



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 05:26 PM EDT

PDB ID : 3K09
Title : Crystal structure of the phosphorylation-site mutant S431D of the KaiC circadian clock protein
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on : 2009-09-24
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

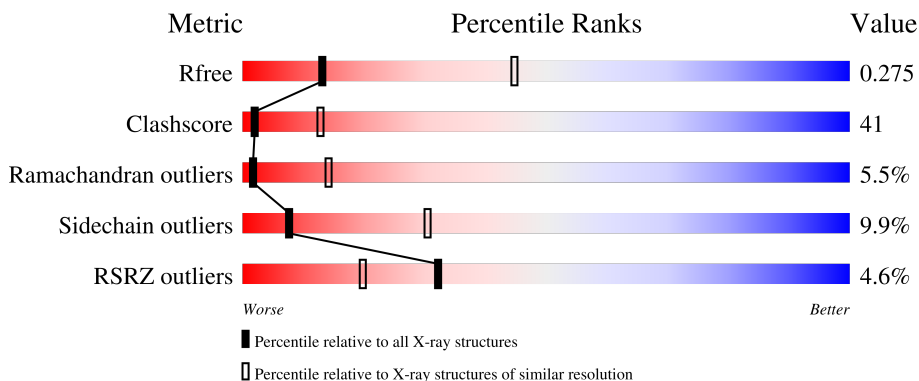
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



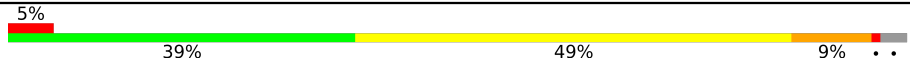
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	519	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
1	B	519	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
1	E	519	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
2	C	519	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
2	D	519	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	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
3	MG	A	702	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23855 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
			Total	C	N	O	P	S			
1	A	506	Total	C	N	O	P	S	0	0	0
			3991	2510	701	764	1	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3876	2440	678	742	1	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3884	2446	679	743	1	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ASP	SER	engineered mutation	UNP Q79PF4
B	431	ASP	SER	engineered mutation	UNP Q79PF4
E	431	ASP	SER	engineered mutation	UNP Q79PF4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	488	Total	C	N	O	S	0	0	0
			3848	2426	674	733	15			
2	D	485	Total	C	N	O	S	0	0	0
			3824	2412	671	726	15			
2	F	506	Total	C	N	O	S	0	0	0
			3987	2510	701	761	15			

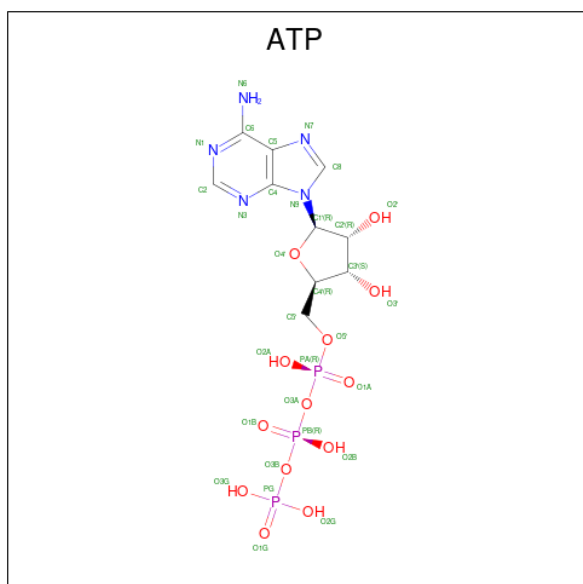
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	431	ASP	SER	engineered mutation	UNP Q79PF4
D	431	ASP	SER	engineered mutation	UNP Q79PF4
F	431	ASP	SER	engineered mutation	UNP Q79PF4

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

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

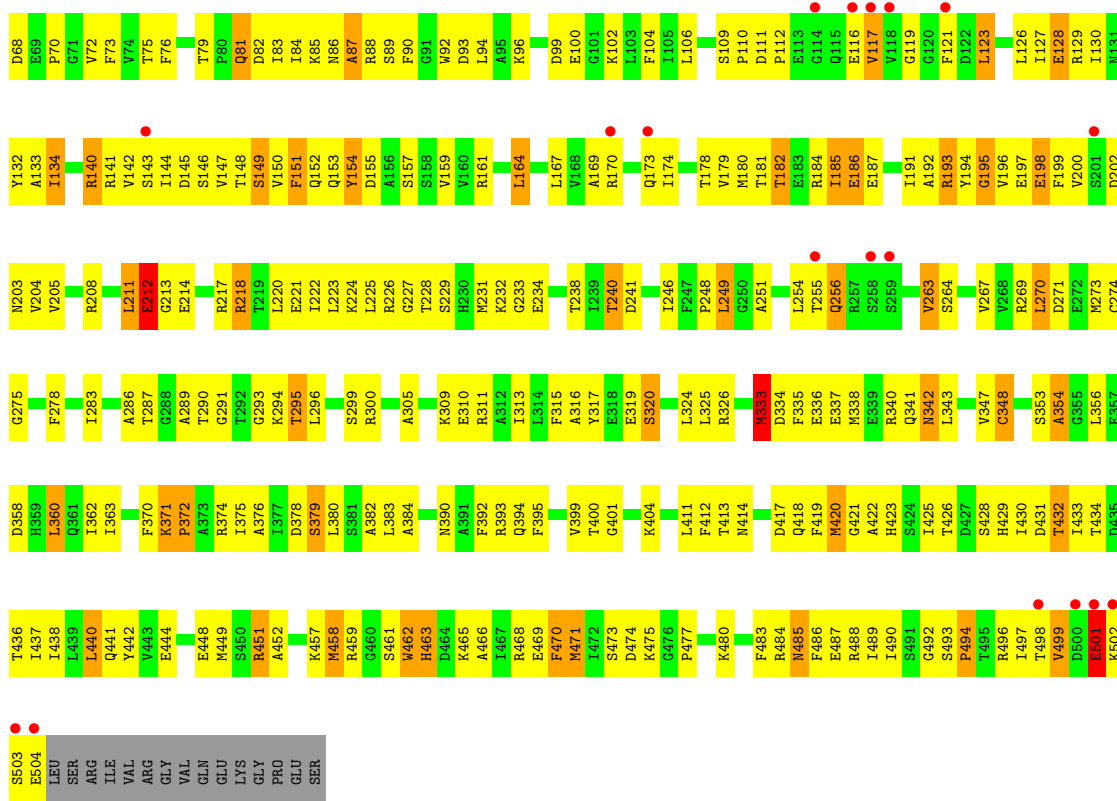
Continued on next page...

Continued from previous page...

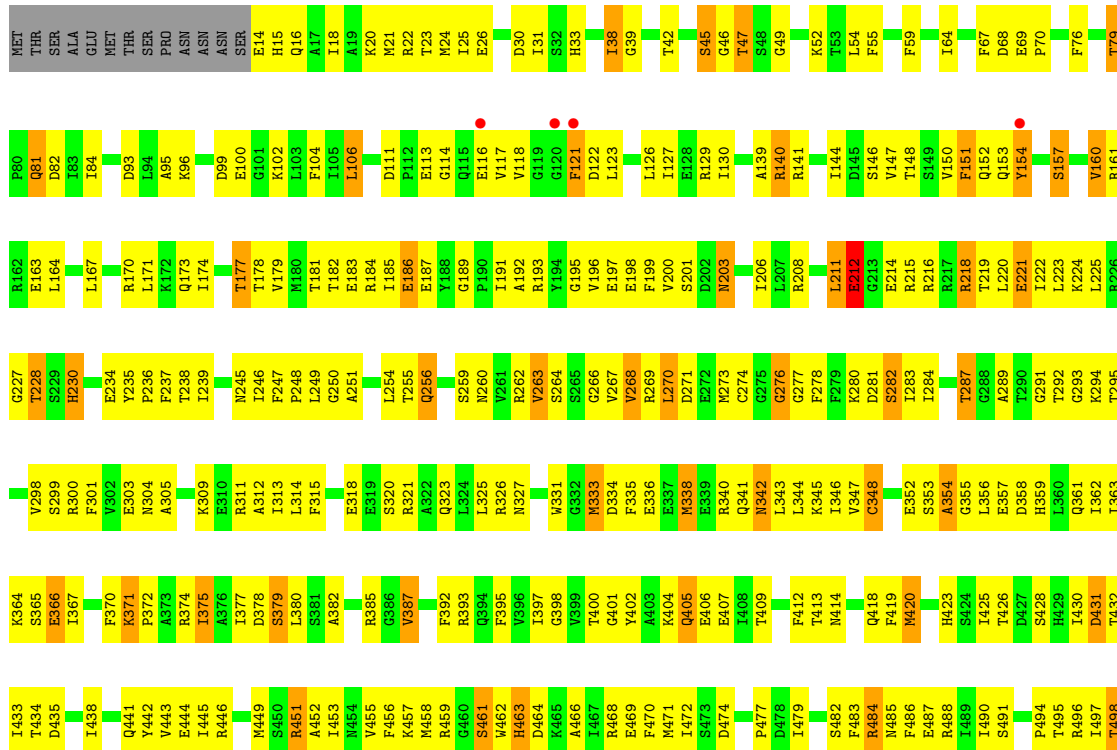
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F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

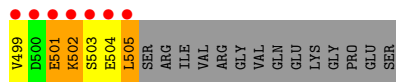
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	5	Total	O	0	0
			5	5		
5	C	5	Total	O	0	0
			5	5		
5	D	10	Total	O	0	0
			10	10		
5	E	7	Total	O	0	0
			7	7		
5	F	19	Total	O	0	0
			19	19		

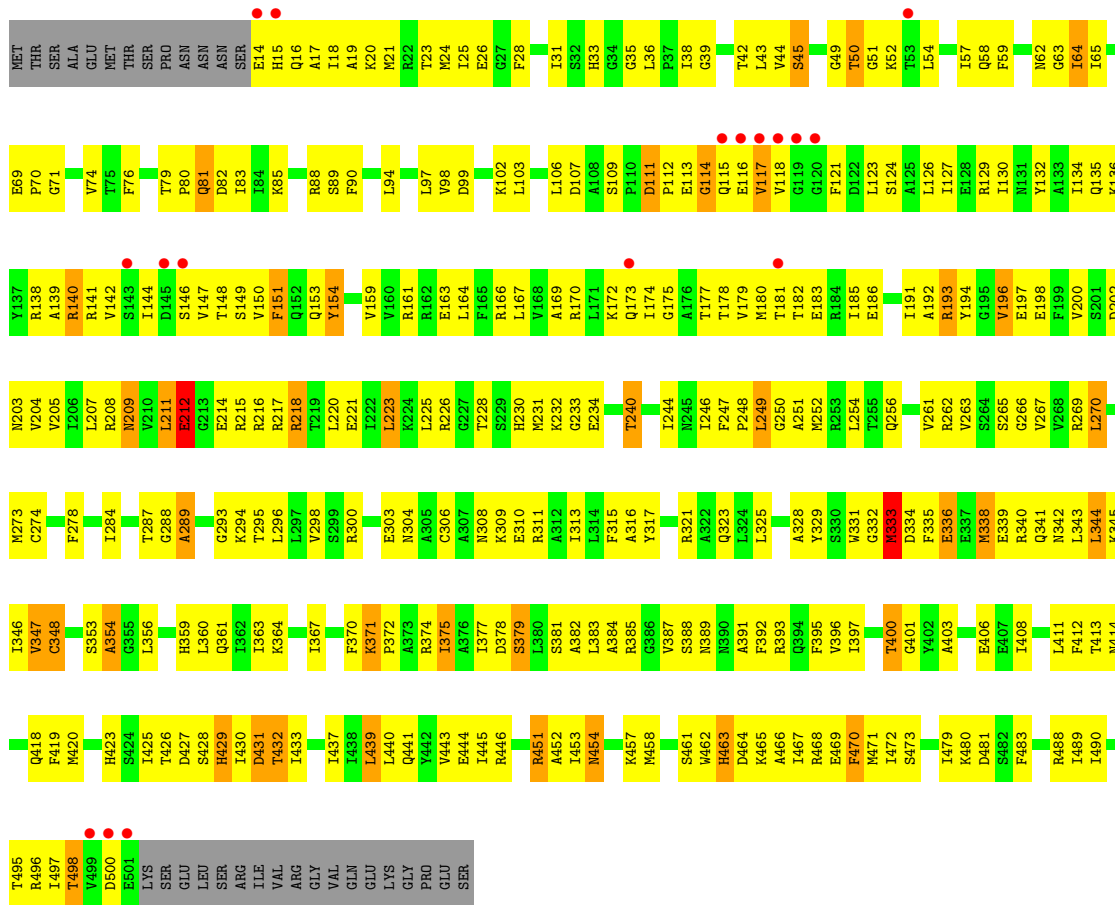


● Molecule 1: Circadian clock protein kinase kaiC

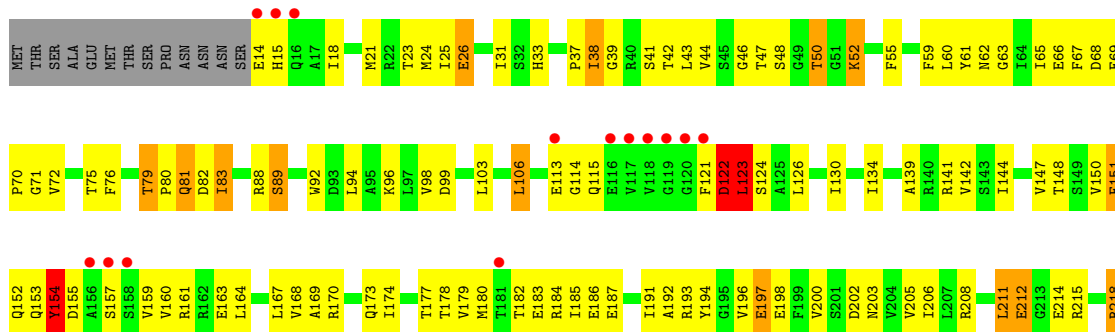




• Molecule 2: Circadian clock protein kinase kaiC



• Molecule 2: Circadian clock protein kinase kaiC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.50Å 135.83Å 204.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.98 – 3.19	Depositor EDS
% Data completeness (in resolution range)	81.4 (30.00-3.20) 90.1 (29.98-3.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.18Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.296 0.219 , 0.275	Depositor DCC
R_{free} test set	5684 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	82.9	Xtrriage
Anisotropy	0.384	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.028 for k,h,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23855	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/4045	0.70	0/5448
1	B	0.41	0/3929	0.66	0/5293
1	E	0.49	0/3937	0.72	1/5304 (0.0%)
2	C	0.44	0/3913	0.68	0/5275
2	D	0.47	0/3889	0.72	0/5242
2	F	0.47	0/4053	0.72	0/5461
All	All	0.45	0/23766	0.70	1/32023 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	380	LEU	N-CA-C	-5.39	96.44	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3991	0	3984	337	0
1	B	3876	0	3861	326	0
1	E	3884	0	3873	337	0
2	C	3848	0	3838	337	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3824	0	3819	332	0
2	F	3987	0	3984	384	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
3	E	4	0	0	0	0
3	F	3	0	0	0	0
4	A	62	0	24	5	0
4	B	62	0	24	7	0
4	C	62	0	24	4	0
4	D	62	0	24	6	0
4	E	62	0	24	6	0
4	F	62	0	24	9	0
5	A	7	0	0	1	0
5	B	5	0	0	2	0
5	C	5	0	0	1	0
5	D	10	0	0	2	0
5	E	7	0	0	1	0
5	F	19	0	0	4	0
All	All	23855	0	23503	1939	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 41.

