
1:K:144:GLY:O	1:K:148:GLY:N	2.47	0.47
1:M:308:ARG:CZ	1:M:308:ARG:HB3	2.44	0.47
1:O:308:ARG:HB3	1:O:308:ARG:CZ	2.44	0.47
1:Q:144:GLY:O	1:Q:148:GLY:N	2.47	0.47
2:D:318:VAL:O	2:D:375:ALA:HA	2.15	0.46
1:E:144:GLY:O	1:E:148:GLY:N	2.47	0.46
1:K:435:VAL:CG1	1:K:435:VAL:O	2.60	0.46
1:C:308:ARG:CZ	1:C:308:ARG:HB3	2.44	0.46
1:E:214:ARG:NH1	2:F:330:GLU:OE2	2.49	0.46
1:K:214:ARG:NH1	2:L:330:GLU:OE2	2.49	0.46
2:N:318:VAL:O	2:N:375:ALA:HA	2.15	0.46
1:Q:214:ARG:NH1	2:R:330:GLU:OE2	2.49	0.46
1:G:308:ARG:HB3	1:G:308:ARG:CZ	2.44	0.46
1:O:36:MET:O	1:O:36:MET:HG3	2.15	0.46
1:C:214:ARG:NH1	2:D:330:GLU:OE2	2.49	0.46
1:G:214:ARG:NH1	2:H:330:GLU:OE2	2.49	0.46
1:I:144:GLY:O	1:I:148:GLY:N	2.47	0.46
1:M:214:ARG:NH1	2:N:330:GLU:OE2	2.49	0.46
6:R:502:TA1:H463	6:R:502:TA1:C26	2.46	0.46
1:A:270:ALA:HA	1:A:377:MET:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ASP:HA	1:E:79:ARG:HG2	1.96	0.46
6:F:502:TA1:C26	6:F:502:TA1:H463	2.46	0.46
1:I:270:ALA:HA	1:I:377:MET:O	2.16	0.46
6:L:502:TA1:H463	6:L:502:TA1:C26	2.46	0.46
1:M:181:VAL:O	1:M:181:VAL:HG12	2.14	0.46
1:M:36:MET:SD	1:M:61:HIS:HB2	2.56	0.46
1:Q:76:ASP:HA	1:Q:79:ARG:HG2	1.96	0.46
1:A:36:MET:HG3	1:A:36:MET:O	2.15	0.46
1:E:36:MET:HG3	1:E:36:MET:O	2.15	0.46
1:K:36:MET:O	1:K:36:MET:HG3	2.15	0.46
2:L:276:THR:OG1	2:L:280:SER:HB2	2.15	0.46
1:O:270:ALA:HA	1:O:377:MET:O	2.16	0.46
1:C:181:VAL:HG12	1:C:181:VAL:O	2.14	0.46
1:C:36:MET:SD	1:C:61:HIS:HB2	2.56	0.46
2:F:276:THR:OG1	2:F:280:SER:HB2	2.15	0.46
2:F:276:THR:HG22	6:F:502:TA1:H162	1.98	0.46
1:G:181:VAL:HG12	1:G:181:VAL:O	2.14	0.46
1:I:36:MET:HG3	1:I:36:MET:O	2.15	0.46
2:P:306:ASP:HA	2:P:307:PRO:HD2	1.81	0.46
2:R:276:THR:OG1	2:R:280:SER:HB2	2.15	0.46
1:G:36:MET:SD	1:G:61:HIS:HB2	2.56	0.46
2:J:276:THR:OG1	2:J:280:SER:HB2	2.15	0.46
1:K:76:ASP:HA	1:K:79:ARG:HG2	1.96	0.46
2:N:177:VAL:HG12	2:N:177:VAL:O	2.16	0.46
1:Q:358:GLU:HA	1:Q:359:PRO:HD3	1.81	0.46
1:Q:36:MET:HG3	1:Q:36:MET:O	2.15	0.46
2:R:276:THR:HG22	6:R:502:TA1:H162	1.98	0.46
2:B:276:THR:OG1	2:B:280:SER:HB2	2.15	0.46
1:G:205:ASP:HB3	1:G:303:VAL:HA	1.98	0.46
2:H:177:VAL:O	2:H:177:VAL:HG12	2.16	0.46
2:J:306:ASP:HA	2:J:307:PRO:HD2	1.81	0.46
1:K:260:VAL:HA	1:K:261:PRO:HD2	1.66	0.46
2:P:276:THR:OG1	2:P:280:SER:HB2	2.15	0.46
1:Q:181:VAL:HG12	1:Q:181:VAL:O	2.14	0.46
2:B:306:ASP:HA	2:B:307:PRO:HD2	1.81	0.46
2:D:177:VAL:O	2:D:177:VAL:HG12	2.16	0.45
1:E:181:VAL:O	1:E:181:VAL:HG12	2.14	0.45
1:G:301:GLN:O	1:G:302:MET:HB2	2.16	0.45
2:H:276:THR:OG1	2:H:280:SER:HB2	2.15	0.45
1:M:205:ASP:HB3	1:M:303:VAL:HA	1.99	0.45
2:P:276:THR:HG22	6:P:502:TA1:H162	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:SD	1:A:61:HIS:HB2	2.56	0.45
1:C:205:ASP:HB3	1:C:303:VAL:HA	1.99	0.45
1:C:270:ALA:HA	1:C:377:MET:O	2.16	0.45
2:D:276:THR:OG1	2:D:280:SER:HB2	2.16	0.45
1:G:270:ALA:HA	1:G:377:MET:O	2.16	0.45
2:L:388:PHE:N	2:L:388:PHE:CD1	2.81	0.45
1:M:270:ALA:HA	1:M:377:MET:O	2.16	0.45
2:N:276:THR:OG1	2:N:280:SER:HB2	2.16	0.45
1:O:36:MET:SD	1:O:61:HIS:HB2	2.56	0.45
1:E:270:ALA:HA	1:E:377:MET:O	2.16	0.45
2:J:177:VAL:HG12	2:J:177:VAL:O	2.16	0.45
2:J:316:ALA:HB3	2:J:378:ILE:HB	1.99	0.45
1:K:181:VAL:HG12	1:K:181:VAL:O	2.14	0.45
1:K:270:ALA:HA	1:K:377:MET:O	2.16	0.45
1:M:301:GLN:O	1:M:302:MET:HB2	2.16	0.45
1:Q:270:ALA:HA	1:Q:377:MET:O	2.16	0.45
2:B:177:VAL:HG12	2:B:177:VAL:O	2.16	0.45
1:C:301:GLN:O	1:C:302:MET:HB2	2.16	0.45
1:E:260:VAL:HA	1:E:261:PRO:HD2	1.66	0.45
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.99	0.45
1:C:345:ASP:HB2	1:C:439:SER:HB2	1.98	0.45
2:F:388:PHE:CD1	2:F:388:PHE:N	2.81	0.45
1:G:345:ASP:HB2	1:G:439:SER:HB2	1.98	0.45
1:I:36:MET:SD	1:I:61:HIS:HB2	2.56	0.45
1:M:345:ASP:HB2	1:M:439:SER:HB2	1.98	0.45
2:P:177:VAL:HG12	2:P:177:VAL:O	2.16	0.45
1:K:205:ASP:HB3	1:K:303:VAL:HA	1.98	0.45
1:M:224:TYR:HA	1:M:227:LEU:HD12	1.98	0.45
1:O:345:ASP:HB2	1:O:439:SER:HB2	1.98	0.45
2:P:316:ALA:HB3	2:P:378:ILE:HB	1.99	0.45
1:A:224:TYR:HA	1:A:227:LEU:HD12	1.98	0.45
1:A:345:ASP:HB2	1:A:439:SER:HB2	1.98	0.45
1:C:304:LYS:HD2	1:C:304:LYS:C	2.37	0.45
1:E:301:GLN:O	1:E:302:MET:HB2	2.16	0.45
1:G:304:LYS:C	1:G:304:LYS:HD2	2.37	0.45
1:I:214:ARG:NH1	2:J:330:GLU:OE2	2.49	0.45
1:K:260:VAL:HG13	1:K:265:GLY:HA3	1.99	0.45
1:K:301:GLN:O	1:K:302:MET:HB2	2.16	0.45
1:M:266:HIS:CG	1:M:266:HIS:O	2.62	0.45
1:O:224:TYR:HA	1:O:227:LEU:HD12	1.98	0.45
1:O:214:ARG:NH1	2:P:330:GLU:OE2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:301:GLN:O	1:Q:302:MET:HB2	2.16	0.45
1:Q:36:MET:SD	1:Q:61:HIS:HB2	2.56	0.45
1:A:214:ARG:NH1	2:B:330:GLU:OE2	2.49	0.45
1:A:260:VAL:HG13	1:A:265:GLY:HA3	1.99	0.45
1:C:224:TYR:HA	1:C:227:LEU:HD12	1.98	0.45
1:E:205:ASP:HB3	1:E:303:VAL:HA	1.99	0.45
1:I:224:TYR:HA	1:I:227:LEU:HD12	1.98	0.45
1:I:260:VAL:HG13	1:I:265:GLY:HA3	1.99	0.45
1:I:205:ASP:HB3	1:I:303:VAL:HA	1.98	0.45
1:K:36:MET:SD	1:K:61:HIS:HB2	2.56	0.45
1:M:304:LYS:HD2	1:M:304:LYS:C	2.37	0.45
1:Q:205:ASP:HB3	1:Q:303:VAL:HA	1.99	0.45
2:R:177:VAL:HG12	2:R:177:VAL:O	2.16	0.45
2:R:388:PHE:CD1	2:R:388:PHE:N	2.81	0.45
2:D:97:SER:OG	2:D:98:GLY:N	2.50	0.45
1:E:260:VAL:HG13	1:E:265:GLY:HA3	1.99	0.45
1:E:36:MET:SD	1:E:61:HIS:HB2	2.56	0.45
1:G:260:VAL:HG13	1:G:265:GLY:HA3	1.99	0.45
1:I:345:ASP:HB2	1:I:439:SER:HB2	1.98	0.45
1:O:260:VAL:HG13	1:O:265:GLY:HA3	1.99	0.45
1:Q:260:VAL:HA	1:Q:261:PRO:HD2	1.66	0.45
1:Q:260:VAL:HG13	1:Q:265:GLY:HA3	1.99	0.45
1:C:260:VAL:HG13	1:C:265:GLY:HA3	1.99	0.45
2:F:177:VAL:O	2:F:177:VAL:HG12	2.16	0.45
1:G:224:TYR:HA	1:G:227:LEU:HD12	1.98	0.45
2:H:97:SER:OG	2:H:98:GLY:N	2.50	0.45
1:I:301:GLN:O	1:I:302:MET:HB2	2.16	0.45
1:M:260:VAL:HG13	1:M:265:GLY:HA3	1.99	0.45
2:N:97:SER:OG	2:N:98:GLY:N	2.50	0.45
1:O:205:ASP:HB3	1:O:303:VAL:HA	1.99	0.45
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.99	0.44
1:E:304:LYS:HD2	1:E:304:LYS:C	2.37	0.44
2:F:305:CYS:SG	2:F:384:ILE:HA	2.58	0.44
1:K:304:LYS:HD2	1:K:304:LYS:C	2.37	0.44
2:L:305:CYS:SG	2:L:384:ILE:HA	2.58	0.44
1:Q:224:TYR:HA	1:Q:227:LEU:HD12	1.98	0.44
1:Q:304:LYS:HD2	1:Q:304:LYS:C	2.37	0.44
1:A:257:THR:O	2:P:404:PHE:CD2	2.71	0.44
1:A:301:GLN:O	1:A:302:MET:HB2	2.16	0.44
1:C:266:HIS:CG	1:C:266:HIS:O	2.62	0.44
2:H:202:TYR:CD1	2:H:202:TYR:N	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:TYR:HA	1:K:227:LEU:HD12	1.98	0.44
