



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 AM UTC

PDB ID : 3K0A / pdb_00003k0a
Title : Crystal structure of the phosphorylation-site mutant S431A of the KaiC circadian clock protein
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on : 2009-09-24
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

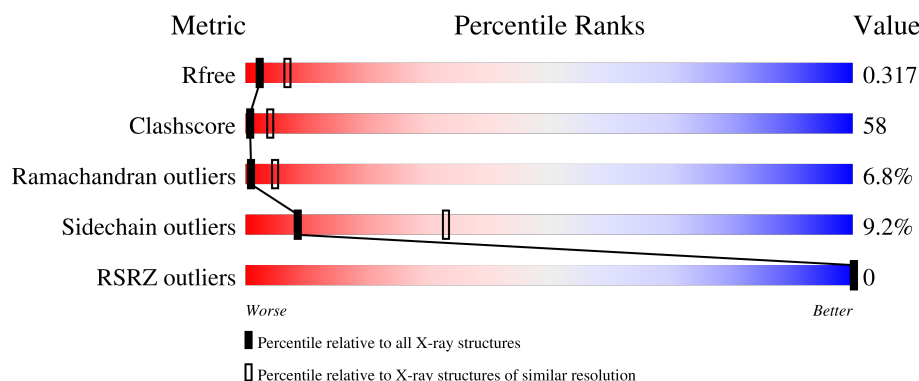
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



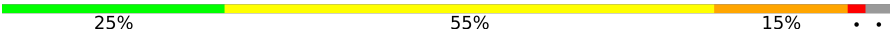
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	519	 27% 58% 11% ..
2	B	519	 27% 56% 11% • 5%
2	C	519	 25% 57% 12% • 6%
2	D	519	 25% 57% 10% • 7%
2	E	519	 28% 54% 12% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	519	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (25%), yellow (55%), and orange (15%). The segments are labeled with their respective percentages. The bar ends with a small red segment and two dots.

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	A	426	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23921 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3992	2509	701	765	2	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ALA	SER	engineered mutation	UNP Q79PF4

- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	491	Total	C	N	O	P	S	0	0	0
			3873	2439	678	740	1	15			
2	C	488	Total	C	N	O	P	S	0	0	0
			3849	2425	674	734	1	15			
2	D	485	Total	C	N	O	P	S	0	0	0
			3825	2411	671	727	1	15			
2	E	492	Total	C	N	O	P	S	0	0	0
			3881	2445	679	741	1	15			
2	F	506	Total	C	N	O	P	S	0	0	0
			3988	2509	701	762	1	15			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	431	ALA	SER	engineered mutation	UNP Q79PF4
C	431	ALA	SER	engineered mutation	UNP Q79PF4
D	431	ALA	SER	engineered mutation	UNP Q79PF4
E	431	ALA	SER	engineered mutation	UNP Q79PF4
F	431	ALA	SER	engineered mutation	UNP Q79PF4

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	Mg 6	0	0
4	B	3	Total 3	Mg 3	0	0
4	C	4	Total 4	Mg 4	0	0
4	D	2	Total 2	Mg 2	0	0
4	E	4	Total 4	Mg 4	0	0
4	F	3	Total 3	Mg 3	0	0

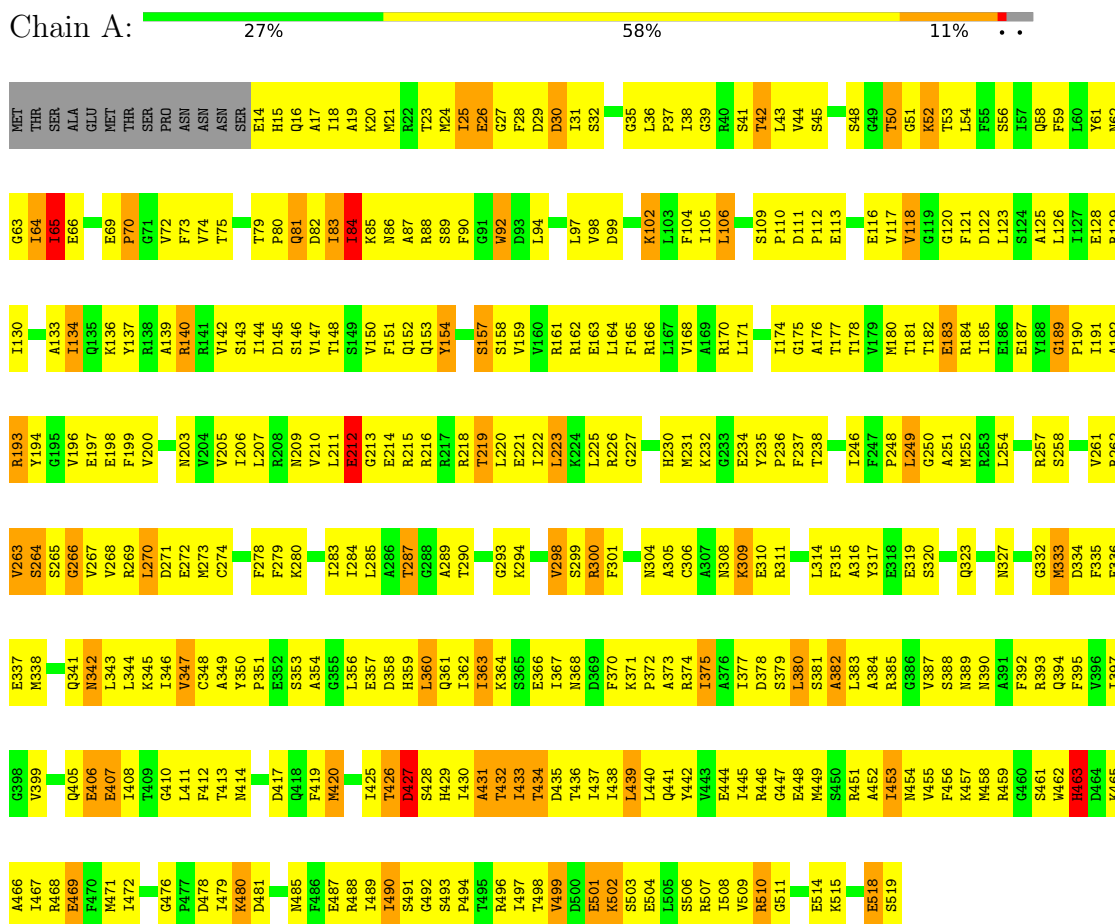
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total 14	O 14	0	0
5	B	20	Total 20	O 20	0	0
5	C	23	Total 23	O 23	0	0
5	D	28	Total 28	O 28	0	0
5	E	15	Total 15	O 15	0	0
5	F	19	Total 19	O 19	0	0

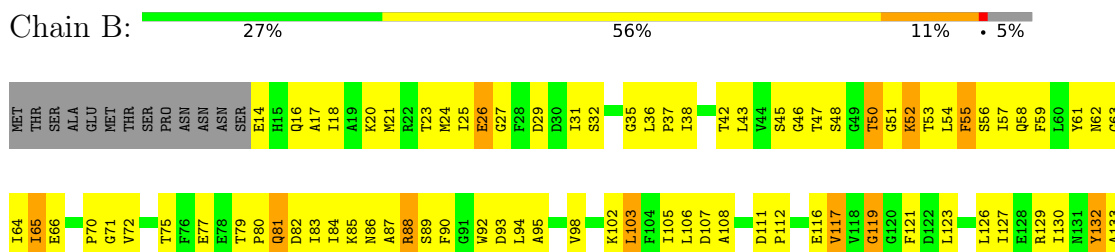
3 Residue-property plots

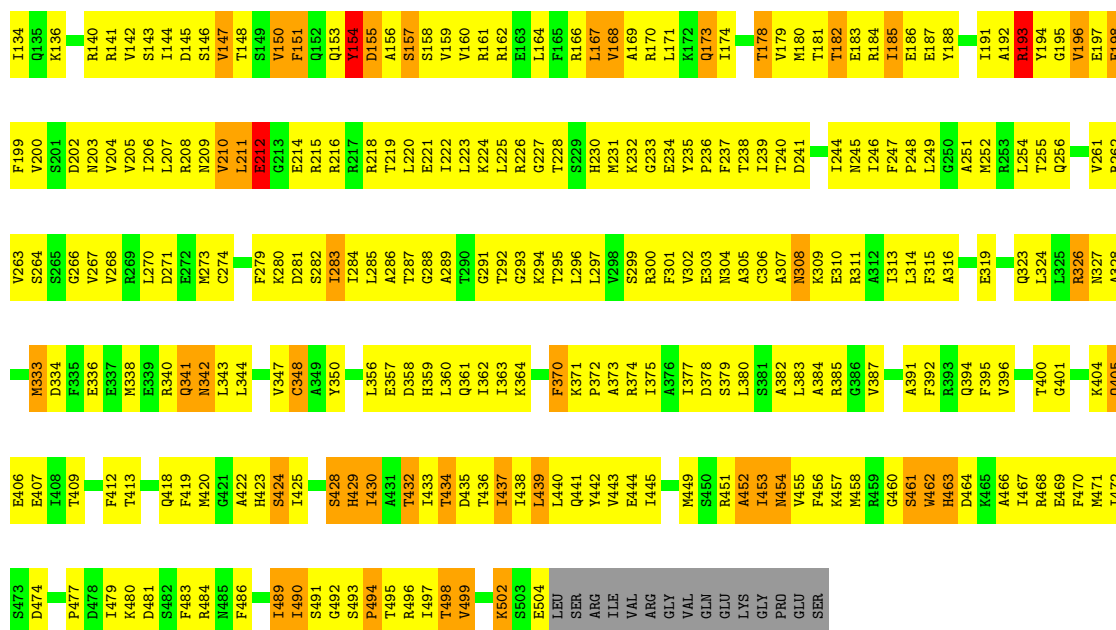
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Circadian clock protein kinase KaiC

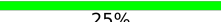
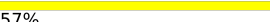


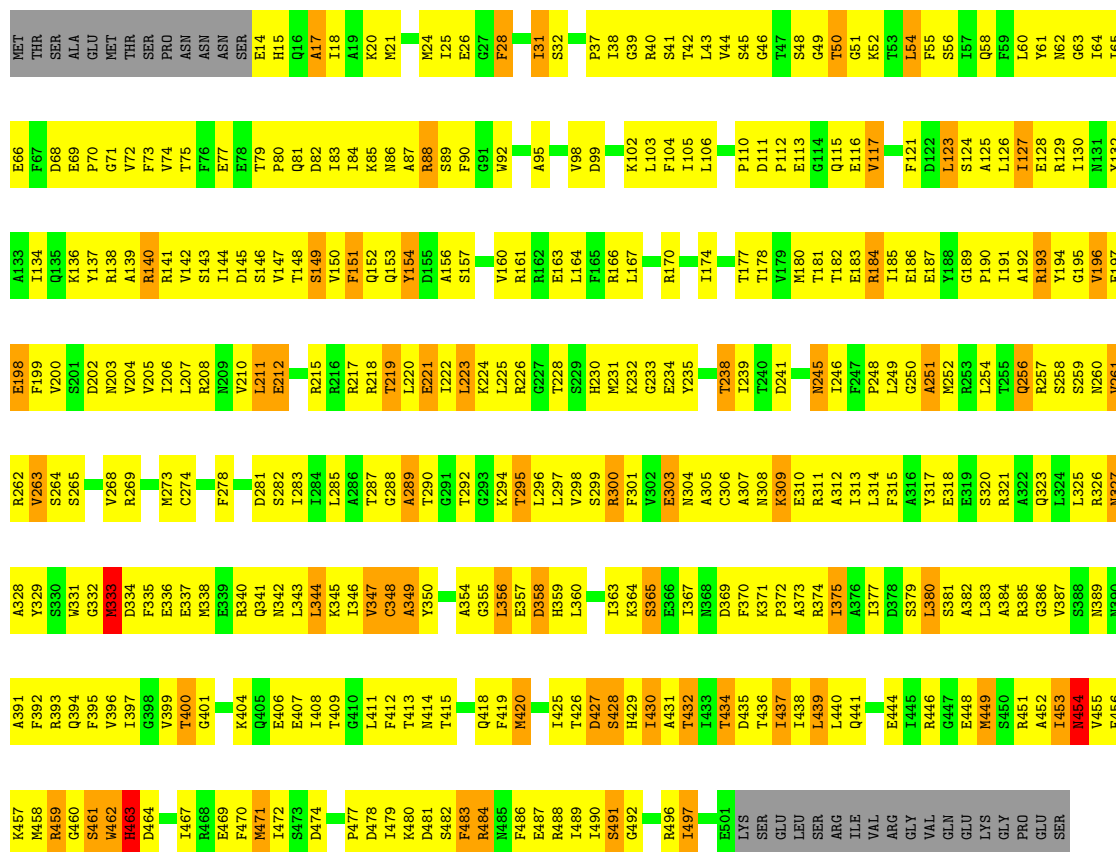
• Molecule 2: Circadian clock protein kinase KaiC





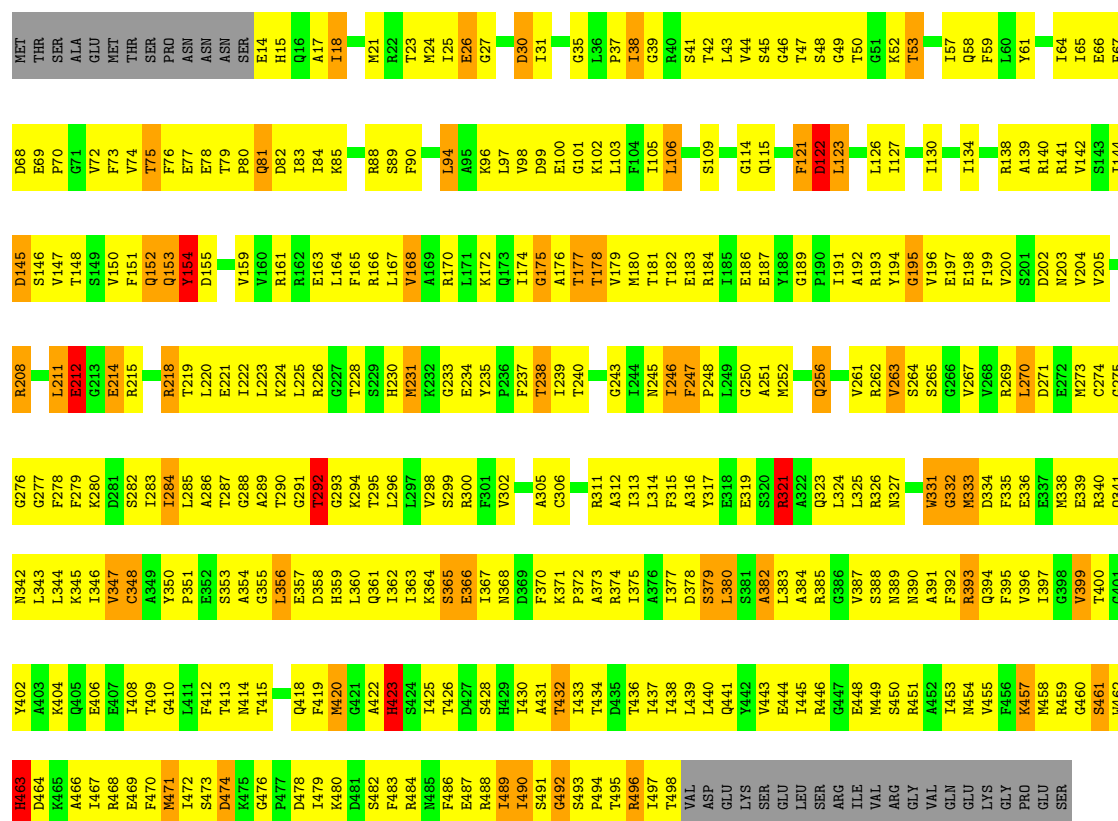
• Molecule 2: Circadian clock protein kinase KaiC

Chain C:  25%  57%  12% • 6%



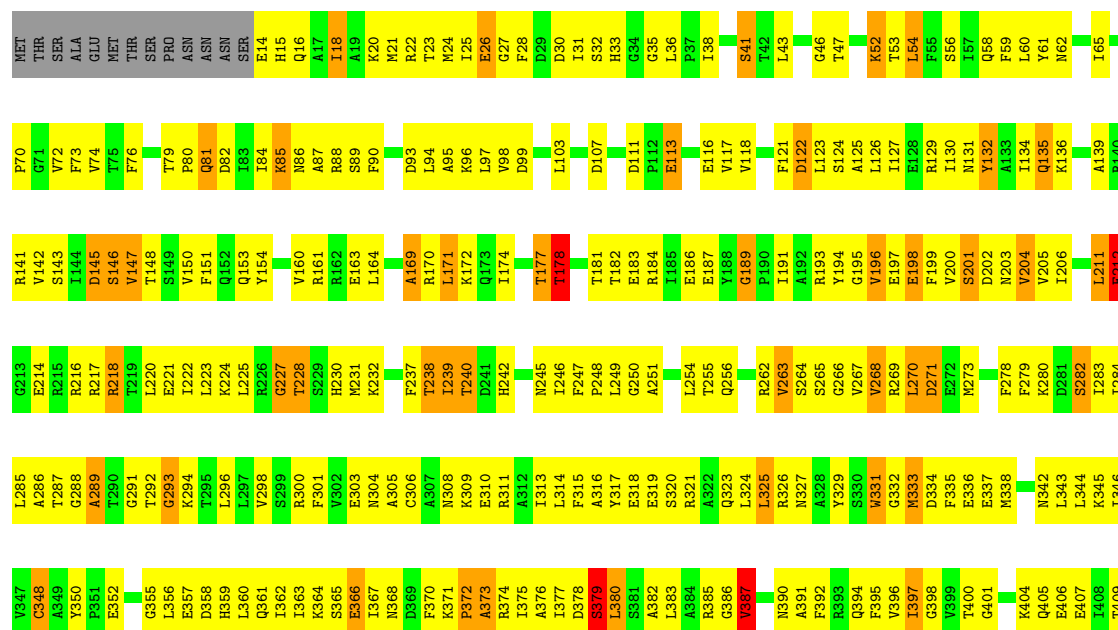
• Molecule 2: Circadian clock protein kinase KaiC

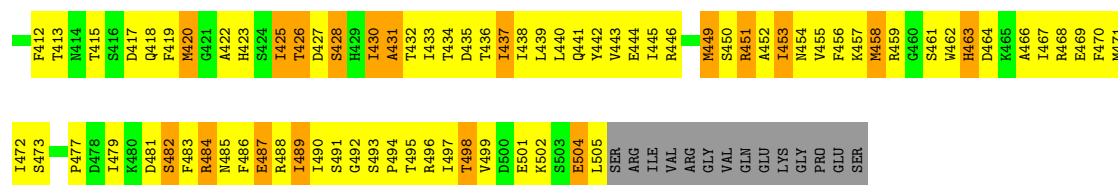
Chain D: 25% 57% 10% • 7%



• Molecule 2: Circadian clock protein kinase KaiC

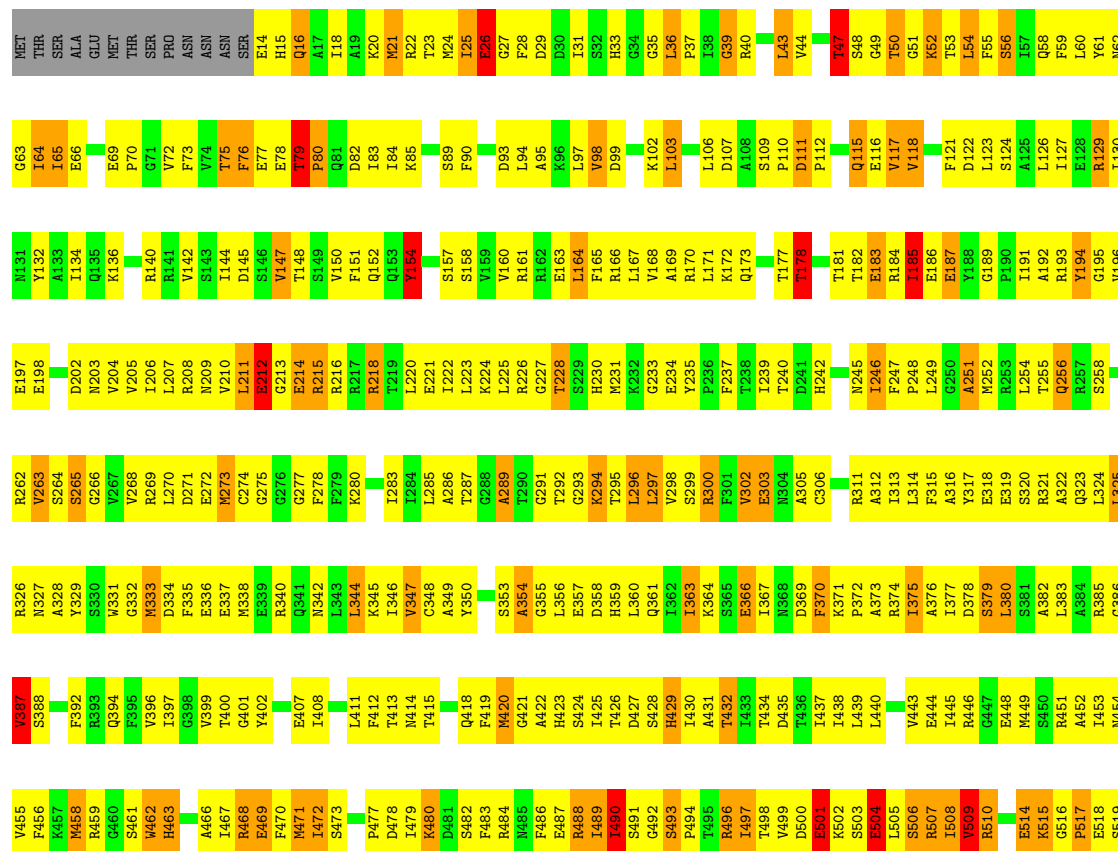
Chain E: 28% 54% 12% • 5%





• Molecule 2: Circadian clock protein kinase KaiC

Chain F: 25% 55% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.23Å 134.96Å 204.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	65.4 (30.00-3.00) 65.2 (30.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.307 0.299 , 0.317	Depositor DCC
R_{free} test set	4953 reflections (9.05%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23921	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.54	0/4034	1.04	23/5431 (0.4%)
2	B	0.50	0/3926	1.00	16/5289 (0.3%)
2	C	0.55	0/3902	1.06	25/5258 (0.5%)
2	D	0.65	1/3878 (0.0%)	1.10	28/5225 (0.5%)
2	E	0.62	0/3934	1.09	21/5300 (0.4%)
2	F	0.66	4/4042 (0.1%)	1.12	32/5444 (0.6%)
All	All	0.59	5/23716 (0.0%)	1.07	145/31947 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	231	MET	SD-CE	-6.45	1.63	1.79
2	F	21	MET	CG-SD	5.51	1.94	1.80
2	F	25	ILE	CA-CB	5.22	1.60	1.53
2	F	64	ILE	CA-CB	5.20	1.60	1.54
2	F	47	THR	CA-CB	5.03	1.61	1.53

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	380	LEU	N-CA-C	-11.27	98.92	112.89
2	E	380	LEU	N-CA-C	-10.20	99.99	111.82
2	F	380	LEU	N-CA-C	-8.77	101.67	111.14
2	D	178	THR	N-CA-C	8.40	123.69	110.17
1	A	380	LEU	N-CA-C	-8.35	102.36	112.54
2	D	373	ALA	N-CA-C	-7.90	104.12	114.31
1	A	84	ILE	N-CA-C	-7.80	104.19	111.45
2	F	178	THR	N-CA-C	7.70	122.56	110.17
2	F	251	ALA	N-CA-C	-7.67	103.65	113.16
2	D	459	ARG	N-CA-C	7.65	120.51	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	LYS	N-CA-C	-7.64	101.64	113.02
2	C	461	SER	N-CA-C	7.50	119.43	108.86
1	A	266	GLY	N-CA-C	-6.96	105.13	114.95
2	E	178	THR	N-CA-C	6.86	120.70	109.72
2	D	482	SER	N-CA-C	6.79	119.73	110.35
2	C	380	LEU	N-CA-C	-6.78	103.90	111.28
2	F	499	VAL	N-CA-C	-6.76	103.46	113.39
1	A	308	ASN	N-CA-C	-6.74	102.36	112.54
2	E	397	ILE	N-CA-C	-6.68	103.28	110.23
2	D	439	LEU	N-CA-C	6.68	119.35	107.80
2	E	493	SER	CA-C-N	6.63	128.12	119.84
2	E	493	SER	C-N-CA	6.63	128.12	119.84
2	E	331	TRP	N-CA-C	-6.60	103.63	112.94
2	D	121	PHE	N-CA-C	-6.59	104.47	113.30
2	C	439	LEU	N-CA-C	6.44	118.90	108.41
2	D	331	TRP	N-CA-C	-6.43	104.06	112.41
2	B	210	VAL	N-CA-C	6.42	118.69	109.51
2	F	373	ALA	N-CA-C	-6.41	104.00	113.61
1	A	290	THR	N-CA-C	-6.39	101.94	110.24
1	A	439	LEU	N-CA-C	6.38	119.30	108.90
2	D	145	ASP	N-CA-C	6.38	119.21	107.99
2	E	147	VAL	N-CA-C	-6.38	103.11	112.04
2	C	427	ASP	N-CA-C	-6.32	105.70	113.41
2	D	53	THR	N-CA-C	-6.26	104.15	110.97
2	D	265	SER	N-CA-C	-6.20	105.71	113.28
2	C	251	ALA	N-CA-C	-6.18	106.96	114.75
2	C	434	THR	N-CA-C	6.17	118.74	110.35
2	B	493	SER	CA-C-N	6.14	127.52	119.84
2	B	493	SER	C-N-CA	6.14	127.52	119.84
2	F	111	ASP	CA-C-N	6.11	126.22	119.87
2	F	111	ASP	C-N-CA	6.11	126.22	119.87
1	A	116	GLU	N-CA-C	6.10	119.60	110.14
2	D	393	ARG	N-CA-C	-6.09	104.65	111.28
2	C	462	TRP	N-CA-C	6.08	117.71	111.14
2	F	16	GLN	N-CA-C	-6.08	99.48	108.79
2	E	204	VAL	N-CA-C	6.08	116.38	106.72
2	F	498	THR	N-CA-C	6.08	118.85	109.07
2	F	22	ARG	N-CA-C	6.07	119.79	110.20
2	F	510	ARG	CB-CA-C	-6.04	109.63	116.63
2	E	489	ILE	N-CA-C	-5.99	104.79	110.42
2	B	196	VAL	N-CA-C	-5.98	105.86	111.48
2	F	79	THR	CA-C-N	5.97	127.30	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	79	THR	C-N-CA	5.97	127.30	119.84
2	C	358	ASP	N-CA-C	5.95	117.64	111.03
2	E	289	ALA	N-CA-C	-5.94	102.53	110.55
2	C	369	ASP	N-CA-C	-5.89	106.42	113.97
2	E	373	ALA	N-CA-C	-5.89	105.94	114.12
2	C	221	GLU	N-CA-C	5.87	117.95	107.80
2	D	382	ALA	N-CA-C	-5.83	106.33	113.50
2	C	54	LEU	N-CA-C	-5.82	104.56	111.03
1	A	493	SER	CA-C-N	5.82	127.20	120.98
1	A	493	SER	C-N-CA	5.82	127.20	120.98
2	C	394	GLN	N-CA-C	-5.82	104.29	111.33
2	B	430	ILE	N-CA-C	-5.81	107.08	112.83
2	C	459	ARG	N-CA-C	5.81	117.61	111.28
2	E	270	LEU	N-CA-C	-5.80	105.09	111.82
2	D	172	LYS	N-CA-C	-5.79	104.56	111.69
2	F	50	THR	N-CA-C	5.78	118.35	111.71
2	F	164	LEU	N-CA-C	-5.77	104.68	110.97
2	D	461	SER	N-CA-C	5.76	118.22	109.63
2	F	39	GLY	N-CA-C	-5.74	106.24	115.08
2	C	365	SER	N-CA-C	5.73	117.33	111.14
2	F	28	PHE	N-CA-C	5.73	118.01	111.02
2	F	147	VAL	N-CA-C	-5.73	104.94	110.72
1	A	476	GLY	CA-C-N	5.72	126.99	119.84
1	A	476	GLY	C-N-CA	5.72	126.99	119.84
2	C	430	ILE	CA-C-O	5.72	123.93	118.90
2	D	204	VAL	N-CA-C	5.70	116.07	107.75
2	C	481	ASP	N-CA-C	5.69	118.50	110.14
2	B	178	THR	N-CA-C	5.67	118.49	109.81
1	A	140	ARG	N-CA-C	-5.65	107.64	114.75
2	F	54	LEU	N-CA-C	-5.64	104.76	111.03
2	D	457	LYS	N-CA-C	5.64	117.10	108.52
2	E	218	ARG	N-CA-C	5.64	117.60	108.41
2	E	430	ILE	N-CA-C	-5.57	107.36	113.43
1	A	373	ALA	N-CA-C	-5.56	106.85	113.97
1	A	306	CYS	N-CA-C	-5.55	106.41	114.12
2	F	36	LEU	N-CA-C	5.53	116.38	109.57
2	F	265	SER	N-CA-C	-5.50	106.61	113.38
2	B	155	ASP	N-CA-C	5.50	118.22	109.81
2	B	173	GLN	N-CA-C	-5.49	104.98	110.97
2	C	204	VAL	N-CA-C	5.49	115.89	107.77
2	D	332	GLY	N-CA-C	-5.49	102.67	112.22
2	F	43	LEU	CA-C-N	-5.49	115.62	122.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	43	LEU	C-N-CA	-5.49	115.62	122.48
2	C	490	ILE	N-CA-C	-5.47	104.21	111.05
2	D	153	GLN	N-CA-C	-5.47	106.66	113.55
1	A	507	ARG	N-CA-C	-5.47	106.11	112.89
2	F	98	VAL	N-CA-C	-5.42	104.09	111.89
2	B	439	LEU	N-CA-C	5.41	117.56	107.99
2	C	437	ILE	CB-CA-C	-5.41	104.30	110.73
1	A	65	ILE	N-CA-C	5.40	120.58	109.34
1	A	102	LYS	N-CA-C	-5.40	106.53	113.23
2	F	185	ILE	N-CA-C	5.38	115.58	110.53
1	A	81	GLN	N-CA-C	-5.37	104.83	111.33
2	F	187	GLU	N-CA-C	5.37	118.05	111.82
1	A	382	ALA	N-CA-C	-5.37	106.57	113.23
2	D	208	ARG	N-CA-C	5.36	117.14	108.41
2	D	38	ILE	N-CA-C	5.34	117.33	109.63
2	E	487	GLU	N-CA-C	-5.34	101.86	110.14
2	D	423	HIS	N-CA-C	5.33	118.62	112.97
2	F	482	SER	N-CA-C	5.33	118.36	110.48
2	B	437	ILE	N-CA-C	5.30	115.15	106.72
2	D	233	GLY	N-CA-C	5.30	119.59	112.17
2	D	138	ARG	N-CA-C	-5.27	104.17	111.28
2	E	171	LEU	N-CA-C	-5.27	105.44	111.07
2	E	268	VAL	N-CA-C	5.26	115.98	110.62
1	A	175	GLY	N-CA-C	-5.26	107.31	115.67
2	F	266	GLY	N-CA-C	-5.26	108.37	115.21
2	B	308	ASN	N-CA-C	-5.25	106.63	112.57
2	E	169	ALA	N-CA-C	5.25	116.85	111.03
2	F	246	ILE	N-CA-C	5.25	117.25	109.17
2	F	369	ASP	N-CA-C	-5.25	106.74	112.72
2	D	480	LYS	CA-C-O	5.24	120.98	117.94
1	A	128	GLU	N-CA-C	-5.23	105.27	110.97
2	B	307	ALA	N-CA-C	-5.22	106.07	112.90
2	B	384	ALA	N-CA-C	-5.21	106.95	113.15
2	C	307	ALA	N-CA-C	-5.20	106.44	112.89
2	D	282	SER	N-CA-C	5.17	117.24	109.23
2	C	454	ASN	N-CA-C	5.15	116.24	108.46
2	C	373	ALA	N-CA-C	-5.13	106.71	113.17
2	E	145	ASP	N-CA-C	5.13	116.66	108.41
2	C	355	GLY	N-CA-C	-5.12	102.78	112.51
2	C	95	ALA	N-CA-C	-5.11	104.98	111.11
2	E	379	SER	N-CA-C	5.11	121.69	110.80
2	B	266	GLY	N-CA-C	-5.11	107.61	114.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	CYS	N-CA-C	-5.10	106.21	112.90
2	F	228	THR	N-CA-C	5.08	115.00	108.34
2	E	437	ILE	N-CA-C	5.07	115.27	107.77
2	C	31	ILE	CB-CA-C	-5.06	105.45	112.24
2	D	321	ARG	N-CA-C	-5.06	105.85	112.23
2	B	373	ALA	N-CA-C	-5.06	106.25	114.09
2	F	355	GLY	N-CA-C	-5.06	104.98	113.02
1	A	176	ALA	N-CA-C	5.06	116.55	108.41
2	D	231	MET	N-CA-C	-5.03	103.41	110.50

There are no chirality outliers.

There are no planarity outliers.

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	3992	0	3983	466	0
2	B	3873	0	3862	467	0
2	C	3849	0	3838	479	0
2	D	3825	0	3820	469	0
2	E	3881	0	3874	478	0
2	F	3988	0	3983	537	0
3	A	62	0	24	8	0
3	B	62	0	24	8	0
3	C	62	0	24	5	0
3	D	62	0	24	13	0
3	E	62	0	24	6	0
3	F	62	0	24	7	0
4	A	6	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	2	0	0	0	0
4	E	4	0	0	0	0
4	F	3	0	0	0	0
5	A	14	0	0	4	0
5	B	20	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	23	0	0	5	0
5	D	28	0	0	7	0
5	E	15	0	0	5	0
5	F	19	0	0	4	0
All	All	23921	0	23504	2755	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 58.

