Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:17 AM GMT

PDB ID	:	2GBL
Title	:	Crystal Structure of Full Length Circadian Clock Protein KaiC with Phosphorylation Sites
Authors	:	Pattanayek, R.; Williams, D.R.; Pattanayek, S.; Xu, Y.; Mori, T.; Johnson, C.H.; Stewart, P.L.; Egli, M.
Deposited on	:	2006-03-10
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

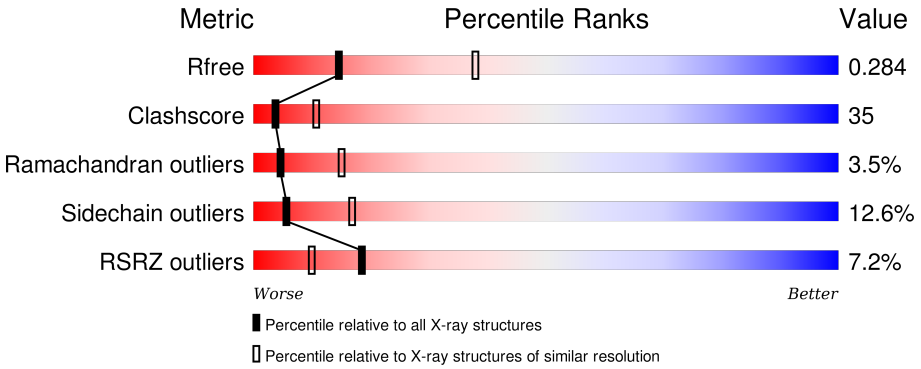
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	519	12% 45% 40% 10% • •
1	B	519	7% 42% 42% 9% • 5%
1	E	519	6% 45% 39% 10% • 5%
1	F	519	7% 45% 41% 10% • •
2	C	519	5% 46% 36% 11% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	519	

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	SEP	A	431	-	-	X	-
1	SEP	B	431	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23872 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
			3994	2509	701	767	2	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3878	2439	678	744	2	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3886	2445	679	745	2	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3994	2509	701	767	2	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
A	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
B	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
B	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
E	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
E	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
F	431	SEP	SER	MODIFIED RESIDUE	UNP Q79PF4
F	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	488	Total	C	N	O	P	S	0	0	0
			3850	2425	674	735	1	15			
2	D	485	Total	C	N	O	P	S	0	0	0
			3826	2411	671	728	1	15			

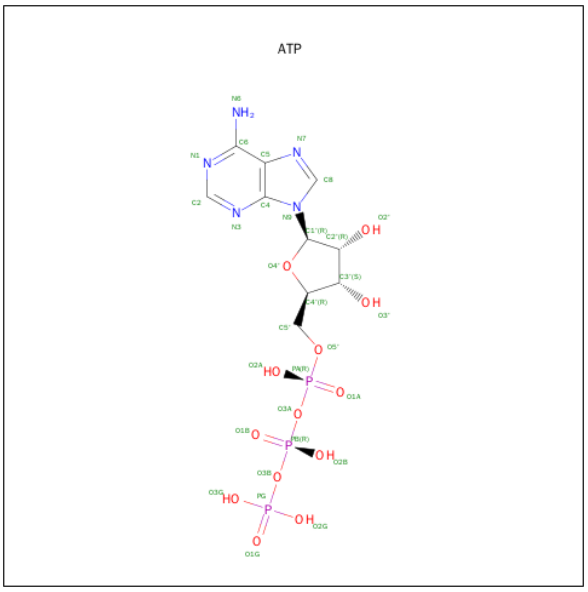
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4
D	432	TPO	THR	MODIFIED RESIDUE	UNP Q79PF4

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 31 10 5 13 3	0	0
4	A	1	Total C N O P 31 10 5 13 3	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

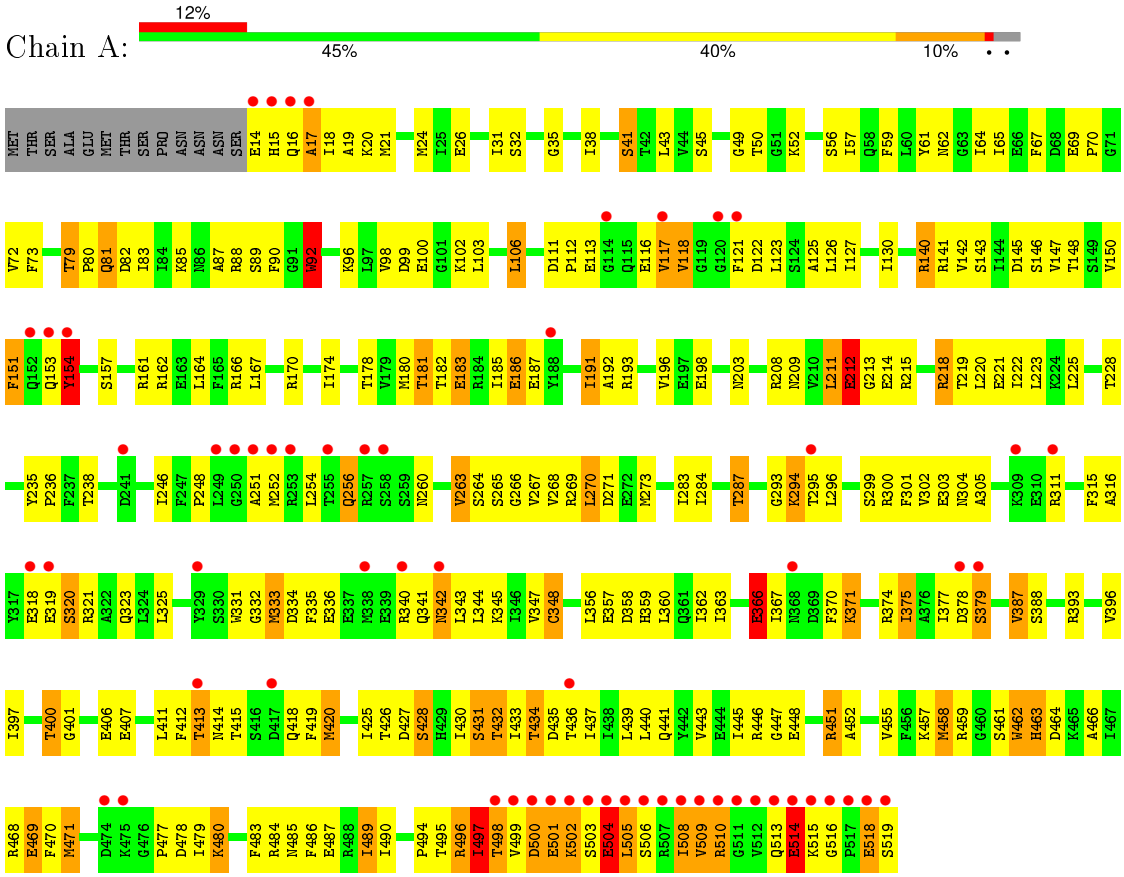
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	5	Total	O	0	0
			5	5		
5	C	7	Total	O	0	0
			7	7		
5	D	13	Total	O	0	0
			13	13		
5	E	10	Total	O	0	0
			10	10		
5	F	23	Total	O	0	0
			23	23		

3 Residue-property plots (i)

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

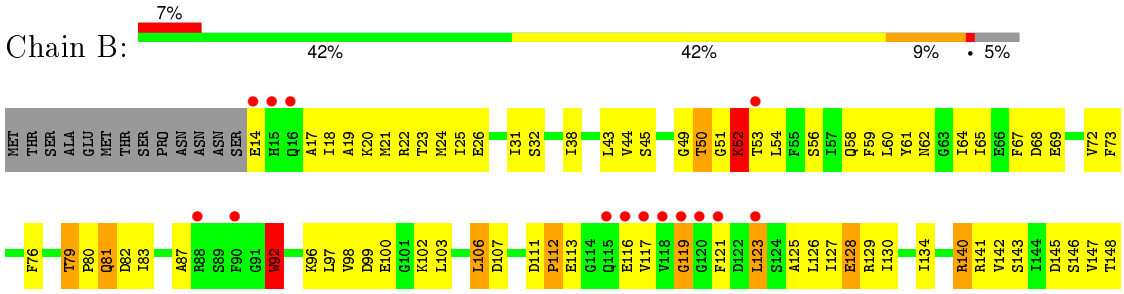
- Molecule 1: Circadian clock protein kinase kaiC

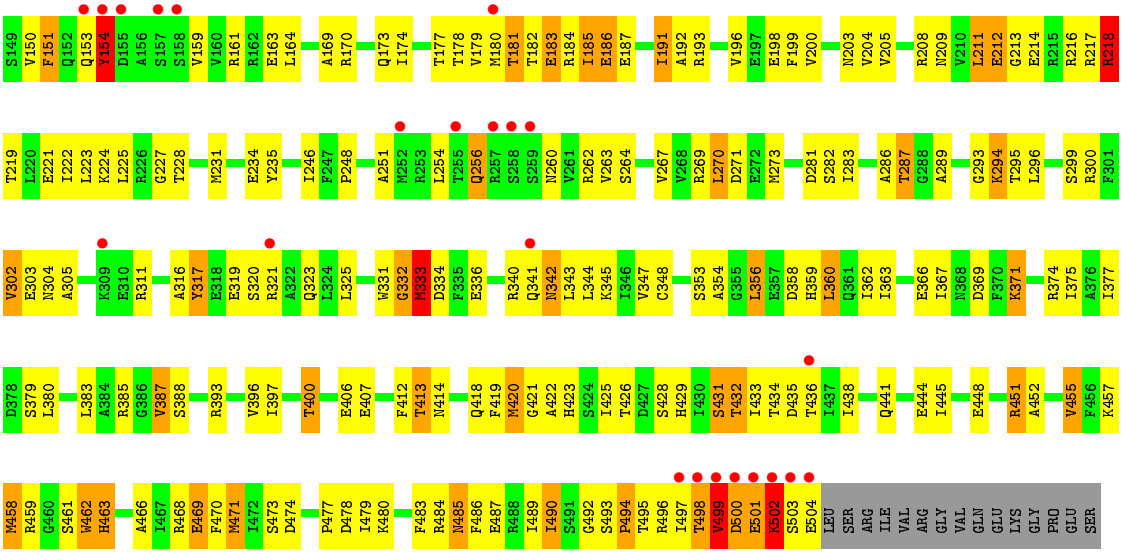
Chain A:



- Molecule 1: Circadian clock protein kinase kaiC

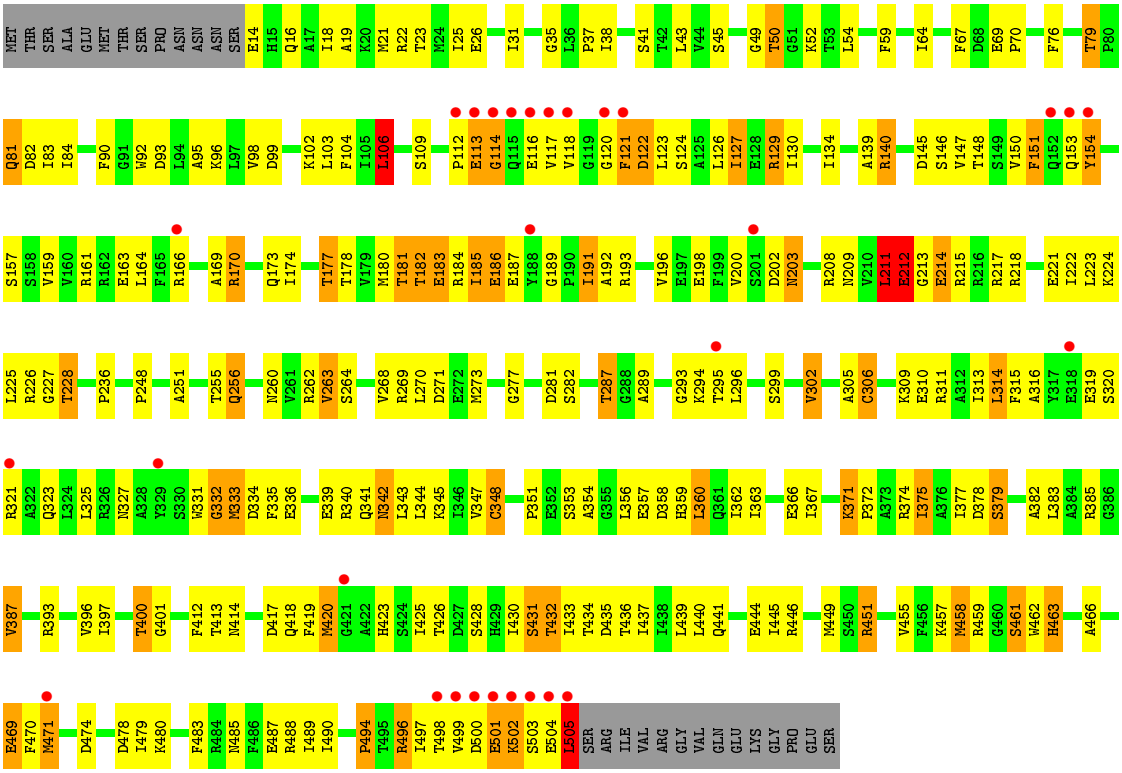
Chain B:





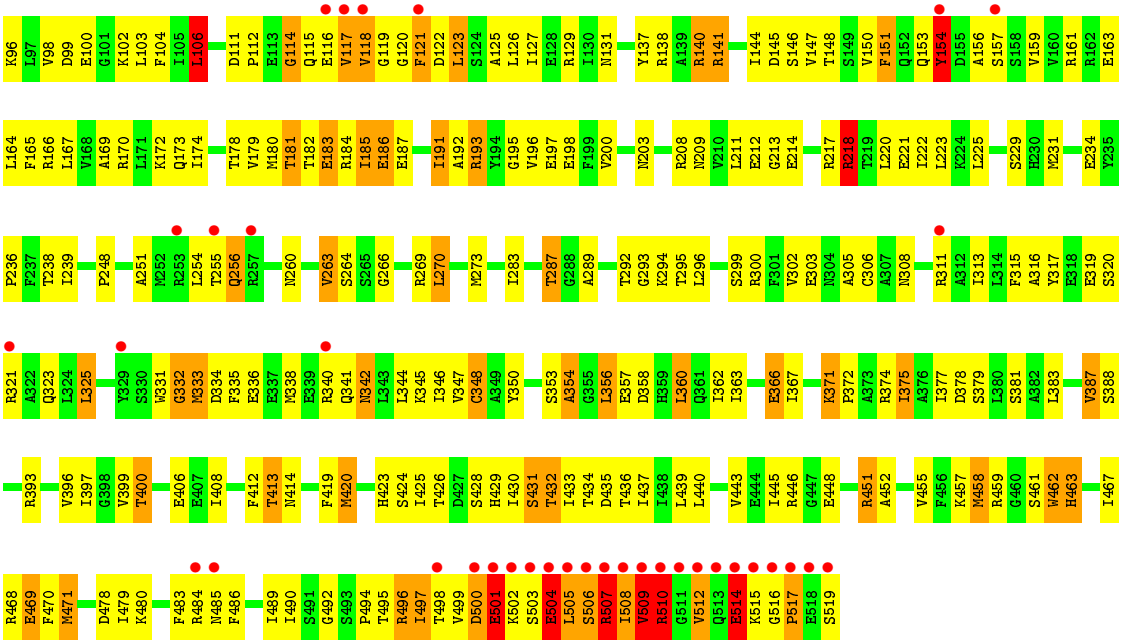
• Molecule 1: Circadian clock protein kinase kaiC

Chain E:



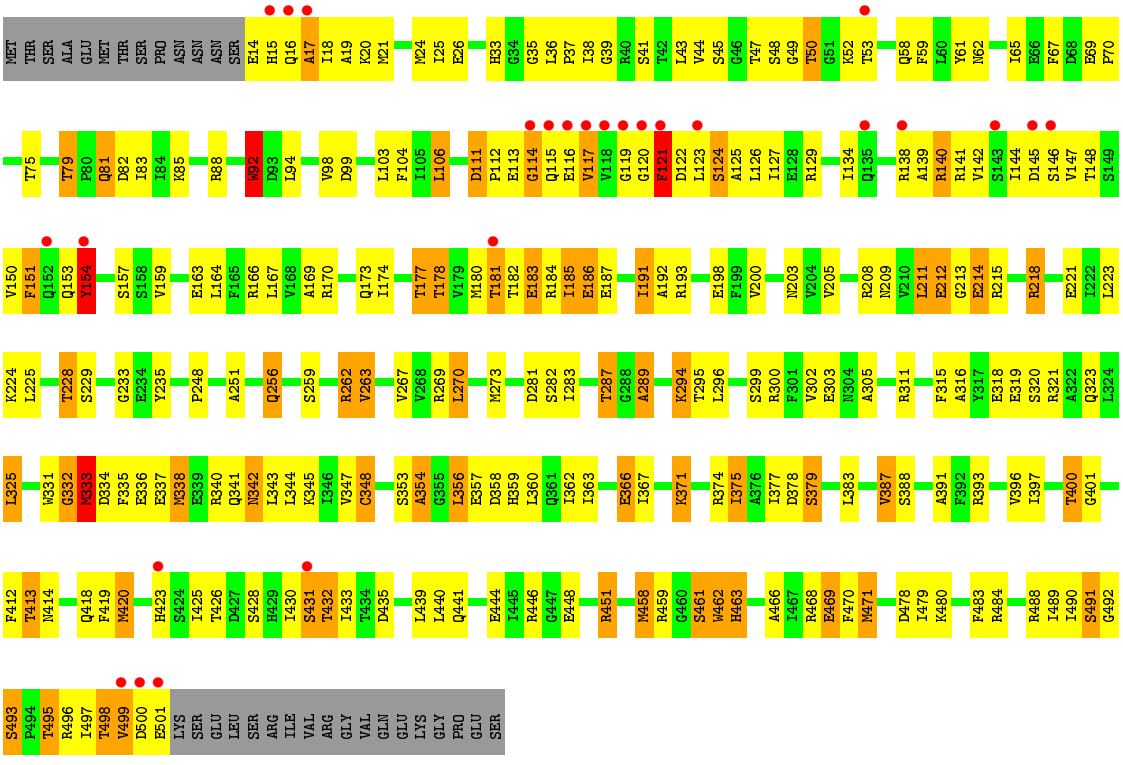
• Molecule 1: Circadian clock protein kinase kaiC

Chain F:



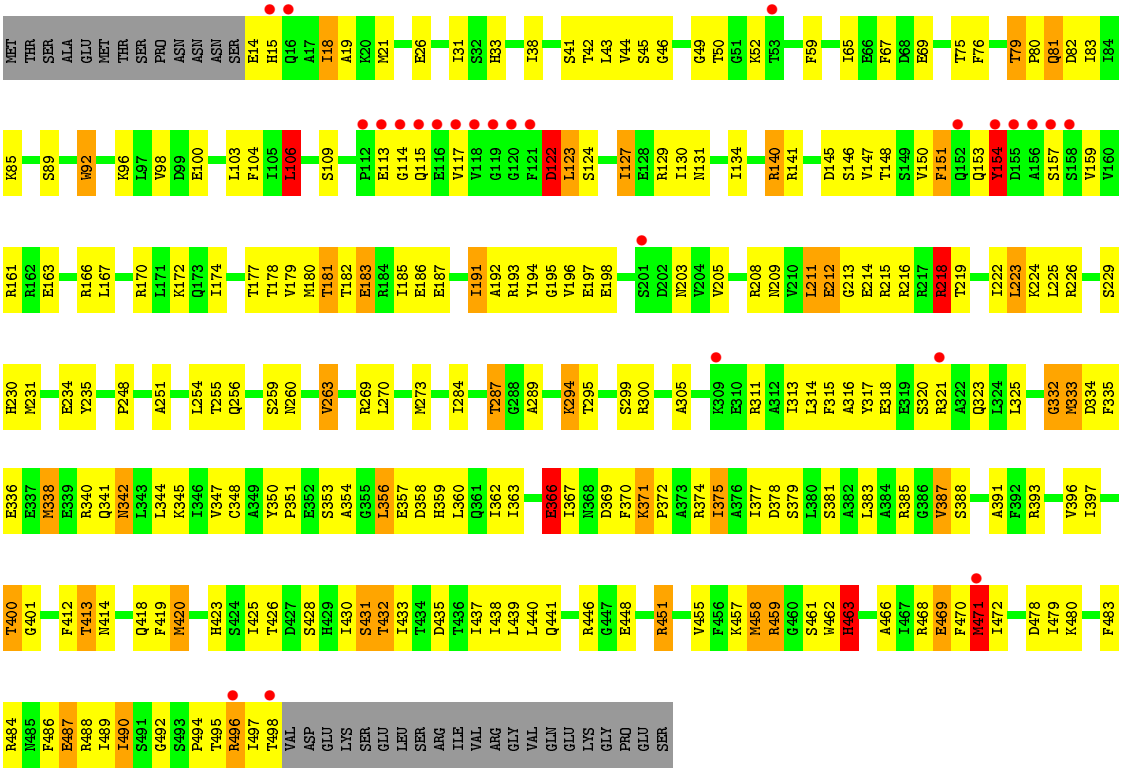
- Molecule 2: Circadian clock protein kinase kaiC

Chain C:



- Molecule 2: Circadian clock protein kinase kaiC

Chain D:


MET THR SER ALA GLU MET THR SER PRO ASN ASN ASN SER E14 H15 Q16 A17 I18 A19 K20 M21 E26 I31 S32 H33 I38 S41 T42 L43 V44 S45 G46 G49 T50 G51 K52 T53 F59 I65 E66 F67 D68 E69 T75 F76 T79 P80 Q81 D82 I83 I84
K85 S89 W92 K96 I97 V98 D99 E100 L103 F104 I105 L106 S109 P112 E113 G114 Q115 E116 V117 V118 G119 G120 F121 D122 L123 S124 I127 E128 R129 I130 N131 I134 R140 R141 D145 S146 V147 T148 S149 V150 F151 Q152 Q153 Y154 D155 A156 S157 S158 V159 V160
R161 R162 E163 R166 L167 R170 L171 K172 Q173 I174 T177 T178 V179 M180 T181 T182 E183 R184 I185 E186 E187 I191 A192 R193 Y194 G195 V196 E197 E198 S201 D202 N203 V204 V205 R208 N209 V210 L211 E212 G213 E214 R215 R216 R217 R218 T219 L222 L223 K224 L225 R226 S229
H230 M231 E234 Y235 P248 A251 L254 T255 Q256 S259 N260 V263 R269 L270 M273 I284 T287 G288 A289 K294 T295 S299 R300 A305 K309 E310 R311 A312 I313 L314 F315 A316 Y317 E318 E319 S320 R321 A322 Q323 L324 L325 G332 M333 D334 F335
E336 E337 M338 E339 R340 Q341 N342 L343 L344 K345 I346 V347 C348 A349 Y350 P351 E352 S353 A354 G355 L356 E357 D358 H359 L360 Q361 I362 I363 E366 I367 N368 D369 F370 K371 P372 A373 R374 I375 A376 I377 D378 S379 L380 S381 A382 L383 A384 R385 G386 V387 S388 A391 F392 R393 V396 I397
T400 G401 F412 T413 N414 Q418 F419 M420 H423 S424 I425 T426 D427 S428 H429 I430 S431 T432 I433 T434 D435 T436 I437 I438 L439 L440 Q441 R446 G447 E448 R451 V455 F456 K457 M458 R459 G460 S461 W462 H463 A466 I467 R468 E469 F470 M471 I472 D478 I479 K480 F483
R484 N485 F486 E487 R488 I489 T490 S491 G492 S493 P494 T495 R496 I497 T498 VAL ASP GLU LYS SER GLU LEU SER ARG ILE VAL ARG GLY VAL GLN GLU LYS GLY PRO GLU SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.87Å 135.58Å 204.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.73 – 2.83	Depositor EDS
% Data completeness (in resolution range)	0.8 (30.00-2.80) 89.7 (29.73-2.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.290 0.232 , 0.284	Depositor DCC
R_{free} test set	4041 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.9	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 87615 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23872	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.00	9/4038 (0.2%)	1.00	3/5437 (0.1%)
1	B	0.89	6/3921 (0.2%)	0.97	8/5282 (0.2%)
1	E	1.06	8/3929 (0.2%)	1.07	9/5293 (0.2%)
1	F	1.02	7/4038 (0.2%)	1.04	9/5437 (0.2%)
2	C	0.91	6/3903 (0.2%)	0.97	4/5259 (0.1%)
2	D	1.03	7/3879 (0.2%)	1.05	7/5226 (0.1%)
All	All	0.99	43/23708 (0.2%)	1.02	40/31934 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	E	0	2
1	F	0	3
2	C	0	2
2	D	0	2
All	All	0	14