All (1939) 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:E:305:ALA:HB2	1:E:374:ARG:HD2	1.16	1.14
1:A:14:GLU:HG3	1:A:15:HIS:H	1.13	1.13
2:F:115:GLN:HG2	2:F:116:GLU:N	1.56	1.13
2:F:115:GLN:HG2	2:F:116:GLU:H	0.97	1.10
1:A:140:ARG:HB3	1:A:140:ARG:HH11	1.14	1.08
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.40	1.04
1:B:140:ARG:HB3	1:B:140:ARG:HH11	1.21	1.03
2:C:313:ILE:HG12	2:C:345:LYS:HB3	1.35	1.03
2:F:305:ALA:HB2	2:F:374:ARG:HD2	1.39	1.02
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.44	0.99
2:F:263:VAL:HG12	2:F:374:ARG:HH21	1.25	0.98
2:F:127:ILE:HD11	2:F:167:LEU:HA	1.42	0.98
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.46	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.46	0.96
2:D:371:LYS:HD2	2:D:371:LYS:O	1.66	0.95
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.30	0.95
2:C:31:ILE:HG23	2:C:231:MET:HB2	1.48	0.94
1:A:140:ARG:HB3	1:A:140:ARG:NH1	1.84	0.92
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.49	0.92
2:D:18:ILE:H	2:D:18:ILE:HD12	1.35	0.92
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.51	0.91
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.32	0.91
1:E:323:GLN:HE22	2:F:459:ARG:HD3	1.34	0.91
1:A:483:PHE:HB2	1:A:489:ILE:HD11	1.51	0.90
1:B:47:THR:O	1:B:50:THR:HG23	1.72	0.90
1:A:207:LEU:HD21	1:A:220:LEU:HD12	1.53	0.90
1:A:425:ILE:HG21	1:A:431:ASP:HB3	1.54	0.90
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.36	0.90
2:F:191:ILE:HG13	2:F:206:ILE:HD11	1.53	0.90
2:F:161:ARG:HB2	2:F:196:VAL:HG11	1.52	0.89
2:F:191:ILE:HB	2:F:198:GLU:HG2	1.54	0.89
1:B:140:ARG:HB3	1:B:140:ARG:NH1	1.88	0.89
1:E:283:ILE:HG13	1:E:400:THR:HG23	1.54	0.89
2:F:191:ILE:HB	2:F:198:GLU:CG	2.03	0.89
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.37	0.88
2:C:371:LYS:O	2:C:371:LYS:HD2	1.73	0.88
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.53	0.88
1:A:425:ILE:HG22	1:A:426:THR:HG23	1.55	0.88
2:C:323:GLN:HE22	2:D:459:ARG:HD3	1.39	0.88
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.38	0.87
1:A:488:ARG:HE	2:F:488:ARG:HH12	1.20	0.87
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.54	0.87
1:E:323:GLN:NE2	2:F:459:ARG:HD3	1.90	0.87
2:C:344:LEU:HD22	2:C:345:LYS:N	1.89	0.87
2:F:140:ARG:HB3	2:F:140:ARG:HH11	1.38	0.87
1:A:379:SER:H	1:A:413:THR:HB	1.39	0.86
1:B:161:ARG:NH2	1:B:199:PHE:HB2	1.91	0.86
2:D:41:SER:HB3	2:D:178:THR:HB	1.57	0.86
2:F:379:SER:H	2:F:413:THR:HB	1.39	0.86
2:D:379:SER:H	2:D:413:THR:HB	1.40	0.86
1:A:318:GLU:OE2	1:B:432:TPO:HG21	1.75	0.86
2:F:47:THR:HG23	5:F:522:HOH:O	1.74	0.85
1:B:497:ILE:HD12	1:B:498:THR:N	1.90	0.85
1:A:14:GLU:CG	1:A:15:HIS:H	1.88	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:SER:H	1:B:181:THR:HB	1.41	0.85
2:D:431:ASP:HA	2:D:434:THR:HG22	1.58	0.85
2:C:45:SER:HB2	2:C:182:THR:HB	1.59	0.85
2:C:344:LEU:HD22	2:C:345:LYS:H	1.42	0.85
2:D:89:SER:HB2	1:E:227:GLY:O	1.77	0.84
1:E:33:HIS:HD2	1:E:230:HIS:HA	1.42	0.84
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.58	0.84
1:B:191:ILE:HB	1:B:198:GLU:CD	1.97	0.84
2:C:287:THR:HG21	2:C:425:ILE:O	1.76	0.84
1:B:170:ARG:O	1:B:174:ILE:HG12	1.78	0.83
1:E:371:LYS:HD2	1:E:371:LYS:O	1.78	0.83
1:A:315:PHE:HE1	1:A:375:ILE:HG12	1.44	0.83
2:D:221:GLU:HG3	2:D:233:GLY:O	1.79	0.83
2:D:214:GLU:HB3	1:E:234:GLU:HB2	1.60	0.83
1:E:418:GLN:HB2	2:F:423:HIS:O	1.79	0.83
1:E:163:GLU:HA	1:E:163:GLU:OE2	1.76	0.83
1:B:492:GLY:O	1:B:494:PRO:HD3	1.79	0.82
2:D:147:VAL:O	2:D:150:VAL:HG12	1.79	0.82
1:A:488:ARG:HE	2:F:488:ARG:NH1	1.78	0.82
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.61	0.82
2:F:50:THR:HA	5:F:534:HOH:O	1.80	0.82
2:D:393:ARG:O	2:D:397:ILE:HG12	1.78	0.82
1:E:263:VAL:CG1	1:E:374:ARG:HH21	1.93	0.81
1:A:140:ARG:HH11	1:A:140:ARG:CB	1.93	0.81
1:B:147:VAL:O	1:B:150:VAL:HG12	1.79	0.81
2:C:94:LEU:O	2:C:98:VAL:HG23	1.80	0.81
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.10	0.81
2:F:515:LYS:HG3	2:F:516:GLY:H	1.45	0.81
1:B:379:SER:OG	1:B:382:ALA:HB2	1.81	0.81
1:E:305:ALA:CB	1:E:374:ARG:HD2	2.08	0.81
2:F:269:ARG:HB3	2:F:479:ILE:HD12	1.60	0.81
2:F:486:PHE:HE2	2:F:496:ARG:HD2	1.45	0.81
2:C:164:LEU:HD11	2:C:197:GLU:HG3	1.62	0.81
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.63	0.81
1:B:140:ARG:HH11	1:B:140:ARG:CB	1.94	0.80
1:A:441:GLN:HE22	1:A:490:ILE:HD13	1.47	0.80
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.44	0.80
2:F:287:THR:HG21	2:F:425:ILE:O	1.82	0.80
2:F:79:THR:HG23	2:F:81:GLN:HG2	1.64	0.79
2:F:115:GLN:CG	2:F:116:GLU:H	1.88	0.79
1:E:425:ILE:HB	1:E:431:ASP:OD2	1.81	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ILE:HG22	1:B:222:ILE:HD12	1.64	0.79
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.82	0.79
1:A:14:GLU:HG3	1:A:15:HIS:N	1.94	0.79
1:A:448:GLU:HG2	1:B:466:ALA:HA	1.62	0.79
1:E:170:ARG:O	1:E:174:ILE:HG12	1.83	0.79
1:B:45:SER:HB3	1:B:182:THR:HB	1.65	0.78
2:F:486:PHE:CE2	2:F:496:ARG:HD2	2.18	0.78
1:B:393:ARG:HH21	1:B:429:HIS:HB2	1.46	0.78
2:D:212:GLU:HG2	2:D:212:GLU:O	1.82	0.78
2:D:496:ARG:HG2	1:E:487:GLU:OE1	1.83	0.78
2:D:379:SER:HA	2:D:413:THR:O	1.82	0.78
2:F:148:THR:HG21	2:F:193:ARG:HD2	1.63	0.78
2:D:262:ARG:HD2	2:D:276:GLY:O	1.84	0.78
2:C:323:GLN:NE2	2:D:459:ARG:HD3	1.98	0.78
2:C:123:LEU:HD22	2:C:127:ILE:HD11	1.64	0.77
2:F:148:THR:CG2	2:F:193:ARG:HD2	2.14	0.77
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.67	0.77
2:F:269:ARG:HG2	2:F:479:ILE:HB	1.66	0.77
2:F:363:ILE:O	2:F:367:ILE:HG13	1.85	0.77
2:C:269:ARG:O	2:C:273:MET:HG3	1.84	0.77
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.19	0.77
2:C:123:LEU:HD21	2:C:167:LEU:HB2	1.66	0.77
2:F:501:GLU:HG3	2:F:502:LYS:H	1.49	0.77
1:B:337:GLU:HB3	1:B:338:MET:HE3	1.67	0.77
1:B:458:MET:HB2	1:B:463:HIS:HD2	1.49	0.77
2:D:315:PHE:CZ	2:D:363:ILE:HG23	2.20	0.77
2:C:495:THR:HA	2:D:487:GLU:OE2	1.84	0.76
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.48	0.76
2:F:263:VAL:CG1	2:F:374:ARG:HH21	1.98	0.76
2:D:332:GLY:O	2:D:333:MET:HG2	1.84	0.76
1:A:433:ILE:HG22	1:A:433:ILE:O	1.85	0.76
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.66	0.76
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.00	0.76
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.67	0.76
1:E:147:VAL:O	1:E:150:VAL:HG12	1.86	0.76
2:C:335:PHE:HA	2:C:338:MET:HG3	1.67	0.76
1:A:18:ILE:H	1:A:18:ILE:HD12	1.50	0.76
1:A:83:ILE:H	1:A:83:ILE:HD12	1.50	0.76
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.66	0.76
2:F:146:SER:H	2:F:181:THR:HG22	1.51	0.75
2:D:256:GLN:HG3	2:D:404:LYS:HD3	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:ARG:NH2	1:E:496:ARG:HH22	1.84	0.75
2:F:115:GLN:CG	2:F:116:GLU:N	2.43	0.75
1:B:147:VAL:HG11	1:B:180:MET:CE	2.16	0.74
2:C:418:GLN:HB2	2:D:423:HIS:O	1.87	0.74
2:F:344:LEU:HD11	2:F:346:ILE:HG13	1.69	0.74
2:C:170:ARG:O	2:C:174:ILE:HG12	1.85	0.74
2:D:130:ILE:O	2:D:134:ILE:HG13	1.87	0.74
1:B:273:MET:O	1:B:463:HIS:HA	1.87	0.74
2:D:114:GLY:O	2:D:115:GLN:HG3	1.87	0.74
1:E:356:LEU:HD11	1:E:387:VAL:HG21	1.68	0.74
1:E:269:ARG:HB3	1:E:479:ILE:HD12	1.68	0.74
2:F:501:GLU:HG3	2:F:502:LYS:N	2.03	0.74
2:C:347:VAL:O	2:C:348:CYS:HB2	1.88	0.74
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.69	0.74
1:E:309:LYS:HA	1:E:343:LEU:HD13	1.68	0.74
2:F:178:THR:HG22	2:F:179:VAL:H	1.53	0.74
1:A:495:THR:HG22	1:A:497:ILE:HG23	1.70	0.74
2:D:46:GLY:HA2	5:D:521:HOH:O	1.87	0.73
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.23	0.73
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.16	0.73
2:D:431:ASP:HA	2:D:434:THR:CG2	2.18	0.73
2:F:371:LYS:O	2:F:371:LYS:HD2	1.88	0.73
1:E:216:ARG:NH2	2:F:223:LEU:HD21	2.03	0.73
2:D:293:GLY:HA2	4:D:901:ATP:O1A	1.89	0.73
2:C:79:THR:HG22	2:C:82:ASP:OD2	1.87	0.73
1:E:81:GLN:NE2	1:E:81:GLN:H	1.87	0.73
1:E:382:ALA:O	1:E:385:ARG:HG3	1.89	0.73
1:A:316:ALA:O	1:A:348:CYS:HA	1.89	0.73
1:A:265:SER:O	1:A:301:PHE:HA	1.89	0.73
1:B:418:GLN:HB2	2:C:423:HIS:O	1.89	0.73
2:D:31:ILE:HA	2:D:231:MET:HG3	1.69	0.73
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.24	0.72
1:E:287:THR:CG2	1:E:414:ASN:HD22	2.02	0.72
1:A:293:GLY:HA2	4:A:901:ATP:O1A	1.89	0.72
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.70	0.72
1:A:299:SER:HB3	1:A:333:MET:HE2	1.71	0.72
2:C:159:VAL:O	2:C:163:GLU:HG2	1.90	0.72
2:D:426:THR:HG22	2:D:428:SER:H	1.54	0.72
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.19	0.72
1:A:21:MET:HE3	1:A:141:ARG:CZ	2.19	0.72
1:A:488:ARG:NE	2:F:488:ARG:HH12	1.87	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:497:ILE:HD12	2:D:497:ILE:O	1.88	0.72
1:B:212:GLU:HG2	1:B:212:GLU:O	1.86	0.72
2:C:396:VAL:HG11	2:C:433:ILE:HD11	1.71	0.72
2:D:347:VAL:O	2:D:348:CYS:HB2	1.90	0.72
2:F:382:ALA:O	2:F:385:ARG:HG3	1.89	0.72
2:F:437:ILE:HD12	2:F:457:LYS:HG2	1.69	0.72
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.54	0.72
1:A:266:GLY:HA3	1:A:300:ARG:O	1.89	0.72
1:A:178:THR:HG22	1:A:179:VAL:N	2.04	0.72
1:B:45:SER:CB	1:B:182:THR:HB	2.19	0.72
1:B:449:MET:CE	2:C:467:ILE:HD11	2.20	0.72
1:E:14:GLU:HG3	1:E:16:GLN:H	1.54	0.72
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.72	0.72
1:A:147:VAL:O	1:A:150:VAL:HG12	1.90	0.72
1:A:298:VAL:HG22	1:A:411:LEU:HD23	1.71	0.72
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.52	0.72
1:B:56:SER:O	1:B:59:PHE:HB3	1.89	0.71
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.55	0.71
2:F:208:ARG:NH2	2:F:221:GLU:OE2	2.22	0.71
2:C:70:PRO:HB2	2:C:139:ALA:HA	1.71	0.71
1:E:294:LYS:HB2	4:E:901:ATP:O1B	1.88	0.71
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.70	0.71
2:F:393:ARG:O	2:F:397:ILE:HG12	1.90	0.71
1:B:283:ILE:HD12	1:B:412:PHE:HE1	1.55	0.71
2:F:127:ILE:CD1	2:F:167:LEU:HA	2.20	0.71
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.20	0.71
2:D:418:GLN:HB2	1:E:423:HIS:O	1.90	0.71
1:E:212:GLU:O	1:E:212:GLU:HG2	1.89	0.71
1:A:61:TYR:CZ	1:A:65:ILE:HG13	2.26	0.71
1:B:25:ILE:HG23	1:B:58:GLN:NE2	2.05	0.71
1:A:211:LEU:HD13	1:A:216:ARG:NE	2.06	0.71
1:A:264:SER:HA	1:A:271:ASP:OD1	1.91	0.71
1:A:305:ALA:CB	1:A:374:ARG:HD2	2.19	0.71
2:F:47:THR:O	2:F:52:LYS:HE2	1.90	0.71
2:F:299:SER:HB3	2:F:333:MET:HE1	1.73	0.71
2:D:484:ARG:HB3	2:D:484:ARG:HH11	1.54	0.71
1:A:211:LEU:O	1:A:212:GLU:HB3	1.89	0.71
2:D:148:THR:HG21	2:D:193:ARG:HD2	1.73	0.70
2:D:192:ALA:HB3	2:D:197:GLU:OE2	1.90	0.70
1:B:44:VAL:HA	1:B:205:VAL:O	1.90	0.70
2:D:31:ILE:HG22	2:D:222:ILE:HD12	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:ILE:HG22	1:E:367:ILE:HD11	1.72	0.70
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.72	0.70
2:D:170:ARG:O	2:D:174:ILE:HG12	1.92	0.70
2:F:191:ILE:HG13	2:F:206:ILE:CD1	2.22	0.70
1:A:451:ARG:HD2	1:A:451:ARG:N	2.06	0.70
1:B:360:LEU:O	1:B:360:LEU:HD22	1.91	0.70
1:E:45:SER:HB2	1:E:182:THR:O	1.92	0.70
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.56	0.69
2:C:25:ILE:HG12	2:C:58:GLN:NE2	2.07	0.69
2:D:264:SER:HA	2:D:271:ASP:OD1	1.92	0.69
2:F:438:ILE:CD1	2:F:455:VAL:HG22	2.21	0.69
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.74	0.69
2:F:443:VAL:HG12	2:F:445:ILE:HG12	1.72	0.69
1:B:263:VAL:HG12	1:B:374:ARG:NH2	2.06	0.69
1:B:31:ILE:HA	1:B:231:MET:SD	2.33	0.69
2:C:45:SER:CB	2:C:182:THR:HB	2.22	0.69
2:D:486:PHE:CE2	2:D:496:ARG:HD3	2.27	0.69
1:B:191:ILE:HB	1:B:198:GLU:CG	2.22	0.69
2:D:218:ARG:HG3	2:D:237:PHE:O	1.93	0.69
2:C:451:ARG:HG2	2:C:451:ARG:HH11	1.57	0.69
1:E:420:MET:HE1	2:F:490:ILE:HG13	1.75	0.69
1:B:150:VAL:HG13	1:B:151:PHE:N	2.08	0.69
2:F:287:THR:CG2	2:F:414:ASN:HD22	2.06	0.69
1:A:438:ILE:HD11	1:A:455:VAL:HG22	1.75	0.69
1:E:140:ARG:HB3	1:E:140:ARG:HH11	1.57	0.69
1:B:286:ALA:HA	1:B:438:ILE:O	1.92	0.69
1:B:358:ASP:O	1:B:362:ILE:HG12	1.93	0.69
1:B:503:SER:O	1:B:504:GLU:HB2	1.94	0.69
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.73	0.69
2:F:336:GLU:HB3	2:F:340:ARG:NH2	2.08	0.69
2:F:44:VAL:HG22	2:F:205:VAL:HB	1.75	0.68
2:C:88:ARG:CZ	2:D:15:HIS:HA	2.23	0.68
2:F:283:ILE:HG23	2:F:412:PHE:CE1	2.28	0.68
2:F:79:THR:HG23	2:F:81:GLN:H	1.58	0.68
1:A:347:VAL:O	1:A:348:CYS:HB2	1.93	0.68
2:D:94:LEU:O	2:D:98:VAL:HG23	1.93	0.68
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.73	0.68
2:F:79:THR:HG22	2:F:82:ASP:H	1.56	0.68
1:E:469:GLU:HB3	1:E:483:PHE:CZ	2.28	0.68
1:B:169:ALA:O	1:B:173:GLN:HG3	1.94	0.68
1:B:202:ASP:HA	1:B:226:ARG:HD2	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:469:GLU:HG3	2:C:480:LYS:HE3	1.74	0.68
1:A:24:MET:HB2	1:A:62:ASN:ND2	2.09	0.68
2:C:202:ASP:HA	2:C:226:ARG:HD2	1.74	0.68
2:C:221:GLU:HG3	2:C:233:GLY:O	1.93	0.68
1:E:433:ILE:O	1:E:433:ILE:HG22	1.92	0.68
1:A:436:THR:HG23	1:A:458:MET:HG2	1.76	0.68
1:B:300:ARG:HA	1:B:333:MET:HE1	1.76	0.68
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.23	0.68
2:D:437:ILE:HD12	2:D:457:LYS:HG2	1.74	0.68
2:F:20:LYS:C	2:F:38:ILE:HD11	2.14	0.68
2:F:347:VAL:O	2:F:348:CYS:HB2	1.93	0.68
2:C:218:ARG:HB3	5:C:522:HOH:O	1.94	0.68
2:D:313:ILE:HD12	2:D:372:PRO:HG2	1.75	0.68
1:A:257:ARG:NH2	1:A:407:GLU:HG2	2.09	0.68
1:A:360:LEU:HD22	1:A:364:LYS:HE3	1.74	0.68
1:E:299:SER:C	1:E:333:MET:HE1	2.14	0.67
1:A:287:THR:HG21	1:A:425:ILE:O	1.94	0.67
1:A:371:LYS:N	1:A:372:PRO:HD3	2.09	0.67
1:B:311:ARG:HD2	1:B:371:LYS:HE3	1.75	0.67
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.21	0.67
2:D:347:VAL:HG12	2:D:348:CYS:N	2.08	0.67
2:D:383:LEU:HD13	2:D:395:PHE:HE2	1.59	0.67
2:F:492:GLY:O	2:F:494:PRO:HD3	1.95	0.67
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.29	0.67
1:A:320:SER:HA	1:B:254:LEU:HG	1.75	0.67
2:C:74:VAL:HG22	2:C:106:LEU:HD23	1.76	0.67
2:C:471:MET:HB3	2:C:480:LYS:NZ	2.09	0.67
2:C:182:THR:HG21	2:C:192:ALA:HB1	1.77	0.67
2:C:315:PHE:CE2	2:C:363:ILE:HA	2.29	0.67
2:C:140:ARG:NH1	2:C:140:ARG:HB3	2.10	0.67
2:F:46:GLY:HA2	2:F:184:ARG:HD2	1.77	0.67
2:F:431:ASP:O	2:F:434:THR:HG22	1.94	0.67
1:A:148:THR:HG21	1:A:193:ARG:HD2	1.75	0.67
2:C:308:ASN:O	2:C:310:GLU:HG3	1.94	0.67
2:D:370:PHE:O	2:D:371:LYS:HG3	1.95	0.67
1:E:152:GLN:HG3	2:F:161:ARG:HH11	1.60	0.67
2:F:461:SER:OG	2:F:462:TRP:N	2.27	0.67
1:A:18:ILE:HD12	1:A:18:ILE:N	2.10	0.67
2:C:18:ILE:HD12	2:C:18:ILE:N	2.10	0.67
2:D:194:TYR:O	2:D:196:VAL:HG23	1.95	0.67
1:A:492:GLY:O	1:A:494:PRO:HD3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:311:ARG:HD2	2:F:371:LYS:HE3	1.77	0.66
2:F:514:GLU:HG2	2:F:519:SER:HB3	1.77	0.66
1:B:458:MET:HB2	1:B:463:HIS:CD2	2.29	0.66
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.61	0.66
2:D:446:ARG:HB3	1:E:484:ARG:HG3	1.77	0.66
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.77	0.66
2:C:444:GLU:OE2	2:D:489:ILE:HG12	1.95	0.66
1:E:148:THR:OG1	1:E:182:THR:HG23	1.95	0.66
2:D:315:PHE:HA	2:D:347:VAL:HB	1.78	0.66
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.59	0.66
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.78	0.66
1:E:446:ARG:NH2	1:E:496:ARG:NH2	2.43	0.66
2:F:294:LYS:N	4:F:901:ATP:O1B	2.27	0.66
1:A:363:ILE:O	1:A:367:ILE:HG13	1.95	0.66
1:B:147:VAL:HG11	1:B:180:MET:HE2	1.77	0.66
2:D:18:ILE:HD13	2:D:228:THR:HG23	1.76	0.66
2:D:79:THR:HG22	2:D:82:ASP:H	1.59	0.66
1:E:191:ILE:HB	1:E:198:GLU:CG	2.25	0.66
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.78	0.66
2:F:57:ILE:HD11	2:F:83:ILE:CG2	2.25	0.66
1:A:274:CYS:HG	1:A:278:PHE:HE2	1.44	0.66
2:C:185:ILE:HD11	2:C:193:ARG:NH1	2.11	0.66
2:C:446:ARG:HA	2:C:496:ARG:NH2	2.11	0.66
2:D:255:THR:O	2:D:255:THR:HG22	1.96	0.66
1:E:214:GLU:HB3	2:F:234:GLU:HB2	1.77	0.66
1:E:504:GLU:OE1	1:E:505:LEU:HD23	1.95	0.66
2:F:293:GLY:HA2	4:F:901:ATP:O1A	1.95	0.66
2:D:487:GLU:OE1	2:D:497:ILE:HG12	1.95	0.66
2:F:79:THR:CG2	2:F:81:GLN:HG2	2.26	0.66
2:F:287:THR:HG23	2:F:414:ASN:HD22	1.59	0.66
2:C:123:LEU:HD13	2:C:166:ARG:HD2	1.76	0.66
2:F:325:LEU:CD2	2:F:335:PHE:HB2	2.26	0.66
2:F:377:ILE:HD12	2:F:412:PHE:HE2	1.60	0.66
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.78	0.66
1:E:23:THR:O	1:E:24:MET:HB2	1.97	0.66
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.77	0.66
2:F:147:VAL:O	2:F:150:VAL:HG12	1.96	0.66
1:B:431:ASP:O	1:B:434:THR:HG22	1.96	0.65
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.61	0.65
1:A:215:ARG:NH1	1:B:232:LYS:O	2.28	0.65
2:F:215:ARG:HA	2:F:215:ARG:NE	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:ILE:HD11	2:F:83:ILE:HG23	1.77	0.65
2:F:280:LYS:NZ	2:F:407:GLU:HB3	2.11	0.65
2:C:359:HIS:O	2:C:363:ILE:HG13	1.96	0.65
2:C:370:PHE:O	2:C:371:LYS:HG3	1.96	0.65
1:A:344:LEU:HD11	1:A:346:ILE:HG13	1.77	0.65
1:B:315:PHE:CE2	1:B:347:VAL:HG21	2.31	0.65
1:E:497:ILE:HG22	1:E:498:THR:H	1.62	0.65
1:E:22:ARG:HD3	5:E:526:HOH:O	1.97	0.65
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.27	0.65
1:B:178:THR:HG22	1:B:179:VAL:N	2.11	0.65
2:C:406:GLU:O	2:C:408:ILE:HG13	1.97	0.65
2:D:197:GLU:H	2:D:197:GLU:CD	2.00	0.65
2:F:283:ILE:HG23	2:F:412:PHE:HE1	1.62	0.65
2:C:430:ILE:O	2:C:432:THR:N	2.28	0.65
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.61	0.65
1:E:426:THR:HG22	1:E:428:SER:H	1.61	0.65
2:F:311:ARG:HD2	2:F:371:LYS:CE	2.27	0.65
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.27	0.65
2:C:54:LEU:HD13	2:C:90:PHE:CZ	2.31	0.65
2:F:93:ASP:OD1	2:F:95:ALA:HB3	1.97	0.65
2:F:515:LYS:HG3	2:F:516:GLY:N	2.10	0.65
1:A:419:PHE:CD2	1:B:425:ILE:HD12	2.32	0.65
2:C:317:TYR:CD2	2:C:383:LEU:HD21	2.32	0.65
2:F:516:GLY:N	2:F:517:PRO:HD2	2.11	0.65
1:E:280:LYS:NZ	1:E:407:GLU:HB3	2.12	0.64
1:E:418:GLN:CB	2:F:423:HIS:O	2.44	0.64
1:E:451:ARG:N	1:E:451:ARG:HD2	2.12	0.64
2:F:178:THR:HG22	2:F:179:VAL:N	2.11	0.64
2:F:300:ARG:NH2	2:F:477:PRO:HD2	2.12	0.64
1:A:24:MET:CB	1:A:62:ASN:HD22	2.07	0.64
2:C:64:ILE:HG22	2:C:65:ILE:N	2.12	0.64
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.12	0.64
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.31	0.64
2:C:44:VAL:HG22	2:C:205:VAL:HB	1.79	0.64
2:C:64:ILE:HG21	2:C:97:LEU:HD13	1.77	0.64
2:D:345:LYS:HZ2	2:D:366:GLU:HG2	1.61	0.64
2:F:377:ILE:CD1	2:F:399:VAL:HG11	2.27	0.64
1:E:225:LEU:HB2	1:E:230:HIS:HD2	1.63	0.64
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.80	0.64
1:E:289:ALA:O	1:E:292:THR:HG23	1.98	0.64
1:E:320:SER:HA	2:F:254:LEU:HG	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.10	0.64
2:C:439:LEU:C	2:C:439:LEU:HD12	2.17	0.64
1:E:335:PHE:HA	1:E:338:MET:HG3	1.79	0.64
1:B:73:PHE:HE2	1:B:83:ILE:HD13	1.63	0.64
1:B:238:THR:HG22	1:B:240:THR:HG22	1.80	0.64
2:F:231:MET:CE	2:F:251:ALA:HB2	2.27	0.64
1:A:418:GLN:HB2	1:B:423:HIS:O	1.97	0.64
1:B:287:THR:HG21	1:B:425:ILE:O	1.97	0.64
1:B:449:MET:HE2	2:C:467:ILE:HD11	1.79	0.64
2:C:396:VAL:HG21	2:C:430:ILE:HD12	1.80	0.64
2:D:41:SER:CB	2:D:178:THR:HB	2.27	0.64
2:D:267:VAL:HG23	2:D:300:ARG:HG2	1.79	0.64
2:D:451:ARG:HG2	2:D:451:ARG:HH11	1.63	0.64
1:A:219:THR:HA	1:A:235:TYR:O	1.98	0.63
2:C:43:LEU:HD11	2:C:182:THR:OG1	1.98	0.63
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.33	0.63
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.79	0.63
1:E:104:PHE:CE2	1:E:106:LEU:HB2	2.34	0.63
1:E:426:THR:HG21	1:E:430:ILE:HG12	1.79	0.63
1:A:254:LEU:HG	2:F:320:SER:HA	1.80	0.63
1:A:191:ILE:HB	1:A:198:GLU:CG	2.28	0.63
2:D:495:THR:HG23	1:E:487:GLU:OE2	1.98	0.63
2:F:426:THR:HG22	2:F:428:SER:H	1.63	0.63
1:B:371:LYS:N	1:B:372:PRO:HD3	2.13	0.63
2:D:286:ALA:O	2:D:294:LYS:HG2	1.98	0.63
1:A:273:MET:O	1:A:463:HIS:HA	1.98	0.63
1:A:458:MET:O	4:F:901:ATP:H3'	1.97	0.63
1:B:73:PHE:CE2	1:B:83:ILE:HD13	2.33	0.63
2:C:220:LEU:HD23	2:C:221:GLU:N	2.13	0.63
1:E:59:PHE:CZ	1:E:141:ARG:HD3	2.34	0.63
1:E:185:ILE:HD11	1:E:193:ARG:NH1	2.13	0.63
1:A:184:ARG:O	1:A:185:ILE:HD13	1.98	0.63
2:C:21:MET:O	2:C:35:GLY:HA3	1.99	0.63
2:D:24:MET:HG3	2:D:66:GLU:HG3	1.80	0.63
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.81	0.63
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.81	0.63
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.25	0.63
2:D:269:ARG:HG2	2:D:479:ILE:HB	1.79	0.63
2:F:344:LEU:HD22	2:F:345:LYS:N	2.13	0.63
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.63	0.62
1:E:451:ARG:HH12	1:E:472:ILE:HD12	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ILE:HG13	1:A:372:PRO:HG2	1.81	0.62
2:F:298:VAL:HA	2:F:411:LEU:CD2	2.27	0.62
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.64	0.62
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.81	0.62
1:B:299:SER:C	1:B:333:MET:HE1	2.20	0.62
1:A:425:ILE:CG2	1:A:431:ASP:HB3	2.27	0.62
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.64	0.62
2:F:80:PRO:HG2	2:F:107:ASP:HB2	1.81	0.62
2:F:334:ASP:OD1	2:F:336:GLU:HB2	1.99	0.62
2:F:504:GLU:O	2:F:505:LEU:HB2	1.98	0.62
2:D:303:GLU:O	2:D:303:GLU:HG2	1.98	0.62
1:E:321:ARG:HG2	1:E:348:CYS:SG	2.40	0.62
2:F:140:ARG:HH11	2:F:140:ARG:CB	2.12	0.62
2:C:440:LEU:HD23	2:C:453:ILE:HG13	1.82	0.62
2:F:283:ILE:HG13	2:F:400:THR:HG23	1.82	0.62
2:C:24:MET:CB	2:C:62:ASN:HD22	2.12	0.62
2:C:382:ALA:O	2:C:385:ARG:HG3	1.98	0.62
2:D:430:ILE:O	2:D:433:ILE:HB	2.00	0.62
2:F:451:ARG:HB3	2:F:470:PHE:CE2	2.34	0.62
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.81	0.62
1:E:435:ASP:HA	1:E:459:ARG:HD2	1.81	0.62
1:E:461:SER:OG	1:E:462:TRP:N	2.28	0.62
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.81	0.62
1:B:379:SER:H	1:B:413:THR:HB	1.65	0.62
1:B:471:MET:HB3	1:B:480:LYS:NZ	2.15	0.62
2:D:304:ASN:HB3	2:D:374:ARG:HH12	1.64	0.62
1:A:284:ILE:HB	1:A:411:LEU:HD12	1.82	0.62
1:B:76:PHE:CZ	1:B:126:LEU:HD21	2.35	0.62
1:E:33:HIS:HD2	1:E:230:HIS:CA	2.10	0.62
2:F:344:LEU:HD22	2:F:345:LYS:H	1.65	0.61
1:A:311:ARG:HA	1:A:343:LEU:O	1.99	0.61
1:E:344:LEU:HD22	1:E:345:LYS:H	1.65	0.61
2:F:371:LYS:O	2:F:371:LYS:CD	2.48	0.61
2:F:377:ILE:HD11	2:F:399:VAL:HG11	1.82	0.61
1:A:24:MET:N	1:A:29:ASP:OD2	2.34	0.61
2:C:389:ASN:HD21	2:C:428:SER:HA	1.66	0.61
2:C:182:THR:HG22	2:C:183:GLU:N	2.15	0.61
2:D:155:ASP:OD1	2:D:159:VAL:HG11	1.98	0.61
2:D:269:ARG:O	2:D:272:GLU:HB2	2.00	0.61
1:E:455:VAL:HG11	1:E:463:HIS:HB2	1.82	0.61
1:B:116:GLU:HG2	1:B:117:VAL:H	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:ARG:CB	2:D:196:VAL:HG11	2.31	0.61
1:E:64:ILE:HD13	1:E:102:LYS:HB3	1.81	0.61
1:B:23:THR:O	1:B:24:MET:HB2	2.01	0.61
2:C:262:ARG:NH2	2:C:461:SER:HB2	2.15	0.61
2:C:419:PHE:O	2:C:420:MET:HB2	2.00	0.61
2:F:248:PRO:HB2	2:F:251:ALA:HB3	1.82	0.61
2:F:439:LEU:O	2:F:440:LEU:HD23	1.99	0.61
1:B:418:GLN:HG3	1:B:418:GLN:O	2.01	0.61
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.35	0.61
1:A:80:PRO:HB2	1:A:81:GLN:NE2	2.16	0.61
2:D:287:THR:HG21	2:D:425:ILE:O	2.00	0.61
1:E:33:HIS:CD2	1:E:230:HIS:HA	2.32	0.61
2:F:38:ILE:N	2:F:38:ILE:HD12	2.16	0.61
2:F:296:LEU:HD13	2:F:331:TRP:CD2	2.36	0.61
1:A:319:GLU:O	1:B:254:LEU:HD21	2.01	0.61
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.15	0.61
2:F:169:ALA:O	2:F:173:GLN:HG3	2.01	0.61
2:F:500:ASP:O	2:F:501:GLU:HB3	2.00	0.61
1:A:360:LEU:CD2	1:A:364:LYS:HE3	2.31	0.60
1:B:436:THR:HG23	1:B:458:MET:HG2	1.83	0.60
2:C:287:THR:HG22	2:C:288:GLY:N	2.16	0.60
2:C:400:THR:HG22	2:C:401:GLY:N	2.16	0.60
2:D:383:LEU:HD13	2:D:395:PHE:CE2	2.35	0.60
1:E:441:GLN:HE22	1:E:490:ILE:HA	1.66	0.60
1:B:32:SER:OG	1:B:35:GLY:HA2	2.01	0.60
2:C:387:VAL:HG12	2:C:391:ALA:HB3	1.83	0.60
2:D:191:ILE:HB	2:D:198:GLU:CG	2.32	0.60
2:D:340:ARG:C	2:D:342:ASN:H	2.04	0.60
1:E:140:ARG:HB3	1:E:140:ARG:NH1	2.15	0.60
1:A:496:ARG:HG3	1:B:487:GLU:OE1	2.02	0.60
2:C:38:ILE:HG22	2:C:39:GLY:N	2.16	0.60
2:C:211:LEU:O	2:C:212:GLU:HB3	1.99	0.60
2:C:471:MET:HB3	2:C:480:LYS:HZ3	1.64	0.60
1:E:283:ILE:HG23	1:E:412:PHE:CE1	2.35	0.60
1:E:347:VAL:O	1:E:348:CYS:HB2	2.01	0.60
1:E:425:ILE:HD11	1:E:456:PHE:CE2	2.36	0.60
2:F:16:GLN:HE22	2:F:33:HIS:HB3	1.66	0.60
2:F:191:ILE:CB	2:F:198:GLU:HG2	2.27	0.60
2:F:303:GLU:OE2	2:F:333:MET:HB3	2.01	0.60
1:E:46:GLY:O	1:E:52:LYS:HE2	2.02	0.60
1:E:353:SER:O	1:E:354:ALA:HB2	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:O	1:B:153:GLN:HG3	2.02	0.60
2:D:334:ASP:OD1	2:D:336:GLU:HB2	2.02	0.60
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.84	0.60
2:D:431:ASP:OD1	2:D:431:ASP:N	2.34	0.60
2:D:461:SER:OG	2:D:462:TRP:N	2.34	0.60
2:F:64:ILE:HG21	2:F:97:LEU:HD13	1.83	0.60
2:F:317:TYR:CD2	2:F:383:LEU:HD21	2.37	0.60
1:A:273:MET:SD	1:A:468:ARG:HD2	2.41	0.60
1:B:65:ILE:O	1:B:65:ILE:HG22	2.01	0.60
1:B:493:SER:HB3	2:C:488:ARG:HG2	1.83	0.60
2:D:350:TYR:CZ	1:E:254:LEU:HD13	2.37	0.60
2:D:371:LYS:N	2:D:372:PRO:HD3	2.16	0.60
1:E:363:ILE:HG22	1:E:367:ILE:CD1	2.31	0.60
2:F:483:PHE:HB3	2:F:486:PHE:CD1	2.37	0.60
2:D:151:PHE:C	2:D:153:GLN:H	2.05	0.60
1:B:300:ARG:HA	1:B:333:MET:CE	2.32	0.60
1:B:337:GLU:HB3	1:B:338:MET:CE	2.31	0.60
2:D:267:VAL:CG2	2:D:300:ARG:HG2	2.32	0.60
1:A:313:ILE:HG13	1:A:372:PRO:CG	2.32	0.60
2:C:240:THR:HG21	2:C:361:GLN:HE22	1.66	0.60
2:C:353:SER:O	2:C:354:ALA:HB2	2.02	0.60
2:F:53:THR:HG23	2:F:145:ASP:OD1	2.01	0.60
1:A:106:LEU:C	1:A:106:LEU:HD12	2.23	0.59
1:E:303:GLU:OE2	1:E:333:MET:HB3	2.02	0.59
1:E:309:LYS:HA	1:E:343:LEU:CD1	2.31	0.59
1:A:178:THR:CG2	1:A:179:VAL:N	2.65	0.59
2:F:20:LYS:C	2:F:38:ILE:CD1	2.71	0.59
2:F:60:LEU:CD1	2:F:73:PHE:HB2	2.32	0.59
1:B:123:LEU:HD13	1:B:123:LEU:O	2.03	0.59
2:C:191:ILE:HB	2:C:198:GLU:HG2	1.83	0.59
1:E:483:PHE:O	1:E:485:ASN:N	2.36	0.59
2:F:325:LEU:HD21	2:F:335:PHE:HB2	1.84	0.59
1:A:483:PHE:HB2	1:A:489:ILE:CD1	2.27	0.59
1:B:150:VAL:HG13	1:B:151:PHE:H	1.67	0.59
1:B:462:TRP:O	1:B:463:HIS:O	2.20	0.59
2:D:314:LEU:O	2:D:314:LEU:HG	2.02	0.59
2:D:344:LEU:HD11	2:D:346:ILE:HG13	1.83	0.59
1:E:192:ALA:HB3	1:E:197:GLU:OE2	2.02	0.59
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.84	0.59
2:F:377:ILE:HD12	2:F:412:PHE:CE2	2.37	0.59
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.31	0.59