All (2755) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:231:MET:HE1	2:D:251:ALA:HB2	1.17	1.15
2:D:379:SER:H	2:D:413:THR:HB	1.13	1.13
2:E:283:ILE:HG13	2:E:400:THR:HG23	1.26	1.13
2:F:25:ILE:HD12	2:F:58:GLN:HE21	1.12	1.13
2:E:164:LEU:HD11	2:E:197:GLU:HG3	1.32	1.12
1:A:72:VAL:HG21	1:A:134:ILE:HD12	1.34	1.09
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.15	1.08
2:C:431:ALA:O	2:C:432:TPO:HG22	1.53	1.08
2:C:41:SER:HB3	2:C:178:THR:HB	1.33	1.07
2:E:18:ILE:HD11	2:E:227:GLY:C	1.81	1.05
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.19	1.03
2:D:148:THR:HG21	2:D:193:ARG:HD2	1.39	1.03
2:E:305:ALA:HB2	2:E:374:ARG:HD2	1.38	1.02
1:A:284:ILE:HD12	1:A:436:THR:HB	1.39	1.02
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.42	1.01
1:A:152:GLN:HG3	2:B:161:ARG:HH11	1.20	1.01
2:E:453:ILE:HG21	2:E:479:ILE:HD12	1.44	1.00
2:C:283:ILE:HG12	2:C:400:THR:HG23	1.40	0.99
2:E:449:MET:HG2	2:F:467:ILE:HD11	1.43	0.97
2:E:446:ARG:HH21	2:E:496:ARG:HH22	1.10	0.97
2:F:305:ALA:HB2	2:F:374:ARG:HD2	1.46	0.97
2:D:218:ARG:CZ	2:D:239:ILE:HD12	1.96	0.96
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.47	0.96
2:D:371:LYS:HD2	2:D:371:LYS:O	1.64	0.95
2:E:431:ALA:O	2:E:434:THR:HG22	1.66	0.95
2:C:371:LYS:O	2:C:371:LYS:HD2	1.67	0.95
2:E:43:LEU:HD23	2:E:204:VAL:HG13	1.48	0.95
2:C:261:VAL:HG12	2:C:262:ARG:H	1.30	0.95
2:D:449:MET:HE3	2:E:467:ILE:HD11	1.46	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:123:LEU:CD2	2:E:127:ILE:HD11	1.97	0.95
2:C:453:ILE:HD13	2:C:454:ASN:N	1.83	0.94
2:E:123:LEU:HD23	2:E:127:ILE:HD11	1.50	0.94
2:F:379:SER:H	2:F:413:THR:HB	1.30	0.94
2:F:359:HIS:O	2:F:363:ILE:HD13	1.66	0.93
2:B:284:ILE:HD12	2:B:436:THR:HB	1.51	0.93
2:C:231:MET:HE1	2:C:251:ALA:HB2	1.49	0.93
2:D:231:MET:CE	2:D:251:ALA:HB2	1.98	0.93
2:E:263:VAL:HG12	2:E:374:ARG:HH21	1.33	0.93
1:A:266:GLY:HA3	1:A:300:ARG:O	1.68	0.92
2:E:418:GLN:HB2	2:F:423:HIS:O	1.67	0.92
2:C:265:SER:O	2:C:301:PHE:HA	1.70	0.92
2:C:471:MET:HE3	2:C:471:MET:O	1.68	0.92
2:B:46:GLY:HA2	2:B:184:ARG:HD3	1.49	0.92
2:C:300:ARG:HA	2:C:333:MET:HE1	1.51	0.91
2:C:25:ILE:HG23	2:C:58:GLN:NE2	1.84	0.91
1:A:359:HIS:O	1:A:363:ILE:HG12	1.70	0.91
2:D:445:ILE:HD13	2:D:450:SER:OG	1.69	0.91
2:E:356:LEU:HD11	2:E:387:VAL:HG21	1.52	0.91
2:B:45:SER:HB2	2:B:182:THR:HB	1.52	0.91
2:D:379:SER:N	2:D:413:THR:HB	1.85	0.91
1:A:379:SER:H	1:A:413:THR:HB	1.35	0.91
2:D:436:THR:HG23	2:D:458:MET:HG2	1.51	0.91
2:F:263:VAL:HG12	2:F:374:ARG:HH21	1.35	0.91
2:C:31:ILE:HG22	2:C:222:ILE:HD12	1.54	0.90
2:C:45:SER:HB3	2:C:182:THR:HB	1.52	0.90
2:D:194:TYR:O	2:D:196:VAL:HG23	1.71	0.90
1:A:327:ASN:HB3	5:A:532:HOH:O	1.70	0.90
2:F:515:LYS:HG3	2:F:516:GLY:H	1.35	0.90
2:F:434:THR:HG21	2:F:437:ILE:HD11	1.52	0.90
2:F:471:MET:HE1	2:F:473:SER:HB3	1.53	0.89
2:F:191:ILE:HB	2:F:198:GLU:HG2	1.54	0.89
2:C:211:LEU:O	2:C:212:GLU:HB3	1.73	0.89
2:D:294:LYS:O	2:D:298:VAL:HG23	1.72	0.89
1:A:14:GLU:HG3	1:A:15:HIS:H	1.36	0.89
2:D:47:THR:O	2:D:50:THR:HG23	1.71	0.89
2:E:313:ILE:HG13	2:E:372:PRO:HG3	1.54	0.89
2:D:64:ILE:HD12	2:D:102:LYS:HB3	1.51	0.89
1:A:314:LEU:HB3	1:A:346:ILE:HD12	1.55	0.89
2:C:261:VAL:HG12	2:C:262:ARG:N	1.86	0.89
2:D:211:LEU:O	2:D:212:GLU:HG3	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:497:ILE:HG22	2:E:498:THR:H	1.38	0.88
2:B:140:ARG:HB3	2:B:140:ARG:NH1	1.89	0.88
2:C:25:ILE:HG23	2:C:58:GLN:HE22	1.37	0.88
2:D:74:VAL:HA	2:D:106:LEU:HB3	1.56	0.88
1:A:226:ARG:HA	5:A:531:HOH:O	1.71	0.88
1:A:265:SER:O	1:A:301:PHE:HA	1.74	0.87
2:F:263:VAL:CG1	2:F:374:ARG:HH21	1.86	0.87
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.09	0.87
1:A:25:ILE:HG13	1:A:58:GLN:NE2	1.89	0.87
1:A:287:THR:CG2	1:A:414:ASN:HD22	1.86	0.87
2:B:379:SER:H	2:B:413:THR:HB	1.39	0.87
2:F:25:ILE:HD12	2:F:58:GLN:NE2	1.89	0.87
2:E:392:PHE:HE2	2:E:430:ILE:HD11	1.37	0.87
2:C:471:MET:HE2	2:C:478:ASP:CB	2.05	0.86
2:F:500:ASP:O	2:F:501:GLU:HB3	1.73	0.86
2:E:313:ILE:HG13	2:E:372:PRO:CG	2.05	0.86
2:F:514:GLU:HG2	2:F:519:SER:HB3	1.55	0.86
2:B:211:LEU:O	2:B:212:GLU:HB3	1.72	0.86
2:E:53:THR:HG23	2:E:145:ASP:OD1	1.76	0.86
2:E:123:LEU:HD13	2:E:163:GLU:OE2	1.74	0.86
2:F:434:THR:CG2	2:F:437:ILE:HD11	2.06	0.86
2:D:64:ILE:HD11	2:D:70:PRO:HA	1.58	0.86
2:C:446:ARG:HG2	2:C:496:ARG:NH2	1.91	0.85
2:D:152:GLN:HG3	2:E:161:ARG:HH11	1.40	0.85
2:C:471:MET:CE	2:C:478:ASP:HB3	2.06	0.85
2:C:471:MET:SD	2:C:478:ASP:HB3	2.15	0.85
3:C:901:ATP:H2'	2:D:458:MET:O	1.77	0.85
2:D:147:VAL:O	2:D:150:VAL:HG12	1.77	0.85
2:C:294:LYS:HG2	2:C:413:THR:HG23	1.58	0.85
2:C:347:VAL:O	2:C:348:CYS:HB2	1.77	0.85
2:F:471:MET:HG3	2:F:478:ASP:HB3	1.59	0.84
2:E:283:ILE:HA	5:E:533:HOH:O	1.77	0.84
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.07	0.84
2:F:394:GLN:HA	2:F:397:ILE:HD12	1.58	0.84
2:D:446:ARG:H	2:D:496:ARG:HH12	1.26	0.84
2:B:193:ARG:HG2	2:B:193:ARG:HH11	1.43	0.84
2:E:123:LEU:O	2:E:127:ILE:HG13	1.78	0.84
2:F:451:ARG:HG2	2:F:451:ARG:HH11	1.43	0.84
2:F:52:LYS:HB2	3:F:903:ATP:O1B	1.78	0.84
2:C:41:SER:CB	2:C:178:THR:HB	2.08	0.83
2:C:364:LYS:HA	2:C:367:ILE:HD12	1.57	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:488:ARG:HH22	2:D:488:ARG:HH21	1.22	0.83
2:D:64:ILE:HG21	2:D:97:LEU:HD13	1.58	0.83
1:A:152:GLN:HG3	2:B:161:ARG:NH1	1.93	0.83
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.61	0.83
2:F:52:LYS:HB3	2:F:181:THR:CG2	2.09	0.83
1:A:350:TYR:CZ	2:B:254:LEU:HD13	2.14	0.83
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.08	0.83
1:A:72:VAL:HG21	1:A:134:ILE:CD1	2.08	0.82
2:C:471:MET:O	2:C:471:MET:CE	2.27	0.82
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.14	0.82
2:B:31:ILE:HG23	2:B:231:MET:HB2	1.61	0.82
2:F:21:MET:HE3	2:F:59:PHE:CZ	2.13	0.82
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.62	0.82
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.59	0.82
2:C:488:ARG:NH2	2:D:488:ARG:HH21	1.77	0.82
2:D:96:LYS:O	2:D:100:GLU:HG3	1.78	0.82
2:F:117:VAL:HA	2:F:154:TYR:OH	1.80	0.82
2:F:486:PHE:HE2	2:F:496:ARG:HH11	1.25	0.82
2:F:285:LEU:HB3	2:F:437:ILE:HD12	1.59	0.82
1:A:467:ILE:HD11	2:F:449:MET:HE3	1.61	0.82
2:C:488:ARG:O	2:C:491:SER:HB3	1.80	0.82
1:A:25:ILE:HG13	1:A:58:GLN:HE21	1.44	0.82
2:C:471:MET:HE2	2:C:478:ASP:N	1.94	0.82
2:F:471:MET:HG2	2:F:480:LYS:HE2	1.59	0.81
2:B:492:GLY:O	2:B:494:PRO:HD3	1.78	0.81
2:C:127:ILE:HD13	2:C:127:ILE:N	1.92	0.81
2:C:471:MET:HE2	2:C:478:ASP:H	1.42	0.81
2:D:24:MET:HE2	2:D:66:GLU:HG3	1.61	0.81
2:E:363:ILE:O	2:E:367:ILE:HG12	1.80	0.81
1:A:211:LEU:O	1:A:212:GLU:HB3	1.81	0.81
2:C:50:THR:HG21	2:C:207:LEU:C	2.05	0.81
2:E:191:ILE:HB	2:E:198:GLU:HG2	1.60	0.81
2:C:221:GLU:HG3	2:C:233:GLY:O	1.81	0.81
2:C:313:ILE:HG12	2:C:345:LYS:HB3	1.63	0.81
1:A:161:ARG:HH11	2:F:152:GLN:HG3	1.46	0.81
2:E:359:HIS:O	2:E:363:ILE:HD13	1.80	0.81
2:D:220:LEU:HD23	2:D:221:GLU:N	1.95	0.81
2:F:191:ILE:HB	2:F:198:GLU:CG	2.10	0.81
2:B:248:PRO:HB2	2:B:251:ALA:HB3	1.62	0.81
1:A:356:LEU:HD11	1:A:387:VAL:HG21	1.60	0.81
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:311:ARG:HA	2:C:343:LEU:O	1.80	0.80
2:F:142:VAL:HB	2:F:178:THR:HG23	1.63	0.80
2:E:345:LYS:NZ	2:E:366:GLU:HG3	1.96	0.80
1:A:323:GLN:HG2	1:A:327:ASN:HD21	1.47	0.80
2:B:216:ARG:HG2	2:C:233:GLY:HA2	1.62	0.80
2:E:58:GLN:HG2	2:E:62:ASN:HD21	1.47	0.80
2:E:379:SER:H	2:E:413:THR:HB	1.43	0.80
2:B:247:PHE:HE2	2:B:364:LYS:HD2	1.47	0.80
2:E:420:MET:HE1	2:F:490:ILE:HG13	1.62	0.80
2:E:191:ILE:HB	2:E:198:GLU:CG	2.12	0.80
1:A:52:LYS:HB3	1:A:181:THR:HG23	1.64	0.79
2:B:430:ILE:HA	2:B:433:ILE:HD13	1.64	0.79
2:B:496:ARG:HG2	2:B:498:THR:HG23	1.65	0.79
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.47	0.79
2:F:514:GLU:CD	2:F:515:LYS:H	1.90	0.79
2:C:287:THR:HG22	2:C:288:GLY:H	1.45	0.79
2:B:239:ILE:CD1	2:B:244:ILE:HG12	2.12	0.79
2:F:248:PRO:HB2	2:F:251:ALA:HB3	1.64	0.79
2:F:194:TYR:O	2:F:196:VAL:HG23	1.82	0.79
1:A:14:GLU:HG3	1:A:16:GLN:OE1	1.83	0.79
2:C:360:LEU:HD21	2:C:364:LYS:HE3	1.63	0.79
1:A:84:ILE:HD13	1:A:94:LEU:HB2	1.64	0.79
1:A:227:GLY:O	2:F:89:SER:HB2	1.83	0.79
2:C:252:MET:HE1	2:C:397:ILE:HG22	1.63	0.79
2:E:33:HIS:HD2	2:E:230:HIS:HA	1.48	0.79
2:E:449:MET:CG	2:F:467:ILE:HD11	2.12	0.79
2:C:471:MET:HE2	2:C:478:ASP:HB3	1.61	0.79
2:E:392:PHE:CE2	2:E:430:ILE:HD11	2.16	0.79
2:D:21:MET:O	2:D:35:GLY:HA3	1.83	0.78
2:F:21:MET:HE2	2:F:177:THR:CG2	2.13	0.78
1:A:284:ILE:CD1	1:A:436:THR:HB	2.12	0.78
2:E:344:LEU:HD22	2:E:345:LYS:H	1.46	0.78
2:B:273:MET:O	2:B:463:HIS:HA	1.83	0.78
2:F:295:THR:HG23	2:F:378:ASP:OD2	1.82	0.78
2:D:202:ASP:HA	2:D:226:ARG:HD2	1.66	0.78
2:D:419:PHE:CE2	2:E:425:ILE:HG12	2.17	0.78
2:E:216:ARG:NH2	2:F:223:LEU:HD21	1.98	0.78
2:F:24:MET:HE2	2:F:66:GLU:OE2	1.84	0.78
2:C:379:SER:H	2:C:413:THR:HB	1.49	0.78
2:C:451:ARG:HG2	2:C:451:ARG:HH11	1.47	0.78
2:C:202:ASP:HA	2:C:226:ARG:HD2	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:LEU:HD12	2:D:127:ILE:HD11	1.66	0.78
2:F:47:THR:HG22	2:F:50:THR:HG23	1.65	0.78
2:B:225:LEU:HD12	2:B:230:HIS:HB3	1.66	0.78
2:F:60:LEU:CD1	2:F:73:PHE:HB2	2.14	0.78
2:C:287:THR:CG2	2:C:414:ASN:HD22	1.96	0.77
2:E:263:VAL:CG1	2:E:374:ARG:HH21	1.97	0.77
1:A:249:LEU:HD13	1:A:394:GLN:HG2	1.66	0.77
2:C:287:THR:HG21	2:C:425:ILE:O	1.83	0.77
2:C:323:GLN:HE21	2:C:327:ASN:HD21	1.33	0.77
2:D:81:GLN:H	2:D:81:GLN:CD	1.92	0.77
2:E:425:ILE:HD12	2:E:439:LEU:HD13	1.65	0.77
2:F:148:THR:HG21	2:F:193:ARG:HD2	1.66	0.77
2:F:375:ILE:HD13	2:F:376:ALA:N	2.00	0.77
2:B:293:GLY:HA2	3:B:901:ATP:O1A	1.84	0.77
2:B:453:ILE:HD13	2:B:454:ASN:N	1.99	0.77
1:A:315:PHE:HE1	1:A:375:ILE:HG13	1.49	0.77
2:E:94:LEU:O	2:E:98:VAL:HG23	1.85	0.77
2:D:438:ILE:HD13	2:D:455:VAL:HG22	1.67	0.77
2:F:285:LEU:HB3	2:F:437:ILE:CD1	2.14	0.77
2:F:305:ALA:CB	2:F:374:ARG:HD2	2.13	0.77
2:B:315:PHE:HE1	2:B:375:ILE:HD11	1.50	0.77
1:A:449:MET:HE2	1:A:449:MET:HA	1.67	0.76
2:B:379:SER:N	2:B:413:THR:HB	1.98	0.76
2:C:432:TPO:HG21	2:C:432:TPO:O1P	1.83	0.76
2:F:21:MET:HE2	2:F:177:THR:HG21	1.67	0.76
2:F:161:ARG:HB2	2:F:196:VAL:HG11	1.65	0.76
1:A:441:GLN:HE22	1:A:490:ILE:HD13	1.49	0.76
2:E:332:GLY:O	2:E:333:MET:HG2	1.85	0.76
2:C:409:THR:HA	5:C:540:HOH:O	1.85	0.76
2:C:471:MET:CE	2:C:478:ASP:CB	2.63	0.76
2:B:316:ALA:HA	2:B:378:ASP:HB3	1.65	0.76
2:B:116:GLU:HG2	2:B:117:VAL:H	1.51	0.76
2:D:152:GLN:HG3	2:E:161:ARG:NH1	2.01	0.76
2:E:132:TYR:HE2	2:E:136:LYS:HD2	1.49	0.76
1:A:79:THR:HG22	1:A:81:GLN:HG2	1.67	0.76
2:E:446:ARG:NH2	2:E:496:ARG:HH22	1.82	0.76
1:A:65:ILE:O	1:A:66:GLU:HG2	1.86	0.76
2:F:509:VAL:HG12	2:F:510:ARG:H	1.51	0.76
2:F:21:MET:HE1	2:F:177:THR:HB	1.67	0.76
1:A:314:LEU:HB3	1:A:346:ILE:CD1	2.15	0.75
2:D:453:ILE:HG21	2:D:479:ILE:HD12	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:471:MET:HE1	2:E:473:SER:OG	1.86	0.75
1:A:471:MET:CG	1:A:478:ASP:HB3	2.16	0.75
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.51	0.75
2:C:448:GLU:HG2	2:D:466:ALA:HB2	1.67	0.75
2:D:164:LEU:HD22	2:D:180:MET:HE1	1.69	0.75
2:B:171:LEU:HD23	2:B:174:ILE:HD12	1.66	0.75
2:B:203:ASN:HB3	2:B:225:LEU:HD23	1.69	0.75
1:A:14:GLU:CG	1:A:15:HIS:H	1.98	0.75
2:C:238:THR:HA	5:C:528:HOH:O	1.86	0.75
2:F:142:VAL:HB	2:F:178:THR:CG2	2.15	0.75
2:F:334:ASP:O	2:F:338:MET:HG2	1.86	0.75
2:F:336:GLU:HB3	2:F:340:ARG:NH2	2.02	0.75
2:C:146:SER:H	2:C:181:THR:HB	1.51	0.75
2:E:238:THR:HB	2:E:361:GLN:HE22	1.52	0.75
2:D:31:ILE:HA	2:D:231:MET:HG3	1.69	0.75
2:E:435:ASP:OD1	2:E:459:ARG:HD2	1.87	0.75
2:F:245:ASN:ND2	2:F:361:GLN:HE21	1.85	0.74
2:D:18:ILE:H	2:D:18:ILE:HD12	1.51	0.74
1:A:147:VAL:O	1:A:150:VAL:HG12	1.87	0.74
2:C:127:ILE:HD13	2:C:127:ILE:H	1.50	0.74
1:A:363:ILE:HG22	1:A:367:ILE:HD11	1.70	0.74
2:D:170:ARG:O	2:D:174:ILE:HG12	1.88	0.74
2:E:320:SER:O	2:E:324:LEU:HB2	1.87	0.74
2:C:261:VAL:CG1	2:C:262:ARG:H	2.00	0.74
2:C:313:ILE:HD11	2:C:370:PHE:HB3	1.70	0.74
2:C:308:ASN:O	2:C:310:GLU:HG3	1.88	0.74
2:E:164:LEU:CD1	2:E:197:GLU:HG3	2.15	0.74
2:E:267:VAL:HG21	2:E:477:PRO:HG3	1.68	0.74
2:B:18:ILE:HB	2:B:228:THR:CG2	2.18	0.73
2:B:347:VAL:O	2:B:348:CYS:HB2	1.87	0.73
2:D:76:PHE:O	2:D:109:SER:HA	1.88	0.73
2:F:245:ASN:ND2	2:F:361:GLN:NE2	2.36	0.73
2:B:454:ASN:HB2	2:B:467:ILE:HD13	1.70	0.73
2:D:347:VAL:O	2:D:348:CYS:HB2	1.86	0.73
2:F:21:MET:HE3	2:F:59:PHE:HZ	1.54	0.73
1:A:508:ILE:HD12	1:A:510:ARG:H	1.52	0.73
2:E:294:LYS:HB3	2:E:413:THR:HG23	1.70	0.73
2:B:187:GLU:OE2	2:B:208:ARG:HA	1.89	0.73
2:B:218:ARG:HD3	2:B:237:PHE:CE1	2.23	0.73
2:C:215:ARG:HA	2:C:215:ARG:HE	1.53	0.73
2:C:287:THR:HG22	2:C:288:GLY:N	2.03	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:441:GLN:HG2	2:C:452:ALA:HB3	1.71	0.73
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.69	0.73
2:E:318:GLU:HG2	2:F:432:TPO:O3P	1.88	0.73
2:E:318:GLU:OE2	2:E:379:SER:HB2	1.87	0.73
2:B:358:ASP:O	2:B:362:ILE:HG12	1.89	0.73
2:B:311:ARG:HG3	2:B:371:LYS:NZ	2.04	0.73
1:A:161:ARG:NH1	2:F:152:GLN:HG3	2.03	0.73
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.24	0.73
2:D:38:ILE:HA	2:D:177:THR:HG23	1.69	0.73
2:E:266:GLY:HA3	2:E:300:ARG:HG3	1.69	0.73
2:D:269:ARG:HG2	2:D:479:ILE:HB	1.70	0.72
2:E:371:LYS:HD2	2:E:371:LYS:O	1.89	0.72
2:F:285:LEU:HD23	2:F:437:ILE:HD12	1.69	0.72
1:A:130:ILE:O	1:A:134:ILE:HD13	1.89	0.72
2:E:470:PHE:HE1	2:E:472:ILE:HD11	1.53	0.72
1:A:51:GLY:HA3	1:A:207:LEU:HD13	1.69	0.72
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.54	0.72
2:E:14:GLU:HG3	2:E:16:GLN:H	1.54	0.72
2:C:24:MET:HE2	2:C:66:GLU:HG3	1.72	0.72
2:C:170:ARG:O	2:C:174:ILE:HG12	1.89	0.72
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.69	0.72
1:A:320:SER:HA	2:B:254:LEU:HG	1.70	0.72
2:B:85:LYS:NZ	2:C:14:GLU:HG2	2.04	0.72
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.53	0.72
2:C:300:ARG:CA	2:C:333:MET:HE1	2.18	0.72
1:A:207:LEU:HD21	1:A:220:LEU:HD12	1.72	0.72
2:D:48:SER:HA	5:D:525:HOH:O	1.89	0.72
2:B:164:LEU:HD22	2:B:180:MET:HE1	1.71	0.72
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.55	0.72
2:D:347:VAL:HG12	2:D:348:CYS:N	2.03	0.72
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.71	0.72
2:C:446:ARG:HG2	2:C:496:ARG:CZ	2.20	0.72
2:F:218:ARG:NH1	2:F:239:ILE:HD12	2.04	0.72
2:B:191:ILE:HB	2:B:198:GLU:CD	2.15	0.72
2:C:31:ILE:HG23	2:C:231:MET:HB2	1.72	0.72
2:C:294:LYS:O	2:C:298:VAL:HG23	1.89	0.72
2:C:497:ILE:HD13	2:C:497:ILE:N	2.05	0.72
2:D:294:LYS:HB3	2:D:413:THR:HG23	1.72	0.72
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.55	0.71
1:A:70:PRO:HA	1:A:102:LYS:O	1.91	0.71
2:D:285:LEU:HD12	2:D:412:PHE:O	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:496:ARG:HG2	2:E:487:GLU:OE1	1.90	0.71
2:F:443:VAL:CG1	2:F:445:ILE:HD11	2.19	0.71
1:A:317:TYR:HA	1:A:349:ALA:O	1.91	0.71
2:C:223:LEU:HD13	2:C:224:LYS:HB3	1.70	0.71
1:A:65:ILE:O	1:A:65:ILE:HG22	1.89	0.71
1:A:211:LEU:O	1:A:212:GLU:CB	2.38	0.71
2:B:21:MET:SD	2:B:141:ARG:NE	2.64	0.71
2:F:313:ILE:CD1	2:F:345:LYS:HB3	2.21	0.71
2:B:451:ARG:HH11	2:B:451:ARG:HG2	1.55	0.71
2:C:436:THR:OG1	2:C:458:MET:HG2	1.90	0.71
2:F:371:LYS:O	2:F:371:LYS:HD2	1.90	0.71
2:C:54:LEU:HD11	2:C:90:PHE:CZ	2.25	0.71
2:C:148:THR:OG1	2:C:182:THR:HG23	1.89	0.71
2:C:221:GLU:HB3	5:C:538:HOH:O	1.90	0.71
2:E:305:ALA:HB2	2:E:374:ARG:CD	2.18	0.71
2:F:191:ILE:CB	2:F:198:GLU:HG2	2.19	0.71
2:B:140:ARG:HB3	2:B:140:ARG:HH11	1.54	0.71
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.25	0.71
2:D:38:ILE:HA	2:D:177:THR:CG2	2.20	0.70
2:E:310:GLU:HB3	2:E:373:ALA:CB	2.20	0.70
1:A:50:THR:HG22	1:A:209:ASN:HB2	1.72	0.70
1:A:273:MET:HE3	1:A:468:ARG:HD2	1.73	0.70
2:D:151:PHE:O	2:D:153:GLN:N	2.20	0.70
2:E:33:HIS:HD2	2:E:230:HIS:CA	2.04	0.70
2:B:256:GLN:OE1	2:B:405:GLN:HB3	1.92	0.70
1:A:453:ILE:HD13	1:A:454:ASN:N	2.06	0.70
2:B:305:ALA:HB2	2:B:374:ARG:HD2	1.74	0.70
2:C:191:ILE:HD12	2:C:191:ILE:H	1.57	0.70
1:A:347:VAL:O	1:A:348:CYS:HB2	1.89	0.70
2:B:45:SER:CB	2:B:182:THR:HB	2.20	0.70
2:E:313:ILE:HD12	2:E:367:ILE:HD13	1.74	0.70
2:F:21:MET:CE	2:F:59:PHE:HZ	2.03	0.70
2:F:23:THR:HB	2:F:25:ILE:HG12	1.72	0.70
1:A:45:SER:HB3	1:A:182:THR:HB	1.74	0.70
2:D:80:PRO:O	2:D:84:ILE:HG12	1.91	0.70
2:F:106:LEU:HD11	2:F:129:ARG:CZ	2.21	0.70
2:D:94:LEU:O	2:D:98:VAL:HG23	1.92	0.70
2:E:417:ASP:HB2	2:E:427:ASP:OD2	1.90	0.70
2:F:132:TYR:CE2	2:F:136:LYS:HD2	2.27	0.70
1:A:73:PHE:HE2	1:A:83:ILE:HD13	1.57	0.70
1:A:451:ARG:H	1:A:451:ARG:HD2	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.74	0.69
2:F:299:SER:C	2:F:333:MET:HE1	2.17	0.69
1:A:487:GLU:OE1	2:F:496:ARG:HG2	1.92	0.69
2:C:425:ILE:HD11	2:C:456:PHE:CE2	2.27	0.69
2:F:335:PHE:HA	2:F:338:MET:CG	2.22	0.69
2:B:193:ARG:HG2	2:B:193:ARG:NH1	2.05	0.69
2:B:308:ASN:O	2:B:310:GLU:HG3	1.93	0.69
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.71	0.69
2:F:160:VAL:HG21	2:F:194:TYR:CD2	2.26	0.69
2:F:303:GLU:OE2	2:F:333:MET:HB3	1.92	0.69
2:B:300:ARG:HA	2:B:333:MET:HE1	1.74	0.69
2:E:401:GLY:O	2:E:405:GLN:HG2	1.92	0.69
2:C:149:SER:HB3	2:D:161:ARG:CZ	2.22	0.69
2:C:440:LEU:CD2	2:C:453:ILE:HG12	2.22	0.69
2:D:53:THR:HG22	2:D:57:ILE:HD11	1.75	0.69
2:D:311:ARG:HD2	2:D:371:LYS:CE	2.08	0.69
2:E:425:ILE:HG22	2:E:425:ILE:O	1.93	0.69
1:A:371:LYS:O	1:A:371:LYS:HD2	1.92	0.69
1:A:407:GLU:OE1	1:A:407:GLU:HA	1.93	0.69
1:A:458:MET:HB2	1:A:463:HIS:HD2	1.57	0.69
2:B:123:LEU:HD13	2:B:123:LEU:O	1.93	0.69
2:B:171:LEU:HA	2:B:174:ILE:HD12	1.73	0.69
2:B:209:ASN:HD22	2:B:218:ARG:HG2	1.58	0.69
2:C:46:GLY:HA2	2:C:184:ARG:HD2	1.73	0.69
2:D:31:ILE:HA	2:D:231:MET:CG	2.23	0.69
2:E:497:ILE:HG22	2:E:498:THR:N	2.07	0.69
2:F:296:LEU:HD21	2:F:477:PRO:HD3	1.75	0.69
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.06	0.69
2:B:418:GLN:HG3	2:B:418:GLN:O	1.93	0.69
2:D:114:GLY:O	2:D:115:GLN:HG3	1.92	0.69
2:D:256:GLN:HG3	2:D:404:LYS:HD3	1.75	0.69
2:E:81:GLN:NE2	2:E:81:GLN:H	1.91	0.69
2:E:325:LEU:HD21	2:E:335:PHE:HB2	1.74	0.69
2:F:515:LYS:HG3	2:F:516:GLY:N	2.08	0.69
2:D:314:LEU:O	2:D:314:LEU:HG	1.93	0.69
2:E:356:LEU:CD2	2:E:392:PHE:HA	2.23	0.69
2:C:261:VAL:CG1	2:C:262:ARG:N	2.56	0.68
2:D:24:MET:HE2	2:D:66:GLU:CG	2.23	0.68
2:E:294:LYS:HB3	2:E:413:THR:CG2	2.23	0.68
2:E:377:ILE:HD12	2:E:412:PHE:HE2	1.58	0.68
2:B:294:LYS:HB3	2:B:413:THR:HG23	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.74	0.68
2:D:377:ILE:HD13	2:D:412:PHE:CE2	2.27	0.68
2:F:262:ARG:HD3	2:F:277:GLY:O	1.92	0.68
2:B:64:ILE:HD11	2:B:70:PRO:HA	1.76	0.68
2:B:441:GLN:HG3	2:B:441:GLN:O	1.94	0.68
2:F:164:LEU:HD11	2:F:197:GLU:HG3	1.75	0.68
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.23	0.68
2:B:338:MET:N	2:B:338:MET:HE2	2.09	0.68
2:C:70:PRO:HB2	2:C:139:ALA:HA	1.75	0.68
2:E:289:ALA:CB	2:E:419:PHE:HA	2.23	0.68
2:F:124:SER:OG	2:F:166:ARG:NH1	2.27	0.68
2:B:429:HIS:HB3	5:B:529:HOH:O	1.93	0.68
2:E:25:ILE:HG23	2:E:58:GLN:NE2	2.08	0.68
2:F:144:ILE:HD13	2:F:167:LEU:HD21	1.73	0.68
2:F:231:MET:SD	2:F:251:ALA:HB2	2.34	0.68
2:C:64:ILE:HG23	2:C:102:LYS:HB3	1.76	0.68
2:C:140:ARG:NH1	2:C:140:ARG:HB3	2.09	0.68
2:E:356:LEU:HD13	2:E:387:VAL:HG11	1.75	0.68
2:F:47:THR:HG22	2:F:50:THR:CG2	2.24	0.68
2:D:31:ILE:HA	2:D:231:MET:SD	2.33	0.68
2:D:61:TYR:O	2:D:65:ILE:HD12	1.93	0.68
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.08	0.68
2:E:470:PHE:CE1	2:E:472:ILE:HD11	2.27	0.68
2:B:377:ILE:HD13	2:B:412:PHE:CE2	2.29	0.68
2:C:71:GLY:O	2:C:103:LEU:HD12	1.94	0.68
2:E:191:ILE:HG23	2:E:206:ILE:HD11	1.76	0.68
2:F:211:LEU:HD12	2:F:215:ARG:O	1.94	0.68
2:C:283:ILE:HD12	2:C:435:ASP:OD2	1.94	0.68
2:E:76:PHE:CZ	2:E:126:LEU:HD21	2.29	0.68
2:E:377:ILE:HD12	2:E:412:PHE:CE2	2.28	0.68
2:B:127:ILE:HA	2:B:130:ILE:HD12	1.75	0.67
2:B:264:SER:HB3	2:B:304:ASN:ND2	2.09	0.67
2:B:444:GLU:O	2:B:494:PRO:HD2	1.94	0.67
2:E:451:ARG:HG2	2:E:451:ARG:HH11	1.59	0.67
2:E:58:GLN:HG2	2:E:62:ASN:ND2	2.09	0.67
2:E:230:HIS:O	2:E:232:LYS:HD2	1.95	0.67
2:F:147:VAL:O	2:F:150:VAL:HG12	1.94	0.67
2:F:313:ILE:HD11	2:F:370:PHE:CD2	2.30	0.67
2:F:432:TPO:HG21	2:F:432:TPO:O1P	1.94	0.67
2:C:261:VAL:O	2:C:262:ARG:HG2	1.95	0.67
2:D:59:PHE:CE2	2:D:141:ARG:HB3	2.29	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.75	0.67
2:F:363:ILE:O	2:F:367:ILE:HG12	1.93	0.67
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.60	0.67
2:B:130:ILE:O	2:B:134:ILE:HG12	1.94	0.67
2:C:25:ILE:HG12	2:C:58:GLN:HE21	1.60	0.67
2:C:31:ILE:HD13	2:C:231:MET:SD	2.34	0.67
2:D:286:ALA:O	2:D:294:LYS:HG2	1.95	0.67
2:D:464:ASP:OD1	2:D:466:ALA:N	2.28	0.67
2:F:21:MET:CE	2:F:177:THR:HB	2.25	0.67
1:A:210:VAL:HG12	1:A:211:LEU:O	1.94	0.67
2:B:25:ILE:HG23	2:B:58:GLN:NE2	2.10	0.67
2:E:273:MET:HE3	2:E:468:ARG:HD2	1.77	0.67
2:F:347:VAL:O	2:F:348:CYS:HB3	1.92	0.67
1:A:451:ARG:NH1	1:A:472:ILE:HD12	2.10	0.67
2:B:441:GLN:NE2	2:B:490:ILE:HD13	2.10	0.67
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.60	0.67
2:F:203:ASN:HB3	2:F:225:LEU:HD23	1.77	0.67
2:F:379:SER:N	2:F:413:THR:HB	2.06	0.67
1:A:311:ARG:HA	1:A:343:LEU:O	1.95	0.67
1:A:488:ARG:HE	2:F:488:ARG:NH1	1.92	0.67
2:B:20:LYS:HB3	2:B:35:GLY:O	1.94	0.66
2:C:21:MET:HE1	2:C:141:ARG:HG2	1.77	0.66
2:D:74:VAL:HG21	2:D:130:ILE:CD1	2.25	0.66
2:D:446:ARG:N	2:D:496:ARG:HH12	1.93	0.66
2:C:18:ILE:HB	2:C:228:THR:HG23	1.77	0.66
2:C:195:GLY:O	2:C:196:VAL:HG23	1.96	0.66
2:D:490:ILE:C	2:D:492:GLY:H	2.02	0.66
2:E:191:ILE:CB	2:E:198:GLU:HG2	2.24	0.66
2:E:321:ARG:HG2	2:E:348:CYS:SG	2.36	0.66
1:A:144:ILE:HD11	1:A:171:LEU:HD11	1.77	0.66
2:F:182:THR:HG21	2:F:192:ALA:HB1	1.77	0.66
2:F:371:LYS:O	2:F:371:LYS:CD	2.43	0.66
2:F:377:ILE:HD12	2:F:412:PHE:CE2	2.31	0.66
1:A:234:GLU:HB2	2:F:214:GLU:HB3	1.76	0.66
2:E:123:LEU:HD21	2:E:127:ILE:HD11	1.75	0.66
2:E:205:VAL:HG22	2:E:222:ILE:HD12	1.76	0.66
1:A:267:VAL:CG1	1:A:270:LEU:HB2	2.25	0.66
2:B:148:THR:HA	2:B:151:PHE:CE1	2.30	0.66
2:D:89:SER:OG	3:D:903:ATP:N6	2.28	0.66
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.76	0.66
2:B:119:GLY:C	2:B:121:PHE:H	2.02	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:171:LEU:HA	2:E:174:ILE:HD12	1.76	0.66
2:F:79:THR:HG22	2:F:82:ASP:OD2	1.96	0.66
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.78	0.66
2:E:316:ALA:CB	2:E:324:LEU:HD11	2.26	0.66
2:F:335:PHE:HA	2:F:338:MET:HG3	1.77	0.66
1:A:426:TPO:O3P	1:A:431:ALA:HB2	1.96	0.66
1:A:492:GLY:O	1:A:494:PRO:HD3	1.96	0.66
2:B:205:VAL:C	2:B:206:ILE:HD12	2.21	0.66
2:E:170:ARG:O	2:E:174:ILE:HG13	1.95	0.66
2:E:269:ARG:HG2	2:E:479:ILE:HB	1.76	0.66
2:E:504:GLU:HG2	2:E:505:LEU:H	1.61	0.66
1:A:323:GLN:HG2	1:A:327:ASN:ND2	2.11	0.66
2:C:287:THR:HG23	2:C:414:ASN:HB3	1.77	0.66
2:E:419:PHE:CE2	2:F:425:ILE:HG13	2.31	0.66
1:A:52:LYS:H	1:A:207:LEU:HD12	1.59	0.66
1:A:98:VAL:HG22	1:A:105:ILE:HD13	1.77	0.66
2:B:146:SER:H	2:B:181:THR:HB	1.60	0.66
2:E:79:THR:HG22	2:E:82:ASP:OD2	1.96	0.66
2:C:74:VAL:HB	2:C:144:ILE:HA	1.79	0.65
2:C:182:THR:HG22	2:C:183:GLU:N	2.10	0.65
2:D:151:PHE:C	2:D:153:GLN:H	2.04	0.65
2:F:396:VAL:HG11	2:F:430:ILE:HG21	1.78	0.65
2:C:299:SER:HB3	2:C:333:MET:HE2	1.78	0.65
2:C:344:LEU:HD22	2:C:345:LYS:N	2.11	0.65
2:C:440:LEU:HD21	2:C:453:ILE:HG12	1.78	0.65
2:C:471:MET:HE3	2:C:471:MET:C	2.21	0.65
2:E:344:LEU:HD13	2:E:345:LYS:N	2.10	0.65
2:E:488:ARG:HB3	2:E:491:SER:OG	1.95	0.65
2:B:145:ASP:HA	2:B:181:THR:HB	1.77	0.65
2:D:264:SER:HA	2:D:271:ASP:OD1	1.96	0.65
2:B:140:ARG:HH11	2:B:140:ARG:CB	2.09	0.65
2:C:334:ASP:O	2:C:338:MET:HG2	1.97	0.65
2:D:287:THR:HG21	2:D:425:ILE:O	1.95	0.65
1:A:21:MET:HE3	1:A:59:PHE:CZ	2.31	0.65
1:A:219:THR:O	1:A:237:PHE:HE2	1.80	0.65
2:B:93:ASP:OD1	2:B:95:ALA:HB3	1.97	0.65
2:D:88:ARG:HG2	2:D:88:ARG:HH11	1.61	0.65
2:D:350:TYR:CE1	2:E:254:LEU:HD13	2.32	0.65
2:B:469:GLU:HB3	2:B:483:PHE:CZ	2.31	0.65
2:F:123:LEU:O	2:F:123:LEU:HD13	1.96	0.65
2:F:169:ALA:O	2:F:173:GLN:HG3	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:VAL:O	2:D:153:GLN:HG3	1.96	0.65
2:F:311:ARG:HG3	2:F:371:LYS:NZ	2.11	0.65
1:A:360:LEU:O	1:A:360:LEU:HD22	1.97	0.65
2:B:148:THR:C	2:B:150:VAL:H	2.04	0.65
2:E:446:ARG:HH21	2:E:496:ARG:NH2	1.89	0.65
2:F:486:PHE:CE2	2:F:496:ARG:HD2	2.32	0.65
1:A:27:GLY:O	1:A:30:ASP:HB2	1.97	0.65
1:A:140:ARG:HA	1:A:140:ARG:HH11	1.62	0.65
1:A:446:ARG:HA	1:A:496:ARG:NH2	2.11	0.65
2:B:79:THR:HG22	2:B:82:ASP:OD2	1.97	0.65
2:B:239:ILE:HD13	2:B:244:ILE:HG12	1.77	0.65
2:B:356:LEU:CD1	2:B:356:LEU:H	2.10	0.65
2:F:294:LYS:HB3	2:F:413:THR:HG23	1.79	0.65
2:C:221:GLU:CG	2:C:233:GLY:O	2.44	0.65
2:F:65:ILE:HD11	2:F:97:LEU:HD11	1.79	0.64
2:C:382:ALA:O	2:C:385:ARG:HG3	1.96	0.64
2:C:415:THR:HG21	2:D:432:TPO:CG2	2.28	0.64
2:D:396:VAL:HG11	2:D:430:ILE:HG21	1.78	0.64
2:F:283:ILE:HG23	2:F:412:PHE:CE1	2.33	0.64
2:B:315:PHE:CE1	2:B:375:ILE:HD11	2.31	0.64
2:B:378:ASP:O	2:B:379:SER:HB3	1.96	0.64
2:D:438:ILE:CD1	2:D:455:VAL:HG22	2.27	0.64
2:E:124:SER:HA	2:E:127:ILE:HD12	1.78	0.64
2:F:31:ILE:HD11	2:F:246:ILE:HG21	1.79	0.64
2:C:392:PHE:O	2:C:395:PHE:HB3	1.97	0.64
2:E:54:LEU:O	2:E:54:LEU:HD12	1.96	0.64
2:F:183:GLU:HG3	2:F:193:ARG:HE	1.63	0.64
2:F:324:LEU:O	2:F:328:ALA:HB2	1.97	0.64
1:A:211:LEU:HG	1:A:212:GLU:H	1.62	0.64
1:A:316:ALA:HB3	1:A:348:CYS:SG	2.37	0.64
2:C:80:PRO:HB3	2:C:105:ILE:HG21	1.79	0.64
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.13	0.64
2:B:80:PRO:HG2	2:B:107:ASP:HB2	1.80	0.64
2:B:185:ILE:HD13	2:B:185:ILE:N	2.13	0.64
2:D:81:GLN:H	2:D:81:GLN:NE2	1.96	0.64
2:B:86:ASN:HD21	2:C:40:ARG:HH22	1.46	0.64
2:B:87:ALA:C	2:B:89:SER:H	2.06	0.64
2:D:218:ARG:NH2	2:D:239:ILE:HD12	2.12	0.64
2:E:18:ILE:HD11	2:E:227:GLY:CA	2.27	0.64
2:F:80:PRO:HG2	2:F:107:ASP:HB2	1.80	0.64
1:A:79:THR:HG22	1:A:81:GLN:H	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:THR:HG22	2:D:183:GLU:N	2.11	0.64
2:D:183:GLU:HB2	2:E:199:PHE:CE1	2.33	0.64
2:D:338:MET:HE2	2:D:338:MET:HA	1.78	0.64
2:B:21:MET:HB2	2:B:38:ILE:HG12	1.79	0.64
2:B:296:LEU:HD21	2:B:477:PRO:HD3	1.80	0.64
2:D:312:ALA:O	2:D:344:LEU:HD22	1.98	0.64
2:E:20:LYS:HE3	2:E:228:THR:HG21	1.80	0.64
2:E:382:ALA:O	2:E:385:ARG:HG3	1.96	0.64
2:B:452:ALA:HA	2:B:469:GLU:HA	1.79	0.64
2:E:148:THR:OG1	2:E:182:THR:HG23	1.98	0.64
2:F:111:ASP:OD1	2:F:112:PRO:HD2	1.98	0.64
2:B:123:LEU:O	2:B:127:ILE:HG13	1.98	0.63
2:C:137:TYR:O	2:C:138:ARG:HB2	1.96	0.63
2:D:315:PHE:HA	2:D:347:VAL:HB	1.80	0.63
2:F:52:LYS:HB3	2:F:181:THR:HG21	1.80	0.63
1:A:207:LEU:CD2	1:A:220:LEU:HD12	2.27	0.63
2:B:164:LEU:CD2	2:B:180:MET:HE1	2.28	0.63
2:C:87:ALA:C	2:C:89:SER:H	2.04	0.63
2:E:21:MET:HE1	2:E:177:THR:HB	1.79	0.63
2:E:76:PHE:HZ	2:E:126:LEU:HD21	1.63	0.63
2:F:300:ARG:NH2	2:F:477:PRO:HD2	2.13	0.63
2:B:377:ILE:HD13	2:B:412:PHE:HE2	1.62	0.63
2:C:384:ALA:HB2	2:C:392:PHE:CZ	2.33	0.63
2:E:362:ILE:O	2:E:365:SER:HB3	1.98	0.63
2:B:52:LYS:H	2:B:207:LEU:HD12	1.63	0.63
2:D:39:GLY:N	2:D:177:THR:HG23	2.13	0.63
2:E:81:GLN:H	2:E:81:GLN:CD	2.05	0.63
2:E:443:VAL:O	2:E:445:ILE:HD12	1.98	0.63
2:F:296:LEU:O	2:F:299:SER:N	2.32	0.63
2:F:516:GLY:N	2:F:517:PRO:HD2	2.14	0.63
2:D:150:VAL:HG13	2:D:151:PHE:N	2.14	0.63
1:A:73:PHE:CE2	1:A:83:ILE:HD13	2.34	0.63
1:A:84:ILE:HD13	1:A:94:LEU:CB	2.29	0.63
2:B:211:LEU:HD13	2:B:216:ARG:CZ	2.28	0.63
2:B:214:GLU:HB3	2:C:234:GLU:HB3	1.81	0.63
2:D:191:ILE:HB	2:D:198:GLU:CG	2.29	0.63
2:D:471:MET:HE2	2:D:478:ASP:HB2	1.79	0.63
1:A:414:ASN:ND2	1:A:426:TPO:HA	2.11	0.63
2:B:184:ARG:HD2	2:B:191:ILE:O	1.99	0.63
2:D:245:ASN:ND2	2:D:361:GLN:HE21	1.95	0.63
2:E:93:ASP:OD2	2:E:96:LYS:HB2	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:247:PHE:CZ	2:E:361:GLN:HB2	2.34	0.63
2:E:263:VAL:HG12	2:E:374:ARG:NH2	2.11	0.63
1:A:45:SER:CB	1:A:182:THR:HB	2.29	0.62
2:B:357:GLU:HG3	2:B:358:ASP:N	2.14	0.62
2:D:489:ILE:HD13	2:D:489:ILE:N	2.14	0.62
2:E:291:GLY:HA3	2:E:442:TYR:OH	1.99	0.62
2:E:334:ASP:OD1	2:E:337:GLU:N	2.31	0.62
2:F:213:GLY:O	2:F:215:ARG:N	2.31	0.62
2:F:311:ARG:HD2	2:F:370:PHE:O	1.98	0.62
1:A:38:ILE:HG22	1:A:39:GLY:N	2.13	0.62
1:A:344:LEU:HD13	1:A:344:LEU:C	2.24	0.62
2:B:24:MET:CB	2:B:62:ASN:HD22	2.13	0.62
2:D:292:THR:HB	2:D:440:LEU:HB3	1.80	0.62
2:F:443:VAL:HG12	2:F:445:ILE:HD11	1.80	0.62
1:A:145:ASP:OD2	1:A:181:THR:HG21	2.00	0.62
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.81	0.62
1:A:471:MET:SD	1:A:478:ASP:HB3	2.39	0.62
2:B:43:LEU:HD11	2:B:182:THR:OG1	1.99	0.62
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.63	0.62
2:B:284:ILE:HD12	2:B:436:THR:CB	2.28	0.62
2:B:425:ILE:H	2:B:425:ILE:HD12	1.63	0.62
2:F:306:CYS:SG	2:F:344:LEU:HB2	2.38	0.62
2:F:98:VAL:HA	2:F:103:LEU:O	1.98	0.62
2:F:197:GLU:OE2	2:F:197:GLU:N	2.29	0.62
2:B:129:ARG:O	2:B:132:TYR:HB3	1.99	0.62
2:D:72:VAL:HG21	2:D:134:ILE:HD13	1.81	0.62
2:D:317:TYR:CE2	2:D:383:LEU:HD11	2.34	0.62
2:E:325:LEU:CD2	2:E:335:PHE:HB2	2.30	0.62
2:F:353:SER:O	2:F:354:ALA:HB2	1.98	0.62
2:B:197:GLU:CD	2:B:197:GLU:H	2.06	0.62
2:B:356:LEU:HD12	2:B:356:LEU:N	2.15	0.62
2:D:267:VAL:HG23	2:D:300:ARG:HG2	1.80	0.62
2:E:249:LEU:HD12	2:E:394:GLN:CD	2.24	0.62
2:F:54:LEU:HD22	2:F:90:PHE:CZ	2.35	0.62
2:F:313:ILE:HG12	2:F:372:PRO:CG	2.30	0.62
2:F:392:PHE:O	2:F:396:VAL:HG23	2.00	0.62
2:B:458:MET:HB2	2:B:463:HIS:HD2	1.64	0.62
2:D:371:LYS:O	2:D:371:LYS:CD	2.46	0.62
2:F:451:ARG:HG2	2:F:451:ARG:NH1	2.12	0.62
2:C:31:ILE:HA	2:C:231:MET:SD	2.40	0.61
2:D:317:TYR:HE2	2:D:383:LEU:HD21	1.61	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:430:ILE:HA	2:D:433:ILE:HD13	1.82	0.61
2:F:344:LEU:HD22	2:F:345:LYS:N	2.14	0.61
2:B:287:THR:HB	2:B:425:ILE:HG23	1.82	0.61
2:C:21:MET:HB2	2:C:38:ILE:HG13	1.83	0.61
2:C:453:ILE:HB	2:C:470:PHE:CD2	2.35	0.61
2:D:178:THR:HG22	2:D:179:VAL:N	2.15	0.61
2:E:53:THR:CG2	2:E:145:ASP:OD1	2.48	0.61
2:F:148:THR:CG2	2:F:193:ARG:HD2	2.29	0.61
2:F:194:TYR:O	2:F:195:GLY:C	2.43	0.61
2:B:112:PRO:O	2:C:166:ARG:HG3	2.00	0.61
2:C:354:ALA:HB1	2:C:358:ASP:HB2	1.81	0.61
2:C:451:ARG:HG2	2:C:451:ARG:NH1	2.14	0.61
2:D:220:LEU:HD23	2:D:220:LEU:C	2.24	0.61
2:F:21:MET:HE3	2:F:59:PHE:CE1	2.35	0.61
2:F:52:LYS:HB3	2:F:181:THR:HG23	1.81	0.61
2:C:217:ARG:HG3	2:C:217:ARG:O	2.00	0.61
2:F:458:MET:SD	2:F:461:SER:HB3	2.40	0.61
2:C:38:ILE:H	2:C:38:ILE:HD12	1.64	0.61
2:D:21:MET:CE	2:D:141:ARG:HG2	2.31	0.61
2:E:356:LEU:HD23	2:E:392:PHE:HA	1.83	0.61
2:F:182:THR:HG21	2:F:192:ALA:CB	2.31	0.61
1:A:56:SER:HB2	1:A:143:SER:HB3	1.81	0.61
2:B:273:MET:HE3	2:B:468:ARG:HD2	1.81	0.61
2:C:150:VAL:HG13	2:C:151:PHE:N	2.15	0.61
2:C:488:ARG:HH22	2:D:488:ARG:NH2	1.97	0.61
2:D:375:ILE:HG22	2:D:377:ILE:CD1	2.29	0.61
2:E:284:ILE:O	2:E:412:PHE:N	2.32	0.61
2:E:323:GLN:HE22	2:F:459:ARG:HH11	1.49	0.61
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.31	0.61
1:A:351:PRO:HG2	1:A:382:ALA:O	2.00	0.61
1:A:377:ILE:HD13	1:A:412:PHE:CE2	2.34	0.61
1:A:426:TPO:HG21	1:A:431:ALA:H	1.65	0.61
1:A:496:ARG:NH1	2:B:497:ILE:HD13	2.16	0.61
2:B:62:ASN:O	2:B:66:GLU:HB2	2.00	0.61
2:E:356:LEU:CD1	2:E:387:VAL:HG11	2.31	0.61
2:E:378:ASP:O	2:E:379:SER:HB3	2.01	0.61
2:C:360:LEU:CD2	2:C:364:LYS:HE3	2.29	0.61
2:E:33:HIS:CD2	2:E:230:HIS:HA	2.32	0.61
1:A:52:LYS:HB3	1:A:181:THR:CG2	2.30	0.61
2:B:31:ILE:HA	2:B:231:MET:SD	2.41	0.61
2:B:497:ILE:O	2:B:499:VAL:N	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:ILE:HD11	2:C:404:LYS:HD2	1.81	0.61
2:D:130:ILE:O	2:D:134:ILE:HG12	2.00	0.61
2:E:266:GLY:CA	2:E:300:ARG:HG3	2.30	0.61
2:E:469:GLU:HB3	2:E:483:PHE:CZ	2.35	0.61
2:F:27:GLY:HA3	2:F:246:ILE:HB	1.81	0.61
1:A:272:GLU:O	1:A:462:TRP:HZ3	1.82	0.61
3:B:901:ATP:C2	2:C:462:TRP:HA	2.36	0.61
2:C:46:GLY:HA2	2:C:184:ARG:CD	2.30	0.61
2:D:23:THR:O	2:D:24:MET:HB2	2.01	0.61
2:D:94:LEU:HD23	2:D:94:LEU:N	2.15	0.61
2:F:248:PRO:CB	2:F:251:ALA:HB3	2.30	0.61
1:A:41:SER:HA	1:A:178:THR:O	2.00	0.60
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.82	0.60
1:A:211:LEU:CG	1:A:212:GLU:H	2.14	0.60
1:A:293:GLY:HA2	3:A:901:ATP:O1A	2.00	0.60
2:C:281:ASP:OD1	2:C:407:GLU:HA	2.01	0.60
2:C:453:ILE:HD13	2:C:454:ASN:H	1.61	0.60
2:D:471:MET:O	2:D:471:MET:HE3	2.00	0.60
2:C:41:SER:HA	2:C:178:THR:O	2.00	0.60
2:C:497:ILE:HD13	2:C:497:ILE:H	1.65	0.60
2:E:130:ILE:O	2:E:134:ILE:HG12	2.01	0.60
2:E:289:ALA:O	2:E:292:THR:HG23	2.01	0.60
2:E:345:LYS:HZ1	2:E:366:GLU:HG3	1.66	0.60
2:B:160:VAL:HG21	2:B:194:TYR:CD1	2.36	0.60
2:C:61:TYR:O	2:C:65:ILE:HG12	2.01	0.60
2:C:248:PRO:C	2:C:250:GLY:H	2.09	0.60
1:A:18:ILE:HD13	2:F:85:LYS:HE3	1.83	0.60
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.66	0.60
3:A:903:ATP:O3'	2:B:224:LYS:HA	2.00	0.60
2:B:218:ARG:HD3	2:B:237:PHE:CZ	2.36	0.60
2:B:264:SER:HA	2:B:271:ASP:OD1	2.01	0.60
2:C:411:LEU:HD12	2:C:412:PHE:N	2.16	0.60
2:F:54:LEU:O	2:F:55:PHE:C	2.44	0.60
2:F:504:GLU:O	2:F:505:LEU:HB2	2.00	0.60
1:A:264:SER:HB3	1:A:304:ASN:ND2	2.16	0.60
2:B:178:THR:HG22	2:B:179:VAL:H	1.65	0.60
2:B:202:ASP:HA	2:B:226:ARG:HD2	1.83	0.60
2:E:171:LEU:HD23	2:E:174:ILE:HD12	1.84	0.60
1:A:80:PRO:HB3	1:A:105:ILE:HG21	1.84	0.60
2:E:171:LEU:HA	2:E:174:ILE:CD1	2.32	0.60
2:E:255:THR:HG22	2:E:255:THR:O	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:278:PHE:CD1	2:E:284:ILE:HD13	2.37	0.60
1:A:380:LEU:HD21	1:A:412:PHE:HD2	1.66	0.60
2:D:388:SER:O	2:D:389:ASN:C	2.43	0.60
2:D:418:GLN:HB2	2:E:423:HIS:O	2.01	0.60
2:F:170:ARG:HB3	2:F:170:ARG:NH1	2.16	0.60
2:F:212:GLU:O	2:F:212:GLU:OE2	2.20	0.60
1:A:299:SER:C	1:A:333:MET:HE1	2.26	0.60
2:B:31:ILE:O	2:B:231:MET:HG3	2.02	0.60
2:C:283:ILE:HD12	2:C:283:ILE:H	1.67	0.60
2:D:46:GLY:O	2:D:52:LYS:HD3	2.02	0.60
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.32	0.60
2:F:344:LEU:HD11	2:F:346:ILE:HG13	1.83	0.60
2:B:210:VAL:HG12	2:B:211:LEU:O	2.01	0.60
2:B:289:ALA:HB2	2:B:419:PHE:HA	1.83	0.60
2:B:432:TPO:O1P	2:B:432:TPO:HG21	2.02	0.60
2:F:318:GLU:HB2	5:F:523:HOH:O	2.00	0.60
2:C:71:GLY:O	2:C:103:LEU:HA	2.02	0.60
2:E:392:PHE:O	2:E:395:PHE:HB3	2.02	0.60
2:F:451:ARG:HB3	2:F:470:PHE:CZ	2.37	0.60
1:A:79:THR:HG23	1:A:80:PRO:HD2	1.83	0.59
1:A:287:THR:HG21	1:A:425:ILE:O	2.02	0.59
1:A:299:SER:O	1:A:333:MET:HE1	2.02	0.59
2:B:36:LEU:HD12	2:B:59:PHE:CE1	2.37	0.59
2:B:178:THR:HG22	2:B:179:VAL:N	2.17	0.59
2:B:183:GLU:HG3	2:B:193:ARG:HD2	1.84	0.59
2:B:435:ASP:O	2:B:457:LYS:HE3	2.02	0.59
2:F:191:ILE:HB	2:F:198:GLU:CD	2.26	0.59
2:F:492:GLY:C	2:F:494:PRO:HD3	2.26	0.59
2:F:514:GLU:HG2	2:F:519:SER:CB	2.30	0.59
2:E:142:VAL:HB	2:E:178:THR:OG1	2.03	0.59
2:F:14:GLU:HG2	5:F:530:HOH:O	2.02	0.59
2:F:94:LEU:HD22	2:F:103:LEU:CD2	2.31	0.59
2:F:317:TYR:HA	2:F:349:ALA:O	2.02	0.59
1:A:433:ILE:HG22	1:A:433:ILE:O	2.02	0.59
2:F:220:LEU:HD23	2:F:221:GLU:N	2.17	0.59
2:F:249:LEU:HD12	2:F:394:GLN:OE1	2.02	0.59
2:B:311:ARG:HG3	2:B:371:LYS:HZ2	1.68	0.59
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.32	0.59
1:A:397:ILE:HD13	1:A:433:ILE:HG21	1.83	0.59
2:B:404:LYS:C	2:B:406:GLU:H	2.11	0.59
2:D:446:ARG:HB3	2:E:484:ARG:CG	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:ILE:CD1	2:F:58:GLN:HG2	2.32	0.59
2:F:379:SER:OG	2:F:382:ALA:HB2	2.02	0.59
1:A:44:VAL:HG22	1:A:205:VAL:HB	1.84	0.59
2:B:85:LYS:HZ2	2:C:14:GLU:HG2	1.67	0.59
2:D:61:TYR:CD1	2:D:65:ILE:HD11	2.37	0.59
2:E:265:SER:HB3	2:E:278:PHE:CZ	2.38	0.59
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.84	0.59
1:A:298:VAL:HG23	1:A:411:LEU:HD23	1.85	0.59
2:C:296:LEU:HD21	2:C:477:PRO:HB3	1.83	0.59
2:D:25:ILE:HG12	2:D:58:GLN:HE21	1.68	0.59
2:D:432:TPO:C	2:D:433:ILE:HD12	2.33	0.59
1:A:147:VAL:HG11	1:A:180:MET:CE	2.29	0.59
2:D:486:PHE:HB3	2:D:489:ILE:CD1	2.33	0.59
2:E:311:ARG:O	2:E:373:ALA:N	2.35	0.59
2:E:461:SER:OG	2:E:462:TRP:N	2.35	0.59
2:F:106:LEU:HD11	2:F:129:ARG:NH2	2.17	0.59
2:F:298:VAL:HG13	2:F:376:ALA:HB1	1.83	0.59
2:F:444:GLU:HB3	2:F:493:SER:HA	1.83	0.59
2:F:484:ARG:HB3	2:F:484:ARG:NH1	2.18	0.59
1:A:310:GLU:O	1:A:343:LEU:HB3	2.01	0.59
2:B:52:LYS:HE3	3:B:903:ATP:O3B	2.03	0.59
2:B:434:THR:CG2	2:B:437:ILE:HD11	2.33	0.59
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.84	0.59
2:D:150:VAL:CG1	2:D:151:PHE:N	2.65	0.59
2:D:296:LEU:HD13	2:D:331:TRP:CE2	2.38	0.59
2:D:332:GLY:O	2:D:333:MET:O	2.21	0.59
2:E:293:GLY:HA2	3:E:901:ATP:O1A	2.01	0.59
2:F:79:THR:HG22	2:F:82:ASP:CG	2.28	0.59
2:B:70:PRO:HA	2:B:102:LYS:O	2.02	0.59
2:D:414:ASN:ND2	2:D:426:THR:HG22	2.18	0.59
2:E:492:GLY:O	2:E:494:PRO:HD3	2.03	0.59
1:A:36:LEU:HD22	1:A:42:THR:HG21	1.84	0.58
2:B:441:GLN:HE22	2:B:490:ILE:HD13	1.68	0.58
2:B:468:ARG:HG2	2:B:468:ARG:HH11	1.68	0.58
2:C:252:MET:CE	2:C:397:ILE:HG22	2.32	0.58
2:D:380:LEU:CD1	2:D:412:PHE:HB3	2.32	0.58
2:D:385:ARG:O	2:D:387:VAL:HG23	2.02	0.58
2:D:471:MET:HE2	2:D:478:ASP:CB	2.32	0.58
2:E:455:VAL:HG11	2:E:463:HIS:HB2	1.83	0.58
2:F:263:VAL:HG12	2:F:374:ARG:NH2	2.11	0.58
2:D:24:MET:HE2	2:D:66:GLU:CD	2.28	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:262:ARG:HD2	2:D:276:GLY:O	2.02	0.58
2:D:345:LYS:NZ	2:D:366:GLU:OE1	2.34	0.58
2:E:170:ARG:HB3	2:E:170:ARG:HH11	1.67	0.58
2:E:383:LEU:HD23	2:E:383:LEU:N	2.18	0.58
2:E:462:TRP:O	2:E:463:HIS:O	2.21	0.58
2:F:16:GLN:HE22	2:F:33:HIS:HB3	1.68	0.58
2:B:284:ILE:CD1	2:B:436:THR:HB	2.30	0.58
2:D:347:VAL:HG12	2:D:348:CYS:H	1.67	0.58
2:D:377:ILE:HG22	2:D:377:ILE:O	2.02	0.58
2:E:28:PHE:N	2:E:246:ILE:HD12	2.19	0.58
2:F:209:ASN:ND2	2:F:216:ARG:HD2	2.19	0.58
2:F:220:LEU:HD23	2:F:220:LEU:C	2.28	0.58
2:F:231:MET:HE1	2:F:251:ALA:HB2	1.85	0.58
2:F:492:GLY:O	2:F:494:PRO:HD3	2.03	0.58
1:A:426:TPO:N	1:A:426:TPO:O1P	2.36	0.58
2:B:291:GLY:HA3	2:B:442:TYR:OH	2.04	0.58
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.85	0.58
2:D:123:LEU:O	2:D:127:ILE:HG13	2.03	0.58
2:E:148:THR:HG21	2:E:183:GLU:CG	2.34	0.58
2:E:221:GLU:HG2	2:E:222:ILE:N	2.18	0.58
2:B:64:ILE:HD12	2:B:102:LYS:HB3	1.83	0.58
2:D:395:PHE:O	2:D:399:VAL:HG23	2.04	0.58
2:E:404:LYS:C	2:E:406:GLU:H	2.10	0.58
2:F:497:ILE:O	2:F:497:ILE:HD13	2.04	0.58
1:A:43:LEU:HD12	1:A:180:MET:O	2.04	0.58
1:A:377:ILE:HD12	1:A:377:ILE:N	2.19	0.58
2:C:69:GLU:HB3	2:C:140:ARG:HB2	1.85	0.58
2:D:218:ARG:CZ	2:D:239:ILE:CD1	2.78	0.58
2:D:443:VAL:HG12	2:D:445:ILE:HD11	1.85	0.58
2:F:377:ILE:HD12	2:F:412:PHE:HE2	1.66	0.58
2:C:38:ILE:HG23	2:C:177:THR:OG1	2.04	0.58
2:D:30:ASP:OD2	2:D:30:ASP:N	2.36	0.58
2:D:85:LYS:HE3	2:E:16:GLN:O	2.03	0.58
2:E:453:ILE:HG21	2:E:479:ILE:CD1	2.27	0.58
2:F:283:ILE:HG23	2:F:412:PHE:HE1	1.67	0.58
2:F:321:ARG:O	2:F:325:LEU:HD12	2.03	0.58
2:B:344:LEU:HD13	2:B:344:LEU:C	2.29	0.58
2:C:344:LEU:HD22	2:C:345:LYS:H	1.67	0.58
2:D:21:MET:HE1	2:D:177:THR:HB	1.86	0.58
2:D:64:ILE:CD1	2:D:70:PRO:HA	2.31	0.58
2:D:267:VAL:HG12	2:D:270:LEU:H	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:440:LEU:HD23	2:F:453:ILE:HG13	1.86	0.58
2:C:63:GLY:HA3	2:C:141:ARG:CZ	2.33	0.58
2:D:79:THR:HG22	2:D:82:ASP:OD2	2.04	0.58
2:E:223:LEU:O	2:E:224:LYS:HB3	2.03	0.58
2:F:471:MET:HG2	2:F:480:LYS:CE	2.33	0.58
2:B:148:THR:HA	2:B:151:PHE:CD1	2.38	0.58
2:B:187:GLU:O	2:B:208:ARG:HD3	2.04	0.58
2:C:50:THR:CG2	2:C:207:LEU:HB3	2.33	0.58
2:C:111:ASP:OD2	2:C:113:GLU:HG2	2.04	0.58
2:E:288:GLY:O	2:E:415:THR:HA	2.04	0.58
2:E:313:ILE:HG13	2:E:372:PRO:HG2	1.84	0.58
2:F:171:LEU:HD13	2:F:178:THR:HG21	1.86	0.58
2:F:426:THR:C	2:F:428:SER:H	2.12	0.58
1:A:425:ILE:HG23	2:F:419:PHE:CE2	2.39	0.57
2:C:314:LEU:HD23	2:C:346:ILE:HD12	1.85	0.57
2:D:496:ARG:NH2	2:E:486:PHE:O	2.37	0.57
2:E:305:ALA:CB	2:E:374:ARG:HD2	2.23	0.57
2:F:443:VAL:O	2:F:445:ILE:HD12	2.04	0.57
2:B:56:SER:HB2	2:B:143:SER:HB3	1.85	0.57
2:B:434:THR:HG21	2:B:437:ILE:HD11	1.85	0.57
2:D:69:GLU:HB3	2:D:140:ARG:HB2	1.86	0.57
2:E:221:GLU:CG	2:E:222:ILE:N	2.67	0.57
2:E:332:GLY:O	2:E:333:MET:O	2.22	0.57
2:F:245:ASN:HD22	2:F:361:GLN:HE21	1.52	0.57
1:A:148:THR:HG21	1:A:183:GLU:HG3	1.85	0.57
1:A:231:MET:HE1	1:A:251:ALA:HB2	1.86	0.57
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.19	0.57
2:B:455:VAL:HG11	2:B:463:HIS:HB2	1.87	0.57
2:B:462:TRP:O	2:B:463:HIS:O	2.20	0.57
2:D:287:THR:HG22	2:D:288:GLY:H	1.68	0.57
2:E:214:GLU:HB3	2:F:234:GLU:HB2	1.85	0.57
1:A:52:LYS:HB2	3:A:903:ATP:O1B	2.04	0.57
1:A:294:LYS:N	3:A:901:ATP:O1B	2.35	0.57
2:F:225:LEU:HB2	2:F:230:HIS:HD2	1.69	0.57
1:A:371:LYS:N	1:A:372:PRO:HD3	2.20	0.57
2:C:287:THR:HG21	2:C:414:ASN:HD22	1.69	0.57
2:C:294:LYS:HD3	2:C:294:LYS:H	1.70	0.57
2:C:360:LEU:O	2:C:360:LEU:HD23	2.04	0.57
2:D:89:SER:HB2	2:E:227:GLY:O	2.04	0.57
2:D:418:GLN:NE2	2:D:422:ALA:HA	2.19	0.57
2:E:231:MET:HE1	2:E:251:ALA:HB2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:247:PHE:HZ	2:E:361:GLN:HB2	1.70	0.57
2:F:317:TYR:OH	2:F:363:ILE:HD11	2.05	0.57
1:A:273:MET:O	1:A:463:HIS:HA	2.03	0.57
2:B:425:ILE:HD11	2:B:456:PHE:CE2	2.39	0.57
2:D:431:ALA:C	2:D:433:ILE:H	2.12	0.57
2:F:202:ASP:HA	2:F:226:ARG:HD2	1.85	0.57
1:A:203:ASN:CG	1:A:225:LEU:HD23	2.30	0.57
1:A:311:ARG:HD2	1:A:371:LYS:NZ	2.19	0.57
1:A:488:ARG:NE	2:F:488:ARG:HH12	2.03	0.57
2:B:285:LEU:HB3	2:B:437:ILE:HD13	1.87	0.57
2:D:67:PHE:O	2:D:68:ASP:HB3	2.03	0.57
2:E:54:LEU:HD22	2:E:90:PHE:CZ	2.39	0.57
2:E:238:THR:HB	2:E:361:GLN:NE2	2.18	0.57
2:B:246:ILE:HD12	2:B:246:ILE:N	2.20	0.57
2:C:248:PRO:O	2:C:250:GLY:N	2.38	0.57
2:C:340:ARG:C	2:C:342:ASN:H	2.13	0.57
2:D:53:THR:HG22	2:D:57:ILE:CD1	2.35	0.57
2:F:246:ILE:HG22	2:F:247:PHE:N	2.19	0.57
1:A:257:ARG:NH2	1:A:407:GLU:HG2	2.20	0.57
1:A:269:ARG:HB3	1:A:479:ILE:HD12	1.86	0.57
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.86	0.57
2:B:88:ARG:HG2	2:B:88:ARG:HH11	1.68	0.57
2:C:289:ALA:HB2	2:C:419:PHE:HA	1.87	0.57
2:D:64:ILE:HD11	2:D:102:LYS:O	2.04	0.57
2:D:351:PRO:HG2	2:D:382:ALA:O	2.05	0.57
2:E:30:ASP:O	2:E:31:ILE:C	2.47	0.57
2:E:296:LEU:HD13	2:E:331:TRP:CE2	2.40	0.57
2:E:396:VAL:HG21	2:E:430:ILE:HD13	1.85	0.57
2:E:437:ILE:CD1	2:E:457:LYS:HE2	2.35	0.57
1:A:52:LYS:HD3	1:A:182:THR:O	2.05	0.57
1:A:388:SER:OG	1:A:389:ASN:N	2.38	0.57
1:A:488:ARG:HE	2:F:488:ARG:HH12	1.53	0.57
2:B:356:LEU:CD1	2:B:356:LEU:N	2.67	0.57
2:C:194:TYR:O	2:C:195:GLY:C	2.46	0.57
2:E:294:LYS:CB	2:E:413:THR:HG23	2.34	0.57
1:A:14:GLU:HG3	1:A:15:HIS:N	2.14	0.56
2:B:35:GLY:O	2:B:36:LEU:C	2.48	0.56
2:C:72:VAL:O	2:C:142:VAL:HG13	2.05	0.56
2:D:486:PHE:HB3	2:D:489:ILE:HD12	1.88	0.56
2:F:115:GLN:CG	2:F:116:GLU:H	2.17	0.56
2:F:245:ASN:HD22	2:F:361:GLN:NE2	2.03	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ALA:O	1:A:348:CYS:HA	2.04	0.56
1:A:501:GLU:O	1:A:503:SER:N	2.37	0.56
2:B:56:SER:O	2:B:59:PHE:HB3	2.06	0.56
2:B:359:HIS:O	2:B:360:LEU:C	2.48	0.56
2:C:147:VAL:O	2:C:150:VAL:HG12	2.05	0.56
2:D:53:THR:HG23	2:D:145:ASP:OD2	2.05	0.56
2:E:444:GLU:OE1	2:F:490:ILE:HG12	2.05	0.56
2:F:130:ILE:O	2:F:134:ILE:HG12	2.05	0.56
1:A:21:MET:HE3	1:A:59:PHE:HZ	1.69	0.56
1:A:432:TPO:HB	2:F:318:GLU:OE2	2.04	0.56
2:B:53:THR:HG23	2:B:145:ASP:OD1	2.06	0.56
2:B:192:ALA:HB3	2:B:197:GLU:OE2	2.05	0.56
2:B:284:ILE:HG23	2:B:436:THR:HB	1.87	0.56
2:B:341:GLN:O	2:B:343:LEU:HG	2.04	0.56
2:C:215:ARG:HA	2:C:215:ARG:NE	2.20	0.56
2:D:21:MET:HE1	2:D:141:ARG:HG2	1.87	0.56
2:D:74:VAL:HG21	2:D:130:ILE:HD13	1.86	0.56
2:D:344:LEU:HD13	2:D:344:LEU:C	2.30	0.56
2:E:205:VAL:HG22	2:E:222:ILE:CD1	2.34	0.56
2:F:317:TYR:CD2	2:F:383:LEU:HD21	2.40	0.56
2:C:103:LEU:HD12	2:C:104:PHE:H	1.70	0.56
2:D:43:LEU:HD21	2:D:197:GLU:CB	2.35	0.56
2:D:436:THR:CG2	2:D:458:MET:HG2	2.32	0.56
2:E:94:LEU:HB3	2:E:103:LEU:CD2	2.35	0.56
2:F:47:THR:HG23	2:F:48:SER:N	2.19	0.56
2:F:161:ARG:HB2	2:F:196:VAL:CG1	2.35	0.56
2:F:213:GLY:C	2:F:215:ARG:H	2.13	0.56
2:F:514:GLU:O	2:F:515:LYS:CB	2.53	0.56
1:A:89:SER:HB2	2:B:227:GLY:O	2.05	0.56
1:A:199:PHE:CE1	2:F:183:GLU:HB2	2.40	0.56
1:A:203:ASN:OD1	1:A:225:LEU:HD23	2.06	0.56
1:A:375:ILE:O	1:A:410:GLY:HA2	2.06	0.56
2:B:449:MET:HE2	2:B:449:MET:HA	1.87	0.56
2:C:37:PRO:HD2	2:C:203:ASN:ND2	2.21	0.56
2:D:18:ILE:HD13	2:D:228:THR:CG2	2.36	0.56
2:E:317:TYR:OH	2:E:363:ILE:HD11	2.06	0.56
2:F:192:ALA:HB1	2:F:197:GLU:OE1	2.06	0.56
2:B:211:LEU:HD13	2:B:216:ARG:NE	2.20	0.56
2:D:283:ILE:HG23	2:D:412:PHE:CE1	2.40	0.56
2:E:131:ASN:O	2:E:135:GLN:HB2	2.05	0.56
2:F:52:LYS:CB	3:F:903:ATP:O1B	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ILE:O	2:B:66:GLU:HG2	2.05	0.56
2:B:126:LEU:O	2:B:130:ILE:HG13	2.06	0.56
2:E:148:THR:CG2	2:E:193:ARG:HD2	2.36	0.56
2:B:87:ALA:C	2:B:89:SER:N	2.61	0.56
2:B:123:LEU:HD12	2:B:166:ARG:HD2	1.88	0.56
2:E:445:ILE:HG22	2:E:446:ARG:HD2	1.87	0.56
2:E:504:GLU:HG2	2:E:505:LEU:N	2.20	0.56
2:F:33:HIS:ND1	2:F:230:HIS:HA	2.21	0.56
1:A:121:PHE:CD1	1:A:122:ASP:N	2.73	0.56
1:A:285:LEU:HB3	1:A:437:ILE:HD13	1.87	0.56
1:A:447:GLY:HA2	2:B:489:ILE:CD1	2.36	0.56
2:C:471:MET:HE2	2:C:478:ASP:CA	2.35	0.56
2:B:370:PHE:O	2:B:371:LYS:HD2	2.06	0.56
2:C:232:LYS:HD2	2:C:232:LYS:N	2.21	0.56
2:C:384:ALA:HB2	2:C:392:PHE:CE1	2.40	0.56
2:C:431:ALA:C	2:C:432:TPO:HG22	2.29	0.56
2:D:68:ASP:OD1	2:D:68:ASP:O	2.23	0.56
2:D:292:THR:HB	2:D:440:LEU:CB	2.36	0.56
2:D:350:TYR:CZ	2:E:254:LEU:HD13	2.41	0.56
2:E:316:ALA:HB2	2:E:324:LEU:HD11	1.88	0.56
2:F:270:LEU:O	2:F:273:MET:HB2	2.05	0.56
2:F:315:PHE:CE2	2:F:347:VAL:HG21	2.41	0.56
1:A:105:ILE:HD12	1:A:105:ILE:N	2.21	0.55
1:A:379:SER:N	1:A:413:THR:HB	2.14	0.55
3:A:901:ATP:H3'	2:B:458:MET:O	2.06	0.55
2:B:216:ARG:HG3	2:C:233:GLY:H	1.71	0.55
2:B:341:GLN:O	2:B:342:ASN:C	2.49	0.55
2:C:220:LEU:HD23	2:C:220:LEU:C	2.31	0.55
2:C:335:PHE:HA	2:C:338:MET:HG3	1.88	0.55
2:C:360:LEU:HD23	2:C:364:LYS:HG3	1.87	0.55
2:E:289:ALA:HB2	2:E:419:PHE:HA	1.87	0.55
2:E:294:LYS:CG	2:E:413:THR:HG23	2.36	0.55
1:A:451:ARG:HD2	1:A:451:ARG:N	2.19	0.55
2:C:313:ILE:HD12	2:C:372:PRO:HG3	1.88	0.55
2:E:41:SER:HB2	2:E:178:THR:HG22	1.87	0.55
2:E:452:ALA:HA	2:E:469:GLU:HA	1.88	0.55
2:F:56:SER:O	2:F:59:PHE:HB3	2.06	0.55
2:F:280:LYS:HZ3	2:F:407:GLU:HB3	1.71	0.55
1:A:159:VAL:O	1:A:163:GLU:HG2	2.07	0.55
1:A:299:SER:C	1:A:301:PHE:H	2.14	0.55
2:C:42:THR:HA	2:C:203:ASN:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:234:GLU:C	2:C:235:TYR:CD1	2.85	0.55
2:D:194:TYR:O	2:D:196:VAL:N	2.40	0.55
2:E:237:PHE:C	2:E:237:PHE:CD1	2.84	0.55
2:E:267:VAL:HG21	2:E:477:PRO:CG	2.36	0.55
2:F:470:PHE:HA	2:F:478:ASP:O	2.06	0.55
2:B:18:ILE:HD12	2:B:18:ILE:N	2.21	0.55
2:B:119:GLY:C	2:B:121:PHE:N	2.61	0.55
2:B:359:HIS:O	2:B:363:ILE:HD13	2.07	0.55
2:B:387:VAL:HG12	2:B:391:ALA:HB3	1.89	0.55
2:C:264:SER:O	2:C:374:ARG:NH2	2.40	0.55
1:A:19:ALA:HB3	1:A:38:ILE:HD12	1.89	0.55
2:B:191:ILE:HB	2:B:198:GLU:CG	2.37	0.55
2:B:195:GLY:HA2	2:B:198:GLU:OE2	2.06	0.55
2:B:247:PHE:CE2	2:B:364:LYS:HD2	2.37	0.55
2:B:357:GLU:CG	2:B:358:ASP:N	2.69	0.55
2:C:296:LEU:HD13	2:C:331:TRP:CE2	2.41	0.55
2:D:191:ILE:CG2	2:D:198:GLU:HG3	2.36	0.55
2:D:191:ILE:HG21	2:D:198:GLU:HG3	1.89	0.55
2:D:393:ARG:O	2:D:397:ILE:HG13	2.07	0.55
2:E:222:ILE:N	5:E:534:HOH:O	2.38	0.55
2:E:371:LYS:O	2:E:371:LYS:CD	2.54	0.55
2:E:501:GLU:O	2:E:502:LYS:HG3	2.06	0.55
1:A:220:LEU:HD13	1:A:246:ILE:HD11	1.89	0.55
2:B:71:GLY:O	2:B:103:LEU:HA	2.07	0.55
2:C:73:PHE:HD1	2:C:143:SER:HB2	1.71	0.55
2:E:197:GLU:OE2	2:E:197:GLU:N	2.30	0.55
2:C:24:MET:CB	2:C:62:ASN:HD22	2.19	0.55
2:C:486:PHE:CE2	2:C:496:ARG:HG2	2.41	0.55
2:D:39:GLY:H	2:D:177:THR:HG23	1.71	0.55
2:D:163:GLU:O	2:D:166:ARG:HB3	2.06	0.55
2:E:279:PHE:HB2	2:E:282:SER:OG	2.07	0.55
2:F:294:LYS:NZ	2:F:415:THR:HG23	2.21	0.55
2:B:18:ILE:HD13	2:B:227:GLY:O	2.07	0.55
2:B:379:SER:OG	2:B:382:ALA:HB2	2.06	0.55
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.37	0.55
2:C:370:PHE:O	2:C:371:LYS:C	2.49	0.55
2:D:445:ILE:HD12	2:D:445:ILE:N	2.22	0.55
2:E:346:ILE:HG22	2:E:348:CYS:SG	2.47	0.55
2:F:64:ILE:HD13	2:F:69:GLU:O	2.07	0.55
1:A:41:SER:OG	1:A:178:THR:HB	2.07	0.55
1:A:509:VAL:O	1:A:509:VAL:HG12	2.08	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:TYR:CE1	2:B:92:TRP:HB2	2.41	0.55
2:B:316:ALA:HB3	2:B:348:CYS:SG	2.47	0.55
2:D:98:VAL:HG21	2:D:105:ILE:HD13	1.88	0.55
2:E:27:GLY:HA3	2:E:246:ILE:HB	1.89	0.55
1:A:363:ILE:O	1:A:367:ILE:HG13	2.07	0.54
2:B:151:PHE:CE2	2:B:160:VAL:HG13	2.42	0.54
2:B:469:GLU:HB3	2:B:483:PHE:CE1	2.42	0.54
2:E:123:LEU:HD23	2:E:127:ILE:CD1	2.30	0.54
2:E:200:VAL:O	2:E:200:VAL:HG12	2.07	0.54
2:F:18:ILE:HG13	2:F:227:GLY:HA3	1.89	0.54
2:F:147:VAL:HG23	2:F:148:THR:N	2.23	0.54
2:F:484:ARG:HB3	2:F:484:ARG:HH11	1.72	0.54
1:A:453:ILE:HD13	1:A:453:ILE:C	2.32	0.54
1:A:514:GLU:C	1:A:515:LYS:HD2	2.32	0.54
2:F:289:ALA:O	2:F:292:THR:HG23	2.06	0.54
1:A:94:LEU:O	1:A:97:LEU:N	2.39	0.54
2:C:25:ILE:HG12	2:C:58:GLN:NE2	2.22	0.54
2:C:187:GLU:OE2	2:C:208:ARG:HA	2.07	0.54
2:E:308:ASN:O	2:E:309:LYS:HB2	2.07	0.54
2:F:378:ASP:O	2:F:379:SER:HB3	2.07	0.54
2:B:50:THR:HB	2:B:207:LEU:CB	2.38	0.54
2:D:154:TYR:O	2:D:154:TYR:HD1	1.90	0.54
2:D:443:VAL:HG12	2:D:445:ILE:CD1	2.37	0.54
2:D:490:ILE:C	2:D:492:GLY:N	2.66	0.54
2:E:437:ILE:HD11	2:E:457:LYS:HE2	1.88	0.54
2:E:451:ARG:HH11	2:E:472:ILE:HD11	1.72	0.54
2:E:497:ILE:CG2	2:E:498:THR:H	2.16	0.54
2:F:313:ILE:HD12	2:F:345:LYS:HB3	1.87	0.54
1:A:211:LEU:HG	1:A:212:GLU:N	2.23	0.54
2:B:436:THR:OG1	2:B:458:MET:HG2	2.08	0.54
2:D:167:LEU:O	2:D:168:VAL:C	2.50	0.54
2:D:184:ARG:HH12	2:D:208:ARG:NH1	2.05	0.54
2:D:471:MET:HE3	2:D:471:MET:C	2.32	0.54
2:D:495:THR:HG23	2:E:487:GLU:OE2	2.06	0.54
2:F:123:LEU:O	2:F:127:ILE:HG12	2.08	0.54
1:A:237:PHE:HB3	1:A:246:ILE:HG12	1.89	0.54
2:B:221:GLU:HG3	2:B:233:GLY:O	2.08	0.54
2:B:311:ARG:HG3	2:B:371:LYS:HZ1	1.71	0.54
2:C:38:ILE:HG22	2:C:39:GLY:N	2.22	0.54
2:D:273:MET:SD	2:D:468:ARG:HD2	2.48	0.54
2:D:362:ILE:O	2:D:365:SER:HB3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:31:ILE:HA	2:E:231:MET:HG3	1.89	0.54
2:E:220:LEU:C	2:E:220:LEU:HD23	2.33	0.54
2:E:472:ILE:HD12	2:E:472:ILE:N	2.23	0.54
2:F:231:MET:CE	2:F:251:ALA:HB2	2.36	0.54
2:F:255:THR:O	2:F:255:THR:HG22	2.06	0.54
1:A:222:ILE:N	1:A:222:ILE:HD12	2.23	0.54
2:B:155:ASP:OD1	2:B:159:VAL:HG11	2.08	0.54
2:B:451:ARG:N	2:B:451:ARG:HD2	2.22	0.54
2:C:63:GLY:HA3	2:C:141:ARG:NH1	2.23	0.54
2:E:292:THR:OG1	2:E:440:LEU:HD12	2.07	0.54
2:E:464:ASP:OD2	2:E:466:ALA:HB3	2.08	0.54
2:F:273:MET:CE	2:F:468:ARG:HD2	2.37	0.54
1:A:111:ASP:C	1:A:113:GLU:H	2.15	0.54
2:B:187:GLU:OE2	2:B:208:ARG:HG2	2.08	0.54
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.89	0.54
2:D:61:TYR:CE1	2:D:65:ILE:HD11	2.43	0.54
2:E:453:ILE:HG23	2:E:453:ILE:O	2.07	0.54
2:D:127:ILE:HD13	2:D:170:ARG:HG3	1.90	0.54
2:D:419:PHE:H	2:D:419:PHE:HD2	1.56	0.54
2:F:303:GLU:CD	2:F:333:MET:HB3	2.33	0.54
2:F:357:GLU:HG3	2:F:358:ASP:N	2.23	0.54
1:A:123:LEU:O	1:A:126:LEU:HB3	2.09	0.54
1:A:161:ARG:NH2	2:F:77:GLU:OE1	2.37	0.54
1:A:358:ASP:O	1:A:362:ILE:HG12	2.07	0.54
2:C:17:ALA:C	2:C:18:ILE:HD12	2.32	0.54
2:C:56:SER:HB2	2:C:143:SER:HB3	1.89	0.54
2:C:215:ARG:HE	2:C:215:ARG:CA	2.18	0.54
2:D:41:SER:HB3	2:D:178:THR:HB	1.89	0.54
2:D:461:SER:OG	2:D:462:TRP:N	2.36	0.54
2:E:153:GLN:O	2:F:158:SER:HB2	2.08	0.54
2:E:385:ARG:O	2:E:387:VAL:HG23	2.08	0.54
2:F:452:ALA:HA	2:F:469:GLU:HA	1.90	0.54
1:A:364:LYS:HA	1:A:367:ILE:HD12	1.91	0.53
1:A:413:THR:HG21	5:A:535:HOH:O	2.07	0.53
2:B:264:SER:HB3	2:B:304:ASN:HD21	1.72	0.53
2:F:39:GLY:O	2:F:172:LYS:HG3	2.08	0.53
2:F:72:VAL:HG21	2:F:134:ILE:HD13	1.90	0.53
2:B:24:MET:HB2	2:B:62:ASN:HD22	1.73	0.53
2:B:211:LEU:HG	2:B:212:GLU:H	1.74	0.53
2:B:433:ILE:HD12	2:B:433:ILE:N	2.23	0.53
2:C:52:LYS:HD2	2:C:182:THR:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:340:ARG:C	2:D:342:ASN:H	2.16	0.53
2:E:273:MET:O	2:E:463:HIS:HB2	2.08	0.53
2:E:294:LYS:HG2	2:E:413:THR:HG23	1.90	0.53
2:E:323:GLN:HG2	2:E:327:ASN:HD21	1.72	0.53
1:A:192:ALA:O	1:A:194:TYR:N	2.41	0.53
1:A:341:GLN:O	1:A:343:LEU:HG	2.08	0.53
1:A:378:ASP:HA	1:A:413:THR:HB	1.91	0.53
2:B:191:ILE:HB	2:B:198:GLU:HG3	1.90	0.53
2:C:283:ILE:HD12	2:C:283:ILE:N	2.23	0.53
2:C:381:SER:O	2:C:384:ALA:N	2.36	0.53
2:C:431:ALA:O	2:C:432:TPO:CG2	2.43	0.53
2:D:446:ARG:HB3	2:E:484:ARG:HG3	1.90	0.53
2:E:170:ARG:HB3	2:E:170:ARG:NH1	2.24	0.53
2:E:287:THR:HG22	2:E:288:GLY:N	2.23	0.53
2:E:451:ARG:HH11	2:E:472:ILE:CD1	2.22	0.53
2:F:377:ILE:CD1	2:F:399:VAL:HG11	2.38	0.53
1:A:64:ILE:HG23	1:A:102:LYS:HB3	1.90	0.53
2:B:140:ARG:NH1	2:B:140:ARG:CB	2.67	0.53
2:B:311:ARG:HD2	2:B:371:LYS:HE3	1.90	0.53
2:C:88:ARG:CZ	2:D:15:HIS:HA	2.36	0.53
2:C:220:LEU:HD23	2:C:221:GLU:N	2.23	0.53
2:C:287:THR:CG2	2:C:288:GLY:H	2.17	0.53
2:E:32:SER:OG	2:E:35:GLY:N	2.42	0.53
2:E:294:LYS:HB2	3:E:901:ATP:O1B	2.08	0.53
2:F:93:ASP:OD1	2:F:95:ALA:HB3	2.07	0.53
1:A:459:ARG:NH1	2:F:319:GLU:HG2	2.23	0.53
1:A:466:ALA:HA	2:F:448:GLU:HG2	1.90	0.53
2:B:204:VAL:HG23	2:B:224:LYS:HG2	1.91	0.53
2:B:326:ARG:HG3	2:C:260:ASN:ND2	2.22	0.53
2:D:64:ILE:CD1	2:D:102:LYS:HB3	2.32	0.53
2:D:316:ALA:C	2:D:317:TYR:HD1	2.16	0.53
2:D:375:ILE:HG22	2:D:377:ILE:HD11	1.91	0.53
2:D:451:ARG:HD2	2:D:451:ARG:N	2.24	0.53
2:E:186:GLU:OE1	2:E:189:GLY:N	2.42	0.53
2:E:264:SER:HB3	2:E:304:ASN:HD21	1.73	0.53
2:F:461:SER:OG	2:F:462:TRP:N	2.41	0.53
1:A:184:ARG:O	1:A:185:ILE:HD13	2.08	0.53
1:A:371:LYS:O	1:A:371:LYS:CD	2.55	0.53
2:C:164:LEU:O	2:C:167:LEU:N	2.42	0.53
2:C:308:ASN:O	2:C:309:LYS:C	2.51	0.53
2:D:18:ILE:HD12	2:D:18:ILE:N	2.19	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:313:ILE:HD11	2:D:370:PHE:HB3	1.91	0.53
2:F:75:THR:OG1	2:F:78:GLU:O	2.23	0.53
1:A:21:MET:CE	1:A:59:PHE:HZ	2.22	0.53
1:A:52:LYS:N	1:A:207:LEU:HD12	2.23	0.53
1:A:121:PHE:HD1	1:A:122:ASP:N	2.07	0.53
2:C:146:SER:C	2:C:148:THR:H	2.14	0.53
2:C:389:ASN:HD21	2:C:428:SER:CB	2.22	0.53
2:D:284:ILE:HD12	2:D:284:ILE:N	2.24	0.53
2:F:31:ILE:HA	2:F:231:MET:HG3	1.90	0.53
2:F:231:MET:HB3	2:F:235:TYR:OH	2.08	0.53
2:F:280:LYS:NZ	2:F:407:GLU:HB3	2.23	0.53
2:F:287:THR:HA	2:F:414:ASN:O	2.08	0.53
2:F:302:VAL:HG12	2:F:303:GLU:N	2.23	0.53
2:F:430:ILE:HG22	2:F:430:ILE:O	2.08	0.53
1:A:230:HIS:CE1	1:A:232:LYS:HE3	2.43	0.53
2:D:37:PRO:HG2	2:D:203:ASN:OD1	2.09	0.53
2:D:294:LYS:N	3:D:901:ATP:O1B	2.42	0.53
2:D:347:VAL:O	2:D:348:CYS:CB	2.56	0.53
2:F:47:THR:O	2:F:52:LYS:HE2	2.08	0.53
2:F:462:TRP:CE3	2:F:463:HIS:N	2.77	0.53
1:A:14:GLU:CG	1:A:15:HIS:N	2.68	0.53
2:B:88:ARG:NH1	2:B:93:ASP:HA	2.23	0.53
2:B:167:LEU:O	2:B:168:VAL:C	2.52	0.53
2:C:223:LEU:HD13	2:C:223:LEU:C	2.33	0.53
2:C:438:ILE:HD12	2:C:438:ILE:N	2.24	0.53
2:D:44:VAL:HG13	2:D:205:VAL:HG12	1.89	0.53
2:D:299:SER:C	2:D:333:MET:HE1	2.34	0.53
2:E:268:VAL:O	2:E:271:ASP:HB2	2.08	0.53
2:E:296:LEU:HD13	2:E:331:TRP:CD2	2.43	0.53
2:E:344:LEU:HD22	2:E:345:LYS:N	2.20	0.53
2:F:418:GLN:NE2	2:F:421:GLY:O	2.41	0.53
1:A:485:ASN:HD22	1:A:498:THR:CG2	2.22	0.53
2:B:304:ASN:HB3	2:B:374:ARG:HH12	1.74	0.53
2:D:194:TYR:O	2:D:195:GLY:C	2.50	0.53
2:D:202:ASP:HA	2:D:226:ARG:CD	2.38	0.53
2:E:326:ARG:HD3	2:F:258:SER:OG	2.09	0.53
2:E:332:GLY:C	2:E:333:MET:HG2	2.33	0.53
2:F:364:LYS:HE2	2:F:402:TYR:CD1	2.43	0.53
2:B:117:VAL:O	2:B:117:VAL:HG12	2.09	0.52
2:C:182:THR:HG22	2:C:183:GLU:H	1.73	0.52
2:D:262:ARG:NH1	2:D:275:GLY:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:443:VAL:O	2:D:445:ILE:HD12	2.09	0.52
2:D:463:HIS:ND1	2:D:464:ASP:O	2.37	0.52
2:E:21:MET:HE3	2:E:141:ARG:NE	2.24	0.52
2:E:47:THR:HG21	2:E:187:GLU:OE1	2.09	0.52
2:E:52:LYS:HB2	2:E:52:LYS:NZ	2.24	0.52
2:E:84:ILE:HG21	2:E:95:ALA:HB2	1.91	0.52
2:F:471:MET:HE1	2:F:473:SER:CB	2.31	0.52
2:B:121:PHE:H	2:B:121:PHE:HD1	1.58	0.52
2:B:326:ARG:O	2:B:328:ALA:N	2.42	0.52
2:B:379:SER:CA	2:B:413:THR:HB	2.39	0.52
2:C:31:ILE:O	2:C:231:MET:HG3	2.09	0.52
2:C:98:VAL:HA	2:C:103:LEU:O	2.09	0.52
2:C:356:LEU:O	2:C:357:GLU:C	2.52	0.52
2:D:353:SER:HA	2:E:250:GLY:O	2.08	0.52
2:E:23:THR:O	2:E:24:MET:HB2	2.07	0.52
2:F:323:GLN:HG2	2:F:327:ASN:HD21	1.73	0.52
1:A:504:GLU:C	1:A:506:SER:H	2.16	0.52
2:C:184:ARG:NH1	2:C:187:GLU:O	2.41	0.52
2:C:202:ASP:CA	2:C:226:ARG:HD2	2.38	0.52
2:C:337:GLU:O	2:C:340:ARG:N	2.42	0.52
2:D:300:ARG:N	2:D:333:MET:HE1	2.25	0.52
2:E:436:THR:OG1	2:E:458:MET:HE2	2.09	0.52
1:A:432:TPO:C	1:A:434:THR:H	2.22	0.52
2:B:379:SER:HA	2:B:413:THR:HB	1.90	0.52
2:C:28:PHE:O	2:C:31:ILE:N	2.37	0.52
2:C:223:LEU:O	2:C:223:LEU:HD22	2.10	0.52
2:C:392:PHE:O	2:C:395:PHE:N	2.43	0.52
2:D:284:ILE:HD12	2:D:284:ILE:H	1.75	0.52
2:E:18:ILE:HD11	2:E:227:GLY:HA3	1.92	0.52
2:F:31:ILE:CD1	2:F:246:ILE:HG21	2.39	0.52
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.45	0.52
1:A:104:PHE:HD2	1:A:133:ALA:HB1	1.75	0.52
2:B:23:THR:N	2:B:29:ASP:OD1	2.28	0.52
2:B:274:CYS:HB3	2:B:458:MET:SD	2.50	0.52
2:D:294:LYS:CB	2:D:413:THR:HG23	2.39	0.52
2:D:316:ALA:C	2:D:317:TYR:CD1	2.88	0.52
1:A:246:ILE:O	1:A:248:PRO:HD3	2.10	0.52
1:A:258:SER:OG	2:F:326:ARG:HD3	2.09	0.52
1:A:407:GLU:OE1	1:A:407:GLU:CA	2.57	0.52
2:B:46:GLY:CA	2:B:184:ARG:HD3	2.32	0.52
2:B:479:ILE:H	2:B:479:ILE:HD12	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:245:ASN:C	2:C:245:ASN:HD22	2.17	0.52
2:D:82:ASP:O	2:D:83:ILE:C	2.52	0.52
2:D:164:LEU:O	2:D:168:VAL:HG23	2.10	0.52
2:D:184:ARG:NH2	2:D:189:GLY:O	2.42	0.52
2:E:444:GLU:OE1	2:F:489:ILE:HB	2.08	0.52
2:F:122:ASP:OD2	2:F:123:LEU:N	2.43	0.52
1:A:61:TYR:CZ	1:A:65:ILE:HG13	2.44	0.52
2:B:246:ILE:O	2:B:248:PRO:HD3	2.09	0.52
2:C:198:GLU:O	2:C:200:VAL:N	2.43	0.52
2:D:49:GLY:O	2:D:218:ARG:NH2	2.43	0.52
2:D:338:MET:HB3	2:D:344:LEU:HB3	1.90	0.52
2:D:418:GLN:HE21	2:D:422:ALA:HA	1.74	0.52
2:C:88:ARG:NH2	2:D:15:HIS:ND1	2.58	0.52
2:C:315:PHE:CE2	2:C:363:ILE:HA	2.44	0.52
2:F:106:LEU:CD1	2:F:129:ARG:NH2	2.73	0.52
2:F:345:LYS:NZ	2:F:366:GLU:OE1	2.41	0.52
2:F:515:LYS:HB3	2:F:517:PRO:HD2	1.92	0.52
1:A:182:THR:HG22	1:A:183:GLU:N	2.25	0.52
1:A:192:ALA:O	1:A:193:ARG:C	2.52	0.52
1:A:317:TYR:HE1	1:A:377:ILE:HG23	1.74	0.52
1:A:436:THR:HG23	1:A:458:MET:HG2	1.92	0.52
2:B:27:GLY:HA3	2:B:246:ILE:O	2.10	0.52
2:C:461:SER:OG	2:C:462:TRP:N	2.43	0.52
2:D:402:TYR:O	2:D:406:GLU:HB2	2.10	0.52
2:E:148:THR:HG21	2:E:183:GLU:HG3	1.90	0.52
2:E:454:ASN:HD21	2:E:456:PHE:HA	1.75	0.52
1:A:20:LYS:HD3	1:A:35:GLY:O	2.10	0.52
1:A:72:VAL:HB	1:A:142:VAL:HG22	1.92	0.52
1:A:452:ALA:HA	1:A:469:GLU:HA	1.92	0.52
1:A:508:ILE:HD12	1:A:510:ARG:N	2.24	0.52
2:B:52:LYS:HE3	3:B:903:ATP:O1B	2.10	0.52
2:B:134:ILE:HG21	2:B:174:ILE:CG2	2.39	0.52
2:C:20:LYS:C	2:C:38:ILE:HD11	2.35	0.52
2:D:375:ILE:CG2	2:D:377:ILE:HD11	2.40	0.52
2:E:310:GLU:HB3	2:E:373:ALA:HB3	1.92	0.52
2:F:300:ARG:N	2:F:333:MET:HE1	2.25	0.52
1:A:194:TYR:O	1:A:196:VAL:HG23	2.09	0.51
1:A:269:ARG:HD2	1:A:272:GLU:OE2	2.10	0.51
2:C:360:LEU:HA	2:C:363:ILE:HD12	1.92	0.51
2:D:23:THR:HB	2:D:25:ILE:HD12	1.91	0.51
2:D:52:LYS:HE3	3:D:903:ATP:O1B	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:GLN:CG	2:E:161:ARG:HH11	2.18	0.51
2:E:70:PRO:HB2	2:E:139:ALA:HA	1.92	0.51
2:E:194:TYR:O	2:E:195:GLY:C	2.53	0.51
2:E:294:LYS:HE3	2:E:415:THR:OG1	2.10	0.51
2:F:126:LEU:O	2:F:129:ARG:HB2	2.10	0.51
1:A:220:LEU:HD23	1:A:220:LEU:C	2.34	0.51
2:B:468:ARG:HG2	2:B:468:ARG:NH1	2.25	0.51
2:C:32:SER:HA	2:C:222:ILE:HD13	1.92	0.51
2:C:454:ASN:OD1	2:C:455:VAL:N	2.43	0.51
2:D:99:ASP:C	2:D:101:GLY:H	2.18	0.51
2:D:284:ILE:HG23	2:D:436:THR:HB	1.90	0.51
2:D:375:ILE:HG22	2:D:377:ILE:HD12	1.90	0.51
1:A:363:ILE:HG22	1:A:367:ILE:CD1	2.39	0.51
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.92	0.51
2:C:287:THR:HG23	2:C:414:ASN:ND2	2.24	0.51
2:C:444:GLU:HB2	2:C:449:MET:CE	2.41	0.51
2:D:208:ARG:HD2	2:D:234:GLU:OE2	2.11	0.51
2:F:25:ILE:HD12	2:F:58:GLN:HG2	1.92	0.51
1:A:211:LEU:CD1	1:A:212:GLU:H	2.24	0.51
2:B:161:ARG:HB2	2:B:196:VAL:HG11	1.92	0.51
2:C:350:TYR:CE1	2:D:252:MET:HE3	2.45	0.51
2:C:363:ILE:O	2:C:364:LYS:C	2.54	0.51
2:C:393:ARG:NH2	2:C:429:HIS:HB2	2.24	0.51
2:D:37:PRO:HD2	2:D:203:ASN:ND2	2.25	0.51
2:D:363:ILE:HG22	2:D:367:ILE:HD13	1.92	0.51
2:D:414:ASN:HD22	2:D:426:THR:HG22	1.75	0.51
2:E:72:VAL:HG21	2:E:134:ILE:HD13	1.92	0.51
2:E:451:ARG:NH1	2:E:472:ILE:HD13	2.25	0.51
1:A:213:GLY:O	1:A:214:GLU:HB2	2.11	0.51
2:B:222:ILE:HD12	2:B:222:ILE:N	2.25	0.51
2:B:311:ARG:HD2	2:B:371:LYS:CE	2.40	0.51
2:C:136:LYS:HG2	2:C:136:LYS:O	2.10	0.51
2:C:331:TRP:NE1	3:C:901:ATP:N7	2.58	0.51
2:C:434:THR:O	2:C:459:ARG:NH2	2.43	0.51
2:D:79:THR:CG2	2:D:82:ASP:OD2	2.59	0.51
2:D:88:ARG:HG2	2:D:88:ARG:NH1	2.23	0.51
2:D:387:VAL:HG12	2:D:388:SER:N	2.25	0.51
2:E:38:ILE:HA	2:E:177:THR:HG23	1.92	0.51
2:E:430:ILE:O	2:E:431:ALA:C	2.53	0.51
2:F:171:LEU:CD1	2:F:178:THR:HG21	2.40	0.51
1:A:383:LEU:C	1:A:385:ARG:H	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:901:ATP:O3'	2:B:457:LYS:HB2	2.10	0.51
2:B:26:GLU:HB3	2:B:245:ASN:OD1	2.11	0.51
2:B:296:LEU:HD21	2:B:477:PRO:HB3	1.92	0.51
2:B:371:LYS:N	2:B:372:PRO:HD3	2.25	0.51
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.76	0.51
2:C:419:PHE:HD1	2:C:420:MET:HG3	1.75	0.51
2:D:31:ILE:CG2	2:D:231:MET:HB2	2.41	0.51
2:D:271:ASP:OD1	2:D:277:GLY:HA2	2.09	0.51
2:D:291:GLY:O	3:D:901:ATP:H4'	2.11	0.51
2:D:338:MET:HB3	2:D:344:LEU:CB	2.41	0.51
2:D:399:VAL:O	2:D:400:THR:C	2.52	0.51
2:E:203:ASN:HB3	2:E:225:LEU:CD2	2.41	0.51
2:F:14:GLU:HG3	2:F:16:GLN:HG3	1.92	0.51
1:A:199:PHE:CZ	2:F:183:GLU:HB2	2.45	0.51
2:B:87:ALA:O	2:B:89:SER:N	2.44	0.51
2:B:148:THR:HA	2:B:151:PHE:HE1	1.76	0.51
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.92	0.51
2:D:237:PHE:HB3	2:D:246:ILE:HD13	1.92	0.51
2:D:289:ALA:O	2:D:294:LYS:NZ	2.44	0.51
2:D:451:ARG:HG2	2:D:451:ARG:HH11	1.75	0.51
2:E:147:VAL:O	2:E:150:VAL:HG12	2.11	0.51
2:F:193:ARG:C	2:F:195:GLY:H	2.19	0.51
1:A:53:THR:O	1:A:56:SER:N	2.43	0.51
1:A:140:ARG:HH11	1:A:140:ARG:CA	2.23	0.51
1:A:266:GLY:O	1:A:300:ARG:HG3	2.11	0.51
2:B:83:ILE:H	2:B:83:ILE:HD12	1.76	0.51
2:B:151:PHE:C	2:B:153:GLN:H	2.19	0.51
2:C:88:ARG:NE	2:D:15:HIS:HA	2.26	0.51
2:C:127:ILE:HD11	2:C:167:LEU:HD13	1.92	0.51
2:E:273:MET:CE	2:E:468:ARG:HD2	2.40	0.51
2:E:367:ILE:HD12	2:E:375:ILE:HD11	1.93	0.51
2:F:94:LEU:O	2:F:95:ALA:C	2.53	0.51
2:F:98:VAL:HG22	2:F:103:LEU:HG	1.92	0.51
2:F:335:PHE:HA	2:F:338:MET:HG2	1.93	0.51
2:B:392:PHE:O	2:B:395:PHE:N	2.44	0.51
2:C:45:SER:CB	2:C:182:THR:HB	2.35	0.51
2:C:86:ASN:O	2:C:89:SER:N	2.43	0.51
2:C:396:VAL:HG11	2:C:430:ILE:HG23	1.92	0.51
2:C:453:ILE:HG21	2:C:479:ILE:HG13	1.93	0.51
2:D:21:MET:HE3	2:D:59:PHE:CZ	2.46	0.51
2:D:52:LYS:N	3:D:903:ATP:O1B	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:ILE:HD12	2:D:144:ILE:N	2.26	0.51
2:D:420:MET:HA	5:D:540:HOH:O	2.10	0.51
2:E:355:GLY:O	2:E:358:ASP:HB2	2.11	0.51
2:F:515:LYS:C	2:F:517:PRO:HD2	2.36	0.51
1:A:360:LEU:O	1:A:364:LYS:HG3	2.11	0.51
2:D:325:LEU:CD2	2:D:335:PHE:HB2	2.41	0.51
2:D:443:VAL:CG1	2:D:445:ILE:HD11	2.41	0.51
2:E:292:THR:HB	2:E:440:LEU:HB3	1.93	0.51
2:F:252:MET:CE	2:F:401:GLY:HA3	2.40	0.51
1:A:61:TYR:C	1:A:63:GLY:N	2.69	0.50
2:B:94:LEU:O	2:B:98:VAL:HG23	2.10	0.50
2:B:170:ARG:O	2:B:173:GLN:HB2	2.12	0.50
2:B:406:GLU:O	2:B:407:GLU:HB2	2.11	0.50
2:B:430:ILE:O	2:B:434:THR:HG22	2.11	0.50
2:D:279:PHE:HE1	2:D:460:GLY:HA3	1.75	0.50
2:F:479:ILE:N	2:F:479:ILE:HD12	2.27	0.50
1:A:145:ASP:O	1:A:146:SER:OG	2.24	0.50
1:A:164:LEU:O	1:A:168:VAL:HG23	2.11	0.50
1:A:487:GLU:HG3	1:A:497:ILE:HD11	1.94	0.50
2:B:50:THR:HB	2:B:207:LEU:HB3	1.93	0.50
2:B:140:ARG:HH11	2:B:140:ARG:CA	2.24	0.50
2:B:443:VAL:HG12	2:B:445:ILE:HD11	1.92	0.50
2:C:359:HIS:O	2:C:363:ILE:HG13	2.10	0.50
2:D:81:GLN:CD	2:D:81:GLN:N	2.64	0.50
2:D:315:PHE:HB3	2:D:317:TYR:HE1	1.77	0.50
2:D:354:ALA:HB3	2:D:359:HIS:CE1	2.46	0.50
2:D:446:ARG:HB3	2:E:484:ARG:HG2	1.93	0.50
2:E:392:PHE:HE2	2:E:430:ILE:CD1	2.15	0.50
2:B:232:LYS:N	2:B:232:LYS:HD2	2.27	0.50
2:B:279:PHE:O	2:B:280:LYS:C	2.54	0.50
2:C:437:ILE:HD12	2:C:457:LYS:HG2	1.93	0.50
2:E:203:ASN:HA	2:E:224:LYS:O	2.11	0.50
2:F:79:THR:HG23	2:F:82:ASP:H	1.77	0.50
2:F:332:GLY:C	2:F:333:MET:HG2	2.35	0.50
1:A:161:ARG:HD2	1:A:196:VAL:HG11	1.94	0.50
1:A:162:ARG:HH11	1:A:162:ARG:HG3	1.76	0.50
1:A:211:LEU:CG	1:A:212:GLU:N	2.73	0.50
2:B:363:ILE:N	2:B:363:ILE:HD12	2.26	0.50
2:C:18:ILE:HD12	2:C:18:ILE:N	2.27	0.50
2:C:111:ASP:O	2:C:113:GLU:N	2.40	0.50
2:D:406:GLU:HB3	2:D:408:ILE:HG12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:191:ILE:HB	2:F:198:GLU:OE2	2.12	0.50
2:F:487:GLU:HG3	2:F:497:ILE:HD12	1.93	0.50
1:A:182:THR:HG22	1:A:183:GLU:O	2.11	0.50
1:A:468:ARG:NH1	1:A:468:ARG:HG2	2.26	0.50
2:B:451:ARG:O	2:B:452:ALA:HB2	2.11	0.50
2:D:72:VAL:CG2	2:D:134:ILE:HD13	2.41	0.50
2:F:44:VAL:HG13	2:F:205:VAL:CG1	2.42	0.50
2:F:206:ILE:O	2:F:207:LEU:HD23	2.11	0.50
2:B:182:THR:HG21	2:B:192:ALA:HB1	1.93	0.50
2:B:470:PHE:HB3	2:B:479:ILE:HA	1.93	0.50
2:C:234:GLU:O	2:C:235:TYR:CD1	2.65	0.50
2:E:221:GLU:HB3	5:E:530:HOH:O	2.10	0.50
2:E:240:THR:C	2:E:242:HIS:H	2.20	0.50
2:F:311:ARG:HG3	2:F:371:LYS:HZ1	1.75	0.50
2:F:313:ILE:HD13	2:F:345:LYS:HB3	1.93	0.50
2:F:514:GLU:OE1	2:F:515:LYS:N	2.38	0.50
2:C:123:LEU:HA	2:C:127:ILE:HD11	1.93	0.50
2:C:219:THR:HB	2:C:234:GLU:HG2	1.93	0.50
2:C:321:ARG:HG2	2:C:348:CYS:SG	2.52	0.50
3:C:901:ATP:O2'	2:D:463:HIS:CD2	2.65	0.50
2:D:182:THR:HG21	2:D:192:ALA:CB	2.41	0.50
2:D:197:GLU:OE2	2:D:197:GLU:N	2.22	0.50
2:D:263:VAL:CG1	2:D:374:ARG:HH21	2.19	0.50
2:D:451:ARG:HD2	2:D:451:ARG:H	1.75	0.50
2:E:438:ILE:HG23	2:E:453:ILE:HD11	1.93	0.50
2:F:205:VAL:HG22	2:F:222:ILE:CD1	2.42	0.50
2:F:231:MET:HE2	2:F:235:TYR:CZ	2.47	0.50
2:F:377:ILE:HD11	2:F:399:VAL:HG11	1.94	0.50
2:F:451:ARG:NH1	2:F:451:ARG:CG	2.75	0.50
1:A:31:ILE:HG22	1:A:231:MET:HB2	1.92	0.50
1:A:490:ILE:O	1:A:490:ILE:HG22	2.12	0.50
2:B:162:ARG:NH1	2:B:162:ARG:HB2	2.27	0.50
2:B:363:ILE:HD12	2:B:363:ILE:H	1.76	0.50
5:B:539:HOH:O	2:C:460:GLY:C	2.55	0.50
2:C:87:ALA:C	2:C:89:SER:N	2.70	0.50
2:D:178:THR:CG2	2:D:179:VAL:N	2.74	0.50
2:D:289:ALA:O	2:D:292:THR:OG1	2.29	0.50
2:E:212:GLU:O	2:E:212:GLU:HG2	2.12	0.50
2:F:72:VAL:CG2	2:F:134:ILE:HD13	2.42	0.50
2:F:418:GLN:HE21	2:F:421:GLY:C	2.20	0.50
1:A:447:GLY:HA2	2:B:489:ILE:HD12	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ARG:HB3	2:B:237:PHE:CZ	2.46	0.50
2:B:222:ILE:CG2	2:B:225:LEU:HG	2.41	0.50
2:C:471:MET:O	2:C:471:MET:HE2	2.09	0.50
2:D:65:ILE:HD12	2:D:65:ILE:N	2.27	0.50
2:E:145:ASP:C	2:E:146:SER:OG	2.54	0.50
2:E:197:GLU:H	2:E:197:GLU:CD	2.19	0.50
2:E:386:GLY:O	2:E:387:VAL:C	2.54	0.50
2:F:115:GLN:CG	2:F:116:GLU:N	2.75	0.50
1:A:444:GLU:O	1:A:445:ILE:HD13	2.12	0.49
1:A:487:GLU:CD	1:A:497:ILE:HD13	2.37	0.49
2:B:170:ARG:O	2:B:174:ILE:HG13	2.12	0.49
2:B:287:THR:HG21	2:B:425:ILE:O	2.12	0.49
2:C:20:LYS:HE2	2:C:228:THR:OG1	2.12	0.49
2:C:269:ARG:O	2:C:273:MET:HG3	2.12	0.49
2:C:344:LEU:HD11	2:C:346:ILE:HD11	1.94	0.49
2:C:393:ARG:O	2:C:397:ILE:HG12	2.12	0.49
2:C:426:THR:HG22	2:C:428:SER:H	1.77	0.49
2:D:224:LYS:O	2:D:225:LEU:HD23	2.12	0.49
2:D:283:ILE:HG13	2:D:400:THR:HG23	1.94	0.49
2:E:314:LEU:HD12	2:E:376:ALA:O	2.12	0.49
2:E:359:HIS:O	2:E:363:ILE:CD1	2.56	0.49
2:F:127:ILE:CD1	2:F:167:LEU:HA	2.42	0.49
2:F:335:PHE:HD2	2:F:338:MET:HG3	1.77	0.49
1:A:90:PHE:HB2	1:A:92:TRP:NE1	2.27	0.49
1:A:134:ILE:HD13	1:A:134:ILE:N	2.27	0.49
2:B:194:TYR:HB2	2:B:197:GLU:OE1	2.12	0.49
2:E:98:VAL:HA	2:E:103:LEU:O	2.13	0.49
2:F:269:ARG:HD2	2:F:272:GLU:OE2	2.11	0.49
2:F:316:ALA:O	2:F:348:CYS:HA	2.12	0.49
1:A:86:ASN:O	1:A:87:ALA:C	2.56	0.49
2:B:203:ASN:HB3	2:B:225:LEU:CD2	2.41	0.49
2:D:27:GLY:O	2:D:31:ILE:HG13	2.13	0.49
2:D:179:VAL:O	2:D:179:VAL:HG12	2.12	0.49
2:D:313:ILE:HG13	2:D:372:PRO:HG3	1.94	0.49
2:E:430:ILE:O	2:E:430:ILE:HG22	2.11	0.49
3:E:903:ATP:O3'	2:F:224:LYS:HB2	2.12	0.49
2:F:115:GLN:HG3	2:F:116:GLU:N	2.27	0.49
1:A:230:HIS:HE1	1:A:232:LYS:HG3	1.78	0.49
2:B:134:ILE:HG21	2:B:174:ILE:HG21	1.94	0.49
2:C:182:THR:CG2	2:C:183:GLU:N	2.75	0.49
2:D:65:ILE:HD12	2:D:65:ILE:H	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:321:ARG:HG2	2:D:348:CYS:SG	2.53	0.49
2:D:375:ILE:HG12	2:D:408:ILE:HG21	1.93	0.49
2:D:380:LEU:HD11	2:D:412:PHE:HB3	1.94	0.49
2:E:52:LYS:HB3	2:E:181:THR:CG2	2.42	0.49
2:F:43:LEU:HD23	2:F:204:VAL:HG13	1.94	0.49
2:F:285:LEU:CB	2:F:437:ILE:HD12	2.36	0.49
2:F:344:LEU:C	2:F:344:LEU:HD13	2.38	0.49
2:F:371:LYS:HD2	2:F:371:LYS:C	2.37	0.49
1:A:82:ASP:O	1:A:85:LYS:N	2.45	0.49
1:A:251:ALA:O	1:A:252:MET:C	2.56	0.49
1:A:370:PHE:C	1:A:372:PRO:HD3	2.38	0.49
2:C:357:GLU:HG3	2:C:358:ASP:N	2.28	0.49
2:C:467:ILE:N	2:C:467:ILE:HD12	2.28	0.49
2:C:482:SER:C	2:C:484:ARG:H	2.20	0.49
2:E:82:ASP:O	2:E:85:LYS:HB3	2.13	0.49
2:F:454:ASN:HB2	2:F:467:ILE:HG23	1.93	0.49
1:A:69:GLU:O	1:A:70:PRO:O	2.31	0.49
1:A:144:ILE:HB	1:A:180:MET:HG2	1.94	0.49
1:A:332:GLY:O	1:A:333:MET:C	2.56	0.49
2:B:52:LYS:H	2:B:207:LEU:CD1	2.26	0.49
2:B:54:LEU:HD23	2:B:239:ILE:HD12	1.95	0.49
2:B:423:HIS:O	2:B:424:SER:HB3	2.11	0.49
2:B:443:VAL:HG12	2:B:445:ILE:CD1	2.43	0.49
2:C:54:LEU:HD11	2:C:90:PHE:CE2	2.46	0.49
2:C:219:THR:CG2	2:C:234:GLU:HG2	2.43	0.49
2:C:371:LYS:O	2:C:371:LYS:CD	2.52	0.49
2:C:426:THR:HG22	2:C:427:ASP:N	2.28	0.49
2:D:155:ASP:OD1	2:D:159:VAL:HG11	2.13	0.49
2:D:334:ASP:OD1	2:D:336:GLU:N	2.46	0.49
2:E:342:ASN:O	2:E:343:LEU:HD23	2.12	0.49
2:F:75:THR:HG21	2:F:80:PRO:HG3	1.94	0.49
2:F:313:ILE:HG12	2:F:372:PRO:HG2	1.95	0.49
2:F:313:ILE:HG22	2:F:314:LEU:N	2.28	0.49
1:A:206:ILE:HD11	1:A:223:LEU:HD12	1.95	0.49
1:A:264:SER:HA	1:A:271:ASP:OD1	2.12	0.49
1:A:468:ARG:HG2	1:A:468:ARG:HH11	1.77	0.49
2:B:316:ALA:O	2:B:348:CYS:HA	2.12	0.49
2:B:326:ARG:C	2:B:328:ALA:H	2.21	0.49
2:C:283:ILE:HD11	2:C:404:LYS:CD	2.42	0.49
2:D:145:ASP:O	2:D:146:SER:HB2	2.12	0.49
2:E:61:TYR:O	2:E:62:ASN:C	2.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:124:SER:HA	2:E:127:ILE:CD1	2.42	0.49
2:E:451:ARG:HH11	2:E:451:ARG:CG	2.25	0.49
2:F:263:VAL:HG11	2:F:374:ARG:HH21	1.76	0.49
2:F:353:SER:O	2:F:354:ALA:CB	2.61	0.49
1:A:38:ILE:CG2	1:A:39:GLY:N	2.76	0.49
1:A:148:THR:OG1	1:A:182:THR:HG23	2.13	0.49
1:A:356:LEU:HD23	1:A:395:PHE:HB2	1.93	0.49
2:B:148:THR:C	2:B:150:VAL:N	2.66	0.49
2:B:191:ILE:HG21	2:B:204:VAL:HG11	1.95	0.49
3:B:901:ATP:H3'	2:C:458:MET:O	2.13	0.49
2:C:38:ILE:HG22	2:C:39:GLY:H	1.76	0.49
2:C:206:ILE:HG21	2:C:208:ARG:NH1	2.27	0.49
2:C:296:LEU:CD2	2:C:472:ILE:HG12	2.42	0.49
2:C:463:HIS:C	2:C:463:HIS:ND1	2.69	0.49
2:D:372:PRO:HG2	2:D:375:ILE:HD11	1.95	0.49
2:E:145:ASP:O	2:E:146:SER:OG	2.28	0.49
2:E:397:ILE:O	2:E:398:GLY:C	2.55	0.49
2:E:419:PHE:HE2	2:F:425:ILE:HG13	1.75	0.49
2:E:505:LEU:O	2:E:505:LEU:HD12	2.13	0.49
2:E:499:VAL:O	2:E:499:VAL:HG12	2.13	0.49
2:F:336:GLU:O	2:F:340:ARG:HG3	2.13	0.49
1:A:145:ASP:HA	1:A:181:THR:HB	1.95	0.49
1:A:351:PRO:C	1:A:353:SER:H	2.21	0.49
2:C:121:PHE:O	2:C:125:ALA:HB3	2.13	0.49
2:C:146:SER:HA	2:C:181:THR:O	2.12	0.49
2:C:239:ILE:N	5:C:528:HOH:O	2.43	0.49
2:C:440:LEU:N	2:C:440:LEU:HD23	2.27	0.49
3:E:903:ATP:O3'	2:F:224:LYS:HA	2.13	0.49
2:F:325:LEU:HD23	2:F:335:PHE:HB2	1.95	0.49
2:F:425:ILE:HG21	2:F:439:LEU:HD13	1.95	0.49
1:A:61:TYR:C	1:A:63:GLY:H	2.19	0.48
1:A:334:ASP:HA	5:A:527:HOH:O	2.12	0.48
2:B:451:ARG:HB3	2:B:470:PHE:CE2	2.47	0.48
2:C:483:PHE:H	2:C:483:PHE:HD1	1.59	0.48
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.41	0.48
2:D:468:ARG:NH1	2:D:468:ARG:HG2	2.28	0.48
2:E:298:VAL:HG13	2:E:376:ALA:HB1	1.95	0.48
2:E:319:GLU:HB2	2:E:324:LEU:HG	1.94	0.48
2:E:352:GLU:OE2	2:E:385:ARG:HD2	2.13	0.48
2:F:82:ASP:HA	2:F:85:LYS:HB3	1.95	0.48
1:A:183:GLU:HB3	2:B:199:PHE:CE1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:SER:C	1:A:301:PHE:N	2.71	0.48
2:B:470:PHE:CB	2:B:479:ILE:HA	2.43	0.48
2:D:41:SER:OG	2:D:168:VAL:HG13	2.13	0.48
2:D:296:LEU:HD13	2:D:331:TRP:CD2	2.47	0.48
2:D:430:ILE:O	2:D:433:ILE:HB	2.13	0.48
2:D:444:GLU:HA	2:D:448:GLU:O	2.13	0.48
2:D:484:ARG:HB3	2:D:484:ARG:HH11	1.77	0.48
2:E:79:THR:HG23	2:E:82:ASP:H	1.78	0.48
2:E:301:PHE:HZ	2:E:409:THR:HG22	1.77	0.48
2:E:320:SER:HA	2:F:254:LEU:HG	1.95	0.48
2:E:371:LYS:O	2:E:372:PRO:O	2.30	0.48
2:E:418:GLN:CB	2:F:423:HIS:O	2.52	0.48
2:F:296:LEU:O	2:F:297:LEU:C	2.55	0.48
2:F:313:ILE:HG12	2:F:372:PRO:HG3	1.95	0.48
1:A:64:ILE:CG2	1:A:102:LYS:HB3	2.44	0.48
1:A:445:ILE:O	1:A:448:GLU:N	2.46	0.48
2:B:194:TYR:O	2:B:196:VAL:HG23	2.13	0.48
2:B:287:THR:OG1	2:B:425:ILE:HG22	2.13	0.48
2:C:406:GLU:O	2:C:408:ILE:HG13	2.13	0.48
2:D:21:MET:HE3	2:D:59:PHE:HZ	1.77	0.48
2:D:220:LEU:HD13	2:D:246:ILE:HD12	1.96	0.48
2:D:354:ALA:HB3	2:D:359:HIS:NE2	2.27	0.48
2:E:221:GLU:CG	2:E:222:ILE:H	2.26	0.48
2:F:293:GLY:O	2:F:294:LYS:C	2.55	0.48
2:F:486:PHE:HD2	2:F:494:PRO:HB2	1.77	0.48
1:A:21:MET:HE2	1:A:177:THR:HG21	1.94	0.48
1:A:390:ASN:OD1	2:F:386:GLY:HA2	2.14	0.48
2:B:150:VAL:CG1	2:B:151:PHE:N	2.76	0.48
2:B:419:PHE:CD2	2:C:425:ILE:HD12	2.49	0.48
2:C:340:ARG:C	2:C:342:ASN:N	2.71	0.48
2:D:472:ILE:N	2:D:472:ILE:HD12	2.28	0.48
3:D:901:ATP:O2'	2:E:463:HIS:NE2	2.44	0.48
1:A:118:VAL:HG23	1:A:118:VAL:O	2.14	0.48
1:A:218:ARG:O	1:A:236:PRO:HA	2.14	0.48
1:A:264:SER:CB	1:A:304:ASN:HD21	2.27	0.48
2:B:218:ARG:O	2:B:236:PRO:HA	2.14	0.48
2:B:283:ILE:HG12	2:B:400:THR:HG23	1.96	0.48
2:B:326:ARG:C	2:B:328:ALA:N	2.71	0.48
2:B:336:GLU:O	2:B:340:ARG:HG3	2.13	0.48
2:C:469:GLU:HB3	2:C:483:PHE:CE1	2.48	0.48
2:D:184:ARG:NH1	2:D:187:GLU:O	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:ILE:HD11	2:F:58:GLN:HG2	1.96	0.48
2:F:489:ILE:HA	2:F:494:PRO:HG3	1.95	0.48
1:A:31:ILE:HA	1:A:231:MET:SD	2.54	0.48
1:A:351:PRO:CG	1:A:382:ALA:O	2.61	0.48
1:A:429:HIS:HB3	5:F:524:HOH:O	2.13	0.48
2:B:88:ARG:HH12	2:B:93:ASP:HA	1.78	0.48
2:B:460:GLY:O	2:B:461:SER:O	2.31	0.48
2:B:492:GLY:C	2:B:494:PRO:HD3	2.38	0.48
2:C:43:LEU:HD12	2:C:180:MET:O	2.13	0.48
2:C:145:ASP:HA	2:C:181:THR:HB	1.95	0.48
2:C:418:GLN:HB2	2:D:423:HIS:O	2.14	0.48
2:D:203:ASN:HB3	2:D:225:LEU:HD22	1.95	0.48
2:E:318:GLU:CD	2:E:379:SER:HB2	2.37	0.48
2:E:451:ARG:NH1	2:E:472:ILE:CD1	2.77	0.48
1:A:270:LEU:O	1:A:273:MET:HB2	2.14	0.48
2:C:49:GLY:O	2:C:218:ARG:NH2	2.40	0.48
2:C:140:ARG:HH11	2:C:140:ARG:CB	2.26	0.48
2:C:263:VAL:HG12	2:C:374:ARG:NH2	2.28	0.48
2:C:285:LEU:HD23	2:C:434:THR:HG21	1.96	0.48
2:D:123:LEU:CD1	2:D:127:ILE:HD11	2.40	0.48
2:E:221:GLU:CB	5:E:530:HOH:O	2.62	0.48
2:E:497:ILE:O	2:E:498:THR:OG1	2.24	0.48
2:F:127:ILE:HD11	2:F:167:LEU:HA	1.95	0.48
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.14	0.48
1:A:425:ILE:HG21	1:A:439:LEU:HD22	1.96	0.48
2:B:193:ARG:HH11	2:B:193:ARG:CG	2.20	0.48
2:B:219:THR:OG1	2:B:234:GLU:OE2	2.29	0.48
2:B:453:ILE:HD13	2:B:453:ILE:C	2.39	0.48
2:C:219:THR:HG22	2:C:235:TYR:C	2.38	0.48
2:C:223:LEU:HD13	2:C:224:LYS:CB	2.39	0.48
2:D:306:CYS:SG	2:D:343:LEU:HB3	2.53	0.48
2:F:147:VAL:CG2	2:F:148:THR:N	2.77	0.48
2:F:311:ARG:HG3	2:F:371:LYS:HZ2	1.76	0.48
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.14	0.48
1:A:430:ILE:H	1:A:430:ILE:HD12	1.78	0.48
2:B:454:ASN:CB	2:B:467:ILE:HD13	2.41	0.48
2:C:75:THR:HG23	2:C:75:THR:O	2.14	0.48
2:C:294:LYS:CG	2:C:413:THR:HG23	2.38	0.48
2:D:18:ILE:HD13	2:D:228:THR:HG22	1.96	0.48
2:D:75:THR:OG1	2:D:78:GLU:O	2.29	0.48
2:E:291:GLY:CA	2:E:442:TYR:OH	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:294:LYS:HB2	3:F:901:ATP:O1B	2.14	0.48
2:F:347:VAL:O	2:F:348:CYS:CB	2.62	0.48
2:F:455:VAL:O	2:F:463:HIS:CE1	2.67	0.48
1:A:52:LYS:CD	1:A:182:THR:O	2.62	0.48
1:A:130:ILE:O	1:A:134:ILE:CD1	2.60	0.48
1:A:289:ALA:HB2	1:A:419:PHE:HA	1.96	0.48
1:A:488:ARG:NE	2:F:488:ARG:NH1	2.58	0.48
2:B:119:GLY:O	2:B:121:PHE:N	2.47	0.48
2:B:285:LEU:HD23	2:B:437:ILE:HD12	1.95	0.48
2:C:86:ASN:O	2:C:87:ALA:C	2.56	0.48
2:C:303:GLU:C	2:C:303:GLU:OE1	2.57	0.48
2:C:340:ARG:O	2:C:342:ASN:N	2.47	0.48
2:D:47:THR:O	2:D:50:THR:CG2	2.53	0.48
2:D:345:LYS:HZ3	2:D:366:GLU:CD	2.18	0.48
2:E:56:SER:HB2	2:E:143:SER:HB3	1.95	0.48
2:F:187:GLU:OE2	2:F:208:ARG:HA	2.13	0.48
2:F:471:MET:HE2	2:F:478:ASP:HB2	1.96	0.48
1:A:183:GLU:HB2	2:B:199:PHE:CZ	2.49	0.47
2:B:18:ILE:HB	2:B:228:THR:HG21	1.94	0.47
2:B:31:ILE:CG2	2:B:222:ILE:HD13	2.44	0.47
2:B:207:LEU:CD2	2:B:220:LEU:HD12	2.44	0.47
2:C:106:LEU:CD2	2:C:130:ILE:HG12	2.44	0.47
2:C:156:ALA:O	2:C:160:VAL:HG23	2.14	0.47
2:C:211:LEU:HD12	2:C:215:ARG:O	2.13	0.47
2:E:46:GLY:HA2	2:E:184:ARG:HD3	1.96	0.47
2:E:94:LEU:O	2:E:95:ALA:C	2.58	0.47
2:E:294:LYS:H	2:E:294:LYS:HD3	1.79	0.47
2:E:504:GLU:CG	2:E:505:LEU:H	2.21	0.47
2:F:185:ILE:HD13	2:F:185:ILE:N	2.29	0.47
2:F:211:LEU:O	2:F:212:GLU:CD	2.57	0.47
2:B:79:THR:OG1	2:B:81:GLN:HG2	2.14	0.47
2:B:90:PHE:HA	2:B:241:ASP:O	2.15	0.47
2:B:193:ARG:NH2	2:C:195:GLY:O	2.47	0.47
2:C:117:VAL:O	2:C:117:VAL:HG12	2.14	0.47
2:C:312:ALA:N	2:C:343:LEU:O	2.44	0.47
2:D:43:LEU:CD2	2:D:197:GLU:HB3	2.44	0.47
2:D:235:TYR:CD2	2:D:248:PRO:HA	2.49	0.47
2:D:273:MET:O	2:D:463:HIS:HA	2.14	0.47
2:D:313:ILE:HG12	2:D:345:LYS:HB3	1.96	0.47
2:E:41:SER:HA	2:E:178:THR:O	2.14	0.47
2:E:199:PHE:C	2:E:201:SER:H	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:470:PHE:HE1	2:E:472:ILE:CD1	2.26	0.47
2:F:332:GLY:O	2:F:333:MET:O	2.31	0.47
2:F:367:ILE:O	2:F:367:ILE:HG22	2.14	0.47
2:F:486:PHE:HE2	2:F:496:ARG:NH1	2.03	0.47
1:A:52:LYS:HE3	3:A:903:ATP:O1B	2.14	0.47
1:A:106:LEU:C	1:A:106:LEU:HD12	2.39	0.47
1:A:309:LYS:HA	1:A:343:LEU:HD13	1.96	0.47
1:A:344:LEU:HD11	1:A:346:ILE:HD11	1.96	0.47
2:B:150:VAL:O	2:B:153:GLN:HG3	2.14	0.47
2:C:381:SER:O	2:C:382:ALA:C	2.57	0.47
2:E:88:ARG:CG	2:E:88:ARG:HH11	2.27	0.47
2:F:382:ALA:O	2:F:385:ARG:HG3	2.15	0.47
1:A:150:VAL:HG13	1:A:151:PHE:CD2	2.49	0.47
1:A:254:LEU:HD13	2:F:350:TYR:CZ	2.50	0.47
1:A:319:GLU:OE1	1:A:327:ASN:ND2	2.47	0.47
2:B:370:PHE:C	2:B:372:PRO:HD3	2.40	0.47
2:D:287:THR:HG22	2:D:288:GLY:N	2.30	0.47
2:E:383:LEU:HD12	2:E:395:PHE:CE2	2.49	0.47
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.14	0.47
2:B:461:SER:OG	2:B:462:TRP:N	2.47	0.47
2:C:191:ILE:HD12	2:C:191:ILE:N	2.24	0.47
2:C:314:LEU:HB3	2:C:346:ILE:HD13	1.96	0.47
2:D:123:LEU:HG	2:D:163:GLU:OE2	2.14	0.47
2:D:237:PHE:CB	2:D:246:ILE:HD13	2.43	0.47
2:F:275:GLY:HA3	2:F:461:SER:OG	2.14	0.47
2:F:503:SER:O	2:F:504:GLU:C	2.57	0.47
1:A:428:SER:OG	1:A:430:ILE:HD11	2.15	0.47
1:A:485:ASN:HD22	1:A:498:THR:HG22	1.80	0.47
2:B:147:VAL:HG11	2:B:180:MET:HE2	1.95	0.47
2:B:204:VAL:HG12	2:B:206:ILE:HD11	1.96	0.47
2:D:31:ILE:HG23	2:D:231:MET:HB2	1.95	0.47
2:D:240:THR:O	2:D:243:GLY:N	2.44	0.47
2:D:313:ILE:CD1	2:D:372:PRO:HG3	2.44	0.47
2:D:388:SER:OG	2:D:391:ALA:HB2	2.14	0.47
2:D:445:ILE:HD11	2:D:483:PHE:HE2	1.79	0.47
2:E:356:LEU:CD1	2:E:356:LEU:H	2.27	0.47
2:F:378:ASP:O	2:F:379:SER:CB	2.63	0.47
1:A:98:VAL:CG2	1:A:105:ILE:HD13	2.44	0.47
1:A:162:ARG:HG3	1:A:162:ARG:NH1	2.28	0.47
1:A:193:ARG:HH21	2:B:199:PHE:HE2	1.62	0.47
1:A:354:ALA:HB1	1:A:358:ASP:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:THR:O	1:A:499:VAL:C	2.56	0.47
1:A:501:GLU:C	1:A:503:SER:H	2.22	0.47
2:B:286:ALA:HA	2:B:438:ILE:O	2.15	0.47
2:B:357:GLU:CG	2:B:358:ASP:H	2.28	0.47
2:B:471:MET:HB3	2:B:480:LYS:HZ1	1.79	0.47
2:C:311:ARG:HB3	2:C:370:PHE:CE2	2.50	0.47
2:C:326:ARG:C	2:C:328:ALA:N	2.70	0.47
2:D:43:LEU:HD21	2:D:197:GLU:HB2	1.96	0.47
2:D:82:ASP:O	2:D:85:LYS:N	2.48	0.47
2:D:121:PHE:N	2:D:121:PHE:CD1	2.82	0.47
2:D:126:LEU:O	2:D:126:LEU:HG	2.14	0.47
2:D:219:THR:HA	2:D:235:TYR:O	2.15	0.47
2:D:315:PHE:HD2	2:D:347:VAL:HG21	1.75	0.47
2:E:334:ASP:OD1	2:E:336:GLU:HB2	2.15	0.47
2:E:335:PHE:HA	2:E:338:MET:HG3	1.96	0.47
2:E:417:ASP:OD1	2:F:429:HIS:ND1	2.48	0.47
2:F:237:PHE:HE1	2:F:239:ILE:HG13	1.80	0.47
2:F:315:PHE:CD2	2:F:363:ILE:HG13	2.50	0.47
2:F:487:GLU:O	2:F:489:ILE:N	2.48	0.47
1:A:458:MET:HB2	1:A:463:HIS:CD2	2.44	0.47
2:D:43:LEU:HD21	2:D:197:GLU:HB3	1.95	0.47
2:D:211:LEU:O	2:D:215:ARG:O	2.33	0.47
2:E:248:PRO:O	2:E:249:LEU:C	2.56	0.47
2:E:269:ARG:HH22	2:E:468:ARG:NH2	2.13	0.47
2:F:18:ILE:HG21	2:F:37:PRO:HB3	1.97	0.47
2:F:300:ARG:HA	2:F:333:MET:HE1	1.97	0.47
2:F:379:SER:O	2:F:382:ALA:HB3	2.15	0.47
2:F:387:VAL:HG13	2:F:388:SER:N	2.29	0.47
1:A:123:LEU:C	1:A:123:LEU:HD13	2.40	0.47
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.96	0.47
2:B:72:VAL:HG21	2:B:134:ILE:HD13	1.97	0.47
2:C:257:ARG:HB3	2:C:407:GLU:OE1	2.15	0.47
2:C:315:PHE:HA	2:C:347:VAL:HB	1.97	0.47
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.96	0.47
2:E:202:ASP:HB2	2:E:203:ASN:ND2	2.29	0.47
2:E:268:VAL:HA	2:E:271:ASP:HB2	1.97	0.47
2:F:194:TYR:CD1	2:F:194:TYR:N	2.81	0.47
2:B:340:ARG:C	2:B:342:ASN:H	2.23	0.47
2:B:350:TYR:CZ	2:C:254:LEU:HD13	2.50	0.47
2:C:60:LEU:CD1	2:C:73:PHE:HB2	2.45	0.47
2:C:90:PHE:N	2:C:90:PHE:CD1	2.83	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.45	0.47
2:C:483:PHE:N	2:C:483:PHE:CD1	2.83	0.47
2:D:98:VAL:HA	2:D:103:LEU:O	2.14	0.47
2:D:182:THR:CG2	2:D:183:GLU:N	2.76	0.47
2:E:427:ASP:O	2:E:428:SER:HB3	2.15	0.47
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.97	0.46
1:A:347:VAL:HG21	1:A:366:GLU:HG2	1.97	0.46
2:C:60:LEU:O	2:C:61:TYR:C	2.56	0.46
2:C:111:ASP:C	2:C:113:GLU:H	2.23	0.46
2:C:411:LEU:HD12	2:C:412:PHE:H	1.80	0.46
2:C:426:THR:HG22	2:C:427:ASP:H	1.79	0.46
2:D:319:GLU:HG2	2:E:459:ARG:NH1	2.30	0.46
2:E:294:LYS:N	3:E:901:ATP:O1B	2.48	0.46
2:E:304:ASN:HB3	2:E:374:ARG:HH12	1.79	0.46
2:E:315:PHE:CE2	2:E:363:ILE:HG13	2.50	0.46
2:F:268:VAL:O	2:F:271:ASP:HB2	2.15	0.46
2:F:387:VAL:CG1	2:F:388:SER:N	2.78	0.46
2:F:466:ALA:C	2:F:467:ILE:HD13	2.41	0.46
2:F:472:ILE:HD12	3:F:901:ATP:C1'	2.45	0.46
1:A:214:GLU:HB3	2:B:234:GLU:HB2	1.97	0.46
1:A:392:PHE:O	1:A:393:ARG:C	2.58	0.46
2:B:64:ILE:HD11	2:B:70:PRO:CA	2.44	0.46
2:C:350:TYR:CZ	2:D:252:MET:HE3	2.51	0.46
2:D:18:ILE:HD13	2:D:228:THR:HG23	1.97	0.46
2:D:154:TYR:O	2:D:154:TYR:CD1	2.68	0.46
2:E:118:VAL:HG12	2:E:122:ASP:OD2	2.15	0.46
2:E:132:TYR:C	2:E:132:TYR:CD2	2.93	0.46
2:F:31:ILE:O	2:F:230:HIS:HB2	2.16	0.46
2:F:118:VAL:O	2:F:118:VAL:HG13	2.15	0.46
2:F:209:ASN:HD21	2:F:216:ARG:HD2	1.80	0.46
2:F:218:ARG:HG3	2:F:237:PHE:O	2.14	0.46
2:F:344:LEU:CD1	2:F:346:ILE:HG13	2.44	0.46
2:F:516:GLY:N	2:F:517:PRO:CD	2.77	0.46
1:A:234:GLU:C	1:A:235:TYR:CD1	2.93	0.46
2:B:52:LYS:HB2	3:B:903:ATP:O1B	2.14	0.46
2:C:51:GLY:O	2:C:54:LEU:HB3	2.16	0.46
2:C:68:ASP:OD1	2:C:68:ASP:O	2.33	0.46
2:C:82:ASP:C	2:C:84:ILE:N	2.72	0.46
2:D:90:PHE:CD1	2:D:90:PHE:N	2.82	0.46
2:D:293:GLY:HA2	3:D:901:ATP:O1A	2.15	0.46
2:D:390:ASN:O	2:D:391:ALA:C	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:393:ARG:NH2	5:D:537:HOH:O	2.47	0.46
2:D:437:ILE:HD12	2:D:457:LYS:HG2	1.97	0.46
2:E:211:LEU:HG	2:E:212:GLU:N	2.30	0.46
2:E:441:GLN:HE22	2:E:490:ILE:HD13	1.80	0.46
2:F:97:LEU:C	2:F:99:ASP:N	2.67	0.46
1:A:154:TYR:O	1:A:154:TYR:HD1	1.98	0.46
1:A:451:ARG:NH2	3:A:901:ATP:O2'	2.48	0.46
1:A:488:ARG:CD	2:F:488:ARG:HH12	2.29	0.46
2:B:383:LEU:C	2:B:385:ARG:H	2.22	0.46
2:B:436:THR:HA	2:B:457:LYS:O	2.15	0.46
2:D:247:PHE:CD1	2:D:247:PHE:N	2.83	0.46
2:D:412:PHE:N	2:D:412:PHE:CD1	2.83	0.46
2:E:471:MET:HE1	2:E:473:SER:CB	2.44	0.46
2:F:21:MET:CE	2:F:177:THR:CB	2.93	0.46
2:F:344:LEU:HD11	2:F:346:ILE:CG1	2.46	0.46
2:F:426:THR:HB	2:F:429:HIS:H	1.80	0.46
1:A:158:SER:O	1:A:159:VAL:C	2.59	0.46
1:A:489:ILE:C	1:A:491:SER:H	2.23	0.46
2:B:245:ASN:ND2	2:B:247:PHE:CZ	2.84	0.46
2:B:280:LYS:O	2:B:409:THR:OG1	2.25	0.46
2:B:469:GLU:HG2	2:B:481:ASP:O	2.16	0.46
2:C:260:ASN:O	2:C:261:VAL:O	2.33	0.46
2:C:313:ILE:HD11	2:C:370:PHE:CB	2.43	0.46
2:C:396:VAL:HG21	2:C:430:ILE:HD12	1.96	0.46
2:C:438:ILE:HD12	2:C:438:ILE:H	1.80	0.46
2:D:134:ILE:HD11	2:D:142:VAL:CG2	2.46	0.46
2:E:160:VAL:HG11	2:E:194:TYR:CD1	2.49	0.46
2:E:186:GLU:OE2	2:E:187:GLU:N	2.48	0.46
2:E:197:GLU:C	2:E:199:PHE:N	2.73	0.46
2:E:311:ARG:HD3	2:E:370:PHE:CE1	2.50	0.46
2:E:358:ASP:O	2:E:362:ILE:HG12	2.15	0.46
2:F:76:PHE:O	2:F:109:SER:HA	2.16	0.46
2:F:97:LEU:C	2:F:99:ASP:H	2.23	0.46
2:F:453:ILE:HG12	2:F:454:ASN:N	2.31	0.46
2:F:514:GLU:O	2:F:515:LYS:HB2	2.14	0.46
1:A:227:GLY:O	2:F:89:SER:CB	2.59	0.46
1:A:266:GLY:C	1:A:300:ARG:HG3	2.41	0.46
1:A:395:PHE:CE2	1:A:399:VAL:HG21	2.51	0.46
2:B:160:VAL:HG21	2:B:194:TYR:CE1	2.50	0.46
2:C:28:PHE:CA	2:C:246:ILE:HD12	2.46	0.46
2:C:146:SER:C	2:C:148:THR:N	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:183:GLU:HB2	2:D:199:PHE:CZ	2.50	0.46
2:C:420:MET:HE3	2:C:492:GLY:O	2.15	0.46
2:D:454:ASN:HB2	2:D:467:ILE:HA	1.97	0.46
2:E:145:ASP:C	2:E:146:SER:HG	2.20	0.46
2:E:164:LEU:HD11	2:E:197:GLU:CG	2.23	0.46
2:E:221:GLU:O	2:E:222:ILE:HD13	2.15	0.46
2:E:468:ARG:HG2	2:E:468:ARG:HH11	1.79	0.46
2:F:163:GLU:HA	2:F:163:GLU:OE2	2.16	0.46
2:F:418:GLN:HG3	2:F:418:GLN:O	2.16	0.46
2:F:426:THR:HB	2:F:429:HIS:HA	1.97	0.46
2:F:431:ALA:HA	2:F:434:THR:CG2	2.46	0.46
1:A:24:MET:HA	1:A:24:MET:HE3	1.97	0.46
2:B:37:PRO:HD2	2:B:203:ASN:ND2	2.31	0.46
2:B:287:THR:HB	2:B:425:ILE:CG2	2.46	0.46
2:B:333:MET:HE3	2:B:333:MET:HB3	1.73	0.46
2:C:52:LYS:N	3:C:903:ATP:O1B	2.48	0.46
2:C:295:THR:HG22	2:C:331:TRP:CZ3	2.51	0.46
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.56	0.46
2:C:311:ARG:HD2	2:C:371:LYS:HE3	1.98	0.46
2:D:191:ILE:HB	2:D:198:GLU:CD	2.40	0.46
2:D:291:GLY:C	2:D:293:GLY:N	2.73	0.46
2:E:470:PHE:CD1	2:E:470:PHE:C	2.94	0.46
1:A:189:GLY:O	1:A:190:PRO:C	2.59	0.46
1:A:200:VAL:O	1:A:200:VAL:HG12	2.15	0.46
1:A:298:VAL:O	1:A:301:PHE:HB3	2.16	0.46
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.46	0.46
2:B:196:VAL:C	2:B:198:GLU:N	2.72	0.46
2:B:326:ARG:HD3	2:C:259:SER:O	2.16	0.46
2:C:193:ARG:HH21	2:D:199:PHE:HE2	1.62	0.46
2:D:363:ILE:O	2:D:367:ILE:HD13	2.16	0.46
2:E:265:SER:CB	2:E:278:PHE:CZ	2.99	0.46
2:E:419:PHE:O	2:E:420:MET:O	2.33	0.46
2:F:396:VAL:HG11	2:F:430:ILE:CG2	2.45	0.46
1:A:211:LEU:HD12	1:A:212:GLU:H	1.81	0.46
1:A:489:ILE:O	1:A:491:SER:N	2.48	0.46
2:B:52:LYS:HE3	3:B:903:ATP:PB	2.56	0.46
2:B:245:ASN:ND2	2:B:247:PHE:CE1	2.84	0.46
2:C:80:PRO:O	2:C:84:ILE:HG12	2.16	0.46
2:C:326:ARG:O	2:C:329:TYR:N	2.49	0.46
2:D:484:ARG:CB	2:D:484:ARG:NH1	2.79	0.46
2:E:31:ILE:HA	2:E:231:MET:CG	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:LYS:HZ3	2:E:366:GLU:HG3	1.78	0.46
2:E:360:LEU:HD13	2:E:360:LEU:C	2.40	0.46
2:E:418:GLN:HG3	2:E:418:GLN:O	2.15	0.46
2:F:79:THR:O	2:F:79:THR:CG2	2.64	0.46
2:F:273:MET:O	2:F:463:HIS:HB2	2.16	0.46
2:F:431:ALA:C	2:F:434:THR:HG22	2.41	0.46
2:F:445:ILE:HG12	2:F:483:PHE:HE2	1.81	0.46
2:F:484:ARG:NH1	2:F:484:ARG:CB	2.78	0.46
1:A:35:GLY:O	1:A:36:LEU:C	2.59	0.46
1:A:375:ILE:HB	1:A:408:ILE:HG21	1.98	0.46
1:A:379:SER:O	1:A:382:ALA:HB3	2.15	0.46
1:A:441:GLN:HE22	1:A:490:ILE:CD1	2.26	0.46
1:A:457:LYS:HB3	2:F:291:GLY:HA3	1.97	0.46
2:B:497:ILE:C	2:B:499:VAL:N	2.74	0.46
2:C:163:GLU:OE2	2:C:163:GLU:HA	2.16	0.46
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.81	0.46
2:D:462:TRP:CE3	2:D:463:HIS:N	2.84	0.46
2:D:470:PHE:CE1	2:D:472:ILE:HD11	2.51	0.46
2:E:197:GLU:C	2:E:199:PHE:H	2.24	0.46
2:E:203:ASN:HB3	2:E:225:LEU:HD22	1.98	0.46
2:E:262:ARG:HH12	2:E:461:SER:HB2	1.81	0.46
2:E:291:GLY:C	2:E:442:TYR:OH	2.60	0.46
2:E:441:GLN:HG3	2:E:452:ALA:HB3	1.97	0.46
2:F:240:THR:C	2:F:242:HIS:H	2.23	0.46
2:F:468:ARG:NH1	2:F:468:ARG:HG2	2.30	0.46
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.30	0.45
1:A:435:ASP:OD1	2:F:323:GLN:NE2	2.46	0.45
2:B:479:ILE:HD12	2:B:479:ILE:N	2.31	0.45
2:B:486:PHE:CE2	2:B:496:ARG:HB2	2.51	0.45
2:C:110:PRO:HB2	2:D:165:PHE:HE2	1.81	0.45
2:C:451:ARG:NH1	2:C:472:ILE:HD12	2.31	0.45
2:D:88:ARG:NE	2:E:15:HIS:HA	2.31	0.45
2:D:291:GLY:N	3:D:901:ATP:O1G	2.49	0.45
2:D:384:ALA:HB2	2:D:392:PHE:CE2	2.51	0.45
2:E:22:ARG:HE	2:E:22:ARG:HB3	1.29	0.45
2:E:74:VAL:HG12	2:E:76:PHE:CE1	2.51	0.45
2:E:313:ILE:CD1	2:E:372:PRO:HG2	2.46	0.45
2:F:240:THR:C	2:F:242:HIS:N	2.72	0.45
2:F:504:GLU:HA	2:F:507:ARG:HE	1.81	0.45
1:A:490:ILE:HG13	2:F:420:MET:HE1	1.97	0.45
2:C:197:GLU:OE2	2:C:197:GLU:N	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:312:ALA:O	2:C:344:LEU:HA	2.16	0.45
2:D:284:ILE:HD12	2:D:410:GLY:O	2.16	0.45
2:E:386:GLY:O	2:E:387:VAL:O	2.33	0.45
2:F:462:TRP:O	2:F:463:HIS:O	2.34	0.45
2:F:488:ARG:O	2:F:491:SER:OG	2.34	0.45
1:A:69:GLU:HB3	1:A:140:ARG:HB2	1.99	0.45
1:A:89:SER:CB	2:B:227:GLY:O	2.64	0.45
2:B:54:LEU:CD2	2:B:244:ILE:HG13	2.47	0.45
2:B:294:LYS:CB	2:B:413:THR:HG23	2.44	0.45
2:B:497:ILE:O	2:B:498:THR:C	2.60	0.45
2:C:63:GLY:CA	2:C:141:ARG:NH1	2.80	0.45
2:C:88:ARG:HG2	2:C:88:ARG:HH11	1.81	0.45
2:C:221:GLU:CD	2:C:233:GLY:O	2.60	0.45
2:C:248:PRO:C	2:C:250:GLY:N	2.71	0.45
2:C:326:ARG:O	2:C:328:ALA:N	2.49	0.45
2:D:38:ILE:HA	2:D:177:THR:HG21	1.98	0.45
2:E:483:PHE:O	2:E:485:ASN:N	2.49	0.45
1:A:153:GLN:O	1:A:154:TYR:HB3	2.17	0.45
1:A:215:ARG:NH2	2:B:234:GLU:O	2.50	0.45
1:A:395:PHE:C	1:A:395:PHE:CD2	2.94	0.45
2:B:88:ARG:HG2	2:B:88:ARG:NH1	2.32	0.45
2:B:88:ARG:HH12	2:B:93:ASP:CB	2.29	0.45
2:B:283:ILE:C	2:B:284:ILE:HD13	2.42	0.45
2:B:334:ASP:OD1	2:B:336:GLU:HB2	2.17	0.45
2:C:44:VAL:O	2:C:44:VAL:HG12	2.15	0.45
2:C:303:GLU:OE1	2:C:304:ASN:N	2.49	0.45
2:C:317:TYR:CE1	2:C:377:ILE:HG23	2.51	0.45
2:C:335:PHE:HA	2:C:338:MET:CG	2.47	0.45
2:D:57:ILE:HG12	2:D:73:PHE:CE1	2.52	0.45
2:D:324:LEU:C	2:D:326:ARG:H	2.24	0.45
2:E:132:TYR:C	2:E:132:TYR:HD2	2.25	0.45
2:E:350:TYR:CE1	2:F:254:LEU:HD13	2.51	0.45
2:F:237:PHE:CD1	2:F:237:PHE:C	2.94	0.45
1:A:230:HIS:CE1	1:A:232:LYS:HG3	2.52	0.45
1:A:254:LEU:HG	2:F:320:SER:HA	1.99	0.45
2:B:214:GLU:OE1	2:C:217:ARG:NH1	2.49	0.45
2:B:227:GLY:O	2:B:228:THR:HG23	2.16	0.45
2:B:285:LEU:HD12	2:B:412:PHE:O	2.17	0.45
2:C:123:LEU:HD11	2:C:163:GLU:HA	1.97	0.45
2:D:497:ILE:HG13	2:D:497:ILE:O	2.17	0.45
2:E:36:LEU:HD23	2:E:36:LEU:HA	1.71	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:280:LYS:HE2	2:E:407:GLU:HB3	1.97	0.45
2:E:287:THR:CG2	2:E:288:GLY:N	2.79	0.45
2:E:313:ILE:CG1	2:E:372:PRO:CG	2.87	0.45
2:F:197:GLU:H	2:F:197:GLU:CD	2.23	0.45
2:B:25:ILE:HG23	2:B:58:GLN:HE22	1.81	0.45
2:B:273:MET:O	2:B:464:ASP:N	2.48	0.45
2:C:191:ILE:H	2:C:191:ILE:CD1	2.25	0.45
2:C:287:THR:CG2	2:C:414:ASN:HB3	2.45	0.45
2:D:164:LEU:HD11	2:D:197:GLU:HG3	1.97	0.45
2:D:286:ALA:O	2:D:294:LYS:CG	2.63	0.45
2:D:306:CYS:SG	2:D:343:LEU:CB	3.05	0.45
2:D:491:SER:C	2:D:493:SER:H	2.24	0.45
2:E:492:GLY:C	2:E:494:PRO:HD3	2.41	0.45
2:F:84:ILE:HD11	2:F:98:VAL:HG21	1.98	0.45
2:F:273:MET:SD	2:F:468:ARG:HD2	2.55	0.45
2:F:509:VAL:HG12	2:F:510:ARG:N	2.26	0.45
2:F:515:LYS:CB	2:F:517:PRO:HD2	2.47	0.45
1:A:123:LEU:O	1:A:123:LEU:HD13	2.16	0.45
1:A:383:LEU:C	1:A:385:ARG:N	2.74	0.45
1:A:489:ILE:C	1:A:491:SER:N	2.75	0.45
2:B:156:ALA:O	2:B:157:SER:C	2.59	0.45
2:B:166:ARG:O	2:B:170:ARG:HG2	2.16	0.45
2:B:296:LEU:HD21	2:B:477:PRO:CD	2.45	0.45
2:B:356:LEU:CD2	2:B:392:PHE:HA	2.46	0.45
2:C:103:LEU:HD12	2:C:104:PHE:N	2.30	0.45
2:C:150:VAL:CG1	2:C:151:PHE:N	2.79	0.45
2:C:439:LEU:C	2:C:440:LEU:HD23	2.41	0.45
2:D:488:ARG:HB3	2:D:491:SER:HB3	1.97	0.45
2:F:508:ILE:O	2:F:508:ILE:HG22	2.17	0.45
2:B:45:SER:OG	2:B:184:ARG:HD2	2.17	0.45
2:B:244:ILE:HG22	2:B:245:ASN:N	2.32	0.45
2:B:437:ILE:O	2:B:437:ILE:HG22	2.17	0.45
2:C:164:LEU:HB3	2:C:200:VAL:HG11	1.98	0.45
2:C:471:MET:H	2:C:471:MET:HG3	1.56	0.45
2:D:79:THR:O	2:D:80:PRO:C	2.58	0.45
2:D:316:ALA:HB3	2:D:348:CYS:SG	2.57	0.45
2:D:473:SER:O	2:D:476:GLY:N	2.50	0.45
2:E:197:GLU:O	2:E:199:PHE:N	2.49	0.45
2:E:451:ARG:NH1	2:E:451:ARG:CG	2.79	0.45
2:F:36:LEU:HA	2:F:37:PRO:HD3	1.81	0.45
2:F:312:ALA:HA	2:F:374:ARG:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:451:ARG:HD2	2:F:451:ARG:N	2.32	0.45
1:A:471:MET:HG2	1:A:478:ASP:HB3	1.95	0.45
2:B:200:VAL:O	2:B:200:VAL:HG12	2.17	0.45
2:B:319:GLU:HG3	5:B:521:HOH:O	2.17	0.45
2:C:144:ILE:HG22	2:C:147:VAL:HG12	1.98	0.45
2:C:281:ASP:O	2:C:282:SER:HB3	2.15	0.45
2:C:296:LEU:O	2:C:299:SER:HB2	2.17	0.45
2:D:72:VAL:HB	2:D:142:VAL:HG22	1.98	0.45
2:D:433:ILE:HD12	2:D:433:ILE:N	2.32	0.45
2:E:171:LEU:O	2:E:174:ILE:N	2.49	0.45
2:E:264:SER:O	2:E:374:ARG:NH2	2.50	0.45
2:E:318:GLU:OE2	2:E:379:SER:CB	2.61	0.45
2:F:64:ILE:HD12	2:F:102:LYS:HB3	1.99	0.45
2:F:504:GLU:HA	2:F:507:ARG:HG3	1.99	0.45
2:F:504:GLU:HB2	2:F:505:LEU:H	1.46	0.45
1:A:23:THR:O	1:A:25:ILE:HD12	2.17	0.45
1:A:165:PHE:O	1:A:166:ARG:C	2.60	0.45
1:A:211:LEU:HD21	2:B:188:TYR:HE2	1.81	0.45
1:A:371:LYS:HD2	1:A:371:LYS:C	2.42	0.45
2:B:147:VAL:CG2	2:B:148:THR:N	2.80	0.45
2:B:216:ARG:CG	2:C:233:GLY:HA2	2.41	0.45
2:C:54:LEU:CD1	2:C:90:PHE:CZ	2.98	0.45
2:C:435:ASP:HA	2:C:459:ARG:HD2	1.99	0.45
2:D:284:ILE:HA	2:D:436:THR:O	2.17	0.45
2:E:107:ASP:C	2:E:107:ASP:OD1	2.59	0.45
2:E:111:ASP:C	2:E:113:GLU:H	2.25	0.45
2:F:283:ILE:HG13	2:F:400:THR:HG23	1.99	0.45
2:F:380:LEU:O	2:F:383:LEU:N	2.46	0.45
1:A:265:SER:O	1:A:300:ARG:O	2.35	0.44
1:A:509:VAL:O	1:A:511:GLY:N	2.50	0.44
2:B:54:LEU:O	2:B:55:PHE:C	2.59	0.44
2:B:90:PHE:HB2	2:B:92:TRP:CE2	2.52	0.44
2:B:147:VAL:HG11	2:B:180:MET:CE	2.47	0.44
2:B:252:MET:HE1	2:B:401:GLY:HA3	1.98	0.44
2:B:334:ASP:O	2:B:338:MET:HG2	2.17	0.44
2:B:463:HIS:HD1	2:B:463:HIS:C	2.25	0.44
2:C:90:PHE:HB2	2:C:92:TRP:CE2	2.51	0.44
2:C:123:LEU:HA	2:C:127:ILE:CD1	2.47	0.44
2:C:134:ILE:CG2	2:C:139:ALA:HB3	2.30	0.44
2:C:174:ILE:HG22	2:C:174:ILE:O	2.17	0.44
2:D:430:ILE:CA	2:D:433:ILE:HD13	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:87:ALA:C	2:E:89:SER:N	2.74	0.44
2:E:338:MET:HB3	2:E:344:LEU:HB2	1.99	0.44
2:F:142:VAL:HB	2:F:178:THR:HG22	1.94	0.44
2:F:272:GLU:C	2:F:274:CYS:N	2.75	0.44
1:A:451:ARG:NH1	1:A:472:ILE:CD1	2.78	0.44
2:B:324:LEU:HD23	2:B:324:LEU:HA	1.81	0.44
2:C:64:ILE:CG2	2:C:102:LYS:HB3	2.47	0.44
2:C:217:ARG:O	2:C:217:ARG:CG	2.65	0.44
2:C:389:ASN:O	2:C:392:PHE:N	2.50	0.44
2:E:96:LYS:O	2:E:99:ASP:N	2.50	0.44
2:E:160:VAL:O	2:E:161:ARG:C	2.60	0.44
2:E:323:GLN:HG2	2:E:327:ASN:ND2	2.32	0.44
1:A:219:THR:HA	1:A:235:TYR:O	2.17	0.44
2:B:64:ILE:HG22	2:B:65:ILE:HD13	1.99	0.44
2:C:124:SER:O	2:C:128:GLU:HG2	2.17	0.44
2:D:164:LEU:HB3	2:D:200:VAL:HG11	1.99	0.44
2:E:264:SER:CB	2:E:304:ASN:HD21	2.30	0.44
2:F:165:PHE:O	2:F:166:ARG:C	2.57	0.44
2:F:286:ALA:HA	2:F:438:ILE:O	2.18	0.44
2:F:298:VAL:HA	2:F:411:LEU:CD2	2.47	0.44
2:F:321:ARG:HG2	2:F:348:CYS:HB3	1.99	0.44
1:A:31:ILE:CG2	1:A:231:MET:HB2	2.47	0.44
1:A:69:GLU:O	1:A:70:PRO:C	2.59	0.44
2:B:240:THR:HG21	2:B:361:GLN:HE22	1.82	0.44
2:B:296:LEU:O	2:B:299:SER:N	2.50	0.44
2:D:222:ILE:O	2:D:222:ILE:HG22	2.17	0.44
2:E:79:THR:O	2:E:80:PRO:C	2.59	0.44
2:E:356:LEU:HD21	2:E:392:PHE:HA	1.98	0.44
2:E:359:HIS:C	2:E:363:ILE:HD13	2.42	0.44
2:E:451:ARG:HG2	2:E:451:ARG:NH1	2.30	0.44
2:F:203:ASN:CB	2:F:225:LEU:HD23	2.47	0.44
2:F:213:GLY:C	2:F:215:ARG:N	2.74	0.44
2:F:517:PRO:HG2	2:F:518:GLU:H	1.82	0.44
1:A:222:ILE:O	1:A:222:ILE:HG22	2.18	0.44
2:B:21:MET:CG	2:B:141:ARG:HH21	2.31	0.44
2:B:161:ARG:NH2	2:B:199:PHE:HB2	2.32	0.44
2:C:50:THR:HG21	2:C:207:LEU:O	2.16	0.44
2:C:332:GLY:O	2:C:333:MET:C	2.61	0.44
2:C:396:VAL:O	2:C:397:ILE:C	2.58	0.44
2:D:288:GLY:O	2:D:415:THR:HA	2.17	0.44
2:D:446:ARG:H	2:D:496:ARG:NH1	2.06	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:903:ATP:O3'	2:E:224:LYS:HB2	2.17	0.44
2:E:24:MET:HA	2:E:24:MET:HE3	2.00	0.44
2:E:81:GLN:CD	2:E:81:GLN:N	2.73	0.44
2:E:118:VAL:HG12	2:E:118:VAL:O	2.18	0.44
2:E:451:ARG:HD3	2:E:472:ILE:CD1	2.48	0.44
3:E:903:ATP:O2'	2:F:230:HIS:NE2	2.48	0.44
2:F:31:ILE:HG23	2:F:231:MET:HB2	1.99	0.44
2:F:170:ARG:HB3	2:F:170:ARG:CZ	2.47	0.44
2:F:356:LEU:O	2:F:357:GLU:C	2.60	0.44
1:A:104:PHE:CD2	1:A:133:ALA:HB1	2.53	0.44
1:A:111:ASP:C	1:A:113:GLU:N	2.76	0.44
1:A:134:ILE:HG23	1:A:139:ALA:HB3	1.98	0.44
1:A:414:ASN:HD21	1:A:426:TPO:HA	1.79	0.44
1:A:425:ILE:O	1:A:426:TPO:HG22	2.18	0.44
2:B:146:SER:O	2:B:147:VAL:C	2.60	0.44
2:B:173:GLN:O	2:B:174:ILE:C	2.60	0.44
2:B:396:VAL:HG21	2:B:430:ILE:HD12	2.00	0.44
2:C:295:THR:HG22	2:C:296:LEU:N	2.32	0.44
2:D:388:SER:OG	2:D:391:ALA:CB	2.66	0.44
2:D:473:SER:O	2:D:474:ASP:C	2.60	0.44
2:E:85:LYS:O	2:E:88:ARG:N	2.48	0.44
2:E:356:LEU:HD12	2:E:356:LEU:N	2.32	0.44
2:F:25:ILE:HG23	2:F:58:GLN:NE2	2.32	0.44
2:F:218:ARG:HE	2:F:218:ARG:HB3	1.55	0.44
2:F:489:ILE:O	2:F:490:ILE:C	2.60	0.44
1:A:51:GLY:HA3	1:A:207:LEU:CD1	2.42	0.44
1:A:284:ILE:HB	1:A:411:LEU:HD12	2.00	0.44
2:B:64:ILE:C	2:B:66:GLU:H	2.25	0.44
2:B:323:GLN:HA	2:C:258:SER:OG	2.18	0.44
2:C:260:ASN:C	2:C:261:VAL:O	2.60	0.44
2:D:89:SER:CB	2:E:227:GLY:O	2.65	0.44
2:F:73:PHE:HE2	2:F:83:ILE:HG12	1.83	0.44
2:F:344:LEU:HD22	2:F:345:LYS:H	1.81	0.44
2:F:379:SER:HA	2:F:413:THR:O	2.18	0.44
2:F:470:PHE:CD1	2:F:470:PHE:C	2.95	0.44
2:F:501:GLU:HG3	2:F:502:LYS:N	2.32	0.44
1:A:136:LYS:HD3	1:A:137:TYR:CE1	2.53	0.44
1:A:508:ILE:HD12	1:A:508:ILE:C	2.43	0.44
2:B:53:THR:O	2:B:57:ILE:HG12	2.17	0.44
2:B:428:SER:O	2:B:429:HIS:HB2	2.17	0.44
2:B:451:ARG:HH11	2:B:451:ARG:CG	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:235:TYR:HD2	2:D:248:PRO:HA	1.83	0.44
2:D:340:ARG:C	2:D:342:ASN:N	2.76	0.44
2:E:47:THR:HG23	5:E:525:HOH:O	2.18	0.44
2:E:94:LEU:HB3	2:E:103:LEU:HD21	1.99	0.44
2:F:256:GLN:H	2:F:256:GLN:HG2	1.50	0.44
1:A:65:ILE:O	1:A:65:ILE:CG2	2.60	0.44
1:A:191:ILE:HB	1:A:198:GLU:CG	2.48	0.44
1:A:463:HIS:CE1	1:A:465:LYS:NZ	2.86	0.44
2:C:48:SER:O	2:D:223:LEU:HD21	2.18	0.44
2:C:425:ILE:HD12	2:C:425:ILE:H	1.83	0.44
2:D:99:ASP:C	2:D:101:GLY:N	2.76	0.44
2:D:222:ILE:CG2	2:D:230:HIS:CD2	3.00	0.44
2:D:338:MET:HE2	2:D:338:MET:CA	2.46	0.44
2:E:24:MET:HB2	2:E:62:ASN:HB3	2.00	0.44
2:E:60:LEU:HD12	2:E:73:PHE:HD1	1.82	0.44
2:E:96:LYS:C	2:E:98:VAL:N	2.74	0.44
2:E:123:LEU:HD23	2:E:123:LEU:C	2.43	0.44
2:E:125:ALA:O	2:E:129:ARG:HG3	2.18	0.44
2:E:335:PHE:O	2:E:338:MET:N	2.51	0.44
2:E:357:GLU:HG3	2:E:358:ASP:N	2.33	0.44
2:F:264:SER:OG	2:F:265:SER:N	2.51	0.44
2:F:445:ILE:O	2:F:446:ARG:HB2	2.17	0.44
2:F:472:ILE:HD12	3:F:901:ATP:O4'	2.18	0.44
1:A:64:ILE:HD12	1:A:102:LYS:O	2.17	0.43
1:A:157:SER:OG	1:A:158:SER:N	2.51	0.43
1:A:439:LEU:HD12	1:A:440:LEU:N	2.33	0.43
2:B:145:ASP:O	2:B:146:SER:OG	2.31	0.43
2:B:313:ILE:HG22	2:B:314:LEU:N	2.33	0.43
2:C:116:GLU:O	2:C:117:VAL:HB	2.17	0.43
2:C:151:PHE:C	2:C:153:GLN:H	2.26	0.43
2:C:386:GLY:HA2	2:D:390:ASN:OD1	2.18	0.43
2:C:435:ASP:O	2:C:457:LYS:HE3	2.17	0.43
2:D:323:GLN:HE21	2:D:327:ASN:HD21	1.64	0.43
2:E:378:ASP:O	2:E:379:SER:CB	2.66	0.43
2:F:25:ILE:O	2:F:27:GLY:N	2.51	0.43
2:F:443:VAL:C	2:F:445:ILE:HD12	2.43	0.43
1:A:335:PHE:O	1:A:338:MET:N	2.51	0.43
1:A:357:GLU:HG3	1:A:358:ASP:N	2.33	0.43
1:A:437:ILE:HB	1:A:456:PHE:HB3	1.99	0.43
1:A:518:GLU:HB2	1:A:519:SER:H	1.48	0.43
2:B:157:SER:OG	2:B:158:SER:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:GLY:HA2	2:B:198:GLU:CD	2.42	0.43
2:B:295:THR:HG21	2:B:319:GLU:OE2	2.18	0.43
2:B:304:ASN:HB3	2:B:374:ARG:NH1	2.32	0.43
2:C:45:SER:HA	2:C:182:THR:O	2.18	0.43
2:C:320:SER:HB3	2:D:256:GLN:HG2	2.01	0.43
2:C:387:VAL:HG12	2:C:391:ALA:HB3	1.99	0.43
2:D:200:VAL:O	2:D:200:VAL:HG12	2.18	0.43
2:D:408:ILE:HG22	2:D:409:THR:N	2.33	0.43
2:E:52:LYS:HB3	2:E:181:THR:HG23	1.99	0.43
2:E:153:GLN:C	2:F:158:SER:HB2	2.42	0.43
2:E:443:VAL:HB	2:E:445:ILE:CD1	2.48	0.43
2:F:21:MET:CE	2:F:59:PHE:CZ	2.84	0.43
1:A:44:VAL:O	1:A:181:THR:HA	2.18	0.43
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.44	0.43
1:A:267:VAL:HG11	1:A:270:LEU:HB2	1.99	0.43
1:A:368:ASN:C	1:A:370:PHE:H	2.25	0.43
1:A:461:SER:OG	1:A:462:TRP:N	2.51	0.43
2:B:21:MET:HG2	2:B:141:ARG:HH21	1.82	0.43
2:B:84:ILE:O	2:B:85:LYS:C	2.62	0.43
2:B:451:ARG:HG2	2:B:451:ARG:NH1	2.27	0.43
2:C:182:THR:CG2	2:C:183:GLU:H	2.31	0.43
2:D:105:ILE:N	2:D:105:ILE:HD12	2.34	0.43
2:D:238:THR:HG23	2:D:358:ASP:OD1	2.17	0.43
2:E:18:ILE:HD11	2:E:228:THR:N	2.27	0.43
2:E:303:GLU:O	2:E:304:ASN:C	2.61	0.43
2:E:313:ILE:HG22	2:E:314:LEU:N	2.32	0.43
2:E:363:ILE:N	2:E:363:ILE:HD12	2.33	0.43
2:F:23:THR:OG1	2:F:29:ASP:OD1	2.32	0.43
1:A:419:PHE:O	1:A:420:MET:O	2.36	0.43
1:A:504:GLU:C	1:A:506:SER:N	2.76	0.43
2:B:162:ARG:CB	2:B:162:ARG:HH11	2.32	0.43
2:B:218:ARG:HB3	2:B:237:PHE:CE2	2.53	0.43
2:C:219:THR:HA	2:C:235:TYR:O	2.18	0.43
2:C:356:LEU:CD1	2:C:356:LEU:N	2.81	0.43
2:D:430:ILE:O	2:D:433:ILE:HD13	2.17	0.43
2:E:160:VAL:HG21	2:E:194:TYR:CG	2.53	0.43
2:E:446:ARG:HE	2:E:496:ARG:NH2	2.16	0.43
2:F:300:ARG:CA	2:F:333:MET:HE1	2.49	0.43
2:F:435:ASP:OD1	2:F:459:ARG:NH1	2.51	0.43
2:B:234:GLU:C	2:B:235:TYR:CD1	2.97	0.43
2:C:127:ILE:CD1	2:C:167:LEU:HD13	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:VAL:C	2:C:152:GLN:H	2.26	0.43
2:D:300:ARG:HA	2:D:333:MET:HE1	1.99	0.43
2:E:43:LEU:HD23	2:E:204:VAL:CG1	2.34	0.43
2:E:323:GLN:NE2	2:F:459:ARG:HD3	2.33	0.43
2:E:323:GLN:HE21	2:F:459:ARG:HD3	1.84	0.43
2:E:329:TYR:O	2:E:332:GLY:N	2.45	0.43
2:F:316:ALA:HB2	2:F:324:LEU:HD11	2.01	0.43
2:F:322:ALA:O	2:F:325:LEU:HB2	2.19	0.43
1:A:109:SER:HA	1:A:110:PRO:HD3	1.81	0.43
2:B:289:ALA:HB1	2:B:419:PHE:HB3	2.00	0.43
2:B:309:LYS:HA	2:B:343:LEU:HD13	2.01	0.43
2:C:184:ARG:HH21	2:C:190:PRO:C	2.26	0.43
2:C:225:LEU:HD23	2:C:225:LEU:HA	1.85	0.43
2:C:296:LEU:HA	2:C:331:TRP:CZ3	2.53	0.43
2:C:300:ARG:HA	2:C:333:MET:CE	2.36	0.43
2:D:174:ILE:O	2:D:176:ALA:N	2.52	0.43
2:D:214:GLU:O	2:D:215:ARG:NE	2.49	0.43
2:E:264:SER:HB3	2:E:304:ASN:ND2	2.33	0.43
2:E:293:GLY:O	2:E:294:LYS:C	2.59	0.43
2:E:425:ILE:HD12	2:E:439:LEU:CD1	2.44	0.43
2:F:70:PRO:HA	2:F:102:LYS:O	2.18	0.43
1:A:82:ASP:O	1:A:84:ILE:N	2.52	0.43
1:A:496:ARG:HH11	2:B:497:ILE:HD13	1.83	0.43
2:B:50:THR:HB	2:B:207:LEU:HB2	1.99	0.43
2:B:385:ARG:NH1	2:C:397:ILE:HD11	2.34	0.43
2:C:129:ARG:O	2:C:132:TYR:HB3	2.18	0.43
2:D:248:PRO:C	2:D:250:GLY:H	2.27	0.43
2:D:367:ILE:HG22	2:D:368:ASN:N	2.33	0.43
2:E:370:PHE:C	2:E:371:LYS:HG3	2.43	0.43
2:F:47:THR:CG2	2:F:48:SER:N	2.81	0.43
2:F:182:THR:HG22	2:F:183:GLU:O	2.19	0.43
2:F:272:GLU:C	2:F:274:CYS:H	2.27	0.43
2:F:431:ALA:HA	2:F:434:THR:HG22	2.00	0.43
1:A:18:ILE:HG21	1:A:37:PRO:HB3	2.00	0.43
2:B:36:LEU:HD22	2:B:42:THR:OG1	2.18	0.43
2:B:206:ILE:HD12	2:B:206:ILE:N	2.34	0.43
2:B:251:ALA:O	2:B:252:MET:C	2.61	0.43
2:B:267:VAL:HG23	2:B:300:ARG:HG2	2.00	0.43
2:B:436:THR:HG23	2:B:458:MET:HG2	2.00	0.43
2:B:439:LEU:HD12	2:B:440:LEU:N	2.34	0.43
2:C:149:SER:HB3	2:D:161:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:313:ILE:HG22	2:C:315:PHE:CE1	2.54	0.43
2:D:42:THR:N	2:D:178:THR:O	2.49	0.43
2:D:453:ILE:CG1	2:D:454:ASN:N	2.82	0.43
2:E:148:THR:HG23	2:E:193:ARG:HD2	1.99	0.43
2:E:380:LEU:HD21	2:E:412:PHE:HD2	1.84	0.43
2:E:469:GLU:HB3	2:E:483:PHE:CE1	2.54	0.43
2:F:115:GLN:OE1	2:F:116:GLU:O	2.37	0.43
2:F:209:ASN:C	2:F:209:ASN:HD22	2.25	0.43
2:F:328:ALA:O	2:F:332:GLY:O	2.37	0.43
2:F:387:VAL:HG11	2:F:392:PHE:HB2	2.00	0.43
1:A:125:ALA:O	1:A:129:ARG:HG3	2.18	0.43
1:A:219:THR:HG22	1:A:235:TYR:C	2.43	0.43
1:A:363:ILE:O	1:A:364:LYS:C	2.62	0.43
1:A:420:MET:HG2	1:A:492:GLY:HA3	2.01	0.43
2:B:52:LYS:HE3	2:B:52:LYS:HB2	1.84	0.43
2:B:359:HIS:C	2:B:363:ILE:HD13	2.44	0.43
2:C:363:ILE:O	2:C:365:SER:N	2.52	0.43
2:D:45:SER:HB2	2:D:182:THR:HB	2.00	0.43
2:D:363:ILE:O	2:D:364:LYS:C	2.62	0.43
2:D:443:VAL:HG21	2:D:489:ILE:HG22	2.01	0.43
2:E:60:LEU:CD1	2:E:73:PHE:HD1	2.32	0.43
2:E:65:ILE:HD12	2:E:65:ILE:N	2.33	0.43
2:E:345:LYS:CE	2:E:366:GLU:HG3	2.49	0.43
2:E:433:ILE:HD12	2:E:433:ILE:N	2.33	0.43
2:F:20:LYS:HB3	2:F:35:GLY:O	2.19	0.43
2:F:111:ASP:CG	2:F:112:PRO:HD2	2.43	0.43
1:A:27:GLY:O	1:A:31:ILE:HG13	2.19	0.43
1:A:334:ASP:OD1	1:A:337:GLU:N	2.45	0.43
1:A:344:LEU:HD11	1:A:346:ILE:CD1	2.49	0.43
2:B:153:GLN:O	2:B:154:TYR:HB3	2.18	0.43
2:B:301:PHE:O	2:B:374:ARG:NH1	2.49	0.43
2:C:52:LYS:HB2	2:C:52:LYS:HE3	1.80	0.43
2:D:38:ILE:CG2	2:D:39:GLY:N	2.82	0.43
2:E:21:MET:SD	2:E:38:ILE:HD13	2.59	0.43
2:F:252:MET:HE3	2:F:401:GLY:HA3	2.01	0.43
2:F:497:ILE:O	2:F:497:ILE:CG1	2.67	0.43
2:F:505:LEU:O	2:F:506:SER:HB3	2.18	0.43
1:A:234:GLU:O	1:A:235:TYR:CD1	2.72	0.42
2:C:83:ILE:O	2:C:83:ILE:HG22	2.17	0.42
2:C:292:THR:HB	2:C:440:LEU:HB3	2.00	0.42
2:C:348:CYS:O	2:C:349:ALA:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:LEU:CD1	2:D:197:GLU:HG3	2.49	0.42
2:D:170:ARG:HH12	2:D:174:ILE:HD11	1.84	0.42
2:D:420:MET:HB3	2:D:492:GLY:HA3	2.01	0.42
2:D:441:GLN:HB2	5:D:540:HOH:O	2.18	0.42
2:E:246:ILE:HG22	2:E:247:PHE:N	2.34	0.42
2:E:315:PHE:HB3	2:E:317:TYR:CE1	2.54	0.42
2:F:65:ILE:O	2:F:66:GLU:HG2	2.19	0.42
2:F:231:MET:HE2	2:F:235:TYR:OH	2.19	0.42
2:F:440:LEU:HD21	2:F:453:ILE:HD12	2.01	0.42
2:F:445:ILE:HD12	2:F:445:ILE:N	2.34	0.42
1:A:442:TYR:HE1	2:B:456:PHE:CZ	2.37	0.42
2:C:295:THR:HG22	2:C:331:TRP:CH2	2.53	0.42
2:D:21:MET:CE	2:D:177:THR:HB	2.49	0.42
2:D:271:ASP:O	2:D:276:GLY:N	2.52	0.42
2:D:462:TRP:CH2	2:D:464:ASP:HA	2.54	0.42
2:E:184:ARG:HD2	2:E:191:ILE:O	2.18	0.42
2:E:426:THR:HG21	2:E:431:ALA:H	1.83	0.42
2:E:486:PHE:HA	2:E:495:THR:O	2.19	0.42
2:F:18:ILE:HD12	2:F:40:ARG:HH12	1.83	0.42
2:F:37:PRO:O	2:F:40:ARG:HB2	2.19	0.42
2:F:285:LEU:CD2	2:F:437:ILE:HD12	2.44	0.42
1:A:361:GLN:C	1:A:363:ILE:N	2.76	0.42
2:B:216:ARG:NE	2:C:221:GLU:OE1	2.47	0.42
2:B:303:GLU:O	2:B:306:CYS:HB2	2.20	0.42
2:B:439:LEU:HD12	2:B:439:LEU:C	2.44	0.42
2:C:150:VAL:HG13	2:C:151:PHE:H	1.84	0.42
2:E:18:ILE:HD12	2:E:228:THR:HG23	2.01	0.42
2:E:404:LYS:C	2:E:406:GLU:N	2.75	0.42
2:F:53:THR:HG1	2:F:145:ASP:CG	2.24	0.42
2:F:247:PHE:HB3	2:F:249:LEU:CD2	2.49	0.42
2:F:294:LYS:HZ1	2:F:415:THR:HG23	1.84	0.42
2:F:331:TRP:HH2	3:F:901:ATP:O2A	2.02	0.42
2:F:357:GLU:HG3	2:F:358:ASP:H	1.84	0.42
2:F:505:LEU:O	2:F:506:SER:CB	2.67	0.42
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.44	0.42
1:A:203:ASN:HB3	1:A:225:LEU:HD23	2.01	0.42
1:A:220:LEU:HD13	1:A:246:ILE:CD1	2.49	0.42
1:A:299:SER:O	1:A:301:PHE:N	2.52	0.42
2:B:51:GLY:O	2:B:54:LEU:N	2.52	0.42
2:C:20:LYS:HA	2:C:38:ILE:HD12	2.01	0.42
2:C:52:LYS:HB3	2:C:181:THR:HG23	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:187:GLU:O	2:C:208:ARG:HD3	2.19	0.42
2:C:404:LYS:C	2:C:406:GLU:H	2.26	0.42
2:D:299:SER:HB3	2:D:335:PHE:HZ	1.84	0.42
2:E:396:VAL:O	2:E:397:ILE:C	2.60	0.42
2:F:204:VAL:HG23	2:F:224:LYS:HG2	2.01	0.42
2:F:220:LEU:HD13	2:F:246:ILE:HD11	2.00	0.42
2:F:468:ARG:HG2	2:F:468:ARG:HH11	1.84	0.42
1:A:52:LYS:HB2	1:A:52:LYS:HE3	1.87	0.42
1:A:85:LYS:O	1:A:88:ARG:HB2	2.19	0.42
1:A:426:TPO:O	1:A:427:ASP:HB2	2.19	0.42
2:B:26:GLU:OE1	2:B:27:GLY:N	2.53	0.42
2:B:281:ASP:O	2:B:282:SER:HB3	2.20	0.42
2:B:356:LEU:H	2:B:356:LEU:HD12	1.77	0.42
2:C:64:ILE:H	2:C:64:ILE:HD12	1.84	0.42
2:C:380:LEU:HD23	2:C:380:LEU:HA	1.87	0.42
2:D:52:LYS:CE	5:D:547:HOH:O	2.67	0.42
2:D:74:VAL:HG13	2:D:106:LEU:HG	2.01	0.42
2:D:311:ARG:CD	2:D:371:LYS:HE3	2.10	0.42
2:E:80:PRO:HD2	2:E:81:GLN:NE2	2.34	0.42
2:E:451:ARG:HG2	2:E:472:ILE:HD11	2.01	0.42
2:F:79:THR:HG23	2:F:79:THR:O	2.19	0.42
2:F:150:VAL:CG1	2:F:151:PHE:N	2.83	0.42
2:F:269:ARG:NH2	2:F:468:ARG:NH2	2.68	0.42
2:F:278:PHE:CZ	2:F:438:ILE:HD11	2.55	0.42
1:A:53:THR:O	1:A:54:LEU:C	2.61	0.42
1:A:267:VAL:HG12	1:A:270:LEU:HB2	1.98	0.42
2:B:65:ILE:O	2:B:65:ILE:HG22	2.20	0.42
2:B:90:PHE:HB2	2:B:92:TRP:CZ2	2.55	0.42
2:B:215:ARG:NE	2:B:215:ARG:HA	2.34	0.42
2:B:247:PHE:HD2	2:B:364:LYS:NZ	2.17	0.42
2:B:294:LYS:N	3:B:901:ATP:O1B	2.52	0.42
2:B:296:LEU:HD22	2:B:472:ILE:HD12	2.01	0.42
2:C:21:MET:HB2	2:C:38:ILE:CG1	2.50	0.42
2:C:85:LYS:HZ2	2:D:14:GLU:HB3	1.83	0.42
2:C:111:ASP:OD2	2:C:113:GLU:CG	2.68	0.42
2:D:41:SER:CB	2:D:178:THR:HB	2.49	0.42
2:E:169:ALA:O	2:E:172:LYS:HB3	2.19	0.42
2:F:191:ILE:HG23	2:F:206:ILE:CD1	2.50	0.42
2:F:332:GLY:O	2:F:333:MET:C	2.62	0.42
1:A:24:MET:HB2	1:A:62:ASN:HB3	2.00	0.42
1:A:380:LEU:C	1:A:382:ALA:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:LYS:O	2:B:371:LYS:HD3	2.20	0.42
2:B:404:LYS:C	2:B:406:GLU:N	2.75	0.42
2:B:502:LYS:HG3	2:B:504:GLU:O	2.20	0.42
2:C:274:CYS:HB3	2:C:458:MET:SD	2.59	0.42
2:C:326:ARG:C	2:C:328:ALA:H	2.28	0.42
2:C:377:ILE:HD11	2:C:399:VAL:HG11	2.01	0.42
2:C:496:ARG:HG3	2:D:487:GLU:OE1	2.20	0.42
2:D:174:ILE:O	2:D:175:GLY:C	2.62	0.42
2:D:261:VAL:HG12	2:D:262:ARG:N	2.35	0.42
2:D:440:LEU:HD22	2:D:470:PHE:CE2	2.55	0.42
3:D:901:ATP:O2G	2:E:459:ARG:NH2	2.50	0.42
2:E:161:ARG:CA	2:E:196:VAL:HG11	2.49	0.42
2:E:451:ARG:N	2:E:451:ARG:HD2	2.34	0.42
2:F:380:LEU:C	2:F:382:ALA:N	2.77	0.42
1:A:25:ILE:O	1:A:25:ILE:HG22	2.19	0.42
1:A:248:PRO:O	1:A:250:GLY:N	2.53	0.42
2:B:296:LEU:CD2	2:B:477:PRO:HB3	2.49	0.42
2:B:356:LEU:H	2:B:356:LEU:HD13	1.84	0.42
2:C:52:LYS:H	2:C:52:LYS:HG3	1.60	0.42
2:C:218:ARG:HD2	5:C:528:HOH:O	2.19	0.42
2:C:431:ALA:HA	2:C:434:THR:HG22	2.01	0.42
2:C:464:ASP:OD1	2:C:464:ASP:C	2.63	0.42
2:D:65:ILE:O	2:D:65:ILE:HG22	2.19	0.42
2:E:195:GLY:HA2	2:E:198:GLU:OE1	2.20	0.42
2:F:289:ALA:HB2	2:F:419:PHE:HA	2.02	0.42
1:A:32:SER:OG	1:A:35:GLY:HA2	2.20	0.42
1:A:209:ASN:ND2	1:A:216:ARG:HB3	2.35	0.42
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.85	0.42
1:A:397:ILE:HD11	1:A:433:ILE:HD13	2.02	0.42
1:A:462:TRP:CE3	1:A:463:HIS:N	2.87	0.42
1:A:463:HIS:ND1	1:A:463:HIS:C	2.77	0.42
2:B:14:GLU:OE2	2:B:16:GLN:HB2	2.19	0.42
2:C:90:PHE:HA	2:C:241:ASP:O	2.20	0.42
2:C:306:CYS:CB	2:C:338:MET:SD	3.07	0.42
2:C:313:ILE:HD12	2:C:372:PRO:CG	2.50	0.42
2:C:471:MET:CE	2:C:478:ASP:HB2	2.47	0.42
2:D:18:ILE:H	2:D:18:ILE:CD1	2.28	0.42
2:D:263:VAL:CG2	2:D:280:LYS:HA	2.50	0.42
2:D:468:ARG:HG2	2:D:468:ARG:HH11	1.83	0.42
2:D:483:PHE:N	2:D:483:PHE:CD1	2.88	0.42
2:E:262:ARG:NH1	2:E:461:SER:HB2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:318:GLU:CG	2:F:432:TPO:O3P	2.63	0.42
2:E:370:PHE:O	2:E:371:LYS:HG3	2.20	0.42
2:F:25:ILE:O	2:F:26:GLU:C	2.62	0.42
2:F:53:THR:OG1	2:F:145:ASP:CG	2.63	0.42
2:F:336:GLU:CD	2:F:340:ARG:HH21	2.27	0.42
2:F:509:VAL:CG1	2:F:510:ARG:H	2.21	0.42
1:A:36:LEU:HD12	1:A:59:PHE:CZ	2.55	0.42
1:A:134:ILE:CD1	1:A:134:ILE:N	2.83	0.42
1:A:389:ASN:ND2	1:A:428:SER:HB2	2.35	0.42
1:A:448:GLU:HG2	2:B:466:ALA:HA	2.01	0.42
2:B:48:SER:OG	2:C:224:LYS:HD3	2.20	0.42
2:B:261:VAL:HG12	2:B:262:ARG:N	2.34	0.42
2:B:455:VAL:HG11	2:B:463:HIS:CB	2.48	0.42
2:C:60:LEU:O	2:C:64:ILE:HD13	2.19	0.42
2:C:300:ARG:NH2	2:C:477:PRO:HD2	2.35	0.42
2:D:223:LEU:HD23	2:D:223:LEU:C	2.45	0.42
2:D:291:GLY:O	2:D:293:GLY:N	2.52	0.42
2:E:245:ASN:ND2	2:E:247:PHE:CE2	2.88	0.42
2:E:306:CYS:HB2	2:E:338:MET:SD	2.59	0.42
2:E:313:ILE:CG1	2:E:372:PRO:HG3	2.37	0.42
2:F:116:GLU:O	2:F:117:VAL:CB	2.67	0.42
2:F:222:ILE:CG2	2:F:225:LEU:HG	2.50	0.42
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.70	0.41
1:A:183:GLU:H	1:A:183:GLU:HG2	1.62	0.41
1:A:480:LYS:HB3	1:A:481:ASP:H	1.64	0.41
2:B:72:VAL:HB	2:B:142:VAL:HG13	2.02	0.41
2:B:83:ILE:HD12	2:B:83:ILE:N	2.35	0.41
2:B:184:ARG:HH22	2:B:187:GLU:C	2.28	0.41
2:B:221:GLU:HG2	2:B:222:ILE:N	2.34	0.41
2:B:287:THR:CG2	2:B:288:GLY:N	2.81	0.41
2:B:383:LEU:HD13	2:B:395:PHE:CE2	2.55	0.41
2:B:418:GLN:O	2:B:422:ALA:HB2	2.19	0.41
2:C:305:ALA:HB2	2:C:374:ARG:HH11	1.85	0.41
2:C:312:ALA:O	2:C:344:LEU:CD2	2.68	0.41
2:E:18:ILE:HD12	2:E:228:THR:OG1	2.20	0.41
2:E:97:LEU:O	2:E:103:LEU:N	2.49	0.41
2:E:356:LEU:H	2:E:356:LEU:HD12	1.85	0.41
2:E:364:LYS:O	2:E:368:ASN:ND2	2.53	0.41
2:E:380:LEU:HD21	2:E:412:PHE:CD2	2.54	0.41
2:E:443:VAL:CG1	2:E:494:PRO:HG2	2.50	0.41
2:F:380:LEU:HD23	2:F:380:LEU:HA	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:THR:C	1:A:25:ILE:N	2.76	0.41
1:A:84:ILE:HA	1:A:94:LEU:HD12	2.02	0.41
1:A:144:ILE:HG22	1:A:147:VAL:HG12	2.02	0.41
1:A:211:LEU:HD12	1:A:212:GLU:N	2.35	0.41
1:A:221:GLU:C	1:A:222:ILE:HD12	2.45	0.41
1:A:344:LEU:HD13	1:A:345:LYS:N	2.35	0.41
1:A:383:LEU:O	1:A:385:ARG:N	2.53	0.41
2:B:31:ILE:HG21	2:B:222:ILE:HD13	2.02	0.41
2:C:64:ILE:HD11	2:C:71:GLY:HA3	2.01	0.41
2:C:79:THR:OG1	2:C:81:GLN:HG2	2.20	0.41
2:C:106:LEU:HD23	2:C:130:ILE:HG12	2.02	0.41
2:C:198:GLU:C	2:C:200:VAL:N	2.77	0.41
2:C:370:PHE:O	2:C:370:PHE:CD2	2.73	0.41
2:D:38:ILE:CA	2:D:177:THR:HG23	2.44	0.41
2:D:47:THR:HG22	2:D:184:ARG:HB2	2.02	0.41
2:E:285:LEU:HG	2:E:286:ALA:N	2.35	0.41
2:E:435:ASP:O	2:E:459:ARG:HG3	2.20	0.41
2:F:375:ILE:HD13	2:F:375:ILE:C	2.44	0.41
2:F:426:THR:C	2:F:428:SER:N	2.75	0.41
2:F:486:PHE:CE2	2:F:496:ARG:CD	3.02	0.41
1:A:19:ALA:O	1:A:38:ILE:HG13	2.21	0.41
1:A:405:GLN:HG3	1:A:406:GLU:N	2.34	0.41
1:A:436:THR:HA	1:A:457:LYS:O	2.20	0.41
2:B:32:SER:OG	2:B:35:GLY:N	2.54	0.41
2:B:140:ARG:HB3	2:B:140:ARG:CZ	2.48	0.41
2:B:211:LEU:HD12	2:B:211:LEU:HA	1.89	0.41
2:B:255:THR:O	2:B:255:THR:HG22	2.19	0.41
2:B:371:LYS:O	2:B:371:LYS:CD	2.69	0.41
2:B:419:PHE:HD2	2:C:425:ILE:HD12	1.85	0.41
2:C:44:VAL:HG22	2:C:205:VAL:HB	2.03	0.41
2:C:142:VAL:O	2:C:178:THR:HA	2.21	0.41
2:D:58:GLN:OE1	2:D:243:GLY:HA3	2.21	0.41
2:D:383:LEU:C	2:D:385:ARG:N	2.77	0.41
2:D:495:THR:HA	2:E:487:GLU:CD	2.44	0.41
2:E:80:PRO:HB2	2:E:81:GLN:NE2	2.35	0.41
2:E:94:LEU:HB3	2:E:103:LEU:HD23	2.01	0.41
1:A:209:ASN:HD21	1:A:216:ARG:HB3	1.85	0.41
1:A:380:LEU:C	1:A:382:ALA:N	2.77	0.41
1:A:502:LYS:HG3	1:A:502:LYS:O	2.21	0.41
2:B:249:LEU:HD12	2:B:394:GLN:CD	2.46	0.41
2:B:263:VAL:HG12	2:B:374:ARG:NH2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ASN:O	2:B:309:LYS:C	2.63	0.41
2:C:198:GLU:C	2:C:200:VAL:H	2.28	0.41
2:D:122:ASP:HB3	2:D:123:LEU:H	1.49	0.41
2:D:144:ILE:HG22	2:D:147:VAL:HG12	2.02	0.41
2:D:211:LEU:O	2:D:212:GLU:CG	2.59	0.41
2:D:353:SER:O	2:D:354:ALA:HB2	2.19	0.41
2:D:355:GLY:O	2:D:358:ASP:HB2	2.20	0.41
2:D:420:MET:HE1	2:E:490:ILE:HG13	2.01	0.41
3:D:903:ATP:O1G	2:E:224:LYS:NZ	2.54	0.41
2:E:54:LEU:HD23	2:E:239:ILE:HG12	2.02	0.41
2:E:199:PHE:C	2:E:201:SER:N	2.77	0.41
2:E:313:ILE:CG1	2:E:372:PRO:HG2	2.49	0.41
2:E:481:ASP:O	2:E:482:SER:O	2.38	0.41
2:F:49:GLY:HA2	3:F:903:ATP:O2B	2.21	0.41
2:F:116:GLU:O	2:F:117:VAL:HB	2.19	0.41
2:F:329:TYR:O	2:F:332:GLY:N	2.43	0.41
2:F:360:LEU:O	2:F:360:LEU:HD22	2.21	0.41
2:F:418:GLN:O	2:F:422:ALA:HB2	2.20	0.41
2:F:487:GLU:O	2:F:488:ARG:C	2.63	0.41
2:F:489:ILE:O	2:F:491:SER:N	2.54	0.41
2:F:490:ILE:C	2:F:492:GLY:N	2.74	0.41
1:A:196:VAL:O	1:A:198:GLU:N	2.53	0.41
1:A:439:LEU:O	1:A:453:ILE:HA	2.19	0.41
2:B:75:THR:O	2:B:108:ALA:HB3	2.20	0.41
2:B:496:ARG:CG	2:B:498:THR:HG23	2.43	0.41
2:C:28:PHE:CE1	2:C:55:PHE:HZ	2.39	0.41
2:C:54:LEU:HD12	2:C:54:LEU:HA	1.83	0.41
2:C:126:LEU:O	2:C:129:ARG:N	2.53	0.41
2:C:278:PHE:N	2:C:278:PHE:CD2	2.87	0.41
2:C:338:MET:HB3	2:C:344:LEU:HB3	2.03	0.41
2:C:444:GLU:OE2	2:D:489:ILE:HG12	2.20	0.41
2:D:220:LEU:C	2:D:220:LEU:CD2	2.93	0.41
2:D:356:LEU:O	2:D:357:GLU:C	2.62	0.41
2:E:85:LYS:HE3	2:F:18:ILE:HD13	2.02	0.41
2:E:375:ILE:HD13	2:E:375:ILE:HA	1.85	0.41
2:E:392:PHE:CE2	2:E:430:ILE:CD1	2.95	0.41
2:F:111:ASP:HA	2:F:112:PRO:HD3	1.83	0.41
2:F:187:GLU:HG3	2:F:208:ARG:HB3	2.02	0.41
2:F:325:LEU:CD2	2:F:335:PHE:HB2	2.50	0.41
2:F:454:ASN:CG	2:F:467:ILE:HD12	2.45	0.41
1:A:84:ILE:HG23	1:A:94:LEU:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:CG2	1:A:366:GLU:HG2	2.50	0.41
1:A:458:MET:SD	1:A:461:SER:HB3	2.61	0.41
2:B:54:LEU:HD13	2:B:90:PHE:CE1	2.55	0.41
2:B:361:GLN:O	2:B:362:ILE:C	2.62	0.41
2:B:385:ARG:NH2	2:C:432:TPO:O2P	2.53	0.41
2:C:192:ALA:HB3	2:C:197:GLU:HB2	2.01	0.41
2:D:484:ARG:HB3	2:D:484:ARG:NH1	2.35	0.41
2:F:132:TYR:CD2	2:F:132:TYR:C	2.98	0.41
2:F:144:ILE:CG2	2:F:147:VAL:HG12	2.50	0.41
2:F:225:LEU:HD23	2:F:225:LEU:HA	1.83	0.41
2:F:245:ASN:HB3	2:F:361:GLN:HE22	1.85	0.41
2:F:246:ILE:CG2	2:F:247:PHE:N	2.84	0.41
2:F:294:LYS:HZ1	2:F:415:THR:CG2	2.33	0.41
2:F:443:VAL:HB	2:F:445:ILE:CD1	2.50	0.41
2:F:500:ASP:O	2:F:501:GLU:CB	2.56	0.41
1:A:90:PHE:CD1	1:A:90:PHE:N	2.89	0.41
1:A:170:ARG:O	1:A:174:ILE:HG12	2.20	0.41
1:A:191:ILE:HD12	1:A:206:ILE:HD11	2.02	0.41
1:A:262:ARG:HA	1:A:278:PHE:O	2.20	0.41
1:A:266:GLY:O	1:A:300:ARG:CG	2.68	0.41
2:B:144:ILE:CG2	2:B:147:VAL:HG12	2.51	0.41
2:B:356:LEU:HD11	2:B:387:VAL:HG21	2.03	0.41
2:B:455:VAL:CG1	2:B:463:HIS:HB2	2.51	0.41
2:B:484:ARG:HB2	5:B:528:HOH:O	2.19	0.41
2:C:32:SER:HB3	2:C:222:ILE:HD11	2.02	0.41
2:C:43:LEU:N	2:C:203:ASN:O	2.47	0.41
2:C:311:ARG:NE	2:C:371:LYS:HE3	2.35	0.41
2:C:317:TYR:HE1	2:C:377:ILE:HG23	1.85	0.41
2:C:438:ILE:CG2	2:C:453:ILE:HD11	2.51	0.41
2:D:181:THR:CG2	5:D:547:HOH:O	2.68	0.41
2:D:288:GLY:HA2	2:D:440:LEU:O	2.20	0.41
2:D:294:LYS:HB2	2:D:294:LYS:HE2	1.85	0.41
2:D:299:SER:HB3	2:D:335:PHE:CZ	2.55	0.41
2:D:299:SER:HB3	2:D:333:MET:HE2	2.02	0.41
2:E:87:ALA:O	2:E:89:SER:N	2.53	0.41
2:E:205:VAL:HG13	2:E:222:ILE:HD13	2.01	0.41
2:E:352:GLU:OE1	2:F:397:ILE:HD13	2.21	0.41
1:A:37:PRO:HG2	1:A:203:ASN:ND2	2.35	0.41
1:A:182:THR:CG2	1:A:183:GLU:N	2.84	0.41
2:B:116:GLU:HG2	2:B:117:VAL:N	2.29	0.41
2:B:490:ILE:O	2:B:491:SER:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:PHE:N	2:C:246:ILE:HD12	2.36	0.41
2:C:70:PRO:HD2	2:C:140:ARG:HG2	2.03	0.41
2:C:123:LEU:HD11	2:C:163:GLU:CA	2.51	0.41
2:C:298:VAL:O	2:C:301:PHE:HB3	2.21	0.41
2:C:318:GLU:OE2	2:D:432:TPO:HB	2.21	0.41
2:C:480:LYS:HB2	2:C:480:LYS:HE3	1.69	0.41
2:E:14:GLU:HG3	2:E:16:GLN:N	2.29	0.41
2:E:27:GLY:O	2:E:28:PHE:C	2.63	0.41
2:E:237:PHE:HB2	2:E:245:ASN:O	2.21	0.41
2:E:371:LYS:HD2	2:E:371:LYS:C	2.46	0.41
2:E:390:ASN:O	2:E:391:ALA:C	2.64	0.41
2:F:273:MET:HE3	2:F:468:ARG:HD2	2.03	0.41
2:F:324:LEU:HD23	2:F:324:LEU:HA	1.93	0.41
2:F:337:GLU:O	2:F:338:MET:C	2.64	0.41
2:F:360:LEU:HD13	2:F:360:LEU:C	2.46	0.41
1:A:51:GLY:O	1:A:52:LYS:C	2.64	0.41
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.56	0.41
1:A:79:THR:O	1:A:82:ASP:HB2	2.21	0.41
1:A:210:VAL:CG1	1:A:211:LEU:O	2.67	0.41
1:A:348:CYS:O	1:A:349:ALA:HB2	2.21	0.41
2:B:24:MET:O	2:B:62:ASN:ND2	2.54	0.41
2:B:379:SER:HA	2:B:413:THR:O	2.21	0.41
2:B:380:LEU:HB3	2:B:392:PHE:HZ	1.86	0.41
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.46	0.41
2:C:487:GLU:N	2:C:497:ILE:HD11	2.36	0.41
2:D:43:LEU:HD11	2:D:182:THR:OG1	2.21	0.41
2:D:150:VAL:CG1	2:D:151:PHE:H	2.34	0.41
2:D:270:LEU:HD21	2:D:438:ILE:HD12	2.02	0.41
2:D:339:GLU:CD	2:D:346:ILE:HD12	2.46	0.41
2:D:397:ILE:HG13	2:D:397:ILE:H	1.66	0.41
2:E:161:ARG:HB2	2:E:196:VAL:HG11	2.02	0.41
2:E:329:TYR:C	2:E:331:TRP:H	2.29	0.41
2:E:344:LEU:HD13	2:E:344:LEU:C	2.46	0.41
2:E:445:ILE:HG22	2:E:445:ILE:O	2.19	0.41
2:E:489:ILE:HD13	2:E:489:ILE:HA	1.89	0.41
2:F:164:LEU:O	2:F:165:PHE:C	2.64	0.41
2:F:271:ASP:O	2:F:272:GLU:C	2.63	0.41
2:F:272:GLU:O	2:F:274:CYS:N	2.54	0.41
2:F:370:PHE:C	2:F:371:LYS:HG3	2.46	0.41
2:F:426:THR:O	2:F:428:SER:N	2.49	0.41
2:F:453:ILE:CG1	2:F:454:ASN:N	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:487:GLU:CD	2:F:497:ILE:HG21	2.46	0.41
2:F:507:ARG:O	2:F:508:ILE:C	2.63	0.41
1:A:52:LYS:O	1:A:53:THR:C	2.63	0.41
1:A:121:PHE:CD1	1:A:121:PHE:C	2.99	0.41
1:A:298:VAL:HG12	1:A:299:SER:N	2.36	0.41
1:A:379:SER:HA	1:A:413:THR:O	2.20	0.41
2:B:61:TYR:O	2:B:64:ILE:N	2.53	0.41
2:B:64:ILE:O	2:B:66:GLU:N	2.51	0.41
2:B:463:HIS:C	2:B:463:HIS:ND1	2.79	0.41
2:B:472:ILE:HD13	2:B:477:PRO:HA	2.03	0.41
2:B:495:THR:O	2:B:496:ARG:C	2.63	0.41
2:C:82:ASP:C	2:C:84:ILE:H	2.28	0.41
2:C:426:THR:HG21	2:C:430:ILE:CG1	2.46	0.41
2:D:114:GLY:C	2:D:115:GLN:HG3	2.46	0.41
2:D:223:LEU:HD23	2:D:223:LEU:O	2.21	0.41
3:D:901:ATP:O3'	2:E:457:LYS:HB2	2.20	0.41
2:E:317:TYR:CD2	2:E:383:LEU:HD21	2.56	0.41
2:F:296:LEU:HG	2:F:297:LEU:N	2.36	0.41
1:A:351:PRO:C	1:A:353:SER:N	2.78	0.40
1:A:488:ARG:HD3	2:F:488:ARG:HH12	1.86	0.40
2:B:21:MET:HE2	2:B:21:MET:HB3	1.95	0.40
2:B:61:TYR:C	2:B:63:GLY:N	2.78	0.40
2:B:61:TYR:HE1	2:B:92:TRP:HB2	1.85	0.40
2:B:82:ASP:O	2:B:83:ILE:C	2.63	0.40
2:B:105:ILE:O	2:B:105:ILE:HG22	2.21	0.40
2:B:169:ALA:O	2:B:173:GLN:HG3	2.21	0.40
2:B:313:ILE:CD1	2:B:372:PRO:HG2	2.51	0.40
2:B:451:ARG:HB3	2:B:452:ALA:H	1.73	0.40
2:C:123:LEU:O	2:C:124:SER:C	2.64	0.40
2:C:256:GLN:H	2:C:256:GLN:HG2	1.60	0.40
2:C:300:ARG:N	2:C:333:MET:HE1	2.36	0.40
2:C:312:ALA:O	2:C:344:LEU:HD22	2.21	0.40
2:D:181:THR:HG21	5:D:547:HOH:O	2.21	0.40
2:E:214:GLU:O	2:F:233:GLY:HA3	2.21	0.40
2:E:420:MET:HE1	2:F:490:ILE:CG1	2.42	0.40
2:F:117:VAL:O	2:F:118:VAL:HB	2.21	0.40
2:F:215:ARG:NE	2:F:215:ARG:HA	2.33	0.40
2:F:455:VAL:HG11	2:F:463:HIS:HB2	2.03	0.40
2:F:484:ARG:CB	2:F:484:ARG:CZ	2.99	0.40
2:F:497:ILE:O	2:F:497:ILE:CD1	2.67	0.40
2:F:504:GLU:C	2:F:506:SER:H	2.28	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PRO:HB2	1:A:251:ALA:CB	2.50	0.40
1:A:488:ARG:N	2:F:444:GLU:OE2	2.54	0.40
2:B:51:GLY:O	2:B:52:LYS:C	2.64	0.40
2:B:287:THR:CB	2:B:425:ILE:CG2	2.99	0.40
2:B:471:MET:HB3	2:B:480:LYS:NZ	2.36	0.40
2:C:88:ARG:HG2	2:C:88:ARG:NH1	2.36	0.40
2:C:148:THR:C	2:C:150:VAL:H	2.29	0.40
2:C:488:ARG:HG3	2:C:488:ARG:HH11	1.85	0.40
2:D:37:PRO:HG2	2:D:203:ASN:CG	2.46	0.40
2:D:263:VAL:O	2:D:278:PHE:N	2.54	0.40
2:D:295:THR:N	3:D:901:ATP:O1B	2.47	0.40
2:E:59:PHE:CZ	2:E:141:ARG:HD3	2.57	0.40
2:F:62:ASN:O	2:F:63:GLY:C	2.63	0.40
2:F:83:ILE:H	2:F:83:ILE:HD12	1.86	0.40
2:F:94:LEU:HD22	2:F:103:LEU:HD22	2.02	0.40
2:F:117:VAL:HG22	5:F:536:HOH:O	2.20	0.40
2:F:231:MET:HB3	2:F:231:MET:HE2	1.92	0.40
2:F:438:ILE:HG23	2:F:453:ILE:HD11	2.04	0.40
2:F:471:MET:CG	2:F:480:LYS:HE2	2.42	0.40
1:A:261:VAL:O	1:A:279:PHE:HA	2.22	0.40
2:B:18:ILE:N	2:B:18:ILE:CD1	2.83	0.40
2:B:121:PHE:N	2:B:121:PHE:CD1	2.89	0.40
2:B:247:PHE:HD2	2:B:364:LYS:HZ2	1.67	0.40
2:B:297:LEU:HD23	2:B:297:LEU:HA	1.79	0.40
2:C:123:LEU:C	2:C:127:ILE:HG12	2.46	0.40
2:C:203:ASN:HB3	2:C:225:LEU:CD2	2.51	0.40
2:C:418:GLN:HG3	2:C:418:GLN:O	2.21	0.40
2:D:41:SER:HA	2:D:178:THR:HB	2.03	0.40
2:E:249:LEU:HD13	2:E:394:GLN:HG2	2.03	0.40
2:E:291:GLY:O	2:E:292:THR:C	2.64	0.40
2:F:79:THR:CG2	2:F:82:ASP:H	2.33	0.40
1:A:230:HIS:O	1:A:232:LYS:HD2	2.22	0.40
1:A:392:PHE:O	1:A:395:PHE:N	2.55	0.40
1:A:489:ILE:H	2:F:444:GLU:CD	2.29	0.40
2:B:133:ALA:HA	2:B:136:LYS:HB3	2.03	0.40
2:B:249:LEU:HD13	2:B:394:GLN:HG2	2.03	0.40
2:C:73:PHE:CD1	2:C:143:SER:HB2	2.54	0.40
2:C:297:LEU:O	2:C:298:VAL:C	2.64	0.40
2:C:483:PHE:HB2	2:C:489:ILE:HD13	2.04	0.40
2:D:161:ARG:CB	2:D:196:VAL:HG11	2.48	0.40
2:E:451:ARG:HB2	2:E:470:PHE:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:51:GLY:O	2:F:52:LYS:C	2.64	0.40
2:F:270:LEU:O	2:F:271:ASP:C	2.64	0.40
2:F:296:LEU:HD13	2:F:331:TRP:CD2	2.56	0.40
2:F:372:PRO:O	2:F:408:ILE:HD12	2.22	0.40
1:A:28:PHE:C	1:A:30:ASP:N	2.79	0.40
1:A:379:SER:C	1:A:381:SER:N	2.79	0.40
2:B:24:MET:HB3	2:B:62:ASN:HD22	1.85	0.40
2:B:164:LEU:HD23	2:B:164:LEU:HA	1.89	0.40
2:B:363:ILE:H	2:B:363:ILE:CD1	2.33	0.40
2:C:161:ARG:HB2	2:C:196:VAL:HG11	2.03	0.40
3:C:903:ATP:HO2'	2:D:230:HIS:CE1	2.40	0.40
2:D:147:VAL:CG2	2:D:148:THR:N	2.82	0.40
2:D:151:PHE:C	2:D:153:GLN:N	2.67	0.40
2:E:163:GLU:OE2	2:E:163:GLU:HA	2.20	0.40
2:E:240:THR:C	2:E:242:HIS:N	2.79	0.40
2:E:301:PHE:O	2:E:374:ARG:NH1	2.54	0.40
2:E:394:GLN:O	2:E:395:PHE:C	2.62	0.40
2:F:18:ILE:HB	2:F:228:THR:CG2	2.51	0.40
2:F:340:ARG:C	2:F:342:ASN:H	2.28	0.40
2:F:387:VAL:CG1	2:F:392:PHE:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/519 (97%)	364 (72%)	98 (20%)	40 (8%)	1	3
2	B	488/519 (94%)	368 (75%)	86 (18%)	34 (7%)	1	4
2	C	485/519 (93%)	371 (76%)	80 (16%)	34 (7%)	1	4
2	D	482/519 (93%)	378 (78%)	83 (17%)	21 (4%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	489/519 (94%)	374 (76%)	86 (18%)	29 (6%)	1	7
2	F	503/519 (97%)	384 (76%)	75 (15%)	44 (9%)	0	3
All	All	2949/3114 (95%)	2239 (76%)	508 (17%)	202 (7%)	1	5

