



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 02:28 AM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.23.2
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) : 2.23.2

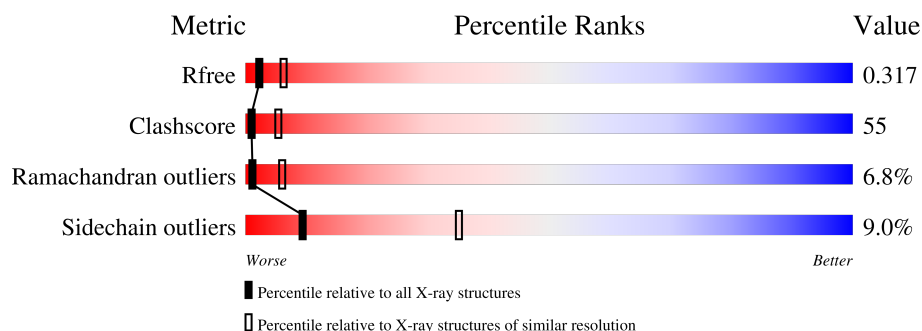
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	519	31% 56% 10% . .
2	B	519	30% 56% 8% . 5%
2	C	519	28% 56% 9% 6%
2	D	519	29% 56% 8% . 7%
2	E	519	29% 56% 9% 5%
2	F	519	28% 56% 13% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

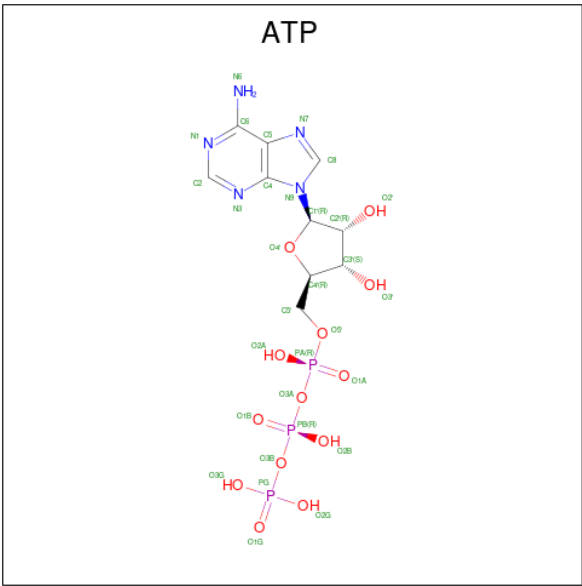
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	491	Total	C	N	O	P	S	0	0	0
			3873	2439	678	740	1	15			
2	C	488	Total	C	N	O	P	S	0	0	0
			3849	2425	674	734	1	15			
2	D	485	Total	C	N	O	P	S	0	0	0
			3825	2411	671	727	1	15			
2	E	492	Total	C	N	O	P	S	0	0	0
			3881	2445	679	741	1	15			
2	F	506	Total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

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

C₁₀H₁₆N₅O₁₃P₃).



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

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

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

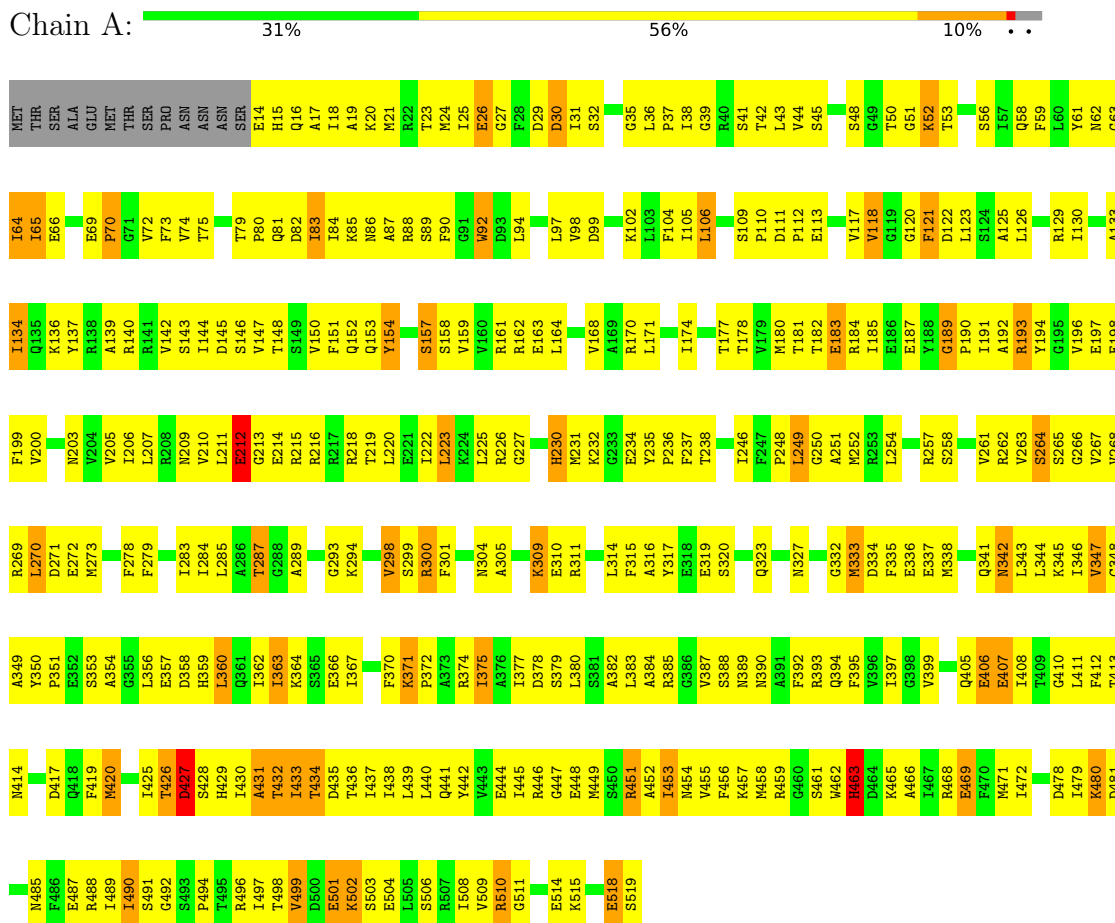
- Molecule 5 is water.

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

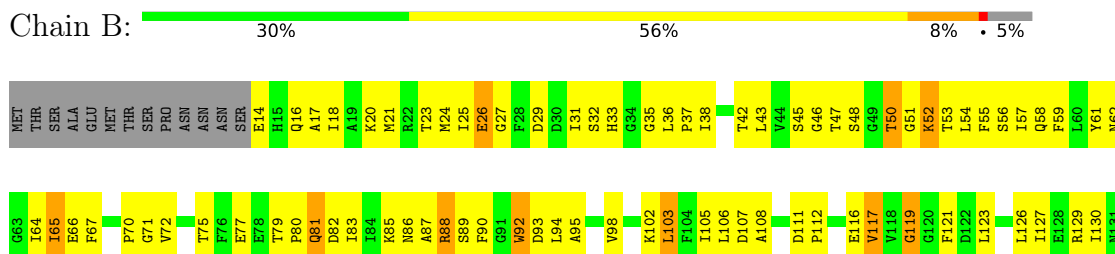
3 Residue-property plots

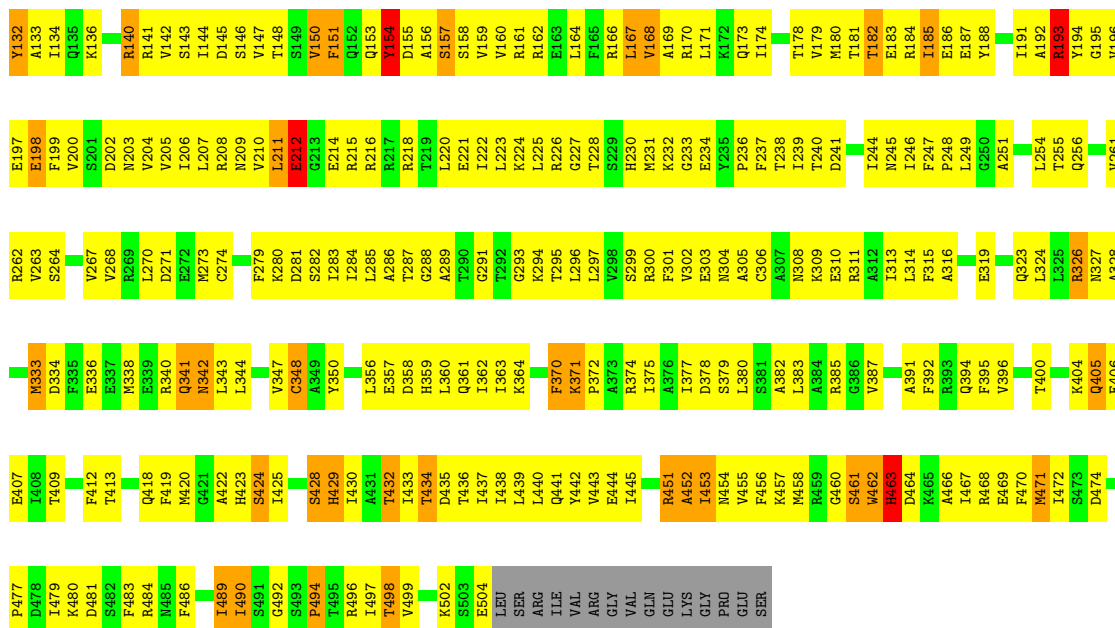
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

• Molecule 1: Circadian clock protein kinase KaiC



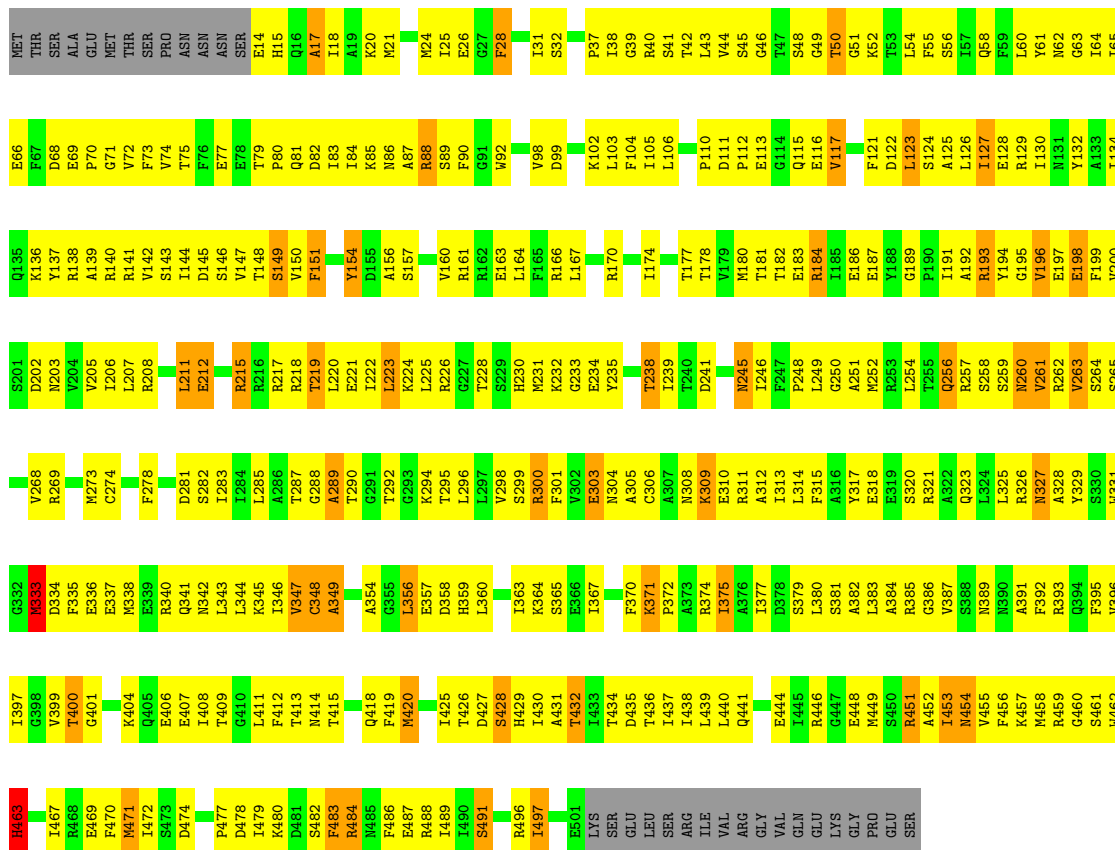
• Molecule 2: Circadian clock protein kinase KaiC