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	TRP	CE3-CZ3	13.50	1.61	1.38
1	A	92	TRP	CE3-CZ3	12.25	1.59	1.38
1	E	92	TRP	CG-CD1	-10.83	1.21	1.36
1	F	92	TRP	CG-CD1	-10.41	1.22	1.36
1	E	92	TRP	CB-CG	-9.45	1.33	1.50
2	C	92	TRP	CG-CD1	-9.41	1.23	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	TRP	CG-CD1	-9.15	1.24	1.36
2	D	92	TRP	CB-CG	-8.34	1.35	1.50
2	C	92	TRP	CE3-CZ3	8.25	1.52	1.38
1	F	92	TRP	CB-CG	-7.39	1.36	1.50
2	D	458	MET	CG-SD	-7.05	1.62	1.81
2	C	92	TRP	CB-CG	-6.83	1.38	1.50
2	D	366	GLU	CD-OE2	6.78	1.33	1.25
1	A	92	TRP	CG-CD1	-6.74	1.27	1.36
2	D	92	TRP	CG-CD1	-6.67	1.27	1.36
1	A	514	GLU	CG-CD	6.38	1.61	1.51
2	C	366	GLU	CD-OE2	6.28	1.32	1.25
1	B	498	THR	CA-CB	6.12	1.69	1.53
1	F	366	GLU	CD-OE2	6.07	1.32	1.25
1	A	508	ILE	CA-CB	6.01	1.68	1.54
1	B	92	TRP	CE2-CZ2	5.97	1.49	1.39
1	F	92	TRP	CE3-CZ3	5.88	1.48	1.38
1	A	92	TRP	CB-CG	-5.82	1.39	1.50
1	F	348	CYS	CB-SG	-5.78	1.72	1.81
1	A	366	GLU	CD-OE2	5.54	1.31	1.25
1	F	509	VAL	C-N	5.49	1.46	1.34
1	E	500	ASP	CB-CG	5.42	1.63	1.51
1	E	310	GLU	CG-CD	5.41	1.60	1.51
1	A	514	GLU	CD-OE2	5.39	1.31	1.25
2	D	183	GLU	CB-CG	-5.34	1.42	1.52
2	C	213	GLY	C-O	-5.32	1.15	1.23
1	A	501	GLU	CB-CG	5.25	1.62	1.52
1	E	357	GLU	CG-CD	5.24	1.59	1.51
2	D	471	MET	CG-SD	5.23	1.94	1.81
1	A	504	GLU	CB-CG	5.14	1.61	1.52
1	E	170	ARG	CG-CD	5.14	1.64	1.51
1	B	52	LYS	N-CA	5.12	1.56	1.46
2	D	357	GLU	CG-CD	5.11	1.59	1.51
1	E	306	CYS	CB-SG	5.07	1.90	1.82
1	E	212	GLU	CG-CD	5.05	1.59	1.51
2	C	357	GLU	CG-CD	5.05	1.59	1.51
1	B	499	VAL	CA-CB	5.05	1.65	1.54
1	F	514	GLU	CG-CD	5.01	1.59	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	216	ARG	NE-CZ-NH1	-10.39	115.10	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	114	GLY	N-CA-C	7.92	132.90	113.10
2	C	213	GLY	N-CA-C	-7.41	94.57	113.10
1	E	500	ASP	CB-CG-OD2	7.16	124.74	118.30
2	D	226	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	E	213	GLY	N-CA-C	-6.74	96.26	113.10
1	F	509	VAL	CA-C-N	-6.70	102.47	117.20
1	E	22	ARG	NE-CZ-NH2	-6.62	116.99	120.30
2	D	218	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	E	505	LEU	CA-CB-CG	6.35	129.90	115.30
1	B	92	TRP	CB-CG-CD1	-6.03	119.16	127.00
2	D	106	LEU	CA-CB-CG	5.99	129.09	115.30
1	E	114	GLY	N-CA-C	5.94	127.95	113.10
1	F	218	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	516	GLY	N-CA-C	-5.92	98.29	113.10
1	A	116	GLU	N-CA-C	5.84	126.78	111.00
1	E	106	LEU	CA-CB-CG	5.82	128.68	115.30
2	C	214	GLU	N-CA-C	-5.69	95.65	111.00
1	B	217	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	F	510	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	F	332	GLY	N-CA-C	-5.59	99.11	113.10
1	B	332	GLY	N-CA-C	-5.51	99.32	113.10
1	E	129	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	C	332	GLY	N-CA-C	-5.48	99.41	113.10
1	B	502	LYS	N-CA-C	-5.47	96.23	111.00
1	B	455	VAL	N-CA-C	-5.40	96.41	111.00
1	F	193	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	216	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	D	332	GLY	N-CA-C	-5.34	99.75	113.10
1	B	92	TRP	CB-CA-C	5.32	121.03	110.40
2	D	218	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	E	332	GLY	N-CA-C	-5.27	99.93	113.10
2	D	459	ARG	C-N-CA	-5.24	111.31	122.30
1	F	141	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	F	512	VAL	O-C-N	-5.20	114.37	122.70
1	B	218	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	F	106	LEU	CA-CB-CG	5.13	127.09	115.30
1	E	214	GLU	N-CA-C	-5.12	97.17	111.00
1	A	497	ILE	N-CA-C	5.05	124.64	111.00
2	C	262	ARG	NE-CZ-NH1	-5.03	117.79	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	SEP	Mainchain
1	A	432	TPO	Mainchain
1	B	317	TYR	Sidechain
1	B	431	SEP	Mainchain
1	B	432	TPO	Mainchain
2	C	235	TYR	Sidechain
2	C	432	TPO	Mainchain
2	D	235	TYR	Sidechain
2	D	432	TPO	Mainchain
1	E	431	SEP	Mainchain
1	E	432	TPO	Mainchain
1	F	431	SEP	Mainchain
1	F	432	TPO	Mainchain
1	F	509	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3994	0	3984	299	0
1	B	3878	0	3862	295	0
1	E	3886	0	3872	282	0
1	F	3994	0	3984	322	0
2	C	3850	0	3837	282	0
2	D	3826	0	3818	275	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	62	0	24	11	0
4	B	62	0	24	8	0
4	C	62	0	24	7	0
4	D	62	0	23	7	0
4	E	62	0	24	6	0
4	F	62	0	24	7	0
5	A	8	0	0	0	0
5	B	5	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	7	0	0	2	0
5	D	13	0	0	2	0
5	E	10	0	0	0	0
5	F	23	0	0	6	0
All	All	23872	0	23500	1663	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 35.