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	65	ILE
1	A	154	TYR
1	A	193	ARG
1	A	212	GLU
1	A	420	MET
1	A	427	ASP
1	A	431	ALA
1	A	463	HIS
1	A	480	LYS
1	A	499	VAL
1	A	502	LYS
2	B	52	LYS
2	B	65	ILE
2	B	154	TYR
2	B	461	SER
2	B	463	HIS
2	B	494	PRO
2	B	498	THR
2	C	17	ALA
2	C	117	VAL
2	C	154	TYR
2	C	198	GLU
2	C	199	PHE
2	C	249	LEU
2	C	261	VAL
2	C	289	ALA
2	C	333	MET
2	C	463	HIS
2	D	17	ALA
2	D	122	ASP
2	D	152	GLN
2	D	154	TYR
2	D	333	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	154	TYR
2	E	333	MET
2	E	372	PRO
2	E	387	VAL
2	E	420	MET
2	E	428	SER
2	E	463	HIS
2	E	482	SER
2	F	26	GLU
2	F	52	LYS
2	F	117	VAL
2	F	118	VAL
2	F	154	TYR
2	F	157	SER
2	F	214	GLU
2	F	333	MET
2	F	387	VAL
2	F	463	HIS
2	F	488	ARG
2	F	504	GLU
2	F	506	SER
2	F	507	ARG
2	F	508	ILE
2	F	515	LYS
1	A	64	ILE
1	A	70	PRO
1	A	187	GLU
1	A	197	GLU
1	A	249	LEU
1	A	264	SER
1	A	268	VAL
1	A	309	LYS
1	A	333	MET
1	A	342	ASN
1	A	417	ASP
1	A	433	ILE
1	A	510	ARG
2	B	106	LEU
2	B	119	GLY
2	B	193	ARG
2	B	212	GLU
2	B	327	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	420	MET
2	B	424	SER
2	B	452	ALA
2	C	115	GLN
2	C	157	SER
2	C	341	GLN
2	C	400	THR
2	D	195	GLY
2	D	463	HIS
2	E	85	LYS
2	E	117	VAL
2	E	122	ASP
2	E	198	GLU
2	E	211	LEU
2	E	348	CYS
2	E	379	SER
2	E	431	ALA
2	E	484	ARG
2	F	47	THR
2	F	129	ARG
2	F	189	GLY
2	F	289	ALA
2	F	296	LEU
2	F	354	ALA
2	F	379	SER
2	F	420	MET
2	F	489	ILE
2	F	501	GLU
2	F	509	VAL
1	A	17	ALA
1	A	26	GLU
2	B	17	ALA
2	B	132	TYR
2	B	167	LEU
2	B	326	ARG
2	B	370	PHE
2	B	405	GLN
2	B	429	HIS
2	C	88	ARG
2	C	112	PRO
2	C	196	VAL
2	C	327	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	349	ALA
2	C	483	PHE
2	C	484	ARG
2	D	26	GLU
2	D	214	GLU
2	D	348	CYS
2	D	420	MET
2	E	26	GLU
2	E	86	ASN
2	E	189	GLY
2	E	422	ALA
2	F	115	GLN
2	F	294	LYS
1	A	83	ILE
1	A	120	GLY
1	A	384	ALA
1	A	490	ILE
2	B	88	ARG
2	B	157	SER
2	C	123	LEU
2	C	348	CYS
2	C	420	MET
2	D	175	GLY
2	D	292	THR
2	D	365	SER
2	D	378	ASP
2	E	212	GLU
2	E	282	SER
2	E	498	THR
2	E	504	GLU
2	F	194	TYR
2	F	211	LEU
2	F	212	GLU
2	F	273	MET
2	F	297	LEU
2	F	480	LYS
1	A	117	VAL
1	A	300	ARG
1	A	501	GLU
2	B	77	GLU
2	B	211	LEU
2	B	341	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	342	ASN
2	B	348	CYS
2	C	77	GLU
2	C	189	GLY
2	C	211	LEU
2	C	309	LYS
2	D	212	GLU
2	D	341	GLN
2	D	379	SER
2	F	61	TYR
2	F	303	GLU
2	F	468	ARG
2	F	490	ILE
1	A	112	PRO
1	A	157	SER
1	A	189	GLY
2	B	55	PHE
2	B	168	VAL
2	C	28	PHE
2	C	193	ARG
2	C	212	GLU
2	C	401	GLY
2	D	168	VAL
2	D	347	VAL
2	E	426	THR
2	F	370	PHE
2	C	268	VAL
2	D	492	GLY
2	E	425	ILE
2	F	110	PRO
2	B	268	VAL
2	E	227	GLY
2	F	80	PRO
1	A	118	VAL
2	B	117	VAL
2	C	347	VAL
2	E	293	GLY
2	F	347	VAL
1	A	347	VAL
1	A	363	ILE
2	B	489	ILE
2	F	517	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/441 (97%)	394 (92%)	35 (8%)	10	37
2	B	417/442 (94%)	386 (93%)	31 (7%)	13	42
2	C	414/442 (94%)	376 (91%)	38 (9%)	8	33
2	D	411/442 (93%)	367 (89%)	44 (11%)	6	26
2	E	418/442 (95%)	382 (91%)	36 (9%)	10	36
2	F	430/442 (97%)	381 (89%)	49 (11%)	5	24
All	All	2519/2651 (95%)	2286 (91%)	233 (9%)	8	33