1:O:301:GLN:O	1:O:302:MET:HB2	2.16	0.44
2:R:305:CYS:SG	2:R:384:ILE:HA	2.58	0.44
2:B:105:LYS:O	2:B:110:GLU:N	2.51	0.44
2:D:202:TYR:CD1	2:D:202:TYR:N	2.85	0.44
1:E:224:TYR:HA	1:E:227:LEU:HD12	1.98	0.44
2:F:313:LEU:HD23	2:F:344:VAL:HG11	2.00	0.44
2:H:388:PHE:CD1	2:H:388:PHE:N	2.81	0.44
2:H:49:ILE:CG2	2:H:53:TYR:HB2	2.47	0.44
1:K:345:ASP:HB2	1:K:439:SER:HB2	1.98	0.44
2:L:177:VAL:HG12	2:L:177:VAL:O	2.16	0.44
2:L:313:LEU:HD23	2:L:344:VAL:HG11	1.99	0.44
2:N:202:TYR:N	2:N:202:TYR:CD1	2.85	0.44
2:N:49:ILE:CG2	2:N:53:TYR:HB2	2.47	0.44
2:R:313:LEU:HD23	2:R:344:VAL:HG11	1.99	0.44
1:G:143:GLY:O	1:G:147:SER:OG	2.20	0.44
2:J:105:LYS:O	2:J:110:GLU:N	2.51	0.44
2:J:305:CYS:SG	2:J:384:ILE:HA	2.57	0.44
1:K:62:VAL:HA	1:K:63:PRO:HD3	1.84	0.44
2:N:105:LYS:O	2:N:110:GLU:N	2.51	0.44
2:N:305:CYS:SG	2:N:384:ILE:HA	2.58	0.44
2:P:105:LYS:O	2:P:110:GLU:N	2.51	0.44
1:Q:345:ASP:HB2	1:Q:439:SER:HB2	1.98	0.44
2:D:105:LYS:O	2:D:110:GLU:N	2.51	0.44
2:D:248:LEU:HB2	2:D:355:VAL:H	1.83	0.44
2:D:49:ILE:CG2	2:D:53:TYR:HB2	2.48	0.44
2:H:248:LEU:HB2	2:H:355:VAL:H	1.83	0.44
2:H:276:THR:HG22	6:H:502:TA1:H162	1.98	0.44
1:O:172:TYR:HA	1:O:173:PRO:HD3	1.87	0.44
2:B:97:SER:OG	2:B:98:GLY:N	2.50	0.44
1:E:345:ASP:HB2	1:E:439:SER:HB2	1.98	0.44
1:G:266:HIS:CG	1:G:266:HIS:O	2.62	0.44
2:H:105:LYS:O	2:H:110:GLU:N	2.51	0.44
2:J:202:TYR:N	2:J:202:TYR:CD1	2.85	0.44
2:J:97:SER:OG	2:J:98:GLY:N	2.50	0.44
2:L:260:VAL:HA	2:L:261:PRO:HD2	1.83	0.44
2:N:248:LEU:HB2	2:N:355:VAL:H	1.83	0.44
2:B:202:TYR:N	2:B:202:TYR:CD1	2.85	0.44
2:B:305:CYS:SG	2:B:384:ILE:HA	2.58	0.44
2:D:305:CYS:SG	2:D:384:ILE:HA	2.58	0.44
2:D:388:PHE:CD1	2:D:388:PHE:N	2.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:ILE:CG2	2:F:53:TYR:HB2	2.47	0.44
1:G:62:VAL:HA	1:G:63:PRO:HD3	1.84	0.44
2:H:260:VAL:HA	2:H:261:PRO:HD2	1.83	0.44
1:I:172:TYR:HA	1:I:173:PRO:HD3	1.87	0.44
2:J:49:ILE:CG2	2:J:53:TYR:HB2	2.47	0.44
2:L:49:ILE:CG2	2:L:53:TYR:HB2	2.48	0.44
6:N:502:TA1:C26	6:N:502:TA1:H463	2.46	0.44
2:P:49:ILE:CG2	2:P:53:TYR:HB2	2.47	0.44
2:P:97:SER:OG	2:P:98:GLY:N	2.50	0.44
2:R:49:ILE:CG2	2:R:53:TYR:HB2	2.47	0.44
2:B:49:ILE:CG2	2:B:53:TYR:HB2	2.48	0.44
1:C:143:GLY:O	1:C:147:SER:OG	2.20	0.44
6:D:502:TA1:H463	6:D:502:TA1:C26	2.46	0.44
2:H:305:CYS:SG	2:H:384:ILE:HA	2.57	0.44
2:J:313:LEU:HD23	2:J:344:VAL:HG11	2.00	0.44
2:P:202:TYR:CD1	2:P:202:TYR:N	2.85	0.44
2:P:305:CYS:SG	2:P:384:ILE:HA	2.58	0.44
2:P:248:LEU:HB2	2:P:355:VAL:H	1.83	0.44
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.88	0.44
2:B:248:LEU:HB2	2:B:355:VAL:H	1.83	0.44
2:D:276:THR:HG22	6:D:502:TA1:H162	1.98	0.44
2:J:248:LEU:HB2	2:J:355:VAL:H	1.83	0.44
1:O:304:LYS:C	1:O:304:LYS:HD2	2.37	0.44
2:R:316:ALA:HB3	2:R:378:ILE:HB	1.99	0.44
1:A:304:LYS:HD2	1:A:304:LYS:C	2.37	0.43
2:B:313:LEU:HD23	2:B:344:VAL:HG11	2.00	0.43
2:D:260:VAL:HA	2:D:261:PRO:HD2	1.83	0.43
1:E:62:VAL:HA	1:E:63:PRO:HD3	1.84	0.43
2:F:316:ALA:HB3	2:F:378:ILE:HB	1.99	0.43
1:I:260:VAL:HA	1:I:261:PRO:HD2	1.66	0.43
1:I:304:LYS:HD2	1:I:304:LYS:C	2.37	0.43
2:L:316:ALA:HB3	2:L:378:ILE:HB	1.99	0.43
2:N:313:LEU:HD23	2:N:344:VAL:HG11	1.99	0.43
2:N:388:PHE:N	2:N:388:PHE:CD1	2.81	0.43
2:P:313:LEU:HD23	2:P:344:VAL:HG11	2.00	0.43
1:I:62:VAL:HA	1:I:63:PRO:HD3	1.84	0.43
2:L:105:LYS:O	2:L:110:GLU:N	2.51	0.43
1:M:121:ARG:HA	1:M:121:ARG:HD3	1.84	0.43
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.99	0.43
2:D:313:LEU:HD23	2:D:344:VAL:HG11	2.00	0.43
2:F:105:LYS:O	2:F:110:GLU:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:260:VAL:HA	2:F:261:PRO:HD2	1.83	0.43
6:H:502:TA1:C26	6:H:502:TA1:H463	2.46	0.43
2:N:276:THR:HG22	6:N:502:TA1:H162	1.98	0.43
2:N:316:ALA:HB3	2:N:378:ILE:HB	1.99	0.43
2:H:316:ALA:HB3	2:H:378:ILE:HB	1.99	0.43
1:I:433:GLU:O	1:I:437:VAL:N	2.50	0.43
2:J:260:VAL:HA	2:J:261:PRO:HD2	1.83	0.43
2:R:105:LYS:O	2:R:110:GLU:N	2.51	0.43
1:A:433:GLU:O	1:A:437:VAL:N	2.50	0.43
2:B:88:ARG:HA	2:B:89:PRO:HD3	1.88	0.43
1:C:62:VAL:HA	1:C:63:PRO:HD3	1.84	0.43
1:G:260:VAL:HA	1:G:261:PRO:HD2	1.66	0.43
2:H:313:LEU:HD23	2:H:344:VAL:HG11	2.00	0.43
2:J:276:THR:HG22	6:J:502:TA1:H162	1.98	0.43
1:O:286:LEU:HB3	1:O:291:ILE:HG13	2.01	0.43
2:P:88:ARG:HA	2:P:89:PRO:HD3	1.88	0.43
1:A:260:VAL:HA	1:A:261:PRO:HD2	1.66	0.43
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.84	0.43
1:C:121:ARG:HD3	1:C:121:ARG:HA	1.84	0.43
1:E:200:CYS:SG	1:E:268:PRO:HG2	2.59	0.43
2:D:404:PHE:CE1	1:G:261:PRO:HB3	2.54	0.43
1:O:433:GLU:O	1:O:437:VAL:N	2.50	0.43
2:R:260:VAL:HA	2:R:261:PRO:HD2	1.83	0.43
1:A:246:GLY:HA3	1:A:356:ASN:HA	2.00	0.43
2:B:260:VAL:HA	2:B:261:PRO:HD2	1.83	0.43
2:B:276:THR:HG22	6:B:502:TA1:H162	1.98	0.43
2:F:202:TYR:CD1	2:F:202:TYR:N	2.85	0.43
1:I:246:GLY:HA3	1:I:356:ASN:HA	2.00	0.43
2:J:88:ARG:HA	2:J:89:PRO:HD3	1.88	0.43
1:K:433:GLU:O	1:K:437:VAL:N	2.50	0.43
2:L:202:TYR:N	2:L:202:TYR:CD1	2.85	0.43
1:M:246:GLY:HA3	1:M:356:ASN:HA	2.00	0.43
2:N:260:VAL:HA	2:N:261:PRO:HD2	1.83	0.43
1:O:246:GLY:HA3	1:O:356:ASN:HA	2.00	0.43
1:Q:200:CYS:SG	1:Q:268:PRO:HG2	2.59	0.43
1:Q:286:LEU:HB3	1:Q:291:ILE:HG13	2.01	0.43
1:Q:62:VAL:HA	1:Q:63:PRO:HD3	1.84	0.43
1:A:286:LEU:HB3	1:A:291:ILE:HG13	2.01	0.43
2:B:62:VAL:HA	2:B:63:PRO:HD3	1.91	0.43
1:C:286:LEU:HB3	1:C:291:ILE:HG13	2.01	0.43
1:E:433:GLU:O	1:E:437:VAL:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:GLY:HA3	1:G:356:ASN:HA	2.00	0.43
1:K:200:CYS:SG	1:K:268:PRO:HG2	2.59	0.43
1:K:286:LEU:HB3	1:K:291:ILE:HG13	2.01	0.43
2:L:276:THR:HG22	6:L:502:TA1:H162	1.98	0.43
1:M:286:LEU:HB3	1:M:291:ILE:HG13	2.01	0.43
2:N:62:VAL:HA	2:N:63:PRO:HD3	1.91	0.43
1:Q:433:GLU:O	1:Q:437:VAL:N	2.50	0.43
2:R:202:TYR:CD1	2:R:202:TYR:N	2.85	0.43
1:C:246:GLY:HA3	1:C:356:ASN:HA	2.00	0.43
1:E:286:LEU:HB3	1:E:291:ILE:HG13	2.01	0.43
1:I:286:LEU:HB3	1:I:291:ILE:HG13	2.01	0.43
1:A:346:TRP:CE2	2:P:401:ARG:CG	3.00	0.43
1:C:260:VAL:HA	1:C:261:PRO:HD2	1.66	0.43
1:G:286:LEU:HB3	1:G:291:ILE:HG13	2.01	0.43
1:M:172:TYR:HA	1:M:173:PRO:HD3	1.87	0.43
2:R:62:VAL:HA	2:R:63:PRO:HD3	1.91	0.43
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.87	0.42
1:E:308:ARG:CZ	1:E:308:ARG:CB	2.97	0.42
1:G:172:TYR:HA	1:G:173:PRO:HD3	1.88	0.42