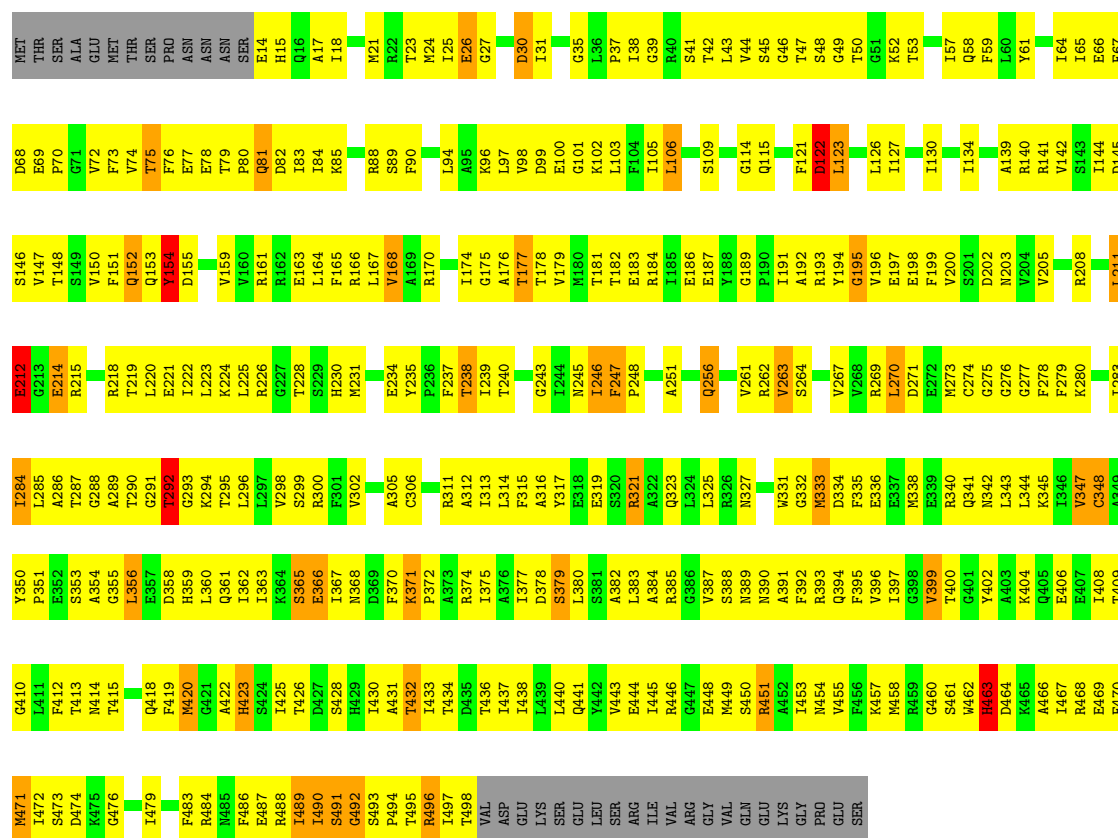
• Molecule 2: Circadian clock protein kinase KaiC

Chain C: 28% 56% 9% 6%



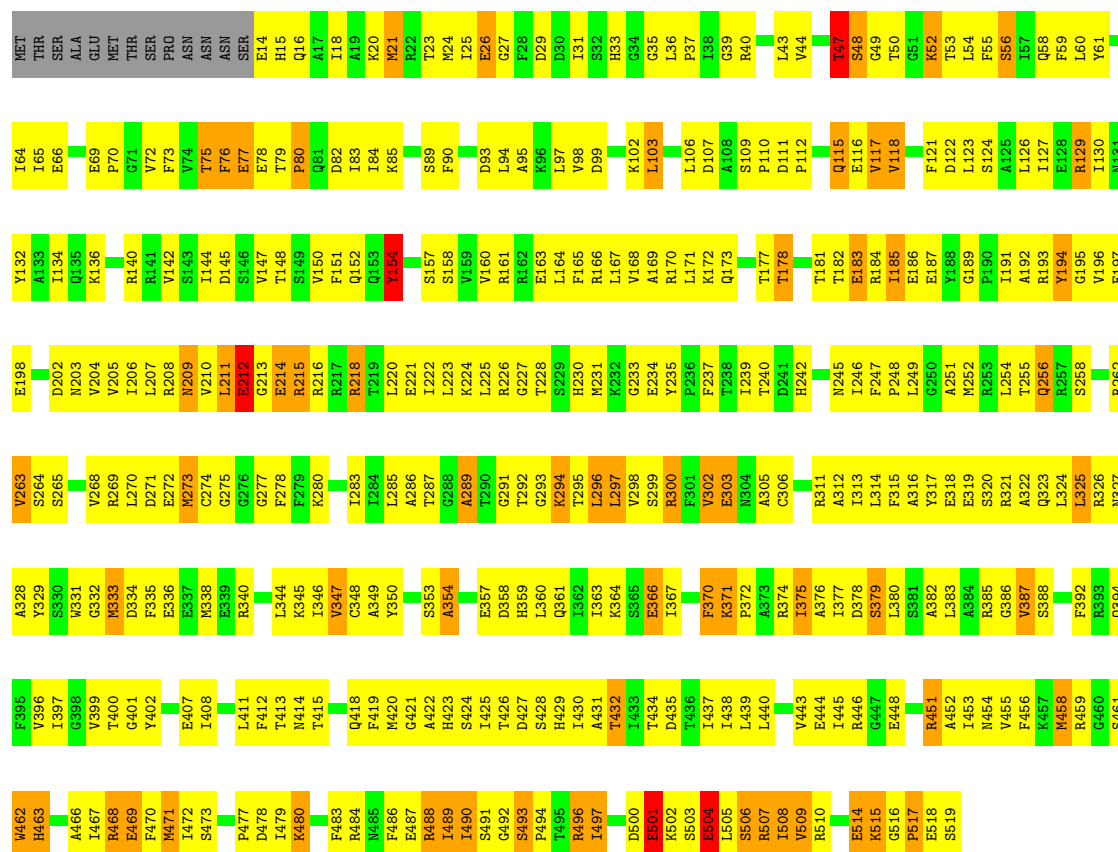
• Molecule 2: Circadian clock protein kinase KaiC

Chain D: 29% 56% 8% 7%





• 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	133.23Å 134.96Å 204.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 48.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	65.4 (30.00-3.00) 64.8 (48.00-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.307 0.300 , 0.317	Depositor DCC
R_{free} test set	4953 reflections (9.05%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	23921	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MG, 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	0/4034	0.67	0/5431
2	B	0.40	0/3926	0.65	0/5289
2	C	0.44	0/3902	0.70	0/5258
2	D	0.50	0/3878	0.74	0/5225
2	E	0.49	0/3934	0.73	1/5300 (0.0%)
2	F	0.51	1/4042 (0.0%)	0.73	0/5444
All	All	0.46	1/23716 (0.0%)	0.71	1/31947 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	21	MET	CG-SD	5.15	1.94	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	208	ARG	NE-CZ-NH1	5.56	123.08	120.30

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	3992	0	3983	439	0
2	B	3873	0	3862	437	0
2	C	3849	0	3838	462	0
2	D	3825	0	3820	445	0
2	E	3881	0	3873	448	0
2	F	3988	0	3983	492	0
3	A	62	0	24	8	0
3	B	62	0	24	8	0
3	C	62	0	24	5	0
3	D	62	0	24	13	0
3	E	62	0	24	6	0
3	F	62	0	24	7	0
4	A	6	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	2	0	0	0	0
4	E	4	0	0	0	0
4	F	3	0	0	0	0
5	A	14	0	0	4	0
5	B	20	0	0	4	0
5	C	23	0	0	5	0
5	D	28	0	0	7	0
5	E	15	0	0	5	0
5	F	19	0	0	4	0
All	All	23921	0	23503	2588	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 55.