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	26	GLU
1	A	29	ASP
1	A	30	ASP
1	A	42	THR
1	A	48	SER
1	A	50	THR
1	A	75	THR
1	A	84	ILE
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	134	ILE
1	A	183	GLU
1	A	212	GLU
1	A	219	THR
1	A	223	LEU
1	A	238	THR
1	A	263	VAL
1	A	270	LEU
1	A	280	LYS
1	A	287	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	298	VAL
1	A	336	GLU
1	A	342	ASN
1	A	360	LEU
1	A	375	ILE
1	A	406	GLU
1	A	407	GLU
1	A	427	ASP
1	A	434	THR
1	A	453	ILE
1	A	463	HIS
1	A	469	GLU
1	A	518	GLU
2	B	26	GLU
2	B	47	THR
2	B	50	THR
2	B	81	GLN
2	B	103	LEU
2	B	111	ASP
2	B	147	VAL
2	B	150	VAL
2	B	151	PHE
2	B	154	TYR
2	B	182	THR
2	B	185	ILE
2	B	186	GLU
2	B	193	ARG
2	B	198	GLU
2	B	212	GLU
2	B	223	LEU
2	B	238	THR
2	B	270	LEU
2	B	283	ILE
2	B	292	THR
2	B	302	VAL
2	B	333	MET
2	B	428	SER
2	B	434	THR
2	B	453	ILE
2	B	454	ASN
2	B	462	TRP
2	B	474	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	490	ILE
2	B	499	VAL
2	C	15	HIS
2	C	26	GLU
2	C	50	THR
2	C	99	ASP
2	C	127	ILE
2	C	140	ARG
2	C	149	SER
2	C	151	PHE
2	C	154	TYR
2	C	184	ARG
2	C	185	ILE
2	C	186	GLU
2	C	210	VAL
2	C	219	THR
2	C	223	LEU
2	C	238	THR
2	C	245	ASN
2	C	256	GLN
2	C	263	VAL
2	C	290	THR
2	C	295	THR
2	C	300	ARG
2	C	303	GLU
2	C	333	MET
2	C	336	GLU
2	C	344	LEU
2	C	356	LEU
2	C	375	ILE
2	C	383	LEU
2	C	428	SER
2	C	449	MET
2	C	453	ILE
2	C	454	ASN
2	C	463	HIS
2	C	471	MET
2	C	474	ASP
2	C	491	SER
2	C	497	ILE
2	D	18	ILE
2	D	26	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	30	ASP
2	D	75	THR
2	D	77	GLU
2	D	81	GLN
2	D	94	LEU
2	D	106	LEU
2	D	122	ASP
2	D	123	LEU
2	D	154	TYR
2	D	177	THR
2	D	186	GLU
2	D	211	LEU
2	D	212	GLU
2	D	218	ARG
2	D	238	THR
2	D	246	ILE
2	D	247	PHE
2	D	256	GLN
2	D	263	VAL
2	D	270	LEU
2	D	274	CYS
2	D	284	ILE
2	D	290	THR
2	D	292	THR
2	D	302	VAL
2	D	321	ARG
2	D	356	LEU
2	D	360	LEU
2	D	366	GLU
2	D	394	GLN
2	D	399	VAL
2	D	423	HIS
2	D	428	SER
2	D	434	THR
2	D	463	HIS
2	D	469	GLU
2	D	471	MET
2	D	474	ASP
2	D	489	ILE
2	D	490	ILE
2	D	496	ARG
2	D	498	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	18	ILE
2	E	26	GLU
2	E	41	SER
2	E	52	LYS
2	E	54	LEU
2	E	81	GLN
2	E	113	GLU
2	E	116	GLU
2	E	121	PHE
2	E	132	TYR
2	E	135	GLN
2	E	146	SER
2	E	151	PHE
2	E	177	THR
2	E	178	THR
2	E	196	VAL
2	E	201	SER
2	E	212	GLU
2	E	217	ARG
2	E	218	ARG
2	E	228	THR
2	E	238	THR
2	E	239	ILE
2	E	240	THR
2	E	256	GLN
2	E	263	VAL
2	E	270	LEU
2	E	271	ASP
2	E	325	LEU
2	E	366	GLU
2	E	387	VAL
2	E	449	MET
2	E	450	SER
2	E	451	ARG
2	E	453	ILE
2	E	458	MET
2	F	15	HIS
2	F	26	GLU
2	F	47	THR
2	F	56	SER
2	F	65	ILE
2	F	75	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	76	PHE
2	F	79	THR
2	F	103	LEU
2	F	121	PHE
2	F	140	ARG
2	F	154	TYR
2	F	168	VAL
2	F	178	THR
2	F	183	GLU
2	F	184	ARG
2	F	185	ILE
2	F	186	GLU
2	F	210	VAL
2	F	212	GLU
2	F	215	ARG
2	F	218	ARG
2	F	256	GLN
2	F	263	VAL
2	F	300	ARG
2	F	302	VAL
2	F	325	LEU
2	F	344	LEU
2	F	363	ILE
2	F	366	GLU
2	F	375	ILE
2	F	387	VAL
2	F	424	SER
2	F	427	ASP
2	F	429	HIS
2	F	456	PHE
2	F	458	MET
2	F	462	TRP
2	F	469	GLU
2	F	471	MET
2	F	472	ILE
2	F	490	ILE
2	F	493	SER
2	F	496	ARG
2	F	497	ILE
2	F	501	GLU
2	F	504	GLU
2	F	509	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	514	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	62	ASN
1	A	131	ASN
1	A	152	GLN
1	A	209	ASN
1	A	304	ASN
1	A	308	ASN
1	A	327	ASN
1	A	368	ASN
1	A	414	ASN
1	A	441	GLN
1	A	454	ASN
1	A	463	HIS
2	B	62	ASN
2	B	209	ASN
2	B	341	GLN
2	B	361	GLN
2	B	394	GLN
2	B	405	GLN
2	B	441	GLN
2	C	33	HIS
2	C	58	GLN
2	C	62	ASN
2	C	81	GLN
2	C	173	GLN
2	C	209	ASN
2	C	245	ASN
2	C	260	ASN
2	C	323	GLN
2	C	342	ASN
2	C	359	HIS
2	C	389	ASN
2	C	414	ASN
2	C	418	GLN
2	C	423	HIS
2	D	33	HIS
2	D	115	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	209	ASN
2	D	245	ASN
2	D	327	ASN
2	D	342	ASN
2	D	394	GLN
2	D	418	GLN
2	D	429	HIS
2	D	441	GLN
2	E	15	HIS
2	E	33	HIS
2	E	81	GLN
2	E	135	GLN
2	E	153	GLN
2	E	209	ASN
2	E	260	ASN
2	E	304	ASN
2	E	323	GLN
2	E	341	GLN
2	E	359	HIS
2	E	361	GLN
2	E	368	ASN
2	E	390	ASN
2	E	429	HIS
2	E	441	GLN
2	E	454	ASN
2	F	16	GLN
2	F	58	GLN
2	F	153	GLN
2	F	209	ASN
2	F	245	ASN
2	F	308	ASN
2	F	327	ASN
2	F	342	ASN
2	F	418	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TPO	D	432	2	8,10,11	1.32	1 (12%)	10,14,16	2.18	1 (10%)
2	TPO	E	432	2	8,10,11	1.92	2 (25%)	10,14,16	2.70	2 (20%)
1	TPO	A	432	1	8,10,11	1.70	3 (37%)	10,14,16	2.84	1 (10%)
2	TPO	B	432	2	8,10,11	1.24	2 (25%)	10,14,16	2.32	2 (20%)
2	TPO	F	432	2	8,10,11	1.91	2 (25%)	10,14,16	2.41	2 (20%)
2	TPO	C	432	2	8,10,11	3.86	5 (62%)	10,14,16	2.15	4 (40%)
1	TPO	A	426	1	8,10,11	1.28	1 (12%)	10,14,16	1.46	1 (10%)