All (1663) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:THR:HB	1:B:431:SEP:O3P	1.37	1.22
2:D:147:VAL:HG11	2:D:180:MET:HE3	1.24	1.20
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.07	1.15
1:A:14:GLU:HG3	1:A:15:HIS:H	1.08	1.11
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.29	1.11
1:A:426:THR:HB	1:A:431:SEP:O2P	1.50	1.10
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.31	1.10
1:B:140:ARG:HH11	1:B:140:ARG:HB3	1.16	1.06
2:D:146:SER:H	2:D:181:THR:HG22	1.20	1.05
1:E:146:SER:H	1:E:181:THR:HG22	1.22	1.04
2:C:21:MET:HE3	2:C:141:ARG:HG2	1.36	1.03
1:E:214:GLU:HB3	1:F:234:GLU:HB2	1.40	1.03
1:F:486:PHE:CE2	1:F:496:ARG:HD2	1.92	1.02
1:B:21:MET:HE1	1:B:141:ARG:HG2	1.42	1.00
2:C:123:LEU:HD12	2:C:163:GLU:OE2	1.61	0.99
1:F:146:SER:H	1:F:181:THR:HG22	1.24	0.99
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.45	0.99
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.29	0.98
2:D:446:ARG:N	2:D:496:ARG:HH12	1.60	0.97
1:B:79:THR:HG22	1:B:82:ASP:H	1.29	0.97
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.31	0.96
2:D:79:THR:HG22	2:D:82:ASP:H	1.25	0.96
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.46	0.95
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.29	0.95
1:F:79:THR:HG22	1:F:82:ASP:H	1.31	0.94
1:E:431:SEP:O	1:E:434:THR:HG22	1.67	0.94
1:F:509:VAL:O	1:F:512:VAL:HG23	1.66	0.94
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.49	0.93
1:B:441:GLN:HE22	1:B:490:ILE:HD13	1.33	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:371:LYS:HD3	2:D:371:LYS:O	1.68	0.93
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.33	0.92
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.00	0.92
2:C:147:VAL:HG11	2:C:180:MET:HE2	1.53	0.91
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.35	0.91
1:B:145:ASP:OD2	1:B:181:THR:HG21	1.72	0.90
1:B:379:SER:HA	1:B:413:THR:HG22	1.54	0.89
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.36	0.89
1:E:123:LEU:HD22	1:E:166:ARG:HD2	1.54	0.89
1:A:147:VAL:HG11	1:A:180:MET:HE2	1.54	0.88
2:C:123:LEU:HD13	2:C:166:ARG:HD2	1.55	0.87
1:F:287:THR:CG2	1:F:414:ASN:HD22	1.85	0.87
2:C:287:THR:CG2	2:C:414:ASN:HD22	1.87	0.87
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.40	0.87
2:D:123:LEU:HD12	2:D:166:ARG:HD2	1.55	0.87
1:B:140:ARG:NH1	1:B:140:ARG:HB3	1.89	0.87
1:E:293:GLY:HA2	4:E:901:ATP:O1A	1.74	0.87
1:A:14:GLU:CG	1:A:15:HIS:H	1.84	0.86
2:D:287:THR:CG2	2:D:414:ASN:HD22	1.87	0.86
1:F:287:THR:HG23	1:F:414:ASN:HB3	1.55	0.86
1:B:431:SEP:O	1:B:434:THR:HG22	1.76	0.86
1:F:45:SER:HB2	1:F:182:THR:HB	1.58	0.86
2:C:146:SER:H	2:C:181:THR:HG22	1.41	0.86
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.58	0.85
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.59	0.85
1:F:426:THR:HG22	1:F:428:SER:H	1.38	0.85
1:A:431:SEP:O	1:A:434:THR:HG22	1.76	0.85
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.40	0.85
1:B:140:ARG:CB	1:B:140:ARG:HH11	1.89	0.85
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.57	0.85
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.57	0.84
1:B:147:VAL:O	1:B:150:VAL:HG12	1.77	0.84
1:F:191:ILE:HB	1:F:198:GLU:CG	2.08	0.84
1:A:287:THR:CG2	1:A:414:ASN:HD22	1.89	0.84
1:F:509:VAL:O	1:F:512:VAL:CG2	2.25	0.84
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.07	0.84
1:F:504:GLU:HB3	1:F:507:ARG:NH2	1.90	0.84
1:E:287:THR:CG2	1:E:414:ASN:HD22	1.90	0.84
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.59	0.84
1:F:145:ASP:OD2	1:F:181:THR:HG21	1.78	0.83
2:D:191:ILE:HB	2:D:198:GLU:CG	2.08	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:LYS:HE3	4:C:903:ATP:O1B	1.78	0.83
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.08	0.83
1:E:146:SER:N	1:E:181:THR:HG22	1.92	0.83
1:A:14:GLU:HG3	1:A:15:HIS:N	1.91	0.83
2:D:446:ARG:H	2:D:496:ARG:HH12	1.20	0.83
2:C:347:VAL:O	2:C:348:CYS:HB2	1.78	0.83
1:A:498:THR:HB	1:A:501:GLU:HG3	1.59	0.83
2:D:146:SER:N	2:D:181:THR:HG22	1.94	0.82
2:C:147:VAL:O	2:C:150:VAL:HG12	1.79	0.82
2:C:182:THR:HG21	2:C:192:ALA:HB1	1.62	0.82
2:C:262:ARG:NH2	2:C:461:SER:HB2	1.93	0.82
1:A:147:VAL:O	1:A:150:VAL:HG12	1.80	0.82
1:A:379:SER:HA	1:A:413:THR:HG22	1.60	0.82
2:C:214:GLU:HB3	2:D:234:GLU:HB2	1.60	0.81
1:F:515:LYS:HG3	1:F:516:GLY:N	1.95	0.81
1:B:191:ILE:HB	1:B:198:GLU:CG	2.10	0.81
2:D:147:VAL:HG11	2:D:180:MET:CE	2.07	0.81
2:D:79:THR:O	2:D:83:ILE:HD12	1.81	0.81
2:C:495:THR:HA	2:D:487:GLU:OE2	1.81	0.80
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.45	0.80
1:A:211:LEU:O	1:A:212:GLU:HB3	1.81	0.80
2:D:315:PHE:CZ	2:D:363:ILE:HG23	2.15	0.80
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.47	0.80
1:E:79:THR:HG22	1:E:82:ASP:H	1.47	0.80
1:F:502:LYS:NZ	1:F:507:ARG:HB3	1.97	0.80
2:D:311:ARG:HD2	2:D:371:LYS:HD2	1.62	0.80
1:F:148:THR:HG21	1:F:183:GLU:HG3	1.64	0.80
1:A:79:THR:HG22	1:A:82:ASP:H	1.47	0.80
2:C:67:PHE:HB2	2:C:69:GLU:HG3	1.61	0.79
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.95	0.79
2:D:446:ARG:H	2:D:496:ARG:NH1	1.80	0.79
1:B:377:ILE:HD12	1:B:412:PHE:CE2	2.18	0.79
2:C:79:THR:HG22	2:C:82:ASP:H	1.48	0.79
1:E:426:THR:HG22	1:E:428:SER:H	1.47	0.79
1:B:471:MET:HB3	1:B:480:LYS:NZ	1.97	0.79
1:E:67:PHE:HB2	1:E:69:GLU:HG3	1.64	0.79
1:E:485:ASN:ND2	1:E:496:ARG:HH11	1.81	0.79
2:D:299:SER:C	2:D:333:MET:HE1	2.03	0.79
1:F:218:ARG:HD2	5:F:906:HOH:O	1.83	0.79
1:F:486:PHE:HE2	1:F:496:ARG:CD	1.94	0.78
1:B:441:GLN:NE2	1:B:490:ILE:HD13	1.97	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ILE:HB	1:B:198:GLU:CD	2.04	0.78
1:F:293:GLY:HA2	4:F:901:ATP:O1A	1.82	0.78
1:A:419:PHE:CD2	1:B:425:ILE:HD12	2.18	0.78
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.48	0.78
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.63	0.78
1:E:461:SER:OG	1:E:462:TRP:N	2.16	0.78
2:D:344:LEU:HD13	2:D:344:LEU:C	2.04	0.78
1:E:14:GLU:HG3	1:E:16:GLN:H	1.48	0.78
1:F:146:SER:N	1:F:181:THR:HG22	1.99	0.78
1:A:41:SER:HB3	1:A:178:THR:HB	1.67	0.77
1:E:147:VAL:O	1:E:150:VAL:HG12	1.84	0.77
1:E:191:ILE:HB	1:E:198:GLU:CG	2.15	0.77
1:A:299:SER:C	1:A:333:MET:HE1	2.05	0.77
1:E:371:LYS:HD2	1:E:371:LYS:O	1.85	0.77
1:B:419:PHE:CD2	2:C:425:ILE:HD12	2.20	0.77
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.49	0.77
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.66	0.76
1:F:420:MET:HA	5:F:915:HOH:O	1.83	0.76
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.67	0.76
1:B:43:LEU:HD11	1:B:182:THR:OG1	1.85	0.76
1:A:426:THR:HG22	1:A:428:SER:H	1.51	0.76
2:C:151:PHE:C	2:C:153:GLN:H	1.89	0.76
1:F:515:LYS:HG3	1:F:516:GLY:H	1.50	0.76
1:B:363:ILE:O	1:B:367:ILE:HG13	1.86	0.76
1:A:371:LYS:O	1:A:371:LYS:HD3	1.86	0.76
1:F:53:THR:HG23	1:F:145:ASP:OD1	1.85	0.75
1:E:146:SER:H	1:E:181:THR:CG2	1.99	0.75
1:A:117:VAL:HA	1:A:154:TYR:OH	1.86	0.75
2:D:287:THR:HG23	2:D:414:ASN:HB3	1.66	0.75
1:F:191:ILE:HB	1:F:198:GLU:CD	2.07	0.75
1:E:371:LYS:CD	1:E:371:LYS:O	2.35	0.75
1:E:334:ASP:OD1	1:E:336:GLU:HB2	1.86	0.75
1:E:140:ARG:HB3	1:E:140:ARG:HH11	1.50	0.75
1:F:439:LEU:HD12	1:F:440:LEU:N	2.01	0.75
4:B:901:ATP:H3'	2:C:458:MET:O	1.86	0.75
2:C:81:GLN:H	2:C:81:GLN:NE2	1.84	0.75
2:D:379:SER:HA	2:D:413:THR:HG22	1.66	0.75
1:B:426:THR:CB	1:B:431:SEP:O3P	2.29	0.75
1:F:185:ILE:HD11	1:F:193:ARG:NH1	2.02	0.75
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.52	0.74
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.00	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:O	1:A:65:ILE:HG22	1.85	0.74
2:D:140:ARG:HH11	2:D:140:ARG:HB3	1.51	0.74
1:B:61:TYR:CE1	1:B:92:TRP:HB2	2.23	0.74
2:D:446:ARG:N	2:D:496:ARG:NH1	2.35	0.74
1:A:316:ALA:O	1:A:348:CYS:HA	1.88	0.74
1:A:426:THR:CB	1:A:431:SEP:O2P	2.32	0.74
1:B:147:VAL:HG11	1:B:180:MET:CE	2.14	0.74
1:E:145:ASP:OD2	1:E:181:THR:HG21	1.86	0.74
1:E:419:PHE:CD2	1:F:425:ILE:HD12	2.23	0.74
1:B:146:SER:H	1:B:181:THR:HG22	1.53	0.74
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.68	0.74
1:F:437:ILE:HD12	1:F:457:LYS:HG2	1.69	0.74
1:E:323:GLN:HE22	1:F:459:ARG:HD3	1.52	0.74
2:D:146:SER:H	2:D:181:THR:CG2	1.99	0.73
1:B:377:ILE:HD12	1:B:412:PHE:HE2	1.53	0.73
1:E:148:THR:HG21	1:E:183:GLU:HG3	1.68	0.73
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.22	0.73
2:D:147:VAL:O	2:D:150:VAL:HG12	1.88	0.73
2:C:79:THR:O	2:C:83:ILE:HD12	1.89	0.73
2:D:419:PHE:CD2	1:E:425:ILE:HD12	2.24	0.73
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.52	0.73
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.69	0.73
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.68	0.73
1:F:140:ARG:NH1	1:F:140:ARG:HB3	2.04	0.73
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.19	0.73
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.70	0.73
2:C:121:PHE:H	2:C:121:PHE:HD1	1.35	0.73
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.71	0.73
1:B:299:SER:C	1:B:333:MET:HE1	2.10	0.72
2:D:148:THR:OG1	2:D:182:THR:HG23	1.89	0.72
2:D:203:ASN:HB3	2:D:225:LEU:HD23	1.70	0.72
1:E:263:VAL:CG1	1:E:374:ARG:HH21	2.02	0.72
2:D:486:PHE:HB2	2:D:489:ILE:HD11	1.71	0.72
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.04	0.72
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.24	0.72
1:F:461:SER:OG	1:F:462:TRP:N	2.21	0.72
1:F:140:ARG:CB	1:F:140:ARG:HH11	2.02	0.72
1:E:191:ILE:HG21	1:E:198:GLU:HG3	1.70	0.72
1:A:145:ASP:OD2	1:A:181:THR:HG21	1.89	0.72
2:D:426:THR:HG22	2:D:428:SER:H	1.52	0.72
1:B:502:LYS:HG3	1:B:504:GLU:O	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:LEU:HD22	2:C:127:ILE:HD11	1.70	0.72
2:C:79:THR:CG2	2:C:81:GLN:HG2	2.19	0.72
2:C:45:SER:HB2	2:C:182:THR:HB	1.71	0.72
1:F:191:ILE:HB	1:F:198:GLU:HG3	1.71	0.72
2:C:218:ARG:HB3	5:C:906:HOH:O	1.89	0.72
2:D:497:ILE:O	2:D:497:ILE:HD12	1.90	0.72
1:E:426:THR:HG22	1:E:428:SER:N	2.04	0.71
1:E:418:GLN:HB2	1:F:423:HIS:O	1.89	0.71
2:D:191:ILE:HB	2:D:198:GLU:HG3	1.70	0.71
1:B:497:ILE:HG13	1:B:498:THR:N	2.04	0.71
2:C:123:LEU:HD21	2:C:167:LEU:HB2	1.72	0.71
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.20	0.71
2:D:21:MET:HE1	2:D:141:ARG:HG2	1.70	0.71
2:C:140:ARG:HB3	2:C:140:ARG:NH1	2.05	0.71
1:A:446:ARG:HA	1:A:496:ARG:NH2	2.05	0.71
2:D:439:LEU:HD12	2:D:440:LEU:N	2.06	0.71
2:C:315:PHE:CZ	2:C:363:ILE:HG23	2.26	0.71
1:F:379:SER:HA	1:F:413:THR:HG22	1.73	0.71
1:B:462:TRP:O	1:B:463:HIS:O	2.08	0.71
2:C:140:ARG:HH11	2:C:140:ARG:CB	2.04	0.71
1:F:299:SER:C	1:F:333:MET:HE1	2.09	0.71
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.55	0.71
1:F:182:THR:HG22	1:F:183:GLU:N	2.06	0.71
1:B:273:MET:O	1:B:463:HIS:HA	1.90	0.71
1:F:147:VAL:HG11	1:F:180:MET:HE2	1.73	0.71
2:C:191:ILE:HB	2:C:198:GLU:CG	2.20	0.70
1:B:169:ALA:O	1:B:173:GLN:HG3	1.91	0.70
1:B:263:VAL:HG12	1:B:374:ARG:NH2	2.06	0.70
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.56	0.70
2:D:31:ILE:HG22	2:D:222:ILE:HD12	1.73	0.70
2:C:451:ARG:HH11	2:C:451:ARG:HG2	1.54	0.70
1:E:123:LEU:CD2	1:E:127:ILE:HD11	2.20	0.70
1:E:19:ALA:O	1:E:38:ILE:HD12	1.91	0.70
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.74	0.70
1:B:498:THR:OG1	2:C:499:VAL:HG21	1.91	0.70
2:D:145:ASP:OD2	2:D:181:THR:HG21	1.92	0.70
2:C:79:THR:HG23	2:C:81:GLN:HG2	1.72	0.70
1:A:266:GLY:HA3	1:A:300:ARG:O	1.91	0.70
2:C:371:LYS:HD3	2:C:371:LYS:O	1.91	0.70
2:C:393:ARG:O	2:C:397:ILE:HG12	1.90	0.70
1:A:451:ARG:NH1	1:A:451:ARG:HG2	1.99	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:VAL:HG11	1:A:180:MET:CE	2.21	0.70
1:A:499:VAL:HG12	1:A:499:VAL:O	1.92	0.70
1:E:273:MET:O	1:E:463:HIS:HA	1.91	0.70
2:C:289:ALA:HB2	2:C:419:PHE:HA	1.72	0.70
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.73	0.70
1:F:378:ASP:OD1	1:F:413:THR:HG21	1.91	0.70
2:C:203:ASN:HB3	2:C:225:LEU:HD23	1.74	0.69
2:C:14:GLU:HG3	2:C:16:GLN:H	1.57	0.69
1:B:65:ILE:HG22	1:B:65:ILE:O	1.91	0.69
1:B:429:HIS:HA	1:B:431:SEP:O1P	1.91	0.69
1:F:347:VAL:O	1:F:348:CYS:HB2	1.92	0.69
2:C:379:SER:HA	2:C:413:THR:HG22	1.73	0.69
1:F:239:ILE:HB	5:F:916:HOH:O	1.91	0.69
2:D:151:PHE:C	2:D:153:GLN:H	1.95	0.69
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.22	0.69
1:B:18:ILE:HB	1:B:228:THR:HG23	1.73	0.69
1:F:147:VAL:O	1:F:150:VAL:HG12	1.92	0.69
2:C:461:SER:OG	2:C:462:TRP:N	2.25	0.69
1:F:21:MET:HE1	1:F:141:ARG:HG2	1.74	0.69
2:D:79:THR:CG2	2:D:81:GLN:HG2	2.22	0.69
1:E:396:VAL:O	1:E:400:THR:HB	1.92	0.69
1:F:502:LYS:HZ1	1:F:507:ARG:HB3	1.55	0.69
2:D:496:ARG:HG2	1:E:487:GLU:OE1	1.92	0.69
1:A:377:ILE:HD12	1:A:412:PHE:HE2	1.58	0.69
1:F:191:ILE:CB	1:F:198:GLU:HG3	2.23	0.69
1:A:89:SER:HB2	1:B:227:GLY:O	1.93	0.69
1:B:334:ASP:OD1	1:B:336:GLU:HB2	1.93	0.69
1:F:81:GLN:H	1:F:81:GLN:NE2	1.91	0.69
1:F:509:VAL:HG12	1:F:510:ARG:H	1.57	0.69
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.75	0.69
2:C:182:THR:HG22	2:C:183:GLU:H	1.57	0.68
1:E:497:ILE:HG22	1:E:498:THR:H	1.58	0.68
1:B:52:LYS:HB2	4:B:903:ATP:O1B	1.93	0.68
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.75	0.68
1:F:334:ASP:OD1	1:F:336:GLU:HB2	1.93	0.68
2:C:287:THR:HG23	2:C:414:ASN:HB3	1.74	0.68
1:A:79:THR:O	1:A:83:ILE:HD12	1.93	0.68
1:A:459:ARG:HD3	1:F:323:GLN:NE2	2.08	0.68
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.74	0.68
1:B:287:THR:CG2	1:B:414:ASN:HD22	2.06	0.68
2:D:295:THR:HG23	2:D:378:ASP:OD2	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:VAL:HG12	2:D:388:SER:N	2.08	0.68
2:C:126:LEU:O	2:C:129:ARG:HB2	1.92	0.68
2:C:146:SER:N	2:C:181:THR:HG22	2.08	0.68
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.58	0.68
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.76	0.68
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.08	0.68
1:A:505:LEU:HD12	1:A:505:LEU:O	1.94	0.68
1:A:18:ILE:HD12	1:A:18:ILE:N	2.08	0.68
2:D:79:THR:HG23	2:D:81:GLN:H	1.59	0.68
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.23	0.68
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.58	0.68
1:F:14:GLU:HG2	5:F:923:HOH:O	1.94	0.67
2:D:370:PHE:O	2:D:371:LYS:HD2	1.94	0.67
1:A:495:THR:HG22	1:A:497:ILE:HG23	1.76	0.67
1:F:504:GLU:HA	1:F:507:ARG:NE	2.09	0.67
1:F:273:MET:O	1:F:463:HIS:HA	1.94	0.67
1:A:363:ILE:O	1:A:367:ILE:HG13	1.94	0.67
2:D:182:THR:HG22	2:D:183:GLU:N	2.09	0.67
1:F:504:GLU:HB3	1:F:507:ARG:CZ	2.24	0.67
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.75	0.67
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.76	0.67
2:D:451:ARG:HH11	2:D:451:ARG:HG2	1.59	0.67
1:B:295:THR:HG21	1:B:319:GLU:OE2	1.94	0.67
1:A:140:ARG:HH11	1:A:140:ARG:CB	2.08	0.67
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.07	0.67
1:A:293:GLY:HA2	4:A:901:ATP:O1A	1.95	0.67
2:C:106:LEU:HD13	2:C:129:ARG:NH2	2.10	0.67
1:B:497:ILE:HD12	1:B:499:VAL:HB	1.74	0.67
1:A:273:MET:O	1:A:463:HIS:HA	1.95	0.67
1:B:497:ILE:HD12	1:B:499:VAL:H	1.60	0.67
2:D:441:GLN:HE22	2:D:490:ILE:HD12	1.60	0.67
2:D:367:ILE:HG12	2:D:375:ILE:HD11	1.76	0.66
1:B:461:SER:OG	1:B:462:TRP:N	2.26	0.66
1:B:81:GLN:H	1:B:81:GLN:NE2	1.93	0.66
1:E:123:LEU:HD22	1:E:166:ARG:CD	2.25	0.66
1:A:64:ILE:HG22	1:A:65:ILE:HD13	1.77	0.66
2:D:316:ALA:O	2:D:348:CYS:HA	1.95	0.66
1:B:106:LEU:C	1:B:106:LEU:HD12	2.16	0.66
1:A:61:TYR:CE1	1:A:92:TRP:HB2	2.31	0.66
2:C:273:MET:O	2:C:463:HIS:HA	1.96	0.66
1:A:24:MET:CB	1:A:62:ASN:HD22	2.08	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:LEU:C	1:E:344:LEU:HD13	2.15	0.66
1:F:371:LYS:CD	1:F:371:LYS:O	2.43	0.66
1:B:119:GLY:C	1:B:121:PHE:H	1.99	0.66
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.19	0.66
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.24	0.66
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.95	0.66
1:E:435:ASP:HA	1:E:459:ARG:HD2	1.76	0.66
1:F:471:MET:HB3	1:F:480:LYS:NZ	2.11	0.66
2:C:371:LYS:CD	2:C:371:LYS:O	2.43	0.66
1:F:363:ILE:O	1:F:367:ILE:HG13	1.96	0.66
1:B:426:THR:HG22	1:B:428:SER:H	1.60	0.66
2:C:106:LEU:C	2:C:106:LEU:HD12	2.16	0.66
1:E:263:VAL:HG12	1:E:374:ARG:NH2	2.09	0.66
2:C:182:THR:HG22	2:C:183:GLU:N	2.10	0.66
2:C:263:VAL:HG12	2:C:374:ARG:HH21	1.61	0.65
2:C:419:PHE:O	2:C:420:MET:HB2	1.95	0.65
2:C:334:ASP:OD1	2:C:336:GLU:HB2	1.97	0.65
2:D:345:LYS:HZ3	2:D:366:GLU:CD	2.00	0.65
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.76	0.65
1:E:359:HIS:O	1:E:363:ILE:HG13	1.97	0.65
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.96	0.65
2:C:470:PHE:HB2	2:C:478:ASP:O	1.96	0.65
1:F:146:SER:H	1:F:181:THR:CG2	2.02	0.65
1:B:293:GLY:HA2	4:B:901:ATP:O1A	1.96	0.65
1:A:459:ARG:HD3	1:F:323:GLN:HE22	1.62	0.65
2:D:344:LEU:HD13	2:D:345:LYS:N	2.12	0.65
1:A:311:ARG:HD2	1:A:371:LYS:HD2	1.78	0.65
2:D:334:ASP:OD1	2:D:336:GLU:HB2	1.96	0.65
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.79	0.65
2:D:486:PHE:CB	2:D:489:ILE:HD11	2.27	0.65
1:A:151:PHE:C	1:A:153:GLN:H	2.00	0.65
2:D:345:LYS:NZ	2:D:366:GLU:HG2	2.10	0.65
1:E:439:LEU:HD12	1:E:440:LEU:N	2.11	0.65
2:D:52:LYS:HE3	4:D:903:ATP:O1B	1.97	0.65
2:D:371:LYS:CD	2:D:371:LYS:O	2.43	0.65
1:F:151:PHE:C	1:F:153:GLN:H	2.00	0.65
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.30	0.65
1:A:146:SER:H	1:A:181:THR:HG22	1.61	0.65
2:D:435:ASP:HA	2:D:459:ARG:HD2	1.79	0.65
1:F:508:ILE:O	1:F:508:ILE:HG22	1.97	0.65
1:B:371:LYS:HD3	1:B:371:LYS:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:GLY:O	2:D:218:ARG:NH2	2.30	0.64
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.79	0.64
1:B:444:GLU:OE2	2:C:489:ILE:HG13	1.97	0.64
2:C:41:SER:HB3	2:C:178:THR:HB	1.78	0.64
2:D:311:ARG:HD2	2:D:371:LYS:CD	2.27	0.64
1:F:432:TPO:HG21	1:F:432:TPO:O3P	1.97	0.64
1:B:79:THR:HG21	1:B:81:GLN:HG2	1.78	0.64
2:D:191:ILE:CB	2:D:198:GLU:HG3	2.28	0.64
1:E:43:LEU:HD11	1:E:182:THR:OG1	1.97	0.64
1:F:79:THR:CG2	1:F:81:GLN:HG2	2.27	0.64
1:E:79:THR:HG23	1:E:81:GLN:HE21	1.61	0.64
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.62	0.64
1:E:148:THR:OG1	1:E:182:THR:HG23	1.97	0.64
1:B:148:THR:HG21	1:B:183:GLU:HG3	1.78	0.64
1:F:311:ARG:HD2	1:F:371:LYS:CE	2.27	0.64
1:A:96:LYS:O	1:A:100:GLU:HG3	1.98	0.64
1:A:334:ASP:OD1	1:A:336:GLU:HB2	1.97	0.64
2:C:18:ILE:HD12	2:C:18:ILE:N	2.11	0.64
1:A:396:VAL:O	1:A:400:THR:HB	1.97	0.64
1:E:462:TRP:O	1:E:463:HIS:O	2.16	0.64
1:E:151:PHE:C	1:E:153:GLN:H	2.01	0.64
1:F:471:MET:HG2	1:F:480:LYS:HE2	1.79	0.64
1:B:311:ARG:HD2	1:B:371:LYS:CE	2.28	0.64
1:F:431:SEP:O	1:F:434:THR:HG22	1.98	0.64
1:F:344:LEU:HD22	1:F:345:LYS:N	2.12	0.64
1:E:186:GLU:OE2	1:E:187:GLU:N	2.30	0.64
2:D:182:THR:HG22	2:D:183:GLU:H	1.61	0.64
2:C:305:ALA:HB2	2:C:374:ARG:CD	2.28	0.64
2:D:400:THR:HG22	2:D:401:GLY:N	2.13	0.64
2:D:469:GLU:HG3	2:D:470:PHE:N	2.13	0.64
1:B:45:SER:HB3	1:B:182:THR:HB	1.79	0.64
1:A:371:LYS:O	1:A:371:LYS:CD	2.45	0.64
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.80	0.64
1:A:315:PHE:CZ	1:A:363:ILE:HG23	2.33	0.64
2:D:393:ARG:O	2:D:397:ILE:HG12	1.98	0.64
2:D:223:LEU:O	2:D:223:LEU:HD22	1.98	0.64
1:B:311:ARG:HD2	1:B:371:LYS:HD2	1.80	0.63
1:A:420:MET:CE	1:B:490:ILE:HG21	2.29	0.63
2:D:345:LYS:HZ3	2:D:366:GLU:CG	2.11	0.63
2:D:313:ILE:CD1	2:D:372:PRO:HG3	2.28	0.63
2:C:170:ARG:O	2:C:174:ILE:HG12	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:MET:CB	1:B:62:ASN:HD22	2.10	0.63
2:C:311:ARG:HD2	2:C:371:LYS:HD2	1.81	0.63
1:F:231:MET:CE	1:F:251:ALA:HB2	2.27	0.63
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.33	0.63
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.34	0.63
2:C:159:VAL:O	2:C:163:GLU:HG2	1.98	0.63
1:F:147:VAL:HG11	1:F:180:MET:CE	2.28	0.63
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.79	0.63
1:E:123:LEU:HD23	1:E:127:ILE:HD11	1.80	0.63
1:F:120:GLY:HA2	1:F:123:LEU:HB2	1.81	0.63
2:C:61:TYR:CE1	2:C:92:TRP:HB2	2.34	0.63
1:A:503:SER:C	1:A:504:GLU:HG3	2.20	0.62
2:C:17:ALA:C	2:C:18:ILE:HD12	2.19	0.62
1:B:151:PHE:C	1:B:153:GLN:H	2.02	0.62
1:E:496:ARG:O	1:E:497:ILE:HD13	1.99	0.62
1:A:21:MET:HE1	1:A:141:ARG:HG2	1.81	0.62
1:A:419:PHE:CD2	1:B:425:ILE:CD1	2.83	0.62
2:C:419:PHE:CD1	2:C:420:MET:HG3	2.34	0.62
1:E:299:SER:C	1:E:333:MET:HE1	2.20	0.62
1:A:52:LYS:HE3	4:A:903:ATP:O1B	2.00	0.62
2:D:340:ARG:O	2:D:342:ASN:N	2.31	0.62
2:D:81:GLN:NE2	2:D:81:GLN:H	1.98	0.62
2:D:311:ARG:HD2	2:D:371:LYS:CE	2.30	0.62
1:B:371:LYS:O	1:B:371:LYS:CD	2.47	0.62
2:D:14:GLU:CD	2:D:15:HIS:H	2.03	0.62
1:E:170:ARG:O	1:E:174:ILE:HG12	1.99	0.62
1:A:14:GLU:HG3	1:A:16:GLN:OE1	1.99	0.62
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.14	0.62
1:F:119:GLY:C	1:F:122:ASP:OD2	2.38	0.62
2:D:14:GLU:OE1	2:D:14:GLU:HA	1.99	0.62
1:A:323:GLN:HE22	1:B:459:ARG:HD3	1.64	0.62
2:D:486:PHE:CE2	2:D:496:ARG:HB3	2.34	0.62
1:E:148:THR:HG21	1:E:183:GLU:CG	2.30	0.62
1:F:31:ILE:HG22	1:F:222:ILE:HD12	1.81	0.62
2:D:377:ILE:HD12	2:D:412:PHE:CE2	2.35	0.62
1:B:146:SER:H	1:B:181:THR:CG2	2.13	0.62
2:C:145:ASP:OD2	2:C:181:THR:HG21	1.99	0.62
1:E:14:GLU:HG3	1:E:16:GLN:N	2.14	0.62
1:F:122:ASP:O	1:F:126:LEU:N	2.32	0.62
1:F:356:LEU:CD2	1:F:387:VAL:HG11	2.30	0.62
1:E:347:VAL:HG12	1:E:348:CYS:N	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:VAL:HG12	1:F:374:ARG:NH2	2.15	0.61
1:B:287:THR:HG21	1:B:425:ILE:O	1.99	0.61
1:E:294:LYS:HB2	4:E:901:ATP:O1B	1.98	0.61
1:A:441:GLN:O	1:A:441:GLN:HG3	2.00	0.61
1:B:170:ARG:O	1:B:174:ILE:HG12	2.00	0.61
2:D:79:THR:HG23	2:D:81:GLN:HE21	1.65	0.61
1:E:79:THR:HG21	1:E:81:GLN:HG2	1.78	0.61
1:E:148:THR:OG1	1:E:182:THR:CG2	2.48	0.61
2:C:203:ASN:HB3	2:C:225:LEU:CD2	2.30	0.61
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.81	0.61
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.15	0.61
1:F:340:ARG:O	1:F:342:ASN:N	2.32	0.61
1:E:161:ARG:HB2	1:E:196:VAL:HG11	1.81	0.61
2:D:446:ARG:H	2:D:496:ARG:HH22	1.47	0.61
2:C:150:VAL:O	2:C:153:GLN:HG3	2.01	0.61
2:C:52:LYS:HD3	2:C:182:THR:O	2.01	0.61
1:F:79:THR:HG23	1:F:81:GLN:HG2	1.82	0.61
2:C:451:ARG:NH1	2:C:451:ARG:HG2	2.15	0.61
2:D:418:GLN:HB2	1:E:423:HIS:O	2.00	0.61
2:C:19:ALA:O	2:C:38:ILE:HD12	2.00	0.61
1:B:146:SER:N	1:B:181:THR:HG22	2.15	0.61
1:B:191:ILE:HB	1:B:198:GLU:HG3	1.83	0.61
1:E:446:ARG:NH2	1:E:496:ARG:NH2	2.49	0.61
1:E:140:ARG:NH1	1:E:140:ARG:HB3	2.15	0.61
1:F:371:LYS:HD3	1:F:371:LYS:O	1.99	0.61
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.83	0.61
2:C:296:LEU:HD13	2:C:331:TRP:CD2	2.36	0.61
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.62	0.61
2:C:148:THR:OG1	2:C:182:THR:HG23	2.01	0.61
1:A:486:PHE:HB2	1:A:489:ILE:HD11	1.82	0.61
2:C:363:ILE:O	2:C:367:ILE:HG13	2.01	0.61
1:A:435:ASP:HA	1:A:459:ARG:HD2	1.81	0.61
2:D:41:SER:HB3	2:D:178:THR:HB	1.83	0.61
2:C:497:ILE:C	2:C:498:THR:HG22	2.21	0.61
1:F:24:MET:HB2	1:F:62:ASN:HD22	1.64	0.61
1:B:418:GLN:HG3	1:B:418:GLN:O	2.00	0.61
1:F:305:ALA:HB2	1:F:374:ARG:CD	2.20	0.61
1:E:159:VAL:O	1:E:163:GLU:HG2	2.01	0.61
2:C:431:SER:O	2:C:432:TPO:HG22	2.00	0.61
1:B:19:ALA:O	1:B:38:ILE:HD12	2.00	0.61
2:C:21:MET:HE3	2:C:141:ARG:CG	2.24	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ILE:HD12	1:B:412:PHE:HE1	1.65	0.61
2:D:347:VAL:O	2:D:348:CYS:HB2	2.00	0.61
1:A:320:SER:HA	1:B:254:LEU:HG	1.82	0.60
1:F:19:ALA:O	1:F:38:ILE:HD12	2.01	0.60
1:A:273:MET:O	1:A:464:ASP:N	2.31	0.60
2:D:231:MET:CE	2:D:251:ALA:HB2	2.31	0.60
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.82	0.60
1:A:16:GLN:O	1:A:17:ALA:O	2.20	0.60
1:A:80:PRO:HD2	1:A:81:GLN:NE2	2.16	0.60
1:A:347:VAL:O	1:A:348:CYS:HB2	2.01	0.60
1:F:123:LEU:HD12	1:F:166:ARG:HD2	1.82	0.60
2:C:396:VAL:HG11	2:C:430:ILE:HG23	1.84	0.60
1:B:493:SER:HB3	2:C:488:ARG:HG2	1.82	0.60
1:B:117:VAL:O	1:B:117:VAL:HG12	2.02	0.60
2:D:130:ILE:O	2:D:134:ILE:HG13	2.00	0.60
2:D:446:ARG:H	2:D:496:ARG:NH2	1.99	0.60
1:F:420:MET:HE3	1:F:492:GLY:HA3	1.83	0.60
2:C:347:VAL:O	2:C:348:CYS:CB	2.45	0.60
1:A:504:GLU:C	1:A:506:SER:H	2.05	0.60
2:C:400:THR:HG22	2:C:401:GLY:N	2.16	0.60
1:E:268:VAL:O	1:E:271:ASP:HB2	2.02	0.60
1:B:469:GLU:HB2	1:B:483:PHE:CZ	2.36	0.60
1:B:379:SER:CA	1:B:413:THR:HG22	2.30	0.60
2:D:140:ARG:HB3	2:D:140:ARG:NH1	2.16	0.60
1:A:126:LEU:HG	1:A:130:ILE:CD1	2.32	0.60
2:D:191:ILE:HB	2:D:198:GLU:CD	2.21	0.60
2:D:79:THR:HG22	2:D:82:ASP:N	2.07	0.60
1:A:420:MET:HE1	1:B:490:ILE:HG21	1.84	0.60
1:F:316:ALA:O	1:F:348:CYS:HA	2.02	0.60
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.84	0.60
2:C:340:ARG:O	2:C:342:ASN:N	2.34	0.59
1:E:436:THR:HG23	1:E:458:MET:HG3	1.83	0.59
1:E:377:ILE:HD12	1:E:412:PHE:HE2	1.67	0.59
2:D:396:VAL:O	2:D:400:THR:HB	2.02	0.59
1:F:378:ASP:HB3	5:F:904:HOH:O	2.02	0.59
2:C:471:MET:HG3	2:C:478:ASP:HB3	1.84	0.59
1:A:418:GLN:HB2	1:B:423:HIS:O	2.02	0.59
2:C:462:TRP:O	2:C:463:HIS:O	2.20	0.59
1:E:315:PHE:CZ	1:E:363:ILE:HG23	2.36	0.59
1:A:514:GLU:HA	1:A:514:GLU:OE1	2.03	0.59
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:VAL:O	1:F:163:GLU:HG2	2.02	0.59
1:F:504:GLU:O	1:F:505:LEU:HB2	2.00	0.59
2:C:318:GLU:OE2	2:D:432:TPO:O1P	2.21	0.59
1:F:123:LEU:O	1:F:127:ILE:HG12	2.02	0.59
1:E:316:ALA:O	1:E:348:CYS:HA	2.03	0.59
1:A:379:SER:H	1:A:413:THR:HB	1.67	0.59
1:E:426:THR:HG21	1:E:430:ILE:HG12	1.85	0.59
1:E:140:ARG:HH11	1:E:140:ARG:CB	2.16	0.59
2:D:131:ASN:OD1	2:D:174:ILE:HD12	2.03	0.59
1:F:218:ARG:HB3	5:F:919:HOH:O	2.03	0.59
1:F:106:LEU:C	1:F:106:LEU:HD12	2.23	0.59
1:B:471:MET:HB3	1:B:480:LYS:HZ3	1.68	0.59
1:F:191:ILE:CG2	1:F:198:GLU:HG3	2.33	0.58
1:E:485:ASN:HD21	1:E:496:ARG:NH1	2.01	0.58
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.85	0.58
1:A:432:TPO:HG22	1:A:432:TPO:O1P	2.02	0.58
2:C:33:HIS:HD2	2:C:229:SER:OG	1.85	0.58
2:C:79:THR:CG2	2:C:82:ASP:H	2.15	0.58
4:A:901:ATP:H3'	1:B:458:MET:O	2.03	0.58
2:C:419:PHE:CD2	2:D:425:ILE:HD12	2.38	0.58
1:E:345:LYS:HZ3	1:E:366:GLU:CD	2.06	0.58
1:A:269:ARG:HG2	1:A:479:ILE:HB	1.85	0.58
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.66	0.58
1:B:264:SER:HB3	1:B:304:ASN:HD21	1.68	0.58
2:D:19:ALA:C	2:D:38:ILE:HD12	2.23	0.58
2:C:294:LYS:HB2	4:C:901:ATP:O1B	2.04	0.58
1:B:65:ILE:O	1:B:65:ILE:CG2	2.52	0.58
1:A:106:LEU:HD12	1:A:106:LEU:C	2.24	0.58
2:D:79:THR:CG2	2:D:82:ASP:H	2.09	0.58
2:C:151:PHE:C	2:C:153:GLN:N	2.55	0.58
1:F:503:SER:O	1:F:504:GLU:O	2.21	0.58
1:E:400:THR:HG22	1:E:401:GLY:N	2.19	0.58
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.85	0.58
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.86	0.58
1:A:513:GLN:HG3	1:A:513:GLN:O	2.04	0.58
2:D:446:ARG:HG3	2:D:496:ARG:NH1	2.18	0.58
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.19	0.58
1:A:461:SER:OG	1:A:462:TRP:N	2.36	0.58
1:B:98:VAL:HA	1:B:103:LEU:O	2.02	0.58
1:A:191:ILE:HB	1:A:198:GLU:CG	2.33	0.58
2:C:344:LEU:HD22	2:C:345:LYS:N	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.37	0.58
1:F:393:ARG:O	1:F:397:ILE:HG12	2.03	0.58
1:A:400:THR:HG22	1:A:401:GLY:N	2.18	0.58
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.86	0.58
1:A:344:LEU:HD13	1:A:344:LEU:C	2.24	0.58
2:D:299:SER:HB3	2:D:333:MET:HE1	1.86	0.58
2:C:147:VAL:HG11	2:C:180:MET:CE	2.32	0.58
2:C:88:ARG:HD3	2:D:15:HIS:O	2.04	0.58
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.38	0.58
1:E:123:LEU:CD1	1:E:163:GLU:OE2	2.52	0.57
1:A:462:TRP:O	1:A:463:HIS:O	2.21	0.57
1:F:295:THR:HG23	1:F:378:ASP:OD2	2.04	0.57
1:E:358:ASP:O	1:E:362:ILE:HG12	2.03	0.57
2:D:79:THR:HG21	2:D:81:GLN:HG2	1.84	0.57
1:A:65:ILE:O	1:A:65:ILE:CG2	2.51	0.57
1:E:41:SER:HB3	1:E:178:THR:HB	1.84	0.57
2:D:345:LYS:NZ	2:D:366:GLU:CG	2.67	0.57
2:C:419:PHE:O	2:C:420:MET:CB	2.51	0.57
1:A:432:TPO:OG1	1:A:433:ILE:HD12	2.04	0.57
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.87	0.57
1:A:448:GLU:HG2	1:B:466:ALA:HA	1.86	0.57
2:D:79:THR:HG23	2:D:81:GLN:HG2	1.86	0.57
1:F:123:LEU:O	1:F:123:LEU:HD13	2.03	0.57
2:C:426:THR:HG22	2:C:428:SER:H	1.70	0.57
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.19	0.57
1:E:81:GLN:H	1:E:81:GLN:NE2	2.02	0.57
2:C:81:GLN:CD	2:C:81:GLN:H	2.05	0.57
1:A:496:ARG:HG3	1:B:487:GLU:OE1	2.04	0.57
1:A:252:MET:HE3	1:F:350:TYR:CE1	2.39	0.57
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.85	0.57
1:E:281:ASP:O	1:E:282:SER:HB3	2.05	0.57
1:E:123:LEU:CD2	1:E:166:ARG:HD2	2.30	0.57
1:F:182:THR:HG22	1:F:183:GLU:H	1.70	0.57
2:C:146:SER:H	2:C:181:THR:CG2	2.16	0.57
1:E:287:THR:HG23	1:E:414:ASN:HB3	1.87	0.57
1:A:182:THR:HG21	1:A:192:ALA:HB1	1.86	0.57
2:C:248:PRO:HB2	2:C:251:ALA:HB3	1.87	0.57
1:E:295:THR:HG23	1:E:378:ASP:OD2	2.05	0.57
2:D:45:SER:HB2	2:D:182:THR:HB	1.87	0.57
2:D:446:ARG:H	2:D:496:ARG:CZ	2.16	0.57
1:F:79:THR:HG23	1:F:81:GLN:H	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:GLU:HB2	1:E:483:PHE:CZ	2.40	0.57
1:A:85:LYS:NZ	1:B:14:GLU:HG3	2.20	0.57
2:C:45:SER:CB	2:C:182:THR:HB	2.35	0.56
1:B:51:GLY:O	1:B:52:LYS:C	2.43	0.56
1:F:451:ARG:HH11	1:F:451:ARG:HG2	1.69	0.56
2:C:444:GLU:OE2	2:D:489:ILE:HG12	2.05	0.56
1:A:21:MET:CE	1:A:59:PHE:CZ	2.88	0.56
1:F:96:LYS:O	1:F:100:GLU:HG3	2.05	0.56
1:F:115:GLN:HG3	1:F:116:GLU:N	2.21	0.56
1:B:150:VAL:O	1:B:153:GLN:HG3	2.05	0.56
2:D:495:THR:HA	1:E:487:GLU:OE2	2.05	0.56
1:E:485:ASN:HD21	1:E:496:ARG:HH11	1.50	0.56
1:B:45:SER:CB	1:B:182:THR:HB	2.35	0.56
1:F:118:VAL:O	1:F:118:VAL:HG13	2.05	0.56
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.87	0.56
1:B:435:ASP:HA	1:B:459:ARG:HD2	1.87	0.56
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.86	0.56
1:A:345:LYS:HZ3	1:A:366:GLU:HG2	1.70	0.56
2:D:96:LYS:O	2:D:100:GLU:HG3	2.05	0.56
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.40	0.56
1:F:484:ARG:NH1	1:F:484:ARG:HB3	2.20	0.56
2:D:151:PHE:C	2:D:153:GLN:N	2.58	0.56
1:A:211:LEU:HD12	1:A:215:ARG:O	2.06	0.56
1:F:150:VAL:O	1:F:153:GLN:HG3	2.06	0.56
2:D:178:THR:HG22	2:D:179:VAL:N	2.20	0.56
2:D:471:MET:HB3	2:D:480:LYS:NZ	2.20	0.56
2:D:67:PHE:HB2	2:D:69:GLU:HG3	1.87	0.56
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.86	0.56
1:B:497:ILE:HG13	1:B:498:THR:H	1.69	0.56
1:E:19:ALA:C	1:E:38:ILE:HD12	2.26	0.56
1:B:294:LYS:HB2	4:B:901:ATP:O1B	2.06	0.56
2:D:354:ALA:HB3	2:D:359:HIS:NE2	2.21	0.56
1:E:449:MET:HE3	1:F:490:ILE:HD11	1.86	0.56
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.41	0.56
1:B:79:THR:CG2	1:B:82:ASP:H	2.11	0.56
1:A:311:ARG:HD2	1:A:371:LYS:CD	2.35	0.56
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.70	0.56
1:B:130:ILE:O	1:B:134:ILE:HG13	2.06	0.56
1:F:436:THR:OG1	1:F:458:MET:HG2	2.06	0.56
1:E:499:VAL:HG12	1:E:499:VAL:O	2.06	0.56
1:A:495:THR:HG22	1:A:497:ILE:CG2	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:VAL:HG22	1:F:122:ASP:HB3	1.88	0.55
4:A:901:ATP:O3'	1:B:457:LYS:HB2	2.06	0.55
1:F:117:VAL:O	1:F:118:VAL:HB	2.06	0.55
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.87	0.55
1:A:501:GLU:O	1:A:503:SER:N	2.39	0.55
2:D:419:PHE:CD2	1:E:425:ILE:CD1	2.88	0.55
2:C:104:PHE:CE2	2:C:106:LEU:HB2	2.41	0.55
2:C:43:LEU:HD11	2:C:182:THR:OG1	2.05	0.55
2:C:49:GLY:O	2:C:218:ARG:NH2	2.39	0.55
2:D:469:GLU:HB2	2:D:483:PHE:CZ	2.42	0.55
1:B:213:GLY:O	1:B:214:GLU:HB2	2.06	0.55
1:E:49:GLY:CA	4:E:903:ATP:O2B	2.53	0.55
2:C:377:ILE:HD12	2:C:412:PHE:CE2	2.42	0.55
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.36	0.55
1:E:123:LEU:HD21	1:E:127:ILE:HD11	1.87	0.55
1:E:496:ARG:HG3	1:E:497:ILE:N	2.21	0.55
2:D:42:THR:HG23	2:D:203:ASN:HB2	1.88	0.55
1:F:294:LYS:N	4:F:901:ATP:O1B	2.40	0.55
1:B:191:ILE:CB	1:B:198:GLU:HG3	2.36	0.55
1:A:433:ILE:HG22	1:A:433:ILE:O	2.06	0.55
1:B:448:GLU:HG2	2:C:466:ALA:HA	1.89	0.55
2:C:356:LEU:HD22	2:C:387:VAL:HG11	1.87	0.55
2:D:140:ARG:HH11	2:D:140:ARG:CB	2.20	0.55
2:C:117:VAL:O	2:C:117:VAL:HG12	2.06	0.55
1:A:393:ARG:O	1:A:397:ILE:HG12	2.06	0.55
1:A:211:LEU:O	1:A:212:GLU:CB	2.52	0.55
1:A:49:GLY:CA	4:A:903:ATP:O2B	2.54	0.55
2:D:377:ILE:HD12	2:D:412:PHE:HE2	1.72	0.55
1:F:340:ARG:C	1:F:342:ASN:H	2.09	0.55
2:C:493:SER:HB3	2:D:488:ARG:HG2	1.89	0.55
2:C:435:ASP:HA	2:C:459:ARG:HD2	1.89	0.55
1:B:340:ARG:C	1:B:342:ASN:H	2.11	0.55
1:B:485:ASN:N	1:B:485:ASN:OD1	2.33	0.55
1:F:501:GLU:HG3	1:F:502:LYS:N	2.22	0.55
1:F:315:PHE:CZ	1:F:363:ILE:HG23	2.41	0.55
1:A:439:LEU:HD12	1:A:440:LEU:N	2.21	0.55
2:C:169:ALA:O	2:C:173:GLN:HG3	2.07	0.55
1:B:184:ARG:HG2	1:B:191:ILE:O	2.06	0.54
2:D:340:ARG:C	2:D:342:ASN:H	2.10	0.54
1:B:360:LEU:HD22	1:B:360:LEU:O	2.07	0.54
1:B:79:THR:O	1:B:83:ILE:HD12	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:148:THR:HG21	2:C:183:GLU:HG3	1.89	0.54
1:E:485:ASN:ND2	1:E:496:ARG:NH1	2.51	0.54
1:B:311:ARG:HD2	1:B:371:LYS:CD	2.37	0.54
1:B:213:GLY:O	1:B:214:GLU:CB	2.55	0.54
2:C:208:ARG:NH2	2:C:221:GLU:OE2	2.40	0.54
1:E:437:ILE:CD1	1:E:457:LYS:HE2	2.37	0.54
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.21	0.54
1:E:147:VAL:HG11	1:E:180:MET:HE2	1.90	0.54
1:B:148:THR:OG1	1:B:182:THR:HG23	2.08	0.54
1:B:451:ARG:HG2	1:B:451:ARG:NH1	2.22	0.54
1:B:159:VAL:O	1:B:163:GLU:HG2	2.08	0.54
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.89	0.54
1:E:121:PHE:CD1	1:E:121:PHE:N	2.74	0.54
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.41	0.54
1:B:21:MET:CE	1:B:141:ARG:HG2	2.27	0.54
1:A:451:ARG:N	1:A:451:ARG:HD2	2.23	0.54
2:C:53:THR:HG23	2:C:145:ASP:OD1	2.06	0.54
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.73	0.54
2:D:387:VAL:CG1	2:D:388:SER:N	2.70	0.54
1:A:148:THR:HG21	1:A:183:GLU:HG3	1.88	0.54
1:A:148:THR:OG1	1:A:182:THR:HG23	2.08	0.54
2:C:356:LEU:CD2	2:C:387:VAL:HG11	2.37	0.54
1:B:340:ARG:O	1:B:342:ASN:N	2.40	0.54
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.89	0.54
1:B:426:THR:HG22	1:B:428:SER:N	2.23	0.54
1:F:504:GLU:HA	1:F:507:ARG:HE	1.73	0.54
1:B:503:SER:O	1:B:504:GLU:HB2	2.06	0.54
2:C:113:GLU:O	2:C:114:GLY:C	2.45	0.54
2:C:300:ARG:N	2:C:333:MET:HE1	2.22	0.54
1:E:471:MET:HB3	1:E:480:LYS:NZ	2.23	0.54
1:A:57:ILE:HD13	1:A:73:PHE:CE1	2.43	0.54
1:E:356:LEU:HD13	1:E:387:VAL:HG21	1.90	0.54
1:B:483:PHE:HB3	1:B:486:PHE:CD1	2.43	0.54
2:D:439:LEU:HD12	2:D:439:LEU:C	2.28	0.54
2:C:18:ILE:HG21	2:C:37:PRO:HB3	1.89	0.54
2:D:127:ILE:HD11	2:D:167:LEU:HA	1.88	0.54
2:D:150:VAL:O	2:D:153:GLN:HG3	2.07	0.54
1:E:123:LEU:O	1:E:127:ILE:CG1	2.55	0.54
1:F:498:THR:HB	1:F:500:ASP:O	2.08	0.54
2:D:191:ILE:CG2	2:D:198:GLU:HG3	2.37	0.54
1:A:79:THR:HG23	1:A:81:GLN:HE21	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LYS:HB2	4:F:901:ATP:O3'	2.07	0.54
1:E:306:CYS:SG	1:E:344:LEU:HB2	2.48	0.54
1:B:38:ILE:HA	1:B:177:THR:CG2	2.37	0.54
1:F:49:GLY:HA2	4:F:903:ATP:O2B	2.07	0.54
1:B:316:ALA:O	1:B:348:CYS:HA	2.08	0.54
2:C:150:VAL:HG13	2:C:151:PHE:N	2.22	0.54
1:F:435:ASP:HA	1:F:459:ARG:HD2	1.89	0.54
1:F:119:GLY:HA2	1:F:122:ASP:OD1	2.08	0.54
1:F:122:ASP:OD2	1:F:123:LEU:N	2.41	0.54
1:B:31:ILE:HG22	1:B:222:ILE:HD12	1.89	0.54
1:E:123:LEU:HD23	1:E:127:ILE:CD1	2.37	0.54
1:A:311:ARG:HA	1:A:343:LEU:O	2.07	0.54
2:D:294:LYS:HB2	4:D:901:ATP:O1B	2.07	0.54
2:D:211:LEU:HD12	2:D:215:ARG:O	2.08	0.54
1:E:50:THR:HG22	1:E:209:ASN:HB2	1.89	0.54
1:E:118:VAL:HG12	1:E:118:VAL:O	2.08	0.54
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.38	0.53
2:D:345:LYS:HZ2	2:D:366:GLU:HG2	1.72	0.53
2:C:323:GLN:HE22	2:D:459:ARG:HD3	1.73	0.53
1:E:489:ILE:HA	1:E:494:PRO:HG3	1.90	0.53
1:E:320:SER:HA	1:F:254:LEU:HG	1.89	0.53
1:A:19:ALA:C	1:A:38:ILE:HD12	2.29	0.53
1:A:510:ARG:HA	1:A:510:ARG:NE	2.23	0.53
2:C:441:GLN:HE22	2:C:490:ILE:HD13	1.73	0.53
1:E:471:MET:HG2	1:E:480:LYS:HE2	1.90	0.53
1:A:264:SER:HA	1:A:271:ASP:OD1	2.08	0.53
1:E:31:ILE:HG22	1:E:222:ILE:HD12	1.90	0.53
1:B:67:PHE:HB2	1:B:69:GLU:HG3	1.89	0.53
1:A:503:SER:O	1:A:504:GLU:HG3	2.08	0.53
2:C:488:ARG:HG3	2:C:488:ARG:HH11	1.71	0.53
1:A:126:LEU:HG	1:A:130:ILE:HD12	1.90	0.53
1:B:358:ASP:O	1:B:362:ILE:HG12	2.09	0.53
1:E:255:THR:O	1:E:255:THR:HG22	2.07	0.53
2:D:255:THR:HG22	2:D:255:THR:O	2.08	0.53
2:C:359:HIS:O	2:C:363:ILE:HG13	2.08	0.53
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.90	0.53
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.89	0.53
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.38	0.53
2:C:433:ILE:HG22	2:C:433:ILE:O	2.08	0.53
1:F:489:ILE:HA	1:F:494:PRO:HG3	1.91	0.53
1:A:419:PHE:O	1:A:420:MET:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG13	1:A:151:PHE:N	2.23	0.53
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.73	0.53
1:F:502:LYS:HZ2	1:F:507:ARG:HB3	1.73	0.53
2:C:211:LEU:O	2:C:212:GLU:HB3	2.08	0.53
2:C:221:GLU:HG3	2:C:233:GLY:O	2.08	0.53
2:D:43:LEU:HD11	2:D:182:THR:OG1	2.08	0.53
1:A:426:THR:HG22	1:A:428:SER:N	2.21	0.53
2:C:123:LEU:O	2:C:126:LEU:N	2.41	0.53
2:C:287:THR:HG21	2:C:425:ILE:O	2.08	0.53
1:F:500:ASP:O	1:F:501:GLU:HB3	2.08	0.53
1:B:119:GLY:C	1:B:121:PHE:N	2.62	0.53
1:B:305:ALA:CB	1:B:374:ARG:HD2	2.32	0.53
2:C:52:LYS:HB2	4:C:903:ATP:O1B	2.09	0.53
1:A:87:ALA:O	1:A:92:TRP:CD1	2.62	0.53
2:C:164:LEU:HB3	2:C:200:VAL:HG11	1.90	0.53
2:D:385:ARG:HG2	1:E:393:ARG:NH1	2.24	0.53
1:B:353:SER:O	1:B:354:ALA:HB2	2.08	0.53
2:C:20:LYS:HE3	2:C:228:THR:HG21	1.91	0.53
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.73	0.53
2:D:81:GLN:CD	2:D:81:GLN:H	2.13	0.53
2:D:353:SER:O	2:D:354:ALA:HB2	2.09	0.53
2:D:359:HIS:O	2:D:363:ILE:HG13	2.09	0.53
1:B:116:GLU:HG2	1:B:117:VAL:H	1.74	0.53
2:C:186:GLU:OE2	2:C:187:GLU:N	2.41	0.53
1:F:52:LYS:HE3	4:F:903:ATP:O1B	2.09	0.53
1:A:332:GLY:O	1:A:333:MET:O	2.27	0.52
1:A:146:SER:N	1:A:181:THR:HG22	2.24	0.52
2:D:451:ARG:HG2	2:D:451:ARG:NH1	2.23	0.52
1:F:311:ARG:HG3	1:F:371:LYS:NZ	2.24	0.52
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.08	0.52
2:D:212:GLU:HG2	2:D:212:GLU:O	2.08	0.52
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.39	0.52
1:F:396:VAL:O	1:F:400:THR:HB	2.10	0.52
1:A:458:MET:O	4:F:901:ATP:H3'	2.10	0.52
1:E:191:ILE:CB	1:E:198:GLU:CG	2.87	0.52
1:F:379:SER:H	1:F:413:THR:HB	1.74	0.52
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.90	0.52
2:C:111:ASP:O	2:C:113:GLU:N	2.38	0.52
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.65	0.52
1:E:123:LEU:O	1:E:127:ILE:HG13	2.09	0.52
1:E:504:GLU:OE1	1:E:505:LEU:HD23	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LYS:O	1:B:100:GLU:HG3	2.09	0.52
2:C:119:GLY:HA2	2:C:122:ASP:OD1	2.09	0.52
2:C:79:THR:C	2:C:83:ILE:HD12	2.29	0.52
1:B:486:PHE:CE2	1:B:496:ARG:HB2	2.45	0.52
1:E:469:GLU:HG3	1:E:470:PHE:N	2.24	0.52
1:F:49:GLY:CA	4:F:903:ATP:O2B	2.56	0.52
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.91	0.52
1:E:191:ILE:HB	1:E:198:GLU:CD	2.29	0.52