All (2588) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:379:SER:H	2:D:413:THR:HB	1.13	1.13
2:E:283:ILE:HG13	2:E:400:THR:HG23	1.26	1.13
2:F:25:ILE:HD12	2:F:58:GLN:HE21	1.12	1.13
2:E:164:LEU:HD11	2:E:197:GLU:HG3	1.32	1.12
1:A:72:VAL:HG21	1:A:134:ILE:HD12	1.34	1.09
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.15	1.08
2:C:431:ALA:O	2:C:432:TPO:HG22	1.53	1.08
2:C:41:SER:HB3	2:C:178:THR:HB	1.33	1.07
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.19	1.03
2:D:148:THR:HG21	2:D:193:ARG:HD2	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:305:ALA:HB2	2:E:374:ARG:HD2	1.38	1.02
1:A:284:ILE:HD12	1:A:436:THR:HB	1.39	1.02
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.42	1.01
1:A:152:GLN:HG3	2:B:161:ARG:HH11	1.20	1.01
2:E:18:ILE:HD11	2:E:227:GLY:C	1.81	1.01
2:E:453:ILE:HG21	2:E:479:ILE:HD12	1.44	1.00
2:C:283:ILE:HG12	2:C:400:THR:HG23	1.40	0.99
2:E:449:MET:HG2	2:F:467:ILE:HD11	1.43	0.97
2:E:446:ARG:HH21	2:E:496:ARG:HH22	1.10	0.97
2:F:305:ALA:HB2	2:F:374:ARG:HD2	1.46	0.97
2:D:218:ARG:CZ	2:D:239:ILE:HD12	1.96	0.96
2:D:371:LYS:HD2	2:D:371:LYS:O	1.64	0.95
2:E:431:ALA:O	2:E:434:THR:HG22	1.66	0.95
2:C:371:LYS:O	2:C:371:LYS:HD2	1.67	0.95
2:E:43:LEU:HD23	2:E:204:VAL:HG13	1.48	0.95
2:C:261:VAL:HG12	2:C:262:ARG:H	1.30	0.95
2:E:123:LEU:CD2	2:E:127:ILE:HD11	1.97	0.95
2:C:453:ILE:HD13	2:C:454:ASN:N	1.83	0.94
2:E:123:LEU:HD23	2:E:127:ILE:HD11	1.50	0.94
2:F:379:SER:H	2:F:413:THR:HB	1.30	0.94
2:F:359:HIS:O	2:F:363:ILE:HD13	1.66	0.93
2:B:284:ILE:HD12	2:B:436:THR:HB	1.51	0.93
2:D:231:MET:CE	2:D:251:ALA:HB2	1.98	0.93
2:E:263:VAL:HG12	2:E:374:ARG:HH21	1.33	0.93
1:A:266:GLY:HA3	1:A:300:ARG:O	1.68	0.92
2:E:418:GLN:HB2	2:F:423:HIS:O	1.67	0.92
2:C:265:SER:O	2:C:301:PHE:HA	1.70	0.92
2:B:46:GLY:HA2	2:B:184:ARG:HD3	1.49	0.92
2:C:25:ILE:HG23	2:C:58:GLN:NE2	1.84	0.91
1:A:359:HIS:O	1:A:363:ILE:HG12	1.70	0.91
2:D:445:ILE:HD13	2:D:450:SER:OG	1.69	0.91
2:E:356:LEU:HD11	2:E:387:VAL:HG21	1.52	0.91
2:B:45:SER:HB2	2:B:182:THR:HB	1.52	0.91
2:D:379:SER:N	2:D:413:THR:HB	1.85	0.91
1:A:379:SER:H	1:A:413:THR:HB	1.35	0.91
2:D:436:THR:HG23	2:D:458:MET:HG2	1.51	0.91
2:F:263:VAL:HG12	2:F:374:ARG:HH21	1.35	0.91
2:C:31:ILE:HG22	2:C:222:ILE:HD12	1.54	0.90
2:C:45:SER:HB3	2:C:182:THR:HB	1.52	0.90
2:D:194:TYR:O	2:D:196:VAL:HG23	1.71	0.90
1:A:327:ASN:HB3	5:A:532:HOH:O	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:515:LYS:HG3	2:F:516:GLY:H	1.35	0.90
2:F:21:MET:HE1	2:F:177:THR:HB	1.53	0.90
2:F:434:THR:HG21	2:F:437:ILE:HD11	1.52	0.90
2:F:191:ILE:HB	2:F:198:GLU:HG2	1.54	0.89
2:C:211:LEU:O	2:C:212:GLU:HB3	1.73	0.89
2:D:294:LYS:O	2:D:298:VAL:HG23	1.72	0.89
1:A:14:GLU:HG3	1:A:15:HIS:H	1.36	0.89
2:D:47:THR:O	2:D:50:THR:HG23	1.71	0.89
2:E:313:ILE:HG13	2:E:372:PRO:HG3	1.54	0.89
2:D:64:ILE:HD12	2:D:102:LYS:HB3	1.51	0.89
1:A:314:LEU:HB3	1:A:346:ILE:HD12	1.55	0.89
2:C:261:VAL:HG12	2:C:262:ARG:N	1.86	0.89
2:D:211:LEU:O	2:D:212:GLU:HG3	1.73	0.88
2:E:497:ILE:HG22	2:E:498:THR:H	1.38	0.88
2:F:21:MET:HE3	2:F:59:PHE:CZ	2.08	0.88
2:B:140:ARG:HB3	2:B:140:ARG:NH1	1.89	0.88
2:C:25:ILE:HG23	2:C:58:GLN:HE22	1.37	0.88
2:D:74:VAL:HA	2:D:106:LEU:HB3	1.56	0.88
1:A:226:ARG:HA	5:A:531:HOH:O	1.71	0.88
1:A:265:SER:O	1:A:301:PHE:HA	1.74	0.87
2:F:263:VAL:CG1	2:F:374:ARG:HH21	1.86	0.87
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.09	0.87
1:A:25:ILE:HG13	1:A:58:GLN:NE2	1.89	0.87
1:A:287:THR:CG2	1:A:414:ASN:HD22	1.86	0.87
2:B:379:SER:H	2:B:413:THR:HB	1.39	0.87
2:F:25:ILE:HD12	2:F:58:GLN:NE2	1.89	0.87
2:E:392:PHE:HE2	2:E:430:ILE:HD11	1.37	0.87
2:F:500:ASP:O	2:F:501:GLU:HB3	1.73	0.86
2:E:313:ILE:HG13	2:E:372:PRO:CG	2.05	0.86
2:F:514:GLU:HG2	2:F:519:SER:HB3	1.55	0.86
2:B:211:LEU:O	2:B:212:GLU:HB3	1.72	0.86
2:E:53:THR:HG23	2:E:145:ASP:OD1	1.76	0.86
2:E:123:LEU:HD13	2:E:163:GLU:OE2	1.74	0.86
2:F:434:THR:CG2	2:F:437:ILE:HD11	2.06	0.86
2:D:64:ILE:HD11	2:D:70:PRO:HA	1.58	0.86
2:C:446:ARG:HG2	2:C:496:ARG:NH2	1.91	0.85
2:C:471:MET:HE2	2:C:478:ASP:H	1.40	0.85
2:D:152:GLN:HG3	2:E:161:ARG:HH11	1.40	0.85
2:C:471:MET:CE	2:C:478:ASP:HB3	2.06	0.85
2:C:471:MET:SD	2:C:478:ASP:HB3	2.15	0.85
3:C:901:ATP:H2'	2:D:458:MET:O	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:VAL:O	2:D:150:VAL:HG12	1.77	0.85
2:C:294:LYS:HG2	2:C:413:THR:HG23	1.58	0.85
2:B:147:VAL:HG11	2:B:180:MET:HE2	1.59	0.85
2:C:347:VAL:O	2:C:348:CYS:HB2	1.77	0.85
2:F:471:MET:HG3	2:F:478:ASP:HB3	1.59	0.84
2:E:283:ILE:HA	5:E:533:HOH:O	1.77	0.84
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.07	0.84
2:F:394:GLN:HA	2:F:397:ILE:HD12	1.58	0.84
2:D:446:ARG:H	2:D:496:ARG:HH12	1.26	0.84
2:B:193:ARG:HG2	2:B:193:ARG:HH11	1.43	0.84
2:E:123:LEU:O	2:E:127:ILE:HG13	1.78	0.84
2:F:451:ARG:HG2	2:F:451:ARG:HH11	1.43	0.84
2:F:52:LYS:HB2	3:F:903:ATP:O1B	1.78	0.84
2:C:41:SER:CB	2:C:178:THR:HB	2.08	0.83
2:C:364:LYS:HA	2:C:367:ILE:HD12	1.57	0.83
2:C:488:ARG:HH22	2:D:488:ARG:HH21	1.22	0.83
2:D:64:ILE:HG21	2:D:97:LEU:HD13	1.58	0.83
1:A:152:GLN:HG3	2:B:161:ARG:NH1	1.93	0.83
2:C:471:MET:CE	2:C:471:MET:O	2.27	0.83
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.61	0.83
2:C:471:MET:HE2	2:C:471:MET:O	1.77	0.83
2:D:231:MET:HE1	2:D:251:ALA:HB2	1.60	0.83
2:F:52:LYS:HB3	2:F:181:THR:CG2	2.09	0.83
1:A:350:TYR:CZ	2:B:254:LEU:HD13	2.14	0.83
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.08	0.83
1:A:72:VAL:HG21	1:A:134:ILE:CD1	2.08	0.82
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.14	0.82
2:B:31:ILE:HG23	2:B:231:MET:HB2	1.61	0.82
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.62	0.82
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.59	0.82
2:C:488:ARG:NH2	2:D:488:ARG:HH21	1.77	0.82
2:D:96:LYS:O	2:D:100:GLU:HG3	1.78	0.82
2:F:117:VAL:HA	2:F:154:TYR:OH	1.80	0.82
2:F:486:PHE:HE2	2:F:496:ARG:HH11	1.25	0.82
2:F:285:LEU:HB3	2:F:437:ILE:HD12	1.59	0.82
2:C:488:ARG:O	2:C:491:SER:HB3	1.80	0.82
1:A:25:ILE:HG13	1:A:58:GLN:HE21	1.44	0.82
2:F:471:MET:HG2	2:F:480:LYS:HE2	1.59	0.81
2:B:492:GLY:O	2:B:494:PRO:HD3	1.78	0.81
2:C:127:ILE:HD13	2:C:127:ILE:N	1.92	0.81
2:E:363:ILE:O	2:E:367:ILE:HG12	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:O	1:A:212:GLU:HB3	1.81	0.81
2:E:191:ILE:HB	2:E:198:GLU:HG2	1.60	0.81
2:C:221:GLU:HG3	2:C:233:GLY:O	1.81	0.81
2:C:313:ILE:HG12	2:C:345:LYS:HB3	1.63	0.81
1:A:161:ARG:HH11	2:F:152:GLN:HG3	1.46	0.81
2:E:359:HIS:O	2:E:363:ILE:HD13	1.80	0.81
2:D:220:LEU:HD23	2:D:221:GLU:N	1.95	0.81
2:F:191:ILE:HB	2:F:198:GLU:CG	2.10	0.81
2:B:248:PRO:HB2	2:B:251:ALA:HB3	1.62	0.81
1:A:356:LEU:HD11	1:A:387:VAL:HG21	1.60	0.81
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.62	0.81
2:C:311:ARG:HA	2:C:343:LEU:O	1.80	0.80
2:F:142:VAL:HB	2:F:178:THR:HG23	1.63	0.80
2:E:345:LYS:NZ	2:E:366:GLU:HG3	1.96	0.80
1:A:323:GLN:HG2	1:A:327:ASN:HD21	1.47	0.80
2:B:216:ARG:HG2	2:C:233:GLY:HA2	1.62	0.80
2:E:58:GLN:HG2	2:E:62:ASN:HD21	1.47	0.80
2:E:379:SER:H	2:E:413:THR:HB	1.43	0.80
2:B:247:PHE:HE2	2:B:364:LYS:HD2	1.47	0.80
2:E:191:ILE:HB	2:E:198:GLU:CG	2.12	0.80
1:A:52:LYS:HB3	1:A:181:THR:HG23	1.64	0.79
2:B:430:ILE:HA	2:B:433:ILE:HD13	1.64	0.79
2:B:496:ARG:HG2	2:B:498:THR:HG23	1.65	0.79
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.47	0.79
2:C:287:THR:HG22	2:C:288:GLY:H	1.45	0.79
2:B:239:ILE:CD1	2:B:244:ILE:HG12	2.12	0.79
2:F:248:PRO:HB2	2:F:251:ALA:HB3	1.64	0.79
2:F:194:TYR:O	2:F:196:VAL:HG23	1.82	0.79
1:A:14:GLU:HG3	1:A:16:GLN:OE1	1.83	0.79
2:C:360:LEU:HD21	2:C:364:LYS:HE3	1.63	0.79
1:A:84:ILE:HD13	1:A:94:LEU:HB2	1.64	0.79
1:A:227:GLY:O	2:F:89:SER:HB2	1.83	0.79
2:E:33:HIS:HD2	2:E:230:HIS:HA	1.48	0.79
2:E:449:MET:CG	2:F:467:ILE:HD11	2.12	0.79
2:E:392:PHE:CE2	2:E:430:ILE:HD11	2.16	0.79