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
2	TPO	D	432	2	-	0/9/11/13	-
2	TPO	E	432	2	-	4/9/11/13	-
1	TPO	A	432	1	-	4/9/11/13	-
2	TPO	B	432	2	-	1/9/11/13	-
2	TPO	F	432	2	-	0/9/11/13	-
2	TPO	C	432	2	-	1/9/11/13	-
1	TPO	A	426	1	-	1/9/11/13	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	432	TPO	P-O2P	6.93	1.80	1.54
2	C	432	TPO	CB-CA	6.59	1.67	1.53
2	F	432	TPO	CG2-CB	-3.89	1.42	1.51
2	E	432	TPO	CG2-CB	-3.73	1.42	1.51
2	C	432	TPO	CA-N	2.88	1.56	1.47
2	C	432	TPO	P-O1P	-2.87	1.41	1.50
2	E	432	TPO	P-O2P	-2.86	1.44	1.54
2	C	432	TPO	P-O3P	2.80	1.65	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	TPO	P-O2P	-2.78	1.44	1.54
2	F	432	TPO	P-O2P	-2.55	1.45	1.54
1	A	432	TPO	P-O3P	2.40	1.63	1.54
1	A	432	TPO	CG2-CB	-2.30	1.46	1.51
1	A	426	TPO	CG2-CB	2.22	1.56	1.51
2	B	432	TPO	P-O2P	-2.20	1.46	1.54
2	D	432	TPO	P-O3P	2.13	1.62	1.54
2	B	432	TPO	P-O3P	2.10	1.62	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	TPO	P-OG1-CB	-8.13	101.22	123.33
2	E	432	TPO	P-OG1-CB	-7.48	102.99	123.33
2	F	432	TPO	P-OG1-CB	-6.54	105.56	123.33
2	B	432	TPO	P-OG1-CB	-6.26	106.32	123.33
2	D	432	TPO	P-OG1-CB	-6.00	107.03	123.33
2	C	432	TPO	O3P-P-O2P	-3.59	94.32	107.80
1	A	426	TPO	P-OG1-CB	-3.48	113.88	123.33
2	C	432	TPO	O3P-P-OG1	3.39	119.07	105.85
2	C	432	TPO	O2P-P-OG1	2.83	116.89	105.85
2	C	432	TPO	OG1-P-O1P	-2.41	100.75	109.33
2	B	432	TPO	CG2-CB-CA	-2.29	108.80	113.26
2	E	432	TPO	O3P-P-OG1	2.26	114.67	105.85
2	F	432	TPO	O3P-P-OG1	2.03	113.74	105.85