1:I:273:ALA:O	1:I:291:ILE:HG23	2.19	0.42
1:K:308:ARG:CB	1:K:308:ARG:CZ	2.97	0.42
1:M:62:VAL:HA	1:M:63:PRO:HD3	1.84	0.42
1:O:260:VAL:HA	1:O:261:PRO:HD2	1.66	0.42
1:A:273:ALA:O	1:A:291:ILE:HG23	2.19	0.42
2:B:182:VAL:HB	2:B:185:TYR:HB2	2.01	0.42
2:F:331:GLN:HA	2:F:331:GLN:OE1	2.20	0.42
1:I:200:CYS:SG	1:I:268:PRO:HG2	2.59	0.42
2:J:182:VAL:HB	2:J:185:TYR:HB2	2.01	0.42
1:M:273:ALA:O	1:M:291:ILE:HG23	2.19	0.42
1:Q:308:ARG:CZ	1:Q:308:ARG:CB	2.97	0.42
1:Q:315:CYS:HB3	1:Q:351:PHE:CD2	2.53	0.42
1:E:218:ASP:OD1	1:E:280:LYS:NZ	2.52	0.42
1:E:315:CYS:HB3	1:E:351:PHE:CD2	2.53	0.42
1:G:121:ARG:HA	1:G:121:ARG:HD3	1.85	0.42
2:H:182:VAL:HB	2:H:185:TYR:HB2	2.01	0.42
1:K:218:ASP:OD1	1:K:280:LYS:NZ	2.52	0.42
1:K:315:CYS:HB3	1:K:351:PHE:CD2	2.53	0.42
2:L:331:GLN:OE1	2:L:331:GLN:HA	2.20	0.42
2:N:182:VAL:HB	2:N:185:TYR:HB2	2.01	0.42
1:O:273:ALA:O	1:O:291:ILE:HG23	2.19	0.42
2:P:260:VAL:HA	2:P:261:PRO:HD2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:62:VAL:HA	2:P:63:PRO:HD3	1.91	0.42
1:Q:218:ASP:OD1	1:Q:280:LYS:NZ	2.52	0.42
2:R:331:GLN:HA	2:R:331:GLN:OE1	2.20	0.42
1:A:200:CYS:SG	1:A:268:PRO:HG2	2.59	0.42
1:C:273:ALA:O	1:C:291:ILE:HG23	2.19	0.42
1:C:315:CYS:HB3	1:C:351:PHE:CD2	2.53	0.42
2:D:182:VAL:HB	2:D:185:TYR:HB2	2.01	0.42
1:G:273:ALA:O	1:G:291:ILE:HG23	2.19	0.42
1:G:315:CYS:HB3	1:G:351:PHE:CD2	2.53	0.42
2:J:331:GLN:OE1	2:J:331:GLN:HA	2.20	0.42
1:O:62:VAL:HA	1:O:63:PRO:HD3	1.84	0.42
2:P:182:VAL:HB	2:P:185:TYR:HB2	2.01	0.42
2:R:105:LYS:HA	2:R:109:THR:OG1	2.20	0.42
2:B:331:GLN:HA	2:B:331:GLN:OE1	2.20	0.42
2:F:105:LYS:HA	2:F:109:THR:OG1	2.20	0.42
1:I:308:ARG:CB	1:I:308:ARG:CZ	2.97	0.42
1:I:402:ARG:HD3	1:I:402:ARG:HA	1.81	0.42
2:L:105:LYS:HA	2:L:109:THR:OG1	2.20	0.42
1:M:315:CYS:HB3	1:M:351:PHE:CD2	2.53	0.42
1:O:200:CYS:SG	1:O:268:PRO:HG2	2.59	0.42
2:P:331:GLN:HA	2:P:331:GLN:OE1	2.20	0.42
2:R:182:VAL:HB	2:R:185:TYR:HB2	2.01	0.42
2:R:248:LEU:HB2	2:R:355:VAL:H	1.83	0.42
1:A:308:ARG:CB	1:A:308:ARG:CZ	2.97	0.42
1:C:200:CYS:SG	1:C:268:PRO:HG2	2.59	0.42
1:C:272:TYR:HD1	1:C:376:CYS:HG	1.67	0.42
2:F:182:VAL:HB	2:F:185:TYR:HB2	2.01	0.42
2:F:248:LEU:HB2	2:F:355:VAL:H	1.83	0.42
1:G:433:GLU:O	1:G:437:VAL:N	2.50	0.42
1:K:246:GLY:HA3	1:K:356:ASN:HA	2.00	0.42
2:L:182:VAL:HB	2:L:185:TYR:HB2	2.01	0.42
1:M:200:CYS:SG	1:M:268:PRO:HG2	2.59	0.42
2:P:288:VAL:N	2:P:289:PRO:CD	2.82	0.42
2:R:85:GLN:N	2:R:85:GLN:CD	2.72	0.42
1:A:218:ASP:OD1	1:A:280:LYS:NZ	2.52	0.42
1:A:402:ARG:HA	1:A:402:ARG:HD3	1.82	0.42
2:B:179:ASP:OD1	1:I:352:LYS:NZ	2.52	0.42
2:B:288:VAL:N	2:B:289:PRO:CD	2.82	0.42
2:B:85:GLN:CD	2:B:85:GLN:N	2.72	0.42
1:C:402:ARG:HA	1:C:402:ARG:HD3	1.82	0.42
1:E:246:GLY:HA3	1:E:356:ASN:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:105:LYS:HA	2:H:109:THR:OG1	2.20	0.42
1:I:218:ASP:OD1	1:I:280:LYS:NZ	2.52	0.42
1:I:315:CYS:HB3	1:I:351:PHE:CD2	2.53	0.42
2:J:288:VAL:N	2:J:289:PRO:CD	2.82	0.42
2:J:85:GLN:N	2:J:85:GLN:CD	2.72	0.42
2:L:85:GLN:N	2:L:85:GLN:CD	2.72	0.42
1:M:272:TYR:HD1	1:M:376:CYS:HG	1.67	0.42
1:M:402:ARG:HD3	1:M:402:ARG:HA	1.81	0.42
1:O:308:ARG:CB	1:O:308:ARG:CZ	2.97	0.42
1:C:433:GLU:O	1:C:437:VAL:N	2.50	0.42
2:F:85:GLN:CD	2:F:85:GLN:N	2.72	0.42
1:G:200:CYS:SG	1:G:268:PRO:HG2	2.59	0.42
1:G:308:ARG:CB	1:G:308:ARG:CZ	2.97	0.42
2:H:288:VAL:N	2:H:289:PRO:CD	2.82	0.42
2:L:248:LEU:HB2	2:L:355:VAL:H	1.83	0.42
1:M:260:VAL:HA	1:M:261:PRO:HD2	1.66	0.42
1:M:433:GLU:O	1:M:437:VAL:N	2.50	0.42
1:O:218:ASP:OD1	1:O:280:LYS:NZ	2.52	0.42
6:P:502:TA1:H463	6:P:502:TA1:C26	2.46	0.42
1:Q:246:GLY:HA3	1:Q:356:ASN:HA	2.00	0.42
2:D:105:LYS:HA	2:D:109:THR:OG1	2.20	0.42
2:D:288:VAL:N	2:D:289:PRO:CD	2.82	0.42
1:G:402:ARG:HD3	1:G:402:ARG:HA	1.82	0.42
1:K:402:ARG:HA	1:K:402:ARG:HD3	1.81	0.42
2:L:262:PHE:HA	2:L:263:PRO:HD3	1.90	0.42
1:A:352:LYS:NZ	2:P:179:ASP:OD1	2.48	0.42
2:P:85:GLN:N	2:P:85:GLN:CD	2.72	0.42
1:A:315:CYS:HB3	1:A:351:PHE:CD2	2.54	0.42
6:B:502:TA1:H463	6:B:502:TA1:C26	2.46	0.42
1:C:218:ASP:OD1	1:C:280:LYS:NZ	2.52	0.42
1:C:308:ARG:CB	1:C:308:ARG:CZ	2.97	0.42
1:E:402:ARG:HD3	1:E:402:ARG:HA	1.82	0.42
1:G:218:ASP:OD1	1:G:280:LYS:NZ	2.52	0.42
2:L:19:LYS:HD2	2:L:19:LYS:HA	1.90	0.42
1:M:218:ASP:OD1	1:M:280:LYS:NZ	2.52	0.42
1:M:308:ARG:CB	1:M:308:ARG:CZ	2.97	0.42
2:N:105:LYS:HA	2:N:109:THR:OG1	2.20	0.42
2:N:288:VAL:N	2:N:289:PRO:CD	2.82	0.42
2:N:40:SER:OG	2:N:41:ASP:N	2.53	0.42
1:O:315:CYS:HB3	1:O:351:PHE:CD2	2.54	0.42
1:Q:35:GLN:HE21	1:Q:37:PRO:HG3	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:ARG:HG3	1:I:346:TRP:CG	2.38	0.41
2:F:168:THR:O	2:F:201:THR:HA	2.20	0.41
2:F:262:PHE:HA	2:F:263:PRO:HD3	1.90	0.41
2:L:168:THR:O	2:L:201:THR:HA	2.20	0.41
1:O:402:ARG:HA	1:O:402:ARG:HD3	1.82	0.41
2:R:168:THR:O	2:R:201:THR:HA	2.20	0.41
1:C:217:LEU:HD23	1:C:217:LEU:HA	1.85	0.41
2:D:331:GLN:HA	2:D:331:GLN:OE1	2.20	0.41
2:D:40:SER:OG	2:D:41:ASP:N	2.53	0.41
1:E:35:GLN:HE21	1:E:37:PRO:HG3	1.85	0.41
2:H:331:GLN:OE1	2:H:331:GLN:HA	2.20	0.41
2:H:40:SER:OG	2:H:41:ASP:N	2.53	0.41
1:K:35:GLN:HE21	1:K:37:PRO:HG3	1.85	0.41
1:Q:402:ARG:HD3	1:Q:402:ARG:HA	1.81	0.41
1:A:35:GLN:HE21	1:A:37:PRO:HG3	1.85	0.41
1:I:35:GLN:HE21	1:I:37:PRO:HG3	1.85	0.41
6:J:502:TA1:H463	6:J:502:TA1:C26	2.46	0.41
2:L:288:VAL:N	2:L:289:PRO:CD	2.82	0.41
2:N:331:GLN:HA	2:N:331:GLN:OE1	2.20	0.41
2:P:104:ALA:O	2:P:108:TYR:HB3	2.21	0.41
1:A:352:LYS:HB2	2:P:179:ASP:O	2.20	0.41
2:B:104:ALA:O	2:B:108:TYR:HB3	2.21	0.41
2:F:104:ALA:O	2:F:108:TYR:HB3	2.21	0.41
2:L:104:ALA:O	2:L:108:TYR:HB3	2.21	0.41
1:O:35:GLN:HE21	1:O:37:PRO:HG3	1.85	0.41
2:R:262:PHE:HA	2:R:263:PRO:HD3	1.90	0.41
2:F:270:PRO:HA	2:F:377:PHE:O	2.21	0.41
2:F:288:VAL:N	2:F:289:PRO:CD	2.82	0.41
1:G:217:LEU:HA	1:G:217:LEU:HD23	1.85	0.41
2:J:104:ALA:O	2:J:108:TYR:HB3	2.21	0.41
2:J:168:THR:O	2:J:201:THR:HA	2.20	0.41
2:L:270:PRO:HA	2:L:377:PHE:O	2.21	0.41
2:R:104:ALA:O	2:R:108:TYR:HB3	2.21	0.41
2:R:270:PRO:HA	2:R:377:PHE:O	2.21	0.41
1:G:35:GLN:HE21	1:G:37:PRO:HG3	1.85	0.41
2:R:288:VAL:N	2:R:289:PRO:CD	2.82	0.41
2:B:168:THR:O	2:B:201:THR:HA	2.20	0.41
1:C:273:ALA:HB3	1:C:295:CYS:SG	2.61	0.41
1:G:273:ALA:HB3	1:G:295:CYS:SG	2.61	0.41
1:I:339:ARG:CG	1:I:339:ARG:O	2.64	0.41