2:D:21:MET:O	2:D:35:GLY:HA3	1.83	0.78
1:A:284:ILE:CD1	1:A:436:THR:HB	2.12	0.78
2:E:344:LEU:HD22	2:E:345:LYS:H	1.46	0.78
2:B:273:MET:O	2:B:463:HIS:HA	1.83	0.78
2:F:295:THR:HG23	2:F:378:ASP:OD2	1.82	0.78
2:D:202:ASP:HA	2:D:226:ARG:HD2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:231:MET:HE3	2:D:251:ALA:HB2	1.65	0.78
2:D:419:PHE:CE2	2:E:425:ILE:HG12	2.17	0.78
2:E:216:ARG:NH2	2:F:223:LEU:HD21	1.98	0.78
2:C:379:SER:H	2:C:413:THR:HB	1.49	0.78
2:C:451:ARG:HG2	2:C:451:ARG:HH11	1.47	0.78
2:C:202:ASP:HA	2:C:226:ARG:HD2	1.65	0.78
2:D:123:LEU:HD12	2:D:127:ILE:HD11	1.66	0.78
2:F:47:THR:HG22	2:F:50:THR:HG23	1.65	0.78
2:B:225:LEU:HD12	2:B:230:HIS:HB3	1.66	0.78
2:F:60:LEU:CD1	2:F:73:PHE:HB2	2.14	0.78
2:C:287:THR:CG2	2:C:414:ASN:HD22	1.96	0.77
2:E:263:VAL:CG1	2:E:374:ARG:HH21	1.97	0.77
1:A:249:LEU:HD13	1:A:394:GLN:HG2	1.66	0.77
2:C:287:THR:HG21	2:C:425:ILE:O	1.83	0.77
2:C:323:GLN:HE21	2:C:327:ASN:HD21	1.33	0.77
2:E:425:ILE:HD12	2:E:439:LEU:HD13	1.65	0.77
2:F:148:THR:HG21	2:F:193:ARG:HD2	1.66	0.77
2:F:375:ILE:HD13	2:F:376:ALA:N	2.00	0.77
2:B:293:GLY:HA2	3:B:901:ATP:O1A	1.84	0.77
2:B:453:ILE:HD13	2:B:454:ASN:N	1.99	0.77
1:A:315:PHE:HE1	1:A:375:ILE:HG13	1.49	0.77
2:E:94:LEU:O	2:E:98:VAL:HG23	1.85	0.77
2:D:438:ILE:HD13	2:D:455:VAL:HG22	1.67	0.77
2:F:285:LEU:HB3	2:F:437:ILE:CD1	2.14	0.77
2:F:305:ALA:CB	2:F:374:ARG:HD2	2.13	0.77
2:C:50:THR:HG21	2:C:207:LEU:C	2.05	0.77
2:B:315:PHE:HE1	2:B:375:ILE:HD11	1.50	0.77
2:B:300:ARG:HA	2:B:333:MET:HE1	1.65	0.76
2:B:379:SER:N	2:B:413:THR:HB	1.98	0.76
2:C:432:TPO:HG21	2:C:432:TPO:O1P	1.83	0.76
2:F:161:ARG:HB2	2:F:196:VAL:HG11	1.65	0.76
1:A:441:GLN:HE22	1:A:490:ILE:HD13	1.49	0.76
2:E:332:GLY:O	2:E:333:MET:HG2	1.85	0.76
2:C:409:THR:HA	5:C:540:HOH:O	1.85	0.76
2:C:471:MET:CE	2:C:478:ASP:CB	2.63	0.76
2:F:21:MET:HE3	2:F:59:PHE:HZ	1.48	0.76
2:B:316:ALA:HA	2:B:378:ASP:HB3	1.65	0.76
2:B:116:GLU:HG2	2:B:117:VAL:H	1.51	0.76
2:D:152:GLN:HG3	2:E:161:ARG:NH1	2.01	0.76
2:E:132:TYR:HE2	2:E:136:LYS:HD2	1.49	0.76
1:A:79:THR:HG22	1:A:81:GLN:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:446:ARG:NH2	2:E:496:ARG:HH22	1.82	0.76
1:A:65:ILE:O	1:A:66:GLU:HG2	1.86	0.76
2:F:509:VAL:HG12	2:F:510:ARG:H	1.51	0.76
1:A:314:LEU:HB3	1:A:346:ILE:CD1	2.15	0.75
2:D:453:ILE:HG21	2:D:479:ILE:HD12	1.67	0.75
1:A:471:MET:CG	1:A:478:ASP:HB3	2.16	0.75
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.51	0.75
2:C:448:GLU:HG2	2:D:466:ALA:HB2	1.67	0.75
2:B:171:LEU:HD23	2:B:174:ILE:HD12	1.66	0.75
2:B:203:ASN:HB3	2:B:225:LEU:HD23	1.69	0.75
1:A:14:GLU:CG	1:A:15:HIS:H	1.98	0.75
2:C:238:THR:HA	5:C:528:HOH:O	1.86	0.75
2:D:347:VAL:O	2:D:348:CYS:HB2	1.86	0.75
2:F:142:VAL:HB	2:F:178:THR:CG2	2.15	0.75
2:F:334:ASP:O	2:F:338:MET:HG2	1.86	0.75
2:F:336:GLU:HB3	2:F:340:ARG:NH2	2.02	0.75
2:C:146:SER:H	2:C:181:THR:HB	1.51	0.75
2:E:238:THR:HB	2:E:361:GLN:HE22	1.52	0.75
2:F:514:GLU:CD	2:F:515:LYS:H	1.90	0.75
2:D:31:ILE:HA	2:D:231:MET:HG3	1.69	0.75
2:E:435:ASP:OD1	2:E:459:ARG:HD2	1.87	0.75
2:F:245:ASN:ND2	2:F:361:GLN:HE21	1.85	0.74
2:D:18:ILE:H	2:D:18:ILE:HD12	1.51	0.74
1:A:147:VAL:O	1:A:150:VAL:HG12	1.87	0.74
2:C:127:ILE:HD13	2:C:127:ILE:H	1.50	0.74
1:A:363:ILE:HG22	1:A:367:ILE:HD11	1.70	0.74
2:D:170:ARG:O	2:D:174:ILE:HG12	1.88	0.74
2:E:320:SER:O	2:E:324:LEU:HB2	1.87	0.74
2:C:261:VAL:CG1	2:C:262:ARG:H	2.00	0.74
2:C:313:ILE:HD11	2:C:370:PHE:HB3	1.70	0.74
2:C:308:ASN:O	2:C:310:GLU:HG3	1.88	0.74
2:E:164:LEU:CD1	2:E:197:GLU:HG3	2.15	0.74
2:E:267:VAL:HG21	2:E:477:PRO:HG3	1.68	0.74
2:B:18:ILE:HB	2:B:228:THR:CG2	2.18	0.73
2:B:347:VAL:O	2:B:348:CYS:HB2	1.87	0.73
2:D:76:PHE:O	2:D:109:SER:HA	1.88	0.73
2:F:245:ASN:ND2	2:F:361:GLN:NE2	2.36	0.73
2:B:454:ASN:HB2	2:B:467:ILE:HD13	1.70	0.73
1:A:508:ILE:HD12	1:A:510:ARG:H	1.52	0.73
2:E:294:LYS:HB3	2:E:413:THR:HG23	1.70	0.73
2:B:187:GLU:OE2	2:B:208:ARG:HA	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ARG:HD3	2:B:237:PHE:CE1	2.23	0.73
2:C:215:ARG:HA	2:C:215:ARG:HE	1.53	0.73
2:C:287:THR:HG22	2:C:288:GLY:N	2.03	0.73
2:C:441:GLN:HG2	2:C:452:ALA:HB3	1.71	0.73
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.69	0.73
2:E:318:GLU:HG2	2:F:432:TPO:O3P	1.88	0.73
2:E:318:GLU:OE2	2:E:379:SER:HB2	1.87	0.73
2:B:358:ASP:O	2:B:362:ILE:HG12	1.89	0.73
2:C:252:MET:HE1	2:C:397:ILE:HG22	1.68	0.73
2:B:311:ARG:HG3	2:B:371:LYS:NZ	2.04	0.73
1:A:161:ARG:NH1	2:F:152:GLN:HG3	2.03	0.73
1:A:299:SER:HB3	1:A:333:MET:HE2	1.70	0.73
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.24	0.73
2:D:38:ILE:HA	2:D:177:THR:HG23	1.69	0.73
2:E:266:GLY:HA3	2:E:300:ARG:HG3	1.69	0.73
2:D:81:GLN:H	2:D:81:GLN:CD	1.92	0.72
2:D:269:ARG:HG2	2:D:479:ILE:HB	1.70	0.72
2:E:371:LYS:HD2	2:E:371:LYS:O	1.89	0.72
2:F:285:LEU:HD23	2:F:437:ILE:HD12	1.69	0.72
1:A:130:ILE:O	1:A:134:ILE:HD13	1.89	0.72
2:E:470:PHE:HE1	2:E:472:ILE:HD11	1.53	0.72
1:A:51:GLY:HA3	1:A:207:LEU:HD13	1.69	0.72
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.54	0.72
2:E:14:GLU:HG3	2:E:16:GLN:H	1.54	0.72
2:C:170:ARG:O	2:C:174:ILE:HG12	1.89	0.72
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.69	0.72
1:A:320:SER:HA	2:B:254:LEU:HG	1.70	0.72
2:B:85:LYS:NZ	2:C:14:GLU:HG2	2.04	0.72
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.53	0.72
1:A:207:LEU:HD21	1:A:220:LEU:HD12	1.72	0.72
2:D:48:SER:HA	5:D:525:HOH:O	1.89	0.72
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.55	0.72
2:C:471:MET:HE2	2:C:478:ASP:N	2.05	0.72
2:D:347:VAL:HG12	2:D:348:CYS:N	2.03	0.72
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.71	0.72
2:C:446:ARG:HG2	2:C:496:ARG:CZ	2.20	0.72
2:F:218:ARG:NH1	2:F:239:ILE:HD12	2.04	0.72
2:C:31:ILE:HG23	2:C:231:MET:HB2	1.72	0.72
2:C:294:LYS:O	2:C:298:VAL:HG23	1.89	0.72
2:C:497:ILE:HD13	2:C:497:ILE:N	2.05	0.72
2:D:294:LYS:HB3	2:D:413:THR:HG23	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.55	0.71
1:A:70:PRO:HA	1:A:102:LYS:O	1.91	0.71
2:D:285:LEU:HD12	2:D:412:PHE:O	1.90	0.71
2:D:496:ARG:HG2	2:E:487:GLU:OE1	1.90	0.71
2:F:443:VAL:CG1	2:F:445:ILE:HD11	2.19	0.71
1:A:317:TYR:HA	1:A:349:ALA:O	1.91	0.71
2:C:223:LEU:HD13	2:C:224:LYS:HB3	1.70	0.71
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.72	0.71
1:A:65:ILE:O	1:A:65:ILE:HG22	1.89	0.71
1:A:211:LEU:O	1:A:212:GLU:CB	2.38	0.71
2:B:21:MET:SD	2:B:141:ARG:NE	2.64	0.71
2:F:313:ILE:CD1	2:F:345:LYS:HB3	2.21	0.71
2:B:451:ARG:HH11	2:B:451:ARG:HG2	1.55	0.71
2:C:436:THR:OG1	2:C:458:MET:HG2	1.90	0.71
2:F:371:LYS:O	2:F:371:LYS:HD2	1.90	0.71
2:C:54:LEU:HD11	2:C:90:PHE:CZ	2.25	0.71
2:C:148:THR:OG1	2:C:182:THR:HG23	1.89	0.71
2:C:221:GLU:HB3	5:C:538:HOH:O	1.90	0.71
2:E:305:ALA:HB2	2:E:374:ARG:CD	2.18	0.71
2:F:191:ILE:CB	2:F:198:GLU:HG2	2.19	0.71
2:B:140:ARG:HB3	2:B:140:ARG:HH11	1.54	0.71
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.25	0.71
2:D:38:ILE:HA	2:D:177:THR:CG2	2.20	0.70
2:E:310:GLU:HB3	2:E:373:ALA:CB	2.20	0.70
1:A:50:THR:HG22	1:A:209:ASN:HB2	1.72	0.70
2:D:151:PHE:O	2:D:153:GLN:N	2.20	0.70
2:E:33:HIS:HD2	2:E:230:HIS:CA	2.04	0.70
2:B:256:GLN:OE1	2:B:405:GLN:HB3	1.92	0.70
1:A:453:ILE:HD13	1:A:454:ASN:N	2.06	0.70
2:B:305:ALA:HB2	2:B:374:ARG:HD2	1.74	0.70
2:C:191:ILE:HD12	2:C:191:ILE:H	1.57	0.70
1:A:347:VAL:O	1:A:348:CYS:HB2	1.89	0.70
2:B:45:SER:CB	2:B:182:THR:HB	2.20	0.70
2:E:313:ILE:HD12	2:E:367:ILE:HD13	1.74	0.70
2:F:21:MET:CE	2:F:59:PHE:HZ	2.03	0.70
2:F:23:THR:HB	2:F:25:ILE:HG12	1.72	0.70
1:A:45:SER:HB3	1:A:182:THR:HB	1.74	0.70
2:D:80:PRO:O	2:D:84:ILE:HG12	1.91	0.70
2:F:106:LEU:HD11	2:F:129:ARG:CZ	2.21	0.70
2:D:94:LEU:O	2:D:98:VAL:HG23	1.92	0.70
2:E:417:ASP:HB2	2:E:427:ASP:OD2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:132:TYR:CE2	2:F:136:LYS:HD2	2.27	0.70
1:A:73:PHE:HE2	1:A:83:ILE:HD13	1.57	0.70