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'	2.03	0.59
1:B:104:PHE:HD2	1:B:133:ALA:HB1	1.67	0.59
1:B:274:CYS:HB3	1:B:458:MET:SD	2.43	0.59
2:D:396:VAL:HG11	2:D:430:ILE:CG2	2.33	0.59
1:A:425:ILE:CG2	1:A:426:THR:HG23	2.32	0.59
2:C:147:VAL:O	2:C:150:VAL:HG12	2.02	0.59
1:E:346:ILE:HG22	1:E:347:VAL:N	2.18	0.59
1:A:207:LEU:CD2	1:A:220:LEU:HD12	2.30	0.59
1:B:170:ARG:HH12	1:B:174:ILE:HD11	1.68	0.59
1:A:136:LYS:HD3	1:A:137:TYR:CE1	2.38	0.59
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.83	0.59
1:E:193:ARG:NH2	2:F:195:GLY:O	2.29	0.59
2:F:80:PRO:CG	2:F:107:ASP:HB2	2.33	0.59
1:A:14:GLU:CG	1:A:15:HIS:N	2.60	0.59
1:B:149:SER:HB3	2:C:161:ARG:NH2	2.18	0.59
2:C:31:ILE:HA	2:C:231:MET:HG3	1.83	0.59
2:C:396:VAL:CG1	2:C:433:ILE:HD11	2.33	0.59
2:D:72:VAL:HB	2:D:142:VAL:HG22	1.85	0.59
2:D:484:ARG:HH11	2:D:484:ARG:CB	2.16	0.59
1:E:334:ASP:OD1	1:E:336:GLU:HB2	2.03	0.59
2:D:363:ILE:O	2:D:367:ILE:HG13	2.02	0.58
2:D:419:PHE:CD2	1:E:425:ILE:HD12	2.37	0.58
2:C:334:ASP:OD1	2:C:336:GLU:HB2	2.03	0.58
1:E:344:LEU:C	1:E:344:LEU:HD13	2.23	0.58
2:F:79:THR:CG2	2:F:82:ASP:H	2.16	0.58
1:B:311:ARG:HD2	1:B:371:LYS:CE	2.34	0.58
1:B:320:SER:HA	2:C:254:LEU:HG	1.84	0.58
2:C:20:LYS:C	2:C:38:ILE:HD11	2.24	0.58
2:C:106:LEU:CD2	2:C:130:ILE:HG12	2.33	0.58
2:D:315:PHE:CE1	2:D:363:ILE:HG23	2.38	0.58
1:A:501:GLU:O	1:A:503:SER:N	2.35	0.58
1:B:451:ARG:HH11	1:B:451:ARG:HG2	1.67	0.58
2:D:495:THR:HA	1:E:487:GLU:OE2	2.03	0.58
1:A:159:VAL:O	1:A:163:GLU:HG2	2.03	0.58
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.34	0.58
1:A:227:GLY:O	2:F:89:SER:HB2	2.02	0.58
1:B:293:GLY:HA2	4:B:901:ATP:O1A	2.03	0.58
2:F:111:ASP:OD1	2:F:112:PRO:HD2	2.03	0.58
1:A:165:PHE:CE2	2:F:110:PRO:HG2	2.39	0.58
4:A:903:ATP:C2	1:B:229:SER:HB3	2.38	0.58
1:B:300:ARG:N	1:B:333:MET:HE1	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:PRO:HA	2:D:83:ILE:HD12	1.84	0.58
1:E:123:LEU:O	1:E:127:ILE:HG13	2.03	0.58
2:F:118:VAL:O	2:F:118:VAL:HG13	2.02	0.58
2:D:312:ALA:O	2:D:344:LEU:HD22	2.04	0.58
1:B:96:LYS:O	1:B:100:GLU:HG3	2.02	0.58
1:B:305:ALA:CB	1:B:374:ARG:HD2	2.29	0.58
1:E:264:SER:H	1:E:374:ARG:NH2	2.02	0.58
2:C:317:TYR:HE1	2:C:377:ILE:HG23	1.69	0.58
2:D:345:LYS:NZ	2:D:366:GLU:HG2	2.18	0.58
1:E:191:ILE:HG22	1:E:192:ALA:N	2.19	0.58
1:E:342:ASN:O	1:E:343:LEU:HD23	2.04	0.58
1:A:423:HIS:O	2:F:418:GLN:HB2	2.04	0.58
1:A:448:GLU:HG2	1:B:466:ALA:CA	2.31	0.58
2:F:464:ASP:OD2	2:F:466:ALA:HB3	2.03	0.58
2:C:296:LEU:HD13	2:C:331:TRP:CD2	2.39	0.57
2:C:393:ARG:O	2:C:397:ILE:HG12	2.03	0.57
2:D:182:THR:HG22	2:D:183:GLU:N	2.19	0.57
2:D:362:ILE:O	2:D:365:SER:HB3	2.03	0.57
1:A:359:HIS:O	1:A:363:ILE:HG13	2.04	0.57
1:B:184:ARG:HD2	1:B:191:ILE:O	2.04	0.57
1:B:194:TYR:O	1:B:195:GLY:C	2.41	0.57
1:B:449:MET:HE3	2:C:467:ILE:HD11	1.85	0.57
1:E:356:LEU:HD12	1:E:356:LEU:N	2.19	0.57
1:E:453:ILE:HG22	1:E:470:PHE:HD2	1.69	0.57
2:F:218:ARG:NH1	2:F:239:ILE:HD12	2.19	0.57
1:A:337:GLU:HG3	1:A:341:GLN:OE1	2.04	0.57
1:B:129:ARG:O	1:B:132:TYR:HB3	2.05	0.57
2:D:191:ILE:CG2	2:D:198:GLU:HG3	2.34	0.57
2:F:134:ILE:HD11	2:F:142:VAL:HG21	1.84	0.57
1:B:291:GLY:HA3	1:B:442:TYR:OH	2.05	0.57
2:C:248:PRO:O	2:C:250:GLY:N	2.37	0.57
1:E:262:ARG:HD2	1:E:276:GLY:O	2.03	0.57
1:E:344:LEU:HD22	1:E:345:LYS:N	2.19	0.57
1:E:445:ILE:O	1:E:446:ARG:HB2	2.05	0.57
2:C:63:GLY:HA3	2:C:141:ARG:CZ	2.34	0.57
2:C:317:TYR:CE2	2:C:383:LEU:HD21	2.39	0.57
2:D:443:VAL:HG12	2:D:445:ILE:HG12	1.86	0.57
1:E:266:GLY:HA2	1:E:304:ASN:HD22	1.70	0.57
1:E:268:VAL:O	1:E:271:ASP:HB2	2.05	0.57
1:B:300:ARG:CA	1:B:333:MET:HE1	2.34	0.57
2:C:451:ARG:HG2	2:C:451:ARG:NH1	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:117:VAL:HG13	2:F:154:TYR:OH	2.04	0.57
1:B:437:ILE:HD12	1:B:457:LYS:HG2	1.86	0.57
2:C:483:PHE:HB2	2:C:489:ILE:HD13	1.85	0.57
2:D:31:ILE:HA	2:D:231:MET:CG	2.34	0.57
2:D:178:THR:HG22	2:D:179:VAL:H	1.70	0.57
2:D:344:LEU:HD13	2:D:344:LEU:C	2.25	0.57
2:D:379:SER:OG	2:D:381:SER:OG	2.21	0.57
2:F:23:THR:O	2:F:24:MET:HB2	2.03	0.57
2:F:151:PHE:CZ	2:F:160:VAL:HG13	2.39	0.57
1:A:323:GLN:HE22	1:B:459:ARG:HD3	1.70	0.57
1:B:211:LEU:O	1:B:212:GLU:HB3	2.03	0.57
1:B:457:LYS:O	1:B:457:LYS:HG3	2.05	0.57
4:C:901:ATP:C2	2:D:462:TRP:HA	2.40	0.57
1:E:152:GLN:HG3	2:F:161:ARG:NH1	2.19	0.57
1:A:80:PRO:HB3	1:A:105:ILE:HG21	1.87	0.57
1:B:289:ALA:CB	1:B:419:PHE:HA	2.34	0.57
2:D:18:ILE:H	2:D:18:ILE:CD1	2.15	0.57
1:E:221:GLU:HG3	1:E:222:ILE:N	2.20	0.57
1:E:499:VAL:O	1:E:499:VAL:HG12	2.02	0.57
1:B:52:LYS:N	4:B:903:ATP:O1B	2.38	0.57
1:B:146:SER:H	1:B:181:THR:CB	2.14	0.57
1:B:294:LYS:N	4:B:901:ATP:O1B	2.33	0.57
2:D:214:GLU:CB	1:E:234:GLU:HB2	2.31	0.57
1:E:38:ILE:HA	1:E:177:THR:HG23	1.86	0.57
1:E:283:ILE:HD12	1:E:412:PHE:HE1	1.70	0.57
1:E:259:SER:N	1:E:281:ASP:OD2	2.38	0.56
1:A:130:ILE:O	1:A:134:ILE:HG13	2.05	0.56
1:A:296:LEU:HD13	1:A:331:TRP:CE2	2.40	0.56
2:C:21:MET:HB2	2:C:38:ILE:HG13	1.87	0.56
2:C:89:SER:HB2	2:D:227:GLY:O	2.05	0.56
2:C:446:ARG:HG2	2:C:496:ARG:CZ	2.35	0.56
2:D:484:ARG:CB	2:D:484:ARG:NH1	2.68	0.56
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.86	0.56
1:E:323:GLN:HE21	1:E:327:ASN:HD21	1.53	0.56
1:B:458:MET:SD	1:B:461:SER:HB3	2.46	0.56
1:E:283:ILE:HD12	1:E:412:PHE:CE1	2.40	0.56
1:E:431:ASP:O	1:E:434:THR:HG22	2.05	0.56
2:F:46:GLY:HA2	2:F:184:ARG:CD	2.35	0.56
2:F:356:LEU:HD11	2:F:387:VAL:HG21	1.87	0.56
2:C:38:ILE:HG23	2:C:177:THR:OG1	2.05	0.56
2:C:54:LEU:HD23	2:C:244:ILE:HG13	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.39	0.56
1:A:225:LEU:O	1:A:226:ARG:C	2.43	0.56
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.87	0.56
1:B:360:LEU:HD23	1:B:399:VAL:HG22	1.87	0.56
1:B:469:GLU:HG2	1:B:480:LYS:HE3	1.87	0.56
2:D:31:ILE:HG23	2:D:231:MET:HB2	1.87	0.56
1:A:161:ARG:HA	1:A:196:VAL:HG11	1.88	0.56
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.40	0.56
2:C:123:LEU:CD2	2:C:167:LEU:HB2	2.36	0.56
2:C:147:VAL:HG11	2:C:180:MET:HE2	1.88	0.56
2:D:211:LEU:O	2:D:215:ARG:O	2.23	0.56
2:D:220:LEU:HD23	2:D:221:GLU:N	2.21	0.56
1:E:362:ILE:O	1:E:365:SER:HB3	2.06	0.56
1:A:193:ARG:NH2	1:B:195:GLY:O	2.26	0.56
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.86	0.56
2:C:300:ARG:HA	2:C:333:MET:HE3	1.87	0.56
1:E:21:MET:HE2	1:E:177:THR:HG21	1.88	0.56
2:F:352:GLU:OE2	2:F:385:ARG:HD2	2.06	0.56
1:A:436:THR:CG2	1:A:458:MET:HG2	2.36	0.56
2:C:336:GLU:OE1	2:C:336:GLU:HA	2.05	0.56
1:E:268:VAL:O	1:E:271:ASP:N	2.38	0.56
1:E:449:MET:CE	2:F:467:ILE:HD11	2.36	0.56
2:F:54:LEU:HD21	2:F:243:GLY:HA2	1.88	0.56
2:F:439:LEU:HD12	2:F:440:LEU:N	2.21	0.56
2:F:514:GLU:O	2:F:515:LYS:CB	2.54	0.56
1:B:249:LEU:HD12	1:B:394:GLN:HG2	1.88	0.56
1:B:315:PHE:HB3	1:B:317:TYR:HE1	1.71	0.56
1:B:392:PHE:O	1:B:395:PHE:HB3	2.06	0.56
2:D:82:ASP:O	2:D:83:ILE:C	2.44	0.56
2:D:151:PHE:O	2:D:153:GLN:N	2.35	0.56
2:D:161:ARG:HB2	2:D:196:VAL:CG1	2.35	0.56
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.36	0.56
2:F:49:GLY:HA2	4:F:903:ATP:O2B	2.05	0.56
2:F:451:ARG:HG2	2:F:451:ARG:HH11	1.70	0.56
1:A:379:SER:HA	1:A:413:THR:O	2.06	0.55
2:C:70:PRO:HA	2:C:102:LYS:O	2.06	0.55
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.21	0.55
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.87	0.55
1:A:377:ILE:HD11	1:A:399:VAL:HG11	1.89	0.55
2:D:431:ASP:O	2:D:432:THR:HG23	2.06	0.55
2:D:436:THR:OG1	2:D:458:MET:HG2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HD21	1:A:412:PHE:HD2	1.72	0.55
1:A:344:LEU:HD13	1:A:344:LEU:C	2.27	0.55
1:B:440:LEU:N	1:B:440:LEU:HD23	2.22	0.55
2:C:248:PRO:C	2:C:250:GLY:H	2.10	0.55
2:C:425:ILE:CG2	2:C:431:ASP:HB3	2.37	0.55
1:E:126:LEU:O	1:E:130:ILE:HG13	2.07	0.55
1:B:196:VAL:O	1:B:200:VAL:HG23	2.06	0.55
2:C:146:SER:H	2:C:181:THR:HB	1.72	0.55
2:C:392:PHE:O	2:C:395:PHE:HB3	2.07	0.55
2:D:169:ALA:O	2:D:173:GLN:HG3	2.05	0.55
2:D:364:LYS:O	2:D:367:ILE:HB	2.05	0.55
2:F:261:VAL:HG12	2:F:262:ARG:N	2.22	0.55
1:A:161:ARG:HD2	1:A:196:VAL:HG13	1.89	0.55
1:A:184:ARG:C	1:A:185:ILE:HD13	2.27	0.55
1:A:382:ALA:O	1:A:385:ARG:HG3	2.07	0.55
1:B:433:ILE:O	1:B:433:ILE:HG22	2.07	0.55
2:C:425:ILE:HG21	2:C:431:ASP:HB3	1.89	0.55
2:C:446:ARG:HG2	2:C:496:ARG:NH2	2.21	0.55
2:D:256:GLN:OE1	2:D:256:GLN:N	2.40	0.55
1:E:504:GLU:HG2	1:E:505:LEU:N	2.22	0.55
2:F:207:LEU:HD21	2:F:220:LEU:HD12	1.88	0.55
1:A:146:SER:H	1:A:181:THR:HB	1.72	0.55
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.88	0.55
1:B:44:VAL:HG22	1:B:205:VAL:HB	1.89	0.55
1:B:269:ARG:O	1:B:273:MET:HG3	2.05	0.55
1:B:419:PHE:CD2	2:C:425:ILE:HD12	2.41	0.55
1:E:347:VAL:HG12	1:E:348:CYS:N	2.22	0.55
2:F:52:LYS:HB3	2:F:181:THR:OG1	2.07	0.55
2:F:94:LEU:O	2:F:98:VAL:HG23	2.07	0.55
2:F:192:ALA:HB3	2:F:197:GLU:OE2	2.07	0.55
2:F:274:CYS:HG	2:F:278:PHE:HE2	1.51	0.55
2:F:311:ARG:HG3	2:F:371:LYS:HZ1	1.70	0.55
2:F:501:GLU:CG	2:F:502:LYS:N	2.70	0.55
1:A:247:PHE:HD2	1:A:364:LYS:HZ2	1.55	0.55
1:A:431:ASP:N	1:A:431:ASP:OD1	2.39	0.55
1:B:117:VAL:O	1:B:117:VAL:HG12	2.07	0.55
1:B:155:ASP:OD1	1:B:159:VAL:HG11	2.07	0.55
1:B:191:ILE:HB	1:B:198:GLU:OE2	2.05	0.55
2:D:24:MET:HB2	2:D:62:ASN:HD22	1.72	0.55
2:D:350:TYR:CE1	1:E:254:LEU:HD13	2.42	0.55
1:A:446:ARG:HG2	1:A:496:ARG:NH1	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:SER:HB2	1:B:143:SER:HB3	1.88	0.55
2:C:44:VAL:HA	2:C:205:VAL:O	2.07	0.55
2:C:267:VAL:HB	2:C:270:LEU:HB2	1.88	0.55
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.87	0.55
2:F:455:VAL:HG11	2:F:463:HIS:HB2	1.88	0.55
1:B:192:ALA:O	1:B:194:TYR:N	2.40	0.55
1:B:441:GLN:HE22	1:B:490:ILE:HA	1.69	0.55
2:C:211:LEU:HA	2:C:216:ARG:HD3	1.89	0.55
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.37	0.55
1:E:255:THR:HG22	1:E:255:THR:O	2.06	0.55
1:A:312:ALA:HA	1:A:374:ARG:O	2.07	0.54
1:A:510:ARG:NE	1:A:510:ARG:HA	2.22	0.54
1:B:150:VAL:CG1	1:B:151:PHE:H	2.21	0.54
2:C:191:ILE:HB	2:C:198:GLU:CG	2.38	0.54
2:C:462:TRP:O	2:C:463:HIS:O	2.25	0.54
1:E:31:ILE:HG22	1:E:222:ILE:CD1	2.37	0.54
1:E:293:GLY:HA2	4:E:901:ATP:O1A	2.07	0.54
1:E:431:ASP:OD1	1:E:431:ASP:N	2.30	0.54
2:F:439:LEU:HD12	2:F:440:LEU:H	1.71	0.54
1:A:419:PHE:HD2	1:B:425:ILE:HD12	1.72	0.54
2:F:458:MET:SD	2:F:461:SER:HB3	2.47	0.54
2:F:471:MET:HE2	2:F:471:MET:O	2.07	0.54
1:A:289:ALA:HB2	1:A:419:PHE:HA	1.90	0.54
1:B:164:LEU:HB3	1:B:200:VAL:HG11	1.89	0.54
2:C:150:VAL:HG13	2:C:151:PHE:N	2.23	0.54
2:C:64:ILE:HD11	2:C:102:LYS:O	2.07	0.54
2:D:23:THR:C	2:D:25:ILE:H	2.10	0.54
2:D:182:THR:HG21	2:D:192:ALA:CB	2.30	0.54
2:C:163:GLU:OE2	2:C:163:GLU:HA	2.08	0.54
2:C:356:LEU:HD22	2:C:387:VAL:HG11	1.90	0.54
2:D:59:PHE:CE2	2:D:141:ARG:HB3	2.42	0.54
1:E:289:ALA:CB	1:E:419:PHE:HA	2.32	0.54
1:E:393:ARG:O	1:E:397:ILE:HG12	2.07	0.54
2:F:170:ARG:O	2:F:174:ILE:HG12	2.07	0.54
2:F:353:SER:O	2:F:354:ALA:HB2	2.07	0.54
1:A:137:TYR:O	1:A:138:ARG:HB2	2.07	0.54
1:A:161:ARG:CA	1:A:196:VAL:HG11	2.37	0.54
2:C:389:ASN:O	2:C:392:PHE:HB3	2.07	0.54
2:D:61:TYR:CZ	2:D:92:TRP:CD1	2.96	0.54
2:D:202:ASP:HA	2:D:226:ARG:HD2	1.90	0.54
1:B:255:THR:HG22	1:B:255:THR:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASP:OD1	1:B:336:GLU:HB2	2.07	0.54
1:B:380:LEU:O	1:B:383:LEU:HB2	2.08	0.54
2:C:80:PRO:HB2	2:C:81:GLN:NE2	2.22	0.54
2:D:313:ILE:CD1	2:D:372:PRO:HG2	2.36	0.54
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.35	0.54
2:D:358:ASP:O	2:D:362:ILE:HG12	2.08	0.54
2:D:431:ASP:C	2:D:432:THR:HG23	2.28	0.54
1:E:248:PRO:O	1:E:251:ALA:N	2.28	0.54
1:E:294:LYS:HG2	1:E:413:THR:HG23	1.89	0.54
1:A:21:MET:HE3	1:A:141:ARG:NE	2.23	0.54
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.90	0.54
2:C:123:LEU:HD12	2:C:163:GLU:OE2	2.08	0.54
1:E:377:ILE:HD12	1:E:412:PHE:HE2	1.71	0.54
1:A:65:ILE:O	1:A:65:ILE:HG22	2.06	0.54
1:B:150:VAL:CG1	1:B:151:PHE:N	2.70	0.54
1:B:249:LEU:CD1	1:B:394:GLN:HG2	2.37	0.54
2:C:295:THR:HB	4:C:901:ATP:PA	2.47	0.54
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.38	0.54
2:F:455:VAL:HB	5:F:525:HOH:O	2.08	0.54
1:A:318:GLU:OE2	1:B:432:TPO:CG2	2.53	0.53
1:A:406:GLU:O	1:A:407:GLU:HB2	2.07	0.53
1:B:68:ASP:O	1:B:70:PRO:HD3	2.08	0.53
1:B:148:THR:HA	1:B:151:PHE:CE1	2.42	0.53
2:C:464:ASP:OD1	2:C:465:LYS:N	2.41	0.53
2:F:269:ARG:HG2	2:F:479:ILE:CB	2.37	0.53
1:A:118:VAL:HG23	1:A:153:GLN:OE1	2.07	0.53
1:B:485:ASN:OD1	1:B:485:ASN:N	2.41	0.53
2:C:182:THR:HG22	2:C:183:GLU:H	1.71	0.53
2:C:313:ILE:HG12	2:C:345:LYS:CB	2.24	0.53
1:E:313:ILE:HG22	1:E:314:LEU:N	2.23	0.53
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.43	0.53
1:A:323:GLN:HG2	1:A:327:ASN:HD21	1.73	0.53
2:D:231:MET:CE	2:D:251:ALA:HB2	2.37	0.53
2:F:73:PHE:C	2:F:73:PHE:CD2	2.82	0.53
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.74	0.53
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.90	0.53
2:D:467:ILE:HG22	2:D:467:ILE:O	2.08	0.53
1:E:262:ARG:HH12	1:E:461:SER:HB2	1.73	0.53
2:F:262:ARG:HD2	2:F:277:GLY:O	2.08	0.53
1:A:21:MET:HE2	1:A:59:PHE:CZ	2.44	0.53
1:B:53:THR:HB	4:B:903:ATP:O1A	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:THR:O	2:C:24:MET:HB2	2.08	0.53
2:C:81:GLN:NE2	2:C:81:GLN:H	2.06	0.53
1:E:267:VAL:HG21	1:E:477:PRO:HG3	1.89	0.53
1:A:299:SER:O	1:A:333:MET:HE1	2.09	0.53
1:A:432:TPO:HG21	1:A:432:TPO:O1P	2.08	0.53
2:D:37:PRO:O	2:D:177:THR:HG23	2.08	0.53
2:D:144:ILE:HD12	2:D:180:MET:HG2	1.90	0.53
1:E:325:LEU:HD21	1:E:335:PHE:HB2	1.89	0.53
2:F:117:VAL:O	2:F:118:VAL:HB	2.07	0.53
2:F:298:VAL:HG22	2:F:411:LEU:CD2	2.39	0.53
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.90	0.53
1:A:488:ARG:HE	2:F:488:ARG:CZ	2.21	0.53
1:B:325:LEU:HD23	1:B:335:PHE:HB2	1.89	0.53
2:D:89:SER:CB	1:E:227:GLY:O	2.55	0.53
2:D:123:LEU:HD11	2:D:163:GLU:HB3	1.90	0.53
2:D:178:THR:HG22	2:D:179:VAL:N	2.23	0.53
2:D:301:PHE:CZ	2:D:374:ARG:HD3	2.44	0.53
1:E:67:PHE:HB2	1:E:69:GLU:HG3	1.90	0.53
1:E:151:PHE:C	1:E:153:GLN:H	2.12	0.53
1:E:363:ILE:O	1:E:367:ILE:HG13	2.09	0.53
1:E:451:ARG:HH12	1:E:472:ILE:CD1	2.21	0.53
1:B:283:ILE:HG22	1:B:434:THR:OG1	2.08	0.53
2:C:379:SER:HA	2:C:413:THR:O	2.09	0.53
2:D:79:THR:CG2	2:D:81:GLN:HG2	2.39	0.53
1:E:273:MET:O	1:E:463:HIS:HA	2.09	0.53
1:A:437:ILE:HD12	1:A:457:LYS:HG2	1.91	0.53
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.39	0.53
2:C:63:GLY:CA	2:C:141:ARG:NH1	2.72	0.53
2:C:161:ARG:HD2	2:C:196:VAL:HG13	1.91	0.53
2:D:273:MET:CE	2:D:468:ARG:HD2	2.39	0.53
2:D:457:LYS:HG3	2:D:457:LYS:O	2.07	0.53
1:E:313:ILE:CD1	1:E:372:PRO:HG2	2.39	0.53
2:F:106:LEU:C	2:F:106:LEU:HD12	2.30	0.53
2:F:298:VAL:HG22	2:F:411:LEU:HD23	1.91	0.53
1:A:430:ILE:O	1:A:432:TPO:N	2.42	0.53
1:B:146:SER:N	1:B:181:THR:HB	2.19	0.53
1:B:150:VAL:C	1:B:152:GLN:H	2.12	0.53
1:B:178:THR:HG22	1:B:179:VAL:H	1.74	0.53
1:B:208:ARG:O	1:B:218:ARG:HA	2.08	0.53
2:C:70:PRO:HG2	2:C:138:ARG:O	2.09	0.53
2:C:340:ARG:O	2:C:342:ASN:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:ARG:HH12	2:D:174:ILE:HD11	1.74	0.53
2:D:294:LYS:O	2:D:297:LEU:HB2	2.09	0.53
1:E:420:MET:CE	2:F:490:ILE:HG13	2.37	0.53
2:F:127:ILE:HD13	2:F:167:LEU:HD12	1.91	0.53
1:A:104:PHE:HD2	1:A:133:ALA:HB1	1.74	0.52
1:A:467:ILE:HD11	2:F:449:MET:CE	2.38	0.52
4:A:903:ATP:N1	1:B:229:SER:HB3	2.25	0.52
1:B:263:VAL:HG23	1:B:278:PHE:O	2.09	0.52
2:C:294:LYS:HG3	2:C:440:LEU:HD12	1.91	0.52
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.92	0.52
1:E:392:PHE:O	1:E:395:PHE:HB3	2.10	0.52
2:F:302:VAL:HG12	2:F:303:GLU:N	2.23	0.52
1:A:191:ILE:HB	1:A:198:GLU:HG3	1.90	0.52
1:B:130:ILE:O	1:B:134:ILE:HG13	2.10	0.52
2:C:461:SER:OG	2:C:462:TRP:N	2.42	0.52
1:E:49:GLY:O	1:E:218:ARG:NH2	2.43	0.52
4:A:903:ATP:O3'	1:B:224:LYS:HB2	2.10	0.52
1:B:184:ARG:HH22	1:B:187:GLU:C	2.13	0.52
1:B:347:VAL:O	1:B:348:CYS:HB2	2.10	0.52
1:B:384:ALA:HB2	1:B:392:PHE:CE1	2.44	0.52
2:C:38:ILE:H	2:C:38:ILE:HD12	1.75	0.52
2:C:63:GLY:HA3	2:C:141:ARG:NH1	2.25	0.52
1:B:79:THR:HG22	1:B:82:ASP:HB2	1.90	0.52
2:C:70:PRO:HD2	2:C:140:ARG:HG2	1.91	0.52
2:C:215:ARG:HA	2:C:215:ARG:HE	1.75	0.52
2:D:430:ILE:O	2:D:433:ILE:HD12	2.09	0.52
1:E:116:GLU:O	1:E:118:VAL:HG23	2.09	0.52
2:F:182:THR:CG2	2:F:183:GLU:N	2.73	0.52
2:F:381:SER:HB3	2:F:414:ASN:OD1	2.10	0.52
1:B:87:ALA:C	1:B:89:SER:H	2.13	0.52
2:D:221:GLU:HG2	2:D:222:ILE:N	2.23	0.52
2:F:344:LEU:HD11	2:F:346:ILE:CG1	2.38	0.52
1:A:63:GLY:HA3	1:A:141:ARG:HD2	1.91	0.52
1:B:36:LEU:HD12	1:B:59:PHE:CE1	2.45	0.52
2:C:371:LYS:O	2:C:371:LYS:CD	2.53	0.52
2:C:468:ARG:NH1	2:C:468:ARG:HG2	2.25	0.52
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.92	0.52
1:E:140:ARG:HH11	1:E:140:ARG:CB	2.22	0.52
1:E:294:LYS:N	4:E:901:ATP:O1B	2.41	0.52
1:E:497:ILE:HG22	1:E:498:THR:N	2.23	0.52
2:D:23:THR:HB	2:D:25:ILE:HD12	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:GLY:HA2	4:D:901:ATP:PA	2.49	0.52
1:E:31:ILE:HG22	1:E:222:ILE:HD12	1.91	0.52
2:F:151:PHE:C	2:F:153:GLN:H	2.13	0.52
2:F:396:VAL:HG11	2:F:430:ILE:CG2	2.40	0.52
1:A:44:VAL:HG22	1:A:205:VAL:HB	1.91	0.52
1:A:218:ARG:O	1:A:236:PRO:HA	2.10	0.52
2:C:142:VAL:O	2:C:178:THR:HA	2.09	0.52
2:C:317:TYR:CE1	2:C:377:ILE:HG23	2.45	0.52
2:D:338:MET:HB3	2:D:344:LEU:HB3	1.92	0.52
1:E:104:PHE:HE2	1:E:106:LEU:HB2	1.73	0.52
2:F:70:PRO:HG2	2:F:139:ALA:HA	1.92	0.52
2:F:224:LYS:HZ1	2:F:226:ARG:CZ	2.21	0.52
2:C:413:THR:O	2:C:413:THR:HG22	2.09	0.52
1:E:501:GLU:O	1:E:502:LYS:HG3	2.09	0.52
1:A:230:HIS:NE2	4:F:903:ATP:O2'	2.42	0.52
2:C:311:ARG:HA	2:C:343:LEU:O	2.09	0.52
1:E:378:ASP:O	1:E:379:SER:HB3	2.10	0.52
2:F:311:ARG:HG3	2:F:371:LYS:NZ	2.25	0.52
1:B:448:GLU:HG2	2:C:466:ALA:HA	1.93	0.51
1:E:280:LYS:HZ1	1:E:407:GLU:HB3	1.75	0.51
2:F:397:ILE:HD13	2:F:433:ILE:HG12	1.91	0.51
1:A:375:ILE:O	1:A:410:GLY:HA2	2.10	0.51
1:B:317:TYR:CE2	1:B:383:LEU:HD21	2.46	0.51
1:E:453:ILE:HG22	1:E:470:PHE:CD2	2.45	0.51
1:B:79:THR:HG23	1:B:82:ASP:H	1.75	0.51
1:B:184:ARG:C	1:B:185:ILE:HD13	2.30	0.51
2:C:79:THR:HG23	2:C:82:ASP:H	1.74	0.51
2:C:88:ARG:NE	2:D:15:HIS:HA	2.25	0.51
2:C:164:LEU:HB3	2:C:200:VAL:HG11	1.91	0.51
2:D:451:ARG:HG2	2:D:451:ARG:NH1	2.26	0.51
1:E:303:GLU:HB2	1:E:333:MET:CE	2.41	0.51
1:B:194:TYR:O	1:B:196:VAL:N	2.43	0.51
1:B:471:MET:HG2	1:B:480:LYS:HZ3	1.76	0.51
2:C:403:ALA:O	2:C:408:ILE:O	2.27	0.51
2:D:340:ARG:C	2:D:342:ASN:N	2.64	0.51
1:E:230:HIS:HD1	1:E:230:HIS:C	2.14	0.51
1:E:263:VAL:HG12	1:E:374:ARG:NH2	2.13	0.51
1:E:264:SER:H	1:E:374:ARG:HH22	1.56	0.51
2:F:164:LEU:O	2:F:165:PHE:C	2.47	0.51
1:A:28:PHE:HB2	1:A:246:ILE:CD1	2.41	0.51
1:A:60:LEU:HD12	1:A:73:PHE:HD1	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:LEU:O	2:C:129:ARG:N	2.43	0.51
2:C:340:ARG:C	2:C:342:ASN:H	2.13	0.51
2:D:248:PRO:HB2	2:D:251:ALA:CB	2.33	0.51
2:F:508:ILE:HG22	2:F:508:ILE:O	2.11	0.51
2:C:21:MET:HE1	2:C:141:ARG:HG2	1.93	0.51
2:D:325:LEU:CD2	2:D:335:PHE:HB2	2.41	0.51
1:E:345:LYS:HE2	1:E:366:GLU:OE1	2.10	0.51
2:F:208:ARG:O	2:F:218:ARG:HA	2.11	0.51
2:F:321:ARG:HG2	2:F:348:CYS:SG	2.51	0.51
1:A:321:ARG:O	1:A:325:LEU:HD12	2.11	0.51
1:A:371:LYS:O	1:A:371:LYS:HD2	2.11	0.51
2:C:468:ARG:HG2	2:C:468:ARG:HH11	1.76	0.51
4:E:903:ATP:O3'	2:F:224:LYS:HB2	2.10	0.51
2:F:31:ILE:HD11	2:F:246:ILE:HG21	1.93	0.51
2:F:504:GLU:HA	2:F:507:ARG:HE	1.76	0.51
2:C:20:LYS:HE3	2:C:228:THR:HG21	1.92	0.51
1:E:397:ILE:CD1	1:E:433:ILE:HG12	2.41	0.51
2:F:218:ARG:HG3	2:F:237:PHE:O	2.09	0.51
1:A:117:VAL:HG22	1:A:154:TYR:OH	2.10	0.51
2:C:19:ALA:O	2:C:38:ILE:HD12	2.10	0.51
2:D:67:PHE:HB2	2:D:69:GLU:HG3	1.93	0.51
2:D:323:GLN:HE21	2:D:327:ASN:HD21	1.58	0.51
1:E:153:GLN:C	2:F:158:SER:HB2	2.32	0.51
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.24	0.51
2:F:451:ARG:HB3	2:F:470:PHE:CZ	2.45	0.51
1:A:220:LEU:HD23	1:A:220:LEU:C	2.31	0.51
1:A:433:ILE:O	1:A:433:ILE:CG2	2.56	0.51
1:B:161:ARG:HH22	1:B:199:PHE:HB2	1.74	0.51
2:D:167:LEU:O	2:D:170:ARG:N	2.44	0.51
2:D:381:SER:HB3	2:D:414:ASN:OD1	2.11	0.51
1:A:18:ILE:HG22	1:A:19:ALA:N	2.25	0.50
2:C:25:ILE:HG12	2:C:58:GLN:HE21	1.76	0.50
2:C:111:ASP:O	2:C:113:GLU:N	2.37	0.50
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.41	0.50
1:E:146:SER:H	1:E:181:THR:HB	1.77	0.50
1:E:359:HIS:O	1:E:363:ILE:HG13	2.12	0.50
2:F:184:ARG:HG2	2:F:191:ILE:O	2.12	0.50
2:F:514:GLU:CD	2:F:515:LYS:H	2.14	0.50
1:A:397:ILE:HD11	2:F:385:ARG:HH12	1.75	0.50
2:C:18:ILE:HB	2:C:228:THR:HG23	1.92	0.50
2:C:178:THR:HG22	2:C:179:VAL:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:247:PHE:HD2	2:C:364:LYS:HZ2	1.59	0.50
2:D:311:ARG:CD	2:D:371:LYS:HE3	2.39	0.50
2:F:60:LEU:HD12	2:F:73:PHE:HB2	1.94	0.50
1:A:344:LEU:HD11	1:A:346:ILE:CG1	2.41	0.50
1:A:396:VAL:HG11	1:A:430:ILE:HG23	1.94	0.50
1:A:397:ILE:HD11	2:F:385:ARG:NH1	2.26	0.50
2:F:21:MET:N	2:F:38:ILE:HD11	2.26	0.50
2:F:344:LEU:CD1	2:F:346:ILE:HG13	2.40	0.50
2:F:500:ASP:CG	2:F:501:GLU:H	2.14	0.50
2:D:122:ASP:O	2:D:123:LEU:C	2.49	0.50
2:D:212:GLU:O	2:D:212:GLU:CG	2.55	0.50
1:E:355:GLY:O	1:E:358:ASP:HB2	2.12	0.50
2:C:49:GLY:O	2:C:218:ARG:NH2	2.43	0.50
2:D:437:ILE:CD1	2:D:457:LYS:HE2	2.41	0.50
1:E:312:ALA:HA	1:E:374:ARG:O	2.11	0.50
2:F:150:VAL:HG13	2:F:151:PHE:N	2.26	0.50
1:A:323:GLN:O	1:A:327:ASN:ND2	2.44	0.50
1:B:144:ILE:HG22	1:B:147:VAL:HG12	1.94	0.50
2:D:269:ARG:HB3	2:D:479:ILE:HD12	1.93	0.50
2:D:304:ASN:HB3	2:D:374:ARG:NH1	2.25	0.50
2:D:441:GLN:HE22	2:D:490:ILE:HD12	1.76	0.50
2:C:185:ILE:HA	5:D:528:HOH:O	2.12	0.50
1:E:281:ASP:O	1:E:282:SER:HB3	2.11	0.50
1:E:451:ARG:HH11	1:E:451:ARG:CG	2.23	0.50
1:B:18:ILE:HB	1:B:228:THR:HG23	1.94	0.50
2:C:126:LEU:O	2:C:129:ARG:HB2	2.12	0.50
2:D:225:LEU:HB2	2:D:230:HIS:HD2	1.77	0.50
2:D:295:THR:HG23	2:D:378:ASP:OD2	2.11	0.50
1:E:67:PHE:CB	1:E:69:GLU:HG3	2.42	0.50
1:E:237:PHE:HB3	1:E:246:ILE:HG12	1.93	0.50
1:A:79:THR:HG22	1:A:82:ASP:H	1.76	0.49
1:A:191:ILE:HB	1:A:198:GLU:CD	2.32	0.49
1:A:344:LEU:HD22	1:A:345:LYS:N	2.27	0.49
1:B:425:ILE:HD12	1:B:425:ILE:H	1.76	0.49
1:E:270:LEU:HD11	1:E:438:ILE:HD12	1.94	0.49
1:E:504:GLU:CG	1:E:505:LEU:H	2.25	0.49
1:B:340:ARG:C	1:B:342:ASN:H	2.15	0.49
2:D:495:THR:HA	1:E:487:GLU:CD	2.32	0.49
2:F:505:LEU:O	2:F:506:SER:CB	2.59	0.49
1:A:21:MET:HE2	1:A:59:PHE:HZ	1.78	0.49
1:B:232:LYS:N	1:B:232:LYS:HD2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:THR:HB	2:C:207:LEU:HB3	1.94	0.49
2:C:140:ARG:HH11	2:C:140:ARG:CB	2.23	0.49
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.77	0.49
2:D:193:ARG:NH2	1:E:195:GLY:O	2.45	0.49
1:E:170:ARG:HD2	1:E:173:GLN:OE1	2.12	0.49
1:E:264:SER:N	1:E:374:ARG:HH22	2.09	0.49
1:E:379:SER:H	1:E:413:THR:HB	1.77	0.49
2:F:122:ASP:OD2	2:F:123:LEU:N	2.45	0.49
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.93	0.49
1:A:344:LEU:HD22	1:A:345:LYS:H	1.75	0.49
1:B:18:ILE:HB	1:B:228:THR:CG2	2.42	0.49
1:B:145:ASP:HA	1:B:181:THR:HB	1.94	0.49
1:B:185:ILE:HD13	1:B:185:ILE:N	2.26	0.49
2:C:164:LEU:CD1	2:C:197:GLU:HG3	2.40	0.49
2:C:389:ASN:HD21	2:C:428:SER:CA	2.25	0.49
2:D:61:TYR:HH	2:D:92:TRP:HD1	1.52	0.49
2:D:418:GLN:HE21	2:D:422:ALA:HA	1.77	0.49
2:D:486:PHE:HE2	2:D:496:ARG:HD3	1.73	0.49
1:E:364:LYS:HE2	1:E:402:TYR:CD1	2.47	0.49
2:F:515:LYS:C	2:F:517:PRO:HD2	2.32	0.49
1:A:18:ILE:H	1:A:18:ILE:CD1	2.23	0.49
1:A:395:PHE:CE2	1:A:399:VAL:HG21	2.47	0.49
1:B:148:THR:HA	1:B:151:PHE:HE1	1.78	0.49
1:B:240:THR:OG1	1:B:241:ASP:N	2.46	0.49
2:C:63:GLY:CA	2:C:141:ARG:CZ	2.90	0.49
2:C:220:LEU:HD23	2:C:220:LEU:C	2.33	0.49
2:C:332:GLY:C	2:C:333:MET:HG2	2.32	0.49
2:D:191:ILE:HG21	2:D:198:GLU:HG3	1.94	0.49
2:D:445:ILE:HA	2:D:496:ARG:HH12	1.77	0.49
1:E:281:ASP:OD1	1:E:407:GLU:OE1	2.30	0.49
1:E:295:THR:O	1:E:298:VAL:HB	2.12	0.49
1:E:443:VAL:HG12	1:E:445:ILE:HG12	1.93	0.49
2:F:286:ALA:HA	2:F:438:ILE:O	2.12	0.49
1:A:363:ILE:HG22	1:A:367:ILE:HD11	1.94	0.49
2:D:314:LEU:O	2:D:314:LEU:CG	2.60	0.49
2:D:451:ARG:NH1	2:D:472:ILE:CD1	2.75	0.49
1:E:451:ARG:HD2	1:E:451:ARG:H	1.78	0.49
2:F:187:GLU:OE2	2:F:208:ARG:HA	2.12	0.49
2:F:312:ALA:HB2	2:F:374:ARG:HB2	1.93	0.49
1:B:221:GLU:HG3	1:B:233:GLY:O	2.12	0.49
2:D:458:MET:HB2	2:D:463:HIS:HD2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:248:PRO:CB	2:F:251:ALA:HB3	2.43	0.49
2:F:489:ILE:HA	2:F:494:PRO:HG3	1.95	0.49
2:C:44:VAL:O	2:C:44:VAL:HG12	2.13	0.49
2:C:116:GLU:O	2:C:117:VAL:HB	2.13	0.49
2:C:381:SER:O	2:C:384:ALA:HB3	2.12	0.49
1:A:437:ILE:HD11	1:A:457:LYS:HE2	1.93	0.49
1:B:45:SER:HB3	1:B:182:THR:CB	2.41	0.49
1:B:212:GLU:O	1:B:212:GLU:CG	2.57	0.49
2:D:148:THR:OG1	2:D:182:THR:HG23	2.13	0.49
2:D:268:VAL:O	2:D:269:ARG:C	2.51	0.49
2:D:451:ARG:NH1	2:D:472:ILE:HD11	2.28	0.49
1:E:81:GLN:H	1:E:81:GLN:CD	2.11	0.49
1:E:121:PHE:CD1	1:E:121:PHE:N	2.80	0.49
1:E:311:ARG:HD3	1:E:370:PHE:CE1	2.48	0.49
1:E:469:GLU:CB	1:E:483:PHE:CZ	2.95	0.49
1:A:150:VAL:HG13	1:A:151:PHE:N	2.28	0.49
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.43	0.49
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.76	0.49
2:C:315:PHE:HE2	2:C:363:ILE:HA	1.75	0.49
2:D:147:VAL:CG2	2:D:148:THR:N	2.75	0.49
1:E:318:GLU:OE2	2:F:432:THR:HB	2.13	0.49
1:E:504:GLU:HG2	1:E:505:LEU:H	1.76	0.49
2:F:500:ASP:O	2:F:501:GLU:CB	2.60	0.49
2:F:515:LYS:CG	2:F:517:PRO:HD2	2.43	0.49
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.94	0.48
1:A:461:SER:OG	1:A:462:TRP:N	2.46	0.48
1:B:144:ILE:CG2	1:B:147:VAL:HG12	2.43	0.48
1:B:283:ILE:HD12	1:B:412:PHE:CE1	2.43	0.48
1:B:316:ALA:O	1:B:348:CYS:HA	2.12	0.48
2:D:287:THR:HG22	2:D:288:GLY:N	2.27	0.48
1:E:355:GLY:H	1:E:358:ASP:HB2	1.78	0.48
2:F:316:ALA:O	2:F:348:CYS:HA	2.12	0.48
1:A:227:GLY:O	2:F:89:SER:CB	2.61	0.48
1:B:496:ARG:CG	1:B:498:THR:HG23	2.29	0.48
2:D:305:ALA:HB2	2:D:374:ARG:CD	2.43	0.48
4:E:903:ATP:O3G	2:F:224:LYS:NZ	2.41	0.48
1:A:211:LEU:HD13	1:A:216:ARG:HE	1.75	0.48
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.26	0.48
1:A:311:ARG:HD2	1:A:371:LYS:NZ	2.28	0.48
1:A:313:ILE:CD1	1:A:372:PRO:HG2	2.42	0.48
1:B:72:VAL:HB	1:B:142:VAL:HG13	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:THR:HG23	1:E:414:ASN:HB3	1.95	0.48
2:F:16:GLN:NE2	2:F:33:HIS:HB3	2.27	0.48
2:F:23:THR:HB	2:F:25:ILE:HG13	1.94	0.48
2:F:269:ARG:HG2	2:F:479:ILE:CG2	2.44	0.48
1:A:294:LYS:HD3	1:A:294:LYS:H	1.76	0.48
2:D:23:THR:HB	2:D:25:ILE:CD1	2.44	0.48
2:D:289:ALA:O	2:D:292:THR:OG1	2.31	0.48
2:D:332:GLY:O	2:D:333:MET:O	2.31	0.48
1:E:325:LEU:HD21	1:E:335:PHE:CB	2.43	0.48
2:F:129:ARG:O	2:F:132:TYR:HB3	2.13	0.48
1:A:83:ILE:HD12	1:A:83:ILE:N	2.25	0.48
2:C:360:LEU:CD2	2:C:364:LYS:HE3	2.43	0.48
2:D:43:LEU:HD11	2:D:182:THR:OG1	2.12	0.48
1:E:47:THR:HG22	1:E:184:ARG:O	2.14	0.48
1:A:178:THR:CG2	1:A:179:VAL:H	2.26	0.48
1:A:220:LEU:N	1:A:235:TYR:O	2.43	0.48
1:B:90:PHE:HB2	1:B:92:TRP:CD2	2.48	0.48
2:C:164:LEU:HD11	2:C:197:GLU:CG	2.39	0.48
2:C:273:MET:CE	2:C:468:ARG:HD2	2.43	0.48
2:D:400:THR:HG22	2:D:401:GLY:N	2.28	0.48
1:B:461:SER:OG	1:B:462:TRP:N	2.47	0.48
1:E:46:GLY:HA2	1:E:184:ARG:HD3	1.96	0.48
1:E:313:ILE:HG13	1:E:372:PRO:HG2	1.95	0.48
1:A:202:ASP:HA	1:A:226:ARG:HD2	1.96	0.48
1:A:392:PHE:O	1:A:395:PHE:N	2.46	0.48
1:A:488:ARG:HE	2:F:488:ARG:NH2	2.11	0.48
1:B:178:THR:CG2	1:B:179:VAL:N	2.77	0.48
2:C:347:VAL:HG12	2:C:348:CYS:N	2.28	0.48
2:C:426:THR:HG22	2:C:427:ASP:N	2.29	0.48
2:D:311:ARG:HD3	2:D:370:PHE:CE1	2.48	0.48
2:D:334:ASP:OD1	2:D:336:GLU:N	2.46	0.48
2:D:340:ARG:O	2:D:342:ASN:N	2.46	0.48
2:F:73:PHE:HE2	2:F:75:THR:HB	1.79	0.48
2:F:244:ILE:HG22	2:F:245:ASN:N	2.28	0.48
1:A:436:THR:HG23	1:A:458:MET:CG	2.42	0.48
1:B:24:MET:CB	1:B:62:ASN:HD22	2.27	0.48
1:B:52:LYS:HB2	4:B:903:ATP:O1B	2.14	0.48
1:B:426:THR:HG22	1:B:428:SER:H	1.79	0.48
1:B:499:VAL:O	1:B:501:GLU:N	2.44	0.48
2:C:118:VAL:O	2:C:118:VAL:HG12	2.14	0.48
2:D:79:THR:HG23	2:D:81:GLN:HG2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:ARG:O	2:D:218:ARG:HA	2.14	0.48
2:D:379:SER:N	2:D:413:THR:HB	2.20	0.48
2:D:420:MET:HE2	2:D:492:GLY:HA3	1.95	0.48
1:E:256:GLN:HG3	1:E:404:LYS:HD3	1.96	0.48
1:E:291:GLY:HA3	1:E:442:TYR:OH	2.13	0.48
2:F:104:PHE:HE2	2:F:106:LEU:HB2	1.79	0.48
2:F:356:LEU:CD1	2:F:387:VAL:HG21	2.43	0.48
1:A:166:ARG:HG3	2:F:112:PRO:O	2.14	0.48
1:A:265:SER:O	1:A:300:ARG:O	2.32	0.48
1:A:315:PHE:HB3	1:A:317:TYR:HE1	1.78	0.48
1:A:470:PHE:CD1	1:A:470:PHE:C	2.87	0.48
1:B:194:TYR:O	1:B:196:VAL:HG23	2.13	0.48
1:B:492:GLY:C	1:B:494:PRO:HD3	2.32	0.48
2:C:64:ILE:CD1	2:C:103:LEU:HB2	2.42	0.48
2:C:82:ASP:O	2:C:83:ILE:C	2.52	0.48
2:C:232:LYS:HD2	2:C:232:LYS:N	2.27	0.48
2:C:353:SER:O	2:C:354:ALA:CB	2.61	0.48
1:E:79:THR:HG22	1:E:82:ASP:CG	2.34	0.48
2:F:142:VAL:HG12	2:F:178:THR:HG23	1.94	0.48
1:A:134:ILE:HG23	1:A:139:ALA:HB3	1.96	0.47
1:A:340:ARG:C	1:A:342:ASN:H	2.18	0.47
1:B:214:GLU:OE2	2:C:217:ARG:NH1	2.46	0.47
1:B:317:TYR:CD2	1:B:383:LEU:HD21	2.49	0.47
2:C:97:LEU:N	2:C:97:LEU:HD23	2.27	0.47
2:C:335:PHE:O	2:C:339:GLU:HG3	2.14	0.47
2:C:439:LEU:HG	2:C:439:LEU:O	2.13	0.47
2:D:430:ILE:C	2:D:431:ASP:O	2.52	0.47
1:E:38:ILE:HA	1:E:177:THR:CG2	2.44	0.47
2:F:79:THR:HG22	2:F:82:ASP:OD2	2.14	0.47
2:F:263:VAL:HG12	2:F:374:ARG:NH2	2.09	0.47
2:F:315:PHE:HE1	2:F:375:ILE:HD11	1.79	0.47
1:A:89:SER:HB2	1:B:227:GLY:O	2.14	0.47
1:A:296:LEU:HD21	1:A:477:PRO:HD3	1.96	0.47
1:B:295:THR:HG21	1:B:319:GLU:OE2	2.13	0.47
1:B:487:GLU:O	1:B:488:ARG:HB2	2.14	0.47
2:C:54:LEU:O	2:C:57:ILE:N	2.47	0.47
2:C:347:VAL:O	2:C:348:CYS:CB	2.58	0.47
2:D:42:THR:HA	2:D:203:ASN:HB2	1.96	0.47
2:D:60:LEU:O	2:D:63:GLY:N	2.47	0.47
2:D:76:PHE:HZ	2:D:126:LEU:CD2	2.27	0.47
2:D:471:MET:CG	2:D:478:ASP:HB3	2.42	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:505:LEU:O	2:F:506:SER:HB3	2.13	0.47
1:A:261:VAL:O	1:A:279:PHE:HA	2.14	0.47
2:D:412:PHE:N	2:D:412:PHE:CD1	2.83	0.47
2:F:44:VAL:O	2:F:181:THR:HA	2.14	0.47
2:F:298:VAL:HA	2:F:411:LEU:HD23	1.94	0.47
1:A:393:ARG:O	1:A:397:ILE:HG12	2.15	0.47
1:A:435:ASP:OD1	2:F:323:GLN:NE2	2.47	0.47
1:B:287:THR:HG23	1:B:414:ASN:ND2	2.21	0.47
2:C:430:ILE:HG23	2:C:433:ILE:HD11	1.96	0.47
2:D:263:VAL:N	2:D:278:PHE:O	2.47	0.47
1:E:14:GLU:CG	1:E:16:GLN:HB2	2.45	0.47
2:C:21:MET:HE1	2:C:141:ARG:NE	2.30	0.47
2:C:151:PHE:C	2:C:153:GLN:H	2.18	0.47
2:C:441:GLN:HE22	2:C:490:ILE:HD13	1.80	0.47
2:D:431:ASP:C	2:D:433:ILE:H	2.17	0.47
1:E:357:GLU:HG3	1:E:358:ASP:N	2.29	0.47
1:A:447:GLY:HA2	1:B:489:ILE:HD12	1.97	0.47
1:B:220:LEU:HD13	1:B:246:ILE:HD11	1.95	0.47
1:B:294:LYS:O	1:B:296:LEU:N	2.47	0.47
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.48	0.47
2:C:179:VAL:O	2:C:179:VAL:HG12	2.13	0.47
2:C:293:GLY:HA2	4:C:901:ATP:O1A	2.13	0.47
2:C:387:VAL:CG1	2:C:391:ALA:HB3	2.44	0.47
2:C:440:LEU:HD22	2:C:470:PHE:CZ	2.49	0.47
2:D:291:GLY:C	2:D:442:TYR:OH	2.53	0.47
2:D:406:GLU:HB3	2:D:408:ILE:HD12	1.97	0.47
2:D:437:ILE:HD11	2:D:457:LYS:HE2	1.97	0.47
1:E:300:ARG:HA	1:E:333:MET:HE1	1.95	0.47
2:F:211:LEU:HD12	2:F:215:ARG:O	2.15	0.47
1:A:80:PRO:HD2	1:A:81:GLN:HE21	1.79	0.47
1:A:419:PHE:O	1:A:420:MET:O	2.32	0.47
1:B:22:ARG:O	1:B:141:ARG:NH2	2.47	0.47
1:B:60:LEU:HA	5:B:521:HOH:O	2.15	0.47
1:B:86:ASN:O	1:B:88:ARG:N	2.47	0.47
4:B:901:ATP:H3'	2:C:458:MET:O	2.15	0.47
2:C:52:LYS:N	4:C:903:ATP:O1B	2.48	0.47
2:C:300:ARG:HA	2:C:333:MET:CE	2.44	0.47
2:C:311:ARG:HD2	2:C:371:LYS:NZ	2.29	0.47
2:D:219:THR:HG22	2:D:236:PRO:HA	1.97	0.47