1:A:52:LYS:N	4:A:903:ATP:O1B	2.34	0.52
1:A:15:HIS:C	1:A:16:GLN:OE1	2.47	0.52
1:B:21:MET:HE3	1:B:141:ARG:NE	2.24	0.52
1:F:191:ILE:HG21	1:F:198:GLU:HG3	1.92	0.52
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.90	0.52
1:A:213:GLY:O	1:A:214:GLU:HB2	2.09	0.52
2:D:106:LEU:C	2:D:106:LEU:HD12	2.30	0.52
1:A:56:SER:HB2	1:A:143:SER:HB3	1.91	0.52
2:D:65:ILE:HG22	2:D:65:ILE:O	2.08	0.52
1:A:419:PHE:CE2	1:B:425:ILE:HD12	2.45	0.52
1:F:231:MET:HE1	1:F:251:ALA:HB2	1.92	0.52
1:F:104:PHE:CE2	1:F:106:LEU:HB2	2.44	0.52
1:B:79:THR:HG23	1:B:81:GLN:HE21	1.74	0.52
1:A:79:THR:HG23	1:A:81:GLN:H	1.75	0.52
1:B:38:ILE:HA	1:B:177:THR:HG23	1.92	0.52
1:A:471:MET:HB3	1:A:480:LYS:NZ	2.24	0.52
1:A:294:LYS:N	4:A:901:ATP:O1B	2.43	0.52
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.39	0.52
1:A:151:PHE:C	1:A:153:GLN:N	2.64	0.51
1:F:191:ILE:CB	1:F:198:GLU:CG	2.81	0.51
2:D:332:GLY:O	2:D:333:MET:O	2.28	0.51
2:C:336:GLU:OE1	2:C:336:GLU:HA	2.10	0.51
1:A:300:ARG:N	1:A:333:MET:HE1	2.25	0.51
1:A:370:PHE:O	1:A:371:LYS:HD2	2.09	0.51
1:B:262:ARG:NH2	1:B:461:SER:HB2	2.25	0.51
1:E:379:SER:H	1:E:413:THR:HB	1.76	0.51
1:F:353:SER:O	1:F:354:ALA:HB2	2.10	0.51
1:B:286:ALA:HA	1:B:438:ILE:O	2.10	0.51
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.91	0.51
2:D:335:PHE:HA	2:D:338:MET:HG3	1.93	0.51
1:E:49:GLY:HA2	4:E:903:ATP:O2B	2.09	0.51
2:D:104:PHE:CE2	2:D:106:LEU:HB2	2.45	0.51
2:D:45:SER:CB	2:D:182:THR:HB	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:LEU:O	1:F:273:MET:HB2	2.10	0.51
1:A:294:LYS:HB2	4:A:901:ATP:O1B	2.10	0.51
1:B:161:ARG:HB2	1:B:196:VAL:CG1	2.40	0.51
2:C:430:ILE:O	2:C:432:TPO:N	2.44	0.51
1:E:437:ILE:HD12	1:E:457:LYS:HE2	1.91	0.51
1:F:170:ARG:O	1:F:174:ILE:HG12	2.10	0.51
1:F:497:ILE:HD12	1:F:497:ILE:C	2.30	0.51
1:A:359:HIS:O	1:A:363:ILE:HG13	2.10	0.51
1:A:340:ARG:O	1:A:342:ASN:N	2.44	0.51
1:B:178:THR:HG22	1:B:179:VAL:N	2.26	0.51
1:F:81:GLN:N	1:F:81:GLN:NE2	2.59	0.51
1:F:148:THR:OG1	1:F:182:THR:HG23	2.11	0.51
2:D:396:VAL:HG11	2:D:430:ILE:HG23	1.91	0.51
1:A:213:GLY:O	1:A:214:GLU:CB	2.59	0.51
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.92	0.51
1:F:501:GLU:HG3	1:F:502:LYS:H	1.75	0.51
1:F:515:LYS:CG	1:F:517:PRO:HD2	2.41	0.51
1:B:148:THR:CG2	1:B:193:ARG:HD2	2.41	0.51
2:C:420:MET:CE	2:D:490:ILE:HG21	2.40	0.51
2:C:323:GLN:NE2	2:D:459:ARG:HD3	2.26	0.51
2:C:299:SER:C	2:C:333:MET:HE1	2.30	0.51
1:E:471:MET:HG3	1:E:478:ASP:HB3	1.93	0.51
1:E:501:GLU:O	1:E:502:LYS:HE3	2.11	0.51
1:F:79:THR:HG23	1:F:81:GLN:HE21	1.76	0.51
1:F:509:VAL:HG12	1:F:510:ARG:N	2.25	0.51
1:F:151:PHE:C	1:F:153:GLN:N	2.63	0.51
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.91	0.51
1:A:166:ARG:HG3	1:F:112:PRO:O	2.11	0.51
1:B:433:ILE:O	1:B:433:ILE:HG22	2.10	0.51
1:F:505:LEU:O	1:F:506:SER:HB3	2.11	0.51
1:B:191:ILE:CG2	1:B:198:GLU:HG3	2.40	0.51
1:E:262:ARG:NH2	1:E:461:SER:HB2	2.26	0.51
2:C:191:ILE:HB	2:C:198:GLU:HG3	1.92	0.51
1:B:49:GLY:O	1:B:218:ARG:NH2	2.44	0.51
1:A:220:LEU:C	1:A:220:LEU:HD23	2.31	0.51
1:B:246:ILE:O	1:B:248:PRO:HD3	2.10	0.51
2:D:80:PRO:HD2	2:D:81:GLN:NE2	2.26	0.50
1:E:191:ILE:CB	1:E:198:GLU:HG3	2.41	0.50
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.11	0.50
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.93	0.50
2:C:123:LEU:HD11	2:C:163:GLU:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:ILE:HB	1:E:198:GLU:HG3	1.92	0.50
1:E:363:ILE:O	1:E:367:ILE:HG13	2.12	0.50
1:F:344:LEU:HD22	1:F:345:LYS:H	1.76	0.50
2:C:344:LEU:HD22	2:C:345:LYS:H	1.75	0.50
1:F:115:GLN:CG	1:F:116:GLU:N	2.74	0.50
2:C:295:THR:HG21	2:C:319:GLU:OE2	2.11	0.50
2:C:120:GLY:O	2:C:122:ASP:N	2.45	0.50
1:F:356:LEU:HD21	1:F:387:VAL:HG11	1.92	0.50
2:D:484:ARG:NH1	2:D:484:ARG:HB3	2.26	0.50
1:A:18:ILE:CD1	1:A:18:ILE:N	2.74	0.50
1:B:79:THR:HG23	1:B:81:GLN:H	1.76	0.50
1:A:425:ILE:HD12	1:F:419:PHE:CE2	2.47	0.50
2:C:79:THR:HG21	2:C:81:GLN:HG2	1.92	0.50
1:A:436:THR:HG23	1:A:458:MET:HG3	1.93	0.50
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.76	0.50
2:D:356:LEU:HD21	2:D:387:VAL:HG11	1.94	0.50
2:D:388:SER:OG	2:D:391:ALA:CB	2.59	0.50
1:F:120:GLY:O	1:F:123:LEU:HB3	2.11	0.50
2:C:340:ARG:C	2:C:342:ASN:H	2.14	0.50
1:F:106:LEU:HD13	1:F:129:ARG:CZ	2.41	0.50
1:F:439:LEU:C	1:F:439:LEU:HD12	2.31	0.50
1:F:406:GLU:HB3	1:F:408:ILE:HG13	1.93	0.50
2:D:419:PHE:CE2	1:E:425:ILE:HD12	2.45	0.50
1:B:31:ILE:HA	1:B:231:MET:SD	2.52	0.50
1:B:126:LEU:HD12	1:B:129:ARG:HD3	1.93	0.50
1:B:81:GLN:CD	1:B:81:GLN:H	2.14	0.50
1:B:61:TYR:CZ	1:B:92:TRP:HB2	2.46	0.50
1:B:436:THR:HG23	1:B:458:MET:HG3	1.94	0.50
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.94	0.50
2:D:273:MET:CE	2:D:468:ARG:HD2	2.42	0.50
1:A:254:LEU:HG	1:F:320:SER:HA	1.94	0.50
2:D:496:ARG:CG	1:E:487:GLU:OE1	2.60	0.50
1:F:148:THR:HG21	1:F:183:GLU:CG	2.38	0.50
1:A:82:ASP:O	1:A:83:ILE:C	2.49	0.50
1:A:295:THR:HG23	1:A:378:ASP:OD2	2.11	0.50
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.94	0.50
1:E:441:GLN:HE22	1:E:490:ILE:HA	1.77	0.50
1:B:433:ILE:CG2	1:B:433:ILE:O	2.60	0.50
1:E:146:SER:CA	1:E:181:THR:HG22	2.41	0.50
1:E:262:ARG:HH22	1:E:461:SER:HB2	1.77	0.50
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ARG:HB2	1:F:196:VAL:CG1	2.41	0.50
1:A:52:LYS:HD3	1:A:182:THR:O	2.11	0.50
2:C:38:ILE:HA	2:C:177:THR:HG23	1.94	0.50
2:D:106:LEU:HD13	2:D:129:ARG:NH2	2.27	0.50
1:B:50:THR:HG22	1:B:209:ASN:HB2	1.94	0.50
1:B:419:PHE:CD2	2:C:425:ILE:CD1	2.92	0.49
2:C:287:THR:HG23	2:C:414:ASN:ND2	2.22	0.49
2:D:347:VAL:O	2:D:348:CYS:CB	2.59	0.49
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.94	0.49
1:B:287:THR:HG23	1:B:414:ASN:HB3	1.94	0.49
1:A:425:ILE:HD12	1:F:419:PHE:CD2	2.46	0.49
2:D:363:ILE:O	2:D:367:ILE:HG13	2.12	0.49
1:F:462:TRP:O	1:F:463:HIS:O	2.29	0.49
1:B:455:VAL:HG11	1:B:463:HIS:HB2	1.93	0.49
1:F:471:MET:CG	1:F:478:ASP:HB3	2.43	0.49
1:A:340:ARG:C	1:A:342:ASN:H	2.15	0.49
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.77	0.49
2:D:191:ILE:CB	2:D:198:GLU:CG	2.87	0.49
1:E:151:PHE:C	1:E:153:GLN:N	2.64	0.49
2:D:313:ILE:HD11	2:D:372:PRO:HG3	1.94	0.49
1:B:418:GLN:HB2	2:C:423:HIS:O	2.12	0.49
1:A:191:ILE:HB	1:A:198:GLU:CD	2.32	0.49
2:D:159:VAL:O	2:D:163:GLU:HG2	2.13	0.49
1:F:79:THR:CG2	1:F:82:ASP:H	2.13	0.49
2:C:52:LYS:N	4:C:903:ATP:O1B	2.43	0.49
2:C:471:MET:HB3	2:C:480:LYS:NZ	2.27	0.49
1:F:121:PHE:O	1:F:125:ALA:N	2.41	0.49
1:A:218:ARG:O	1:A:236:PRO:HA	2.13	0.49
1:E:347:VAL:O	1:E:348:CYS:HB2	2.12	0.49
2:C:111:ASP:OD1	2:C:113:GLU:HG2	2.12	0.49
2:D:148:THR:OG1	2:D:182:THR:CG2	2.59	0.49
1:E:294:LYS:N	4:E:901:ATP:O1B	2.43	0.49
1:B:191:ILE:HG21	1:B:198:GLU:HG3	1.94	0.49
1:B:377:ILE:HD12	1:B:412:PHE:CD2	2.46	0.49
4:B:903:ATP:O3'	2:C:224:LYS:HB2	2.13	0.49
2:C:396:VAL:O	2:C:400:THR:HB	2.13	0.49
1:A:433:ILE:CG2	1:A:433:ILE:O	2.61	0.49
1:F:131:ASN:OD1	1:F:174:ILE:HD12	2.13	0.49
2:C:70:PRO:HG2	2:C:138:ARG:O	2.11	0.49
1:F:65:ILE:HG22	1:F:65:ILE:O	2.12	0.49
2:D:79:THR:HG23	2:D:81:GLN:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:ILE:CD1	1:F:457:LYS:HE2	2.42	0.49
2:D:289:ALA:HB2	2:D:419:PHE:HA	1.93	0.49
1:F:471:MET:HB3	1:F:480:LYS:HZ3	1.77	0.49
2:C:38:ILE:HA	2:C:177:THR:CG2	2.42	0.49
1:B:347:VAL:O	1:B:348:CYS:HB2	2.12	0.49
1:F:20:LYS:C	1:F:38:ILE:HD11	2.32	0.49
1:F:19:ALA:C	1:F:38:ILE:HD12	2.33	0.49
1:A:267:VAL:O	1:A:271:ASP:OD2	2.31	0.49
1:B:219:THR:HA	1:B:235:TYR:O	2.11	0.49
2:D:151:PHE:O	2:D:153:GLN:N	2.41	0.49
1:A:17:ALA:C	1:A:18:ILE:HD12	2.33	0.49
2:C:419:PHE:HD1	2:C:420:MET:HG3	1.76	0.49
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.48	0.49
1:E:348:CYS:HB3	1:F:254:LEU:HD23	1.95	0.49
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.93	0.49
1:B:396:VAL:O	1:B:400:THR:HB	2.13	0.49
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.47	0.49
1:E:79:THR:HG23	1:E:81:GLN:H	1.77	0.49
1:F:340:ARG:C	1:F:342:ASN:N	2.65	0.49
2:C:332:GLY:O	2:C:333:MET:O	2.30	0.49
1:A:471:MET:HG2	1:A:480:LYS:HE2	1.94	0.49
2:D:461:SER:OG	2:D:462:TRP:N	2.45	0.49
1:B:281:ASP:O	1:B:282:SER:HB3	2.12	0.49
2:C:495:THR:HG22	2:D:487:GLU:OE2	2.12	0.48
1:F:311:ARG:HD2	1:F:371:LYS:HD2	1.95	0.48
1:A:419:PHE:HD1	1:A:420:MET:HG3	1.77	0.48
1:E:123:LEU:HD23	1:E:127:ILE:CG1	2.43	0.48
2:D:263:VAL:CG1	2:D:374:ARG:HH21	2.22	0.48
2:C:81:GLN:CD	2:C:81:GLN:N	2.66	0.48
1:A:127:ILE:HD11	1:A:167:LEU:CD1	2.41	0.48
1:A:19:ALA:O	1:A:38:ILE:HD12	2.13	0.48
2:D:98:VAL:HA	2:D:103:LEU:O	2.14	0.48
1:E:169:ALA:O	1:E:173:GLN:HG3	2.13	0.48
2:C:305:ALA:CB	2:C:374:ARG:HD2	2.38	0.48
1:F:426:THR:CG2	1:F:428:SER:OG	2.61	0.48
2:C:311:ARG:HD2	2:C:371:LYS:CD	2.43	0.48
1:F:356:LEU:HD22	1:F:387:VAL:HG11	1.96	0.48
1:E:185:ILE:HD11	1:E:193:ARG:NH1	2.29	0.48
2:C:98:VAL:HA	2:C:103:LEU:O	2.13	0.48
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.95	0.48
1:E:417:ASP:O	1:F:424:SER:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:THR:O	1:F:83:ILE:HD12	2.13	0.48
1:F:426:THR:HG21	1:F:430:ILE:HG12	1.95	0.48
2:C:49:GLY:CA	4:C:903:ATP:O2B	2.61	0.48
1:E:311:ARG:HD2	1:E:371:LYS:CE	2.43	0.48
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.47	0.48
1:F:471:MET:HB3	1:F:480:LYS:HZ1	1.77	0.48
2:C:58:GLN:HG3	2:C:92:TRP:CH2	2.49	0.48
1:F:169:ALA:O	1:F:173:GLN:HG3	2.12	0.48
1:F:203:ASN:HB3	1:F:225:LEU:CD2	2.37	0.48
2:C:469:GLU:HB2	2:C:483:PHE:CZ	2.48	0.48
2:C:44:VAL:HA	2:C:205:VAL:O	2.14	0.48
1:F:182:THR:CG2	1:F:183:GLU:N	2.75	0.48
2:C:67:PHE:CB	2:C:69:GLU:HG3	2.40	0.48
2:D:299:SER:HB3	2:D:333:MET:CE	2.43	0.48
1:B:311:ARG:HA	1:B:343:LEU:O	2.13	0.48
1:E:186:GLU:HB3	1:E:189:GLY:HA3	1.96	0.48
2:C:311:ARG:HA	2:C:343:LEU:O	2.14	0.48
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.42	0.48
2:C:41:SER:HA	2:C:178:THR:O	2.13	0.48
1:E:21:MET:CE	1:E:59:PHE:CZ	2.97	0.48
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.44	0.48
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.46	0.48
1:B:294:LYS:N	4:B:901:ATP:O1B	2.47	0.48
1:F:311:ARG:HG3	1:F:371:LYS:HZ1	1.78	0.48
2:D:323:GLN:NE2	1:E:459:ARG:HD3	2.28	0.48
2:D:174:ILE:HG22	2:D:174:ILE:O	2.13	0.48
1:B:264:SER:HA	1:B:271:ASP:OD1	2.13	0.48
2:D:468:ARG:NH1	2:D:468:ARG:HG2	2.28	0.48
1:A:387:VAL:HG12	1:A:388:SER:N	2.28	0.48
1:E:332:GLY:O	1:E:333:MET:O	2.32	0.48
1:F:484:ARG:HH11	1:F:484:ARG:HB3	1.79	0.48
1:E:18:ILE:HD11	1:E:227:GLY:C	2.34	0.48
1:B:123:LEU:HD13	1:B:127:ILE:HD11	1.96	0.48
2:D:430:ILE:O	2:D:432:TPO:N	2.47	0.48
1:E:18:ILE:CG1	1:E:228:THR:HG23	2.43	0.48
1:A:121:PHE:O	1:A:125:ALA:HB2	2.14	0.48
2:C:263:VAL:CG1	2:C:374:ARG:HH21	2.27	0.47
2:D:19:ALA:O	2:D:38:ILE:HD12	2.14	0.47
1:B:323:GLN:NE2	2:C:459:ARG:HD3	2.29	0.47
1:F:514:GLU:HB3	1:F:519:SER:HB3	1.96	0.47
1:F:325:LEU:CD2	1:F:335:PHE:HB2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLN:O	1:A:154:TYR:CB	2.62	0.47
1:F:426:THR:HG22	1:F:428:SER:N	2.18	0.47
1:A:89:SER:CB	1:B:227:GLY:O	2.59	0.47
2:D:81:GLN:CD	2:D:81:GLN:N	2.68	0.47
1:F:504:GLU:HB3	1:F:507:ARG:HH21	1.75	0.47
1:E:336:GLU:HA	1:E:336:GLU:OE1	2.15	0.47
2:D:21:MET:CE	2:D:59:PHE:CZ	2.98	0.47
1:A:98:VAL:HA	1:A:103:LEU:O	2.13	0.47
1:A:502:LYS:O	1:A:502:LYS:HG3	2.14	0.47
1:B:111:ASP:O	1:B:113:GLU:N	2.47	0.47
2:D:122:ASP:HB3	2:D:123:LEU:H	1.44	0.47
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.49	0.47
1:E:345:LYS:NZ	1:E:366:GLU:CG	2.77	0.47
1:E:271:ASP:OD1	1:E:277:GLY:HA2	2.14	0.47
2:D:213:GLY:O	2:D:214:GLU:HB2	2.14	0.47
2:C:354:ALA:HB1	2:C:358:ASP:HB2	1.95	0.47
1:A:49:GLY:HA2	4:A:903:ATP:O2B	2.15	0.47
1:B:125:ALA:O	1:B:129:ARG:HG3	2.15	0.47
1:B:211:LEU:O	1:B:212:GLU:HB3	2.13	0.47
2:C:320:SER:HA	2:D:254:LEU:HG	1.95	0.47
1:B:25:ILE:HG12	1:B:58:GLN:NE2	2.30	0.47
1:F:420:MET:HE3	1:F:420:MET:HB3	1.79	0.47
1:E:148:THR:HG1	1:E:182:THR:HG23	1.77	0.47
1:E:313:ILE:HD11	1:E:372:PRO:HG3	1.97	0.47
1:A:170:ARG:O	1:A:174:ILE:HG12	2.15	0.47
1:F:317:TYR:CD2	1:F:383:LEU:HD21	2.49	0.47
4:D:903:ATP:O3'	1:E:224:LYS:HB2	2.15	0.47
1:F:81:GLN:CD	1:F:81:GLN:N	2.68	0.47
1:A:486:PHE:CD2	1:A:496:ARG:HA	2.50	0.47
1:F:311:ARG:HD2	1:F:371:LYS:NZ	2.29	0.47
2:D:323:GLN:HE22	1:E:459:ARG:HD3	1.79	0.47
1:F:117:VAL:HG13	1:F:154:TYR:OH	2.15	0.47
1:A:45:SER:CB	1:A:182:THR:HB	2.43	0.47
2:D:412:PHE:N	2:D:412:PHE:CD1	2.83	0.47
1:B:387:VAL:HG12	1:B:388:SER:N	2.28	0.47
1:E:76:PHE:HZ	1:E:126:LEU:CD2	2.28	0.47
1:E:444:GLU:OE1	1:F:490:ILE:HG12	2.13	0.47
1:B:212:GLU:HG2	1:B:212:GLU:O	2.15	0.47
2:C:468:ARG:HG2	2:C:468:ARG:HH11	1.79	0.47
1:E:104:PHE:CE2	1:E:106:LEU:HB2	2.50	0.47
1:A:32:SER:HB3	1:A:222:ILE:HD11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:VAL:CG2	2:D:148:THR:N	2.77	0.47
1:B:150:VAL:HG13	1:B:151:PHE:N	2.29	0.47
1:B:21:MET:HE3	1:B:141:ARG:CZ	2.45	0.47
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.50	0.47
1:F:65:ILE:O	1:F:65:ILE:CG2	2.61	0.47
2:D:350:TYR:O	2:D:351:PRO:C	2.50	0.47
2:D:269:ARG:HB3	2:D:479:ILE:HD12	1.97	0.47
2:D:52:LYS:HD3	2:D:182:THR:O	2.15	0.47
1:E:487:GLU:O	1:E:488:ARG:HB2	2.15	0.47
1:F:184:ARG:HG2	1:F:191:ILE:O	2.15	0.47
1:E:52:LYS:HD3	1:E:182:THR:O	2.14	0.47
1:A:268:VAL:O	1:A:271:ASP:HB2	2.15	0.47
1:E:79:THR:O	1:E:83:ILE:HD12	2.15	0.47
1:B:182:THR:HG22	1:B:183:GLU:N	2.30	0.47
1:A:146:SER:H	1:A:181:THR:CG2	2.27	0.47
1:E:344:LEU:HD22	1:E:345:LYS:N	2.30	0.47
1:A:182:THR:HG22	1:A:183:GLU:N	2.30	0.47
2:C:497:ILE:O	2:C:498:THR:HG22	2.15	0.47
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.44	0.47
1:F:197:GLU:H	1:F:197:GLU:CD	2.17	0.47
1:B:60:LEU:HD12	1:B:73:PHE:HB2	1.97	0.47
1:E:305:ALA:HB2	1:E:374:ARG:CD	2.31	0.46
1:B:441:GLN:HE22	1:B:490:ILE:HA	1.79	0.46
2:D:299:SER:CB	2:D:333:MET:HE1	2.45	0.46
2:C:50:THR:HG22	2:C:209:ASN:HB2	1.97	0.46
2:D:150:VAL:HG13	2:D:151:PHE:N	2.29	0.46
1:F:486:PHE:CE2	1:F:496:ARG:CD	2.80	0.46
1:A:420:MET:HB3	1:A:420:MET:HE3	1.84	0.46
1:A:150:VAL:CG1	1:A:151:PHE:N	2.78	0.46
1:B:419:PHE:CE2	2:C:425:ILE:HD12	2.49	0.46
2:C:214:GLU:O	2:C:215:ARG:NH2	2.48	0.46
1:F:104:PHE:HE2	1:F:106:LEU:HB2	1.80	0.46
2:C:353:SER:O	2:C:354:ALA:HB2	2.14	0.46
1:A:186:GLU:OE2	1:A:187:GLU:N	2.49	0.46
1:A:164:LEU:HA	1:A:164:LEU:HD23	1.69	0.46
1:A:487:GLU:OE1	1:F:496:ARG:HD3	2.16	0.46
1:B:300:ARG:N	1:B:333:MET:HE1	2.30	0.46
1:E:345:LYS:HZ3	1:E:366:GLU:CG	2.28	0.46
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.30	0.46
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.97	0.46
1:F:266:GLY:O	1:F:300:ARG:CG	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:LEU:O	1:F:360:LEU:HD22	2.15	0.46
1:B:164:LEU:HA	1:B:164:LEU:HD23	1.66	0.46
1:A:430:ILE:O	1:A:431:SEP:C	2.63	0.46
2:C:367:ILE:HG12	2:C:375:ILE:CD1	2.46	0.46
1:F:180:MET:HB3	1:F:180:MET:HE2	1.72	0.46
2:C:191:ILE:HB	2:C:198:GLU:CD	2.35	0.46
2:C:377:ILE:HD12	2:C:412:PHE:HE2	1.79	0.46
1:B:125:ALA:O	1:B:128:GLU:HB2	2.15	0.46
1:A:490:ILE:HD13	1:A:490:ILE:HA	1.84	0.46
1:B:80:PRO:HD2	1:B:81:GLN:NE2	2.30	0.46
2:D:305:ALA:HB2	2:D:374:ARG:CD	2.38	0.46
1:E:311:ARG:HA	1:E:343:LEU:O	2.16	0.46
2:C:471:MET:CG	2:C:478:ASP:HB3	2.46	0.46
1:E:49:GLY:O	1:E:218:ARG:NH2	2.49	0.46
1:A:518:GLU:HB2	1:A:519:SER:H	1.55	0.46
1:E:340:ARG:O	1:E:342:ASN:N	2.49	0.46
1:F:264:SER:O	1:F:374:ARG:NH2	2.47	0.46
1:E:79:THR:HG23	1:E:81:GLN:NE2	2.30	0.46
1:B:419:PHE:HD1	1:B:420:MET:HG3	1.80	0.46
1:B:469:GLU:HG3	1:B:470:PHE:N	2.29	0.46
1:A:497:ILE:O	1:A:497:ILE:CD1	2.64	0.46
2:C:451:ARG:NH1	2:C:451:ARG:CG	2.78	0.46
1:B:18:ILE:HB	1:B:228:THR:CG2	2.44	0.46
2:D:340:ARG:C	2:D:342:ASN:N	2.68	0.46
1:A:191:ILE:HG21	1:A:198:GLU:HG3	1.97	0.46
1:B:429:HIS:HA	1:B:431:SEP:O3P	2.16	0.46
1:A:287:THR:HG21	1:A:425:ILE:O	2.16	0.46
1:A:447:GLY:HA2	1:B:489:ILE:HD12	1.96	0.46
1:F:144:ILE:CG2	1:F:147:VAL:HG12	2.46	0.46
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.45	0.46
1:F:137:TYR:O	1:F:138:ARG:HB2	2.16	0.46
1:B:151:PHE:C	1:B:153:GLN:N	2.68	0.46
1:E:147:VAL:HG11	1:E:180:MET:CE	2.46	0.46
1:B:52:LYS:HD3	1:B:182:THR:O	2.16	0.46
1:B:23:THR:O	1:B:24:MET:HB2	2.16	0.46
1:B:64:ILE:HG21	1:B:97:LEU:HD13	1.97	0.46
1:F:38:ILE:HG22	1:F:39:GLY:N	2.30	0.46
1:B:323:GLN:HE22	2:C:459:ARG:HD3	1.79	0.46
1:F:111:ASP:HA	1:F:112:PRO:HD3	1.66	0.46
1:F:514:GLU:CB	1:F:519:SER:HB3	2.46	0.46
1:F:358:ASP:O	1:F:362:ILE:HG12	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:GLN:H	1:F:256:GLN:HG2	1.45	0.46
1:E:81:GLN:H	1:E:81:GLN:CD	2.19	0.46
1:A:504:GLU:C	1:A:506:SER:N	2.68	0.46
2:D:426:THR:HG21	2:D:430:ILE:HG12	1.97	0.46
1:B:492:GLY:O	1:B:494:PRO:HD3	2.16	0.46
1:F:469:GLU:HG3	1:F:470:PHE:N	2.31	0.46
2:C:387:VAL:HG12	2:C:388:SER:N	2.31	0.46
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.97	0.46
1:E:313:ILE:CD1	1:E:372:PRO:HG3	2.46	0.46
2:C:448:GLU:HG2	2:D:466:ALA:HA	1.98	0.46
1:A:50:THR:HG22	1:A:209:ASN:HB2	1.98	0.46
2:D:396:VAL:HG12	2:D:433:ILE:HG21	1.98	0.45
1:A:45:SER:HB3	1:A:182:THR:HB	1.97	0.45
1:A:161:ARG:HB2	1:A:196:VAL:CG1	2.47	0.45
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.98	0.45
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.98	0.45
2:C:185:ILE:HA	5:D:912:HOH:O	2.15	0.45
1:F:509:VAL:CG1	1:F:510:ARG:H	2.08	0.45
2:C:150:VAL:CG1	2:C:151:PHE:N	2.80	0.45
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.97	0.45
1:E:18:ILE:HD13	1:E:227:GLY:HA3	1.96	0.45
2:C:187:GLU:O	2:C:208:ARG:HD3	2.16	0.45
1:E:116:GLU:O	1:E:118:VAL:HG23	2.16	0.45
1:E:313:ILE:CD1	1:E:372:PRO:CG	2.94	0.45
1:A:485:ASN:N	1:A:485:ASN:OD1	2.39	0.45
1:F:446:ARG:H	1:F:496:ARG:NH2	2.15	0.45
1:E:166:ARG:O	1:E:169:ALA:HB3	2.16	0.45
1:A:455:VAL:HG11	1:A:463:HIS:CB	2.39	0.45
1:E:483:PHE:HB2	1:E:489:ILE:HD11	1.98	0.45
1:E:393:ARG:O	1:E:397:ILE:HG12	2.17	0.45
1:A:72:VAL:O	1:A:142:VAL:HA	2.16	0.45
1:A:487:GLU:OE1	1:F:495:THR:HA	2.16	0.45
1:A:436:THR:OG1	1:A:458:MET:HG2	2.17	0.45
2:D:338:MET:H	2:D:338:MET:HG2	1.58	0.45
2:C:14:GLU:CG	2:C:16:GLN:HB2	2.46	0.45
1:E:344:LEU:HD22	1:E:345:LYS:H	1.82	0.45
1:E:345:LYS:NZ	1:E:366:GLU:HG2	2.31	0.45
2:C:446:ARG:HA	2:C:496:ARG:NH2	2.31	0.45
1:B:345:LYS:HZ2	1:B:366:GLU:HG2	1.82	0.45
1:A:415:THR:HG21	1:B:432:TPO:CG2	2.47	0.45
2:D:52:LYS:N	4:D:903:ATP:O1B	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:LEU:O	2:C:124:SER:C	2.54	0.45
1:B:296:LEU:HD13	1:B:331:TRP:CD2	2.52	0.45
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.98	0.45
1:B:186:GLU:OE2	1:B:187:GLU:N	2.49	0.45
2:D:146:SER:CA	2:D:181:THR:HG22	2.45	0.45
1:A:455:VAL:CG1	1:A:463:HIS:HB2	2.39	0.45
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.97	0.45
1:E:140:ARG:HA	1:E:140:ARG:HD2	1.62	0.45
1:B:56:SER:HB2	1:B:143:SER:HB3	1.99	0.45
1:E:146:SER:HA	1:E:181:THR:O	2.17	0.45
1:B:141:ARG:HB2	5:B:905:HOH:O	2.16	0.45
1:F:79:THR:HG21	1:F:81:GLN:HG2	1.98	0.45
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.99	0.45
4:E:901:ATP:H3'	1:F:458:MET:O	2.17	0.45
1:E:147:VAL:CG2	1:E:148:THR:N	2.79	0.45
2:D:344:LEU:C	2:D:344:LEU:CD1	2.77	0.45
1:A:496:ARG:O	1:A:497:ILE:HG23	2.16	0.45
1:F:336:GLU:OE1	1:F:336:GLU:HA	2.17	0.45
2:D:388:SER:OG	2:D:391:ALA:HB2	2.15	0.45
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.32	0.45
2:C:19:ALA:C	2:C:38:ILE:HD12	2.37	0.45
1:F:451:ARG:NH1	1:F:451:ARG:HG2	2.32	0.45
2:C:433:ILE:CG2	2:C:433:ILE:O	2.64	0.45
1:A:471:MET:HG3	1:A:478:ASP:HB3	1.97	0.45
2:D:468:ARG:HH11	2:D:468:ARG:HG2	1.80	0.45
1:A:318:GLU:OE2	1:B:432:TPO:HB	2.16	0.45
1:E:353:SER:O	1:E:354:ALA:HB2	2.17	0.45
1:B:21:MET:CE	1:B:59:PHE:CZ	3.00	0.45
1:B:379:SER:H	1:B:413:THR:CG2	2.30	0.45
1:A:153:GLN:O	1:A:154:TYR:CG	2.70	0.45
1:A:266:GLY:O	1:A:300:ARG:CG	2.65	0.45
1:B:483:PHE:HB2	1:B:489:ILE:HD11	1.99	0.45
1:A:504:GLU:O	1:A:506:SER:N	2.49	0.45
2:D:338:MET:HB2	2:D:344:LEU:HB3	1.99	0.45
1:B:499:VAL:C	1:B:501:GLU:H	2.21	0.45
1:F:332:GLY:O	1:F:333:MET:O	2.35	0.45
1:E:345:LYS:HZ2	1:E:366:GLU:HG2	1.81	0.45
2:C:488:ARG:NH1	2:C:488:ARG:HG3	2.31	0.45
2:D:448:GLU:HG2	1:E:466:ALA:HA	1.98	0.45
1:F:186:GLU:OE2	1:F:187:GLU:N	2.50	0.45
1:F:504:GLU:CA	1:F:507:ARG:HE	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:O	1:A:463:HIS:CA	2.63	0.44
2:D:379:SER:H	2:D:413:THR:HB	1.82	0.44
1:A:432:TPO:O1P	1:A:432:TPO:CG2	2.65	0.44
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.98	0.44
1:A:219:THR:HA	1:A:235:TYR:O	2.17	0.44
2:D:311:ARG:HG3	2:D:371:LYS:NZ	2.31	0.44
1:B:22:ARG:NH2	1:B:24:MET:SD	2.90	0.44
1:A:146:SER:HA	1:A:181:THR:O	2.17	0.44
1:B:500:ASP:O	1:B:503:SER:HB2	2.17	0.44
1:A:469:GLU:HG3	1:A:470:PHE:N	2.31	0.44
1:B:487:GLU:O	1:B:494:PRO:HA	2.17	0.44
2:C:18:ILE:CD1	2:C:18:ILE:N	2.80	0.44
1:F:127:ILE:HD11	1:F:167:LEU:HD12	1.99	0.44
1:E:295:THR:HG21	1:E:319:GLU:OE2	2.17	0.44
2:C:164:LEU:HD23	2:C:164:LEU:HA	1.70	0.44
2:C:358:ASP:O	2:C:362:ILE:HG12	2.17	0.44
1:B:344:LEU:C	1:B:344:LEU:HD13	2.38	0.44
1:B:302:VAL:HG13	1:B:344:LEU:HD23	2.00	0.44
2:D:300:ARG:N	2:D:333:MET:HE1	2.31	0.44
2:D:432:TPO:O1P	2:D:432:TPO:HG21	2.17	0.44
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.46	0.44
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.47	0.44
1:B:126:LEU:C	1:B:128:GLU:N	2.68	0.44
1:E:193:ARG:NH2	1:F:195:GLY:O	2.27	0.44
2:D:318:GLU:OE2	1:E:432:TPO:HB	2.17	0.44
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.47	0.44
1:F:287:THR:HG23	1:F:414:ASN:ND2	2.30	0.44
1:F:46:GLY:HA2	1:F:184:ARG:HD2	1.99	0.44
1:B:191:ILE:CB	1:B:198:GLU:CG	2.87	0.44
1:E:396:VAL:HG11	1:E:430:ILE:CG2	2.48	0.44
1:E:45:SER:HB2	1:E:182:THR:HB	1.99	0.44
2:D:231:MET:HE1	2:D:251:ALA:HB2	1.99	0.44
2:D:451:ARG:NH1	2:D:472:ILE:HD12	2.32	0.44
1:F:311:ARG:HD2	1:F:371:LYS:CD	2.48	0.44
2:D:170:ARG:O	2:D:174:ILE:HG12	2.17	0.44
1:A:191:ILE:CG2	1:A:198:GLU:HG3	2.47	0.44
2:C:94:LEU:O	2:C:98:VAL:HG23	2.17	0.44
1:E:123:LEU:HD13	1:E:163:GLU:OE2	2.16	0.44
1:A:273:MET:SD	1:A:468:ARG:HD2	2.57	0.44
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.48	0.44
2:C:123:LEU:O	2:C:125:ALA:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:LEU:HD23	1:E:127:ILE:HG13	1.99	0.44
1:E:485:ASN:OD1	1:E:485:ASN:N	2.42	0.44
1:F:299:SER:HB3	1:F:333:MET:HE1	1.99	0.44
1:B:204:VAL:HG23	1:B:224:LYS:HG2	2.00	0.44
1:F:20:LYS:O	1:F:38:ILE:HD11	2.17	0.44
1:F:178:THR:HG22	1:F:179:VAL:N	2.33	0.44
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.99	0.44
1:B:107:ASP:C	1:B:107:ASP:OD1	2.56	0.44
1:F:255:THR:O	1:F:255:THR:HG22	2.17	0.44
1:A:14:GLU:CG	1:A:15:HIS:N	2.57	0.44
1:F:81:GLN:H	1:F:81:GLN:CD	2.19	0.44
1:B:51:GLY:O	1:B:54:LEU:N	2.50	0.44
2:C:426:THR:HG22	2:C:428:SER:N	2.33	0.44
2:C:294:LYS:N	4:C:901:ATP:O1B	2.50	0.44
1:F:33:HIS:HD2	1:F:229:SER:OG	1.99	0.44
2:D:33:HIS:HD2	2:D:229:SER:OG	2.01	0.44
2:C:21:MET:HE1	2:C:59:PHE:CZ	2.52	0.44
1:A:452:ALA:HA	1:A:468:ARG:O	2.17	0.44
1:F:371:LYS:HD2	1:F:371:LYS:O	2.17	0.44
2:D:148:THR:HG21	2:D:193:ARG:HD2	2.00	0.44
2:D:79:THR:HG23	2:D:81:GLN:NE2	2.33	0.44
1:E:496:ARG:C	1:E:497:ILE:HD13	2.38	0.44
1:F:295:THR:HG21	1:F:319:GLU:OE2	2.17	0.44
1:B:340:ARG:C	1:B:342:ASN:N	2.71	0.44
1:F:313:ILE:HG13	1:F:372:PRO:HG3	2.00	0.44
1:E:164:LEU:HD23	1:E:164:LEU:HA	1.65	0.44
2:C:75:THR:HG23	2:C:75:THR:O	2.18	0.44
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.48	0.43
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.18	0.43
1:B:359:HIS:O	1:B:363:ILE:HG13	2.18	0.43
1:A:496:ARG:O	1:A:497:ILE:CG2	2.66	0.43
2:C:116:GLU:O	2:C:117:VAL:HB	2.17	0.43
2:D:455:VAL:HG11	2:D:463:HIS:HB2	1.99	0.43
2:C:439:LEU:HD12	2:C:440:LEU:N	2.32	0.43
1:F:217:ARG:HH21	1:F:236:PRO:HB3	1.82	0.43
1:E:217:ARG:HH21	1:E:236:PRO:HB3	1.83	0.43
1:F:468:ARG:NH1	1:F:468:ARG:HG2	2.33	0.43
2:D:344:LEU:HD22	2:D:345:LYS:H	1.83	0.43
2:D:21:MET:CE	2:D:141:ARG:HG2	2.44	0.43
4:A:901:ATP:C5	1:B:461:SER:O	2.71	0.43
1:F:123:LEU:HA	1:F:123:LEU:HD22	1.90	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PHE:CZ	1:B:126:LEU:HD21	2.53	0.43
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.99	0.43
2:D:197:GLU:CD	2:D:197:GLU:H	2.19	0.43
2:C:120:GLY:C	2:C:122:ASP:N	2.71	0.43
1:E:79:THR:HG23	1:E:81:GLN:CG	2.36	0.43
1:A:499:VAL:CG1	1:A:499:VAL:O	2.64	0.43
1:A:514:GLU:HB3	1:A:515:LYS:HD2	2.00	0.43
1:F:452:ALA:HB1	1:F:467:ILE:HG22	1.99	0.43
1:A:357:GLU:HG3	1:A:358:ASP:N	2.33	0.43
2:C:418:GLN:HB2	2:D:423:HIS:O	2.18	0.43
1:E:70:PRO:HB2	1:E:139:ALA:HA	2.00	0.43
1:F:220:LEU:C	1:F:220:LEU:HD23	2.39	0.43
2:D:437:ILE:HD12	2:D:457:LYS:HG2	1.99	0.43
2:C:121:PHE:HB3	2:C:125:ALA:HB3	2.01	0.43
1:E:445:ILE:O	1:E:446:ARG:HB2	2.18	0.43
1:B:52:LYS:N	4:B:903:ATP:O1B	2.51	0.43
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.48	0.43
2:D:426:THR:HG22	2:D:428:SER:N	2.28	0.43
1:B:164:LEU:HB3	1:B:200:VAL:HG11	2.00	0.43
2:D:420:MET:HE3	2:D:492:GLY:HA3	1.99	0.43
1:B:146:SER:HA	1:B:181:THR:HG22	2.01	0.43
1:F:191:ILE:HG12	1:F:198:GLU:HG2	2.00	0.43
1:B:471:MET:HE3	1:B:473:SER:OG	2.18	0.43
2:D:345:LYS:NZ	2:D:366:GLU:OE1	2.43	0.43
2:C:419:PHE:CD2	2:D:425:ILE:CD1	3.01	0.43
2:D:46:GLY:HA2	5:D:904:HOH:O	2.17	0.43
2:D:153:GLN:O	2:D:154:TYR:CB	2.65	0.43
1:A:305:ALA:HB2	1:A:374:ARG:CD	2.33	0.43
1:B:184:ARG:C	1:B:185:ILE:HD13	2.38	0.43
1:A:49:GLY:O	1:A:218:ARG:NH2	2.52	0.43
2:C:121:PHE:N	2:C:121:PHE:CD1	2.78	0.43
1:E:419:PHE:O	1:E:420:MET:O	2.36	0.43
1:F:127:ILE:CD1	1:F:167:LEU:HD12	2.48	0.43
1:F:156:ALA:O	1:F:159:VAL:HG23	2.19	0.43
2:D:65:ILE:O	2:D:65:ILE:CG2	2.67	0.43
1:A:325:LEU:CD2	1:A:335:PHE:HB2	2.49	0.43
1:B:126:LEU:C	1:B:128:GLU:H	2.21	0.43
2:D:269:ARG:HG2	2:D:479:ILE:HB	2.01	0.43
1:E:23:THR:C	1:E:25:ILE:H	2.22	0.43
1:A:265:SER:O	1:A:301:PHE:HA	2.18	0.43
1:E:211:LEU:HD12	1:E:215:ARG:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:47:THR:O	2:C:48:SER:C	2.54	0.43
2:D:92:TRP:CD1	2:D:92:TRP:N	2.83	0.43
1:A:487:GLU:HG2	1:F:496:ARG:CZ	2.48	0.43
1:F:43:LEU:HD11	1:F:182:THR:OG1	2.18	0.43
2:C:193:ARG:NH2	2:D:195:GLY:O	2.28	0.43
2:C:315:PHE:CE1	2:C:363:ILE:HG23	2.52	0.43
2:D:31:ILE:HA	2:D:231:MET:SD	2.59	0.43
2:C:419:PHE:CE2	2:D:425:ILE:HD12	2.54	0.43
2:C:340:ARG:C	2:C:342:ASN:N	2.71	0.43
1:E:489:ILE:O	1:E:490:ILE:C	2.56	0.43
1:A:57:ILE:CD1	1:A:73:PHE:CE1	3.02	0.43
1:B:44:VAL:HG22	1:B:205:VAL:HB	2.01	0.43
2:C:484:ARG:HB3	2:C:484:ARG:NH1	2.34	0.43
2:C:88:ARG:HD3	2:D:15:HIS:C	2.40	0.43
1:F:451:ARG:HB3	1:F:470:PHE:CE2	2.54	0.43
1:F:443:VAL:HG12	1:F:445:ILE:HG12	2.01	0.43
1:E:383:LEU:HA	1:E:383:LEU:HD23	1.82	0.43
1:B:332:GLY:O	1:B:333:MET:O	2.37	0.43
1:A:445:ILE:HD12	1:A:486:PHE:CZ	2.54	0.43
1:E:302:VAL:HG13	1:E:344:LEU:HD23	2.00	0.43
2:C:396:VAL:HG11	2:C:430:ILE:CG2	2.47	0.43
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.51	0.43
2:C:267:VAL:HB	2:C:270:LEU:HB2	2.01	0.43
1:E:433:ILE:HG22	1:E:433:ILE:O	2.18	0.43
1:B:146:SER:CA	1:B:181:THR:HG22	2.48	0.42
2:D:381:SER:HB3	2:D:414:ASN:OD1	2.19	0.42
2:C:148:THR:HG1	2:C:182:THR:HG23	1.84	0.42
1:F:344:LEU:HD13	1:F:344:LEU:C	2.40	0.42
1:A:162:ARG:CZ	1:F:116:GLU:HG2	2.49	0.42
2:C:151:PHE:O	2:C:153:GLN:N	2.44	0.42
1:A:425:ILE:CD1	1:F:419:PHE:CD2	3.01	0.42
2:D:191:ILE:HG21	2:D:198:GLU:HG3	2.00	0.42
2:C:214:GLU:O	2:C:215:ARG:NE	2.53	0.42
1:B:471:MET:HG3	1:B:478:ASP:HB3	2.01	0.42
1:E:43:LEU:HD12	1:E:43:LEU:HA	1.82	0.42
1:B:299:SER:HB3	1:B:333:MET:HE1	2.01	0.42
2:C:489:ILE:O	2:C:492:GLY:N	2.46	0.42
2:C:142:VAL:O	2:C:178:THR:HA	2.19	0.42
1:E:347:VAL:O	1:E:348:CYS:CB	2.65	0.42
2:C:283:ILE:HD12	2:C:412:PHE:HE1	1.84	0.42
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:ASP:CG	1:F:112:PRO:HD2	2.40	0.42
2:C:468:ARG:HG2	2:C:468:ARG:NH1	2.33	0.42
1:E:54:LEU:HD13	1:E:90:PHE:CE1	2.54	0.42
2:D:496:ARG:HE	1:E:487:GLU:HG2	1.84	0.42
1:B:490:ILE:HD13	1:B:490:ILE:HA	1.76	0.42
2:C:263:VAL:HG12	2:C:374:ARG:NH2	2.33	0.42
1:E:273:MET:O	1:E:463:HIS:CA	2.63	0.42
2:D:85:LYS:NZ	1:E:14:GLU:HB3	2.34	0.42
1:A:332:GLY:O	1:A:333:MET:C	2.58	0.42
1:B:501:GLU:HB2	1:B:502:LYS:H	1.38	0.42
1:B:262:ARG:HH22	1:B:461:SER:HB2	1.84	0.42
2:C:191:ILE:CG2	2:C:198:GLU:HG3	2.49	0.42
2:C:378:ASP:OD1	2:C:413:THR:HG21	2.18	0.42
1:F:31:ILE:HG22	1:F:222:ILE:CD1	2.48	0.42
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.33	0.42
1:E:64:ILE:HD13	1:E:102:LYS:HB3	2.01	0.42
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.82	0.42
2:D:18:ILE:H	2:D:18:ILE:HD12	1.83	0.42
1:E:311:ARG:HD2	1:E:371:LYS:HE3	2.02	0.42
2:D:140:ARG:HD2	2:D:140:ARG:HA	1.82	0.42
1:B:418:GLN:CG	1:B:418:GLN:O	2.67	0.42
2:C:337:GLU:OE1	2:C:340:ARG:NH1	2.52	0.42
2:C:114:GLY:O	2:C:115:GLN:HB3	2.19	0.42
1:A:31:ILE:HD11	1:A:246:ILE:HG21	2.01	0.42
1:B:452:ALA:HA	1:B:468:ARG:O	2.19	0.42
1:F:338:MET:H	1:F:338:MET:HG2	1.68	0.42
1:A:498:THR:HB	1:A:501:GLU:CG	2.41	0.42
1:E:184:ARG:HG2	1:E:191:ILE:O	2.20	0.42
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.55	0.42
1:E:38:ILE:HA	1:E:177:THR:HG23	2.01	0.42
2:C:344:LEU:HD13	2:C:344:LEU:C	2.40	0.42
1:E:18:ILE:CD1	1:E:227:GLY:HA3	2.50	0.42
1:E:501:GLU:O	1:E:502:LYS:CE	2.67	0.42
1:B:256:GLN:H	1:B:256:GLN:HG2	1.54	0.42
2:D:370:PHE:O	2:D:371:LYS:CD	2.67	0.42
1:A:503:SER:C	1:A:504:GLU:CG	2.88	0.42
1:E:147:VAL:HG23	1:E:148:THR:N	2.34	0.42
1:F:292:THR:HB	1:F:440:LEU:HB3	2.02	0.42
1:E:419:PHE:CD2	1:F:425:ILE:CD1	3.00	0.42
1:A:21:MET:CE	1:A:59:PHE:HZ	2.30	0.42
1:E:378:ASP:OD1	1:E:413:THR:HG21	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:469:GLU:HB2	1:F:483:PHE:CZ	2.54	0.42
1:F:484:ARG:CB	1:F:484:ARG:NH1	2.82	0.42
1:E:256:GLN:HG2	1:E:256:GLN:H	1.52	0.42
1:B:21:MET:HE2	1:B:59:PHE:CZ	2.54	0.42
1:F:367:ILE:HG12	1:F:375:ILE:HD11	2.02	0.42
1:E:76:PHE:O	1:E:109:SER:HA	2.19	0.42
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.50	0.42
1:A:443:VAL:CG1	1:A:494:PRO:HG2	2.50	0.42
2:D:153:GLN:O	2:D:154:TYR:CG	2.72	0.42
1:F:504:GLU:CA	1:F:507:ARG:NE	2.81	0.42
1:F:507:ARG:O	1:F:508:ILE:C	2.58	0.42
2:C:211:LEU:HD12	2:C:215:ARG:O	2.20	0.42
2:C:311:ARG:HD2	2:C:371:LYS:NZ	2.35	0.42
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.55	0.42
1:F:38:ILE:CG2	1:F:39:GLY:N	2.83	0.42
2:D:89:SER:HB2	1:E:227:GLY:O	2.19	0.42
1:E:164:LEU:HB3	1:E:200:VAL:HG11	2.02	0.42
1:B:317:TYR:CD2	1:B:383:LEU:HD21	2.55	0.42
1:F:302:VAL:HG12	1:F:303:GLU:N	2.35	0.42
1:F:433:ILE:N	1:F:433:ILE:HD12	2.35	0.42
1:A:406:GLU:O	1:A:407:GLU:HB2	2.19	0.42
1:F:98:VAL:HA	1:F:103:LEU:O	2.20	0.42
2:C:121:PHE:O	2:C:122:ASP:C	2.58	0.42
1:E:264:SER:O	1:E:374:ARG:NH2	2.51	0.42
2:D:219:THR:HB	2:D:234:GLU:HB3	2.02	0.42
1:B:273:MET:O	1:B:463:HIS:CA	2.63	0.42
2:C:14:GLU:HG3	2:C:16:GLN:HB2	2.01	0.42
1:B:119:GLY:O	1:B:121:PHE:N	2.53	0.42
1:F:23:THR:O	1:F:24:MET:HB2	2.20	0.42
1:E:379:SER:HA	1:E:413:THR:HG22	2.01	0.42
2:C:281:ASP:O	2:C:282:SER:HB3	2.20	0.42
1:A:70:PRO:HA	1:A:102:LYS:O	2.19	0.42
2:D:182:THR:CG2	2:D:183:GLU:N	2.80	0.42
2:C:123:LEU:HA	2:C:123:LEU:HD23	1.79	0.42
1:B:81:GLN:CD	1:B:81:GLN:N	2.73	0.42
1:A:80:PRO:HD2	1:A:81:GLN:HE21	1.82	0.42
1:B:492:GLY:C	1:B:494:PRO:HD3	2.41	0.42
2:C:419:PHE:CG	2:C:419:PHE:O	2.72	0.42
1:F:161:ARG:CB	1:F:196:VAL:HG11	2.46	0.42
1:E:21:MET:O	1:E:35:GLY:HA3	2.20	0.42
1:E:106:LEU:HD13	1:E:129:ARG:CZ	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.54	0.42
1:E:130:ILE:O	1:E:134:ILE:HG13	2.19	0.42
1:F:213:GLY:O	1:F:214:GLU:HB2	2.19	0.42
2:C:383:LEU:HD23	2:C:383:LEU:HA	1.85	0.42
2:D:187:GLU:O	2:D:208:ARG:HD3	2.20	0.41
1:A:426:THR:HG22	1:A:427:ASP:N	2.35	0.41
1:B:53:THR:HG23	1:B:145:ASP:OD1	2.20	0.41
1:B:419:PHE:O	1:B:420:MET:O	2.38	0.41
2:C:214:GLU:O	2:C:215:ARG:CZ	2.68	0.41
1:E:455:VAL:HG11	1:E:463:HIS:HB2	2.01	0.41
1:A:311:ARG:HD2	1:A:371:LYS:NZ	2.35	0.41
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.54	0.41
1:F:379:SER:CA	1:F:413:THR:HG22	2.46	0.41
1:B:106:LEU:CD1	1:B:106:LEU:C	2.88	0.41
1:E:345:LYS:NZ	1:E:366:GLU:OE1	2.53	0.41
1:B:311:ARG:HD2	1:B:371:LYS:HE3	2.02	0.41
2:C:489:ILE:C	2:C:491:SER:N	2.71	0.41
1:F:165:PHE:O	1:F:166:ARG:C	2.57	0.41
2:D:194:TYR:O	2:D:196:VAL:HG23	2.19	0.41
2:D:273:MET:O	2:D:463:HIS:HA	2.19	0.41
1:B:219:THR:HB	1:B:234:GLU:HB3	2.02	0.41
1:E:382:ALA:O	1:E:385:ARG:HG3	2.20	0.41
1:A:486:PHE:CE2	1:A:496:ARG:HA	2.55	0.41
1:F:238:THR:HG22	1:F:239:ILE:N	2.35	0.41
1:F:367:ILE:HG12	1:F:375:ILE:CD1	2.50	0.41
1:F:387:VAL:HG12	1:F:388:SER:N	2.36	0.41
2:C:38:ILE:HG22	2:C:39:GLY:N	2.35	0.41
1:A:85:LYS:O	1:A:88:ARG:HB2	2.20	0.41
2:C:332:GLY:O	2:C:333:MET:C	2.58	0.41
1:A:256:GLN:HG2	1:A:256:GLN:H	1.52	0.41
1:E:371:LYS:HD3	1:E:371:LYS:O	2.17	0.41
1:B:87:ALA:HB1	1:B:92:TRP:HE1	1.85	0.41
2:C:489:ILE:O	2:C:490:ILE:C	2.57	0.41
1:A:510:ARG:HD2	1:A:510:ARG:N	2.35	0.41
1:B:72:VAL:O	1:B:142:VAL:HA	2.21	0.41
2:D:75:THR:HG23	2:D:75:THR:O	2.19	0.41
1:F:485:ASN:N	1:F:485:ASN:OD1	2.48	0.41
2:C:21:MET:O	2:C:35:GLY:HA3	2.20	0.41
1:F:42:THR:HG23	1:F:203:ASN:HB2	2.02	0.41
2:D:33:HIS:CD2	2:D:230:HIS:HA	2.55	0.41
1:B:421:GLY:O	1:B:422:ALA:C	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HD3	1:A:35:GLY:O	2.19	0.41
2:C:256:GLN:HG2	2:C:256:GLN:H	1.48	0.41
1:F:287:THR:HG23	1:F:414:ASN:CB	2.38	0.41
1:B:420:MET:HE3	1:B:420:MET:HB3	1.74	0.41
1:F:396:VAL:HG11	1:F:430:ILE:HG23	2.01	0.41
2:D:315:PHE:CE2	2:D:363:ILE:HG23	2.53	0.41
1:E:323:GLN:HE21	1:E:327:ASN:HD21	1.68	0.41
1:F:164:LEU:HD11	1:F:197:GLU:HG3	2.01	0.41
1:B:393:ARG:O	1:B:397:ILE:HG12	2.20	0.41
1:F:200:VAL:O	1:F:200:VAL:HG12	2.19	0.41
2:D:49:GLY:HA2	4:D:903:ATP:O2B	2.20	0.41
1:A:396:VAL:HG11	1:A:430:ILE:HG23	2.03	0.41
1:E:180:MET:HB3	1:E:180:MET:HE2	1.79	0.41
1:A:296:LEU:HD21	1:A:477:PRO:HD3	2.02	0.41
1:F:127:ILE:HD11	1:F:167:LEU:CD1	2.50	0.41
1:A:345:LYS:NZ	1:A:366:GLU:HG2	2.35	0.41
2:D:495:THR:HG23	1:E:487:GLU:OE2	2.21	0.41
1:E:289:ALA:CB	1:E:419:PHE:HA	2.45	0.41
1:E:315:PHE:HE1	1:E:375:ILE:CD1	2.34	0.41
1:E:412:PHE:N	1:E:412:PHE:CD1	2.88	0.41
2:D:41:SER:HA	2:D:178:THR:O	2.21	0.41
1:E:76:PHE:CZ	1:E:126:LEU:CD2	3.03	0.41
1:F:68:ASP:OD2	1:F:102:LYS:NZ	2.49	0.41
2:C:65:ILE:HG22	2:C:65:ILE:O	2.20	0.41
1:E:360:LEU:HD22	1:E:360:LEU:O	2.21	0.41
1:B:153:GLN:O	1:B:154:TYR:CB	2.69	0.41
1:F:140:ARG:HD2	1:F:140:ARG:HA	1.96	0.41
2:C:153:GLN:O	2:C:154:TYR:CG	2.74	0.41
1:F:419:PHE:O	1:F:420:MET:HB2	2.19	0.41
1:F:508:ILE:O	1:F:508:ILE:CG2	2.67	0.41
2:C:82:ASP:O	2:C:83:ILE:C	2.59	0.41
2:D:21:MET:CE	2:D:59:PHE:HZ	2.33	0.41
1:E:161:ARG:CB	1:E:196:VAL:HG11	2.49	0.41
1:E:483:PHE:CB	1:E:489:ILE:HD11	2.51	0.41
1:A:471:MET:HE2	1:A:478:ASP:CB	2.50	0.41
1:F:306:CYS:C	1:F:308:ASN:N	2.72	0.41
1:B:68:ASP:OD2	1:B:102:LYS:HE3	2.20	0.41
1:A:400:THR:CG2	1:A:401:GLY:N	2.83	0.41
1:B:141:ARG:HD2	5:B:905:HOH:O	2.19	0.41
4:B:901:ATP:C5	2:C:461:SER:O	2.74	0.41
1:E:122:ASP:HB3	1:E:123:LEU:H	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ILE:CD1	1:F:193:ARG:NH1	2.80	0.41
1:F:46:GLY:HA2	1:F:184:ARG:CD	2.51	0.41
1:F:506:SER:O	1:F:507:ARG:O	2.39	0.41
2:D:224:LYS:O	2:D:225:LEU:HD23	2.21	0.41
2:C:182:THR:CG2	2:C:183:GLU:N	2.79	0.41
1:A:436:THR:HG23	1:A:458:MET:CG	2.51	0.41
1:E:150:VAL:HG13	1:E:151:PHE:N	2.36	0.41
1:E:182:THR:HG21	1:E:192:ALA:HB1	2.02	0.41
1:E:336:GLU:O	1:E:339:GLU:HB2	2.21	0.41
1:B:385:ARG:HG2	2:C:393:ARG:NH1	2.35	0.41
2:C:471:MET:HB3	2:C:480:LYS:HZ3	1.85	0.41
4:A:903:ATP:O3'	1:B:224:LYS:HB2	2.21	0.41
2:C:338:MET:HB2	2:C:344:LEU:HB3	2.03	0.41
1:E:449:MET:HE3	1:F:467:ILE:HD11	2.02	0.41
2:C:387:VAL:CG1	2:C:391:ALA:HB3	2.51	0.41
1:E:471:MET:HB3	1:E:480:LYS:HZ1	1.84	0.41
1:B:32:SER:HB3	1:B:222:ILE:HD11	2.02	0.41
2:D:50:THR:HG22	2:D:209:ASN:HB2	2.03	0.41
2:D:114:GLY:O	2:D:115:GLN:HG3	2.21	0.41
1:E:113:GLU:HB3	1:E:114:GLY:H	1.75	0.41
1:E:98:VAL:HA	1:E:103:LEU:O	2.21	0.41
1:B:484:ARG:NH1	1:B:484:ARG:HB3	2.35	0.41
2:D:208:ARG:O	2:D:218:ARG:HA	2.21	0.41
2:D:49:GLY:CA	4:D:903:ATP:O2B	2.69	0.41
1:E:123:LEU:HD12	1:E:163:GLU:OE2	2.20	0.41
2:C:79:THR:HG23	2:C:81:GLN:HE21	1.86	0.41
1:F:455:VAL:HG11	1:F:463:HIS:CB	2.48	0.41
2:C:420:MET:HE3	2:C:420:MET:HB3	1.69	0.41
1:A:505:LEU:CD1	1:A:505:LEU:O	2.65	0.41
1:A:21:MET:CE	1:A:59:PHE:CE1	3.04	0.41
1:A:484:ARG:CZ	1:A:484:ARG:CB	2.99	0.41
1:A:340:ARG:C	1:A:342:ASN:N	2.74	0.41
1:B:406:GLU:O	1:B:407:GLU:HB2	2.20	0.41
1:B:79:THR:C	1:B:83:ILE:HD12	2.41	0.40
1:B:79:THR:HG23	1:B:81:GLN:CG	2.42	0.40
1:B:441:GLN:HG3	1:B:441:GLN:O	2.21	0.40
1:F:508:ILE:CD1	1:F:508:ILE:H	2.34	0.40
1:F:437:ILE:HD11	1:F:457:LYS:HE2	2.03	0.40
1:B:445:ILE:HD12	1:B:486:PHE:CZ	2.56	0.40
2:C:184:ARG:HG2	2:C:191:ILE:O	2.20	0.40
1:E:344:LEU:HD13	1:E:345:LYS:N	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:ILE:HD11	1:F:399:VAL:HG11	2.03	0.40
1:A:148:THR:HG1	1:A:182:THR:HG23	1.84	0.40
1:A:183:GLU:CB	1:B:199:PHE:CE1	3.04	0.40
1:F:484:ARG:CB	1:F:484:ARG:CZ	2.99	0.40
1:A:284:ILE:HB	1:A:411:LEU:HD12	2.02	0.40
1:A:362:ILE:HG22	1:A:362:ILE:O	2.21	0.40
2:C:120:GLY:C	2:C:122:ASP:H	2.24	0.40
2:D:287:THR:HA	2:D:414:ASN:O	2.22	0.40
1:F:516:GLY:N	1:F:517:PRO:HD2	2.36	0.40
2:D:315:PHE:CE1	2:D:363:ILE:HG23	2.56	0.40
2:D:471:MET:CG	2:D:478:ASP:HB3	2.51	0.40
1:B:76:PHE:HZ	1:B:126:LEU:HD21	1.84	0.40
1:F:266:GLY:HA3	1:F:300:ARG:O	2.22	0.40
1:F:357:GLU:HG3	1:F:358:ASP:N	2.36	0.40
1:A:111:ASP:C	1:A:113:GLU:H	2.24	0.40
4:C:903:ATP:O3G	2:D:224:LYS:NZ	2.50	0.40
1:F:429:HIS:HA	1:F:431:SEP:O1P	2.21	0.40
2:C:269:ARG:NE	5:C:909:HOH:O	2.33	0.40
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.86	0.40
1:E:314:LEU:C	1:E:314:LEU:HD12	2.42	0.40
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.98	0.40
1:B:19:ALA:C	1:B:38:ILE:HD12	2.41	0.40
1:F:93:ASP:OD2	1:F:96:LYS:HB2	2.22	0.40
2:D:294:LYS:N	4:D:901:ATP:O1B	2.54	0.40
2:D:438:ILE:CD1	2:D:455:VAL:HG22	2.52	0.40
2:D:462:TRP:O	2:D:463:HIS:O	2.40	0.40
2:D:76:PHE:O	2:D:109:SER:HA	2.21	0.40
1:A:140:ARG:HD2	1:A:140:ARG:HA	1.84	0.40
2:C:316:ALA:O	2:C:348:CYS:HA	2.22	0.40
1:A:437:ILE:CD1	1:A:457:LYS:HE2	2.52	0.40
1:E:306:CYS:O	1:E:309:LYS:N	2.42	0.40
2:C:25:ILE:HG23	2:C:58:GLN:NE2	2.36	0.40
2:D:44:VAL:HA	2:D:205:VAL:O	2.21	0.40
2:D:314:LEU:C	2:D:314:LEU:HD12	2.42	0.40
2:D:358:ASP:O	2:D:362:ILE:HG12	2.21	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%)	442 (88%)	39 (8%)	21 (4%)	3	11
1	B	487/519 (94%)	431 (88%)	44 (9%)	12 (2%)	7	24
1	E	488/519 (94%)	422 (86%)	49 (10%)	17 (4%)	4	15
1	F	502/519 (97%)	443 (88%)	38 (8%)	21 (4%)	3	11
2	C	485/519 (93%)	436 (90%)	30 (6%)	19 (4%)	4	12
2	D	482/519 (93%)	433 (90%)	37 (8%)	12 (2%)	7	24
All	All	2946/3114 (95%)	2607 (88%)	237 (8%)	102 (4%)	4	15