1:I:222:PRO:HG2	2:J:326:LYS:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:27:GLU:HA	2:J:369:ARG:NE	2.36	0.41
1:M:273:ALA:HB3	1:M:295:CYS:SG	2.61	0.41
2:N:85:GLN:CD	2:N:85:GLN:N	2.72	0.41
2:P:105:LYS:HA	2:P:109:THR:OG1	2.20	0.41
2:P:168:THR:O	2:P:201:THR:HA	2.20	0.41
2:R:40:SER:OG	2:R:41:ASP:N	2.53	0.41
1:A:273:ALA:HB3	1:A:295:CYS:SG	2.61	0.41
1:A:339:ARG:CG	1:A:339:ARG:O	2.64	0.41
1:A:222:PRO:HG2	2:B:326:LYS:HB2	2.03	0.41
1:C:35:GLN:HE21	1:C:37:PRO:HG3	1.85	0.41
2:F:40:SER:OG	2:F:41:ASP:N	2.53	0.41
1:I:273:ALA:HB3	1:I:295:CYS:SG	2.61	0.41
2:J:270:PRO:HA	2:J:377:PHE:O	2.20	0.41
1:O:273:ALA:HB3	1:O:295:CYS:SG	2.61	0.41
1:O:222:PRO:HG2	2:P:326:LYS:HB2	2.03	0.41
2:B:105:LYS:HA	2:B:109:THR:OG1	2.20	0.41
2:B:270:PRO:HA	2:B:377:PHE:O	2.21	0.41
2:B:27:GLU:HA	2:B:369:ARG:NE	2.36	0.41
1:M:35:GLN:HE21	1:M:37:PRO:HG3	1.85	0.41
1:M:222:PRO:HG2	2:N:326:LYS:HB2	2.03	0.41
2:P:270:PRO:HA	2:P:377:PHE:O	2.21	0.41
1:Q:222:PRO:HG2	2:R:326:LYS:HB2	2.03	0.41
2:R:27:GLU:HA	2:R:369:ARG:NE	2.36	0.41
1:E:346:TRP:CE2	2:R:401:ARG:CG	3.00	0.41
1:C:222:PRO:HG2	2:D:326:LYS:HB2	2.03	0.41
1:E:222:PRO:HG2	2:F:326:LYS:HB2	2.03	0.41
1:E:273:ALA:O	1:E:291:ILE:HG23	2.19	0.41
2:F:27:GLU:HA	2:F:369:ARG:NE	2.36	0.41
2:J:262:PHE:HA	2:J:263:PRO:HD3	1.90	0.41
1:K:143:GLY:O	1:K:147:SER:OG	2.20	0.41
1:K:222:PRO:HG2	2:L:326:LYS:HB2	2.03	0.41
2:P:27:GLU:HA	2:P:369:ARG:NE	2.36	0.41
1:Q:273:ALA:O	1:Q:291:ILE:HG23	2.19	0.41
1:C:358:GLU:HA	1:C:359:PRO:HD3	1.81	0.41
2:D:347:ILE:HB	2:D:350:ASN:OD1	2.21	0.41
2:F:185:TYR:OH	2:F:399:PHE:HA	2.21	0.41
1:G:222:PRO:HG2	2:H:326:LYS:HB2	2.03	0.41
2:H:104:ALA:O	2:H:108:TYR:HB3	2.21	0.41
2:H:347:ILE:HB	2:H:350:ASN:OD1	2.21	0.41
2:J:105:LYS:HA	2:J:109:THR:OG1	2.20	0.41
1:K:273:ALA:O	1:K:291:ILE:HG23	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:168:THR:O	2:N:201:THR:HA	2.20	0.41
2:N:347:ILE:HB	2:N:350:ASN:OD1	2.21	0.41
1:O:339:ARG:O	1:O:339:ARG:CG	2.64	0.41
1:Q:273:ALA:HB3	1:Q:295:CYS:SG	2.61	0.41
2:D:104:ALA:O	2:D:108:TYR:HB3	2.21	0.40
1:E:273:ALA:HB3	1:E:295:CYS:SG	2.61	0.40
2:F:97:SER:OG	2:F:98:GLY:N	2.50	0.40
2:H:168:THR:O	2:H:201:THR:HA	2.20	0.40
2:L:27:GLU:HA	2:L:369:ARG:NE	2.36	0.40
2:L:97:SER:OG	2:L:98:GLY:N	2.50	0.40
1:O:217:LEU:HA	1:O:217:LEU:HD23	1.85	0.40
2:R:185:TYR:OH	2:R:399:PHE:HA	2.22	0.40
2:R:97:SER:OG	2:R:98:GLY:N	2.50	0.40
2:B:262:PHE:HA	2:B:263:PRO:HD3	1.90	0.40
2:B:347:ILE:HB	2:B:350:ASN:OD1	2.21	0.40
2:D:185:TYR:OH	2:D:399:PHE:HA	2.22	0.40
2:D:168:THR:O	2:D:201:THR:HA	2.20	0.40
2:H:185:TYR:OH	2:H:399:PHE:HA	2.22	0.40
2:J:40:SER:OG	2:J:41:ASP:N	2.53	0.40
2:L:183:GLU:N	2:L:184:PRO:CD	2.84	0.40
2:L:185:TYR:OH	2:L:399:PHE:HA	2.22	0.40
2:R:183:GLU:N	2:R:184:PRO:CD	2.84	0.40
1:C:138:PHE:N	1:C:138:PHE:CD1	2.90	0.40
2:D:183:GLU:N	2:D:184:PRO:CD	2.84	0.40
1:E:138:PHE:CD1	1:E:138:PHE:N	2.90	0.40
1:E:143:GLY:O	1:E:147:SER:OG	2.20	0.40
2:F:183:GLU:N	2:F:184:PRO:CD	2.84	0.40
2:H:183:GLU:N	2:H:184:PRO:CD	2.84	0.40
2:H:85:GLN:N	2:H:85:GLN:CD	2.72	0.40
1:K:138:PHE:N	1:K:138:PHE:CD1	2.90	0.40
1:K:273:ALA:HB3	1:K:295:CYS:SG	2.61	0.40
1:M:138:PHE:CD1	1:M:138:PHE:N	2.90	0.40
2:N:104:ALA:O	2:N:108:TYR:HB3	2.21	0.40
2:N:183:GLU:N	2:N:184:PRO:CD	2.84	0.40
2:N:185:TYR:OH	2:N:399:PHE:HA	2.22	0.40
2:P:347:ILE:HB	2:P:350:ASN:OD1	2.21	0.40
1:Q:36:MET:HA	1:Q:37:PRO:HD3	1.42	0.40
2:B:40:SER:OG	2:B:41:ASP:N	2.53	0.40
1:E:183:GLU:N	1:E:184:PRO:CD	2.84	0.40
1:G:138:PHE:CD1	1:G:138:PHE:N	2.90	0.40
2:H:140:SER:O	2:H:147:SER:HB2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:270:PRO:HA	2:H:377:PHE:O	2.21	0.40
2:H:338:LYS:NZ	2:J:127:GLU:OE2	2.54	0.40
2:J:347:ILE:HB	2:J:350:ASN:OD1	2.21	0.40
2:L:40:SER:OG	2:L:41:ASP:N	2.53	0.40
2:P:19:LYS:HA	2:P:19:LYS:HD2	1.90	0.40
1:Q:183:GLU:N	1:Q:184:PRO:CD	2.84	0.40
1:E:352:LYS:NZ	2:R:179:ASP:OD2	2.52	0.40
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.04	0.40
1:C:339:ARG:CG	1:C:339:ARG:O	2.64	0.40
2:D:140:SER:O	2:D:147:SER:HB2	2.22	0.40
1:E:381:THR:OG1	1:E:382:THR:N	2.54	0.40
1:G:339:ARG:O	1:G:339:ARG:CG	2.64	0.40
2:H:214:PHE:O	2:H:218:LYS:HA	2.22	0.40
2:H:262:PHE:HA	2:H:263:PRO:HD3	1.90	0.40
1:K:183:GLU:N	1:K:184:PRO:CD	2.84	0.40
1:K:381:THR:OG1	1:K:382:THR:N	2.54	0.40
1:M:180:ALA:HB3	1:M:183:GLU:HG3	2.04	0.40
1:M:358:GLU:HA	1:M:359:PRO:HD3	1.81	0.40
2:N:140:SER:O	2:N:147:SER:HB2	2.22	0.40
2:N:214:PHE:O	2:N:218:LYS:HA	2.22	0.40
2:P:262:PHE:HA	2:P:263:PRO:HD3	1.90	0.40
1:Q:138:PHE:N	1:Q:138:PHE:CD1	2.90	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	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	20	63
1	C	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	20	63
1	E	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	20	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	20	63
1	I	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	20	63
1	K	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	20	63
1	M	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	20	63
1	O	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	20	63
1	Q	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	20	63
2	B	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	D	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	F	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	H	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	J	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	L	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	N	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	P	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	R	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	32	74
All	All	7632/7794 (98%)	7290 (96%)	288 (4%)	54 (1%)	30	68

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASP
1	A	274	PRO
1	A	342	GLN
2	B	50	ASN
1	C	98	ASP
1	C	274	PRO
1	C	342	GLN
2	D	50	ASN
1	E	98	ASP
1	E	274	PRO
1	E	342	GLN
2	F	50	ASN
1	G	98	ASP
1	G	274	PRO
1	G	342	GLN
2	H	50	ASN
1	I	98	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	274	PRO
1	I	342	GLN
2	J	50	ASN
1	K	98	ASP
1	K	274	PRO
1	K	342	GLN
2	L	50	ASN
1	M	98	ASP
1	M	274	PRO
1	M	342	GLN
2	N	50	ASN
1	O	98	ASP
1	O	274	PRO
1	O	342	GLN
2	P	50	ASN
1	Q	98	ASP
1	Q	274	PRO
1	Q	342	GLN
2	R	50	ASN
1	A	348	PRO