2:D:287:THR:HG23	2:D:414:ASN:ND2	2.26	0.47
1:E:79:THR:CG2	1:E:82:ASP:H	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:GLU:HB3	1:E:483:PHE:CE1	2.49	0.47
1:A:27:GLY:O	1:A:30:ASP:N	2.42	0.47
1:A:142:VAL:HG12	1:A:143:SER:N	2.29	0.47
1:A:316:ALA:CB	1:A:324:LEU:HD11	2.45	0.47
2:C:121:PHE:HD1	2:C:121:PHE:H	1.62	0.47
2:C:453:ILE:HG12	2:C:454:ASN:N	2.30	0.47
2:D:371:LYS:O	2:D:371:LYS:CD	2.52	0.47
2:D:446:ARG:H	2:D:496:ARG:HH12	1.63	0.47
1:E:353:SER:O	1:E:354:ALA:CB	2.63	0.47
2:F:387:VAL:HG12	2:F:388:SER:N	2.29	0.47
1:A:60:LEU:CD1	1:A:73:PHE:HD1	2.28	0.47
1:A:324:LEU:O	1:A:328:ALA:HB2	2.15	0.47
1:A:371:LYS:O	1:A:371:LYS:CD	2.62	0.47
1:B:483:PHE:O	1:B:485:ASN:N	2.48	0.47
2:D:44:VAL:HA	2:D:205:VAL:O	2.13	0.47
2:F:19:ALA:O	2:F:38:ILE:HD13	2.14	0.47
2:F:220:LEU:HD23	2:F:220:LEU:C	2.35	0.47
2:F:269:ARG:O	2:F:273:MET:HG3	2.15	0.47
1:A:79:THR:O	1:A:82:ASP:N	2.48	0.47
1:A:245:ASN:ND2	1:A:247:PHE:CZ	2.82	0.47
1:A:371:LYS:HD2	1:A:371:LYS:C	2.35	0.47
1:A:455:VAL:O	1:A:463:HIS:CE1	2.68	0.47
1:B:273:MET:CE	1:B:468:ARG:HD2	2.45	0.47
1:B:340:ARG:O	1:B:342:ASN:N	2.48	0.47
2:D:261:VAL:HG12	2:D:262:ARG:N	2.30	0.47
1:E:123:LEU:HD13	1:E:163:GLU:OE2	2.14	0.47
2:F:14:GLU:HG3	2:F:16:GLN:HG3	1.97	0.47
2:F:144:ILE:HD13	2:F:167:LEU:HD21	1.97	0.47
2:F:154:TYR:O	2:F:154:TYR:HD1	1.98	0.47
2:F:313:ILE:HG13	2:F:372:PRO:CG	2.45	0.47
1:A:452:ALA:HA	1:A:468:ARG:O	2.14	0.46
2:C:287:THR:HG22	2:C:288:GLY:H	1.78	0.46
1:E:433:ILE:O	1:E:433:ILE:CG2	2.62	0.46
2:F:396:VAL:HG11	2:F:430:ILE:HG21	1.96	0.46
1:A:161:ARG:NH2	2:F:149:SER:HB3	2.30	0.46
1:A:440:LEU:CD2	1:A:453:ILE:HG13	2.44	0.46
1:B:121:PHE:H	1:B:121:PHE:HD1	1.62	0.46
1:B:294:LYS:HD3	4:B:901:ATP:O1B	2.16	0.46
2:C:340:ARG:C	2:C:342:ASN:N	2.67	0.46
1:E:299:SER:O	1:E:333:MET:HE1	2.15	0.46
2:F:194:TYR:N	2:F:194:TYR:CD1	2.83	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.97	0.46
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.31	0.46
1:B:186:GLU:OE2	1:B:187:GLU:N	2.49	0.46
1:B:421:GLY:O	1:B:422:ALA:C	2.53	0.46
2:C:106:LEU:HD23	2:C:130:ILE:HG12	1.97	0.46
2:D:296:LEU:HA	2:D:331:TRP:CZ3	2.50	0.46
2:D:332:GLY:C	2:D:333:MET:HG2	2.34	0.46
2:F:270:LEU:O	2:F:273:MET:HB2	2.16	0.46
1:B:214:GLU:HA	2:C:234:GLU:HB2	1.98	0.46
2:C:38:ILE:CG2	2:C:39:GLY:N	2.78	0.46
2:C:287:THR:CG2	2:C:414:ASN:HD22	2.18	0.46
2:D:294:LYS:HE3	2:D:414:ASN:O	2.16	0.46
1:E:52:LYS:HD2	1:E:181:THR:HG23	1.97	0.46
1:E:442:TYR:CE1	2:F:456:PHE:CZ	3.03	0.46
2:F:123:LEU:O	2:F:123:LEU:HD13	2.14	0.46
1:A:195:GLY:O	2:F:193:ARG:NH2	2.43	0.46
1:A:441:GLN:HB2	5:A:522:HOH:O	2.15	0.46
1:B:64:ILE:HD11	1:B:102:LYS:O	2.16	0.46
2:D:88:ARG:NE	1:E:15:HIS:HA	2.30	0.46
2:D:338:MET:HB3	2:D:344:LEU:CB	2.46	0.46
1:E:191:ILE:HG13	1:E:206:ILE:HD11	1.96	0.46
1:E:248:PRO:O	1:E:250:GLY:N	2.48	0.46
2:F:306:CYS:SG	2:F:344:LEU:HB2	2.56	0.46
2:F:340:ARG:C	2:F:342:ASN:H	2.19	0.46
1:A:178:THR:HG22	1:A:179:VAL:H	1.81	0.46
1:A:259:SER:O	2:F:326:ARG:HD3	2.15	0.46
1:A:433:ILE:HD12	1:A:433:ILE:N	2.30	0.46
1:A:488:ARG:O	1:A:494:PRO:HA	2.15	0.46
1:A:499:VAL:O	1:A:500:ASP:HB2	2.16	0.46
2:C:51:GLY:O	2:C:52:LYS:C	2.53	0.46
2:D:163:GLU:HA	2:D:163:GLU:OE2	2.16	0.46
2:D:305:ALA:O	2:D:310:GLU:O	2.34	0.46
2:F:268:VAL:O	2:F:269:ARG:C	2.54	0.46
2:F:280:LYS:HZ3	2:F:407:GLU:HB3	1.81	0.46
2:F:312:ALA:HA	2:F:374:ARG:O	2.16	0.46
1:A:298:VAL:CG2	1:A:411:LEU:HD23	2.42	0.46
1:B:76:PHE:HZ	1:B:126:LEU:HD21	1.78	0.46
1:B:379:SER:OG	1:B:382:ALA:CB	2.57	0.46
2:C:42:THR:HA	2:C:203:ASN:HB2	1.97	0.46
2:C:214:GLU:C	2:C:215:ARG:HE	2.19	0.46
2:D:380:LEU:N	2:D:413:THR:O	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:385:ARG:HA	1:E:393:ARG:HH12	1.81	0.46
1:E:14:GLU:HG3	1:E:16:GLN:N	2.28	0.46
1:E:157:SER:O	1:E:160:VAL:HB	2.16	0.46
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.43	0.46
1:E:484:ARG:HG2	1:E:484:ARG:O	2.15	0.46
2:F:270:LEU:O	2:F:273:MET:N	2.49	0.46
1:B:51:GLY:O	1:B:54:LEU:HB3	2.16	0.46
1:B:220:LEU:HD13	1:B:246:ILE:CD1	2.46	0.46
2:C:367:ILE:CD1	2:C:375:ILE:CD1	2.94	0.46
2:C:440:LEU:HA	2:C:452:ALA:O	2.15	0.46
2:D:363:ILE:O	2:D:364:LYS:C	2.55	0.46
1:E:118:VAL:O	1:E:118:VAL:HG12	2.16	0.46
1:E:164:LEU:O	1:E:167:LEU:N	2.49	0.46
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.98	0.46
2:F:269:ARG:O	2:F:272:GLU:HB2	2.16	0.46
2:F:357:GLU:HG3	2:F:358:ASP:N	2.30	0.46
1:A:72:VAL:HG23	1:A:139:ALA:CB	2.46	0.46
1:A:466:ALA:HA	2:F:448:GLU:HG2	1.98	0.46
1:B:21:MET:HB2	1:B:38:ILE:HG12	1.97	0.46
1:B:23:THR:HB	1:B:25:ILE:HG13	1.96	0.46
1:B:60:LEU:O	1:B:61:TYR:C	2.54	0.46
2:C:274:CYS:HG	2:C:278:PHE:HE2	1.64	0.46
2:C:443:VAL:HG12	2:C:445:ILE:HG12	1.98	0.46
2:D:151:PHE:C	2:D:153:GLN:N	2.69	0.46
2:D:419:PHE:O	2:D:420:MET:O	2.34	0.46
1:E:311:ARG:HD2	1:E:371:LYS:HE3	1.97	0.46
1:E:444:GLU:OE1	2:F:490:ILE:HG12	2.15	0.46
2:F:131:ASN:OD1	2:F:174:ILE:HD12	2.16	0.46
2:F:191:ILE:CB	2:F:198:GLU:CG	2.87	0.46
2:F:329:TYR:HA	2:F:332:GLY:O	2.16	0.46
2:F:438:ILE:HD13	2:F:455:VAL:HG22	1.98	0.46
1:B:86:ASN:O	1:B:89:SER:N	2.47	0.45
1:B:273:MET:C	1:B:275:GLY:H	2.19	0.45
1:B:313:ILE:HG13	1:B:372:PRO:HG3	1.97	0.45
2:D:320:SER:HB3	1:E:256:GLN:HG2	1.98	0.45
2:D:430:ILE:O	2:D:431:ASP:C	2.54	0.45
1:E:497:ILE:O	1:E:498:THR:OG1	2.24	0.45
2:F:419:PHE:O	2:F:420:MET:O	2.33	0.45
1:B:49:GLY:O	1:B:218:ARG:NH2	2.48	0.45
1:B:151:PHE:C	1:B:153:GLN:H	2.18	0.45
1:E:280:LYS:HZ3	1:E:407:GLU:HB3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:154:TYR:O	2:F:154:TYR:CD1	2.69	0.45
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.51	0.45
2:C:338:MET:H	2:C:338:MET:HG2	1.47	0.45
2:D:164:LEU:HD22	2:D:180:MET:HE1	1.99	0.45
1:E:52:LYS:O	1:E:55:PHE:HB3	2.16	0.45
2:F:345:LYS:HZ3	2:F:366:GLU:HG3	1.80	0.45
1:A:371:LYS:N	1:A:372:PRO:CD	2.78	0.45
1:B:264:SER:HA	1:B:271:ASP:OD1	2.17	0.45
2:C:392:PHE:O	2:C:395:PHE:N	2.42	0.45
1:E:464:ASP:OD2	1:E:466:ALA:HB3	2.16	0.45
2:F:116:GLU:O	2:F:117:VAL:HB	2.16	0.45
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.98	0.45
2:C:225:LEU:HB2	2:C:230:HIS:CD2	2.52	0.45
1:E:230:HIS:C	1:E:230:HIS:ND1	2.69	0.45
1:E:264:SER:N	1:E:374:ARG:NH2	2.64	0.45
1:E:462:TRP:CE3	1:E:463:HIS:N	2.85	0.45
2:F:504:GLU:HA	2:F:507:ARG:NE	2.32	0.45
1:A:313:ILE:CG1	1:A:372:PRO:HG2	2.46	0.45
1:A:334:ASP:O	1:A:338:MET:HG2	2.17	0.45
1:B:213:GLY:O	1:B:214:GLU:HB2	2.16	0.45
1:B:436:THR:CG2	1:B:458:MET:HG2	2.46	0.45
1:B:452:ALA:HA	1:B:468:ARG:O	2.17	0.45
2:D:468:ARG:HG2	2:D:468:ARG:HH11	1.81	0.45
1:E:208:ARG:HB2	1:E:219:THR:OG1	2.16	0.45
2:F:49:GLY:CA	4:F:903:ATP:O2B	2.64	0.45
2:F:65:ILE:O	2:F:65:ILE:HG22	2.17	0.45
2:F:142:VAL:O	2:F:178:THR:HA	2.15	0.45
2:F:420:MET:HA	5:F:532:HOH:O	2.16	0.45
2:F:425:ILE:HG22	2:F:426:THR:OG1	2.17	0.45
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.46	0.45
1:B:289:ALA:O	1:B:290:THR:C	2.53	0.45
1:B:315:PHE:HB3	1:B:317:TYR:CE1	2.50	0.45
2:C:107:ASP:C	2:C:107:ASP:OD1	2.55	0.45
2:C:215:ARG:HA	2:C:215:ARG:NE	2.30	0.45
2:C:225:LEU:HD12	2:C:230:HIS:HB3	1.98	0.45
2:C:418:GLN:HG3	2:C:418:GLN:O	2.17	0.45
2:C:437:ILE:CD1	2:C:457:LYS:HE2	2.47	0.45
1:E:219:THR:HA	1:E:235:TYR:O	2.16	0.45
2:F:308:ASN:O	2:F:309:LYS:HB2	2.16	0.45
1:A:69:GLU:OE1	1:A:141:ARG:NH2	2.48	0.45
1:A:157:SER:O	1:A:160:VAL:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:NE	2:F:488:ARG:HH22	2.15	0.45
1:B:200:VAL:O	1:B:200:VAL:HG12	2.17	0.45
1:B:313:ILE:HG21	1:B:315:PHE:CZ	2.51	0.45
2:C:76:PHE:O	2:C:109:SER:HA	2.16	0.45
2:C:261:VAL:HG12	2:C:262:ARG:N	2.32	0.45
2:D:164:LEU:CD2	2:D:180:MET:HE1	2.46	0.45
2:D:353:SER:O	2:D:354:ALA:HB2	2.16	0.45
1:E:20:LYS:HE3	1:E:228:THR:HG21	1.98	0.45
1:E:419:PHE:O	1:E:420:MET:HB2	2.16	0.45
2:F:38:ILE:HD12	2:F:38:ILE:H	1.82	0.45
2:F:79:THR:HG23	2:F:81:GLN:N	2.28	0.45
2:F:215:ARG:NE	2:F:215:ARG:CA	2.77	0.45
2:F:455:VAL:O	2:F:455:VAL:HG12	2.17	0.45
1:A:518:GLU:HB2	1:A:519:SER:H	1.54	0.45
1:B:376:ALA:HA	1:B:411:LEU:O	2.17	0.45
2:C:262:ARG:HH22	2:C:461:SER:CB	2.30	0.45
2:C:308:ASN:O	2:C:310:GLU:N	2.50	0.45
2:D:344:LEU:CD1	2:D:346:ILE:HG13	2.47	0.45
1:E:371:LYS:O	1:E:371:LYS:CD	2.57	0.45
1:A:18:ILE:HG21	1:A:37:PRO:HB3	1.99	0.45
1:A:170:ARG:HD2	1:A:173:GLN:OE1	2.16	0.45
1:A:440:LEU:HD23	1:A:453:ILE:HG13	1.99	0.45
2:C:18:ILE:HB	2:C:228:THR:CG2	2.45	0.45
2:C:33:HIS:CD2	2:C:230:HIS:HA	2.52	0.45
2:C:79:THR:HG23	2:C:81:GLN:HG2	1.99	0.45
2:D:264:SER:OG	2:D:265:SER:N	2.50	0.45
2:D:294:LYS:O	2:D:297:LEU:N	2.50	0.45
2:F:59:PHE:CD2	2:F:179:VAL:HG21	2.52	0.45
2:F:302:VAL:CG1	2:F:303:GLU:N	2.80	0.45
2:F:325:LEU:HD21	2:F:335:PHE:CB	2.46	0.45
2:F:486:PHE:CB	2:F:489:ILE:HD11	2.47	0.45
1:A:370:PHE:C	1:A:372:PRO:HD3	2.37	0.44
2:C:194:TYR:O	2:C:196:VAL:HG23	2.17	0.44
1:E:203:ASN:HA	1:E:224:LYS:O	2.16	0.44
2:F:299:SER:C	2:F:333:MET:HE1	2.37	0.44
2:F:347:VAL:O	2:F:348:CYS:CB	2.63	0.44
2:F:504:GLU:HB2	2:F:505:LEU:H	1.48	0.44
1:A:104:PHE:CD2	1:A:133:ALA:HB1	2.52	0.44
1:A:184:ARG:NH2	1:A:186:GLU:O	2.50	0.44
1:A:261:VAL:CG1	1:A:262:ARG:N	2.79	0.44
1:A:364:LYS:O	1:A:367:ILE:HB	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ARG:O	1:A:497:ILE:HG23	2.17	0.44
2:C:52:LYS:N	2:C:207:LEU:HD12	2.32	0.44
2:C:113:GLU:O	2:C:114:GLY:C	2.56	0.44
2:C:150:VAL:CG1	2:C:151:PHE:N	2.80	0.44
2:C:348:CYS:HB3	2:D:254:LEU:HB3	1.99	0.44
2:D:79:THR:CG2	2:D:82:ASP:H	2.28	0.44
2:F:111:ASP:CG	2:F:112:PRO:HD2	2.38	0.44
2:F:145:ASP:OD2	2:F:181:THR:HG21	2.17	0.44
2:F:197:GLU:OE2	2:F:197:GLU:N	2.36	0.44
2:F:329:TYR:O	2:F:332:GLY:N	2.50	0.44
1:A:502:LYS:HG3	1:A:502:LYS:O	2.17	0.44
1:B:191:ILE:HD12	1:B:191:ILE:N	2.32	0.44
1:B:238:THR:CG2	1:B:240:THR:HG22	2.47	0.44
2:C:18:ILE:N	2:C:18:ILE:CD1	2.79	0.44
2:C:117:VAL:O	2:C:117:VAL:HG12	2.18	0.44
2:C:360:LEU:HD21	2:C:364:LYS:HE3	1.99	0.44
2:D:183:GLU:HB2	1:E:199:PHE:CZ	2.52	0.44
2:D:206:ILE:HD11	2:D:223:LEU:HD12	1.99	0.44
1:E:291:GLY:HA3	1:E:442:TYR:HH	1.82	0.44
1:E:340:ARG:O	1:E:342:ASN:N	2.51	0.44
2:F:104:PHE:CE2	2:F:106:LEU:HB2	2.51	0.44
1:A:131:ASN:O	1:A:132:TYR:C	2.55	0.44
1:B:84:ILE:HA	1:B:94:LEU:HD12	1.99	0.44
4:D:903:ATP:O3'	1:E:224:LYS:HB2	2.17	0.44
1:E:164:LEU:HD11	1:E:197:GLU:CG	2.47	0.44
2:F:379:SER:HB3	2:F:382:ALA:HB2	2.00	0.44
2:F:514:GLU:O	2:F:515:LYS:HB3	2.17	0.44
1:A:56:SER:HB2	1:A:143:SER:HB3	1.98	0.44
1:A:79:THR:O	1:A:83:ILE:HD12	2.17	0.44
1:B:51:GLY:O	1:B:52:LYS:C	2.56	0.44
1:B:185:ILE:HD11	1:B:193:ARG:HG3	1.99	0.44
2:C:50:THR:HG23	2:C:209:ASN:HB2	2.00	0.44
2:C:69:GLU:HA	2:C:70:PRO:HD3	1.90	0.44
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.99	0.44
2:C:215:ARG:HE	2:C:215:ARG:CA	2.31	0.44
2:C:344:LEU:HD11	2:C:346:ILE:HG13	1.99	0.44
2:D:262:ARG:NH1	2:D:275:GLY:O	2.51	0.44
2:D:313:ILE:HG13	2:D:372:PRO:HG3	2.00	0.44
1:E:46:GLY:H	1:E:52:LYS:HD3	1.81	0.44
1:E:356:LEU:HD12	1:E:356:LEU:H	1.82	0.44
1:E:446:ARG:HH21	1:E:496:ARG:NH2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:115:GLN:HE21	2:F:115:GLN:HB3	1.54	0.44
2:F:184:ARG:HH12	2:F:187:GLU:C	2.20	0.44
2:F:264:SER:O	2:F:374:ARG:NH2	2.51	0.44
2:F:516:GLY:N	2:F:517:PRO:CD	2.80	0.44
1:A:65:ILE:O	1:A:65:ILE:CG2	2.65	0.44
1:A:83:ILE:H	1:A:83:ILE:CD1	2.26	0.44
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.99	0.44
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.89	0.44
1:B:401:GLY:O	1:B:404:LYS:N	2.51	0.44
2:C:225:LEU:HD23	2:C:225:LEU:HA	1.78	0.44
2:C:419:PHE:O	2:C:420:MET:CB	2.65	0.44
2:D:47:THR:O	2:D:50:THR:OG1	2.21	0.44
2:D:65:ILE:O	2:D:65:ILE:HG22	2.17	0.44
2:D:98:VAL:HA	2:D:103:LEU:O	2.18	0.44
2:D:225:LEU:HD12	2:D:230:HIS:HB3	2.00	0.44
2:D:419:PHE:O	2:D:420:MET:HB2	2.18	0.44
1:E:300:ARG:N	1:E:333:MET:HE1	2.31	0.44
1:E:346:ILE:CG2	1:E:347:VAL:N	2.80	0.44
1:B:256:GLN:H	1:B:256:GLN:HG2	1.55	0.44
1:B:291:GLY:HA3	1:B:442:TYR:HH	1.81	0.44
1:E:315:PHE:CD2	1:E:347:VAL:HG21	2.53	0.44
2:F:292:THR:HB	2:F:440:LEU:HB3	2.00	0.44
2:F:313:ILE:CD1	2:F:372:PRO:HG2	2.48	0.44
1:A:79:THR:O	1:A:82:ASP:HB2	2.17	0.44
1:A:211:LEU:HG	1:A:212:GLU:H	1.82	0.44
1:A:323:GLN:HE21	1:A:327:ASN:HD21	1.64	0.44
1:A:462:TRP:CE3	1:A:463:HIS:N	2.86	0.44
2:C:42:THR:O	2:C:180:MET:HB2	2.18	0.44
2:C:85:LYS:HZ3	2:D:14:GLU:HB3	1.82	0.44
2:D:221:GLU:HG3	2:D:233:GLY:C	2.38	0.44
1:E:274:CYS:C	1:E:276:GLY:H	2.21	0.44
1:E:344:LEU:HD13	1:E:345:LYS:N	2.32	0.44
2:F:224:LYS:HZ1	2:F:226:ARG:NE	2.16	0.44
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.99	0.44
1:B:463:HIS:CE1	1:B:465:LYS:HZ2	2.35	0.44
1:B:463:HIS:CE1	1:B:465:LYS:NZ	2.85	0.44
2:C:14:GLU:HG3	2:C:16:GLN:H	1.83	0.44
2:D:359:HIS:O	2:D:363:ILE:HG13	2.17	0.44
1:E:42:THR:HG23	1:E:203:ASN:HB2	1.99	0.44
1:E:401:GLY:O	1:E:405:GLN:HG2	2.18	0.44
2:F:31:ILE:CD1	2:F:246:ILE:HG21	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:96:LYS:O	2:F:99:ASP:HB2	2.18	0.44
2:F:300:ARG:CZ	2:F:477:PRO:HD2	2.47	0.44
2:F:387:VAL:HG12	2:F:388:SER:O	2.18	0.44
1:A:31:ILE:O	1:A:222:ILE:HD12	2.18	0.43
1:A:407:GLU:OE1	1:A:407:GLU:HA	2.18	0.43
1:B:197:GLU:O	1:B:200:VAL:N	2.41	0.43
1:B:417:ASP:HB3	2:C:429:HIS:CE1	2.52	0.43
2:C:64:ILE:HD11	2:C:102:LYS:C	2.38	0.43
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.57	0.43
2:C:457:LYS:O	2:C:457:LYS:HG3	2.17	0.43
2:D:41:SER:HB3	2:D:178:THR:CB	2.39	0.43
2:D:52:LYS:HD2	2:D:182:THR:O	2.18	0.43
2:D:435:ASP:HA	2:D:459:ARG:HD2	1.99	0.43
1:E:167:LEU:O	1:E:171:LEU:HD12	2.18	0.43
1:E:248:PRO:HB2	1:E:251:ALA:CB	2.45	0.43
1:E:367:ILE:HG12	1:E:375:ILE:HD11	2.00	0.43
2:F:150:VAL:CG1	2:F:151:PHE:N	2.80	0.43
2:F:431:ASP:OD1	2:F:431:ASP:N	2.43	0.43
2:F:483:PHE:CD1	2:F:483:PHE:N	2.86	0.43
1:A:268:VAL:O	1:A:271:ASP:HB2	2.17	0.43
1:B:52:LYS:HB2	1:B:52:LYS:HE3	1.85	0.43
1:B:75:THR:HG23	1:B:75:THR:O	2.18	0.43
1:B:444:GLU:OE2	2:C:489:ILE:HG13	2.18	0.43
2:C:321:ARG:HG2	2:C:348:CYS:SG	2.57	0.43
2:C:360:LEU:HD23	2:C:364:LYS:HG3	2.00	0.43
2:D:76:PHE:HZ	2:D:126:LEU:HD21	1.82	0.43
2:D:197:GLU:OE2	2:D:197:GLU:N	2.43	0.43
2:D:367:ILE:HG12	2:D:375:ILE:HD11	2.00	0.43
1:E:419:PHE:CD2	2:F:425:ILE:HD12	2.53	0.43
1:E:444:GLU:O	1:E:494:PRO:HD2	2.18	0.43
2:F:59:PHE:CE2	2:F:179:VAL:HG23	2.53	0.43
2:F:295:THR:HB	4:F:901:ATP:PA	2.58	0.43
2:F:344:LEU:C	2:F:344:LEU:HD13	2.39	0.43
1:A:147:VAL:HG11	1:A:180:MET:HE2	1.99	0.43
2:C:89:SER:CB	2:D:227:GLY:O	2.66	0.43
2:C:208:ARG:O	2:C:218:ARG:HA	2.18	0.43
2:C:240:THR:HG21	2:C:361:GLN:NE2	2.32	0.43
2:C:247:PHE:HB3	2:C:249:LEU:HD21	2.00	0.43
2:D:294:LYS:N	4:D:901:ATP:O1B	2.43	0.43
2:D:401:GLY:O	2:D:405:GLN:HG2	2.18	0.43
1:E:356:LEU:N	1:E:356:LEU:CD1	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:298:VAL:HA	2:F:411:LEU:HD21	1.99	0.43
1:A:261:VAL:HG12	1:A:262:ARG:N	2.33	0.43
2:C:412:PHE:N	2:C:412:PHE:CD1	2.87	0.43
2:D:81:GLN:CD	2:D:81:GLN:H	2.22	0.43
2:D:96:LYS:O	2:D:99:ASP:N	2.51	0.43
2:D:299:SER:C	2:D:333:MET:HE1	2.39	0.43
2:D:396:VAL:HG11	2:D:430:ILE:HG21	2.00	0.43
1:E:140:ARG:HA	1:E:140:ARG:HD2	1.86	0.43
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.49	0.43
2:F:121:PHE:HD2	2:F:121:PHE:HA	1.73	0.43
2:F:363:ILE:HG22	2:F:367:ILE:HD11	1.99	0.43
2:F:462:TRP:O	2:F:463:HIS:O	2.37	0.43
2:C:123:LEU:HD11	2:C:163:GLU:O	2.18	0.43
1:E:426:THR:HG21	1:E:430:ILE:CG1	2.47	0.43
1:E:496:ARG:O	1:E:497:ILE:HD13	2.18	0.43
2:F:294:LYS:HE2	2:F:294:LYS:HB2	1.89	0.43
2:F:332:GLY:O	2:F:333:MET:O	2.37	0.43
2:F:371:LYS:HD2	2:F:371:LYS:C	2.39	0.43
1:B:161:ARG:NH2	1:B:199:PHE:CB	2.74	0.43
1:B:208:ARG:NE	1:B:234:GLU:OE2	2.45	0.43
1:B:356:LEU:HD23	1:B:395:PHE:HB2	2.01	0.43
2:D:299:SER:HB3	2:D:333:MET:CE	2.49	0.43
1:E:25:ILE:HD12	1:E:55:PHE:CE1	2.53	0.43
2:F:164:LEU:HD11	2:F:197:GLU:HG3	2.01	0.43
1:A:153:GLN:O	1:A:154:TYR:CB	2.67	0.43
2:C:446:ARG:HG2	2:C:496:ARG:NH1	2.33	0.43
2:D:106:LEU:HD23	2:D:130:ILE:HG12	2.01	0.43
2:D:206:ILE:HG21	2:D:208:ARG:NH1	2.34	0.43
2:D:231:MET:HB3	2:D:235:TYR:OH	2.19	0.43
1:E:195:GLY:C	1:E:198:GLU:OE1	2.57	0.43
1:E:264:SER:O	1:E:374:ARG:NH2	2.52	0.43
1:E:326:ARG:HD3	2:F:258:SER:OG	2.19	0.43
2:F:73:PHE:C	2:F:73:PHE:HD2	2.22	0.43
2:F:231:MET:SD	2:F:251:ALA:HB2	2.59	0.43
2:F:335:PHE:HA	2:F:338:MET:HG3	2.01	0.43
2:F:445:ILE:HG13	2:F:483:PHE:HE2	1.82	0.43
1:A:84:ILE:O	1:A:87:ALA:HB3	2.19	0.43
1:A:210:VAL:HG12	1:A:211:LEU:O	2.18	0.43
1:A:316:ALA:HB3	1:A:348:CYS:SG	2.59	0.43
1:A:463:HIS:O	1:A:465:LYS:HE2	2.19	0.43
1:A:489:ILE:H	2:F:444:GLU:CD	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:PHE:O	1:B:420:MET:O	2.36	0.43
2:C:471:MET:CE	2:C:473:SER:HB3	2.49	0.43
2:D:41:SER:OG	2:D:168:VAL:HG13	2.18	0.43
2:D:200:VAL:O	2:D:200:VAL:HG12	2.19	0.43
2:D:392:PHE:O	2:D:395:PHE:N	2.50	0.43
1:E:356:LEU:H	1:E:356:LEU:CD1	2.31	0.43
1:E:363:ILE:CG2	1:E:367:ILE:HD11	2.44	0.43
2:F:54:LEU:O	2:F:55:PHE:C	2.57	0.43
2:F:79:THR:CG2	2:F:82:ASP:OD2	2.67	0.43
1:A:147:VAL:HG11	1:A:180:MET:CE	2.48	0.43
1:B:87:ALA:C	1:B:89:SER:N	2.71	0.43
1:B:294:LYS:C	1:B:296:LEU:N	2.70	0.43
2:C:204:VAL:HG11	2:C:223:LEU:HD12	2.00	0.43
2:D:208:ARG:NE	2:D:234:GLU:OE2	2.51	0.43
1:E:178:THR:CG2	1:E:179:VAL:N	2.80	0.43
1:E:352:GLU:C	1:E:354:ALA:H	2.22	0.43
1:E:392:PHE:O	1:E:395:PHE:N	2.52	0.43
1:E:468:ARG:HA	1:E:482:SER:HA	2.01	0.43
1:E:486:PHE:HA	1:E:495:THR:O	2.19	0.43
2:F:183:GLU:HG3	2:F:193:ARG:HE	1.83	0.43
1:A:49:GLY:CA	4:A:903:ATP:O2B	2.66	0.43
1:A:207:LEU:HD22	1:A:237:PHE:CE2	2.53	0.43
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.83	0.43
1:A:446:ARG:HG2	1:A:496:ARG:CZ	2.49	0.43
1:B:184:ARG:CD	1:B:191:ILE:O	2.66	0.43
2:C:295:THR:O	2:C:298:VAL:HB	2.18	0.43
2:D:88:ARG:HD3	1:E:15:HIS:C	2.39	0.43
2:D:153:GLN:O	2:D:154:TYR:CB	2.67	0.43
1:A:402:TYR:O	1:A:406:GLU:HB2	2.18	0.42
1:B:20:LYS:HG2	1:B:35:GLY:O	2.19	0.42
2:C:426:THR:HG22	2:C:428:SER:H	1.84	0.42
2:D:430:ILE:O	2:D:431:ASP:O	2.36	0.42
1:E:313:ILE:CG1	1:E:372:PRO:CG	2.93	0.42
1:E:462:TRP:O	1:E:463:HIS:O	2.37	0.42
2:F:377:ILE:CD1	2:F:412:PHE:HE2	2.31	0.42
2:F:380:LEU:CD1	2:F:412:PHE:HB3	2.49	0.42
2:F:513:GLN:OE1	2:F:513:GLN:HA	2.19	0.42
1:A:237:PHE:HA	1:A:245:ASN:O	2.18	0.42
1:A:504:GLU:C	1:A:506:SER:N	2.72	0.42
1:B:217:ARG:NH2	1:B:394:GLN:OE1	2.52	0.42
2:C:136:LYS:O	2:C:136:LYS:HG2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:370:PHE:C	2:D:372:PRO:HD3	2.39	0.42
2:D:446:ARG:N	2:D:496:ARG:HH12	2.16	0.42
1:E:164:LEU:HD11	1:E:197:GLU:HG3	2.02	0.42
1:E:451:ARG:NH1	1:E:451:ARG:CG	2.78	0.42
2:F:56:SER:O	2:F:59:PHE:HB3	2.19	0.42
2:F:443:VAL:HG12	2:F:445:ILE:CG1	2.47	0.42
1:B:334:ASP:O	1:B:338:MET:HG2	2.18	0.42
1:B:371:LYS:N	1:B:372:PRO:CD	2.80	0.42
1:B:392:PHE:O	1:B:395:PHE:N	2.45	0.42
1:E:336:GLU:OE1	1:E:336:GLU:HA	2.19	0.42
1:E:452:ALA:HA	1:E:469:GLU:HA	2.00	0.42
2:F:451:ARG:HH11	2:F:451:ARG:CG	2.33	0.42
1:A:111:ASP:O	1:A:113:GLU:N	2.49	0.42
1:A:111:ASP:C	1:A:113:GLU:H	2.23	0.42
1:A:211:LEU:CD1	1:A:216:ARG:HG2	2.49	0.42
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.31	0.42
1:A:488:ARG:HE	2:F:488:ARG:HH22	1.65	0.42
1:B:62:ASN:O	1:B:66:GLU:HB2	2.19	0.42
1:B:267:VAL:HB	1:B:270:LEU:HB2	2.01	0.42
1:B:309:LYS:HA	1:B:343:LEU:HD13	2.00	0.42
1:B:473:SER:C	1:B:475:LYS:H	2.22	0.42
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.84	0.42
2:C:173:GLN:C	2:C:175:GLY:H	2.23	0.42
2:C:437:ILE:HD11	2:C:457:LYS:HE2	2.01	0.42
2:D:193:ARG:NH1	2:D:193:ARG:HG2	2.34	0.42
1:E:301:PHE:HZ	1:E:409:THR:HG22	1.84	0.42
2:F:64:ILE:HD11	2:F:102:LYS:O	2.19	0.42
2:F:451:ARG:NH1	2:F:472:ILE:HD12	2.35	0.42
1:B:220:LEU:C	1:B:220:LEU:HD23	2.40	0.42
2:C:211:LEU:O	2:C:212:GLU:CB	2.65	0.42
2:C:378:ASP:O	2:C:379:SER:CB	2.67	0.42
2:D:371:LYS:N	2:D:372:PRO:CD	2.82	0.42
2:D:468:ARG:HG2	2:D:468:ARG:NH1	2.34	0.42
1:E:449:MET:HE3	2:F:467:ILE:HD11	2.00	0.42
2:F:497:ILE:O	2:F:497:ILE:HG13	2.19	0.42
1:A:150:VAL:CG1	1:A:151:PHE:N	2.81	0.42
1:B:61:TYR:O	1:B:64:ILE:N	2.52	0.42
1:B:178:THR:CG2	1:B:179:VAL:H	2.32	0.42
1:B:248:PRO:HB2	1:B:251:ALA:CB	2.47	0.42
1:B:425:ILE:HD12	1:B:425:ILE:N	2.35	0.42
2:C:433:ILE:O	2:C:433:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:THR:C	2:D:25:ILE:N	2.73	0.42
2:D:323:GLN:HE22	1:E:459:ARG:HD3	1.84	0.42
1:E:113:GLU:HB3	1:E:114:GLY:H	1.62	0.42
1:A:52:LYS:HD2	1:A:181:THR:HG23	2.01	0.42
1:A:256:GLN:O	2:F:322:ALA:HB3	2.19	0.42
1:A:323:GLN:HG2	1:A:327:ASN:ND2	2.35	0.42
1:A:487:GLU:OE1	2:F:495:THR:HA	2.19	0.42
1:A:488:ARG:HD3	2:F:488:ARG:HH22	1.85	0.42
1:A:504:GLU:C	1:A:506:SER:H	2.22	0.42
1:B:106:LEU:HG	1:B:106:LEU:O	2.20	0.42
1:B:283:ILE:HD13	1:B:283:ILE:HA	1.88	0.42
1:B:311:ARG:HG3	1:B:371:LYS:NZ	2.34	0.42
2:C:28:PHE:O	2:C:31:ILE:N	2.48	0.42
2:C:182:THR:CG2	2:C:183:GLU:N	2.82	0.42
2:C:266:GLY:HA3	2:C:300:ARG:HG3	2.00	0.42
2:D:68:ASP:OD1	2:D:68:ASP:O	2.37	0.42
2:D:295:THR:HG21	2:D:319:GLU:OE2	2.20	0.42
2:D:488:ARG:HB3	2:D:491:SER:HB3	2.02	0.42
1:E:67:PHE:O	1:E:68:ASP:C	2.58	0.42
2:F:79:THR:HA	2:F:80:PRO:HD3	1.93	0.42
2:F:153:GLN:O	2:F:154:TYR:HB3	2.19	0.42
2:F:500:ASP:CG	2:F:501:GLU:N	2.73	0.42
1:A:146:SER:HA	1:A:181:THR:O	2.20	0.42
1:A:469:GLU:O	1:A:470:PHE:HB3	2.19	0.42
2:C:129:ARG:O	2:C:132:TYR:HB3	2.20	0.42
2:C:389:ASN:ND2	2:C:428:SER:HA	2.32	0.42
1:E:96:LYS:O	1:E:100:GLU:HG3	2.19	0.42
2:F:287:THR:HG23	2:F:414:ASN:HB3	2.02	0.42
2:F:364:LYS:O	2:F:367:ILE:N	2.51	0.42
2:F:492:GLY:C	2:F:494:PRO:HD3	2.40	0.42
1:A:392:PHE:O	1:A:393:ARG:C	2.58	0.42
1:A:439:LEU:HD12	1:A:440:LEU:N	2.35	0.42
2:C:174:ILE:HG22	2:C:174:ILE:O	2.19	0.42
2:C:211:LEU:HD12	2:C:215:ARG:O	2.20	0.42
2:C:246:ILE:HG22	2:C:247:PHE:N	2.35	0.42
2:D:323:GLN:O	2:D:324:LEU:C	2.58	0.42
2:D:328:ALA:O	2:D:332:GLY:O	2.38	0.42
2:D:463:HIS:ND1	2:D:463:HIS:C	2.73	0.42
2:F:379:SER:N	2:F:413:THR:HB	2.20	0.42
1:A:54:LEU:CD2	1:A:244:ILE:HG13	2.50	0.42
1:B:25:ILE:HG23	1:B:58:GLN:HE21	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HD23	1:B:94:LEU:HA	1.89	0.42
1:B:104:PHE:HD2	1:B:133:ALA:CB	2.31	0.42
1:B:109:SER:HA	1:B:110:PRO:HD3	1.87	0.42
1:B:220:LEU:HD23	1:B:221:GLU:N	2.35	0.42
1:B:238:THR:HG22	1:B:240:THR:CG2	2.48	0.42
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.50	0.42
2:C:328:ALA:O	2:C:329:TYR:C	2.58	0.42
2:C:388:SER:O	2:C:389:ASN:C	2.58	0.42
2:C:471:MET:HE3	2:C:473:SER:HB3	2.02	0.42
1:E:79:THR:HG22	1:E:82:ASP:H	1.85	0.42
1:E:284:ILE:O	1:E:412:PHE:HD1	2.02	0.42
2:F:185:ILE:HD11	2:F:193:ARG:NH1	2.34	0.42
2:F:291:GLY:HA3	2:F:442:TYR:OH	2.19	0.42
1:A:84:ILE:HA	1:A:94:LEU:HD12	2.02	0.41
1:A:211:LEU:HD12	1:A:216:ARG:HG2	2.01	0.41
1:B:37:PRO:HG2	5:B:522:HOH:O	2.20	0.41
1:B:213:GLY:O	1:B:214:GLU:CB	2.68	0.41
1:B:340:ARG:C	1:B:342:ASN:N	2.73	0.41
2:C:121:PHE:CD1	2:C:121:PHE:N	2.87	0.41
2:C:287:THR:HG23	2:C:414:ASN:ND2	2.18	0.41
2:C:471:MET:N	2:C:480:LYS:HZ1	2.18	0.41
2:D:21:MET:HE1	2:D:177:THR:HB	2.02	0.41
2:D:38:ILE:CG2	2:D:39:GLY:N	2.83	0.41
2:D:150:VAL:HG13	2:D:151:PHE:N	2.35	0.41
2:D:387:VAL:HG12	2:D:388:SER:N	2.35	0.41
1:E:161:ARG:HB2	1:E:196:VAL:HG11	2.01	0.41
2:F:21:MET:HE3	2:F:141:ARG:HD3	2.02	0.41
2:F:52:LYS:HE3	4:F:903:ATP:O1B	2.20	0.41
2:F:345:LYS:HE2	2:F:366:GLU:OE1	2.19	0.41
2:F:471:MET:HG2	2:F:480:LYS:NZ	2.35	0.41
1:B:70:PRO:HA	1:B:102:LYS:O	2.20	0.41
1:B:146:SER:H	1:B:181:THR:CG2	2.34	0.41
1:B:291:GLY:CA	1:B:442:TYR:OH	2.68	0.41
2:C:451:ARG:NH1	2:C:472:ILE:HD12	2.35	0.41
2:D:313:ILE:CD1	2:D:372:PRO:CG	2.98	0.41
1:E:21:MET:HE1	1:E:177:THR:HB	2.00	0.41
1:E:111:ASP:C	1:E:113:GLU:H	2.23	0.41
1:E:225:LEU:HD23	1:E:225:LEU:HA	1.90	0.41
1:E:247:PHE:CZ	1:E:361:GLN:HB2	2.55	0.41
2:F:104:PHE:CD1	2:F:137:TYR:CE1	3.08	0.41
2:F:389:ASN:HD21	2:F:428:SER:HA	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:O	1:A:100:GLU:HG3	2.20	0.41
1:A:298:VAL:O	1:A:301:PHE:HB3	2.21	0.41
2:C:59:PHE:O	2:C:141:ARG:NH1	2.51	0.41
2:C:289:ALA:HB2	2:C:419:PHE:HA	2.02	0.41
1:E:79:THR:O	1:E:82:ASP:N	2.54	0.41
1:E:200:VAL:O	1:E:200:VAL:HG12	2.19	0.41
2:F:328:ALA:O	2:F:332:GLY:O	2.38	0.41
1:A:31:ILE:H	1:A:31:ILE:HG13	1.66	0.41
1:A:64:ILE:HG21	1:A:97:LEU:HD22	2.02	0.41
1:A:419:PHE:CD2	1:B:425:ILE:CD1	3.02	0.41
1:B:60:LEU:O	1:B:63:GLY:N	2.53	0.41
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.86	0.41
1:B:295:THR:HG23	1:B:378:ASP:OD2	2.21	0.41
2:C:265:SER:HB3	2:C:278:PHE:CZ	2.55	0.41
2:C:284:ILE:HB	2:C:411:LEU:HD13	2.02	0.41
2:D:182:THR:CG2	2:D:183:GLU:N	2.82	0.41
1:E:76:PHE:HE1	1:E:144:ILE:HG23	1.85	0.41
1:E:211:LEU:HD12	1:E:215:ARG:O	2.20	0.41
2:F:273:MET:O	2:F:463:HIS:HA	2.20	0.41
2:F:273:MET:O	2:F:463:HIS:HB2	2.21	0.41
1:A:386:GLY:HA2	1:B:390:ASN:OD1	2.19	0.41
1:A:451:ARG:HG2	1:A:451:ARG:NH1	2.34	0.41
1:B:45:SER:HB2	1:B:182:THR:HB	1.98	0.41
1:B:93:ASP:OD2	1:B:96:LYS:HB2	2.20	0.41
1:B:451:ARG:H	1:B:451:ARG:HD2	1.84	0.41
2:C:88:ARG:HD3	2:D:15:HIS:C	2.41	0.41
2:C:371:LYS:N	2:C:372:PRO:HD3	2.35	0.41
2:D:33:HIS:CD2	2:D:230:HIS:HA	2.55	0.41
1:E:54:LEU:CD2	1:E:239:ILE:HG23	2.51	0.41
1:E:378:ASP:O	1:E:379:SER:CB	2.68	0.41
2:F:486:PHE:HB3	2:F:489:ILE:HD11	2.02	0.41
1:A:438:ILE:HD13	1:A:438:ILE:HA	1.89	0.41
1:B:44:VAL:HG13	1:B:205:VAL:HG12	2.01	0.41
2:C:54:LEU:CD1	2:C:90:PHE:CZ	3.03	0.41
2:C:214:GLU:HB3	2:D:234:GLU:HB2	2.01	0.41
2:C:354:ALA:HB3	2:C:359:HIS:CE1	2.56	0.41
2:D:55:PHE:HA	2:D:244:ILE:HD12	2.02	0.41
2:D:151:PHE:CE1	2:D:160:VAL:HG13	2.55	0.41
2:D:184:ARG:NH1	2:D:187:GLU:O	2.47	0.41
2:D:192:ALA:HB3	2:D:197:GLU:CD	2.41	0.41
1:E:230:HIS:ND1	1:E:230:HIS:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:LYS:C	1:E:406:GLU:H	2.24	0.41
1:E:426:THR:HG22	1:E:428:SER:N	2.30	0.41
2:F:79:THR:HG22	2:F:82:ASP:CB	2.51	0.41
2:F:117:VAL:HA	2:F:154:TYR:OH	2.21	0.41
2:F:127:ILE:HD12	2:F:170:ARG:HB2	2.03	0.41
2:F:311:ARG:CG	2:F:371:LYS:NZ	2.83	0.41
2:F:364:LYS:O	2:F:367:ILE:HB	2.20	0.41
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.51	0.41
1:A:52:LYS:HB3	1:A:181:THR:HG23	2.03	0.41
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.85	0.41
1:A:302:VAL:HG21	1:A:314:LEU:HB2	2.02	0.41
1:A:437:ILE:CD1	1:A:457:LYS:HE2	2.51	0.41
1:B:75:THR:HG21	1:B:83:ILE:HD11	2.02	0.41
1:B:106:LEU:C	1:B:106:LEU:HD12	2.41	0.41
1:B:426:THR:HG22	1:B:428:SER:N	2.35	0.41
1:B:473:SER:C	1:B:475:LYS:N	2.74	0.41
2:C:182:THR:HG21	2:C:192:ALA:CB	2.47	0.41
2:D:274:CYS:SG	2:D:458:MET:SD	3.18	0.41
2:D:360:LEU:HD21	2:D:364:LYS:HE3	2.03	0.41
1:E:216:ARG:HH21	2:F:223:LEU:HD21	1.84	0.41
1:E:248:PRO:C	1:E:250:GLY:N	2.72	0.41
2:F:398:GLY:O	2:F:399:VAL:C	2.58	0.41
1:A:220:LEU:HD23	1:A:220:LEU:O	2.21	0.41
1:A:315:PHE:HD1	1:A:376:ALA:O	2.03	0.41
1:A:379:SER:C	1:A:381:SER:N	2.72	0.41
2:C:52:LYS:HE3	2:C:52:LYS:HB2	1.89	0.41
2:C:439:LEU:HD12	2:C:440:LEU:N	2.35	0.41
2:D:48:SER:OG	1:E:224:LYS:HE2	2.21	0.41
2:D:52:LYS:N	4:D:903:ATP:O1B	2.54	0.41
2:D:284:ILE:HG23	2:D:436:THR:CG2	2.51	0.41
2:F:270:LEU:HD21	2:F:438:ILE:HD12	2.01	0.41
1:A:21:MET:CE	1:A:59:PHE:CZ	3.04	0.41
1:A:130:ILE:HG22	1:A:134:ILE:HD11	2.03	0.41
1:B:150:VAL:C	1:B:152:GLN:N	2.74	0.41
1:B:204:VAL:HG23	1:B:224:LYS:HG2	2.03	0.41
1:B:305:ALA:O	1:B:310:GLU:O	2.39	0.41
1:B:370:PHE:C	1:B:372:PRO:HD3	2.41	0.41
2:C:360:LEU:HD23	2:C:360:LEU:O	2.20	0.41
2:C:497:ILE:C	2:C:498:THR:HG22	2.40	0.41
2:D:46:GLY:O	2:D:183:GLU:HA	2.20	0.41
2:D:60:LEU:HD22	2:D:71:GLY:HA3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:PHE:N	2:D:278:PHE:CD2	2.86	0.41
2:D:436:THR:HA	2:D:457:LYS:O	2.20	0.41
1:E:79:THR:HG22	1:E:82:ASP:OD2	2.21	0.41
1:E:294:LYS:HB3	1:E:413:THR:HG23	2.03	0.41
1:E:331:TRP:NE1	4:E:901:ATP:N7	2.67	0.41
2:F:211:LEU:HA	2:F:216:ARG:HD3	2.02	0.41
2:F:283:ILE:CD1	2:F:400:THR:HG23	2.50	0.41
2:F:311:ARG:HD3	2:F:370:PHE:CE2	2.56	0.41
2:F:387:VAL:CG1	2:F:388:SER:N	2.84	0.41
2:F:430:ILE:O	2:F:431:ASP:C	2.59	0.41
1:A:123:LEU:HD22	1:A:123:LEU:HA	1.97	0.41
1:A:147:VAL:HG21	1:A:180:MET:CE	2.51	0.41
1:B:248:PRO:O	1:B:251:ALA:N	2.53	0.41
1:B:430:ILE:O	1:B:430:ILE:HG22	2.21	0.41
2:C:57:ILE:HD13	2:C:57:ILE:HA	1.88	0.41
2:C:252:MET:HE2	2:C:252:MET:HB3	1.88	0.41
2:C:480:LYS:HB3	2:C:481:ASP:H	1.50	0.41
2:D:121:PHE:CD1	2:D:121:PHE:N	2.89	0.41
2:D:299:SER:HB3	2:D:333:MET:HE2	2.04	0.41
2:D:344:LEU:HD13	2:D:345:LYS:N	2.36	0.41
2:D:402:TYR:O	2:D:405:GLN:HG2	2.20	0.41
1:E:126:LEU:O	1:E:129:ARG:HB2	2.21	0.41
1:E:218:ARG:O	1:E:236:PRO:HA	2.21	0.41
1:E:267:VAL:O	1:E:270:LEU:N	2.52	0.41
1:E:294:LYS:O	1:E:295:THR:C	2.59	0.41
1:E:397:ILE:HD11	1:E:433:ILE:HG12	2.03	0.41
1:E:488:ARG:O	1:E:491:SER:OG	2.29	0.41
2:F:43:LEU:HB2	2:F:201:SER:OG	2.21	0.41
2:F:127:ILE:HG21	2:F:170:ARG:HG3	2.03	0.41
1:A:378:ASP:O	1:A:379:SER:HB3	2.21	0.40
1:B:287:THR:CG2	1:B:414:ASN:HD22	2.24	0.40
2:C:316:ALA:O	2:C:348:CYS:HA	2.21	0.40
2:D:76:PHE:CZ	2:D:126:LEU:HD21	2.56	0.40
1:E:67:PHE:O	1:E:69:GLU:HG3	2.21	0.40
1:E:163:GLU:OE2	1:E:163:GLU:CA	2.55	0.40
2:F:275:GLY:HA2	2:F:462:TRP:HE3	1.86	0.40
2:F:315:PHE:CZ	2:F:363:ILE:HG23	2.56	0.40
1:A:157:SER:OG	1:A:158:SER:N	2.53	0.40
1:A:367:ILE:HG12	1:A:375:ILE:CD1	2.51	0.40
1:A:484:ARG:CZ	1:A:484:ARG:CB	2.99	0.40
1:B:84:ILE:O	1:B:85:LYS:C	2.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:C	1:B:128:GLU:N	2.75	0.40
2:C:71:GLY:O	2:C:103:LEU:HA	2.21	0.40
2:C:114:GLY:O	2:C:115:GLN:HB3	2.21	0.40
2:C:169:ALA:O	2:C:172:LYS:N	2.54	0.40
2:C:287:THR:CG2	2:C:288:GLY:N	2.83	0.40
2:C:294:LYS:HE2	2:C:294:LYS:HB2	1.90	0.40
2:D:88:ARG:HH11	2:D:88:ARG:HG2	1.86	0.40
2:F:147:VAL:HG23	2:F:148:THR:N	2.35	0.40
2:F:153:GLN:O	2:F:154:TYR:CB	2.69	0.40
2:F:261:VAL:CG1	2:F:262:ARG:N	2.84	0.40
1:A:22:ARG:CZ	1:A:24:MET:SD	3.10	0.40
1:B:170:ARG:HD2	1:B:173:GLN:OE1	2.21	0.40
1:B:383:LEU:HD13	1:B:395:PHE:CE2	2.56	0.40
2:C:240:THR:CG2	2:C:361:GLN:HE22	2.33	0.40
2:C:248:PRO:HB2	2:C:251:ALA:HB3	2.04	0.40
2:D:179:VAL:O	2:D:179:VAL:HG12	2.20	0.40
2:D:469:GLU:HG3	2:D:470:PHE:N	2.33	0.40
1:E:435:ASP:O	1:E:457:LYS:HE3	2.21	0.40
2:F:335:PHE:O	2:F:338:MET:HB2	2.21	0.40
1:A:267:VAL:HB	1:A:270:LEU:HB2	2.03	0.40
1:A:344:LEU:HD13	1:A:345:LYS:N	2.36	0.40
1:A:467:ILE:HD11	2:F:449:MET:HE3	2.02	0.40
1:A:506:SER:HB2	1:A:509:VAL:HA	2.03	0.40
1:B:353:SER:O	1:B:354:ALA:HB2	2.21	0.40
2:C:248:PRO:C	2:C:250:GLY:N	2.73	0.40
2:C:396:VAL:O	2:C:397:ILE:C	2.60	0.40
2:D:352:GLU:OE1	2:D:385:ARG:NH1	2.54	0.40
1:E:39:GLY:H	1:E:177:THR:HG23	1.86	0.40
1:E:186:GLU:OE2	1:E:187:GLU:N	2.54	0.40
2:F:334:ASP:OD1	2:F:336:GLU:N	2.55	0.40
2:C:304:ASN:OD1	2:C:374:ARG:NH2	2.54	0.40
2:C:332:GLY:O	2:C:333:MET:O	2.39	0.40
2:D:315:PHE:HB3	2:D:317:TYR:HE1	1.87	0.40
2:D:441:GLN:NE2	2:D:490:ILE:HD12	2.36	0.40
2:D:451:ARG:NH2	4:D:901:ATP:O3'	2.49	0.40
1:E:291:GLY:C	1:E:442:TYR:OH	2.60	0.40
1:E:379:SER:OG	1:E:382:ALA:N	2.53	0.40
2:F:269:ARG:HH22	2:F:468:ARG:NH2	2.19	0.40
2:F:359:HIS:O	2:F:363:ILE:HG13	2.22	0.40
2:F:471:MET:HG2	2:F:480:LYS:HZ3	1.86	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	503/519 (97%)	389 (77%)	83 (16%)	31 (6%)	1	11
1	B	488/519 (94%)	383 (78%)	71 (14%)	34 (7%)	1	8
1	E	489/519 (94%)	396 (81%)	66 (14%)	27 (6%)	2	14
2	C	486/519 (94%)	394 (81%)	69 (14%)	23 (5%)	2	17
2	D	483/519 (93%)	396 (82%)	68 (14%)	19 (4%)	3	22
2	F	504/519 (97%)	411 (82%)	65 (13%)	28 (6%)	2	14
All	All	2953/3114 (95%)	2369 (80%)	422 (14%)	162 (6%)	2	14