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	154	TYR
1	A	211	LEU
1	A	333	MET
1	A	387	VAL
1	A	463	HIS
1	A	502	LYS
1	A	509	VAL
1	B	52	LYS
1	B	154	TYR
1	B	333	MET
1	B	341	GLN
1	B	387	VAL
1	B	463	HIS
2	C	17	ALA
2	C	112	PRO
2	C	117	VAL
2	C	124	SER
2	C	154	TYR
2	C	333	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	341	GLN
2	C	431	SER
2	C	463	HIS
2	D	122	ASP
2	D	154	TYR
2	D	333	MET
2	D	387	VAL
2	D	431	SER
2	D	463	HIS
1	E	122	ASP
1	E	154	TYR
1	E	211	LEU
1	E	333	MET
1	E	420	MET
1	E	463	HIS
1	E	502	LYS
1	F	118	VAL
1	F	154	TYR
1	F	333	MET
1	F	463	HIS
1	F	501	GLU
1	F	504	GLU
1	F	506	SER
1	F	507	ARG
1	F	508	ILE
1	F	509	VAL
1	A	117	VAL
1	A	157	SER
1	A	341	GLN
1	A	500	ASP
1	A	505	LEU
1	B	17	ALA
1	B	119	GLY
1	B	211	LEU
1	B	420	MET
2	C	121	PHE
2	C	379	SER
2	C	387	VAL
2	D	18	ILE
2	D	113	GLU
2	D	341	GLN
2	D	420	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	117	VAL
1	E	120	GLY
1	E	341	GLN
1	E	387	VAL
1	F	114	GLY
1	F	117	VAL
1	F	211	LEU
1	F	341	GLN
1	F	510	ARG
1	A	379	SER
1	A	420	MET
1	B	112	PRO
2	C	114	GLY
2	C	211	LEU
2	C	289	ALA
1	E	157	SER
1	F	157	SER
1	F	420	MET
1	A	480	LYS
1	A	504	GLU
2	C	354	ALA
2	C	499	VAL
2	D	211	LEU
1	E	379	SER
1	B	494	PRO
2	C	157	SER
1	E	348	CYS
1	F	354	ALA
1	F	500	ASP
1	F	517	PRO
1	A	212	GLU
1	A	348	CYS
2	C	348	CYS
2	D	157	SER
1	E	212	GLU
1	E	494	PRO
1	A	112	PRO
1	A	497	ILE
1	F	387	VAL
1	E	112	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/442 (97%)	373 (87%)	57 (13%)	5	14
1	B	417/442 (94%)	364 (87%)	53 (13%)	5	16
1	E	418/442 (95%)	368 (88%)	50 (12%)	6	19
1	F	430/442 (97%)	381 (89%)	49 (11%)	7	21
2	C	415/443 (94%)	358 (86%)	57 (14%)	4	13
2	D	412/443 (93%)	360 (87%)	52 (13%)	5	17
All	All	2522/2654 (95%)	2204 (87%)	318 (13%)	5	17