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	432	TPO	N-CA-CB-CG2
1	A	432	TPO	N-CA-CB-OG1
1	A	432	TPO	C-CA-CB-CG2
1	A	432	TPO	O-C-CA-CB
2	C	432	TPO	N-CA-CB-OG1
2	E	432	TPO	N-CA-CB-CG2
2	E	432	TPO	N-CA-CB-OG1
2	E	432	TPO	C-CA-CB-CG2
2	E	432	TPO	O-C-CA-CB
1	A	426	TPO	CG2-CB-OG1-P
2	B	432	TPO	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	432	TPO	3	0
1	A	432	TPO	2	0
2	B	432	TPO	1	0
2	F	432	TPO	3	0
2	C	432	TPO	5	0
1	A	426	TPO	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 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	ATP	B	903	4	32,33,33	1.09	2 (6%)	48,52,52	2.05	11 (22%)
3	ATP	E	901	4	32,33,33	1.09	2 (6%)	48,52,52	2.19	14 (29%)
3	ATP	E	903	4	32,33,33	1.27	2 (6%)	48,52,52	2.06	14 (29%)
3	ATP	D	903	4	32,33,33	1.16	4 (12%)	48,52,52	2.10	11 (22%)
3	ATP	A	903	4	32,33,33	1.09	4 (12%)	48,52,52	1.97	11 (22%)
3	ATP	F	901	4	32,33,33	1.11	3 (9%)	48,52,52	2.06	12 (25%)
3	ATP	A	901	4	32,33,33	1.16	4 (12%)	48,52,52	2.02	11 (22%)
3	ATP	D	901	4	32,33,33	1.25	3 (9%)	48,52,52	2.09	12 (25%)
3	ATP	C	901	4	32,33,33	1.10	3 (9%)	48,52,52	2.12	13 (27%)
3	ATP	C	903	4	32,33,33	0.96	1 (3%)	48,52,52	2.07	13 (27%)
3	ATP	F	903	4	32,33,33	1.21	3 (9%)	48,52,52	2.14	14 (29%)
3	ATP	B	901	4	32,33,33	1.23	4 (12%)	48,52,52	2.07	12 (25%)