1	C	348	PRO
1	E	348	PRO
1	G	348	PRO
1	I	348	PRO
1	K	348	PRO
1	M	348	PRO
1	O	348	PRO
1	Q	348	PRO
2	B	73	GLY
2	D	73	GLY
2	F	73	GLY
2	H	73	GLY
2	J	73	GLY
2	L	73	GLY
2	N	73	GLY
2	P	73	GLY
2	R	73	GLY

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	360/368 (98%)	360 (100%)	0	100	100
1	C	360/368 (98%)	360 (100%)	0	100	100
1	E	360/368 (98%)	360 (100%)	0	100	100
1	G	360/368 (98%)	360 (100%)	0	100	100
1	I	360/368 (98%)	360 (100%)	0	100	100
1	K	360/368 (98%)	360 (100%)	0	100	100
1	M	360/368 (98%)	360 (100%)	0	100	100
1	O	360/368 (98%)	360 (100%)	0	100	100
1	Q	360/368 (98%)	360 (100%)	0	100	100
2	B	367/368 (100%)	367 (100%)	0	100	100
2	D	367/368 (100%)	367 (100%)	0	100	100
2	F	367/368 (100%)	367 (100%)	0	100	100
2	H	367/368 (100%)	367 (100%)	0	100	100
2	J	367/368 (100%)	367 (100%)	0	100	100
2	L	367/368 (100%)	367 (100%)	0	100	100
2	N	367/368 (100%)	367 (100%)	0	100	100
2	P	367/368 (100%)	367 (100%)	0	100	100
2	R	367/368 (100%)	367 (100%)	0	100	100
All	All	6543/6624 (99%)	6543 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	35	GLN
1	A	102	ASN
2	B	96	GLN
2	B	228	ASN
1	C	31	GLN
1	C	35	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	102	ASN
2	D	228	ASN
1	E	31	GLN
1	E	35	GLN
1	E	102	ASN
2	F	228	ASN
1	G	31	GLN
1	G	35	GLN
1	G	102	ASN
2	H	96	GLN
2	H	228	ASN
1	I	31	GLN
1	I	35	GLN
1	I	102	ASN
2	J	96	GLN
2	J	228	ASN
1	K	31	GLN
1	K	35	GLN
1	K	102	ASN
2	L	96	GLN
2	L	228	ASN
1	M	31	GLN
1	M	35	GLN
1	M	102	ASN
2	N	228	ASN
1	O	31	GLN
1	O	35	GLN
1	O	102	ASN
2	P	96	GLN
2	P	228	ASN
1	Q	31	GLN
1	Q	35	GLN
1	Q	102	ASN
2	R	96	GLN
2	R	228	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 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$
3	GTP	A	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	4 (14%)
5	GDP	B	501	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	11 (42%)
6	TA1	B	502	-	68,68,68	1.98	20 (29%)	105,105,105	1.33	8 (7%)
3	GTP	C	501	4	27,34,34	1.51	4 (14%)	27,54,54	2.15	4 (14%)
5	GDP	D	501	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	10 (38%)
6	TA1	D	502	-	68,68,68	1.98	20 (29%)	105,105,105	1.33	8 (7%)
3	GTP	E	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	4 (14%)
5	GDP	F	501	-	25,30,30	2.73	8 (32%)	26,47,47	3.66	11 (42%)
6	TA1	F	502	-	68,68,68	1.98	20 (29%)	105,105,105	1.33	8 (7%)
3	GTP	G	501	4	27,34,34	1.51	4 (14%)	27,54,54	2.15	5 (18%)
5	GDP	H	501	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	10 (38%)
6	TA1	H	502	-	68,68,68	1.98	21 (30%)	105,105,105	1.33	8 (7%)
3	GTP	I	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.14	4 (14%)
5	GDP	J	501	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	10 (38%)
6	TA1	J	502	-	68,68,68	1.98	20 (29%)	105,105,105	1.33	8 (7%)
3	GTP	K	501	4	27,34,34	1.51	4 (14%)	27,54,54	2.14	4 (14%)
5	GDP	L	501	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	11 (42%)
6	TA1	L	502	-	68,68,68	1.98	20 (29%)	105,105,105	1.33	8 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	M	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	4 (14%)
5	GDP	N	501	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	11 (42%)
6	TA1	N	502	-	68,68,68	1.97	20 (29%)	105,105,105	1.33	8 (7%)
3	GTP	O	501	4	27,34,34	1.51	4 (14%)	27,54,54	2.16	5 (18%)
5	GDP	P	501	-	25,30,30	2.73	8 (32%)	26,47,47	3.66	10 (38%)
6	TA1	P	502	-	68,68,68	1.98	20 (29%)	105,105,105	1.32	8 (7%)
3	GTP	Q	501	4	27,34,34	1.51	4 (14%)	27,54,54	2.15	5 (18%)
5	GDP	R	501	-	25,30,30	2.73	8 (32%)	26,47,47	3.65	10 (38%)
6	TA1	R	502	-	68,68,68	1.97	20 (29%)	105,105,105	1.33	8 (7%)

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
3	GTP	A	501	4	-	0/18/38/38	0/3/3/3
5	GDP	B	501	-	-	0/12/32/32	0/3/3/3
6	TA1	B	502	-	-	0/41/127/127	0/5/7/7
3	GTP	C	501	4	-	0/18/38/38	0/3/3/3
5	GDP	D	501	-	-	0/12/32/32	0/3/3/3
6	TA1	D	502	-	-	0/41/127/127	0/5/7/7
3	GTP	E	501	4	-	0/18/38/38	0/3/3/3
5	GDP	F	501	-	-	0/12/32/32	0/3/3/3
6	TA1	F	502	-	-	0/41/127/127	0/5/7/7
3	GTP	G	501	4	-	0/18/38/38	0/3/3/3
5	GDP	H	501	-	-	0/12/32/32	0/3/3/3
6	TA1	H	502	-	-	0/41/127/127	0/5/7/7
3	GTP	I	501	4	-	0/18/38/38	0/3/3/3
5	GDP	J	501	-	-	0/12/32/32	0/3/3/3
6	TA1	J	502	-	-	0/41/127/127	0/5/7/7
3	GTP	K	501	4	-	0/18/38/38	0/3/3/3
5	GDP	L	501	-	-	0/12/32/32	0/3/3/3
6	TA1	L	502	-	-	0/41/127/127	0/5/7/7
3	GTP	M	501	4	-	0/18/38/38	0/3/3/3
5	GDP	N	501	-	-	0/12/32/32	0/3/3/3
6	TA1	N	502	-	-	0/41/127/127	0/5/7/7
3	GTP	O	501	4	-	0/18/38/38	0/3/3/3
5	GDP	P	501	-	-	0/12/32/32	0/3/3/3
6	TA1	P	502	-	-	0/41/127/127	0/5/7/7
3	GTP	Q	501	4	-	0/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	R	501	-	-	0/12/32/32	0/3/3/3
6	TA1	R	502	-	-	0/41/127/127	0/5/7/7

All (285) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	TA1	C07-C06	-5.13	1.25	1.38
6	F	502	TA1	C07-C06	-5.13	1.25	1.38
6	N	502	TA1	C07-C06	-5.13	1.25	1.38
6	H	502	TA1	C07-C06	-5.12	1.25	1.38
6	P	502	TA1	C07-C06	-5.12	1.25	1.38
6	J	502	TA1	C07-C06	-5.12	1.25	1.38
6	R	502	TA1	C07-C06	-5.12	1.25	1.38
6	D	502	TA1	C07-C06	-5.11	1.25	1.38
6	L	502	TA1	C07-C06	-5.08	1.25	1.38
5	F	501	GDP	PB-O2B	-3.56	1.40	1.54
5	L	501	GDP	PB-O2B	-3.56	1.40	1.54
5	P	501	GDP	PB-O2B	-3.56	1.40	1.54
5	R	501	GDP	PB-O2B	-3.55	1.40	1.54
5	D	501	GDP	PB-O2B	-3.55	1.40	1.54
5	N	501	GDP	PB-O2B	-3.55	1.40	1.54
5	B	501	GDP	PB-O2B	-3.54	1.40	1.54
5	H	501	GDP	PB-O2B	-3.54	1.40	1.54
5	J	501	GDP	PB-O2B	-3.54	1.40	1.54
6	P	502	TA1	C04-C03	-2.37	1.44	1.49
6	R	502	TA1	C04-C03	-2.36	1.44	1.49
6	J	502	TA1	C04-C03	-2.35	1.44	1.49
6	D	502	TA1	C04-C03	-2.34	1.44	1.49
6	F	502	TA1	C04-C03	-2.34	1.44	1.49
6	B	502	TA1	C04-C03	-2.34	1.44	1.49
6	H	502	TA1	C04-C03	-2.34	1.44	1.49
6	N	502	TA1	C04-C03	-2.33	1.44	1.49
6	L	502	TA1	C04-C03	-2.32	1.44	1.49
3	O	501	GTP	C8-N7	-2.02	1.30	1.34
3	Q	501	GTP	C8-N7	-2.01	1.30	1.34
3	G	501	GTP	C8-N7	-2.01	1.30	1.34
3	K	501	GTP	C8-N7	-2.01	1.30	1.34
3	C	501	GTP	C8-N7	-2.00	1.30	1.34
6	H	502	TA1	C08-C07	2.00	1.42	1.38
6	F	502	TA1	C10-C02	2.01	1.62	1.57
6	B	502	TA1	C10-C02	2.02	1.62	1.57
6	P	502	TA1	C10-C02	2.03	1.62	1.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	502	TA1	C10-C02	2.03	1.62	1.57
6	N	502	TA1	C10-C02	2.03	1.62	1.57
6	H	502	TA1	C10-C02	2.03	1.62	1.57