All (318) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	41	SER
1	A	79	THR
1	A	81	GLN
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	118	VAL
1	A	123	LEU
1	A	140	ARG
1	A	151	PHE
1	A	154	TYR
1	A	181	THR
1	A	183	GLU
1	A	185	ILE
1	A	186	GLU
1	A	191	ILE
1	A	193	ARG
1	A	212	GLU
1	A	218	ARG
1	A	223	LEU
1	A	228	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	238	THR
1	A	256	GLN
1	A	260	ASN
1	A	263	VAL
1	A	270	LEU
1	A	287	THR
1	A	294	LYS
1	A	302	VAL
1	A	303	GLU
1	A	320	SER
1	A	321	ARG
1	A	342	ASN
1	A	360	LEU
1	A	366	GLU
1	A	371	LYS
1	A	375	ILE
1	A	400	THR
1	A	413	THR
1	A	428	SER
1	A	434	THR
1	A	451	ARG
1	A	458	MET
1	A	462	TRP
1	A	469	GLU
1	A	471	MET
1	A	489	ILE
1	A	496	ARG
1	A	498	THR
1	A	500	ASP
1	A	504	GLU
1	A	508	ILE
1	A	509	VAL
1	A	510	ARG
1	A	514	GLU
1	A	518	GLU
1	B	26	GLU
1	B	50	THR
1	B	79	THR
1	B	81	GLN
1	B	92	TRP
1	B	99	ASP
1	B	106	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	112	PRO
1	B	123	LEU
1	B	128	GLU
1	B	140	ARG
1	B	151	PHE
1	B	154	TYR
1	B	181	THR
1	B	183	GLU
1	B	185	ILE
1	B	186	GLU
1	B	191	ILE
1	B	212	GLU
1	B	218	ARG
1	B	223	LEU
1	B	256	GLN
1	B	260	ASN
1	B	270	LEU
1	B	287	THR
1	B	294	LYS
1	B	302	VAL
1	B	303	GLU
1	B	320	SER
1	B	321	ARG
1	B	325	LEU
1	B	333	MET
1	B	342	ASN
1	B	356	LEU
1	B	360	LEU
1	B	369	ASP
1	B	371	LYS
1	B	375	ILE
1	B	400	THR
1	B	413	THR
1	B	451	ARG
1	B	458	MET
1	B	462	TRP
1	B	469	GLU
1	B	471	MET
1	B	474	ASP
1	B	485	ASN
1	B	490	ILE
1	B	495	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	499	VAL
1	B	500	ASP
1	B	501	GLU
1	B	502	LYS
2	C	15	HIS
2	C	26	GLU
2	C	50	THR
2	C	79	THR
2	C	81	GLN
2	C	92	TRP
2	C	99	ASP
2	C	106	LEU
2	C	111	ASP
2	C	121	PHE
2	C	140	ARG
2	C	151	PHE
2	C	154	TYR
2	C	177	THR
2	C	178	THR
2	C	181	THR
2	C	183	GLU
2	C	185	ILE
2	C	186	GLU
2	C	191	ILE
2	C	212	GLU
2	C	218	ARG
2	C	223	LEU
2	C	228	THR
2	C	256	GLN
2	C	259	SER
2	C	263	VAL
2	C	270	LEU
2	C	287	THR
2	C	294	LYS
2	C	302	VAL
2	C	303	GLU
2	C	321	ARG
2	C	325	LEU
2	C	333	MET
2	C	338	MET
2	C	342	ASN
2	C	356	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	360	LEU
2	C	366	GLU
2	C	371	LYS
2	C	375	ILE
2	C	400	THR
2	C	413	THR
2	C	420	MET
2	C	451	ARG
2	C	458	MET
2	C	461	SER
2	C	462	TRP
2	C	469	GLU
2	C	471	MET
2	C	491	SER
2	C	493	SER
2	C	495	THR
2	C	498	THR
2	C	500	ASP
2	C	501	GLU
2	D	26	GLU
2	D	79	THR
2	D	81	GLN
2	D	106	LEU
2	D	117	VAL
2	D	122	ASP
2	D	123	LEU
2	D	124	SER
2	D	127	ILE
2	D	140	ARG
2	D	151	PHE
2	D	154	TYR
2	D	172	LYS
2	D	177	THR
2	D	181	THR
2	D	185	ILE
2	D	186	GLU
2	D	191	ILE
2	D	212	GLU
2	D	218	ARG
2	D	223	LEU
2	D	256	GLN
2	D	259	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	260	ASN
2	D	263	VAL
2	D	270	LEU
2	D	284	ILE
2	D	287	THR
2	D	294	LYS
2	D	320	SER
2	D	321	ARG
2	D	325	LEU
2	D	338	MET
2	D	342	ASN
2	D	356	LEU
2	D	360	LEU
2	D	366	GLU
2	D	369	ASP
2	D	371	LYS
2	D	375	ILE
2	D	400	THR
2	D	413	THR
2	D	431	SER
2	D	451	ARG
2	D	458	MET
2	D	463	HIS
2	D	469	GLU
2	D	471	MET
2	D	487	GLU
2	D	490	ILE
2	D	496	ARG
2	D	498	THR
1	E	26	GLU
1	E	37	PRO
1	E	50	THR
1	E	79	THR
1	E	81	GLN
1	E	99	ASP
1	E	106	LEU
1	E	113	GLU
1	E	121	PHE
1	E	124	SER
1	E	127	ILE
1	E	140	ARG
1	E	151	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	154	TYR
1	E	177	THR
1	E	181	THR
1	E	182	THR
1	E	183	GLU
1	E	185	ILE
1	E	186	GLU
1	E	191	ILE
1	E	203	ASN
1	E	211	LEU
1	E	212	GLU
1	E	223	LEU
1	E	228	THR
1	E	256	GLN
1	E	260	ASN
1	E	263	VAL
1	E	270	LEU
1	E	287	THR
1	E	302	VAL
1	E	314	LEU
1	E	321	ARG
1	E	342	ASN
1	E	351	PRO
1	E	360	LEU
1	E	371	LYS
1	E	375	ILE
1	E	400	THR
1	E	451	ARG
1	E	458	MET
1	E	461	SER
1	E	469	GLU
1	E	471	MET
1	E	474	ASP
1	E	496	ARG
1	E	501	GLU
1	E	503	SER
1	E	505	LEU
1	F	26	GLU
1	F	45	SER
1	F	79	THR
1	F	81	GLN
1	F	99	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	106	LEU
1	F	121	PHE
1	F	123	LEU
1	F	140	ARG
1	F	151	PHE
1	F	154	TYR
1	F	172	LYS
1	F	181	THR
1	F	183	GLU
1	F	185	ILE
1	F	186	GLU
1	F	191	ILE
1	F	212	GLU
1	F	218	ARG
1	F	223	LEU
1	F	256	GLN
1	F	260	ASN
1	F	263	VAL
1	F	270	LEU
1	F	287	THR
1	F	321	ARG
1	F	325	LEU
1	F	342	ASN
1	F	356	LEU
1	F	360	LEU
1	F	366	GLU
1	F	371	LYS
1	F	375	ILE
1	F	381	SER
1	F	400	THR
1	F	413	THR
1	F	451	ARG
1	F	458	MET
1	F	462	TRP
1	F	469	GLU
1	F	471	MET
1	F	496	ARG
1	F	497	ILE
1	F	499	VAL
1	F	501	GLU
1	F	504	GLU
1	F	505	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	507	ARG
1	F	514	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	33	HIS
1	A	62	ASN
1	A	81	GLN
1	A	209	ASN
1	A	245	ASN
1	A	323	GLN
1	A	368	ASN
1	A	414	ASN
1	A	441	GLN
1	B	16	GLN
1	B	62	ASN
1	B	81	GLN
1	B	209	ASN
1	B	260	ASN
1	B	304	ASN
1	B	361	GLN
1	B	368	ASN
1	B	414	ASN
1	B	441	GLN
2	C	33	HIS
2	C	62	ASN
2	C	81	GLN
2	C	209	ASN
2	C	256	GLN
2	C	323	GLN
2	C	368	ASN
2	C	389	ASN
2	C	414	ASN
2	C	441	GLN
2	D	33	HIS
2	D	81	GLN
2	D	209	ASN
2	D	304	ASN
2	D	368	ASN
2	D	389	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	414	ASN
2	D	441	GLN
1	E	33	HIS
1	E	81	GLN
1	E	209	ASN
1	E	256	GLN
1	E	304	ASN
1	E	323	GLN
1	E	361	GLN
1	E	368	ASN
1	E	414	ASN
1	E	441	GLN
1	E	454	ASN
1	F	33	HIS
1	F	62	ASN
1	F	81	GLN
1	F	115	GLN
1	F	209	ASN
1	F	256	GLN
1	F	368	ASN
1	F	414	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 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	$\#\|Z\| > 2$
1	SEP	A	431	1	8,9,10	5.79	4 (50%)	8,12,14	4.81	5 (62%)
1	TPO	A	432	1	8,10,11	5.77	5 (62%)	7,14,16	2.54	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SEP	B	431	1	8,9,10	5.63	4 (50%)	8,12,14	4.04	5 (62%)
1	TPO	B	432	1	8,10,11	5.98	5 (62%)	7,14,16	2.32	4 (57%)
2	TPO	C	432	2	8,10,11	6.16	5 (62%)	7,14,16	3.57	4 (57%)
2	TPO	D	432	2	8,10,11	5.28	6 (75%)	7,14,16	3.16	3 (42%)
1	SEP	E	431	1	8,9,10	5.84	5 (62%)	8,12,14	2.59	6 (75%)
1	TPO	E	432	1	8,10,11	5.08	6 (75%)	7,14,16	2.72	3 (42%)
1	SEP	F	431	1	8,9,10	5.85	5 (62%)	8,12,14	3.54	3 (37%)
1	TPO	F	432	1	8,10,11	5.68	6 (75%)	7,14,16	3.11	6 (85%)