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	VAL
1	A	154	TYR
1	A	157	SER
1	A	387	VAL
1	A	420	MET
1	A	431	ASP
1	A	463	HIS
1	A	500	ASP
1	A	502	LYS
1	B	17	ALA
1	B	154	TYR
1	B	193	ARG
1	B	420	MET
1	B	463	HIS
1	B	494	PRO
2	C	17	ALA
2	C	117	VAL
2	C	154	TYR
2	C	249	LEU
2	C	309	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	333	MET
2	C	431	ASP
2	C	463	HIS
2	D	122	ASP
2	D	154	TYR
2	D	333	MET
2	D	387	VAL
2	D	463	HIS
1	E	122	ASP
1	E	154	TYR
1	E	157	SER
1	E	333	MET
1	E	354	ALA
1	E	463	HIS
1	E	484	ARG
2	F	118	VAL
2	F	154	TYR
2	F	278	PHE
2	F	333	MET
2	F	420	MET
2	F	463	HIS
2	F	501	GLU
2	F	504	GLU
2	F	506	SER
2	F	507	ARG
2	F	508	ILE
2	F	509	VAL
2	F	515	LYS
1	A	198	GLU
1	A	333	MET
1	A	480	LYS
1	A	499	VAL
1	A	509	VAL
1	B	87	ALA
1	B	119	GLY
1	B	195	GLY
1	B	211	LEU
1	B	341	GLN
1	B	379	SER
1	B	484	ARG
2	C	112	PRO
2	C	289	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	341	GLN
2	C	354	ALA
2	C	379	SER
2	D	113	GLU
2	D	211	LEU
2	D	420	MET
2	D	431	ASP
1	E	117	VAL
1	E	211	LEU
1	E	268	VAL
1	E	277	GLY
1	E	278	PHE
1	E	379	SER
1	E	498	THR
2	F	117	VAL
2	F	157	SER
2	F	211	LEU
2	F	480	LYS
1	A	26	GLU
1	A	65	ILE
1	A	193	ARG
1	A	211	LEU
1	B	61	TYR
1	B	112	PRO
1	B	198	GLU
1	B	295	THR
1	B	501	GLU
2	C	348	CYS
2	C	429	HIS
2	D	26	GLU
2	D	152	GLN
2	D	341	GLN
1	E	341	GLN
1	E	405	GLN
1	E	420	MET
2	F	47	THR
2	F	431	ASP
2	F	500	ASP
1	A	17	ALA
1	A	149	SER
1	B	26	GLU
1	B	33	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	149	SER
1	B	167	LEU
1	B	249	LEU
1	B	326	ARG
1	B	354	ALA
1	B	372	PRO
2	C	211	LEU
1	E	249	LEU
1	E	502	LYS
2	F	212	GLU
2	F	354	ALA
2	F	379	SER
1	A	112	PRO
1	A	120	GLY
1	A	212	GLU
1	A	309	LYS
1	B	333	MET
1	B	348	CYS
2	C	124	SER
2	C	149	SER
2	C	193	ARG
2	C	212	GLU
2	D	123	LEU
2	D	494	PRO
1	E	212	GLU
2	F	26	GLU
2	F	152	GLN
1	A	167	LEU
1	A	348	CYS
1	A	510	ARG
1	B	52	LYS
1	B	157	SER
1	B	212	GLU
2	C	114	GLY
2	C	347	VAL
2	D	52	LYS
2	D	157	SER
1	E	160	VAL
1	E	276	GLY
1	E	282	SER
1	E	348	CYS
1	E	387	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	398	GLY
2	F	341	GLN
1	A	497	ILE
1	B	117	VAL
2	D	83	ILE
2	D	268	VAL
1	E	189	GLY
2	F	398	GLY
1	A	91	GLY
1	A	433	ILE
1	A	64	ILE
2	C	196	VAL
2	F	517	PRO
1	B	134	ILE
1	B	363	ILE
2	D	347	VAL