6	D	502	TA1	C10-C02	2.04	1.62	1.57
3	I	501	GTP	O4'-C1'	2.04	1.44	1.41
6	L	502	TA1	C10-C02	2.06	1.62	1.57
6	R	502	TA1	C10-C02	2.06	1.62	1.57
3	O	501	GTP	O4'-C1'	2.10	1.44	1.41
3	K	501	GTP	O4'-C1'	2.10	1.44	1.41
3	G	501	GTP	O4'-C1'	2.11	1.44	1.41
3	C	501	GTP	O4'-C1'	2.11	1.44	1.41
6	L	502	TA1	C37-C29	2.12	1.54	1.51
3	E	501	GTP	O4'-C1'	2.12	1.44	1.41
6	N	502	TA1	C37-C29	2.12	1.54	1.51
6	P	502	TA1	C41-C42	2.13	1.43	1.38
3	A	501	GTP	O4'-C1'	2.13	1.44	1.41
3	Q	501	GTP	O4'-C1'	2.13	1.44	1.41
5	F	501	GDP	O3'-C3'	2.14	1.47	1.43
3	M	501	GTP	O4'-C1'	2.14	1.44	1.41
6	J	502	TA1	C41-C42	2.14	1.43	1.38
6	B	502	TA1	C37-C29	2.14	1.54	1.51
6	B	502	TA1	C41-C42	2.14	1.43	1.38
5	L	501	GDP	O3'-C3'	2.15	1.47	1.43
5	N	501	GDP	O3'-C3'	2.15	1.47	1.43
6	H	502	TA1	C41-C42	2.15	1.43	1.38
5	D	501	GDP	O3'-C3'	2.16	1.47	1.43
5	B	501	GDP	O3'-C3'	2.16	1.47	1.43
6	D	502	TA1	C41-C42	2.16	1.43	1.38
5	R	501	GDP	O3'-C3'	2.16	1.47	1.43
6	F	502	TA1	C41-C42	2.16	1.43	1.38
5	J	501	GDP	O3'-C3'	2.16	1.47	1.43
6	D	502	TA1	C37-C29	2.16	1.54	1.51
5	H	501	GDP	O3'-C3'	2.17	1.47	1.43
6	R	502	TA1	C41-C42	2.17	1.43	1.38
6	H	502	TA1	C37-C29	2.17	1.54	1.51
6	F	502	TA1	C37-C29	2.17	1.54	1.51
6	P	502	TA1	C37-C29	2.17	1.54	1.51
5	P	501	GDP	O3'-C3'	2.18	1.48	1.43
6	R	502	TA1	C37-C29	2.18	1.54	1.51
6	J	502	TA1	C37-C29	2.18	1.54	1.51
6	L	502	TA1	C41-C42	2.19	1.43	1.38
6	R	502	TA1	C18-C20	2.19	1.62	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502	TA1	C16-C15	2.19	1.56	1.52
6	H	502	TA1	C16-C15	2.19	1.56	1.52
6	H	502	TA1	C18-C20	2.20	1.62	1.56
6	N	502	TA1	C41-C42	2.20	1.43	1.38
6	D	502	TA1	C18-C20	2.20	1.62	1.56
6	N	502	TA1	C18-C20	2.20	1.62	1.56
6	R	502	TA1	C16-C15	2.21	1.56	1.52
6	D	502	TA1	C16-C15	2.21	1.56	1.52
6	F	502	TA1	C16-C15	2.21	1.56	1.52
6	B	502	TA1	C18-C20	2.21	1.62	1.56
6	N	502	TA1	C16-C15	2.21	1.56	1.52
6	J	502	TA1	C18-C20	2.21	1.62	1.56
6	B	502	TA1	C16-C15	2.21	1.56	1.52
6	P	502	TA1	C16-C15	2.21	1.56	1.52
6	F	502	TA1	C18-C20	2.22	1.62	1.56
6	P	502	TA1	C18-C20	2.22	1.62	1.56
6	L	502	TA1	C18-C20	2.22	1.62	1.56
6	J	502	TA1	C16-C15	2.23	1.57	1.52
6	F	502	TA1	C01-C45	2.24	1.66	1.56
6	J	502	TA1	C01-C45	2.24	1.66	1.56
6	H	502	TA1	C01-C45	2.24	1.66	1.56
6	P	502	TA1	C01-C45	2.24	1.66	1.56
6	L	502	TA1	C01-C45	2.24	1.66	1.56
6	D	502	TA1	C01-C45	2.25	1.66	1.56
6	B	502	TA1	C01-C45	2.25	1.66	1.56
6	J	502	TA1	C11-C10	2.26	1.61	1.55
6	R	502	TA1	C01-C45	2.26	1.66	1.56
6	L	502	TA1	C11-C10	2.26	1.61	1.55
6	D	502	TA1	C11-C10	2.27	1.61	1.55
6	F	502	TA1	C11-C10	2.27	1.61	1.55
6	N	502	TA1	C01-C45	2.27	1.66	1.56
6	N	502	TA1	C11-C10	2.27	1.61	1.55
6	H	502	TA1	C11-C10	2.27	1.61	1.55
6	B	502	TA1	C11-C10	2.28	1.61	1.55
6	P	502	TA1	C11-C10	2.28	1.61	1.55
6	R	502	TA1	C11-C10	2.29	1.61	1.55
6	J	502	TA1	C26-C25	2.46	1.56	1.51
6	H	502	TA1	C26-C25	2.47	1.56	1.51
6	D	502	TA1	C26-C25	2.47	1.56	1.51
6	P	502	TA1	C26-C25	2.47	1.56	1.51
6	F	502	TA1	C26-C25	2.49	1.56	1.51
5	L	501	GDP	C5-C4	2.49	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	502	TA1	C26-C25	2.50	1.56	1.51
5	H	501	GDP	C5-C4	2.50	1.46	1.40
6	L	502	TA1	C26-C25	2.50	1.56	1.51
6	R	502	TA1	C26-C25	2.50	1.56	1.51
5	D	501	GDP	C5-C4	2.51	1.46	1.40
5	B	501	GDP	C5-C4	2.51	1.46	1.40
5	R	501	GDP	C5-C4	2.51	1.46	1.40
5	J	501	GDP	C5-C4	2.51	1.46	1.40
6	B	502	TA1	C43-C26	2.52	1.58	1.52
6	N	502	TA1	C43-C26	2.52	1.58	1.52
6	L	502	TA1	C43-C26	2.53	1.58	1.52
6	H	502	TA1	C43-C26	2.53	1.58	1.52
6	B	502	TA1	C26-C25	2.53	1.56	1.51
5	N	501	GDP	C5-C4	2.53	1.46	1.40
5	F	501	GDP	C5-C4	2.53	1.46	1.40
5	P	501	GDP	C5-C4	2.53	1.46	1.40
6	J	502	TA1	C43-C26	2.54	1.58	1.52
6	R	502	TA1	C43-C26	2.54	1.58	1.52
6	D	502	TA1	C43-C26	2.54	1.58	1.52
6	F	502	TA1	C43-C26	2.54	1.58	1.52
6	P	502	TA1	C43-C26	2.57	1.58	1.52
6	F	502	TA1	C43-C01	2.89	1.60	1.54
6	R	502	TA1	C43-C01	2.89	1.60	1.54
6	N	502	TA1	C43-C01	2.92	1.60	1.54
6	D	502	TA1	C43-C01	2.92	1.60	1.54
6	P	502	TA1	C43-C01	2.92	1.60	1.54
6	H	502	TA1	C43-C01	2.92	1.60	1.54
6	L	502	TA1	C43-C01	2.93	1.60	1.54
6	B	502	TA1	C43-C01	2.94	1.60	1.54
6	J	502	TA1	C43-C01	2.94	1.60	1.54
6	B	502	TA1	C25-C24	3.03	1.39	1.34
6	F	502	TA1	C25-C24	3.03	1.39	1.34
6	R	502	TA1	C25-C24	3.03	1.39	1.34
6	N	502	TA1	C25-C24	3.04	1.39	1.34
6	H	502	TA1	C25-C24	3.04	1.39	1.34
6	D	502	TA1	C25-C24	3.06	1.39	1.34
6	L	502	TA1	C25-C24	3.06	1.39	1.34
6	P	502	TA1	C25-C24	3.08	1.39	1.34
6	J	502	TA1	C25-C24	3.08	1.39	1.34
6	R	502	TA1	C46-C45	3.12	1.60	1.53
6	N	502	TA1	C46-C45	3.14	1.60	1.53
6	D	502	TA1	C46-C45	3.14	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	502	TA1	C46-C45	3.15	1.60	1.53
6	J	502	TA1	C46-C45	3.15	1.60	1.53
6	B	502	TA1	C46-C45	3.15	1.60	1.53
6	P	502	TA1	C46-C45	3.16	1.60	1.53
6	L	502	TA1	C46-C45	3.16	1.60	1.53
6	F	502	TA1	C46-C45	3.16	1.60	1.53
6	F	502	TA1	O02-C03	3.37	1.41	1.34
6	P	502	TA1	O02-C03	3.38	1.41	1.34
6	H	502	TA1	O02-C03	3.39	1.41	1.34
6	D	502	TA1	O02-C03	3.41	1.41	1.34
6	P	502	TA1	C45-C24	3.41	1.61	1.54
6	J	502	TA1	O02-C03	3.42	1.41	1.34
6	N	502	TA1	O02-C03	3.42	1.41	1.34
6	R	502	TA1	O02-C03	3.42	1.41	1.34
6	B	502	TA1	O02-C03	3.43	1.41	1.34
6	L	502	TA1	O02-C03	3.44	1.41	1.34
6	H	502	TA1	C45-C24	3.44	1.61	1.54
6	N	502	TA1	C45-C24	3.44	1.61	1.54
6	R	502	TA1	C45-C24	3.44	1.61	1.54
6	D	502	TA1	C45-C24	3.45	1.61	1.54
6	B	502	TA1	C45-C24	3.45	1.61	1.54
6	F	502	TA1	C45-C24	3.45	1.61	1.54
6	J	502	TA1	C45-C24	3.47	1.61	1.54
5	H	501	GDP	C8-N7	3.47	1.41	1.34
5	R	501	GDP	C8-N7	3.48	1.41	1.34
6	L	502	TA1	C45-C24	3.48	1.61	1.54
5	L	501	GDP	C8-N7	3.48	1.41	1.34
6	R	502	TA1	C36-C31	3.49	1.45	1.39
5	B	501	GDP	C8-N7	3.49	1.41	1.34
5	D	501	GDP	C8-N7	3.49	1.41	1.34
5	N	501	GDP	C8-N7	3.50	1.41	1.34
6	N	502	TA1	C36-C31	3.50	1.45	1.39
6	J	502	TA1	C36-C31	3.50	1.45	1.39
6	B	502	TA1	C36-C31	3.52	1.45	1.39
6	D	502	TA1	C36-C31	3.53	1.45	1.39
6	F	502	TA1	C36-C31	3.53	1.45	1.39
6	P	502	TA1	C36-C31	3.53	1.45	1.39
5	F	501	GDP	C8-N7	3.53	1.41	1.34
5	P	501	GDP	C8-N7	3.54	1.41	1.34
5	J	501	GDP	C8-N7	3.54	1.41	1.34
6	L	502	TA1	C36-C31	3.54	1.45	1.39
6	H	502	TA1	C36-C31	3.54	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	PB-O1B	3.83	1.63	1.50
5	N	501	GDP	PB-O1B	3.84	1.63	1.50
5	D	501	GDP	PB-O1B	3.85	1.63	1.50