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
1	SEP	A	431	1	-	0/6/8/10	0/0/0/0
1	TPO	A	432	1	-	0/8/11/13	0/0/0/0
1	SEP	B	431	1	-	0/6/8/10	0/0/0/0
1	TPO	B	432	1	-	0/8/11/13	0/0/0/0
2	TPO	C	432	2	-	0/8/11/13	0/0/0/0
2	TPO	D	432	2	-	0/8/11/13	0/0/0/0
1	SEP	E	431	1	-	0/6/8/10	0/0/0/0
1	TPO	E	432	1	-	0/8/11/13	0/0/0/0
1	SEP	F	431	1	-	0/6/8/10	0/0/0/0
1	TPO	F	432	1	-	0/8/11/13	0/0/0/0

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	432	TPO	CB-CA	-5.15	1.44	1.54
1	F	432	TPO	CB-CA	-2.59	1.49	1.54
1	F	432	TPO	CA-N	2.06	1.54	1.47
2	D	432	TPO	CB-CA	2.22	1.58	1.54
1	F	431	SEP	CB-CA	2.25	1.59	1.52
2	C	432	TPO	CA-N	2.28	1.55	1.47
1	B	432	TPO	CA-N	2.31	1.55	1.47
1	E	432	TPO	CA-N	2.52	1.55	1.47
1	E	431	SEP	CB-CA	2.93	1.61	1.52
2	D	432	TPO	CA-N	2.96	1.57	1.47
1	A	432	TPO	CA-N	3.40	1.58	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	432	TPO	P-O3P	5.03	1.72	1.54
1	F	431	SEP	P-OG	5.04	1.77	1.60
1	E	432	TPO	P-O3P	5.20	1.73	1.54
1	A	431	SEP	P-OG	5.33	1.78	1.60
1	A	432	TPO	P-O2P	5.45	1.74	1.54
1	E	432	TPO	P-OG1	5.51	1.76	1.60
1	F	432	TPO	P-O3P	5.77	1.75	1.54
1	F	431	SEP	P-O3P	5.77	1.75	1.54
2	D	432	TPO	P-O2P	5.85	1.75	1.54
1	F	432	TPO	P-O2P	6.10	1.76	1.54
1	B	431	SEP	P-OG	6.13	1.80	1.60
1	B	432	TPO	P-OG1	6.44	1.79	1.60
1	E	432	TPO	P-O2P	6.53	1.78	1.54
1	F	432	TPO	P-OG1	6.67	1.80	1.60
1	A	432	TPO	P-OG1	7.08	1.81	1.60
2	C	432	TPO	P-O2P	7.43	1.81	1.54
1	B	432	TPO	P-O2P	7.53	1.81	1.54
1	B	431	SEP	P-O2P	7.57	1.81	1.54
1	B	431	SEP	P-O3P	7.77	1.82	1.54
1	A	431	SEP	P-O1P	7.77	1.76	1.51
1	A	431	SEP	P-O2P	7.78	1.82	1.54
1	E	431	SEP	P-O3P	7.79	1.82	1.54
2	C	432	TPO	P-O3P	7.99	1.83	1.54
1	E	431	SEP	P-OG	8.01	1.87	1.60
2	C	432	TPO	P-OG1	8.16	1.84	1.60
1	E	431	SEP	P-O2P	8.25	1.84	1.54
1	E	431	SEP	P-O1P	8.29	1.78	1.51
1	E	432	TPO	P-O1P	8.33	1.78	1.51
1	A	432	TPO	P-O3P	8.35	1.84	1.54
2	D	432	TPO	P-OG1	8.40	1.85	1.60
1	B	432	TPO	P-O3P	8.44	1.85	1.54
2	D	432	TPO	P-O1P	8.67	1.79	1.51
1	F	431	SEP	P-O2P	9.05	1.87	1.54
1	B	431	SEP	P-O1P	9.70	1.83	1.51
1	A	432	TPO	P-O1P	10.15	1.84	1.51
1	B	432	TPO	P-O1P	10.49	1.85	1.51
2	C	432	TPO	P-O1P	10.51	1.85	1.51
1	A	431	SEP	P-O3P	10.71	1.93	1.54
1	F	431	SEP	P-O1P	11.24	1.88	1.51
1	F	432	TPO	P-O1P	11.35	1.88	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	432	TPO	C-CA-N	-6.90	95.41	109.83
2	C	432	TPO	C-CA-N	-6.15	96.98	109.83
1	F	431	SEP	O-C-CA	-5.81	110.37	125.49
1	A	431	SEP	O-C-CA	-5.79	110.41	125.49
2	C	432	TPO	O-C-CA	-5.51	110.90	125.44
1	F	432	TPO	CG2-CB-CA	-5.10	102.79	113.17
1	B	431	SEP	O-C-CA	-4.77	113.08	125.49
1	E	432	TPO	O-C-CA	-4.72	112.98	125.44
1	A	432	TPO	O-C-CA	-4.69	113.05	125.44
1	E	432	TPO	CG2-CB-CA	-4.59	103.82	113.17
1	B	432	TPO	O-C-CA	-4.50	113.56	125.44
1	E	431	SEP	O-C-CA	-4.36	114.14	125.49
1	B	431	SEP	O3P-P-O1P	-4.02	97.62	110.58
2	D	432	TPO	O-C-CA	-3.99	114.89	125.44
1	F	432	TPO	O-C-CA	-3.97	114.95	125.44
1	A	432	TPO	CG2-CB-CA	-3.81	105.42	113.17
1	B	431	SEP	OG-P-O1P	-3.30	98.74	107.14
1	F	432	TPO	O2P-P-O1P	-2.38	102.91	110.58
1	E	431	SEP	O2P-P-O1P	-2.19	103.52	110.58
1	E	431	SEP	O3P-P-O1P	-2.19	103.53	110.58
1	A	431	SEP	O3P-P-OG	-2.15	100.37	106.56
2	D	432	TPO	OG1-P-O1P	-2.10	101.85	107.11
1	B	432	TPO	C-CA-N	-2.03	105.59	109.83
1	F	432	TPO	O3P-P-O2P	2.05	115.18	107.38
1	A	432	TPO	O3P-P-O1P	2.07	117.25	110.58
1	B	432	TPO	OG1-P-O1P	2.12	112.40	107.11
1	A	431	SEP	OG-P-O1P	2.19	112.71	107.14
2	C	432	TPO	CG2-CB-CA	2.20	117.65	113.17
1	F	432	TPO	C-CA-N	2.34	114.72	109.83
1	E	431	SEP	O3P-P-OG	2.38	113.42	106.56
1	B	432	TPO	O3P-P-O1P	2.45	118.48	110.58
1	F	431	SEP	O3P-P-OG	2.47	113.67	106.56
1	E	431	SEP	O2P-P-OG	2.50	113.76	106.56
1	E	432	TPO	O3P-P-O1P	2.51	118.65	110.58
1	F	432	TPO	O3P-P-O1P	2.68	119.20	110.58
1	E	431	SEP	OG-CB-CA	3.30	111.09	108.27
2	C	432	TPO	O3P-P-O1P	3.63	122.27	110.58
1	A	431	SEP	O2P-P-OG	4.44	119.34	106.56
1	B	431	SEP	OG-CB-CA	6.05	113.44	108.27
1	B	431	SEP	O3P-P-OG	6.42	125.06	106.56
1	F	431	SEP	OG-CB-CA	7.44	114.62	108.27
1	A	431	SEP	OG-CB-CA	10.81	117.50	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	431	SEP	4	0
1	A	432	TPO	3	0
1	B	431	SEP	5	0
1	B	432	TPO	2	0
2	C	432	TPO	2	0
2	D	432	TPO	3	0
1	E	431	SEP	1	0
1	E	432	TPO	1	0
1	F	431	SEP	2	0
1	F	432	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
4	ATP	A	901	3	24,33,33	1.49	4 (16%)	31,52,52	2.61	7 (22%)
4	ATP	A	903	-	24,33,33	1.58	5 (20%)	31,52,52	2.62	8 (25%)
4	ATP	B	901	3	24,33,33	1.49	5 (20%)	31,52,52	2.70	7 (22%)
4	ATP	B	903	-	24,33,33	1.73	3 (12%)	31,52,52	3.06	12 (38%)
4	ATP	C	901	3	24,33,33	1.45	4 (16%)	31,52,52	2.56	8 (25%)
4	ATP	C	903	-	24,33,33	1.24	2 (8%)	31,52,52	2.90	8 (25%)
4	ATP	D	901	3	24,33,33	1.51	5 (20%)	31,52,52	2.67	6 (19%)
4	ATP	D	903	-	24,33,33	1.73	5 (20%)	31,52,52	3.08	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ATP	E	901	3	24,33,33	1.55	3 (12%)	31,52,52	2.73	6 (19%)
4	ATP	E	903	-	24,33,33	1.66	9 (37%)	31,52,52	2.87	10 (32%)
4	ATP	F	901	3	24,33,33	1.50	5 (20%)	31,52,52	2.67	7 (22%)
4	ATP	F	903	-	24,33,33	1.40	4 (16%)	31,52,52	2.73	7 (22%)