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	431/443 (97%)	387 (90%)	44 (10%)	7 29
1	B	418/443 (94%)	381 (91%)	37 (9%)	9 35
1	E	419/443 (95%)	373 (89%)	46 (11%)	6 26
2	C	416/444 (94%)	380 (91%)	36 (9%)	10 37
2	D	413/444 (93%)	372 (90%)	41 (10%)	8 30
2	F	432/444 (97%)	386 (89%)	46 (11%)	6 27
All	All	2529/2661 (95%)	2279 (90%)	250 (10%)	8 30

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	33	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	38	ILE
1	A	75	THR
1	A	79	THR
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	118	VAL
1	A	121	PHE
1	A	123	LEU
1	A	140	ARG
1	A	151	PHE
1	A	154	TYR
1	A	158	SER
1	A	182	THR
1	A	185	ILE
1	A	186	GLU
1	A	201	SER
1	A	209	ASN
1	A	212	GLU
1	A	218	ARG
1	A	223	LEU
1	A	256	GLN
1	A	260	ASN
1	A	263	VAL
1	A	270	LEU
1	A	287	THR
1	A	303	GLU
1	A	342	ASN
1	A	360	LEU
1	A	371	LYS
1	A	375	ILE
1	A	428	SER
1	A	431	ASP
1	A	434	THR
1	A	451	ARG
1	A	462	TRP
1	A	470	PHE
1	A	471	MET
1	A	500	ASP
1	A	508	ILE
1	A	509	VAL
1	A	518	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	26	GLU
1	B	81	GLN
1	B	99	ASP
1	B	111	ASP
1	B	123	LEU
1	B	128	GLU
1	B	140	ARG
1	B	151	PHE
1	B	154	TYR
1	B	164	LEU
1	B	182	THR
1	B	185	ILE
1	B	186	GLU
1	B	212	GLU
1	B	218	ARG
1	B	223	LEU
1	B	240	THR
1	B	256	GLN
1	B	263	VAL
1	B	270	LEU
1	B	320	SER
1	B	333	MET
1	B	342	ASN
1	B	360	LEU
1	B	371	LYS
1	B	375	ILE
1	B	440	LEU
1	B	451	ARG
1	B	458	MET
1	B	462	TRP
1	B	470	PHE
1	B	471	MET
1	B	474	ASP
1	B	485	ASN
1	B	499	VAL
1	B	501	GLU
1	B	502	LYS
2	C	15	HIS
2	C	26	GLU
2	C	45	SER
2	C	50	THR
2	C	64	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	81	GLN
2	C	99	ASP
2	C	111	ASP
2	C	135	GLN
2	C	140	ARG
2	C	151	PHE
2	C	154	TYR
2	C	186	GLU
2	C	209	ASN
2	C	212	GLU
2	C	218	ARG
2	C	223	LEU
2	C	240	THR
2	C	256	GLN
2	C	263	VAL
2	C	270	LEU
2	C	303	GLU
2	C	333	MET
2	C	336	GLU
2	C	338	MET
2	C	344	LEU
2	C	371	LYS
2	C	375	ILE
2	C	400	THR
2	C	432	THR
2	C	439	LEU
2	C	451	ARG
2	C	454	ASN
2	C	470	PHE
2	C	498	THR
2	C	500	ASP
2	D	26	GLU
2	D	38	ILE
2	D	50	THR
2	D	75	THR
2	D	79	THR
2	D	81	GLN
2	D	89	SER
2	D	106	LEU
2	D	122	ASP
2	D	123	LEU
2	D	124	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	151	PHE
2	D	154	TYR
2	D	185	ILE
2	D	186	GLU
2	D	197	GLU
2	D	212	GLU
2	D	218	ARG
2	D	223	LEU
2	D	240	THR
2	D	256	GLN
2	D	263	VAL
2	D	270	LEU
2	D	284	ILE
2	D	292	THR
2	D	321	ARG
2	D	342	ASN
2	D	356	LEU
2	D	360	LEU
2	D	371	LYS
2	D	375	ILE
2	D	428	SER
2	D	431	ASP
2	D	451	ARG
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	30	ASP
1	E	38	ILE
1	E	45	SER
1	E	47	THR
1	E	79	THR
1	E	81	GLN
1	E	99	ASP
1	E	106	LEU
1	E	121	PHE
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	183	GLU
1	E	186	GLU
1	E	201	SER
1	E	203	ASN
1	E	212	GLU
1	E	218	ARG
1	E	220	LEU
1	E	221	GLU
1	E	223	LEU
1	E	228	THR
1	E	230	HIS
1	E	238	THR
1	E	245	ASN
1	E	256	GLN
1	E	260	ASN
1	E	263	VAL
1	E	270	LEU
1	E	287	THR
1	E	338	MET
1	E	342	ASN
1	E	366	GLU
1	E	371	LYS
1	E	375	ILE
1	E	431	ASP
1	E	451	ARG
1	E	458	MET
1	E	461	SER
1	E	471	MET
1	E	474	ASP
1	E	501	GLU
1	E	503	SER
1	E	505	LEU
2	F	15	HIS
2	F	26	GLU
2	F	33	HIS
2	F	53	THR
2	F	73	PHE
2	F	77	GLU
2	F	79	THR
2	F	99	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	106	LEU
2	F	115	GLN
2	F	121	PHE
2	F	140	ARG
2	F	151	PHE
2	F	154	TYR
2	F	181	THR
2	F	183	GLU
2	F	186	GLU
2	F	209	ASN
2	F	212	GLU
2	F	218	ARG
2	F	225	LEU
2	F	256	GLN
2	F	263	VAL
2	F	270	LEU
2	F	287	THR
2	F	300	ARG
2	F	302	VAL
2	F	321	ARG
2	F	325	LEU
2	F	360	LEU
2	F	371	LYS
2	F	379	SER
2	F	424	SER
2	F	431	ASP
2	F	451	ARG
2	F	458	MET
2	F	462	TRP
2	F	469	GLU
2	F	471	MET
2	F	496	ARG
2	F	501	GLU
2	F	504	GLU
2	F	507	ARG
2	F	509	VAL
2	F	514	GLU
2	F	515	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	62	ASN
1	A	81	GLN
1	A	209	ASN
1	A	323	GLN
1	A	414	ASN
1	A	441	GLN
1	B	15	HIS
1	B	62	ASN
1	B	209	ASN
1	B	256	GLN
1	B	323	GLN
1	B	361	GLN
1	B	368	ASN
1	B	414	ASN
1	B	441	GLN
2	C	33	HIS
2	C	58	GLN
2	C	62	ASN
2	C	81	GLN
2	C	209	ASN
2	C	323	GLN
2	C	361	GLN
2	C	389	ASN
2	C	414	ASN
2	C	429	HIS
2	C	441	GLN
2	D	33	HIS
2	D	62	ASN
2	D	209	ASN
2	D	323	GLN
2	D	361	GLN
2	D	418	GLN
2	D	441	GLN
1	E	15	HIS
1	E	33	HIS
1	E	81	GLN
1	E	245	ASN
1	E	304	ASN
1	E	323	GLN
1	E	327	ASN
1	E	361	GLN
1	E	368	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	414	ASN
1	E	418	GLN
1	E	429	HIS
1	E	441	GLN
2	F	16	GLN
2	F	115	GLN
2	F	209	ASN
2	F	368	ASN
2	F	389	ASN
2	F	414	ASN
2	F	418	GLN
2	F	454	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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	TPO	A	432	1	8,10,11	0.92	0	10,14,16	1.75	2 (20%)
1	TPO	E	432	1	8,10,11	1.18	0	10,14,16	1.91	2 (20%)
1	TPO	B	432	1	8,10,11	0.86	0	10,14,16	1.50	2 (20%)

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	TPO	A	432	1	-	1/9/11/13	-
1	TPO	E	432	1	-	2/9/11/13	-
1	TPO	B	432	1	-	5/9/11/13	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	432	TPO	P-OG1-CB	-5.12	107.75	123.21
1	A	432	TPO	P-OG1-CB	-4.37	110.02	123.21
1	B	432	TPO	CG2-CB-CA	-3.24	106.77	113.16
1	A	432	TPO	CG2-CB-CA	-2.80	107.65	113.16
1	B	432	TPO	P-OG1-CB	-2.59	115.40	123.21
1	E	432	TPO	CG2-CB-CA	-2.32	108.58	113.16

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	432	TPO	2	0
1	B	432	TPO	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 20 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	B	901	-	26,33,33	1.26	4 (15%)	31,52,52	1.67	4 (12%)
4	ATP	B	903	3	26,33,33	1.28	3 (11%)	31,52,52	1.86	7 (22%)
4	ATP	F	901	3	26,33,33	1.37	3 (11%)	31,52,52	1.73	5 (16%)
4	ATP	A	901	3	26,33,33	1.34	3 (11%)	31,52,52	1.75	6 (19%)
4	ATP	E	903	3	26,33,33	1.30	3 (11%)	31,52,52	1.97	6 (19%)
4	ATP	D	901	3	26,33,33	1.30	3 (11%)	31,52,52	1.75	7 (22%)
4	ATP	E	901	3	26,33,33	1.34	1 (3%)	31,52,52	1.82	5 (16%)
4	ATP	A	903	3	26,33,33	1.23	3 (11%)	31,52,52	1.85	7 (22%)
4	ATP	F	903	3	26,33,33	1.32	1 (3%)	31,52,52	1.85	6 (19%)
4	ATP	C	901	3	26,33,33	1.26	2 (7%)	31,52,52	1.78	7 (22%)
4	ATP	D	903	3	26,33,33	1.43	5 (19%)	31,52,52	1.89	6 (19%)
4	ATP	C	903	3	26,33,33	1.35	3 (11%)	31,52,52	1.79	4 (12%)

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	B	901	-	-	5/18/38/38	0/3/3/3
4	ATP	B	903	3	-	8/18/38/38	0/3/3/3
4	ATP	F	901	3	-	8/18/38/38	0/3/3/3
4	ATP	A	901	3	-	7/18/38/38	0/3/3/3
4	ATP	E	903	3	-	8/18/38/38	0/3/3/3
4	ATP	D	901	3	-	7/18/38/38	0/3/3/3
4	ATP	E	901	3	-	6/18/38/38	0/3/3/3
4	ATP	A	903	3	-	8/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	F	903	3	-	7/18/38/38	0/3/3/3
4	ATP	C	901	3	-	8/18/38/38	0/3/3/3
4	ATP	D	903	3	-	10/18/38/38	0/3/3/3
4	ATP	C	903	3	-	7/18/38/38	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	903	ATP	C2-N3	4.99	1.40	1.32
4	F	901	ATP	C2-N3	4.49	1.39	1.32
4	E	903	ATP	C2-N3	4.42	1.39	1.32
4	E	901	ATP	C2-N3	4.32	1.39	1.32
4	D	903	ATP	C2-N3	4.29	1.39	1.32
4	A	901	ATP	C2-N3	4.25	1.38	1.32
4	B	903	ATP	C2-N3	4.01	1.38	1.32
4	C	901	ATP	C2-N3	3.96	1.38	1.32
4	D	901	ATP	C2-N3	3.87	1.38	1.32
4	C	903	ATP	C2-N3	3.56	1.37	1.32
4	A	903	ATP	C2-N3	3.51	1.37	1.32
4	F	901	ATP	O4'-C1'	3.02	1.45	1.41
4	C	903	ATP	C2'-C1'	-2.93	1.49	1.53
4	A	903	ATP	O4'-C1'	2.93	1.45	1.41
4	B	901	ATP	C2-N3	2.92	1.36	1.32
4	D	903	ATP	C4-N3	2.62	1.39	1.35
4	E	903	ATP	O4'-C1'	2.60	1.44	1.41
4	B	901	ATP	C2-N1	2.55	1.38	1.33
4	B	903	ATP	O4'-C1'	2.54	1.44	1.41
4	A	901	ATP	O4'-C1'	2.53	1.44	1.41
4	B	901	ATP	O4'-C1'	2.48	1.44	1.41
4	A	903	ATP	C2-N1	2.35	1.38	1.33
4	D	903	ATP	C2-N1	2.34	1.38	1.33
4	D	901	ATP	C2-N1	2.31	1.38	1.33
4	B	901	ATP	C4-N3	2.30	1.38	1.35
4	D	901	ATP	O4'-C1'	2.29	1.44	1.41
4	D	903	ATP	O4'-C1'	2.27	1.44	1.41
4	E	903	ATP	C8-N7	-2.20	1.30	1.34
4	C	901	ATP	O4'-C1'	2.15	1.44	1.41
4	B	903	ATP	C2-N1	2.11	1.37	1.33
4	A	901	ATP	C2'-C1'	-2.08	1.50	1.53
4	D	903	ATP	C2'-C1'	-2.07	1.50	1.53
4	C	903	ATP	C2-N1	2.02	1.37	1.33
4	F	901	ATP	C2-N1	2.01	1.37	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	903	ATP	N3-C2-N1	-5.88	119.49	128.68
4	E	903	ATP	N3-C2-N1	-5.79	119.63	128.68
4	B	901	ATP	N3-C2-N1	-5.69	119.79	128.68
4	E	901	ATP	N3-C2-N1	-5.68	119.81	128.68
4	C	903	ATP	N3-C2-N1	-5.66	119.84	128.68
4	A	903	ATP	N3-C2-N1	-5.61	119.90	128.68
4	C	901	ATP	N3-C2-N1	-5.56	119.99	128.68
4	A	901	ATP	N3-C2-N1	-5.55	120.00	128.68
4	B	903	ATP	N3-C2-N1	-5.52	120.05	128.68
4	D	901	ATP	N3-C2-N1	-5.46	120.14	128.68
4	F	901	ATP	N3-C2-N1	-5.45	120.16	128.68
4	F	903	ATP	N3-C2-N1	-5.41	120.23	128.68
4	E	903	ATP	C4-C5-N7	-4.81	104.38	109.40
4	F	903	ATP	C4-C5-N7	-4.67	104.54	109.40
4	B	903	ATP	C4-C5-N7	-4.42	104.80	109.40
4	D	903	ATP	C5-C6-N6	4.37	126.99	120.35
4	F	901	ATP	C5-C6-N6	4.25	126.81	120.35
4	C	903	ATP	C5-C6-N6	4.24	126.79	120.35
4	B	903	ATP	C5-C6-N6	4.21	126.75	120.35
4	E	903	ATP	C5-C6-N6	4.11	126.59	120.35
4	C	903	ATP	C4-C5-N7	-3.95	105.28	109.40
4	F	901	ATP	C4-C5-N7	-3.95	105.28	109.40
4	C	901	ATP	C5-C6-N6	3.95	126.35	120.35
4	E	901	ATP	C4-C5-N7	-3.92	105.32	109.40
4	E	901	ATP	C5-C6-N6	3.86	126.22	120.35
4	A	901	ATP	C4-C5-N7	-3.86	105.38	109.40
4	D	903	ATP	C4-C5-N7	-3.82	105.41	109.40
4	A	901	ATP	C5-C6-N6	3.81	126.15	120.35
4	A	903	ATP	C4-C5-N7	-3.78	105.46	109.40
4	C	901	ATP	C4-C5-N7	-3.73	105.51	109.40
4	B	901	ATP	C4-C5-N7	-3.69	105.55	109.40
4	D	901	ATP	C4-C5-N7	-3.69	105.56	109.40
4	B	901	ATP	C5-C6-N6	3.65	125.89	120.35
4	D	901	ATP	C5-C6-N6	3.64	125.88	120.35
4	F	903	ATP	C5-C6-N6	3.63	125.87	120.35
4	A	903	ATP	PB-O3B-PG	-3.53	120.72	132.83
4	A	903	ATP	C5-C6-N6	3.33	125.41	120.35
4	E	903	ATP	PB-O3B-PG	-3.28	121.59	132.83
4	D	903	ATP	PB-O3B-PG	-3.01	122.48	132.83
4	E	901	ATP	C3'-C2'-C1'	2.66	104.98	100.98
4	D	901	ATP	C3'-C2'-C1'	2.63	104.94	100.98
4	A	903	ATP	O2G-PG-O3B	-2.60	95.93	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	903	ATP	C3'-C2'-C1'	2.50	104.74	100.98
4	A	901	ATP	PB-O3B-PG	-2.48	124.30	132.83
4	F	903	ATP	PB-O3B-PG	-2.45	124.41	132.83
4	B	903	ATP	N6-C6-N1	-2.45	113.49	118.57
4	C	901	ATP	C3'-C2'-C1'	2.44	104.66	100.98
4	F	901	ATP	O2'-C2'-C3'	2.42	119.65	111.82
4	D	903	ATP	N6-C6-N1	-2.38	113.64	118.57
4	E	903	ATP	N6-C6-N1	-2.36	113.67	118.57
4	B	901	ATP	O2'-C2'-C3'	2.35	119.43	111.82
4	C	901	ATP	PB-O3B-PG	-2.33	124.85	132.83
4	B	903	ATP	C3'-C2'-C1'	2.31	104.46	100.98
4	D	901	ATP	PB-O3B-PG	-2.30	124.94	132.83
4	B	903	ATP	PB-O3B-PG	-2.28	124.99	132.83
4	C	901	ATP	N6-C6-N1	-2.22	113.97	118.57
4	F	901	ATP	N6-C6-N1	-2.22	113.97	118.57
4	E	903	ATP	O2'-C2'-C3'	2.20	118.95	111.82
4	A	903	ATP	O2'-C2'-C3'	2.20	118.95	111.82
4	C	903	ATP	N6-C6-N1	-2.19	114.03	118.57
4	C	901	ATP	O2'-C2'-C3'	2.17	118.85	111.82
4	B	903	ATP	O2'-C2'-C3'	2.17	118.84	111.82
4	D	901	ATP	C2'-C3'-C4'	2.17	106.86	102.64
4	F	903	ATP	N6-C6-N1	-2.15	114.11	118.57
4	D	903	ATP	O2G-PG-O3B	2.15	111.84	104.64
4	E	901	ATP	N6-C6-N1	-2.14	114.14	118.57
4	A	901	ATP	N6-C6-N1	-2.13	114.16	118.57
4	D	901	ATP	N6-C6-N1	-2.11	114.19	118.57
4	A	901	ATP	C3'-C2'-C1'	2.07	104.09	100.98
4	A	903	ATP	O3B-PG-O1G	2.05	122.54	111.19

There are no chirality outliers.

All (89) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

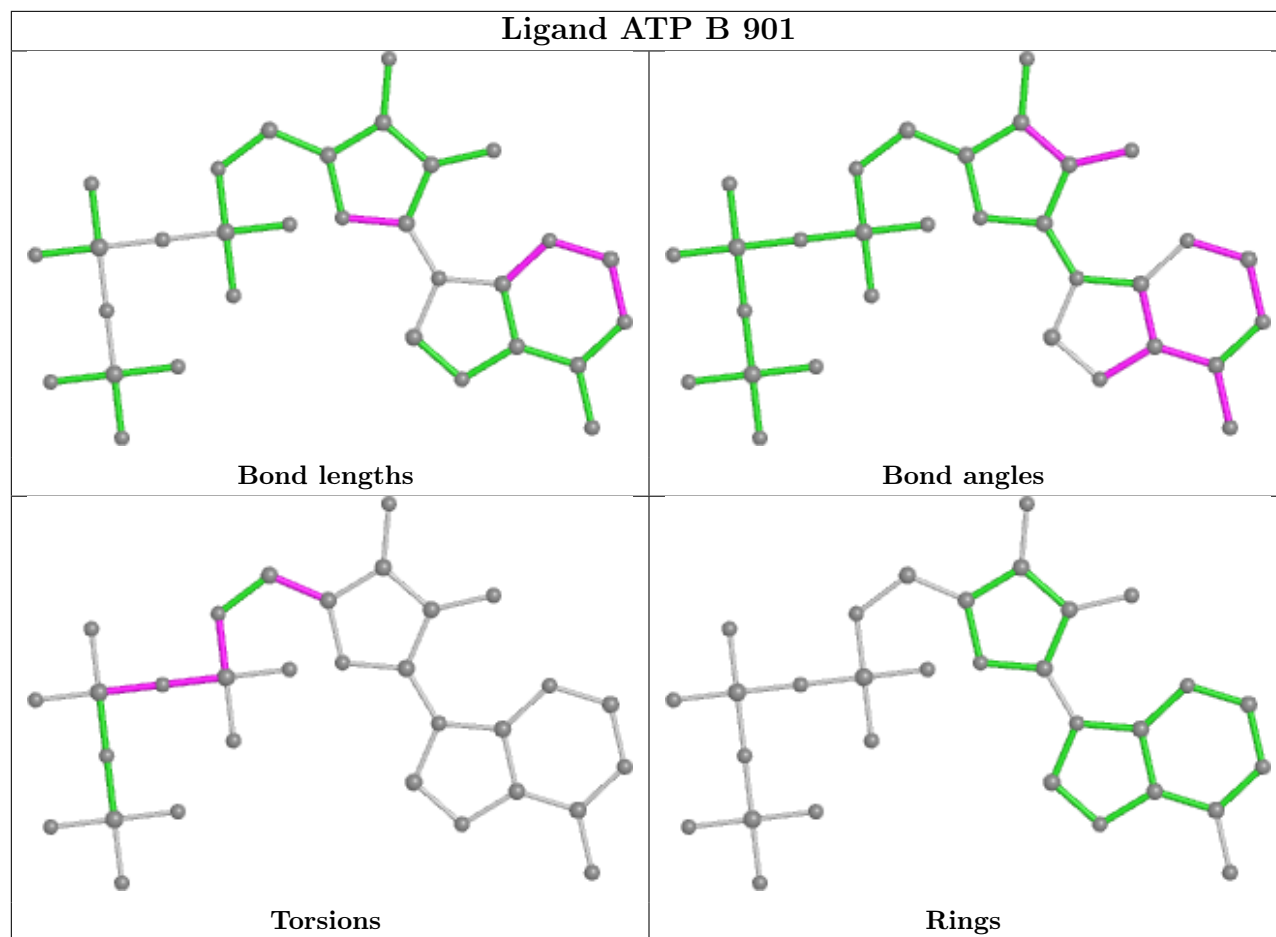
Mol	Chain	Res	Type	Atoms
4	A	901	ATP	PA-O3A-PB-O2B
4	B	901	ATP	PA-O3A-PB-O2B
4	B	903	ATP	PA-O3A-PB-O2B
4	C	901	ATP	PA-O3A-PB-O2B
4	C	903	ATP	PA-O3A-PB-O2B
4	D	901	ATP	PA-O3A-PB-O2B
4	D	903	ATP	PA-O3A-PB-O2B
4	E	901	ATP	PA-O3A-PB-O2B
4	E	903	ATP	PA-O3A-PB-O2B
4	F	901	ATP	PA-O3A-PB-O2B
4	F	903	ATP	PA-O3A-PB-O2B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

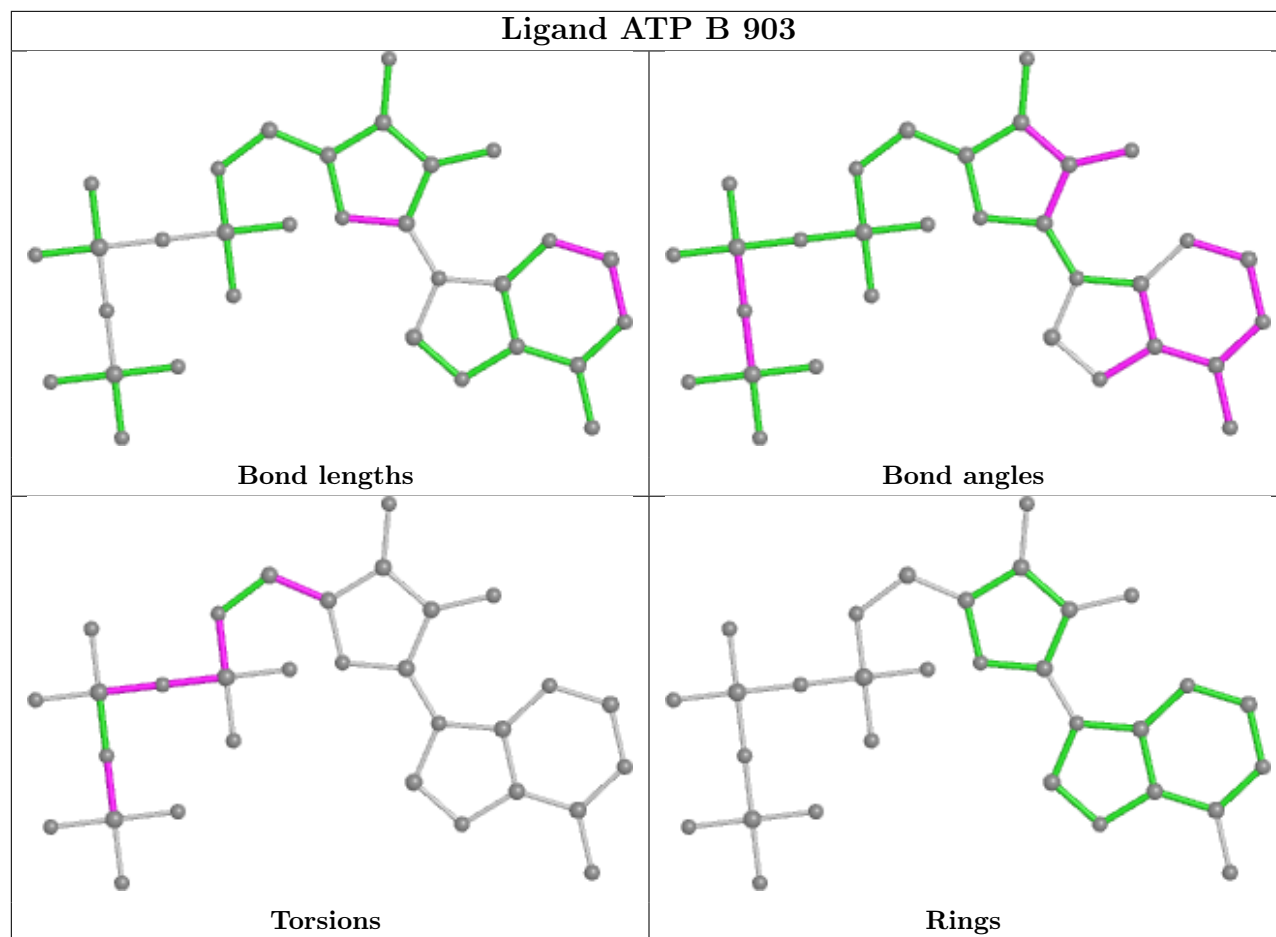
There are no ring outliers.