1:A:451:ARG:H	1:A:451:ARG:HD2	1.57	0.69
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.74	0.69
1:A:487:GLU:OE1	2:F:496:ARG:HG2	1.92	0.69
2:C:425:ILE:HD11	2:C:456:PHE:CE2	2.27	0.69
2:F:335:PHE:HA	2:F:338:MET:CG	2.22	0.69
2:B:193:ARG:HG2	2:B:193:ARG:NH1	2.05	0.69
2:B:308:ASN:O	2:B:310:GLU:HG3	1.93	0.69
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.71	0.69
2:F:160:VAL:HG21	2:F:194:TYR:CD2	2.26	0.69
2:F:303:GLU:OE2	2:F:333:MET:HB3	1.92	0.69
2:E:401:GLY:O	2:E:405:GLN:HG2	1.92	0.69
2:C:149:SER:HB3	2:D:161:ARG:CZ	2.22	0.69
2:C:440:LEU:CD2	2:C:453:ILE:HG12	2.22	0.69
2:D:53:THR:HG22	2:D:57:ILE:HD11	1.75	0.69
2:D:311:ARG:HD2	2:D:371:LYS:CE	2.08	0.69
2:E:425:ILE:HG22	2:E:425:ILE:O	1.93	0.69
1:A:371:LYS:O	1:A:371:LYS:HD2	1.92	0.69
1:A:407:GLU:OE1	1:A:407:GLU:HA	1.93	0.69
1:A:458:MET:HB2	1:A:463:HIS:HD2	1.57	0.69
2:B:123:LEU:HD13	2:B:123:LEU:O	1.93	0.69
2:B:171:LEU:HA	2:B:174:ILE:HD12	1.73	0.69
2:B:209:ASN:HD22	2:B:218:ARG:HG2	1.58	0.69
2:C:46:GLY:HA2	2:C:184:ARG:HD2	1.73	0.69
2:D:31:ILE:HA	2:D:231:MET:CG	2.23	0.69
2:E:497:ILE:HG22	2:E:498:THR:N	2.07	0.69
2:F:296:LEU:HD21	2:F:477:PRO:HD3	1.75	0.69
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.06	0.69
2:B:418:GLN:HG3	2:B:418:GLN:O	1.93	0.69
2:D:114:GLY:O	2:D:115:GLN:HG3	1.92	0.69
2:D:256:GLN:HG3	2:D:404:LYS:HD3	1.75	0.69
2:E:81:GLN:NE2	2:E:81:GLN:H	1.91	0.69
2:E:325:LEU:HD21	2:E:335:PHE:HB2	1.74	0.69
2:F:515:LYS:HG3	2:F:516:GLY:N	2.08	0.69
2:D:314:LEU:O	2:D:314:LEU:HG	1.93	0.69
2:E:356:LEU:CD2	2:E:392:PHE:HA	2.23	0.69
2:C:261:VAL:CG1	2:C:262:ARG:N	2.56	0.68
2:E:294:LYS:HB3	2:E:413:THR:CG2	2.23	0.68
2:E:377:ILE:HD12	2:E:412:PHE:HE2	1.58	0.68
2:B:294:LYS:HB3	2:B:413:THR:HG23	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.74	0.68
2:D:377:ILE:HD13	2:D:412:PHE:CE2	2.27	0.68
2:F:262:ARG:HD3	2:F:277:GLY:O	1.92	0.68
2:B:64:ILE:HD11	2:B:70:PRO:HA	1.76	0.68
2:B:441:GLN:HG3	2:B:441:GLN:O	1.94	0.68
2:F:164:LEU:HD11	2:F:197:GLU:HG3	1.75	0.68
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.23	0.68
2:C:70:PRO:HB2	2:C:139:ALA:HA	1.75	0.68
2:E:289:ALA:CB	2:E:419:PHE:HA	2.23	0.68
2:F:124:SER:OG	2:F:166:ARG:NH1	2.27	0.68
2:B:429:HIS:HB3	5:B:529:HOH:O	1.93	0.68
2:E:25:ILE:HG23	2:E:58:GLN:NE2	2.08	0.68
2:F:144:ILE:HD13	2:F:167:LEU:HD21	1.73	0.68
2:F:231:MET:SD	2:F:251:ALA:HB2	2.34	0.68
2:C:64:ILE:HG23	2:C:102:LYS:HB3	1.76	0.68
2:C:140:ARG:NH1	2:C:140:ARG:HB3	2.09	0.68
2:E:356:LEU:HD13	2:E:387:VAL:HG11	1.75	0.68
2:F:47:THR:HG22	2:F:50:THR:CG2	2.24	0.68
2:D:31:ILE:HA	2:D:231:MET:SD	2.33	0.68
2:D:61:TYR:O	2:D:65:ILE:HD12	1.93	0.68
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.08	0.68
2:E:470:PHE:CE1	2:E:472:ILE:HD11	2.27	0.68
2:B:377:ILE:HD13	2:B:412:PHE:CE2	2.29	0.68
2:C:71:GLY:O	2:C:103:LEU:HD12	1.94	0.68
2:E:191:ILE:HG23	2:E:206:ILE:HD11	1.76	0.68
2:F:211:LEU:HD12	2:F:215:ARG:O	1.94	0.68
2:C:283:ILE:HD12	2:C:435:ASP:OD2	1.94	0.68
2:E:76:PHE:CZ	2:E:126:LEU:HD21	2.29	0.68
2:E:377:ILE:HD12	2:E:412:PHE:CE2	2.28	0.68
2:B:127:ILE:HA	2:B:130:ILE:HD12	1.75	0.67
2:B:264:SER:HB3	2:B:304:ASN:ND2	2.09	0.67
2:B:444:GLU:O	2:B:494:PRO:HD2	1.94	0.67
2:E:451:ARG:HG2	2:E:451:ARG:HH11	1.59	0.67
2:E:58:GLN:HG2	2:E:62:ASN:ND2	2.09	0.67
2:E:230:HIS:O	2:E:232:LYS:HD2	1.95	0.67
2:F:147:VAL:O	2:F:150:VAL:HG12	1.94	0.67
2:F:313:ILE:HD11	2:F:370:PHE:CD2	2.30	0.67
2:F:432:TPO:HG21	2:F:432:TPO:O1P	1.94	0.67
2:C:261:VAL:O	2:C:262:ARG:HG2	1.95	0.67
2:D:59:PHE:CE2	2:D:141:ARG:HB3	2.29	0.67
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:363:ILE:O	2:F:367:ILE:HG12	1.93	0.67
2:B:191:ILE:HB	2:B:198:GLU:CD	2.15	0.67
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.60	0.67
2:B:130:ILE:O	2:B:134:ILE:HG12	1.94	0.67
2:C:25:ILE:HG12	2:C:58:GLN:HE21	1.60	0.67
2:C:31:ILE:HD13	2:C:231:MET:SD	2.34	0.67
2:D:286:ALA:O	2:D:294:LYS:HG2	1.95	0.67
2:D:464:ASP:OD1	2:D:466:ALA:N	2.28	0.67
2:F:21:MET:CE	2:F:177:THR:HB	2.25	0.67
1:A:210:VAL:HG12	1:A:211:LEU:O	1.94	0.67
2:B:25:ILE:HG23	2:B:58:GLN:NE2	2.10	0.67
2:F:347:VAL:O	2:F:348:CYS:HB3	1.92	0.67
1:A:451:ARG:NH1	1:A:472:ILE:HD12	2.10	0.67
2:B:441:GLN:NE2	2:B:490:ILE:HD13	2.10	0.67
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.60	0.67
2:F:203:ASN:HB3	2:F:225:LEU:HD23	1.77	0.67
2:F:379:SER:N	2:F:413:THR:HB	2.06	0.67
1:A:311:ARG:HA	1:A:343:LEU:O	1.95	0.67
1:A:488:ARG:HE	2:F:488:ARG:NH1	1.92	0.67
2:F:21:MET:HE2	2:F:177:THR:HG21	1.76	0.67
2:B:20:LYS:HB3	2:B:35:GLY:O	1.94	0.66
2:D:74:VAL:HG21	2:D:130:ILE:CD1	2.25	0.66
2:D:446:ARG:N	2:D:496:ARG:HH12	1.93	0.66
2:C:18:ILE:HB	2:C:228:THR:HG23	1.77	0.66
2:C:195:GLY:O	2:C:196:VAL:HG23	1.96	0.66
2:E:191:ILE:CB	2:E:198:GLU:HG2	2.24	0.66
2:E:321:ARG:HG2	2:E:348:CYS:SG	2.36	0.66
2:F:21:MET:HE2	2:F:177:THR:CG2	2.25	0.66
1:A:144:ILE:HD11	1:A:171:LEU:HD11	1.77	0.66
2:F:182:THR:HG21	2:F:192:ALA:HB1	1.77	0.66
2:F:371:LYS:O	2:F:371:LYS:CD	2.43	0.66
2:F:377:ILE:HD12	2:F:412:PHE:CE2	2.31	0.66
1:A:234:GLU:HB2	2:F:214:GLU:HB3	1.76	0.66
2:E:123:LEU:HD21	2:E:127:ILE:HD11	1.75	0.66
2:E:205:VAL:HG22	2:E:222:ILE:HD12	1.76	0.66
1:A:267:VAL:CG1	1:A:270:LEU:HB2	2.25	0.66
2:B:148:THR:HA	2:B:151:PHE:CE1	2.30	0.66
2:D:89:SER:OG	3:D:903:ATP:N6	2.28	0.66
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.76	0.66
2:E:171:LEU:HA	2:E:174:ILE:HD12	1.76	0.66
2:F:79:THR:HG22	2:F:82:ASP:OD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.78	0.66
2:E:316:ALA:CB	2:E:324:LEU:HD11	2.26	0.66
2:F:335:PHE:HA	2:F:338:MET:HG3	1.77	0.66
1:A:426:TPO:O3P	1:A:431:ALA:HB2	1.96	0.66
1:A:492:GLY:O	1:A:494:PRO:HD3	1.96	0.66
2:E:170:ARG:O	2:E:174:ILE:HG13	1.95	0.66
2:E:269:ARG:HG2	2:E:479:ILE:HB	1.76	0.66
2:E:504:GLU:HG2	2:E:505:LEU:H	1.61	0.66
1:A:323:GLN:HG2	1:A:327:ASN:ND2	2.11	0.66
2:C:287:THR:HG23	2:C:414:ASN:HB3	1.77	0.66
2:E:419:PHE:CE2	2:F:425:ILE:HG13	2.31	0.66
1:A:52:LYS:H	1:A:207:LEU:HD12	1.59	0.66
1:A:98:VAL:HG22	1:A:105:ILE:HD13	1.77	0.66
2:B:146:SER:H	2:B:181:THR:HB	1.60	0.66
2:E:79:THR:HG22	2:E:82:ASP:OD2	1.96	0.66
2:C:74:VAL:HB	2:C:144:ILE:HA	1.79	0.65
2:C:182:THR:HG22	2:C:183:GLU:N	2.10	0.65
2:F:396:VAL:HG11	2:F:430:ILE:HG21	1.78	0.65
2:C:344:LEU:HD22	2:C:345:LYS:N	2.11	0.65
2:C:440:LEU:HD21	2:C:453:ILE:HG12	1.78	0.65
2:E:344:LEU:HD13	2:E:345:LYS:N	2.10	0.65
2:E:488:ARG:HB3	2:E:491:SER:OG	1.95	0.65
2:B:145:ASP:HA	2:B:181:THR:HB	1.77	0.65
2:D:264:SER:HA	2:D:271:ASP:OD1	1.96	0.65
2:B:140:ARG:HH11	2:B:140:ARG:CB	2.09	0.65
2:C:334:ASP:O	2:C:338:MET:HG2	1.97	0.65
2:D:287:THR:HG21	2:D:425:ILE:O	1.95	0.65
1:A:219:THR:O	1:A:237:PHE:HE2	1.80	0.65
2:B:93:ASP:OD1	2:B:95:ALA:HB3	1.97	0.65
2:D:88:ARG:HG2	2:D:88:ARG:HH11	1.61	0.65
2:D:350:TYR:CE1	2:E:254:LEU:HD13	2.32	0.65
2:B:469:GLU:HB3	2:B:483:PHE:CZ	2.31	0.65
2:D:182:THR:HG22	2:D:183:GLU:N	2.11	0.65
2:F:123:LEU:O	2:F:123:LEU:HD13	1.96	0.65
2:F:169:ALA:O	2:F:173:GLN:HG3	1.97	0.65
2:D:150:VAL:O	2:D:153:GLN:HG3	1.96	0.65
2:F:311:ARG:HG3	2:F:371:LYS:NZ	2.11	0.65
1:A:360:LEU:O	1:A:360:LEU:HD22	1.97	0.65
2:C:300:ARG:N	2:C:333:MET:HE1	2.12	0.65
2:E:446:ARG:HH21	2:E:496:ARG:NH2	1.89	0.65
2:F:486:PHE:CE2	2:F:496:ARG:HD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:O	1:A:30:ASP:HB2	1.97	0.65
1:A:140:ARG:HA	1:A:140:ARG:HH11	1.62	0.65
1:A:446:ARG:HA	1:A:496:ARG:NH2	2.11	0.65
2:B:79:THR:HG22	2:B:82:ASP:OD2	1.97	0.65
2:B:239:ILE:HD13	2:B:244:ILE:HG12	1.77	0.65
2:B:356:LEU:CD1	2:B:356:LEU:H	2.10	0.65
2:B:378:ASP:O	2:B:379:SER:HB3	1.96	0.65
2:F:294:LYS:HB3	2:F:413:THR:HG23	1.79	0.65
2:C:221:GLU:CG	2:C:233:GLY:O	2.44	0.65
2:F:65:ILE:HD11	2:F:97:LEU:HD11	1.79	0.64
2:C:382:ALA:O	2:C:385:ARG:HG3	1.96	0.64
2:C:415:THR:HG21	2:D:432:TPO:CG2	2.28	0.64