5	R	501	GDP	PB-O1B	3.85	1.63	1.50
5	H	501	GDP	PB-O1B	3.85	1.63	1.50
5	F	501	GDP	PB-O1B	3.85	1.63	1.50
5	P	501	GDP	PB-O1B	3.86	1.63	1.50
5	L	501	GDP	PB-O1B	3.86	1.63	1.50
5	J	501	GDP	PB-O1B	3.86	1.63	1.50
3	G	501	GTP	PG-O3B	3.87	1.66	1.60
3	Q	501	GTP	PG-O3B	3.87	1.66	1.60
3	O	501	GTP	PG-O3B	3.88	1.66	1.60
3	A	501	GTP	PG-O3B	3.88	1.66	1.60
3	M	501	GTP	PG-O3B	3.90	1.66	1.60
3	E	501	GTP	PG-O3B	3.90	1.66	1.60
3	C	501	GTP	PG-O3B	3.90	1.66	1.60
3	K	501	GTP	PG-O3B	3.92	1.66	1.60
3	I	501	GTP	PG-O3B	3.92	1.66	1.60
5	B	501	GDP	O6-C6	4.14	1.34	1.24
5	R	501	GDP	O6-C6	4.14	1.35	1.24
5	J	501	GDP	O6-C6	4.14	1.35	1.24
5	L	501	GDP	O6-C6	4.15	1.35	1.24
5	D	501	GDP	O6-C6	4.16	1.35	1.24
5	N	501	GDP	O6-C6	4.17	1.35	1.24
5	P	501	GDP	O6-C6	4.17	1.35	1.24
5	F	501	GDP	O6-C6	4.18	1.35	1.24
5	H	501	GDP	O6-C6	4.18	1.35	1.24
6	F	502	TA1	C18-C10	4.30	1.69	1.57
6	L	502	TA1	C18-C10	4.30	1.69	1.57
6	P	502	TA1	C18-C10	4.31	1.69	1.57
6	D	502	TA1	C18-C10	4.32	1.69	1.57
6	H	502	TA1	C18-C10	4.33	1.69	1.57
6	N	502	TA1	C18-C10	4.33	1.69	1.57
6	R	502	TA1	C18-C10	4.34	1.69	1.57
6	J	502	TA1	C18-C10	4.34	1.69	1.57
6	B	502	TA1	C18-C10	4.35	1.69	1.57
6	R	502	TA1	C09-C04	4.50	1.46	1.39
6	H	502	TA1	C09-C04	4.50	1.46	1.39
6	P	502	TA1	C09-C04	4.50	1.46	1.39
6	D	502	TA1	C09-C04	4.51	1.46	1.39
6	N	502	TA1	C09-C04	4.51	1.46	1.39
6	J	502	TA1	C09-C04	4.51	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	TA1	C09-C04	4.51	1.46	1.39
6	F	502	TA1	C09-C04	4.53	1.46	1.39
6	L	502	TA1	C09-C04	4.57	1.46	1.39
3	M	501	GTP	C6-N1	4.70	1.41	1.33
3	Q	501	GTP	C6-N1	4.73	1.41	1.33
3	O	501	GTP	C6-N1	4.75	1.41	1.33
3	C	501	GTP	C6-N1	4.76	1.41	1.33
3	A	501	GTP	C6-N1	4.76	1.41	1.33
3	G	501	GTP	C6-N1	4.77	1.41	1.33
3	K	501	GTP	C6-N1	4.77	1.41	1.33
3	I	501	GTP	C6-N1	4.79	1.41	1.33
3	E	501	GTP	C6-N1	4.80	1.41	1.33
6	J	502	TA1	C08-C09	5.79	1.50	1.38
6	L	502	TA1	C08-C09	5.80	1.50	1.38
6	R	502	TA1	C08-C09	5.80	1.50	1.38
6	B	502	TA1	C08-C09	5.81	1.50	1.38
6	N	502	TA1	C08-C09	5.81	1.50	1.38
6	D	502	TA1	C08-C09	5.83	1.50	1.38
6	H	502	TA1	C08-C09	5.83	1.50	1.38
6	P	502	TA1	C08-C09	5.83	1.50	1.38
6	F	502	TA1	C08-C09	5.86	1.50	1.38
5	N	501	GDP	O4'-C1'	6.21	1.49	1.41
5	B	501	GDP	O4'-C1'	6.21	1.49	1.41
5	D	501	GDP	O4'-C1'	6.22	1.49	1.41
5	J	501	GDP	O4'-C1'	6.23	1.49	1.41
5	H	501	GDP	O4'-C1'	6.23	1.49	1.41
5	P	501	GDP	O4'-C1'	6.24	1.49	1.41
5	F	501	GDP	O4'-C1'	6.25	1.49	1.41
5	L	501	GDP	O4'-C1'	6.26	1.49	1.41
5	R	501	GDP	O4'-C1'	6.30	1.50	1.41
5	P	501	GDP	C2-N1	7.53	1.49	1.35
5	J	501	GDP	C2-N1	7.53	1.49	1.35
5	R	501	GDP	C2-N1	7.53	1.49	1.35
5	H	501	GDP	C2-N1	7.54	1.49	1.35
5	L	501	GDP	C2-N1	7.54	1.49	1.35
5	D	501	GDP	C2-N1	7.55	1.49	1.35
5	B	501	GDP	C2-N1	7.56	1.49	1.35
5	N	501	GDP	C2-N1	7.56	1.49	1.35
5	F	501	GDP	C2-N1	7.56	1.49	1.35

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	501	GDP	C6-C5-C4	-11.54	109.37	120.84
5	F	501	GDP	C6-C5-C4	-11.53	109.38	120.84
5	P	501	GDP	C6-C5-C4	-11.51	109.40	120.84
5	J	501	GDP	C6-C5-C4	-11.51	109.40	120.84
5	D	501	GDP	C6-C5-C4	-11.51	109.40	120.84
5	B	501	GDP	C6-C5-C4	-11.50	109.40	120.84
5	L	501	GDP	C6-C5-C4	-11.50	109.41	120.84
5	H	501	GDP	C6-C5-C4	-11.48	109.42	120.84
5	R	501	GDP	C6-C5-C4	-11.46	109.44	120.84
3	O	501	GTP	C5-C6-N1	-7.10	113.37	123.48
3	A	501	GTP	C5-C6-N1	-7.09	113.39	123.48
3	G	501	GTP	C5-C6-N1	-7.08	113.41	123.48
3	C	501	GTP	C5-C6-N1	-7.07	113.41	123.48
3	I	501	GTP	C5-C6-N1	-7.07	113.41	123.48
3	E	501	GTP	C5-C6-N1	-7.07	113.41	123.48
3	Q	501	GTP	C5-C6-N1	-7.06	113.43	123.48
3	K	501	GTP	C5-C6-N1	-7.06	113.43	123.48
3	M	501	GTP	C5-C6-N1	-7.04	113.46	123.48
5	J	501	GDP	N2-C2-N1	-5.89	107.81	117.24
5	N	501	GDP	N2-C2-N1	-5.89	107.82	117.24
5	H	501	GDP	N2-C2-N1	-5.89	107.83	117.24
5	R	501	GDP	N2-C2-N1	-5.87	107.86	117.24
5	D	501	GDP	N2-C2-N1	-5.87	107.86	117.24
5	B	501	GDP	N2-C2-N1	-5.87	107.86	117.24
5	P	501	GDP	N2-C2-N1	-5.86	107.87	117.24
5	L	501	GDP	N2-C2-N1	-5.85	107.89	117.24
5	F	501	GDP	N2-C2-N1	-5.84	107.89	117.24
5	H	501	GDP	C4-C5-N7	-5.03	104.55	109.41
5	L	501	GDP	C4-C5-N7	-5.01	104.57	109.41
5	B	501	GDP	C4-C5-N7	-4.99	104.59	109.41
5	P	501	GDP	C4-C5-N7	-4.99	104.59	109.41
5	N	501	GDP	C4-C5-N7	-4.98	104.60	109.41
5	F	501	GDP	C4-C5-N7	-4.98	104.60	109.41
5	R	501	GDP	C4-C5-N7	-4.98	104.60	109.41
5	D	501	GDP	C4-C5-N7	-4.98	104.60	109.41
5	F	501	GDP	N3-C2-N1	-4.97	120.20	127.46
5	L	501	GDP	N3-C2-N1	-4.96	120.21	127.46
5	B	501	GDP	N3-C2-N1	-4.95	120.22	127.46
5	P	501	GDP	N3-C2-N1	-4.94	120.24	127.46
5	J	501	GDP	C4-C5-N7	-4.94	104.64	109.41
5	D	501	GDP	N3-C2-N1	-4.94	120.25	127.46
5	H	501	GDP	N3-C2-N1	-4.93	120.25	127.46
5	J	501	GDP	N3-C2-N1	-4.93	120.25	127.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	501	GDP	N3-C2-N1	-4.92	120.27	127.46
5	N	501	GDP	N3-C2-N1	-4.91	120.28	127.46
6	L	502	TA1	C08-C09-C04	-4.88	114.61	120.35
6	F	502	TA1	C08-C09-C04	-4.87	114.63	120.35
6	B	502	TA1	C08-C09-C04	-4.85	114.65	120.35
6	D	502	TA1	C08-C09-C04	-4.84	114.65	120.35
6	R	502	TA1	C08-C09-C04	-4.84	114.66	120.35
6	N	502	TA1	C08-C09-C04	-4.83	114.66	120.35
6	P	502	TA1	C08-C09-C04	-4.83	114.67	120.35
6	J	502	TA1	C08-C09-C04	-4.83	114.67	120.35
6	H	502	TA1	C08-C09-C04	-4.82	114.68	120.35
6	L	502	TA1	C09-C04-C03	-3.99	111.41	120.39
6	B	502	TA1	C09-C04-C03	-3.98	111.43	120.39
6	F	502	TA1	C09-C04-C03	-3.97	111.45	120.39
6	N	502	TA1	C09-C04-C03	-3.97	111.45	120.39
6	D	502	TA1	C09-C04-C03	-3.97	111.46	120.39
6	J	502	TA1	C09-C04-C03	-3.97	111.46	120.39
6	H	502	TA1	C09-C04-C03	-3.96	111.47	120.39
6	R	502	TA1	C09-C04-C03	-3.96	111.47	120.39
6	P	502	TA1	C09-C04-C03	-3.94	111.53	120.39
3	Q	501	GTP	N3-C2-N1	-3.19	122.80	127.46
3	O	501	GTP	N3-C2-N1	-3.19	122.81	127.46
3	M	501	GTP	N3-C2-N1	-3.18	122.81	127.46
3	E	501	GTP	N3-C2-N1	-3.18	122.81	127.46
3	K	501	GTP	N3-C2-N1	-3.17	122.83	127.46
3	C	501	GTP	N3-C2-N1	-3.16	122.85	127.46
3	G	501	GTP	N3-C2-N1	-3.16	122.85	127.46
3	A	501	GTP	N3-C2-N1	-3.15	122.86	127.46
3	I	501	GTP	N3-C2-N1	-3.14	122.88	127.46
6	B	502	TA1	O04-C11-C14	-2.73	101.81	108.14
6	F	502	TA1	O04-C11-C14	-2.73	101.83	108.14
6	H	502	TA1	O04-C11-C14	-2.72	101.84	108.14
6	P	502	TA1	O04-C11-C14	-2.72	101.84	108.14