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	ATP	B	903	4	-	9/22/38/38	0/3/3/3
3	ATP	E	901	4	-	7/22/38/38	0/3/3/3
3	ATP	E	903	4	-	7/22/38/38	0/3/3/3
3	ATP	D	903	4	-	9/22/38/38	0/3/3/3
3	ATP	A	903	4	-	7/22/38/38	0/3/3/3
3	ATP	F	901	4	-	6/22/38/38	0/3/3/3
3	ATP	A	901	4	-	6/22/38/38	0/3/3/3
3	ATP	D	901	4	-	6/22/38/38	0/3/3/3
3	ATP	C	901	4	-	10/22/38/38	0/3/3/3
3	ATP	C	903	4	-	8/22/38/38	0/3/3/3
3	ATP	F	903	4	-	9/22/38/38	0/3/3/3
3	ATP	B	901	4	-	6/22/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	903	ATP	PB-O3B	-3.97	1.55	1.59
3	D	903	ATP	PB-O3B	-3.01	1.56	1.59
3	E	901	ATP	C2-N3	2.98	1.39	1.33
3	C	901	ATP	C2-N3	2.95	1.39	1.33
3	F	903	ATP	C2-N3	2.93	1.39	1.33
3	B	901	ATP	PB-O3A	2.91	1.62	1.59
3	D	901	ATP	C2-N3	2.74	1.38	1.33
3	F	901	ATP	C2-N3	2.74	1.38	1.33
3	B	903	ATP	C2-N3	2.64	1.38	1.33
3	D	901	ATP	C2-N1	2.62	1.38	1.33
3	B	903	ATP	C1'-N9	2.54	1.53	1.46
3	A	901	ATP	C2-N3	2.49	1.38	1.33
3	A	903	ATP	C1'-N9	2.46	1.53	1.46
3	D	903	ATP	C2-N3	2.44	1.38	1.33
3	C	901	ATP	O4'-C4'	-2.40	1.39	1.45
3	A	901	ATP	C1'-N9	2.40	1.53	1.46
3	B	901	ATP	C2-N3	2.35	1.38	1.33
3	B	901	ATP	PA-O3A	2.35	1.62	1.59
3	A	901	ATP	PB-O3B	-2.35	1.57	1.59
3	F	903	ATP	C2-N1	2.34	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	ATP	C1'-N9	2.32	1.52	1.46
3	D	903	ATP	C4-N3	2.26	1.38	1.34
3	E	901	ATP	C2-N1	2.26	1.38	1.33
3	C	901	ATP	C2-N1	2.23	1.37	1.33
3	D	901	ATP	C4-N3	2.21	1.38	1.34
3	F	901	ATP	C2-N1	2.20	1.37	1.33
3	A	903	ATP	C2-N3	2.18	1.37	1.33
3	E	903	ATP	C2-N3	2.17	1.37	1.33
3	F	903	ATP	PB-O3A	-2.13	1.57	1.59
3	A	901	ATP	C2-N1	2.13	1.37	1.33
3	F	901	ATP	C4-N3	2.12	1.38	1.34
3	C	903	ATP	C2-N3	2.10	1.37	1.33
3	A	903	ATP	C2-N1	2.08	1.37	1.33
3	A	903	ATP	C5-N7	-2.07	1.35	1.39
3	D	903	ATP	C2-N1	2.02	1.37	1.33

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	903	ATP	N3-C2-N1	-5.83	119.76	128.58
3	F	901	ATP	N3-C2-N1	-5.76	119.86	128.58
3	D	901	ATP	N3-C2-N1	-5.72	119.92	128.58
3	C	903	ATP	N3-C2-N1	-5.65	120.03	128.58
3	B	901	ATP	N3-C2-N1	-5.64	120.05	128.58
3	E	901	ATP	N3-C2-N1	-5.61	120.09	128.58
3	F	903	ATP	N3-C2-N1	-5.55	120.18	128.58
3	E	903	ATP	N3-C2-N1	-5.52	120.23	128.58
3	A	901	ATP	N3-C2-N1	-5.49	120.28	128.58
3	A	903	ATP	N3-C2-N1	-5.48	120.29	128.58
3	C	901	ATP	N3-C2-N1	-5.46	120.31	128.58
3	B	903	ATP	N3-C2-N1	-5.46	120.31	128.58
3	B	903	ATP	C5-N7-C8	5.36	111.87	103.45
3	B	901	ATP	C5-N7-C8	5.32	111.81	103.45
3	D	901	ATP	C5-N7-C8	5.28	111.74	103.45
3	A	901	ATP	C5-N7-C8	5.27	111.73	103.45
3	A	903	ATP	C5-N7-C8	5.27	111.72	103.45
3	E	901	ATP	C5-N7-C8	5.24	111.68	103.45
3	C	901	ATP	C5-N7-C8	5.22	111.66	103.45
3	F	903	ATP	C5-N7-C8	5.21	111.63	103.45
3	C	901	ATP	C4-C5-N7	-5.09	104.77	110.58
3	C	903	ATP	C5-N7-C8	5.06	111.41	103.45
3	F	903	ATP	C4-C5-N7	-4.99	104.87	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	901	ATP	C5-N7-C8	4.99	111.29	103.45
3	D	903	ATP	C5-N7-C8	4.98	111.28	103.45
3	D	903	ATP	N9-C8-N7	-4.97	106.89	113.94
3	A	901	ATP	C4-C5-N7	-4.96	104.91	110.58
3	B	901	ATP	C4-C5-N7	-4.93	104.94	110.58
3	E	901	ATP	C4-C5-N7	-4.93	104.95	110.58
3	B	903	ATP	C4-C5-N7	-4.91	104.97	110.58
3	F	901	ATP	C4-C5-N7	-4.89	104.99	110.58
3	E	903	ATP	C5-N7-C8	4.81	111.01	103.45
3	C	903	ATP	N9-C8-N7	-4.81	107.12	113.94
3	B	901	ATP	N9-C8-N7	-4.80	107.12	113.94
3	C	903	ATP	C4-C5-N7	-4.74	105.17	110.58
3	E	901	ATP	N9-C8-N7	-4.73	107.22	113.94
3	D	903	ATP	C4-C5-N7	-4.64	105.28	110.58
3	B	903	ATP	N9-C8-N7	-4.63	107.37	113.94
3	E	903	ATP	N9-C8-N7	-4.59	107.42	113.94
3	E	903	ATP	C4-C5-N7	-4.57	105.36	110.58
3	A	903	ATP	C4-C5-N7	-4.54	105.39	110.58
3	F	903	ATP	N9-C8-N7	-4.53	107.50	113.94
3	D	901	ATP	C4-C5-N7	-4.51	105.42	110.58
3	A	903	ATP	N9-C8-N7	-4.50	107.55	113.94
3	C	901	ATP	N9-C8-N7	-4.49	107.57	113.94
3	A	901	ATP	N9-C8-N7	-4.40	107.70	113.94
3	D	901	ATP	N9-C8-N7	-4.21	107.97	113.94
3	F	901	ATP	N9-C8-N7	-4.14	108.06	113.94
3	F	903	ATP	O2B-PB-O3B	3.60	116.99	107.27
3	F	903	ATP	O3A-PB-O1B	-3.59	99.91	110.70
3	F	901	ATP	C5-C4-N3	-3.47	121.94	126.72
3	C	901	ATP	C5-C4-N3	-3.38	122.06	126.72
3	A	901	ATP	C5-C4-N3	-3.35	122.10	126.72
3	E	901	ATP	C5-C4-N3	-3.35	122.11	126.72
3	D	903	ATP	C6-C5-N7	3.34	138.53	132.09
3	B	903	ATP	C5-C4-N3	-3.31	122.16	126.72
3	E	901	ATP	C2-N3-C4	3.29	119.86	111.83
3	D	901	ATP	O2B-PB-O3B	3.29	116.16	107.27
3	F	903	ATP	C5-C4-N3	-3.25	122.24	126.72
3	E	901	ATP	O2B-PB-O3B	3.25	116.06	107.27
3	D	903	ATP	C2-N3-C4	3.25	119.76	111.83
3	C	901	ATP	C2-N3-C4	3.23	119.73	111.83
3	D	903	ATP	C2'-C1'-N9	3.22	121.30	113.30
3	C	903	ATP	C5-C4-N3	-3.20	122.31	126.72
3	A	901	ATP	C2-N3-C4	3.19	119.62	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	ATP	C5-C4-N3	-3.17	122.35	126.72
3	B	903	ATP	C2-N3-C4	3.16	119.56	111.83
3	D	901	ATP	C5-C4-N3	-3.16	122.36	126.72
3	F	901	ATP	C2-N3-C4	3.16	119.54	111.83
3	B	901	ATP	C2'-C1'-N9	3.13	121.07	113.30
3	E	903	ATP	C6-C5-N7	3.12	138.11	132.09
3	B	901	ATP	O2B-PB-O3B	3.12	115.71	107.27
3	F	903	ATP	C2-N3-C4	3.12	119.45	111.83
3	C	901	ATP	O2B-PB-O3B	3.12	115.70	107.27
3	D	903	ATP	C4-N9-C8	3.09	108.98	105.74
3	C	901	ATP	O4'-C1'-N9	-3.08	102.17	108.09
3	C	903	ATP	C2-N3-C4	3.08	119.35	111.83
3	B	901	ATP	C2-N3-C4	3.07	119.33	111.83
3	B	901	ATP	C5-C4-N3	-3.07	122.49	126.72
3	E	903	ATP	C2-N3-C4	3.05	119.28	111.83
3	E	901	ATP	O3A-PB-O1B	-3.04	101.56	110.70
3	E	901	ATP	C6-C5-N7	3.01	137.89	132.09
3	E	903	ATP	C2'-C1'-N9	3.00	120.76	113.30
3	B	901	ATP	C6-C5-N7	3.00	137.88	132.09
3	A	903	ATP	C2-N3-C4	2.99	119.13	111.83
3	A	901	ATP	O2B-PB-O3B	2.97	115.31	107.27
3	E	903	ATP	C5-C4-N3	-2.95	122.66	126.72
3	B	903	ATP	C6-C5-N7	2.94	137.76	132.09
3	C	903	ATP	C6-C5-N7	2.94	137.76	132.09
3	A	901	ATP	C6-C5-N7	2.93	137.73	132.09
3	C	901	ATP	C6-C5-N7	2.92	137.72	132.09
3	D	901	ATP	O4'-C1'-N9	-2.91	102.50	108.09
3	D	901	ATP	C2-N3-C4	2.91	118.93	111.83
3	F	903	ATP	C2'-C1'-N9	2.89	120.48	113.30
3	D	901	ATP	C2'-C1'-N9	2.85	120.39	113.30
3	B	903	ATP	C2'-C1'-N9	2.83	120.34	113.30
3	F	903	ATP	C6-C5-N7	2.82	137.53	132.09
3	E	901	ATP	O4'-C1'-N9	-2.79	102.73	108.09
3	F	901	ATP	O2B-PB-O3B	2.77	114.77	107.27
3	C	903	ATP	O2B-PB-O3B	2.75	114.70	107.27
3	A	903	ATP	C2'-C1'-N9	2.72	120.07	113.30
3	D	903	ATP	C5-C4-N3	-2.71	122.98	126.72
3	F	901	ATP	C6-C5-N7	2.61	137.13	132.09
3	E	901	ATP	C2'-C1'-N9	2.60	119.75	113.30
3	A	903	ATP	O2B-PB-O3B	2.58	114.26	107.27
3	F	901	ATP	C2'-C1'-N9	2.58	119.71	113.30
3	E	901	ATP	C4-N9-C8	2.55	108.42	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	ATP	C4-N9-C8	2.55	108.41	105.74
3	E	903	ATP	C4-N9-C8	2.54	108.40	105.74
3	E	903	ATP	O4'-C1'-N9	-2.53	103.23	108.09
3	D	901	ATP	O3B-PB-O1B	-2.51	103.15	110.70
3	A	901	ATP	C2'-C1'-N9	2.51	119.53	113.30
3	D	901	ATP	O3A-PB-O1B	-2.49	103.22	110.70
3	D	901	ATP	C6-C5-N7	2.49	136.89	132.09
3	C	901	ATP	C4-N9-C8	2.48	108.35	105.74
3	F	903	ATP	O3B-PB-O1B	-2.43	103.39	110.70
3	F	903	ATP	O4'-C1'-N9	-2.43	103.43	108.09
3	A	903	ATP	C6-C5-N7	2.41	136.74	132.09
3	C	901	ATP	C2'-C1'-N9	2.40	119.28	113.30
3	C	901	ATP	O2'-C2'-C3'	2.30	119.20	111.82
3	F	903	ATP	C4-N9-C8	2.29	108.14	105.74
3	B	901	ATP	C4-N9-C8	2.28	108.13	105.74
3	F	903	ATP	O2G-PG-O3B	2.27	112.26	104.64
3	E	903	ATP	O2B-PB-O3B	2.27	113.41	107.27
3	E	901	ATP	O3B-PB-O1B	-2.24	103.96	110.70
3	B	903	ATP	O2'-C2'-C3'	2.21	118.92	111.82
3	D	903	ATP	O4'-C1'-N9	-2.20	103.86	108.09
3	F	901	ATP	O2'-C2'-C3'	2.19	118.85	111.82
3	B	903	ATP	O2G-PG-O3B	2.19	111.97	104.64
3	A	901	ATP	O3B-PB-O1B	-2.18	104.14	110.70
3	C	901	ATP	O2G-PG-O3B	2.15	111.86	104.64
3	C	903	ATP	O3A-PB-O1B	-2.15	104.24	110.70
3	B	901	ATP	O3B-PB-O1B	-2.14	104.26	110.70
3	A	903	ATP	O2G-PG-O3B	2.13	111.78	104.64
3	A	903	ATP	O3A-PB-O1B	-2.09	104.41	110.70
3	B	903	ATP	O2B-PB-O3B	2.09	112.93	107.27
3	E	903	ATP	N6-C6-N1	-2.08	113.75	118.38
3	E	901	ATP	O2'-C2'-C3'	2.08	118.48	111.82
3	C	903	ATP	C3'-C2'-C1'	2.08	105.39	101.46
3	B	901	ATP	O2'-C2'-C3'	2.07	118.45	111.82
3	F	901	ATP	O3B-PB-O1B	-2.05	104.54	110.70
3	C	903	ATP	N6-C6-N1	-2.05	113.81	118.38
3	E	903	ATP	C2'-C3'-C4'	2.04	106.56	102.61
3	A	901	ATP	C5-C4-N9	2.04	108.03	105.81
3	C	903	ATP	O3B-PB-O1B	-2.02	104.61	110.70
3	F	901	ATP	O4'-C1'-N9	-2.02	104.21	108.09
3	E	903	ATP	O2G-PG-O3B	2.02	111.40	104.64
3	D	903	ATP	N6-C6-N1	-2.01	113.89	118.38

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	C3'-C4'-C5'-O5'
3	A	903	ATP	PB-O3B-PG-O3G
3	A	903	ATP	C5'-O5'-PA-O1A
3	B	901	ATP	C5'-O5'-PA-O1A
3	B	903	ATP	PB-O3B-PG-O3G
3	B	903	ATP	O4'-C4'-C5'-O5'
3	C	901	ATP	C5'-O5'-PA-O2A
3	C	901	ATP	C5'-O5'-PA-O3A
3	C	903	ATP	PB-O3B-PG-O3G
3	C	903	ATP	PB-O3A-PA-O5'
3	C	903	ATP	C5'-O5'-PA-O1A
3	C	903	ATP	O4'-C4'-C5'-O5'
3	C	903	ATP	C3'-C4'-C5'-O5'
3	D	901	ATP	C5'-O5'-PA-O3A
3	D	903	ATP	PB-O3B-PG-O3G
3	D	903	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	C5'-O5'-PA-O3A
3	E	903	ATP	C5'-O5'-PA-O1A
3	E	903	ATP	C5'-O5'-PA-O3A
3	F	901	ATP	C5'-O5'-PA-O1A
3	F	901	ATP	C5'-O5'-PA-O3A
3	F	901	ATP	C3'-C4'-C5'-O5'
3	F	903	ATP	C5'-O5'-PA-O1A
3	F	903	ATP	C5'-O5'-PA-O3A
3	F	903	ATP	O4'-C4'-C5'-O5'
3	A	903	ATP	C3'-C4'-C5'-O5'
3	B	901	ATP	C3'-C4'-C5'-O5'
3	B	903	ATP	C3'-C4'-C5'-O5'
3	C	901	ATP	C3'-C4'-C5'-O5'
3	D	901	ATP	C3'-C4'-C5'-O5'
3	D	903	ATP	C3'-C4'-C5'-O5'
3	E	901	ATP	C3'-C4'-C5'-O5'
3	E	903	ATP	C3'-C4'-C5'-O5'
3	F	903	ATP	C3'-C4'-C5'-O5'
3	A	901	ATP	O4'-C4'-C5'-O5'
3	B	901	ATP	O4'-C4'-C5'-O5'
3	C	901	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	O4'-C4'-C5'-O5'
3	E	903	ATP	O4'-C4'-C5'-O5'
3	F	901	ATP	O4'-C4'-C5'-O5'
3	D	901	ATP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	903	ATP	O4'-C4'-C5'-O5'
3	F	903	ATP	PB-O3B-PG-O1G
3	B	903	ATP	PB-O3A-PA-O1A
3	A	901	ATP	PB-O3A-PA-O5'
3	A	903	ATP	PB-O3A-PA-O5'
3	B	901	ATP	PB-O3A-PA-O5'
3	B	903	ATP	PB-O3A-PA-O5'
3	C	901	ATP	PB-O3A-PA-O5'
3	D	901	ATP	PB-O3A-PA-O5'
3	D	903	ATP	PB-O3A-PA-O5'
3	E	901	ATP	PB-O3A-PA-O5'
3	E	903	ATP	PB-O3A-PA-O5'
3	F	901	ATP	PB-O3A-PA-O5'
3	F	903	ATP	PB-O3A-PA-O5'
3	A	901	ATP	PA-O3A-PB-O2B
3	A	903	ATP	PA-O3A-PB-O2B
3	B	901	ATP	PA-O3A-PB-O2B
3	B	903	ATP	PA-O3A-PB-O2B
3	C	901	ATP	PA-O3A-PB-O2B
3	C	903	ATP	PA-O3A-PB-O2B
3	D	901	ATP	PA-O3A-PB-O2B
3	D	903	ATP	PA-O3A-PB-O2B
3	E	901	ATP	PA-O3A-PB-O2B
3	E	903	ATP	PA-O3A-PB-O2B
3	F	901	ATP	PA-O3A-PB-O2B
3	F	903	ATP	PA-O3A-PB-O2B
3	A	901	ATP	C5'-O5'-PA-O3A
3	B	903	ATP	C5'-O5'-PA-O1A
3	C	901	ATP	C5'-O5'-PA-O1A
3	D	901	ATP	C5'-O5'-PA-O1A
3	D	903	ATP	C5'-O5'-PA-O1A
3	E	901	ATP	C5'-O5'-PA-O1A
3	C	901	ATP	PB-O3A-PA-O2A
3	B	903	ATP	PB-O3B-PG-O1G
3	D	903	ATP	PB-O3B-PG-O1G
3	C	901	ATP	PB-O3B-PG-O2G
3	C	901	ATP	PB-O3B-PG-O3G
3	D	903	ATP	PB-O3B-PG-O2G
3	B	901	ATP	C4'-C5'-O5'-PA
3	A	903	ATP	PB-O3A-PA-O2A
3	B	903	ATP	PA-O3A-PB-O1B
3	D	903	ATP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	903	ATP	PA-O3A-PB-O1B
3	F	903	ATP	PB-O3A-PA-O2A
3	C	903	ATP	PB-O3A-PA-O1A
3	C	903	ATP	PB-O3A-PA-O2A
3	E	901	ATP	PA-O3A-PB-O1B
3	F	903	ATP	PA-O3A-PB-O1B

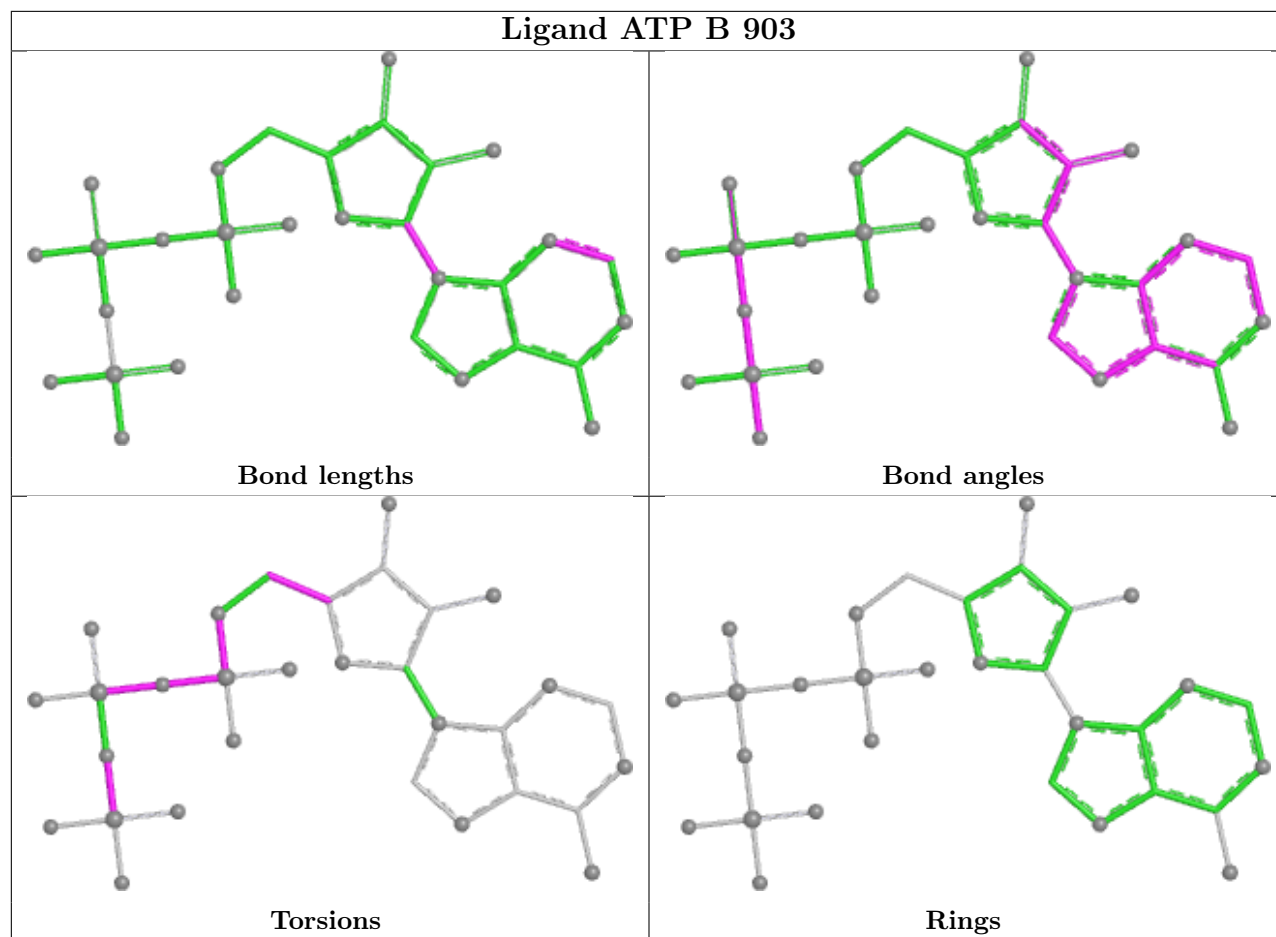
There are no ring outliers.

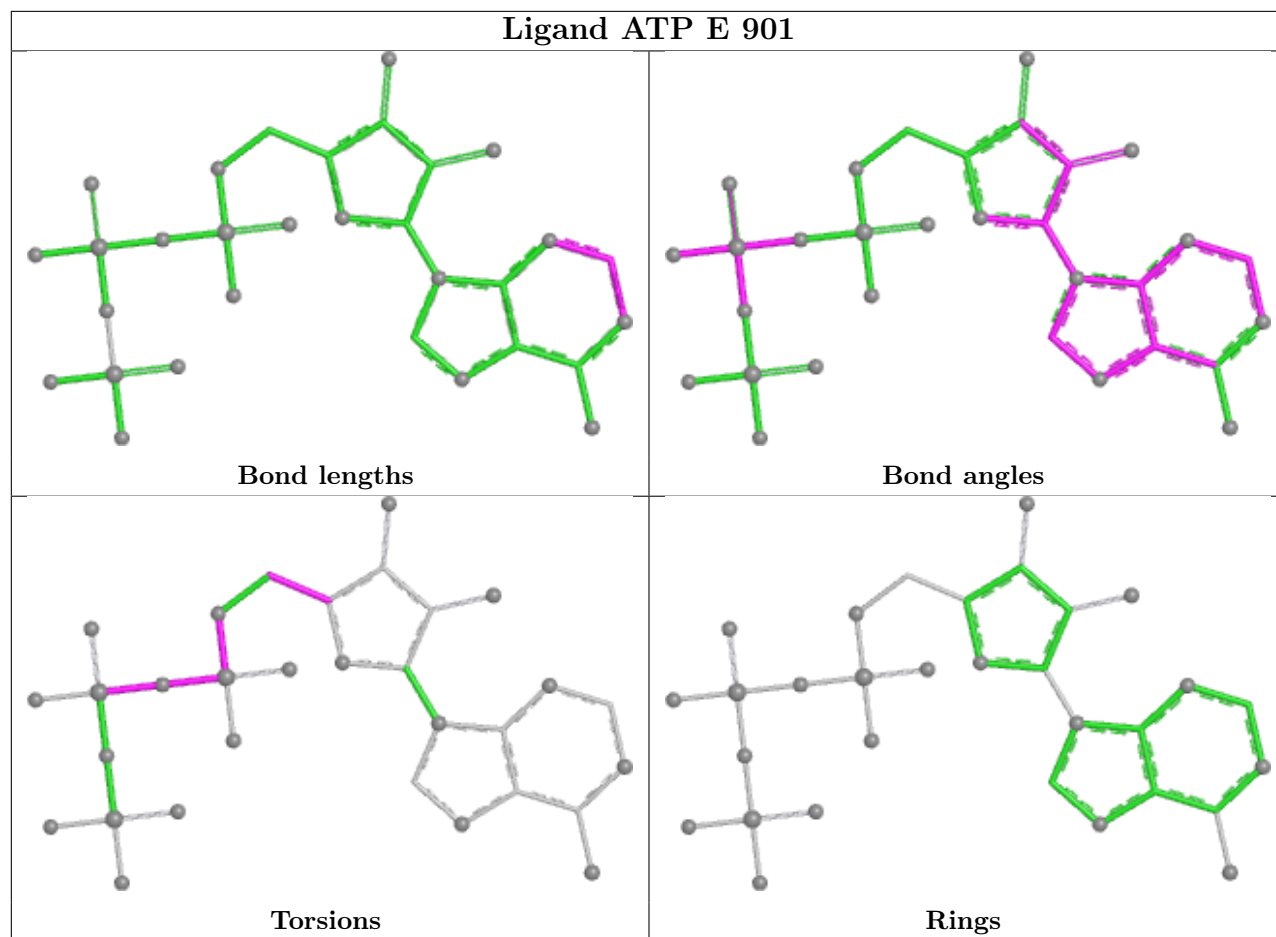
12 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	903	ATP	4	0
3	E	901	ATP	3	0
3	E	903	ATP	3	0
3	D	903	ATP	5	0
3	A	903	ATP	3	0
3	F	901	ATP	4	0
3	A	901	ATP	5	0
3	D	901	ATP	8	0
3	C	901	ATP	3	0
3	C	903	ATP	2	0
3	F	903	ATP	3	0
3	B	901	ATP	4	0

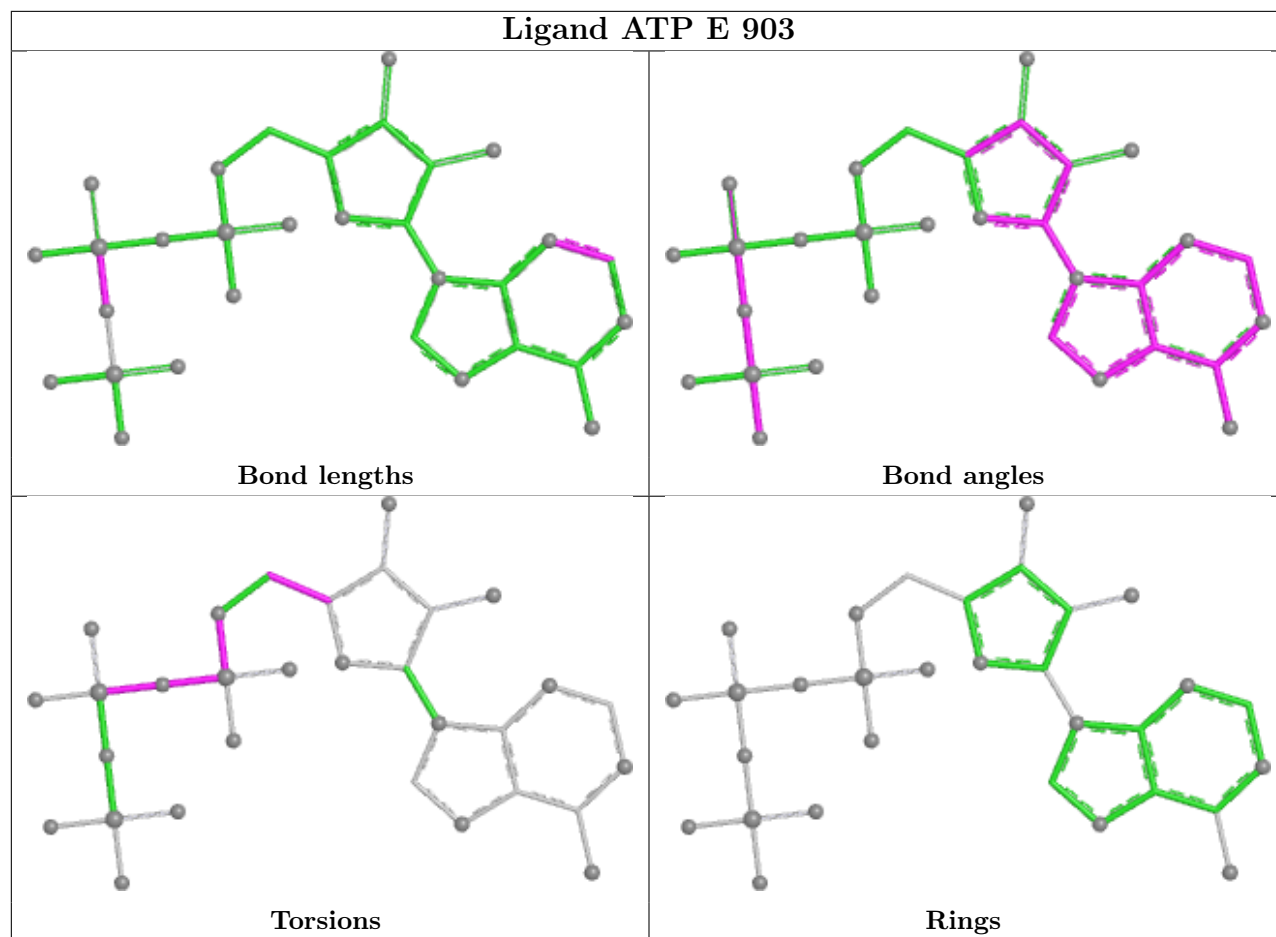
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