2:D:396:VAL:HG11	2:D:430:ILE:HG21	1.78	0.64
2:F:283:ILE:HG23	2:F:412:PHE:CE1	2.33	0.64
2:B:315:PHE:CE1	2:B:375:ILE:HD11	2.31	0.64
2:D:438:ILE:CD1	2:D:455:VAL:HG22	2.27	0.64
2:E:124:SER:HA	2:E:127:ILE:HD12	1.78	0.64
2:F:31:ILE:HD11	2:F:246:ILE:HG21	1.79	0.64
2:C:392:PHE:O	2:C:395:PHE:HB3	1.97	0.64
2:E:54:LEU:O	2:E:54:LEU:HD12	1.96	0.64
2:F:183:GLU:HG3	2:F:193:ARG:HE	1.63	0.64
2:F:324:LEU:O	2:F:328:ALA:HB2	1.97	0.64
1:A:211:LEU:HG	1:A:212:GLU:H	1.62	0.64
1:A:316:ALA:HB3	1:A:348:CYS:SG	2.37	0.64
2:C:80:PRO:HB3	2:C:105:ILE:HG21	1.79	0.64
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.13	0.64
2:B:80:PRO:HG2	2:B:107:ASP:HB2	1.80	0.64
2:B:185:ILE:HD13	2:B:185:ILE:N	2.13	0.64
2:D:81:GLN:H	2:D:81:GLN:NE2	1.96	0.64
2:B:86:ASN:HD21	2:C:40:ARG:HH22	1.46	0.64
2:D:218:ARG:NH2	2:D:239:ILE:HD12	2.12	0.64
2:E:18:ILE:HD11	2:E:227:GLY:CA	2.27	0.64
2:F:80:PRO:HG2	2:F:107:ASP:HB2	1.80	0.64
1:A:79:THR:HG22	1:A:81:GLN:H	1.61	0.64
2:D:183:GLU:HB2	2:E:199:PHE:CE1	2.33	0.64
2:B:21:MET:HB2	2:B:38:ILE:HG12	1.79	0.64
2:B:296:LEU:HD21	2:B:477:PRO:HD3	1.80	0.64
2:D:312:ALA:O	2:D:344:LEU:HD22	1.98	0.64
2:E:20:LYS:HE3	2:E:228:THR:HG21	1.80	0.64
2:E:382:ALA:O	2:E:385:ARG:HG3	1.96	0.64
2:B:452:ALA:HA	2:B:469:GLU:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:148:THR:OG1	2:E:182:THR:HG23	1.98	0.64
2:F:111:ASP:OD1	2:F:112:PRO:HD2	1.98	0.64
2:B:123:LEU:O	2:B:127:ILE:HG13	1.98	0.63
2:C:137:TYR:O	2:C:138:ARG:HB2	1.96	0.63
2:D:315:PHE:HA	2:D:347:VAL:HB	1.80	0.63
2:F:52:LYS:HB3	2:F:181:THR:HG21	1.80	0.63
1:A:207:LEU:CD2	1:A:220:LEU:HD12	2.27	0.63
2:E:76:PHE:HZ	2:E:126:LEU:HD21	1.63	0.63
2:F:300:ARG:NH2	2:F:477:PRO:HD2	2.13	0.63
2:B:377:ILE:HD13	2:B:412:PHE:HE2	1.62	0.63
2:C:384:ALA:HB2	2:C:392:PHE:CZ	2.33	0.63
2:E:362:ILE:O	2:E:365:SER:HB3	1.98	0.63
2:B:52:LYS:H	2:B:207:LEU:HD12	1.63	0.63
2:D:39:GLY:N	2:D:177:THR:HG23	2.13	0.63
2:E:443:VAL:O	2:E:445:ILE:HD12	1.98	0.63
2:F:296:LEU:O	2:F:299:SER:N	2.32	0.63
2:F:516:GLY:N	2:F:517:PRO:HD2	2.14	0.63
2:D:150:VAL:HG13	2:D:151:PHE:N	2.14	0.63
1:A:73:PHE:CE2	1:A:83:ILE:HD13	2.34	0.63
1:A:84:ILE:HD13	1:A:94:LEU:CB	2.29	0.63
2:B:211:LEU:HD13	2:B:216:ARG:CZ	2.28	0.63
2:B:214:GLU:HB3	2:C:234:GLU:HB3	1.81	0.63
2:D:191:ILE:HB	2:D:198:GLU:CG	2.29	0.63
2:D:490:ILE:C	2:D:492:GLY:H	2.02	0.63
1:A:414:ASN:ND2	1:A:426:TPO:HA	2.11	0.63
2:B:184:ARG:HD2	2:B:191:ILE:O	1.99	0.63
2:D:245:ASN:ND2	2:D:361:GLN:HE21	1.95	0.63
2:E:93:ASP:OD2	2:E:96:LYS:HB2	1.99	0.63
2:E:247:PHE:CZ	2:E:361:GLN:HB2	2.34	0.63
2:E:263:VAL:HG12	2:E:374:ARG:NH2	2.11	0.63
2:F:21:MET:HE3	2:F:59:PHE:CE1	2.34	0.63
1:A:45:SER:CB	1:A:182:THR:HB	2.29	0.62
2:B:357:GLU:HG3	2:B:358:ASP:N	2.14	0.62
2:D:489:ILE:HD13	2:D:489:ILE:N	2.14	0.62
2:E:291:GLY:HA3	2:E:442:TYR:OH	1.99	0.62
2:E:334:ASP:OD1	2:E:337:GLU:N	2.31	0.62
2:F:213:GLY:O	2:F:215:ARG:N	2.31	0.62
2:F:311:ARG:HD2	2:F:370:PHE:O	1.98	0.62
1:A:21:MET:HE2	1:A:177:THR:HG21	1.81	0.62
1:A:38:ILE:HG22	1:A:39:GLY:N	2.13	0.62
1:A:147:VAL:HG11	1:A:180:MET:CE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:MET:CB	2:B:62:ASN:HD22	2.13	0.62
2:D:292:THR:HB	2:D:440:LEU:HB3	1.80	0.62
2:F:443:VAL:HG12	2:F:445:ILE:HD11	1.80	0.62
1:A:145:ASP:OD2	1:A:181:THR:HG21	2.00	0.62
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.81	0.62
1:A:471:MET:SD	1:A:478:ASP:HB3	2.39	0.62
2:B:43:LEU:HD11	2:B:182:THR:OG1	1.99	0.62
2:C:471:MET:O	2:C:471:MET:HE3	2.00	0.62
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.63	0.62
2:B:284:ILE:HD12	2:B:436:THR:CB	2.28	0.62
2:B:425:ILE:H	2:B:425:ILE:HD12	1.63	0.62
2:F:306:CYS:SG	2:F:344:LEU:HB2	2.38	0.62
2:F:98:VAL:HA	2:F:103:LEU:O	1.98	0.62
2:F:197:GLU:OE2	2:F:197:GLU:N	2.29	0.62
2:B:129:ARG:O	2:B:132:TYR:HB3	1.99	0.62
2:D:72:VAL:HG21	2:D:134:ILE:HD13	1.81	0.62
2:D:317:TYR:CE2	2:D:383:LEU:HD11	2.34	0.62
2:E:325:LEU:CD2	2:E:335:PHE:HB2	2.30	0.62
2:F:353:SER:O	2:F:354:ALA:HB2	1.98	0.62
2:B:356:LEU:HD12	2:B:356:LEU:N	2.15	0.62
2:D:267:VAL:HG23	2:D:300:ARG:HG2	1.80	0.62
2:F:54:LEU:HD22	2:F:90:PHE:CZ	2.35	0.62
2:F:313:ILE:HG12	2:F:372:PRO:CG	2.30	0.62
2:F:392:PHE:O	2:F:396:VAL:HG23	2.00	0.62
2:B:458:MET:HB2	2:B:463:HIS:HD2	1.64	0.62
2:D:371:LYS:O	2:D:371:LYS:CD	2.46	0.62
2:F:451:ARG:HG2	2:F:451:ARG:NH1	2.12	0.62
2:B:205:VAL:C	2:B:206:ILE:HD12	2.21	0.61
2:C:31:ILE:HA	2:C:231:MET:SD	2.40	0.61
2:D:317:TYR:HE2	2:D:383:LEU:HD21	1.61	0.61
2:D:430:ILE:HA	2:D:433:ILE:HD13	1.82	0.61
2:F:344:LEU:HD22	2:F:345:LYS:N	2.14	0.61
2:B:287:THR:HB	2:B:425:ILE:HG23	1.82	0.61
2:C:21:MET:HB2	2:C:38:ILE:HG13	1.83	0.61
2:C:453:ILE:HB	2:C:470:PHE:CD2	2.35	0.61
2:D:178:THR:HG22	2:D:179:VAL:N	2.15	0.61
2:E:53:THR:CG2	2:E:145:ASP:OD1	2.48	0.61
2:F:148:THR:CG2	2:F:193:ARG:HD2	2.29	0.61
2:B:112:PRO:O	2:C:166:ARG:HG3	2.00	0.61
2:C:354:ALA:HB1	2:C:358:ASP:HB2	1.81	0.61
2:C:451:ARG:HG2	2:C:451:ARG:NH1	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:52:LYS:HB3	2:F:181:THR:HG23	1.81	0.61
2:B:119:GLY:C	2:B:121:PHE:H	2.02	0.61
2:C:217:ARG:HG3	2:C:217:ARG:O	2.00	0.61
2:F:458:MET:SD	2:F:461:SER:HB3	2.40	0.61
2:C:38:ILE:H	2:C:38:ILE:HD12	1.64	0.61
2:D:21:MET:CE	2:D:141:ARG:HG2	2.31	0.61
2:E:356:LEU:HD23	2:E:392:PHE:HA	1.83	0.61
2:F:182:THR:HG21	2:F:192:ALA:CB	2.31	0.61
1:A:56:SER:HB2	1:A:143:SER:HB3	1.81	0.61
2:C:150:VAL:HG13	2:C:151:PHE:N	2.15	0.61
2:C:488:ARG:HH22	2:D:488:ARG:NH2	1.97	0.61
2:D:375:ILE:HG22	2:D:377:ILE:CD1	2.29	0.61
2:E:284:ILE:O	2:E:412:PHE:N	2.32	0.61
2:E:323:GLN:HE22	2:F:459:ARG:HH11	1.49	0.61
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.31	0.61
1:A:351:PRO:HG2	1:A:382:ALA:O	2.00	0.61
1:A:377:ILE:HD13	1:A:412:PHE:CE2	2.34	0.61
1:A:426:TPO:HG21	1:A:431:ALA:H	1.65	0.61
1:A:496:ARG:NH1	2:B:497:ILE:HD13	2.16	0.61
2:B:62:ASN:O	2:B:66:GLU:HB2	2.00	0.61
2:D:445:ILE:HD13	2:D:450:SER:HG	1.63	0.61
2:E:356:LEU:CD1	2:E:387:VAL:HG11	2.31	0.61
2:E:378:ASP:O	2:E:379:SER:HB3	2.01	0.61
2:C:360:LEU:CD2	2:C:364:LYS:HE3	2.29	0.61
2:E:33:HIS:CD2	2:E:230:HIS:HA	2.32	0.61
1:A:52:LYS:HB3	1:A:181:THR:CG2	2.30	0.61
2:B:31:ILE:HA	2:B:231:MET:SD	2.41	0.61
2:B:497:ILE:O	2:B:499:VAL:N	2.34	0.61
2:C:283:ILE:HD11	2:C:404:LYS:HD2	1.81	0.61
2:D:130:ILE:O	2:D:134:ILE:HG12	2.00	0.61
2:D:151:PHE:C	2:D:153:GLN:H	2.04	0.61
2:E:266:GLY:CA	2:E:300:ARG:HG3	2.30	0.61
2:E:469:GLU:HB3	2:E:483:PHE:CZ	2.35	0.61
2:F:27:GLY:HA3	2:F:246:ILE:HB	1.81	0.61
1:A:272:GLU:O	1:A:462:TRP:HZ3	1.82	0.61
3:B:901:ATP:C2	2:C:462:TRP:HA	2.36	0.61
2:C:46:GLY:HA2	2:C:184:ARG:CD	2.30	0.61
2:D:23:THR:O	2:D:24:MET:HB2	2.01	0.61
2:D:94:LEU:HD23	2:D:94:LEU:N	2.15	0.61
2:F:248:PRO:CB	2:F:251:ALA:HB3	2.30	0.61
1:A:41:SER:HA	1:A:178:THR:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.82	0.60
1:A:211:LEU:CG	1:A:212:GLU:H	2.14	0.60
1:A:293:GLY:HA2	3:A:901:ATP:O1A	2.00	0.60
2:C:281:ASP:OD1	2:C:407:GLU:HA	2.01	0.60
2:C:453:ILE:HD13	2:C:454:ASN:H	1.61	0.60
2:C:41:SER:HA	2:C:178:THR:O	2.00	0.60
2:C:497:ILE:HD13	2:C:497:ILE:H	1.65	0.60
2:E:130:ILE:O	2:E:134:ILE:HG12	2.01	0.60
2:E:289:ALA:O	2:E:292:THR:HG23	2.01	0.60
2:E:345:LYS:HZ1	2:E:366:GLU:HG3	1.66	0.60
2:B:160:VAL:HG21	2:B:194:TYR:CD1	2.36	0.60
2:C:61:TYR:O	2:C:65:ILE:HG12	2.01	0.60
1:A:18:ILE:HD13	2:F:85:LYS:HE3	1.83	0.60
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.66	0.60
3:A:903:ATP:O3'	2:B:224:LYS:HA	2.00	0.60
2:B:148:THR:C	2:B:150:VAL:H	2.04	0.60
2:B:218:ARG:HD3	2:B:237:PHE:CZ	2.36	0.60
2:B:264:SER:HA	2:B:271:ASP:OD1	2.01	0.60
2:C:411:LEU:HD12	2:C:412:PHE:N	2.16	0.60
2:F:504:GLU:O	2:F:505:LEU:HB2	2.00	0.60
1:A:264:SER:HB3	1:A:304:ASN:ND2	2.16	0.60
2:B:178:THR:HG22	2:B:179:VAL:H	1.65	0.60
2:B:202:ASP:HA	2:B:226:ARG:HD2	1.83	0.60
2:C:471:MET:HE2	2:C:478:ASP:HB3	1.83	0.60