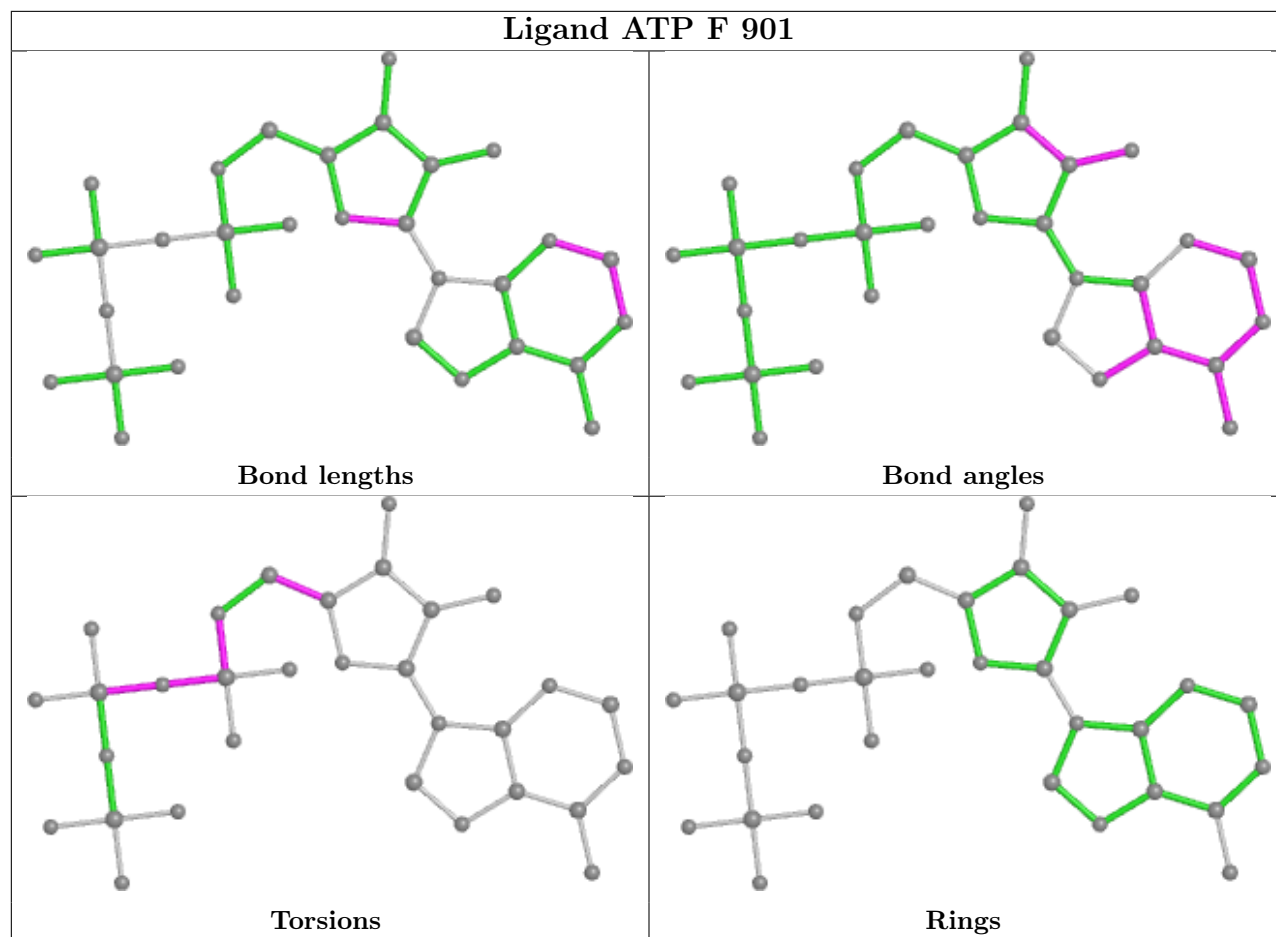
12 monomers are involved in 37 short contacts:

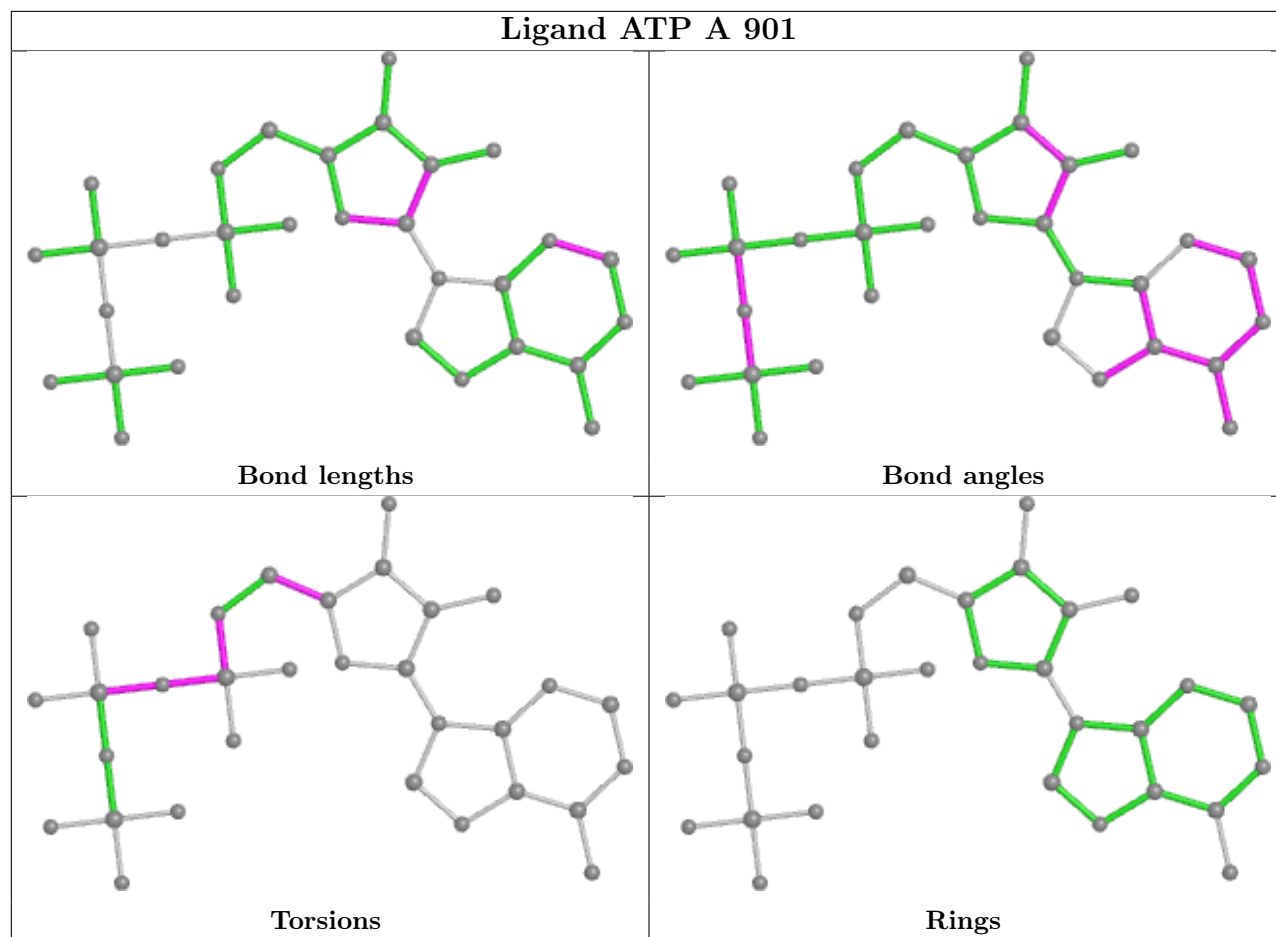
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901	ATP	4	0
4	B	903	ATP	3	0
4	F	901	ATP	5	0
4	A	901	ATP	1	0
4	E	903	ATP	2	0
4	D	901	ATP	4	0
4	E	901	ATP	4	0
4	A	903	ATP	4	0
4	F	903	ATP	4	0
4	C	901	ATP	3	0
4	D	903	ATP	2	0
4	C	903	ATP	1	0

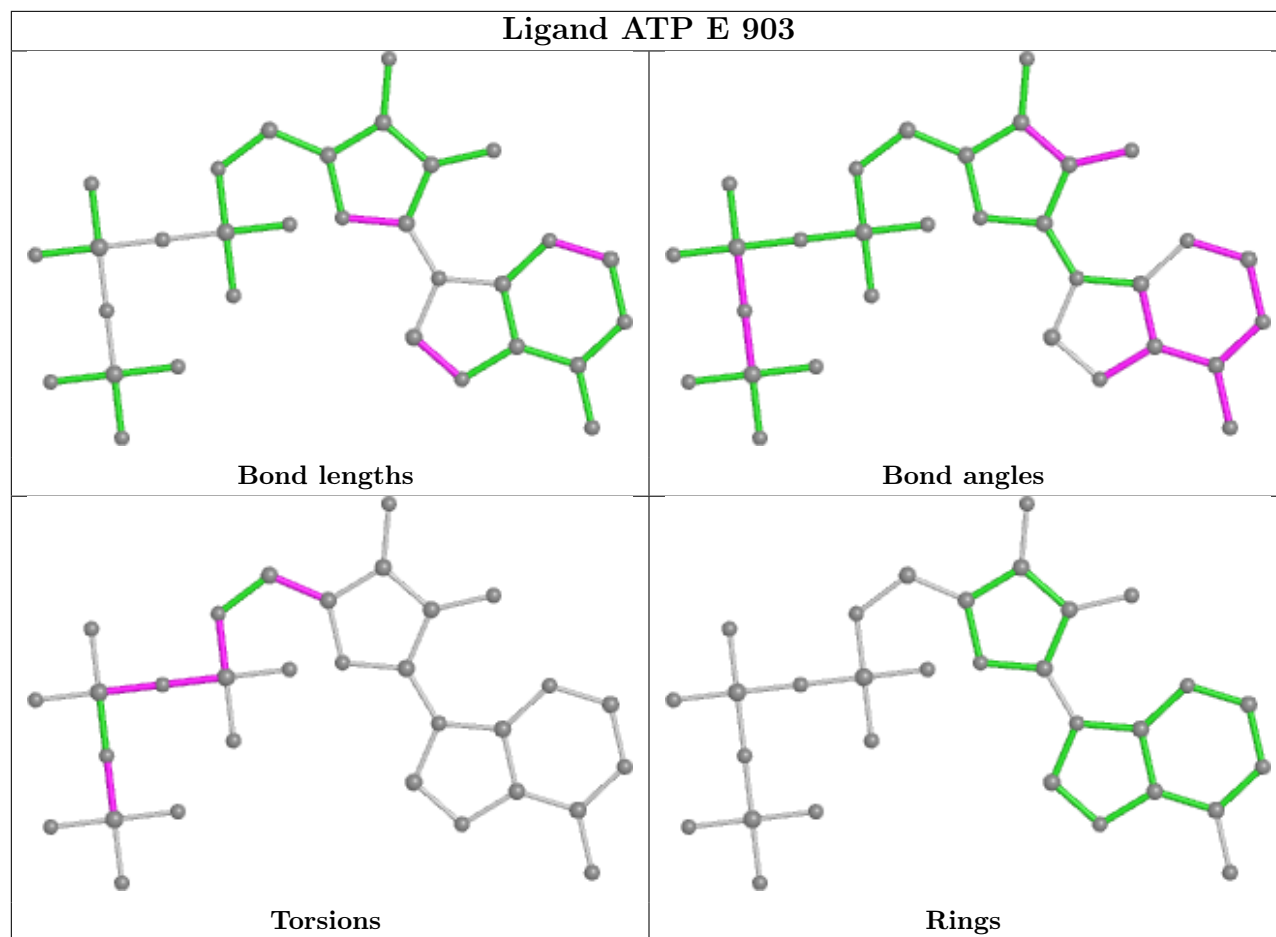
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