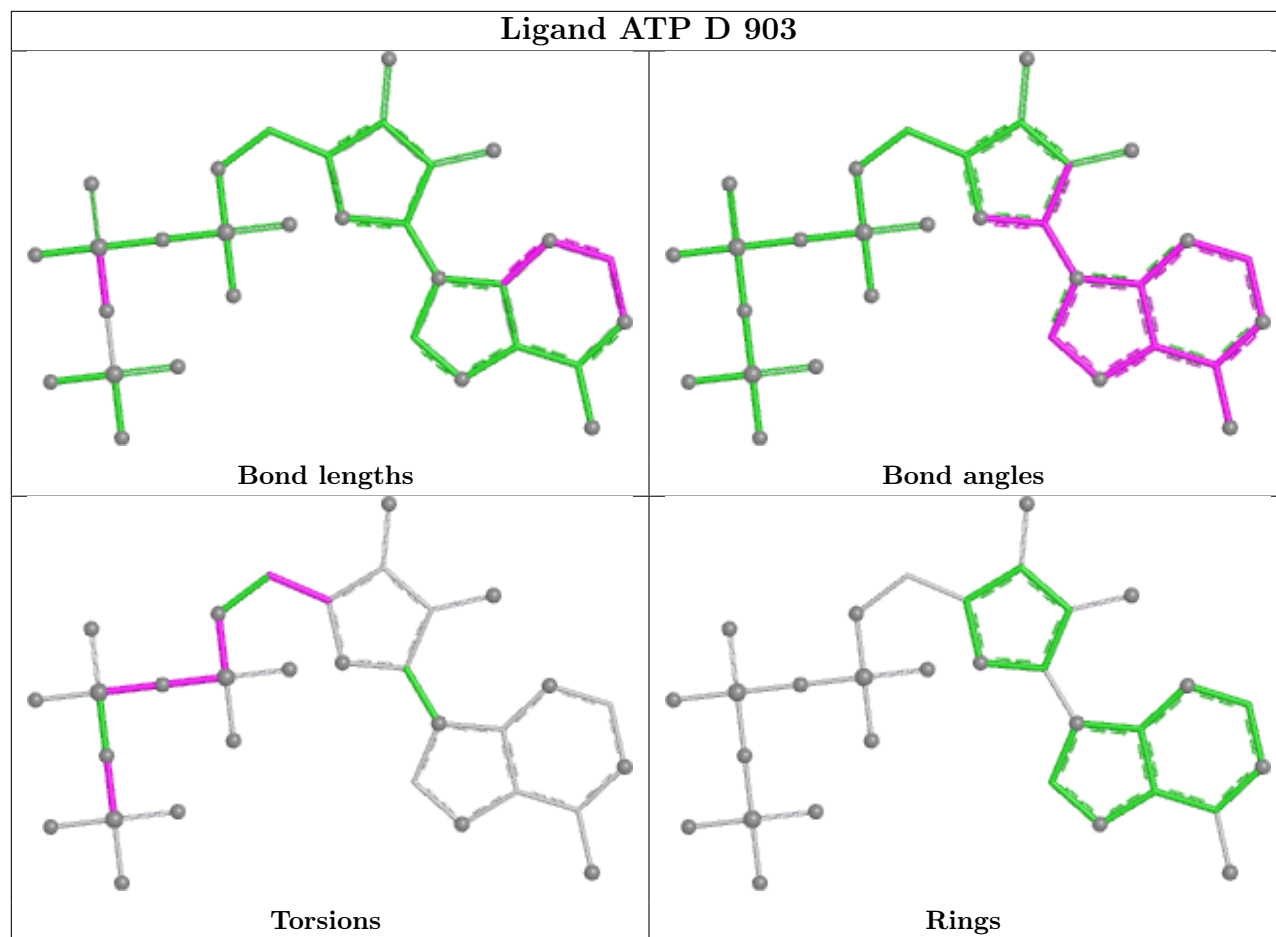
Ligand ATP B 903



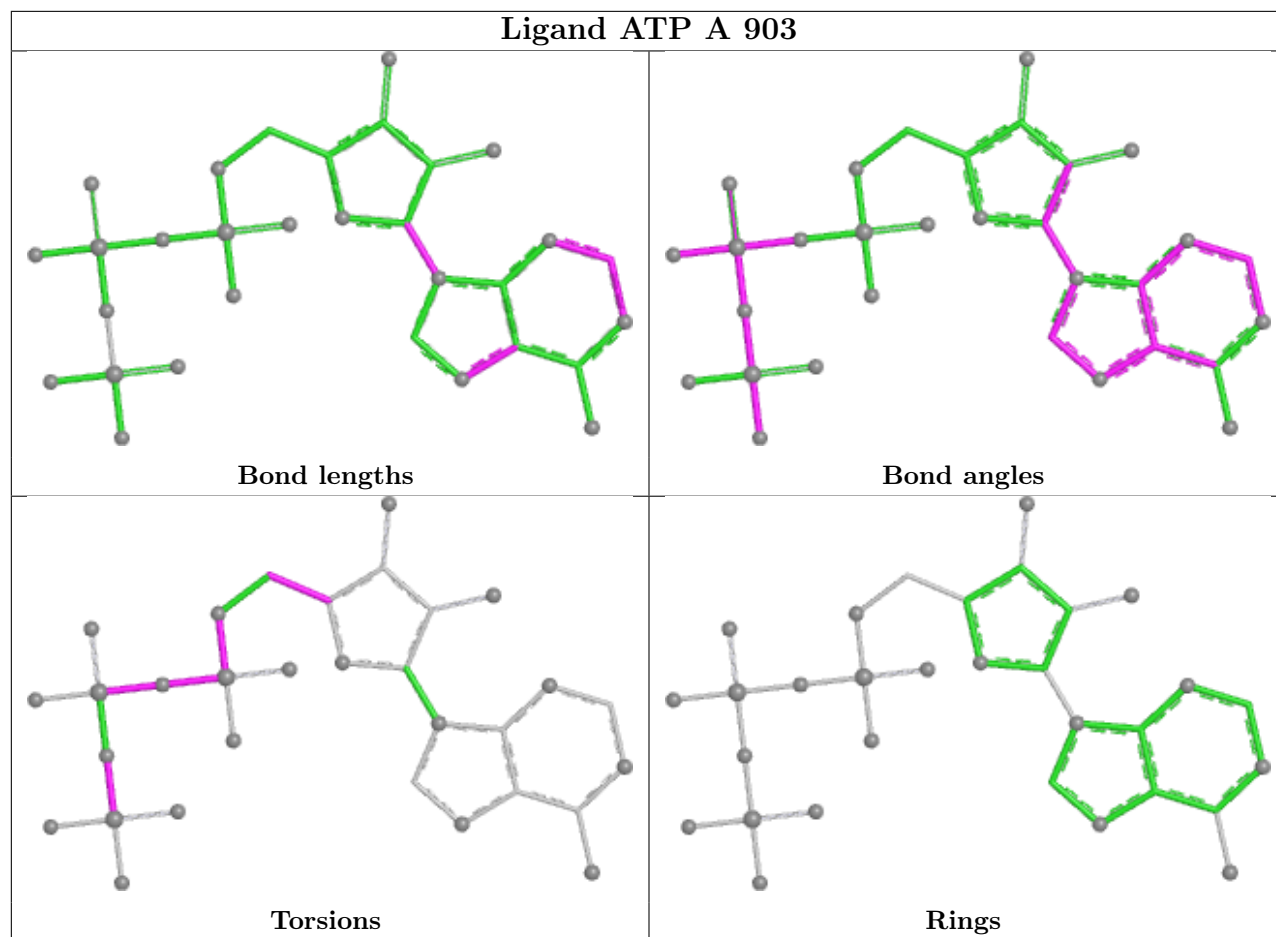


Ligand ATP E 903

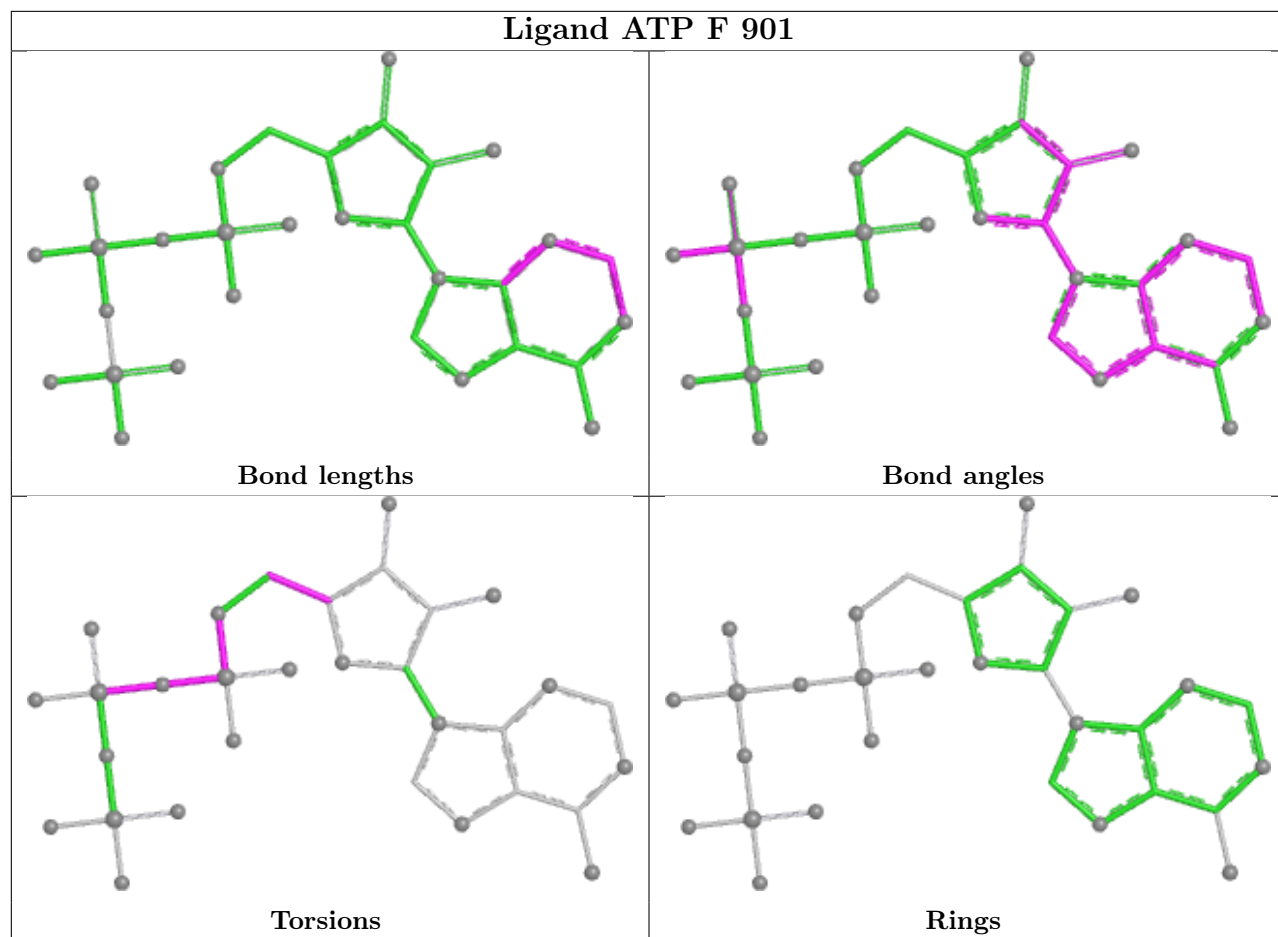




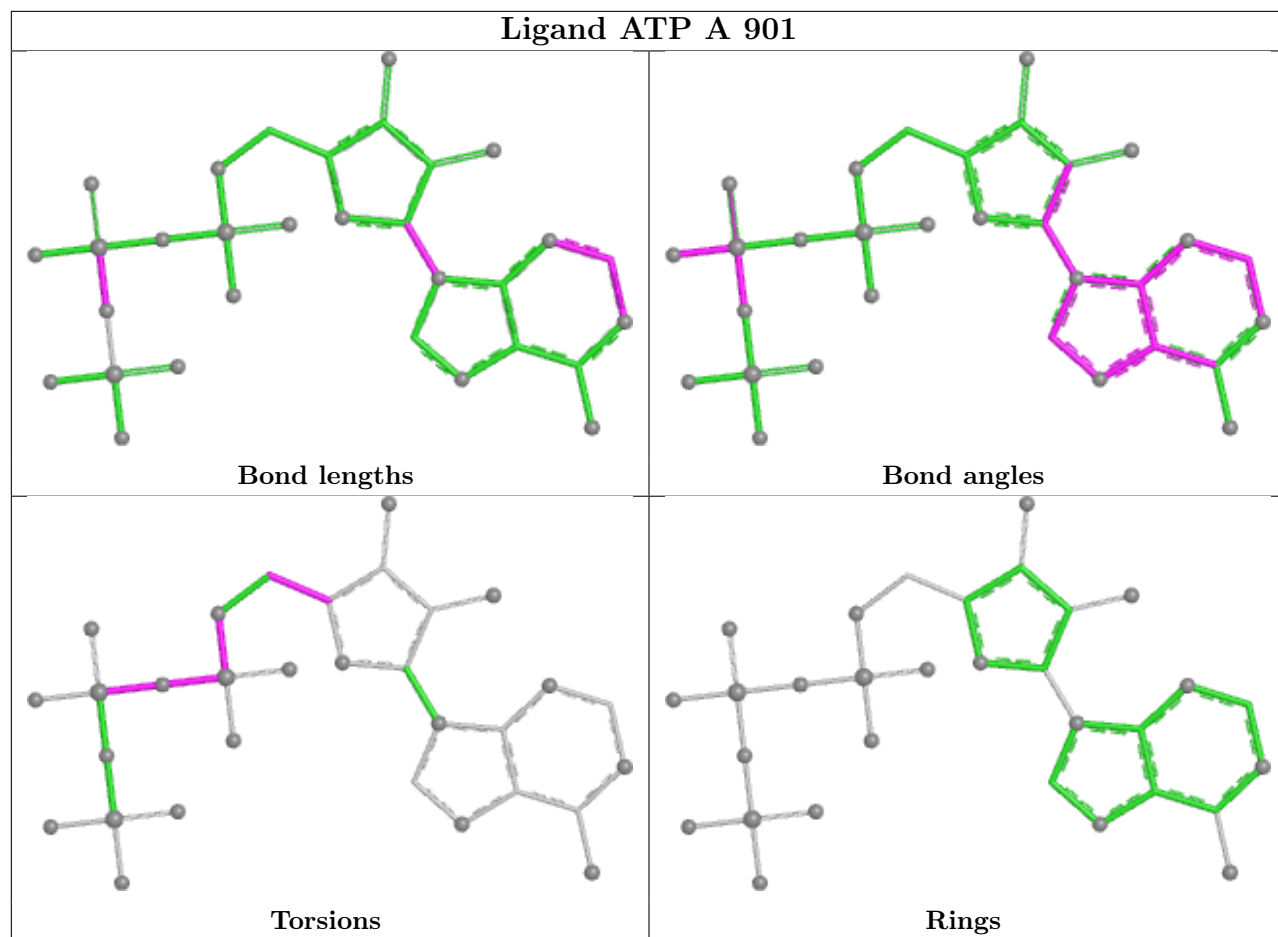
Ligand ATP A 903

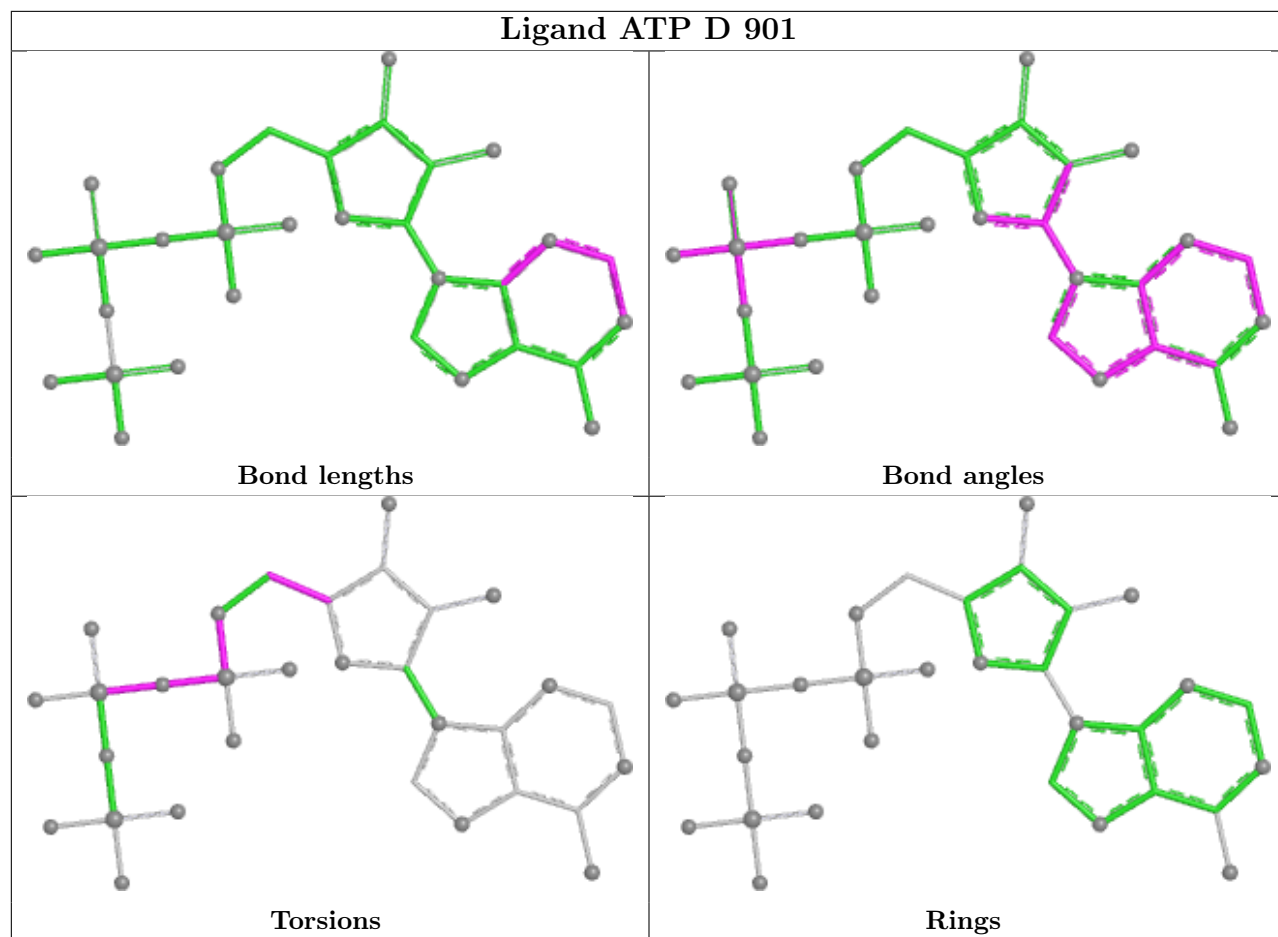


Ligand ATP F 901

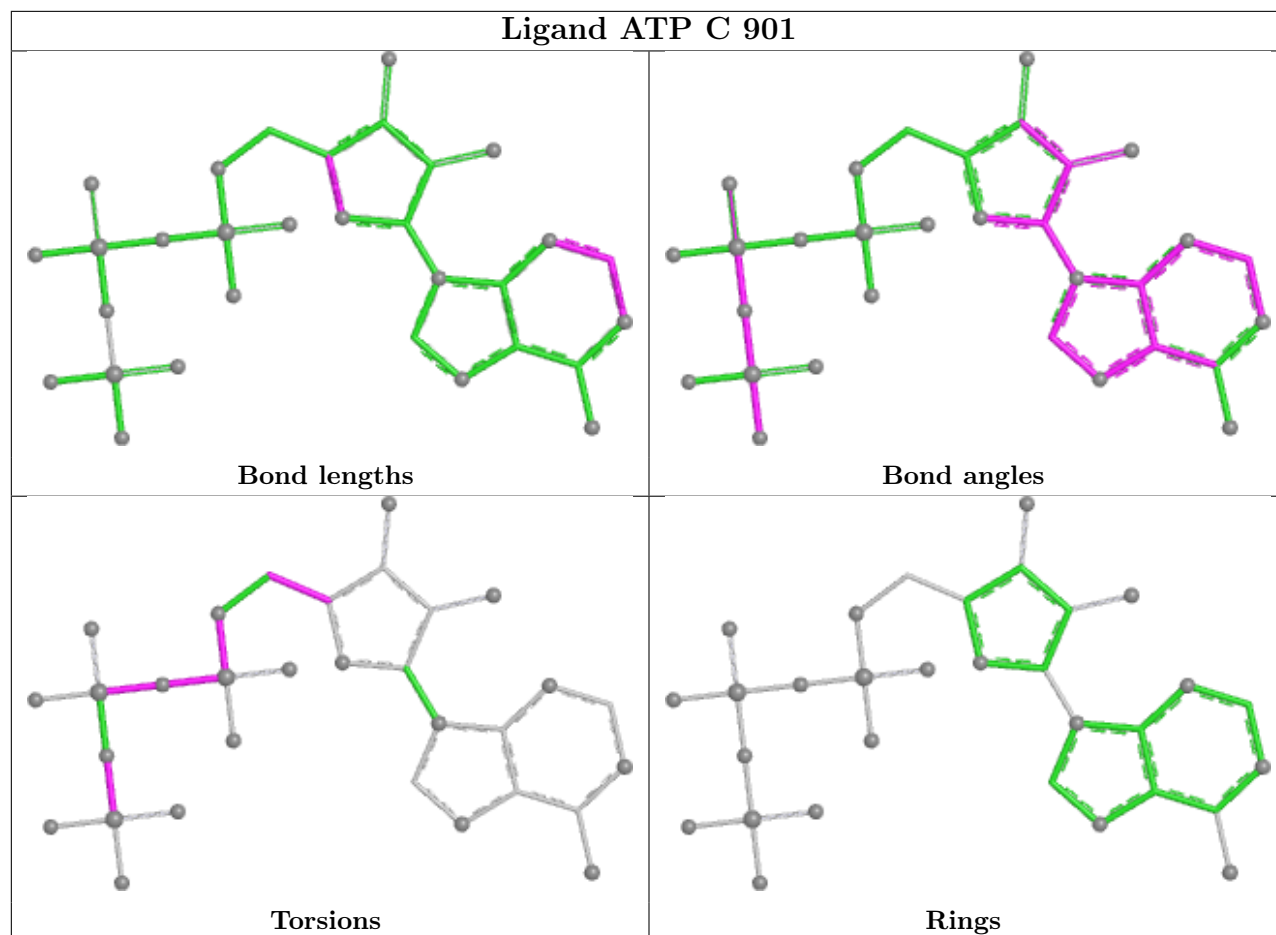


Ligand ATP A 901

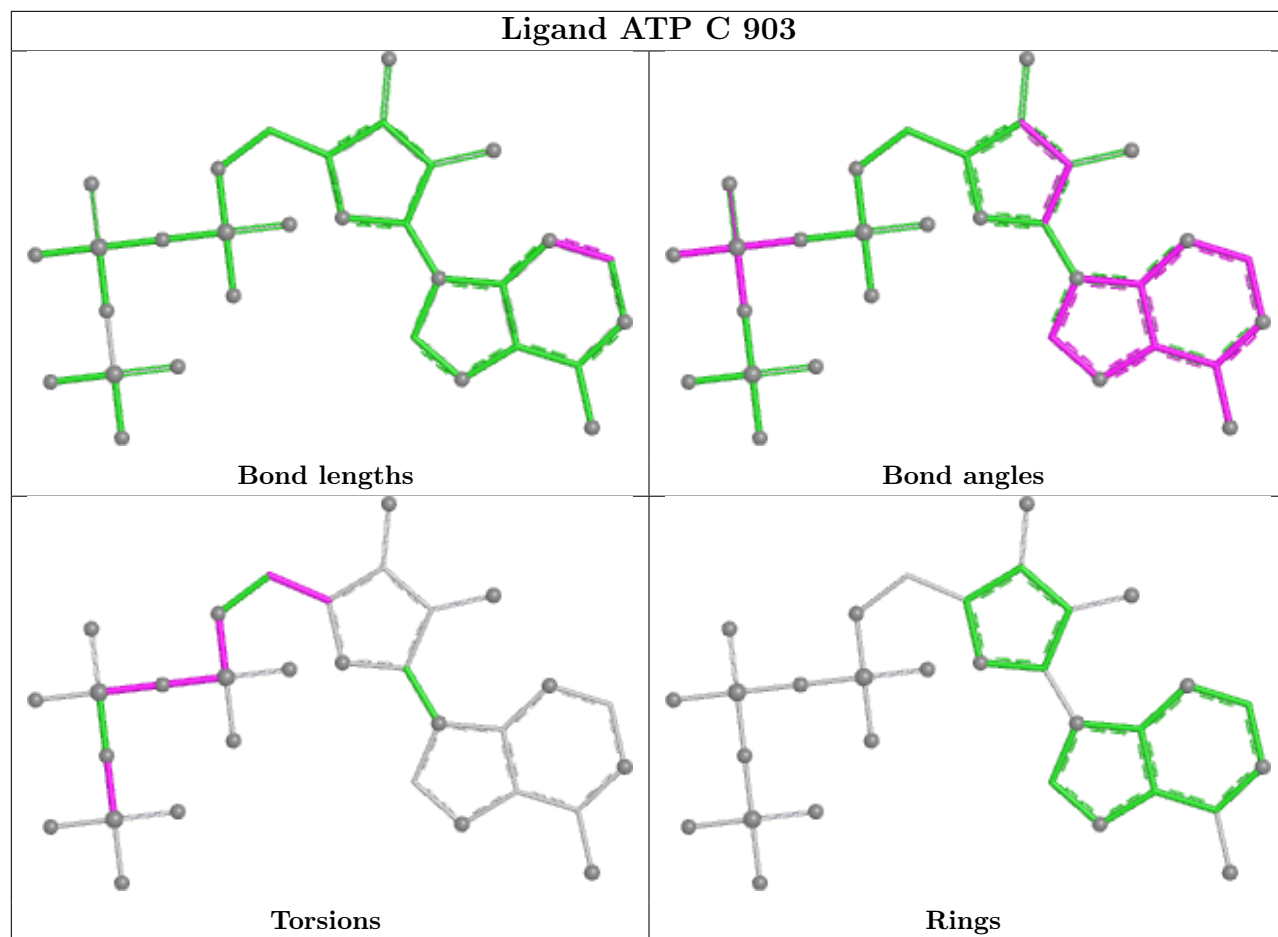




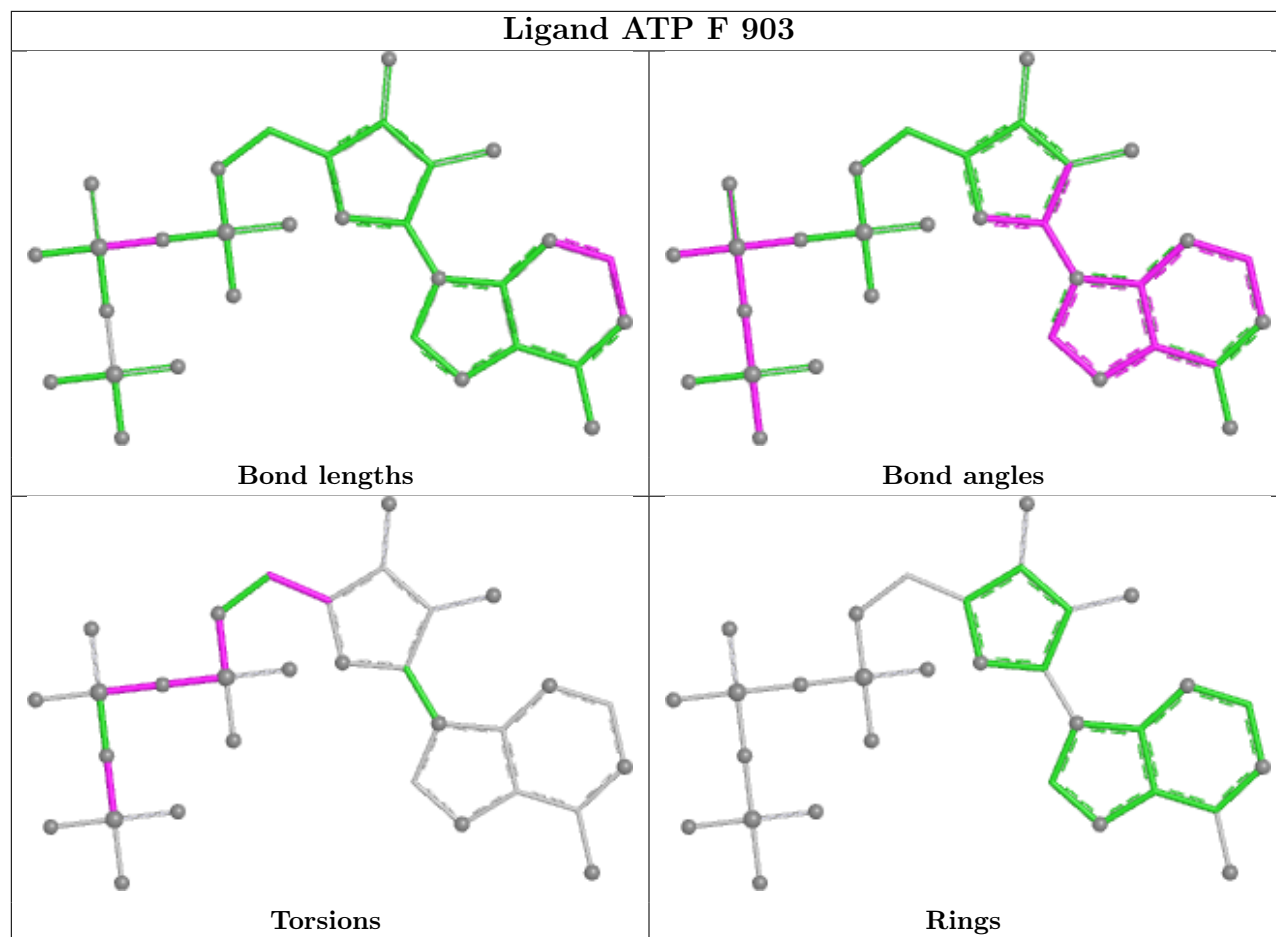
Ligand ATP C 901

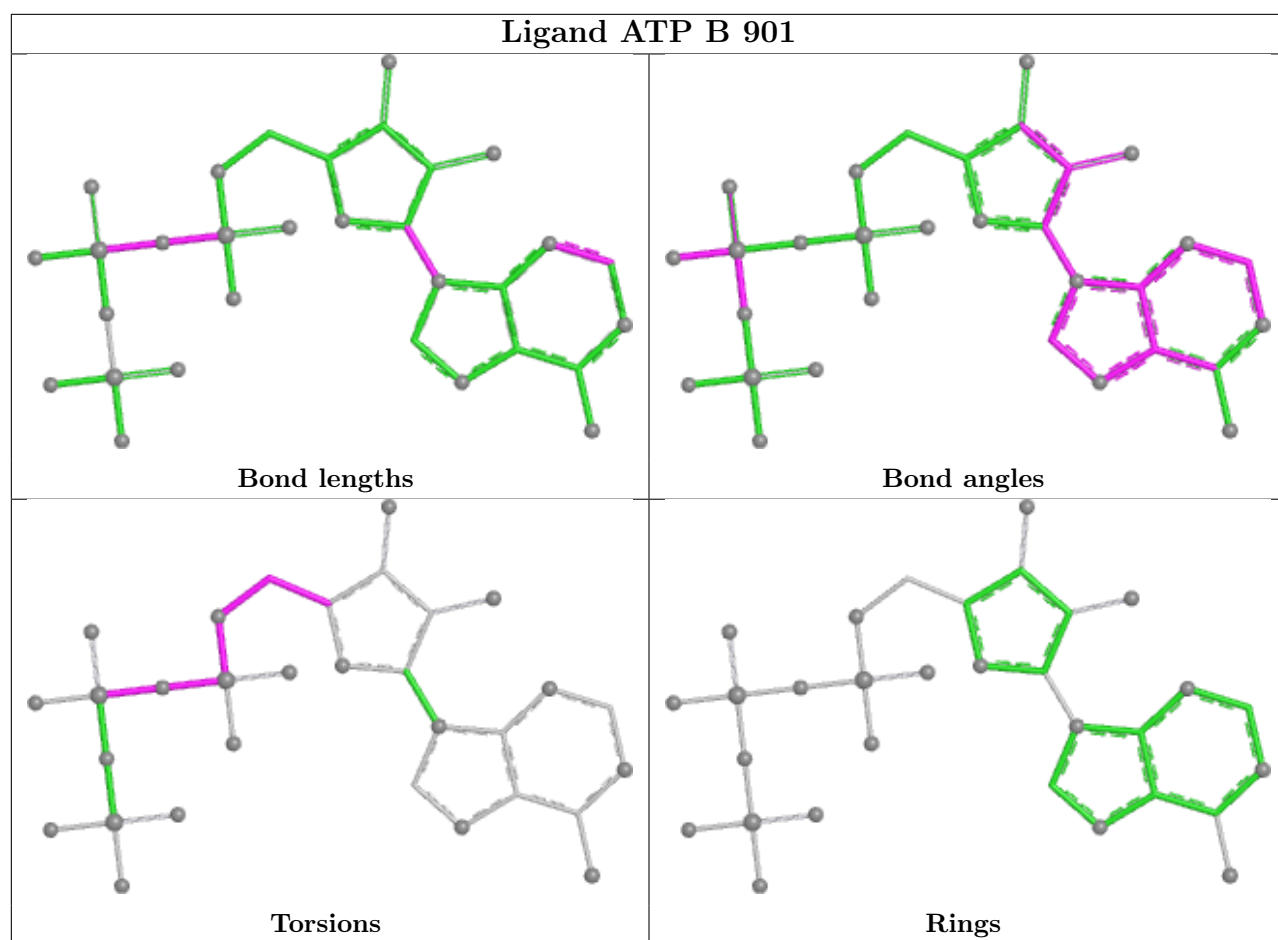


Ligand ATP C 903



Ligand ATP F 903





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	504/519 (97%)	-1.34	0 100 100	11, 72, 132, 152	0
2	B	490/519 (94%)	-1.31	0 100 100	29, 75, 131, 163	0
2	C	487/519 (93%)	-1.36	0 100 100	10, 58, 125, 165	0
2	D	484/519 (93%)	-1.51	0 100 100	2, 41, 95, 146	0
2	E	491/519 (94%)	-1.51	0 100 100	2, 47, 107, 148	0
2	F	505/519 (97%)	-1.45	0 100 100	1, 55, 120, 141	0
All	All	2961/3114 (95%)	-1.41	0 100 100	1, 59, 123, 165	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	A	426	11/12	0.99	0.04	92,94,101,101	0
1	TPO	A	432	11/12	0.99	0.03	64,66,74,75	0
2	TPO	B	432	11/12	0.99	0.03	53,56,58,59	0
2	TPO	D	432	11/12	0.99	0.03	40,49,61,61	0
2	TPO	E	432	11/12	0.99	0.05	31,41,50,50	0
2	TPO	F	432	11/12	0.99	0.03	47,52,56,60	0
2	TPO	C	432	11/12	1.00	0.02	20,21,34,43	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	702	1/1	0.98	0.12	125,125,125,125	0
3	ATP	B	903	31/31	0.99	0.03	58,64,70,72	0
3	ATP	A	903	31/31	0.99	0.03	38,51,56,58	0
4	MG	A	521	1/1	0.99	0.06	58,58,58,58	0
4	MG	C	701	1/1	0.99	0.07	60,60,60,60	0
4	MG	E	520	1/1	0.99	0.04	17,17,17,17	0
4	MG	E	702	1/1	0.99	0.04	15,15,15,15	0
4	MG	F	701	1/1	0.99	0.03	21,21,21,21	0
4	MG	F	802	1/1	0.99	0.03	46,46,46,46	0
3	ATP	E	903	31/31	1.00	0.02	12,19,30,31	0
3	ATP	F	901	31/31	1.00	0.02	67,76,77,77	0
3	ATP	F	903	31/31	1.00	0.03	22,29,33,34	0
4	MG	A	801	1/1	1.00	0.03	15,15,15,15	0
4	MG	A	802	1/1	1.00	0.04	45,45,45,45	0
4	MG	A	701	1/1	1.00	0.03	24,24,24,24	0
3	ATP	B	901	31/31	1.00	0.02	48,51,57,59	0
3	ATP	A	901	31/31	1.00	0.02	63,77,85,86	0
4	MG	A	520	1/1	1.00	0.02	92,92,92,92	0
4	MG	B	801	1/1	1.00	0.02	21,21,21,21	0
4	MG	B	802	1/1	1.00	0.03	37,37,37,37	0
4	MG	B	701	1/1	1.00	0.01	24,24,24,24	0
4	MG	C	801	1/1	1.00	0.03	12,12,12,12	0
4	MG	C	802	1/1	1.00	0.02	18,18,18,18	0
3	ATP	C	901	31/31	1.00	0.02	24,30,37,38	0
4	MG	C	702	1/1	1.00	0.03	74,74,74,74	0
4	MG	D	802	1/1	1.00	0.03	21,21,21,21	0
4	MG	D	702	1/1	1.00	0.03	63,63,63,63	0
4	MG	E	701	1/1	1.00	0.02	27,27,27,27	0
4	MG	E	801	1/1	1.00	0.04	66,66,66,66	0
3	ATP	C	903	31/31	1.00	0.02	37,45,69,70	0
3	ATP	D	901	31/31	1.00	0.03	32,43,48,49	0
3	ATP	D	903	31/31	1.00	0.02	11,20,29,30	0

Continued on next page...

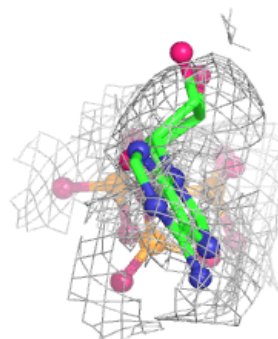
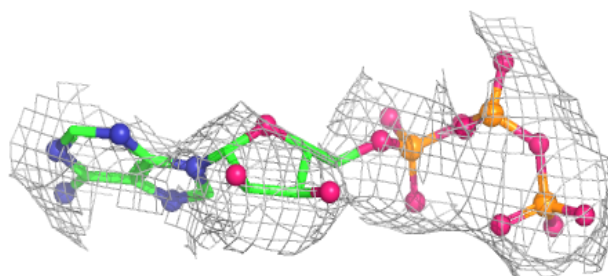
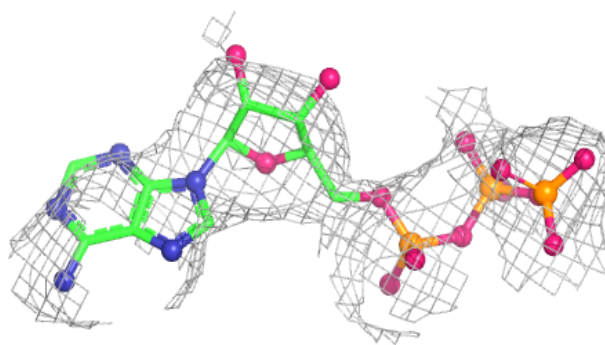
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	F	520	1/1	1.00	0.04	36,36,36,36	0
3	ATP	E	901	31/31	1.00	0.02	47,56,66,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

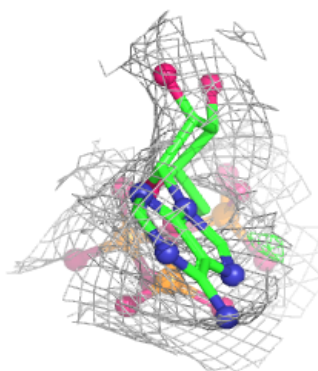
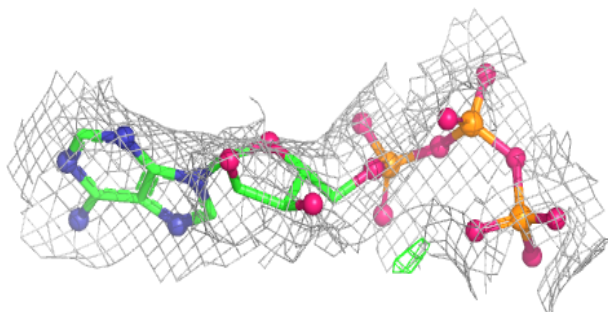
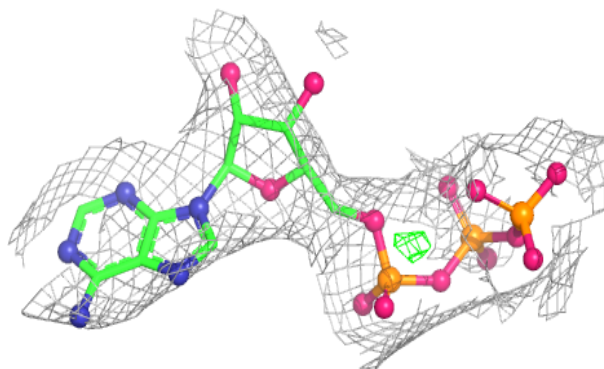
Electron density around ATP B 903:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

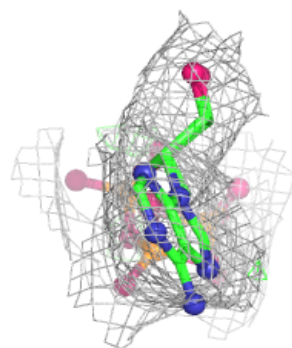
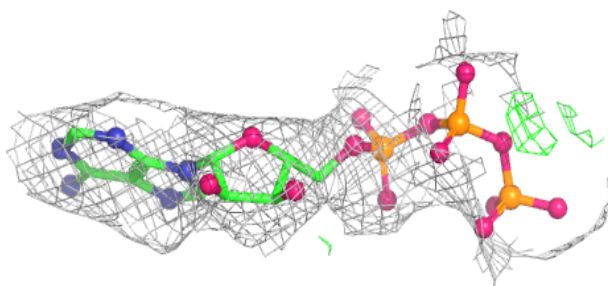
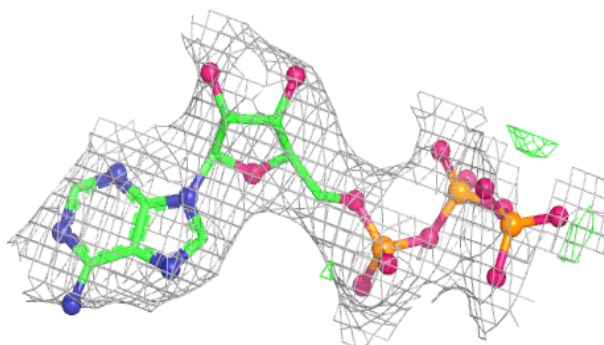


Electron density around ATP A 903:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

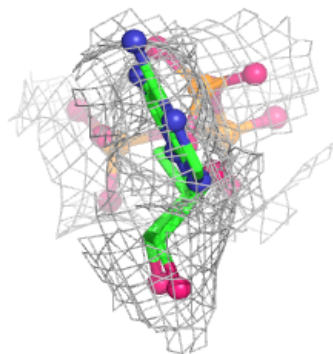
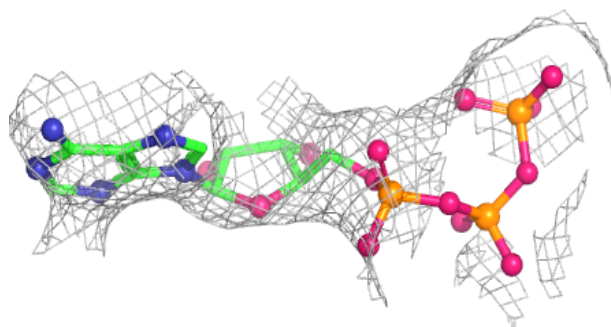
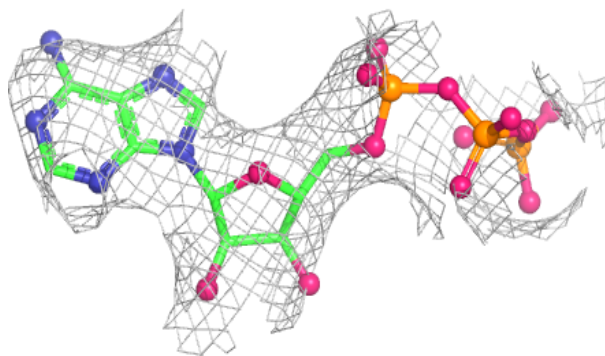
**Electron density around ATP E 903:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

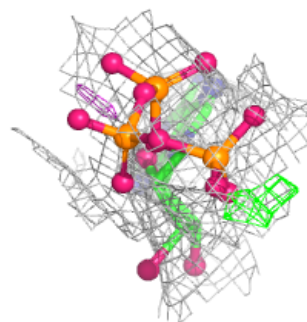
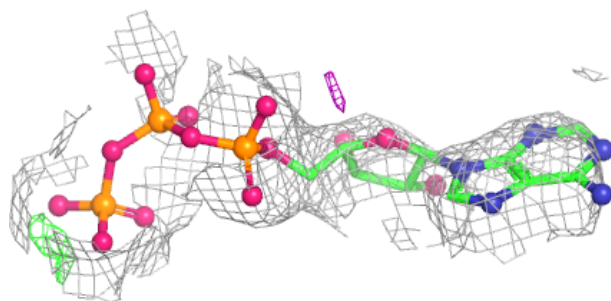
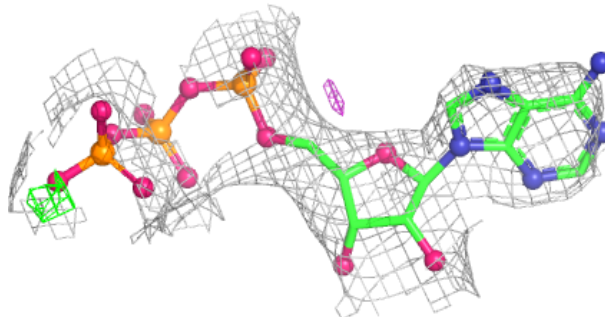


Electron density around ATP F 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

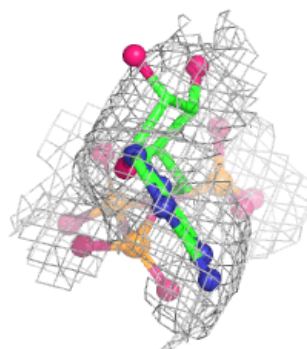
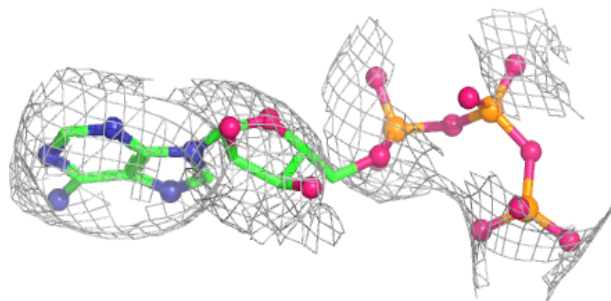
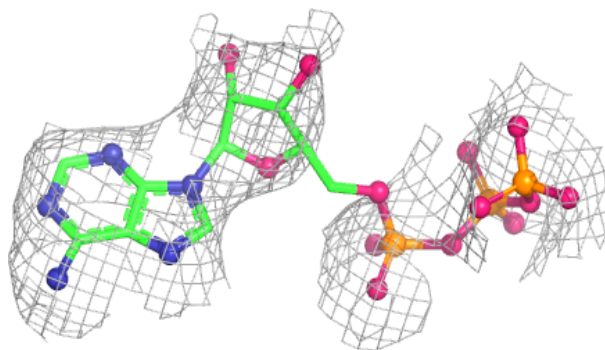
**Electron density around ATP F 903:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

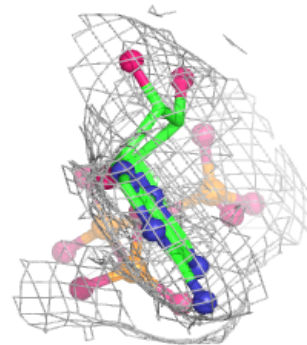
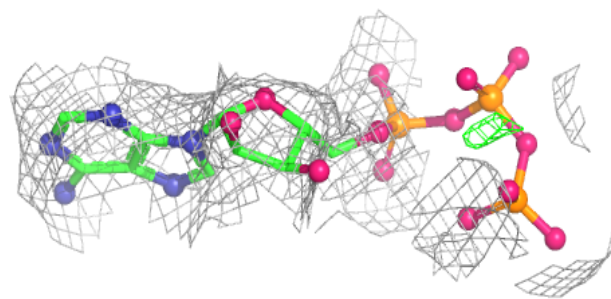
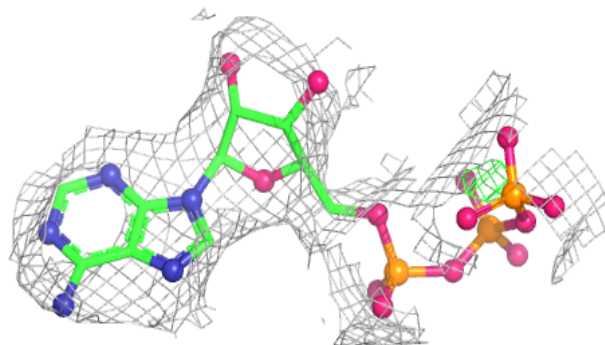


Electron density around ATP B 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

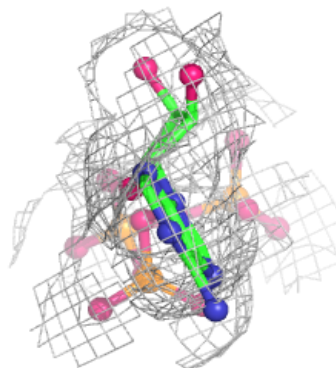
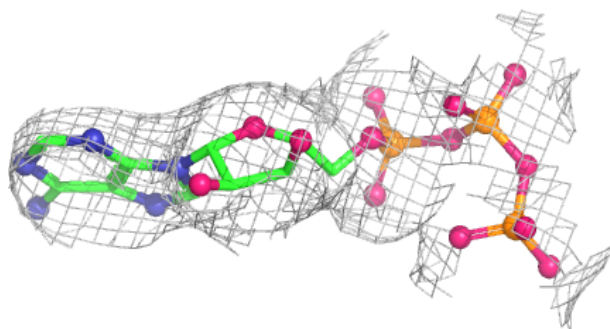
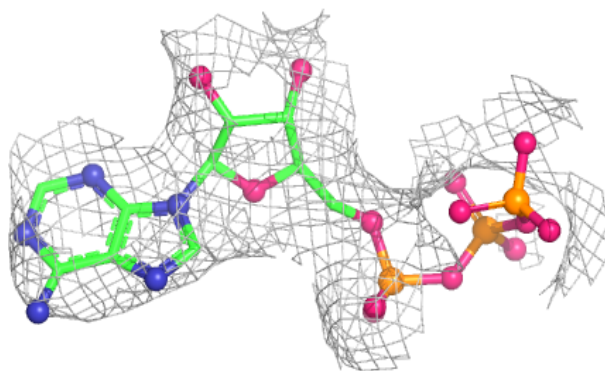
**Electron density around ATP A 901:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

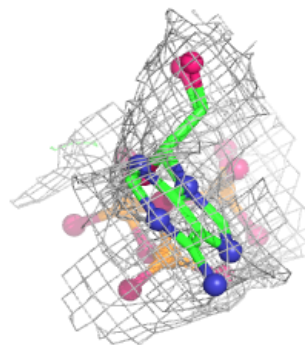
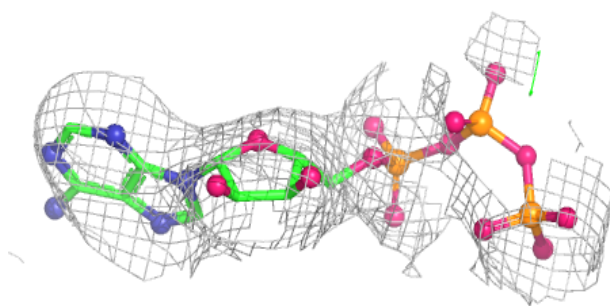
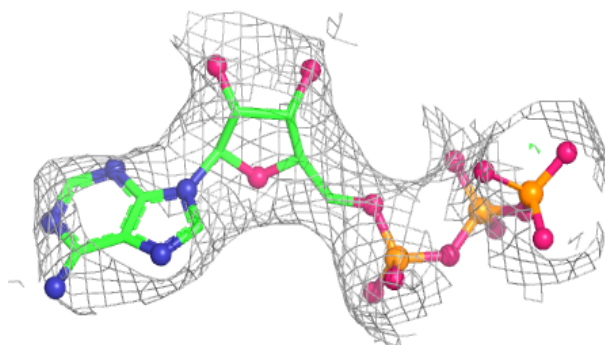


Electron density around ATP C 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

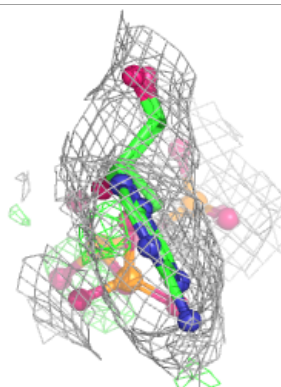
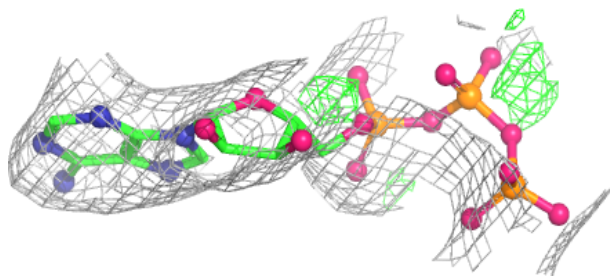
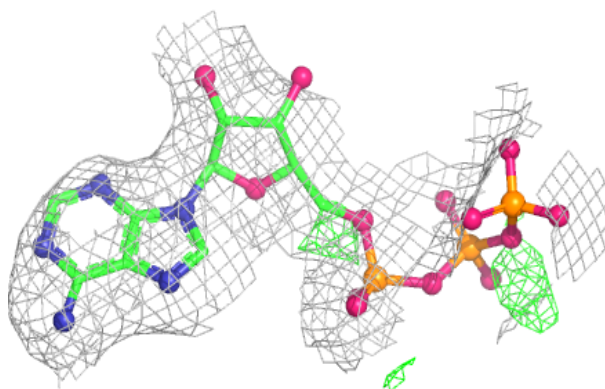
**Electron density around ATP C 903:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

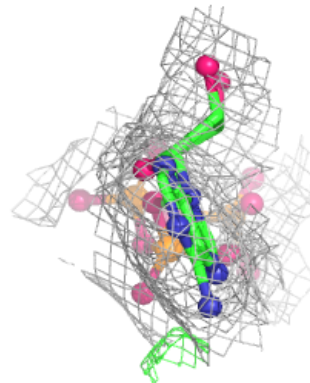
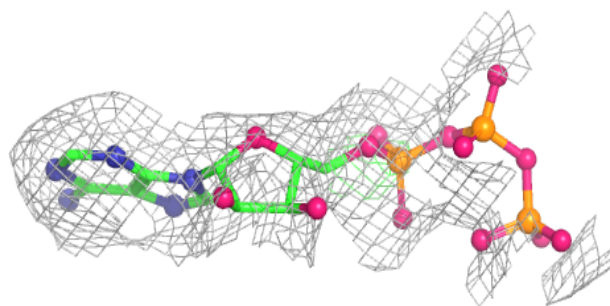
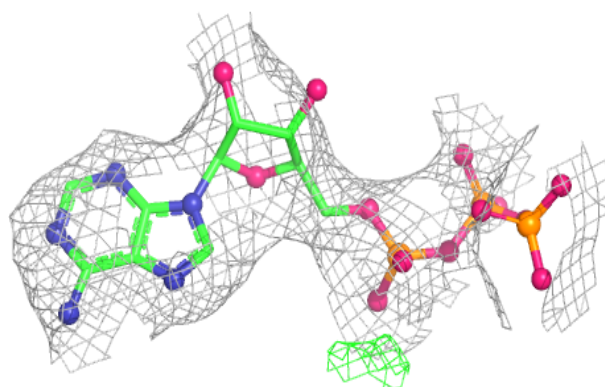


Electron density around ATP D 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

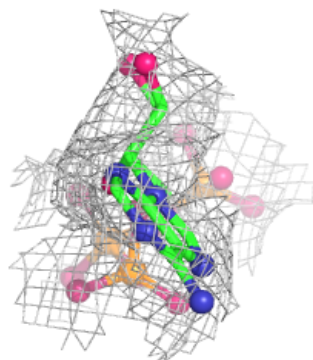
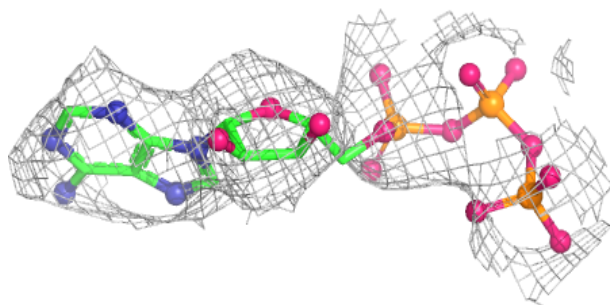
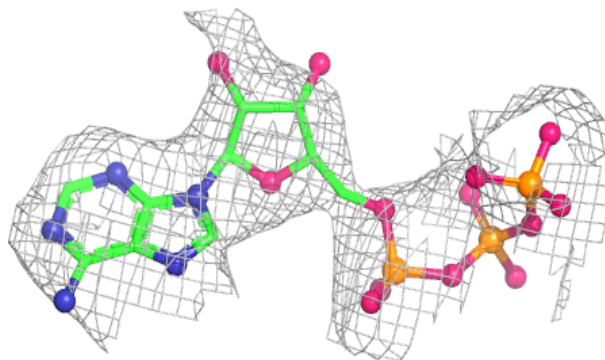
**Electron density around ATP D 903:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP E 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.