6	N	502	TA1	O04-C11-C14	-2.72	101.84	108.14
6	D	502	TA1	O04-C11-C14	-2.72	101.84	108.14
6	J	502	TA1	O04-C11-C14	-2.72	101.85	108.14
6	L	502	TA1	O04-C11-C14	-2.72	101.85	108.14
6	R	502	TA1	O04-C11-C14	-2.71	101.86	108.14
3	M	501	GTP	C6-C5-C4	-2.52	118.34	120.84
3	O	501	GTP	C6-C5-C4	-2.49	118.37	120.84
3	E	501	GTP	C6-C5-C4	-2.47	118.39	120.84
3	Q	501	GTP	C6-C5-C4	-2.47	118.39	120.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	GTP	C6-C5-C4	-2.47	118.39	120.84
3	K	501	GTP	C6-C5-C4	-2.46	118.40	120.84
3	G	501	GTP	C6-C5-C4	-2.45	118.41	120.84
3	I	501	GTP	C6-C5-C4	-2.43	118.43	120.84
3	A	501	GTP	C6-C5-C4	-2.42	118.44	120.84
5	N	501	GDP	O4'-C4'-C3'	-2.01	101.16	105.17
5	L	501	GDP	O4'-C4'-C3'	-2.01	101.17	105.17
5	F	501	GDP	O4'-C4'-C3'	-2.01	101.17	105.17
5	B	501	GDP	O4'-C4'-C3'	-2.00	101.18	105.17
3	Q	501	GTP	O5'-C5'-C4'	2.00	116.10	109.00
3	G	501	GTP	O5'-C5'-C4'	2.00	116.11	109.00
3	O	501	GTP	O5'-C5'-C4'	2.00	116.11	109.00
5	B	501	GDP	O3B-PB-O2B	2.07	115.98	107.61
5	F	501	GDP	O3B-PB-O2B	2.08	116.00	107.61
5	J	501	GDP	O3B-PB-O2B	2.08	116.02	107.61
5	R	501	GDP	O3B-PB-O2B	2.09	116.03	107.61
5	L	501	GDP	O3B-PB-O2B	2.09	116.04	107.61
5	H	501	GDP	O3B-PB-O2B	2.09	116.05	107.61
5	D	501	GDP	O3B-PB-O2B	2.09	116.05	107.61
5	N	501	GDP	O3B-PB-O2B	2.09	116.06	107.61
5	P	501	GDP	O3B-PB-O2B	2.10	116.07	107.61
5	H	501	GDP	O2'-C2'-C3'	2.34	119.33	111.83
5	N	501	GDP	O2'-C2'-C3'	2.35	119.34	111.83
5	D	501	GDP	O2'-C2'-C3'	2.35	119.36	111.83
5	J	501	GDP	O2'-C2'-C3'	2.35	119.37	111.83
5	P	501	GDP	O2'-C2'-C3'	2.35	119.37	111.83
5	F	501	GDP	O2'-C2'-C3'	2.35	119.37	111.83
5	L	501	GDP	O2'-C2'-C3'	2.36	119.38	111.83
5	B	501	GDP	O2'-C2'-C3'	2.36	119.38	111.83
5	R	501	GDP	O2'-C2'-C3'	2.36	119.40	111.83
6	B	502	TA1	O01-C01-C43	2.48	113.41	106.86
6	J	502	TA1	O01-C01-C43	2.48	113.41	106.86
6	H	502	TA1	O01-C01-C43	2.48	113.42	106.86
6	P	502	TA1	O01-C01-C43	2.49	113.43	106.86
6	D	502	TA1	O01-C01-C43	2.49	113.43	106.86
6	F	502	TA1	O01-C01-C43	2.50	113.45	106.86
6	R	502	TA1	O01-C01-C43	2.50	113.46	106.86
6	L	502	TA1	O01-C01-C43	2.51	113.48	106.86
6	N	502	TA1	O01-C01-C43	2.51	113.49	106.86
6	L	502	TA1	C45-C01-C02	2.56	115.06	111.85
6	F	502	TA1	C45-C01-C02	2.56	115.07	111.85
6	N	502	TA1	C45-C01-C02	2.58	115.08	111.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	502	TA1	C45-C01-C02	2.58	115.09	111.85
6	H	502	TA1	C45-C01-C02	2.58	115.09	111.85
6	D	502	TA1	C45-C01-C02	2.60	115.11	111.85
6	J	502	TA1	C45-C01-C02	2.60	115.11	111.85
6	B	502	TA1	C45-C01-C02	2.60	115.12	111.85
6	R	502	TA1	C45-C01-C02	2.60	115.12	111.85
6	L	502	TA1	C17-C18-C20	2.83	109.79	102.33
6	P	502	TA1	C17-C18-C20	2.83	109.80	102.33
6	F	502	TA1	C17-C18-C20	2.84	109.81	102.33
6	J	502	TA1	C17-C18-C20	2.84	109.81	102.33
6	B	502	TA1	C17-C18-C20	2.84	109.83	102.33
6	D	502	TA1	C17-C18-C20	2.84	109.83	102.33
6	H	502	TA1	C17-C18-C20	2.85	109.84	102.33
6	R	502	TA1	C17-C18-C20	2.85	109.85	102.33
6	N	502	TA1	C17-C18-C20	2.86	109.87	102.33
5	P	501	GDP	C2'-C3'-C4'	3.48	109.40	102.62
5	J	501	GDP	C2'-C3'-C4'	3.49	109.41	102.62
5	H	501	GDP	C2'-C3'-C4'	3.49	109.41	102.62
5	D	501	GDP	C2'-C3'-C4'	3.49	109.42	102.62
5	N	501	GDP	C2'-C3'-C4'	3.49	109.42	102.62
5	B	501	GDP	C2'-C3'-C4'	3.49	109.42	102.62
5	F	501	GDP	C2'-C3'-C4'	3.50	109.43	102.62
5	L	501	GDP	C2'-C3'-C4'	3.50	109.43	102.62
5	R	501	GDP	C2'-C3'-C4'	3.50	109.44	102.62
6	P	502	TA1	C05-C04-C03	3.55	128.40	120.39
5	B	501	GDP	C2-N3-C4	3.56	119.31	115.16
5	N	501	GDP	C2-N3-C4	3.56	119.31	115.16
5	D	501	GDP	C2-N3-C4	3.56	119.31	115.16
5	R	501	GDP	C2-N3-C4	3.56	119.32	115.16
5	J	501	GDP	C2-N3-C4	3.56	119.32	115.16
6	D	502	TA1	C05-C04-C03	3.57	128.43	120.39
6	R	502	TA1	C05-C04-C03	3.57	128.43	120.39
6	J	502	TA1	C05-C04-C03	3.57	128.43	120.39
6	H	502	TA1	C05-C04-C03	3.57	128.43	120.39
5	F	501	GDP	C2-N3-C4	3.57	119.33	115.16
6	B	502	TA1	C05-C04-C03	3.57	128.44	120.39
5	H	501	GDP	C2-N3-C4	3.58	119.33	115.16
6	F	502	TA1	C05-C04-C03	3.58	128.45	120.39
5	L	501	GDP	C2-N3-C4	3.58	119.33	115.16
5	P	501	GDP	C2-N3-C4	3.58	119.33	115.16
6	N	502	TA1	C05-C04-C03	3.58	128.45	120.39
6	L	502	TA1	C05-C04-C03	3.59	128.47	120.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	501	GDP	C4'-O4'-C1'	3.99	114.01	109.77
5	P	501	GDP	C4'-O4'-C1'	3.99	114.02	109.77
5	H	501	GDP	C4'-O4'-C1'	4.00	114.02	109.77
5	F	501	GDP	C4'-O4'-C1'	4.00	114.03	109.77
5	R	501	GDP	C4'-O4'-C1'	4.00	114.03	109.77
5	D	501	GDP	C4'-O4'-C1'	4.00	114.03	109.77
5	L	501	GDP	C4'-O4'-C1'	4.01	114.04	109.77
5	N	501	GDP	C4'-O4'-C1'	4.01	114.04	109.77
5	B	501	GDP	C4'-O4'-C1'	4.04	114.07	109.77
6	P	502	TA1	C07-C06-C05	5.21	127.37	120.21
6	N	502	TA1	C07-C06-C05	5.23	127.39	120.21
6	L	502	TA1	C07-C06-C05	5.23	127.40	120.21
6	D	502	TA1	C07-C06-C05	5.24	127.41	120.21
6	B	502	TA1	C07-C06-C05	5.25	127.42	120.21
6	J	502	TA1	C07-C06-C05	5.25	127.42	120.21
6	R	502	TA1	C07-C06-C05	5.25	127.43	120.21
6	H	502	TA1	C07-C06-C05	5.26	127.44	120.21
6	F	502	TA1	C07-C06-C05	5.27	127.45	120.21
3	I	501	GTP	C6-N1-C2	5.89	124.54	116.06
3	K	501	GTP	C6-N1-C2	5.90	124.55	116.06
3	M	501	GTP	C6-N1-C2	5.91	124.57	116.06
3	E	501	GTP	C6-N1-C2	5.92	124.57	116.06
3	Q	501	GTP	C6-N1-C2	5.92	124.57	116.06
3	C	501	GTP	C6-N1-C2	5.92	124.58	116.06
3	G	501	GTP	C6-N1-C2	5.93	124.59	116.06
3	A	501	GTP	C6-N1-C2	5.93	124.59	116.06
3	O	501	GTP	C6-N1-C2	5.97	124.64	116.06
5	R	501	GDP	N2-C2-N3	7.64	131.86	117.75
5	P	501	GDP	N2-C2-N3	7.65	131.88	117.75
5	D	501	GDP	N2-C2-N3	7.66	131.88	117.75
5	N	501	GDP	N2-C2-N3	7.66	131.89	117.75
5	L	501	GDP	N2-C2-N3	7.66	131.89	117.75
5	F	501	GDP	N2-C2-N3	7.66	131.90	117.75
5	B	501	GDP	N2-C2-N3	7.67	131.91	117.75
5	H	501	GDP	N2-C2-N3	7.67	131.91	117.75
5	J	501	GDP	N2-C2-N3	7.68	131.92	117.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	GDP	2	0
6	B	502	TA1	4	0
5	D	501	GDP	2	0
6	D	502	TA1	4	0
5	F	501	GDP	2	0
6	F	502	TA1	4	0
5	H	501	GDP	2	0
6	H	502	TA1	4	0
5	J	501	GDP	2	0
6	J	502	TA1	4	0
5	L	501	GDP	2	0
6	L	502	TA1	4	0
5	N	501	GDP	2	0
6	N	502	TA1	4	0
5	P	501	GDP	2	0
6	P	502	TA1	4	0
5	R	501	GDP	2	0
6	R	502	TA1	4	0

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.