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
4	ATP	A	901	3	-	0/18/38/38	0/3/3/3
4	ATP	A	903	-	-	0/18/38/38	0/3/3/3
4	ATP	B	901	3	-	0/18/38/38	0/3/3/3
4	ATP	B	903	-	-	0/18/38/38	0/3/3/3
4	ATP	C	901	3	-	0/18/38/38	0/3/3/3
4	ATP	C	903	-	-	0/18/38/38	0/3/3/3
4	ATP	D	901	3	-	0/18/38/38	0/3/3/3
4	ATP	D	903	-	-	0/18/38/38	0/3/3/3
4	ATP	E	901	3	-	0/18/38/38	0/3/3/3
4	ATP	E	903	-	-	0/18/38/38	0/3/3/3
4	ATP	F	901	3	-	0/18/38/38	0/3/3/3
4	ATP	F	903	-	-	0/18/38/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	903	ATP	O4'-C4'	-3.96	1.35	1.45
4	C	901	ATP	PB-O1B	-3.35	1.38	1.51
4	C	903	ATP	O4'-C4'	-3.29	1.37	1.45
4	D	903	ATP	PB-O2B	-3.12	1.41	1.54
4	D	903	ATP	PB-O1B	-3.11	1.39	1.51
4	E	903	ATP	PB-O1B	-2.80	1.40	1.51
4	D	901	ATP	O2'-C2'	-2.61	1.36	1.43
4	F	903	ATP	PB-O1B	-2.59	1.41	1.51
4	B	901	ATP	PB-O1B	-2.55	1.41	1.51
4	E	901	ATP	PB-O1B	-2.47	1.42	1.51
4	F	901	ATP	PB-O1B	-2.47	1.42	1.51
4	E	903	ATP	O4'-C4'	-2.37	1.39	1.45
4	E	903	ATP	C2'-C3'	-2.37	1.46	1.53
4	E	903	ATP	PA-O1A	-2.36	1.42	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	ATP	PB-O1B	-2.32	1.42	1.51
4	E	903	ATP	C8-N7	-2.18	1.30	1.34
4	A	903	ATP	PB-O2B	-2.15	1.45	1.54
4	F	903	ATP	C6-N6	-2.15	1.28	1.34
4	A	903	ATP	PB-O1B	-2.12	1.43	1.51
4	E	903	ATP	C5-N7	-2.11	1.32	1.39
4	C	901	ATP	PB-O2B	-2.09	1.46	1.54
4	D	903	ATP	PA-O1A	-2.06	1.43	1.51
4	D	901	ATP	PB-O1B	-2.06	1.43	1.51
4	E	903	ATP	PB-O2B	-2.04	1.46	1.54
4	E	903	ATP	O2'-C2'	-2.02	1.38	1.43
4	C	901	ATP	O4'-C4'	-2.01	1.40	1.45
4	F	901	ATP	O4'-C1'	2.05	1.43	1.41
4	E	903	ATP	C2-N3	2.07	1.35	1.32
4	B	901	ATP	O4'-C1'	2.12	1.43	1.41
4	A	901	ATP	C2-N1	2.13	1.38	1.33
4	D	901	ATP	C3'-C4'	2.36	1.59	1.53
4	F	903	ATP	C2-N1	2.42	1.38	1.33
4	F	901	ATP	C2-N1	2.53	1.38	1.33
4	C	903	ATP	C2-N3	2.55	1.36	1.32
4	D	901	ATP	C2-N3	2.55	1.36	1.32
4	B	901	ATP	C2-N3	2.56	1.36	1.32
4	D	901	ATP	O4'-C1'	2.75	1.44	1.41
4	B	901	ATP	C4-N3	2.82	1.39	1.35
4	F	901	ATP	C4-N3	2.83	1.39	1.35
4	B	903	ATP	C4-N3	2.91	1.39	1.35
4	A	903	ATP	O4'-C1'	2.97	1.45	1.41
4	E	901	ATP	C4-N3	3.06	1.40	1.35
4	A	903	ATP	C2-N3	3.18	1.37	1.32
4	A	903	ATP	C2-N1	3.30	1.40	1.33
4	A	901	ATP	O4'-C1'	3.34	1.45	1.41
4	B	901	ATP	C2-N1	3.41	1.40	1.33
4	D	903	ATP	C2-N3	3.50	1.38	1.32
4	A	901	ATP	C2-N3	3.51	1.38	1.32
4	F	903	ATP	C2-N3	3.53	1.38	1.32
4	F	901	ATP	C2-N3	3.62	1.38	1.32
4	C	901	ATP	C2-N3	3.90	1.39	1.32
4	B	903	ATP	C2-N3	4.23	1.39	1.32
4	E	901	ATP	C2-N3	4.28	1.39	1.32
4	B	903	ATP	O4'-C1'	5.09	1.47	1.41

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	903	ATP	N3-C2-N1	-12.95	118.98	128.89
4	B	901	ATP	N3-C2-N1	-12.42	119.38	128.89
4	C	903	ATP	N3-C2-N1	-12.40	119.40	128.89
4	E	901	ATP	N3-C2-N1	-12.27	119.50	128.89
4	D	901	ATP	N3-C2-N1	-12.19	119.56	128.89
4	D	903	ATP	N3-C2-N1	-12.04	119.68	128.89
4	F	901	ATP	N3-C2-N1	-11.86	119.81	128.89
4	E	903	ATP	N3-C2-N1	-11.74	119.91	128.89
4	A	901	ATP	N3-C2-N1	-11.39	120.17	128.89
4	C	901	ATP	N3-C2-N1	-10.74	120.67	128.89
4	A	903	ATP	N3-C2-N1	-10.60	120.78	128.89
4	F	903	ATP	N3-C2-N1	-10.60	120.78	128.89
4	D	903	ATP	C4-C5-N7	-5.68	104.26	109.48
4	F	903	ATP	C4-C5-N7	-5.00	104.88	109.48
4	C	901	ATP	C4-C5-N7	-4.90	104.97	109.48
4	A	903	ATP	C4-C5-N7	-4.74	105.12	109.48
4	A	901	ATP	C4-C5-N7	-4.54	105.31	109.48
4	F	901	ATP	C4-C5-N7	-4.39	105.44	109.48
4	E	901	ATP	C4-C5-N7	-4.34	105.48	109.48
4	B	903	ATP	C4-C5-N7	-4.08	105.73	109.48
4	C	903	ATP	C4-C5-N7	-4.04	105.76	109.48
4	E	903	ATP	C4-C5-N7	-3.92	105.88	109.48
4	B	901	ATP	C4-C5-N7	-3.36	106.39	109.48
4	D	901	ATP	C4-C5-N7	-3.28	106.46	109.48
4	A	903	ATP	C1'-N9-C4	-3.20	122.11	126.94
4	B	903	ATP	N6-C6-N1	-3.12	112.51	119.20
4	E	901	ATP	N6-C6-N1	-2.86	113.06	119.20
4	B	903	ATP	C1'-N9-C4	-2.80	122.72	126.94
4	A	903	ATP	N6-C6-N1	-2.78	113.23	119.20
4	F	903	ATP	N6-C6-N1	-2.75	113.31	119.20
4	C	903	ATP	O5'-PA-O1A	-2.53	99.79	109.62
4	F	901	ATP	N6-C6-N1	-2.48	113.89	119.20
4	E	903	ATP	O3G-PG-O1G	-2.31	103.16	110.58
4	C	903	ATP	C1'-N9-C4	-2.29	123.48	126.94
4	D	903	ATP	N6-C6-N1	-2.20	114.49	119.20
4	D	903	ATP	C1'-N9-C4	-2.17	123.66	126.94
4	A	901	ATP	N6-C6-N1	-2.12	114.66	119.20
4	B	903	ATP	PB-O3B-PG	-2.10	125.63	132.67
4	E	903	ATP	N6-C6-N1	-2.08	114.75	119.20
4	B	903	ATP	O5'-PA-O1A	-2.06	101.60	109.62
4	D	903	ATP	O5'-PA-O1A	-2.02	101.78	109.62
4	A	903	ATP	O2B-PB-O3B	2.06	114.42	105.09
4	C	903	ATP	O2G-PG-O1G	2.06	117.22	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	903	ATP	O2B-PB-O3A	2.07	114.49	105.09
4	B	903	ATP	O2G-PG-O1G	2.12	117.41	110.58
4	D	903	ATP	C4'-O4'-C1'	2.13	112.06	109.72
4	A	901	ATP	O2'-C2'-C3'	2.16	118.86	111.83
4	B	903	ATP	O2B-PB-O3A	2.16	114.91	105.09
4	A	903	ATP	PA-O3A-PB	2.17	138.81	132.73
4	B	901	ATP	O2B-PB-O3A	2.17	114.94	105.09
4	B	901	ATP	O2'-C2'-C3'	2.18	118.92	111.83
4	E	901	ATP	O2'-C2'-C3'	2.19	118.93	111.83
4	F	903	ATP	O2B-PB-O3B	2.31	115.56	105.09
4	D	903	ATP	O2G-PG-O1G	2.31	118.01	110.58
4	E	903	ATP	O2B-PB-O3B	2.35	115.74	105.09
4	C	901	ATP	PA-O3A-PB	2.36	139.34	132.73
4	B	903	ATP	O4'-C1'-N9	2.37	113.05	108.10
4	D	901	ATP	O2B-PB-O3A	2.45	116.21	105.09
4	C	901	ATP	O2B-PB-O3A	2.50	116.42	105.09
4	F	903	ATP	O2G-PG-O1G	2.52	118.68	110.58
4	C	901	ATP	C2'-C1'-N9	2.52	118.14	114.29
4	A	901	ATP	O2B-PB-O3B	2.52	116.53	105.09
4	E	903	ATP	O2G-PG-O1G	2.54	118.75	110.58
4	D	903	ATP	PA-O3A-PB	2.54	139.86	132.73
4	D	901	ATP	C2'-C1'-N9	2.54	118.17	114.29
4	F	901	ATP	O2B-PB-O3B	2.56	116.70	105.09
4	C	901	ATP	O2'-C2'-C3'	2.58	120.22	111.83
4	C	903	ATP	O2B-PB-O3B	2.61	116.93	105.09
4	D	903	ATP	O2B-PB-O3B	2.68	117.25	105.09
4	B	901	ATP	C2'-C1'-N9	2.69	118.40	114.29
4	E	903	ATP	PA-O3A-PB	2.71	140.34	132.73
4	F	901	ATP	C2'-C1'-N9	2.71	118.44	114.29
4	B	903	ATP	O2'-C2'-C3'	2.75	120.77	111.83
4	F	901	ATP	O2'-C2'-C3'	2.82	121.01	111.83
4	A	903	ATP	C2'-C1'-N9	2.95	118.79	114.29
4	B	901	ATP	O2B-PB-O3B	2.99	118.66	105.09
4	B	903	ATP	O2B-PB-O3B	3.03	118.86	105.09
4	A	901	ATP	C2'-C1'-N9	3.12	119.06	114.29
4	C	901	ATP	O2B-PB-O3B	3.13	119.30	105.09
4	E	901	ATP	C2'-C1'-N9	3.23	119.23	114.29
4	B	901	ATP	O3A-PA-O5'	3.24	111.54	102.94
4	C	903	ATP	C2'-C1'-N9	3.27	119.28	114.29
4	A	901	ATP	O3A-PA-O5'	3.32	111.74	102.94
4	D	901	ATP	O2B-PB-O3B	3.33	120.21	105.09
4	E	901	ATP	O3A-PA-O5'	3.34	111.81	102.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	901	ATP	O3A-PA-O5'	3.56	112.38	102.94
4	D	901	ATP	O3A-PA-O5'	3.62	112.53	102.94
4	C	901	ATP	O3A-PA-O5'	3.70	112.74	102.94
4	A	903	ATP	O3A-PA-O5'	4.10	113.80	102.94
4	F	903	ATP	C2'-C1'-N9	4.40	121.01	114.29
4	E	903	ATP	C2'-C1'-N9	4.52	121.19	114.29
4	E	903	ATP	O3A-PA-O5'	5.48	117.48	102.94
4	B	903	ATP	O3A-PA-O5'	5.58	117.75	102.94
4	F	903	ATP	O3A-PA-O5'	5.66	117.96	102.94
4	D	903	ATP	O3A-PA-O5'	5.72	118.12	102.94
4	D	903	ATP	C2'-C1'-N9	5.81	123.17	114.29
4	C	903	ATP	O3A-PA-O5'	6.15	119.25	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	ATP	6	0
4	A	903	ATP	5	0
4	B	901	ATP	5	0
4	B	903	ATP	3	0
4	C	901	ATP	2	0
4	C	903	ATP	5	0
4	D	901	ATP	2	0
4	D	903	ATP	5	0
4	E	901	ATP	4	0
4	E	903	ATP	2	0
4	F	901	ATP	4	0
4	F	903	ATP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	504/519 (97%)	0.43	60 (11%) 6 3	30, 77, 128, 155	0
1	B	489/519 (94%)	0.33	37 (7%) 17 9	41, 83, 129, 161	0
1	E	490/519 (94%)	-0.04	29 (5%) 26 16	21, 61, 107, 156	0
1	F	504/519 (97%)	0.16	36 (7%) 19 10	21, 69, 115, 159	0
2	C	487/519 (93%)	0.08	26 (5%) 30 20	34, 73, 125, 161	0
2	D	484/519 (93%)	-0.10	25 (5%) 31 20	27, 59, 110, 161	0
All	All	2958/3114 (94%)	0.15	213 (7%) 18 10	21, 71, 122, 161	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	PRO	8.1
1	F	117	VAL	8.1
1	B	117	VAL	7.9
2	D	121	PHE	7.7
1	E	503	SER	7.6
1	F	517	PRO	7.5
1	A	518	GLU	7.4
1	F	516	GLY	7.4
1	E	505	LEU	7.2
2	D	120	GLY	7.2
2	C	118	VAL	7.1
1	F	519	SER	7.1
1	A	519	SER	7.0
1	A	506	SER	6.8
2	D	117	VAL	6.6
1	B	500	ASP	6.5
1	B	118	VAL	6.5
1	A	503	SER	6.4
2	D	118	VAL	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	116	GLU	6.3
1	A	257	ARG	6.3
1	A	511	GLY	6.2
1	A	508	ILE	6.0
1	A	507	ARG	5.9
2	D	119	GLY	5.8
1	B	121	PHE	5.8
1	A	516	GLY	5.7
1	B	498	THR	5.7
1	E	154	TYR	5.7
1	F	154	TYR	5.6
1	E	499	VAL	5.6
1	F	506	SER	5.5
1	A	515	LYS	5.5
1	F	515	LYS	5.5
1	A	251	ALA	5.3
1	F	509	VAL	5.2
1	F	518	GLU	5.2
2	C	499	VAL	5.2
1	A	513	GLN	5.2
1	A	509	VAL	5.2
1	B	154	TYR	5.0
2	C	117	VAL	5.0
1	B	503	SER	5.0
1	E	500	ASP	4.9
1	B	119	GLY	4.9
1	F	513	GLN	4.9
1	A	514	GLU	4.9
1	A	152	GLN	4.8
2	C	501	GLU	4.8
1	A	258	SER	4.8
1	A	120	GLY	4.7
1	B	258	SER	4.6
1	B	255	THR	4.6
1	B	158	SER	4.6
1	A	500	ASP	4.6
1	A	512	VAL	4.6
1	A	498	THR	4.6
1	F	512	VAL	4.5
1	E	501	GLU	4.4
1	E	121	PHE	4.4
1	A	510	ARG	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	120	GLY	4.3
1	A	252	MET	4.3
1	F	514	GLU	4.3
1	B	16	GLN	4.1
1	F	500	ASP	4.1
1	A	295	THR	4.1
1	B	321	ARG	4.1
1	F	507	ARG	4.1
1	B	504	GLU	4.1
1	A	502	LYS	4.0
2	D	113	GLU	4.0
1	A	121	PHE	4.0
2	D	498	THR	4.0
2	C	423	HIS	3.9
1	F	503	SER	3.9
1	F	505	LEU	3.9
1	B	157	SER	3.8
2	C	500	ASP	3.8
2	D	158	SER	3.8
1	E	504	GLU	3.8
1	F	508	ILE	3.8
1	A	504	GLU	3.7
1	F	510	ARG	3.7
1	B	15	HIS	3.7
2	C	53	THR	3.7
1	E	153	GLN	3.7
1	F	311	ARG	3.7
1	B	115	GLN	3.7
1	F	511	GLY	3.6
1	A	505	LEU	3.6
1	B	499	VAL	3.6
2	C	154	TYR	3.6
2	C	15	HIS	3.5
1	A	368	ASN	3.4
2	C	119	GLY	3.4
1	E	152	GLN	3.4
1	A	475	LYS	3.4
1	B	120	GLY	3.4
1	E	117	VAL	3.4
1	B	502	LYS	3.4
1	B	501	GLU	3.3
1	A	114	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	115	GLN	3.3
1	A	311	ARG	3.3
1	E	321	ARG	3.3
1	F	121	PHE	3.3
2	C	121	PHE	3.3
2	C	152	GLN	3.2
1	E	115	GLN	3.2
2	D	53	THR	3.2
1	F	255	THR	3.2
1	B	257	ARG	3.2
1	A	249	LEU	3.2
2	C	17	ALA	3.1
1	A	153	GLN	3.1
1	A	318	GLU	3.1
1	F	321	ARG	3.1
1	F	504	GLU	3.1
1	A	253	ARG	3.1
2	D	16	GLN	3.1
2	D	112	PRO	3.1
1	A	117	VAL	3.0
2	D	471	MET	3.0
1	B	53	THR	3.0
2	D	154	TYR	3.0
1	A	154	TYR	2.9
1	B	88	ARG	2.9
1	F	329	TYR	2.9
1	A	329	TYR	2.9
1	E	116	GLU	2.9
1	A	499	VAL	2.9
1	A	338	MET	2.8
1	A	15	HIS	2.8
1	F	501	GLU	2.8
1	E	502	LYS	2.8
1	B	252	MET	2.8
1	A	17	ALA	2.8
2	C	116	GLU	2.8
1	F	157	SER	2.8
1	A	501	GLU	2.8
1	F	485	ASN	2.8
2	C	145	ASP	2.8
1	A	188	TYR	2.8
2	D	115	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	15	HIS	2.7
1	A	14	GLU	2.7
1	A	255	THR	2.7
1	A	16	GLN	2.7
1	F	253	ARG	2.7
1	B	259	SER	2.7
2	D	114	GLY	2.7
1	F	118	VAL	2.7
1	E	112	PRO	2.7
1	A	309	LYS	2.7
1	E	113	GLU	2.7
1	E	498	THR	2.6
1	E	329	TYR	2.6
1	E	118	VAL	2.6
1	F	502	LYS	2.6
1	F	340	ARG	2.6
2	C	143	SER	2.5
1	A	241	ASP	2.5
1	A	417	ASP	2.5
2	D	152	GLN	2.5
2	C	16	GLN	2.5
1	E	120	GLY	2.5
2	D	496	ARG	2.4
2	C	114	GLY	2.4
1	A	319	GLU	2.4
1	B	497	ILE	2.4
1	A	474	ASP	2.4
2	D	116	GLU	2.4
1	A	378	ASP	2.4
1	F	484	ARG	2.4
1	B	123	LEU	2.4
1	F	498	THR	2.4
1	B	341	GLN	2.4
1	B	155	ASP	2.3
1	E	166	ARG	2.3
1	A	250	GLY	2.3
2	C	146	SER	2.3
1	E	421	GLY	2.3
1	E	471	MET	2.3
2	D	157	SER	2.3
1	B	153	GLN	2.3
2	C	431	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	181	THR	2.3
1	B	90	PHE	2.2
1	F	257	ARG	2.2
1	B	436	THR	2.2
1	A	340	ARG	2.2
2	C	138	ARG	2.2
1	B	180	MET	2.2
1	B	309	LYS	2.2
1	A	413	THR	2.2
1	A	342	ASN	2.2
1	B	14	GLU	2.2
2	D	156	ALA	2.2
2	D	201	SER	2.2
1	E	295	THR	2.2
2	D	309	LYS	2.1
1	A	436	THR	2.1
2	C	123	LEU	2.1
1	A	379	SER	2.1
2	D	321	ARG	2.1
2	C	135	GLN	2.1
2	D	155	ASP	2.1
1	F	116	GLU	2.1
1	E	201	SER	2.1
1	E	114	GLY	2.0
1	E	318	GLU	2.0
1	E	188	TYR	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	B	431	10/11	0.80	0.30	-	4,82,87,88	0
1	SEP	A	431	10/11	0.78	0.30	-	4,79,81,84	0
1	TPO	B	432	11/12	0.85	0.27	-	3,19,83,84	0
1	TPO	F	432	11/12	0.76	0.32	-	3,10,75,76	0
2	TPO	D	432	11/12	0.77	0.31	-	3,9,61,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	TPO	C	432	11/12	0.76	0.27	-	3,10,78,79	0
1	TPO	A	432	11/12	0.80	0.28	-	3,19,82,83	0
1	TPO	E	432	11/12	0.83	0.22	-	3,10,59,61	0
1	SEP	F	431	10/11	0.62	0.38	-	4,80,83,83	0
1	SEP	E	431	10/11	0.71	0.33	-	4,57,60,61	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	ATP	D	903	31/31	0.94	0.25	1.32	42,54,77,81	0
4	ATP	E	903	31/31	0.96	0.23	1.18	42,54,77,80	0
4	ATP	F	903	31/31	0.94	0.22	1.14	42,54,76,80	0
3	MG	B	802	1/1	0.81	0.29	1.03	73,73,73,73	0
4	ATP	D	901	31/31	0.95	0.23	0.93	53,66,89,104	0
4	ATP	B	901	31/31	0.92	0.22	0.60	62,73,109,116	0
4	ATP	F	901	31/31	0.88	0.25	0.55	74,90,114,121	0
4	ATP	C	901	31/31	0.95	0.19	0.49	48,55,97,110	0
4	ATP	A	901	31/31	0.84	0.32	0.48	75,89,103,112	0
4	ATP	E	901	31/31	0.90	0.24	0.23	61,77,101,113	0
4	ATP	C	903	31/31	0.92	0.22	0.23	43,54,77,81	0
4	ATP	A	903	31/31	0.88	0.22	0.16	42,54,76,81	0
4	ATP	B	903	31/31	0.89	0.18	-0.55	43,54,77,81	0
3	MG	E	805	1/1	0.98	0.08	-	19,19,19,19	0
3	MG	D	804	1/1	0.91	0.17	-	19,19,19,19	0
3	MG	F	806	1/1	0.98	0.13	-	19,19,19,19	0
3	MG	C	803	1/1	0.89	0.12	-	19,19,19,19	0
3	MG	A	801	1/1	0.96	0.12	-	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.