2:E:171:LEU:HD23	2:E:174:ILE:HD12	1.84	0.60
1:A:80:PRO:HB3	1:A:105:ILE:HG21	1.84	0.60
2:E:171:LEU:HA	2:E:174:ILE:CD1	2.32	0.60
2:E:255:THR:HG22	2:E:255:THR:O	2.01	0.60
2:E:278:PHE:CD1	2:E:284:ILE:HD13	2.37	0.60
1:A:380:LEU:HD21	1:A:412:PHE:HD2	1.66	0.60
2:D:418:GLN:HB2	2:E:423:HIS:O	2.01	0.60
2:F:170:ARG:HB3	2:F:170:ARG:NH1	2.16	0.60
2:F:212:GLU:O	2:F:212:GLU:OE2	2.20	0.60
2:B:31:ILE:O	2:B:231:MET:HG3	2.02	0.60
2:C:283:ILE:HD12	2:C:283:ILE:H	1.67	0.60
2:D:46:GLY:O	2:D:52:LYS:HD3	2.02	0.60
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.32	0.60
2:F:344:LEU:HD11	2:F:346:ILE:HG13	1.83	0.60
2:B:210:VAL:HG12	2:B:211:LEU:O	2.01	0.60
2:B:289:ALA:HB2	2:B:419:PHE:HA	1.83	0.60
2:B:432:TPO:O1P	2:B:432:TPO:HG21	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:318:GLU:HB2	5:F:523:HOH:O	2.00	0.60
2:B:247:PHE:HD2	2:B:364:LYS:HZ2	1.49	0.60
2:C:71:GLY:O	2:C:103:LEU:HA	2.02	0.60
2:E:392:PHE:O	2:E:395:PHE:HB3	2.02	0.60
2:F:451:ARG:HB3	2:F:470:PHE:CZ	2.37	0.60
1:A:79:THR:HG23	1:A:80:PRO:HD2	1.83	0.59
1:A:287:THR:HG21	1:A:425:ILE:O	2.02	0.59
2:B:36:LEU:HD12	2:B:59:PHE:CE1	2.37	0.59
2:B:178:THR:HG22	2:B:179:VAL:N	2.17	0.59
2:B:183:GLU:HG3	2:B:193:ARG:HD2	1.84	0.59
2:B:435:ASP:O	2:B:457:LYS:HE3	2.02	0.59
2:F:514:GLU:HG2	2:F:519:SER:CB	2.30	0.59
2:E:142:VAL:HB	2:E:178:THR:OG1	2.03	0.59
2:F:14:GLU:HG2	5:F:530:HOH:O	2.02	0.59
2:F:94:LEU:HD22	2:F:103:LEU:CD2	2.31	0.59
2:F:317:TYR:HA	2:F:349:ALA:O	2.02	0.59
1:A:433:ILE:HG22	1:A:433:ILE:O	2.02	0.59
2:F:220:LEU:HD23	2:F:221:GLU:N	2.17	0.59
2:F:249:LEU:HD12	2:F:394:GLN:OE1	2.02	0.59
2:B:311:ARG:HG3	2:B:371:LYS:HZ2	1.68	0.59
2:C:87:ALA:C	2:C:89:SER:H	2.04	0.59
2:D:21:MET:HE1	2:D:141:ARG:HG2	1.84	0.59
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.32	0.59
1:A:397:ILE:HD13	1:A:433:ILE:HG21	1.83	0.59
2:D:446:ARG:HB3	2:E:484:ARG:CG	2.32	0.59
2:F:25:ILE:CD1	2:F:58:GLN:HG2	2.32	0.59
2:F:379:SER:OG	2:F:382:ALA:HB2	2.02	0.59
1:A:44:VAL:HG22	1:A:205:VAL:HB	1.84	0.59
2:D:61:TYR:CD1	2:D:65:ILE:HD11	2.37	0.59
2:E:265:SER:HB3	2:E:278:PHE:CZ	2.38	0.59
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.84	0.59
1:A:298:VAL:HG23	1:A:411:LEU:HD23	1.85	0.59
2:C:296:LEU:HD21	2:C:477:PRO:HB3	1.83	0.59
2:D:25:ILE:HG12	2:D:58:GLN:HE21	1.68	0.59
2:D:30:ASP:OD2	2:D:30:ASP:N	2.36	0.59
2:D:432:TPO:C	2:D:433:ILE:HD12	2.33	0.59
2:D:486:PHE:HB3	2:D:489:ILE:CD1	2.33	0.59
2:E:311:ARG:O	2:E:373:ALA:N	2.35	0.59
2:E:461:SER:OG	2:E:462:TRP:N	2.35	0.59
2:F:106:LEU:HD11	2:F:129:ARG:NH2	2.17	0.59
2:F:298:VAL:HG13	2:F:376:ALA:HB1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:444:GLU:HB3	2:F:493:SER:HA	1.83	0.59
2:F:484:ARG:HB3	2:F:484:ARG:NH1	2.18	0.59
1:A:310:GLU:O	1:A:343:LEU:HB3	2.01	0.59
2:B:52:LYS:HE3	3:B:903:ATP:O3B	2.03	0.59
2:B:434:THR:CG2	2:B:437:ILE:HD11	2.33	0.59
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.84	0.59
2:D:150:VAL:CG1	2:D:151:PHE:N	2.65	0.59
2:D:296:LEU:HD13	2:D:331:TRP:CE2	2.38	0.59
2:D:332:GLY:O	2:D:333:MET:O	2.21	0.59
2:E:293:GLY:HA2	3:E:901:ATP:O1A	2.01	0.59
2:B:70:PRO:HA	2:B:102:LYS:O	2.02	0.59
2:D:414:ASN:ND2	2:D:426:THR:HG22	2.18	0.59
2:E:492:GLY:O	2:E:494:PRO:HD3	2.03	0.59
1:A:36:LEU:HD22	1:A:42:THR:HG21	1.84	0.58
2:B:441:GLN:HE22	2:B:490:ILE:HD13	1.68	0.58
2:B:468:ARG:HG2	2:B:468:ARG:HH11	1.68	0.58
2:C:252:MET:CE	2:C:397:ILE:HG22	2.32	0.58
2:D:380:LEU:CD1	2:D:412:PHE:HB3	2.32	0.58
2:D:385:ARG:O	2:D:387:VAL:HG23	2.02	0.58
2:E:455:VAL:HG11	2:E:463:HIS:HB2	1.83	0.58
2:F:263:VAL:HG12	2:F:374:ARG:NH2	2.11	0.58
2:D:262:ARG:HD2	2:D:276:GLY:O	2.02	0.58
2:D:345:LYS:NZ	2:D:366:GLU:OE1	2.34	0.58
2:E:81:GLN:H	2:E:81:GLN:CD	2.05	0.58
2:E:170:ARG:HB3	2:E:170:ARG:HH11	1.67	0.58
2:E:383:LEU:HD23	2:E:383:LEU:N	2.18	0.58
2:E:462:TRP:O	2:E:463:HIS:O	2.21	0.58
2:F:16:GLN:HE22	2:F:33:HIS:HB3	1.68	0.58
2:B:284:ILE:CD1	2:B:436:THR:HB	2.30	0.58
2:D:347:VAL:HG12	2:D:348:CYS:H	1.67	0.58
2:D:377:ILE:HG22	2:D:377:ILE:O	2.02	0.58
2:E:28:PHE:N	2:E:246:ILE:HD12	2.19	0.58
2:F:209:ASN:ND2	2:F:216:ARG:HD2	2.19	0.58
2:F:492:GLY:O	2:F:494:PRO:HD3	2.03	0.58
1:A:426:TPO:N	1:A:426:TPO:O1P	2.36	0.58
2:B:291:GLY:HA3	2:B:442:TYR:OH	2.04	0.58
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.85	0.58
2:D:123:LEU:O	2:D:127:ILE:HG13	2.03	0.58
2:E:148:THR:HG21	2:E:183:GLU:CG	2.34	0.58
2:E:221:GLU:HG2	2:E:222:ILE:N	2.18	0.58
2:B:64:ILE:HD12	2:B:102:LYS:HB3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:PHE:O	2:D:399:VAL:HG23	2.04	0.58
2:F:497:ILE:O	2:F:497:ILE:HD13	2.04	0.58
1:A:43:LEU:HD12	1:A:180:MET:O	2.04	0.58
1:A:377:ILE:HD12	1:A:377:ILE:N	2.19	0.58
2:C:56:SER:HG	2:C:73:PHE:HE1	1.52	0.58
2:C:69:GLU:HB3	2:C:140:ARG:HB2	1.85	0.58
2:D:218:ARG:CZ	2:D:239:ILE:CD1	2.78	0.58
2:D:443:VAL:HG12	2:D:445:ILE:HD11	1.85	0.58
2:F:377:ILE:HD12	2:F:412:PHE:HE2	1.66	0.58
2:C:38:ILE:HG23	2:C:177:THR:OG1	2.04	0.58
2:D:85:LYS:HE3	2:E:16:GLN:O	2.03	0.58
2:E:453:ILE:HG21	2:E:479:ILE:CD1	2.27	0.58
2:F:283:ILE:HG23	2:F:412:PHE:HE1	1.67	0.58
2:F:321:ARG:O	2:F:325:LEU:HD12	2.03	0.58
1:A:344:LEU:HD13	1:A:344:LEU:C	2.24	0.58
2:C:344:LEU:HD22	2:C:345:LYS:H	1.67	0.58
2:D:64:ILE:CD1	2:D:70:PRO:HA	2.31	0.58
2:D:267:VAL:HG12	2:D:270:LEU:H	1.69	0.58
2:F:440:LEU:HD23	2:F:453:ILE:HG13	1.86	0.58
2:B:85:LYS:HZ1	2:C:14:GLU:HG2	1.69	0.58
2:C:63:GLY:HA3	2:C:141:ARG:CZ	2.33	0.58
2:D:79:THR:HG22	2:D:82:ASP:OD2	2.04	0.58
2:E:223:LEU:O	2:E:224:LYS:HB3	2.03	0.58
2:F:471:MET:HG2	2:F:480:LYS:CE	2.33	0.58
2:B:148:THR:HA	2:B:151:PHE:CD1	2.38	0.58
2:B:187:GLU:O	2:B:208:ARG:HD3	2.04	0.58
2:C:50:THR:CG2	2:C:207:LEU:HB3	2.33	0.58
2:C:111:ASP:OD2	2:C:113:GLU:HG2	2.04	0.58
2:E:288:GLY:O	2:E:415:THR:HA	2.04	0.58
2:E:313:ILE:HG13	2:E:372:PRO:HG2	1.84	0.58
2:F:171:LEU:HD13	2:F:178:THR:HG21	1.86	0.58
1:A:425:ILE:HG23	2:F:419:PHE:CE2	2.39	0.57
2:C:314:LEU:HD23	2:C:346:ILE:HD12	1.85	0.57
2:D:496:ARG:NH2	2:E:486:PHE:O	2.37	0.57
2:E:305:ALA:CB	2:E:374:ARG:HD2	2.23	0.57
2:F:443:VAL:O	2:F:445:ILE:HD12	2.04	0.57
2:B:56:SER:HB2	2:B:143:SER:HB3	1.85	0.57
2:B:434:THR:HG21	2:B:437:ILE:HD11	1.85	0.57
2:D:69:GLU:HB3	2:D:140:ARG:HB2	1.86	0.57
2:E:221:GLU:CG	2:E:222:ILE:N	2.67	0.57
2:E:332:GLY:O	2:E:333:MET:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:245:ASN:HD22	2:F:361:GLN:HE21	1.52	0.57
1:A:148:THR:HG21	1:A:183:GLU:HG3	1.85	0.57
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.19	0.57
2:B:455:VAL:HG11	2:B:463:HIS:HB2	1.87	0.57
2:B:462:TRP:O	2:B:463:HIS:O	2.20	0.57
2:D:287:THR:HG22	2:D:288:GLY:H	1.68	0.57
2:E:214:GLU:HB3	2:F:234:GLU:HB2	1.85	0.57
1:A:52:LYS:HB2	3:A:903:ATP:O1B	2.04	0.57
1:A:294:LYS:N	3:A:901:ATP:O1B	2.35	0.57
2:F:225:LEU:HB2	2:F:230:HIS:HD2	1.69	0.57
2:F:246:ILE:HG22	2:F:247:PHE:N	2.19	0.57
1:A:371:LYS:N	1:A:372:PRO:HD3	2.20	0.57
2:B:87:ALA:C	2:B:89:SER:H	2.06	0.57
2:C:287:THR:HG21	2:C:414:ASN:HD22	1.69	0.57
2:C:294:LYS:HD3	2:C:294:LYS:H	1.70	0.57
2:C:360:LEU:O	2:C:360:LEU:HD23	2.04	0.57
2:D:89:SER:HB2	2:E:227:GLY:O	2.04	0.57
2:D:418:GLN:NE2	2:D:422:ALA:HA	2.19	0.57
2:E:247:PHE:HZ	2:E:361:GLN:HB2	1.70	0.57
2:F:317:TYR:OH	2:F:363:ILE:HD11	2.05	0.57
1:A:273:MET:O	1:A:463:HIS:HA	2.03	0.57
2:B:197:GLU:CD	2:B:197:GLU:H	2.06	0.57
2:B:425:ILE:HD11	2:B:456:PHE:CE2	2.39	0.57
2:E:249:LEU:HD12	2:E:394:GLN:CD	2.24	0.57
2:F:202:ASP:HA	2:F:226:ARG:HD2	1.85	0.57
1:A:311:ARG:HD2	1:A:371:LYS:NZ	2.19	0.57
1:A:488:ARG:NE	2:F:488:ARG:HH12	2.03	0.57
2:B:285:LEU:HB3	2:B:437:ILE:HD13	1.87	0.57
2:D:67:PHE:O	2:D:68:ASP:HB3	2.03	0.57
2:E:54:LEU:HD22	2:E:90:PHE:CZ	2.39	0.57
2:E:238:THR:HB	2:E:361:GLN:NE2	2.18	0.57
2:B:246:ILE:HD12	2:B:246:ILE:N	2.20	0.57
2:C:248:PRO:O	2:C:250:GLY:N	2.38	0.57
2:D:53:THR:HG22	2:D:57:ILE:CD1	2.35	0.57