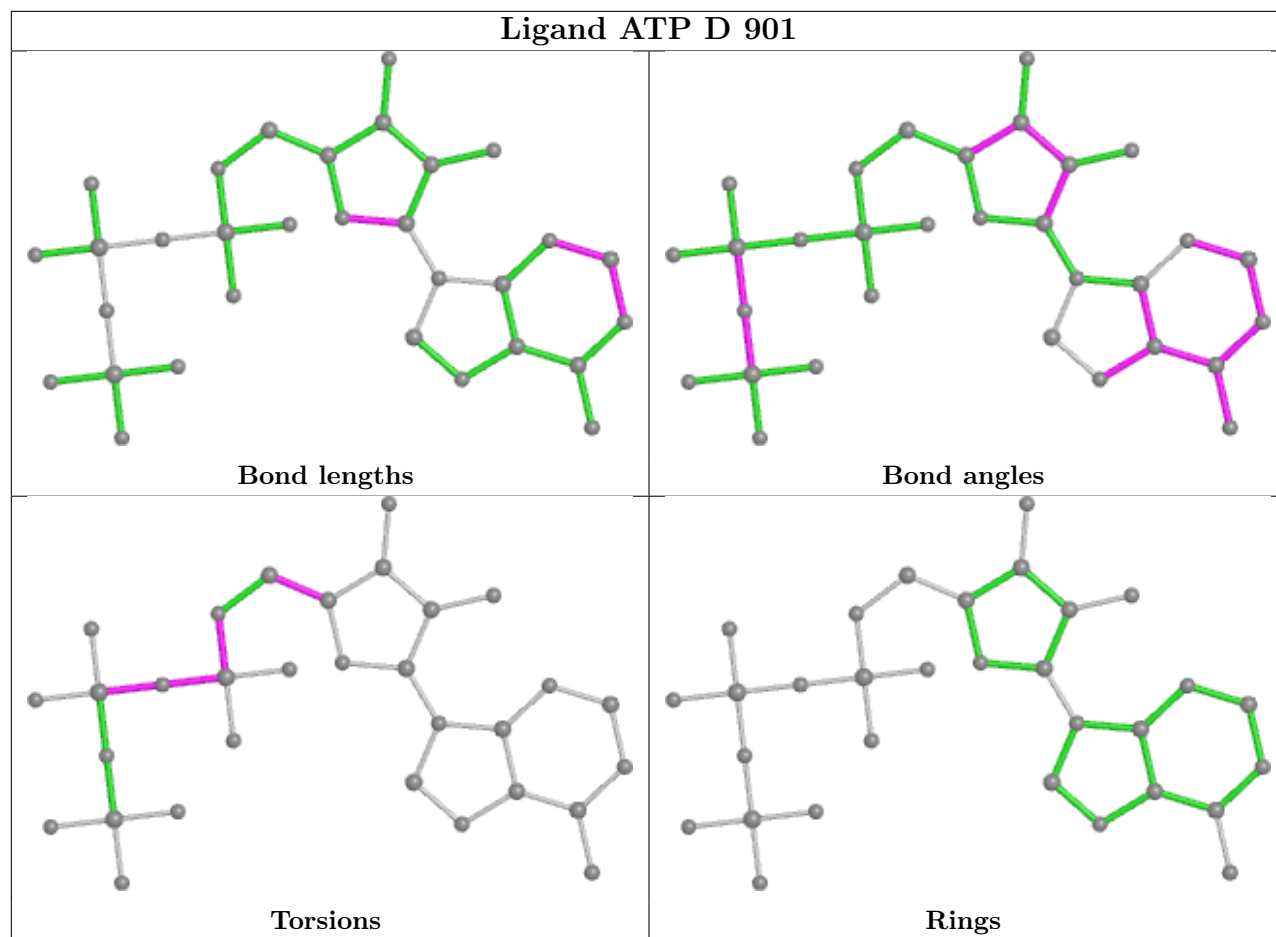


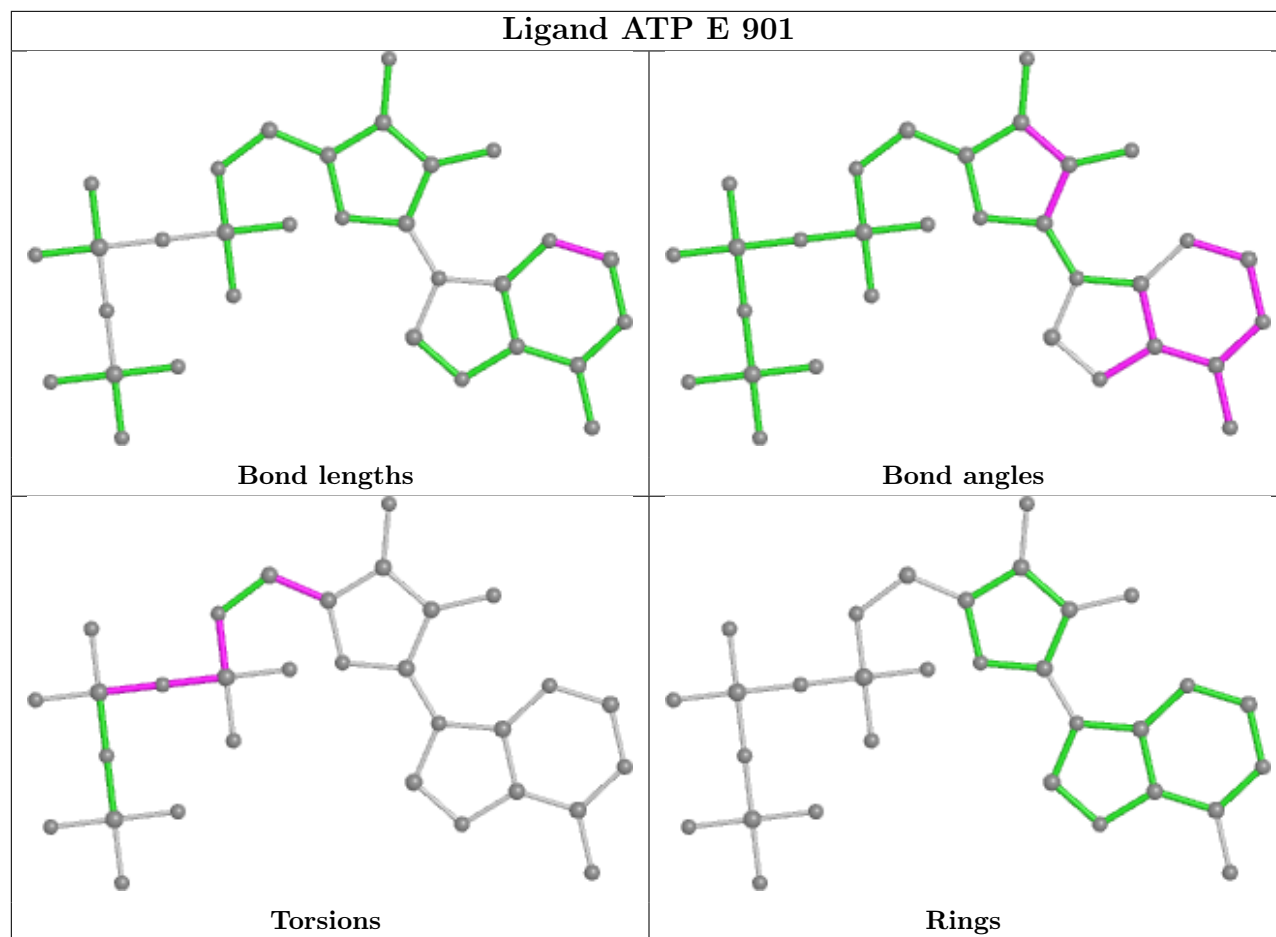


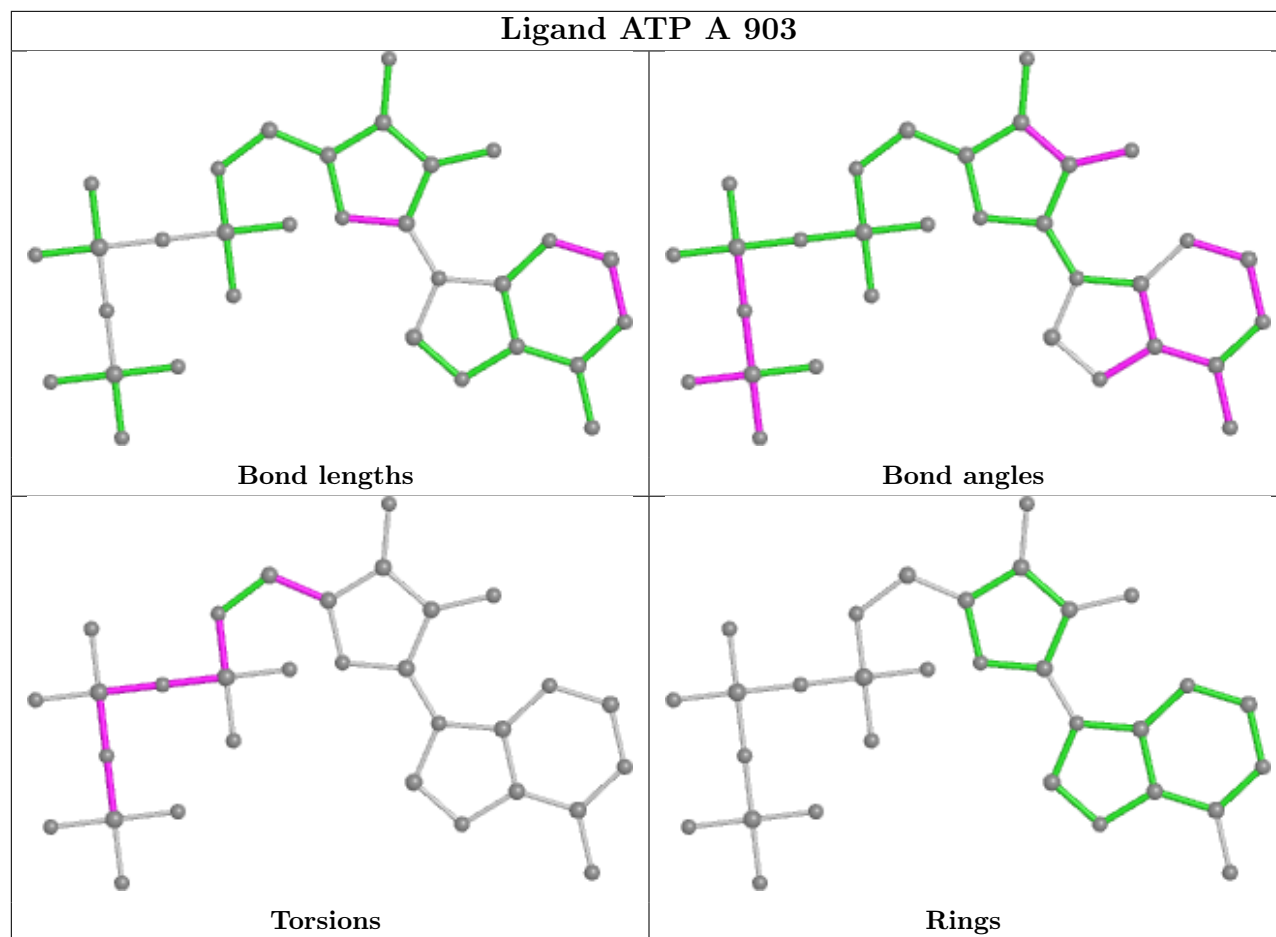


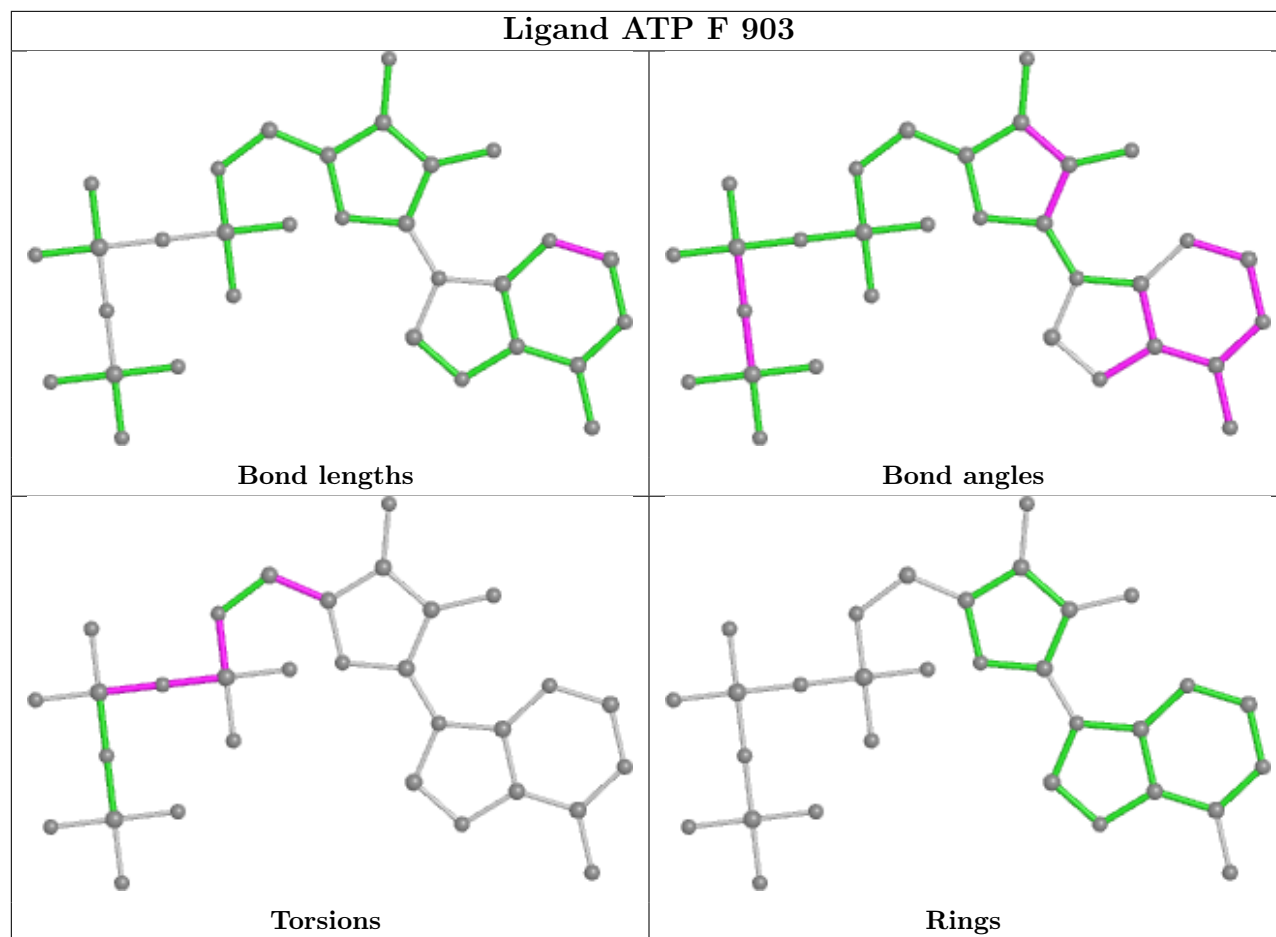


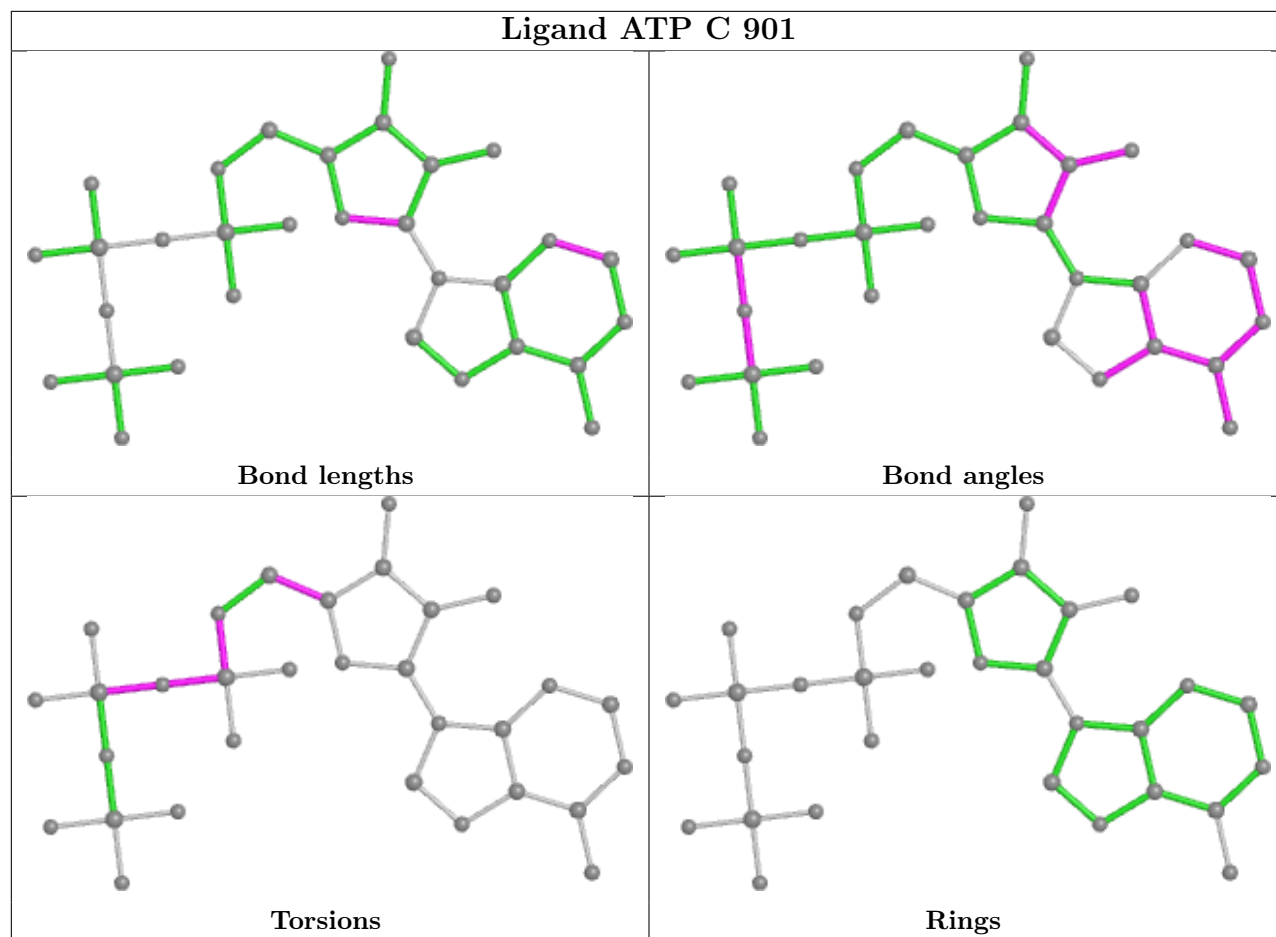


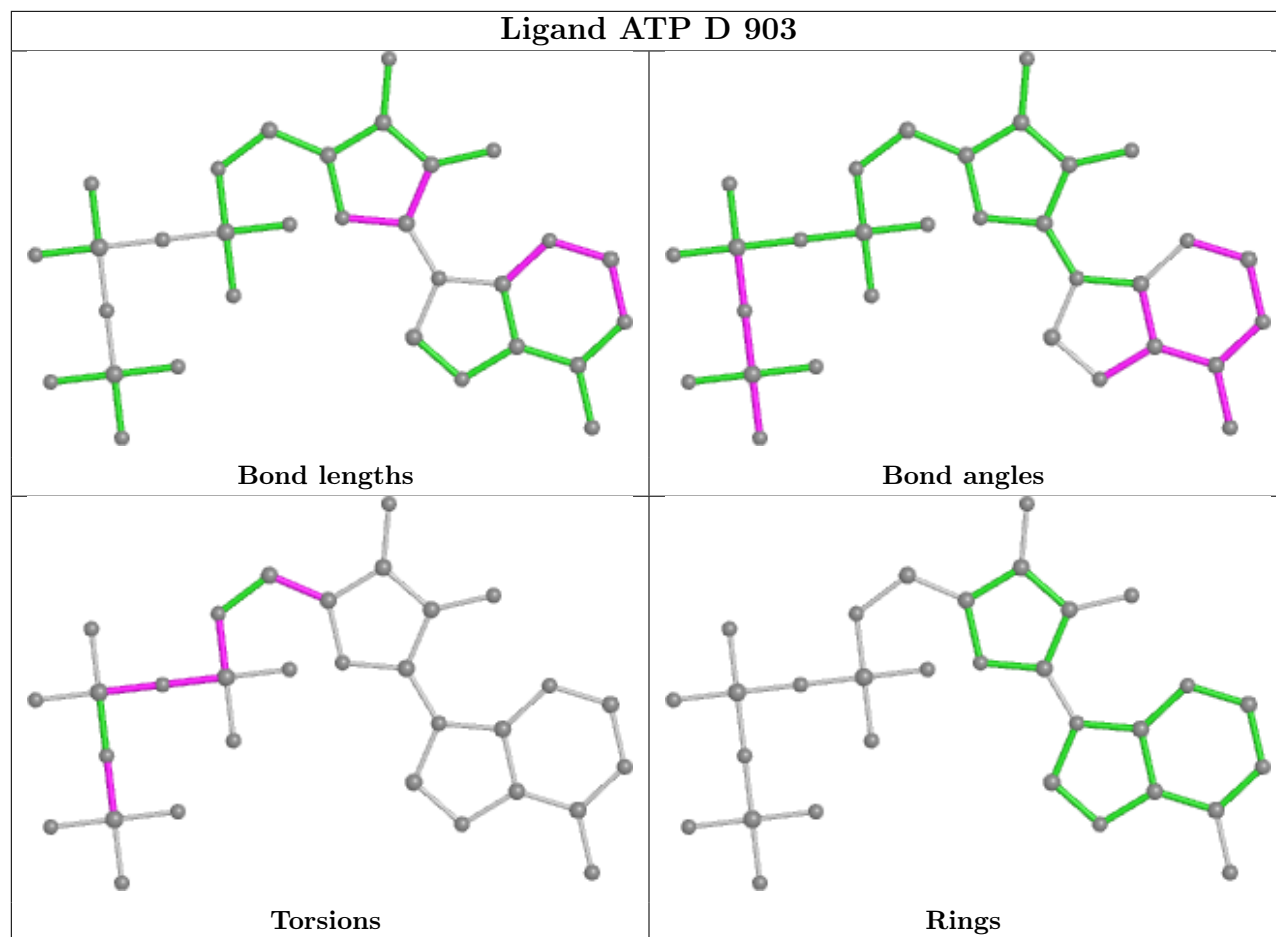


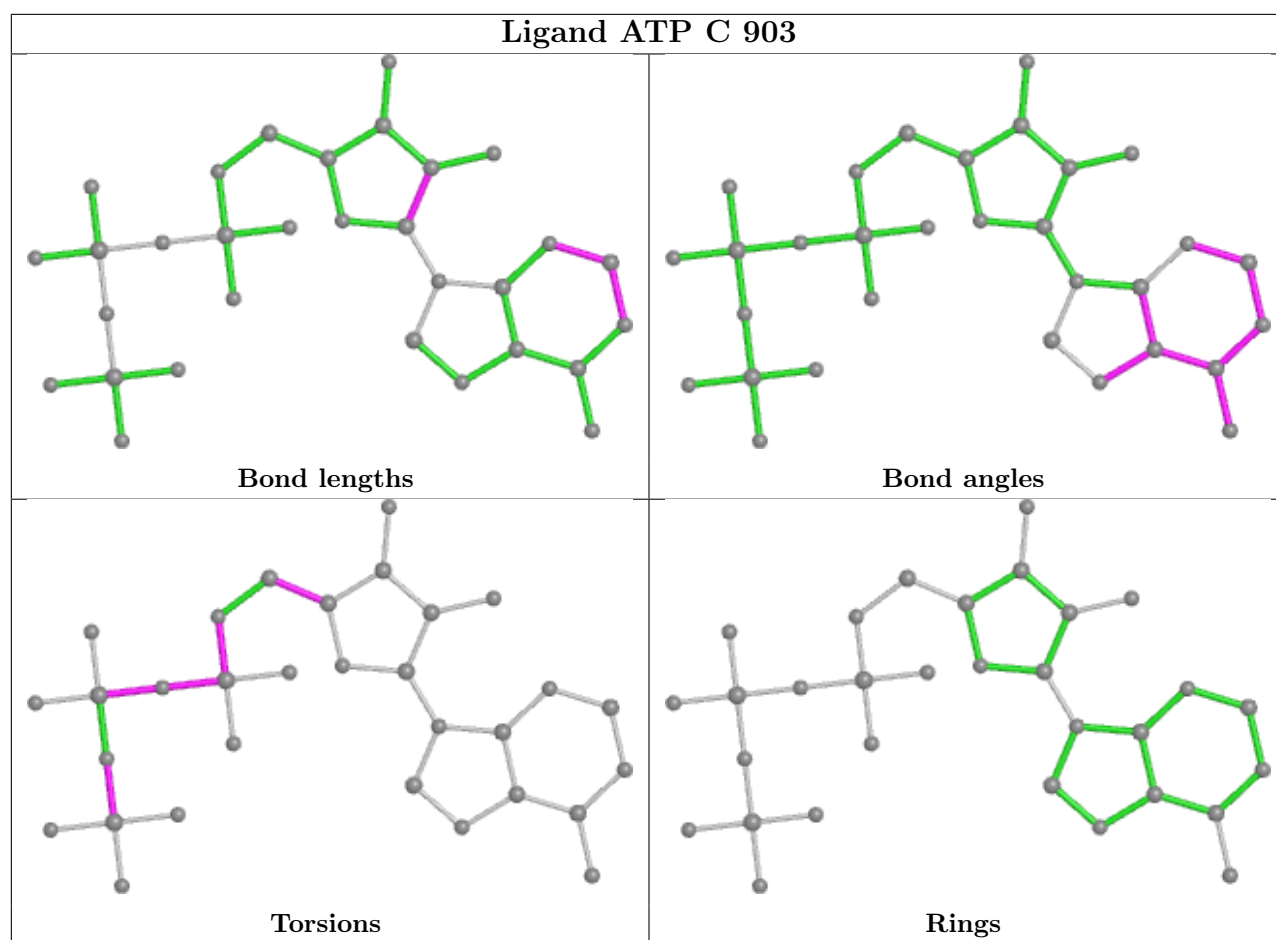












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	505/519 (97%)	0.14	46 (9%) 9 5	30, 83, 129, 159	0
1	B	490/519 (94%)	0.05	20 (4%) 37 24	43, 85, 130, 165	0
1	E	491/519 (94%)	-0.19	11 (2%) 62 48	8, 65, 118, 160	0
2	C	488/519 (94%)	-0.08	17 (3%) 44 28	25, 73, 127, 169	0
2	D	485/519 (93%)	-0.26	15 (3%) 49 32	17, 60, 115, 158	0
2	F	506/519 (97%)	-0.04	28 (5%) 25 14	11, 73, 125, 146	0
All	All	2965/3114 (95%)	-0.06	137 (4%) 32 20	8, 73, 126, 169	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	517	PRO	7.2
1	A	519	SER	6.7
1	A	518	GLU	6.3
2	F	500	ASP	6.3
2	C	500	ASP	6.2
1	A	517	PRO	5.8
1	A	506	SER	5.6
1	E	116	GLU	5.5
2	F	519	SER	5.5
1	A	508	ILE	5.2
2	F	516	GLY	5.1
2	F	513	GLN	5.1
2	C	501	GLU	5.0
2	C	118	VAL	5.0
1	A	511	GLY	5.0
1	A	117	VAL	4.9
1	B	16	GLN	4.8
1	B	121	PHE	4.8
2	F	503	SER	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	500	ASP	4.8
2	F	518	GLU	4.7
1	E	500	ASP	4.6
1	B	117	VAL	4.6
2	F	509	VAL	4.6
1	E	503	SER	4.5
2	C	117	VAL	4.4
2	D	158	SER	4.3
1	B	15	HIS	4.2
1	A	258	SER	4.2
2	F	507	ARG	4.1
2	D	121	PHE	4.1
1	A	253	ARG	4.0
2	D	113	GLU	4.0
1	A	514	GLU	4.0
1	A	516	GLY	4.0
1	B	498	THR	3.9
2	F	515	LYS	3.9
1	B	258	SER	3.8
1	A	507	ARG	3.8
1	A	295	THR	3.8
2	C	119	GLY	3.8
2	F	504	GLU	3.8
1	A	16	GLN	3.7
1	A	500	ASP	3.7
2	D	157	SER	3.6
2	C	143	SER	3.6
1	E	154	TYR	3.6
1	A	503	SER	3.6
2	D	14	GLU	3.5
2	C	145	ASP	3.5
1	A	515	LYS	3.5
2	D	118	VAL	3.5
1	B	255	THR	3.4
2	F	505	LEU	3.4
1	A	513	GLN	3.4
2	F	255	THR	3.4
2	F	512	VAL	3.3
1	A	14	GLU	3.3
2	F	511	GLY	3.3
2	F	506	SER	3.3
1	E	504	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	17	ALA	3.3
1	B	503	SER	3.2
1	A	509	VAL	3.2
1	E	501	GLU	3.1
2	D	15	HIS	3.1
2	D	119	GLY	3.0
1	B	118	VAL	3.0
2	C	115	GLN	2.9
2	D	117	VAL	2.9
2	F	502	LYS	2.9
1	E	502	LYS	2.9
1	A	256	GLN	2.9
2	F	508	ILE	2.8
1	A	15	HIS	2.8
1	B	501	GLU	2.8
2	F	501	GLU	2.8
2	D	16	GLN	2.8
2	C	116	GLU	2.7
1	A	502	LYS	2.7
1	A	496	ARG	2.7
1	E	499	VAL	2.7
1	A	115	GLN	2.7
2	C	173	GLN	2.6
2	D	156	ALA	2.6
1	B	504	GLU	2.6
2	C	499	VAL	2.6
1	E	505	LEU	2.5
2	F	119	GLY	2.5
2	C	181	THR	2.5
1	A	152	GLN	2.5
1	A	501	GLU	2.5
2	F	498	THR	2.4
1	A	378	ASP	2.4
2	C	120	GLY	2.4
1	A	257	ARG	2.4
1	A	504	GLU	2.4
2	F	257	ARG	2.4
1	A	254	LEU	2.4
1	A	498	THR	2.4
2	F	120	GLY	2.4
2	F	334	ASP	2.4
1	B	201	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	499	VAL	2.3
1	E	120	GLY	2.3
1	A	255	THR	2.3
1	B	173	GLN	2.3
1	A	505	LEU	2.3
2	D	120	GLY	2.3
1	B	116	GLU	2.3
2	D	475	LYS	2.2
1	A	116	GLU	2.2
1	A	510	ARG	2.2
1	B	114	GLY	2.2
1	A	121	PHE	2.2
1	A	120	GLY	2.2
1	A	259	SER	2.2
1	A	114	GLY	2.2
1	B	502	LYS	2.2
2	F	154	TYR	2.2
2	D	116	GLU	2.2
1	B	259	SER	2.2
2	F	514	GLU	2.2
1	A	512	VAL	2.1
1	E	121	PHE	2.1
1	A	499	VAL	2.1
2	C	146	SER	2.1
1	B	170	ARG	2.1
2	D	181	THR	2.1
1	A	410	GLY	2.1
2	C	15	HIS	2.1
2	F	448	GLU	2.0
1	A	143	SER	2.0
1	A	249	LEU	2.0
2	C	53	THR	2.0
2	C	14	GLU	2.0
1	B	143	SER	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TPO	B	432	11/12	0.77	0.34	84,94,104,105	0
1	TPO	A	432	11/12	0.84	0.21	82,90,97,97	0
1	TPO	E	432	11/12	0.94	0.19	61,68,76,76	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

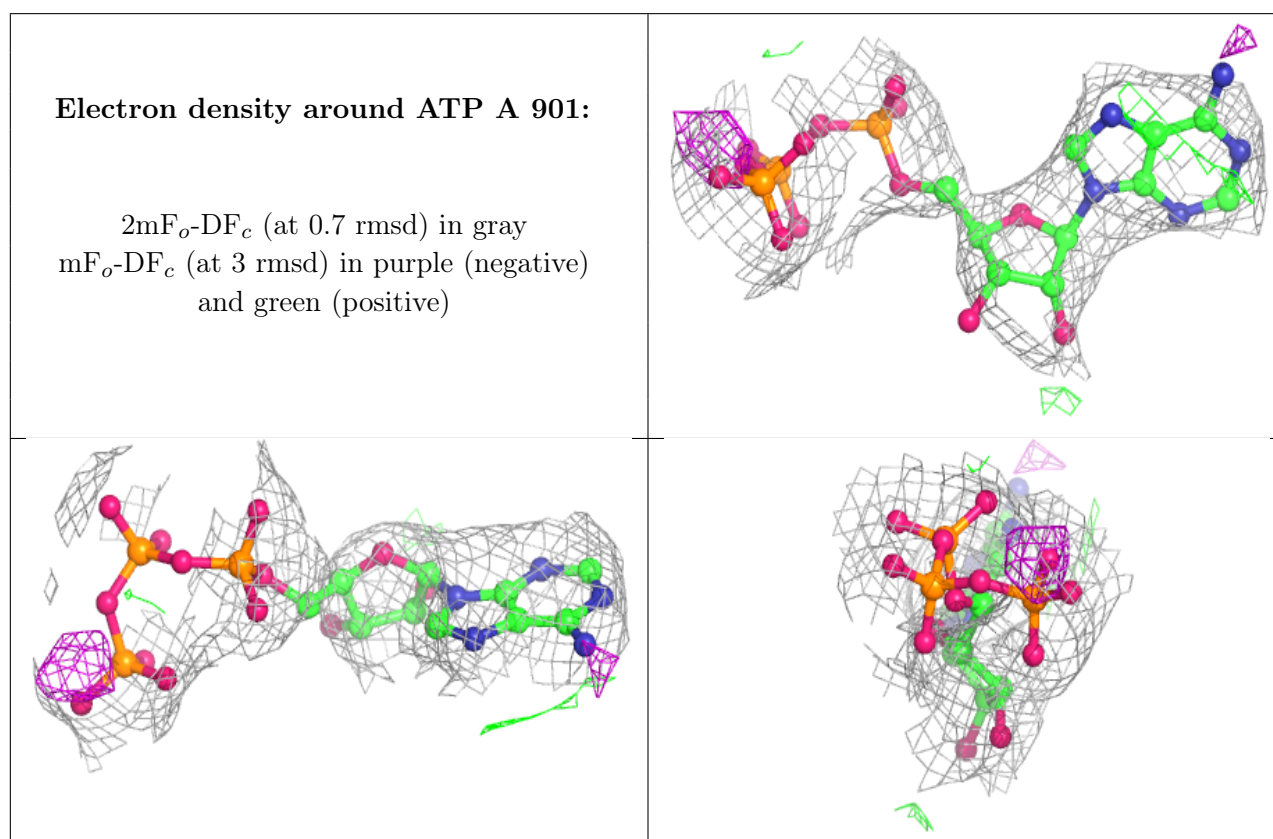
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	702	1/1	0.68	0.62	90,90,90,90	0
3	MG	E	801	1/1	0.72	0.20	25,25,25,25	0
3	MG	C	801	1/1	0.76	0.40	28,28,28,28	0
3	MG	C	701	1/1	0.82	1.17	112,112,112,112	0
3	MG	D	520	1/1	0.83	0.37	25,25,25,25	0
3	MG	A	801	1/1	0.84	0.22	26,26,26,26	0
3	MG	C	702	1/1	0.88	1.16	104,104,104,104	0
4	ATP	A	901	31/31	0.88	0.26	72,82,84,84	0
4	ATP	F	901	31/31	0.88	0.28	93,98,104,104	0
4	ATP	A	903	31/31	0.89	0.25	57,60,67,68	0
4	ATP	E	901	31/31	0.90	0.24	68,74,77,77	0
4	ATP	B	903	31/31	0.90	0.24	62,69,79,80	0
4	ATP	D	903	31/31	0.91	0.27	36,41,61,63	0
4	ATP	B	901	31/31	0.92	0.24	62,71,84,84	0
3	MG	E	702	1/1	0.93	0.36	18,18,18,18	0
4	ATP	C	901	31/31	0.93	0.19	47,54,68,69	0
4	ATP	E	903	31/31	0.93	0.23	24,31,51,52	0
4	ATP	C	903	31/31	0.93	0.21	45,49,77,80	0
4	ATP	D	901	31/31	0.94	0.24	58,63,70,70	0
4	ATP	F	903	31/31	0.94	0.20	27,33,45,47	0
3	MG	E	520	1/1	0.96	0.33	42,42,42,42	0
3	MG	F	702	1/1	0.96	0.22	19,19,19,19	0
3	MG	A	520	1/1	0.97	0.39	113,113,113,113	0
3	MG	E	701	1/1	0.97	0.94	91,91,91,91	0
3	MG	B	701	1/1	0.97	0.61	69,69,69,69	0
3	MG	C	802	1/1	0.97	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

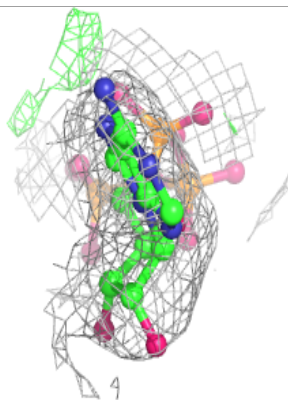
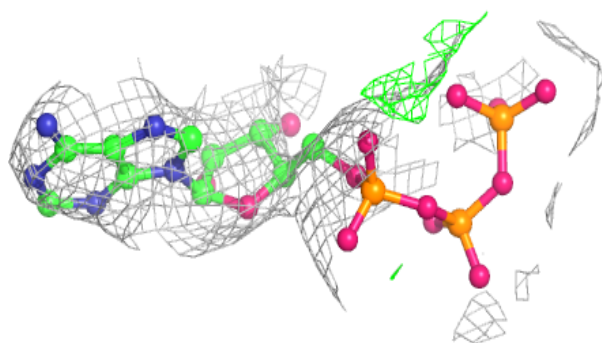
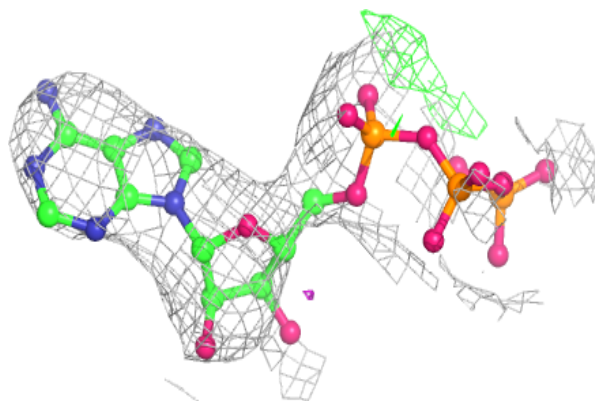
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	F	701	1/1	0.97	0.39	60,60,60,60	0
3	MG	A	701	1/1	0.97	0.51	75,75,75,75	0
3	MG	F	801	1/1	0.98	0.36	40,40,40,40	0
3	MG	D	801	1/1	0.98	0.08	26,26,26,26	0
3	MG	A	802	1/1	0.98	0.42	44,44,44,44	0
3	MG	D	702	1/1	0.99	0.70	90,90,90,90	0

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

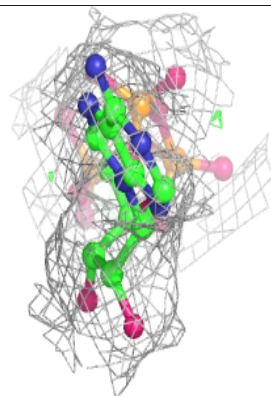
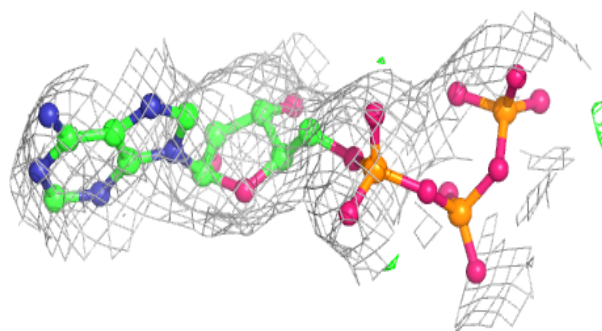
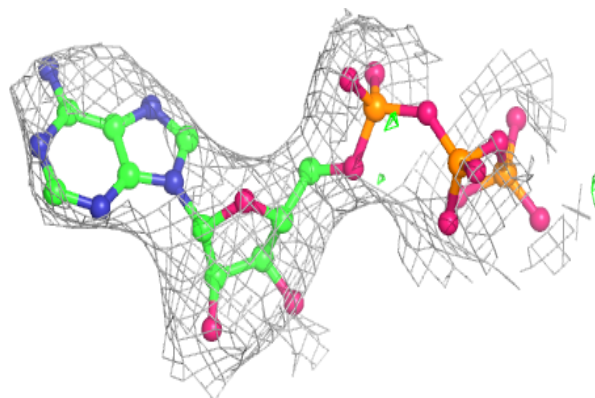


Electron density around ATP F 901:

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

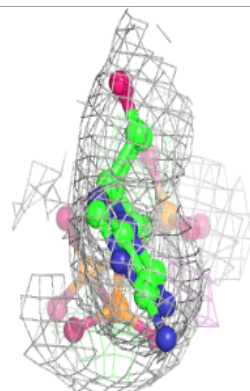
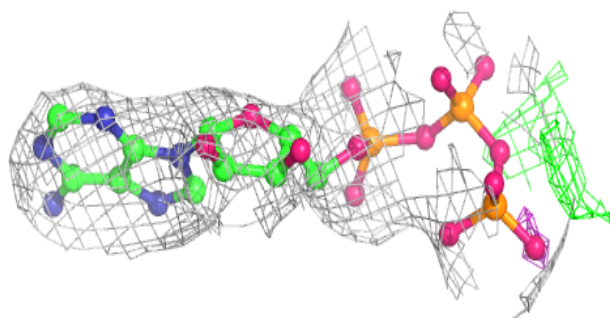
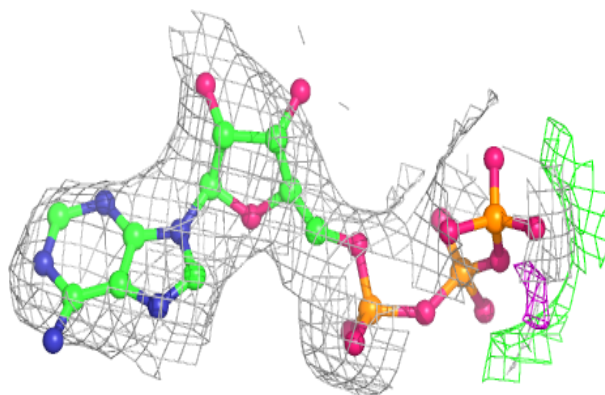
**Electron density around ATP A 903:**

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

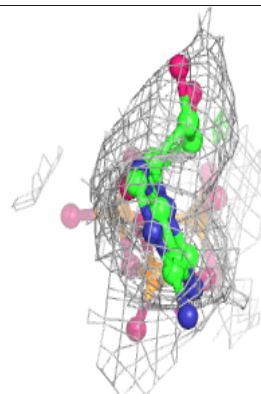
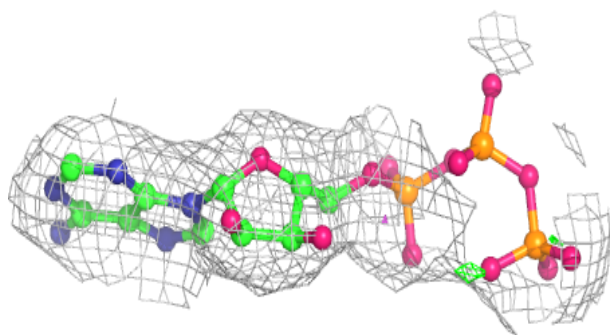
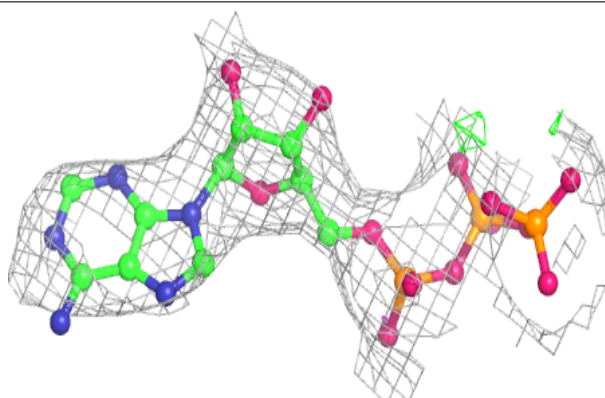


Electron density around ATP E 901:

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

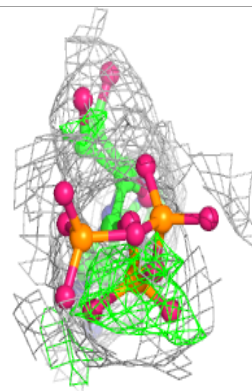
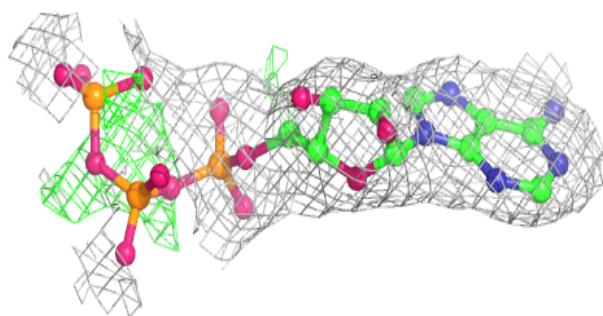
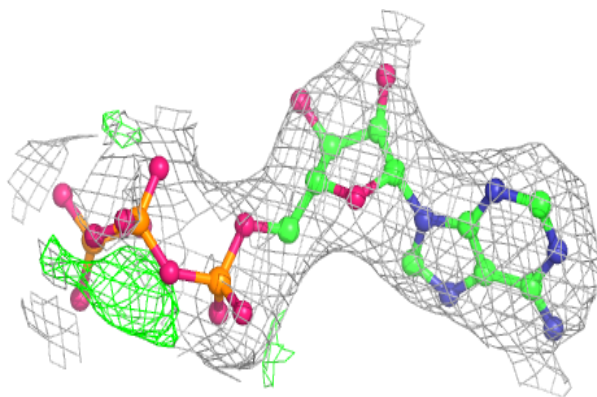
**Electron density around ATP B 903:**

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

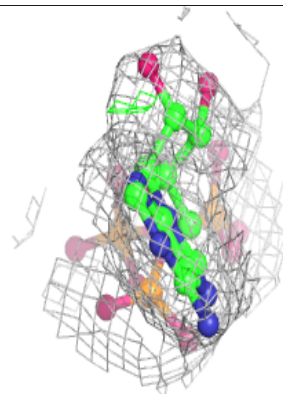
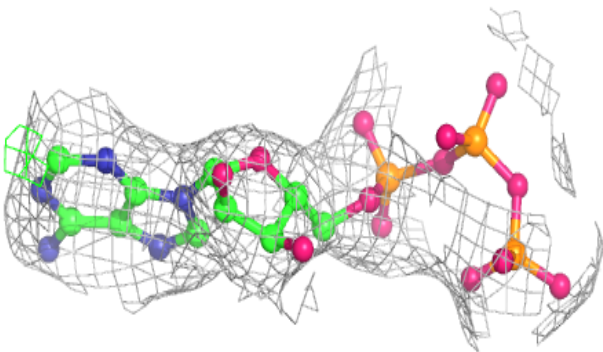
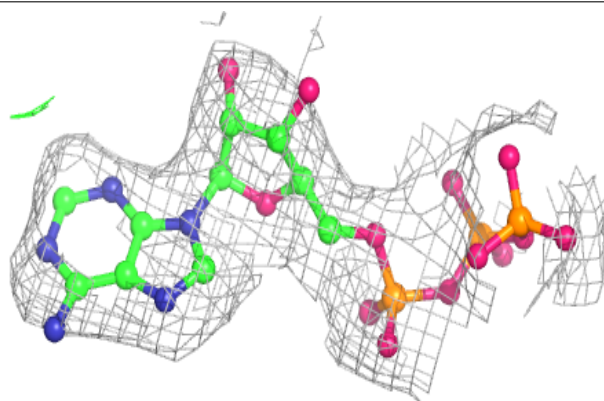


Electron density around ATP D 903:

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

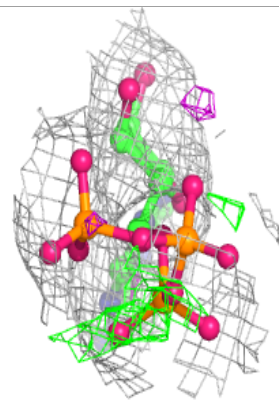
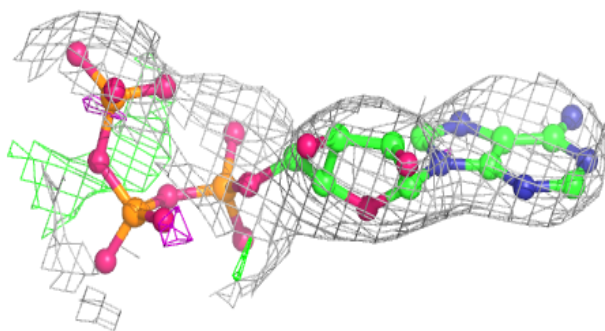
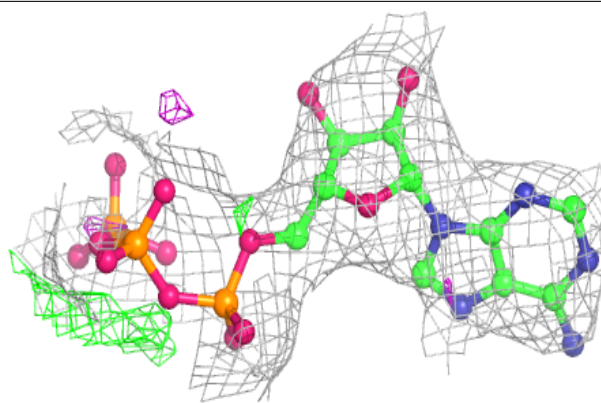
**Electron density around ATP B 901:**

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

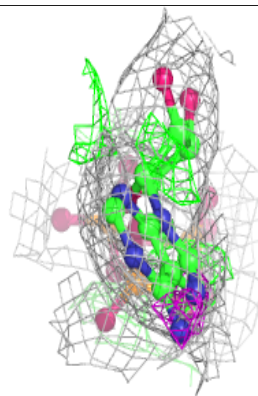
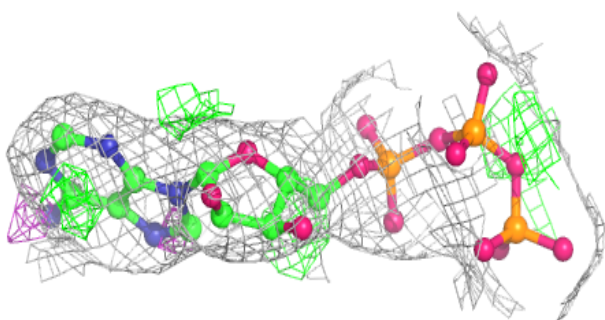
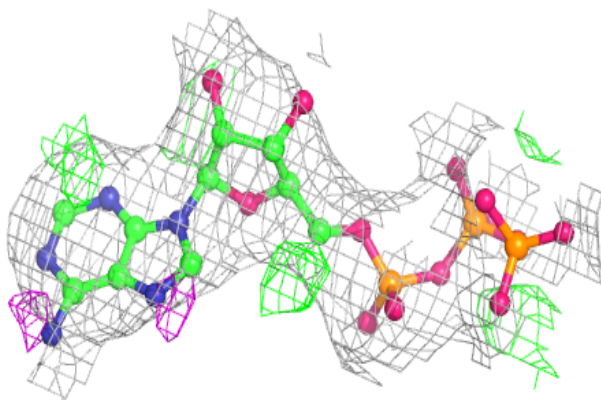


Electron density around ATP C 901:

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

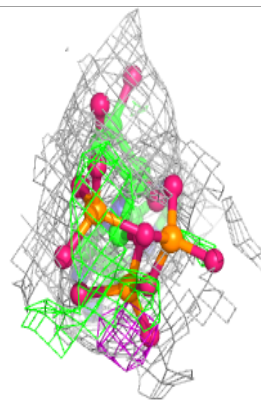
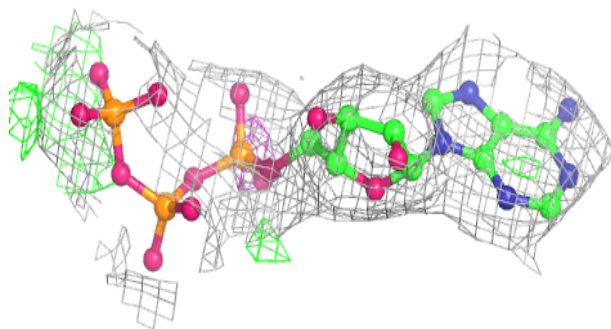
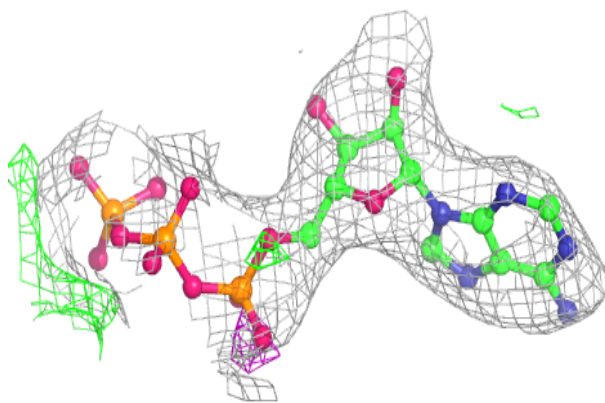
**Electron density around ATP E 903:**

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

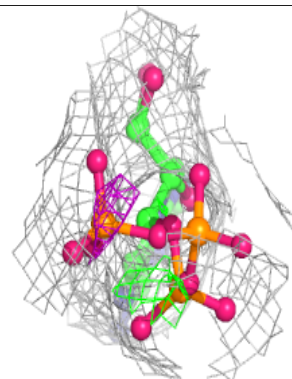
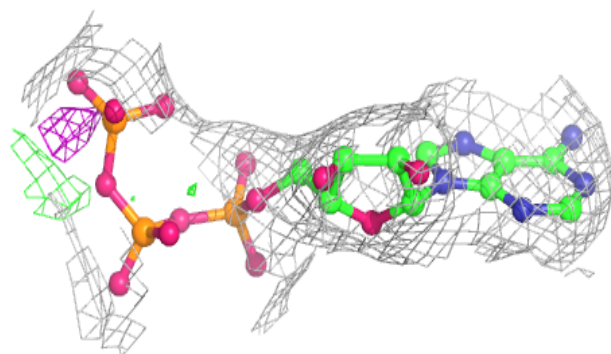
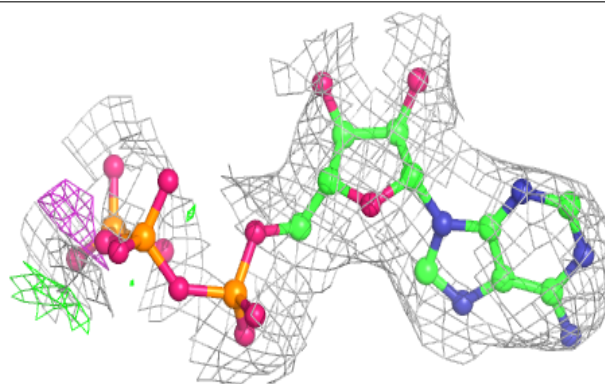


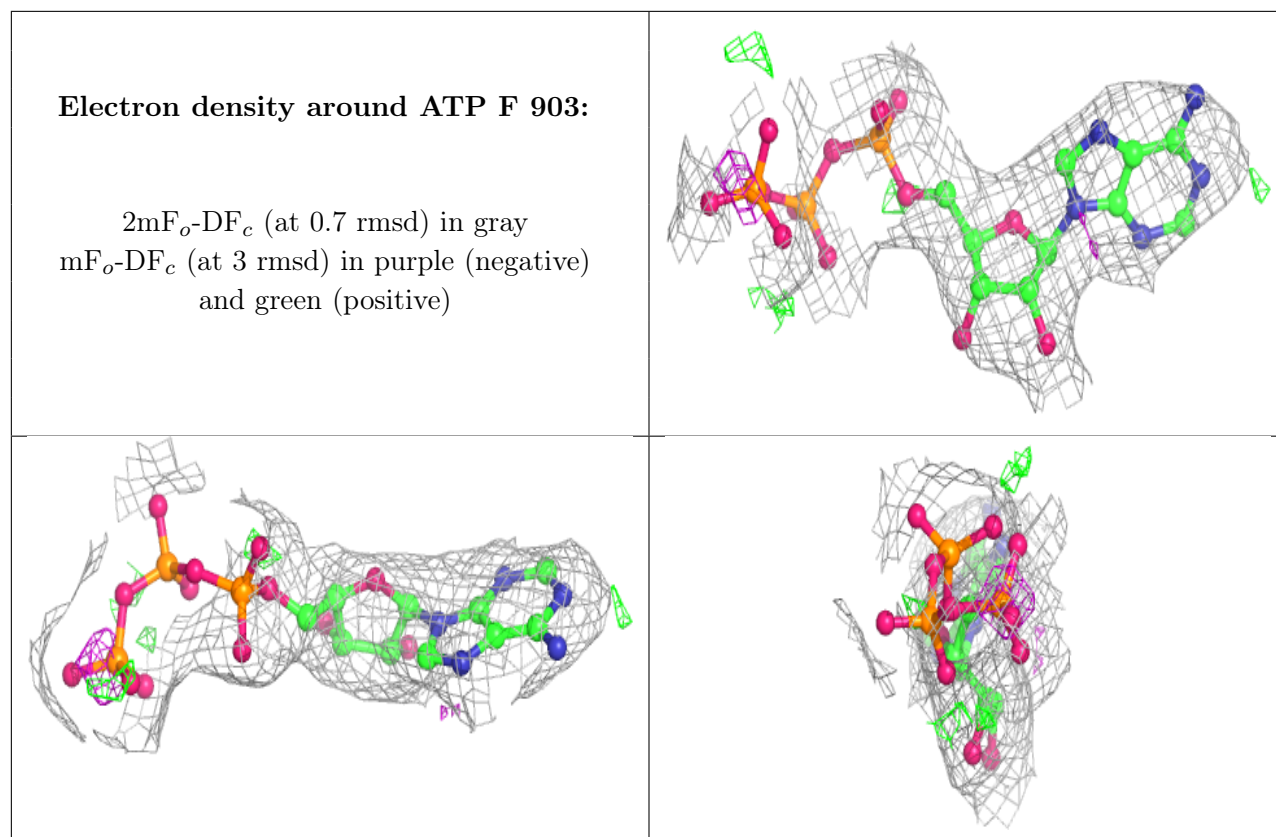
Electron density around ATP C 903:

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

**Electron density around ATP D 901:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.