1:A:257:ARG:NH2	1:A:407:GLU:HG2	2.20	0.57
1:A:269:ARG:HB3	1:A:479:ILE:HD12	1.86	0.57
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.86	0.57
2:B:88:ARG:HG2	2:B:88:ARG:HH11	1.68	0.57
2:C:289:ALA:HB2	2:C:419:PHE:HA	1.87	0.57
2:C:471:MET:HE2	2:C:478:ASP:CB	2.35	0.57
2:D:64:ILE:HD11	2:D:102:LYS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:351:PRO:HG2	2:D:382:ALA:O	2.05	0.57
2:E:296:LEU:HD13	2:E:331:TRP:CE2	2.40	0.57
2:E:396:VAL:HG21	2:E:430:ILE:HD13	1.85	0.57
2:E:437:ILE:CD1	2:E:457:LYS:HE2	2.35	0.57
1:A:52:LYS:HD3	1:A:182:THR:O	2.05	0.57
1:A:388:SER:OG	1:A:389:ASN:N	2.38	0.57
1:A:488:ARG:HE	2:F:488:ARG:HH12	1.53	0.57
2:B:356:LEU:CD1	2:B:356:LEU:N	2.67	0.57
2:D:220:LEU:HD23	2:D:220:LEU:C	2.24	0.57
2:E:294:LYS:CB	2:E:413:THR:HG23	2.34	0.57
2:F:194:TYR:O	2:F:195:GLY:C	2.43	0.57
1:A:14:GLU:HG3	1:A:15:HIS:N	2.14	0.56
2:C:72:VAL:O	2:C:142:VAL:HG13	2.05	0.56
2:D:486:PHE:HB3	2:D:489:ILE:HD12	1.88	0.56
2:F:115:GLN:CG	2:F:116:GLU:H	2.17	0.56
2:F:245:ASN:HD22	2:F:361:GLN:NE2	2.03	0.56
1:A:316:ALA:O	1:A:348:CYS:HA	2.04	0.56
1:A:501:GLU:O	1:A:503:SER:N	2.37	0.56
2:B:56:SER:O	2:B:59:PHE:HB3	2.06	0.56
2:C:147:VAL:O	2:C:150:VAL:HG12	2.05	0.56
2:D:53:THR:HG23	2:D:145:ASP:OD2	2.05	0.56
2:E:444:GLU:OE1	2:F:490:ILE:HG12	2.05	0.56
2:F:130:ILE:O	2:F:134:ILE:HG12	2.05	0.56
1:A:432:TPO:HB	2:F:318:GLU:OE2	2.04	0.56
2:B:53:THR:HG23	2:B:145:ASP:OD1	2.06	0.56
2:B:192:ALA:HB3	2:B:197:GLU:OE2	2.05	0.56
2:B:284:ILE:HG23	2:B:436:THR:HB	1.87	0.56
2:B:341:GLN:O	2:B:343:LEU:HG	2.04	0.56
2:C:215:ARG:HA	2:C:215:ARG:NE	2.20	0.56
2:D:74:VAL:HG21	2:D:130:ILE:HD13	1.86	0.56
2:E:205:VAL:HG22	2:E:222:ILE:CD1	2.34	0.56
2:F:311:ARG:HG3	2:F:371:LYS:HZ2	1.69	0.56
2:F:317:TYR:CD2	2:F:383:LEU:HD21	2.40	0.56
2:C:103:LEU:HD12	2:C:104:PHE:H	1.70	0.56
2:D:24:MET:HE2	2:D:66:GLU:HG3	1.87	0.56
2:D:43:LEU:HD21	2:D:197:GLU:CB	2.35	0.56
2:D:436:THR:CG2	2:D:458:MET:HG2	2.32	0.56
2:E:94:LEU:HB3	2:E:103:LEU:CD2	2.35	0.56
2:F:47:THR:HG23	2:F:48:SER:N	2.19	0.56
2:F:161:ARG:HB2	2:F:196:VAL:CG1	2.35	0.56
2:F:514:GLU:O	2:F:515:LYS:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SER:HB2	2:B:227:GLY:O	2.05	0.56
1:A:199:PHE:CE1	2:F:183:GLU:HB2	2.40	0.56
1:A:203:ASN:OD1	1:A:225:LEU:HD23	2.06	0.56
1:A:375:ILE:O	1:A:410:GLY:HA2	2.06	0.56
2:C:37:PRO:HD2	2:C:203:ASN:ND2	2.21	0.56
2:D:18:ILE:HD13	2:D:228:THR:CG2	2.36	0.56
2:E:317:TYR:OH	2:E:363:ILE:HD11	2.06	0.56
2:F:192:ALA:HB1	2:F:197:GLU:OE1	2.06	0.56
2:B:211:LEU:HD13	2:B:216:ARG:NE	2.20	0.56
2:D:283:ILE:HG23	2:D:412:PHE:CE1	2.40	0.56
2:E:131:ASN:O	2:E:135:GLN:HB2	2.05	0.56
2:F:52:LYS:CB	3:F:903:ATP:O1B	2.53	0.56
2:B:65:ILE:O	2:B:66:GLU:HG2	2.05	0.56
2:B:126:LEU:O	2:B:130:ILE:HG13	2.06	0.56
2:D:21:MET:HE1	2:D:177:THR:HB	1.88	0.56
2:E:148:THR:CG2	2:E:193:ARG:HD2	2.36	0.56
2:B:123:LEU:HD12	2:B:166:ARG:HD2	1.88	0.56
2:E:445:ILE:HG22	2:E:446:ARG:HD2	1.87	0.56
2:E:504:GLU:HG2	2:E:505:LEU:N	2.20	0.56
2:F:33:HIS:ND1	2:F:230:HIS:HA	2.21	0.56
1:A:121:PHE:CD1	1:A:122:ASP:N	2.73	0.56
1:A:285:LEU:HB3	1:A:437:ILE:HD13	1.87	0.56
1:A:447:GLY:HA2	2:B:489:ILE:CD1	2.36	0.56
2:C:248:PRO:C	2:C:250:GLY:H	2.09	0.56
2:B:370:PHE:O	2:B:371:LYS:HD2	2.06	0.56
2:C:232:LYS:HD2	2:C:232:LYS:N	2.21	0.56
2:C:384:ALA:HB2	2:C:392:PHE:CE1	2.40	0.56
2:D:68:ASP:OD1	2:D:68:ASP:O	2.23	0.56
2:D:292:THR:HB	2:D:440:LEU:CB	2.36	0.56
2:D:350:TYR:CZ	2:E:254:LEU:HD13	2.41	0.56
2:E:316:ALA:HB2	2:E:324:LEU:HD11	1.88	0.56
2:F:54:LEU:O	2:F:55:PHE:C	2.44	0.56
2:F:270:LEU:O	2:F:273:MET:HB2	2.05	0.56
2:F:315:PHE:CE2	2:F:347:VAL:HG21	2.41	0.56
1:A:105:ILE:HD12	1:A:105:ILE:N	2.21	0.55
1:A:145:ASP:O	1:A:146:SER:OG	2.24	0.55
1:A:379:SER:N	1:A:413:THR:HB	2.14	0.55
3:A:901:ATP:H3'	2:B:458:MET:O	2.06	0.55
2:B:216:ARG:HG3	2:C:233:GLY:H	1.71	0.55
2:C:335:PHE:HA	2:C:338:MET:HG3	1.88	0.55
2:C:360:LEU:HD23	2:C:364:LYS:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:289:ALA:HB2	2:E:419:PHE:HA	1.87	0.55
2:E:294:LYS:CG	2:E:413:THR:HG23	2.36	0.55
1:A:451:ARG:HD2	1:A:451:ARG:N	2.19	0.55
2:C:313:ILE:HD12	2:C:372:PRO:HG3	1.88	0.55
2:E:41:SER:HB2	2:E:178:THR:HG22	1.87	0.55
2:E:452:ALA:HA	2:E:469:GLU:HA	1.88	0.55
2:F:56:SER:O	2:F:59:PHE:HB3	2.06	0.55
1:A:159:VAL:O	1:A:163:GLU:HG2	2.07	0.55
2:C:42:THR:HA	2:C:203:ASN:HB2	1.88	0.55
2:D:194:TYR:O	2:D:196:VAL:N	2.40	0.55
2:D:388:SER:O	2:D:389:ASN:C	2.43	0.55
2:E:267:VAL:HG21	2:E:477:PRO:CG	2.36	0.55
2:F:470:PHE:HA	2:F:478:ASP:O	2.06	0.55
2:B:18:ILE:HD12	2:B:18:ILE:N	2.21	0.55
2:B:359:HIS:O	2:B:363:ILE:HD13	2.07	0.55
2:B:387:VAL:HG12	2:B:391:ALA:HB3	1.89	0.55
2:C:264:SER:O	2:C:374:ARG:NH2	2.40	0.55
2:F:255:THR:O	2:F:255:THR:HG22	2.06	0.55
1:A:19:ALA:HB3	1:A:38:ILE:HD12	1.89	0.55
2:B:191:ILE:HB	2:B:198:GLU:CG	2.37	0.55
2:B:195:GLY:HA2	2:B:198:GLU:OE2	2.06	0.55
2:B:247:PHE:CE2	2:B:364:LYS:HD2	2.37	0.55
2:B:357:GLU:CG	2:B:358:ASP:N	2.69	0.55
2:C:296:LEU:HD13	2:C:331:TRP:CE2	2.41	0.55
2:C:300:ARG:HA	2:C:333:MET:CE	2.36	0.55
2:D:191:ILE:CG2	2:D:198:GLU:HG3	2.36	0.55
2:D:191:ILE:HG21	2:D:198:GLU:HG3	1.89	0.55
2:D:393:ARG:O	2:D:397:ILE:HG13	2.07	0.55
2:E:222:ILE:N	5:E:534:HOH:O	2.38	0.55
2:E:308:ASN:O	2:E:309:LYS:HB2	2.07	0.55
2:E:371:LYS:O	2:E:371:LYS:CD	2.54	0.55
2:E:501:GLU:O	2:E:502:LYS:HG3	2.06	0.55
2:F:191:ILE:HB	2:F:198:GLU:CD	2.26	0.55
2:F:231:MET:HE3	2:F:251:ALA:HB2	1.87	0.55
1:A:220:LEU:HD13	1:A:246:ILE:HD11	1.89	0.55
2:B:71:GLY:O	2:B:103:LEU:HA	2.07	0.55
2:C:73:PHE:HD1	2:C:143:SER:HB2	1.71	0.55
2:E:197:GLU:OE2	2:E:197:GLU:N	2.30	0.55
2:C:24:MET:CB	2:C:62:ASN:HD22	2.19	0.55
2:C:486:PHE:CE2	2:C:496:ARG:HG2	2.41	0.55
2:D:39:GLY:H	2:D:177:THR:HG23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:GLU:O	2:D:166:ARG:HB3	2.06	0.55
2:E:279:PHE:HB2	2:E:282:SER:OG	2.07	0.55
2:F:294:LYS:NZ	2:F:415:THR:HG23	2.21	0.55
2:B:18:ILE:HD13	2:B:227:GLY:O	2.07	0.55
2:B:379:SER:OG	2:B:382:ALA:HB2	2.06	0.55
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.37	0.55
2:D:445:ILE:HD12	2:D:445:ILE:N	2.22	0.55
2:E:346:ILE:HG22	2:E:348:CYS:SG	2.47	0.55
2:F:64:ILE:HD13	2:F:69:GLU:O	2.07	0.55
2:F:492:GLY:C	2:F:494:PRO:HD3	2.26	0.55
1:A:41:SER:OG	1:A:178:THR:HB	2.07	0.55
1:A:509:VAL:O	1:A:509:VAL:HG12	2.08	0.55
2:B:61:TYR:CE1	2:B:92:TRP:HB2	2.41	0.55
2:B:316:ALA:HB3	2:B:348:CYS:SG	2.47	0.55
2:D:98:VAL:HG21	2:D:105:ILE:HD13	1.88	0.55
2:E:27:GLY:HA3	2:E:246:ILE:HB	1.89	0.55
1:A:363:ILE:O	1:A:367:ILE:HG13	2.07	0.54
2:B:151:PHE:CE2	2:B:160:VAL:HG13	2.42	0.54
2:B:469:GLU:HB3	2:B:483:PHE:CE1	2.42	0.54
2:E:123:LEU:HD23	2:E:127:ILE:CD1	2.30	0.54
2:E:200:VAL:O	2:E:200:VAL:HG12	2.07	0.54
2:E:404:LYS:C	2:E:406:GLU:H	2.10	0.54
2:F:18:ILE:HG13	2:F:227:GLY:HA3	1.89	0.54
2:F:147:VAL:HG23	2:F:148:THR:N	2.23	0.54
2:F:484:ARG:HB3	2:F:484:ARG:HH11	1.72	0.54
2:D:449:MET:HE2	2:E:467:ILE:HD11	1.89	0.54
2:F:289:ALA:O	2:F:292:THR:HG23	2.06	0.54
1:A:94:LEU:O	1:A:97:LEU:N	2.39	0.54
2:C:25:ILE:HG12	2:C:58:GLN:NE2	2.22	0.54
2:C:187:GLU:OE2	2:C:208:ARG:HA	2.07	0.54
2:F:378:ASP:O	2:F:379:SER:HB3	2.07	0.54
2:B:50:THR:HB	2:B:207:LEU:CB	2.38	0.54
2:B:404:LYS:C	2:B:406:GLU:H	2.11	0.54
2:D:154:TYR:O	2:D:154:TYR:HD1	1.90	0.54
2:D:443:VAL:HG12	2:D:445:ILE:CD1	2.37	0.54
2:E:437:ILE:HD11	2:E:457:LYS:HE2	1.88	0.54
2:E:451:ARG:HH11	2:E:472:ILE:HD11	1.72	0.54
2:E:497:ILE:CG2	2:E:498:THR:H	2.16	0.54
2:F:313:ILE:HD12	2:F:345:LYS:HB3	1.87	0.54
1:A:211:LEU:HG	1:A:212:GLU:N	2.23	0.54
2:B:436:THR:OG1	2:B:458:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:ARG:HH12	2:D:208:ARG:NH1	2.05	0.54
2:D:495:THR:HG23	2:E:487:GLU:OE2	2.06	0.54
2:F:79:THR:HG22	2:F:82:ASP:CG	2.28	0.54
2:F:123:LEU:O	2:F:127:ILE:HG12	2.08	0.54
1:A:237:PHE:HB3	1:A:246:ILE:HG12	1.89	0.54
2:B:221:GLU:HG3	2:B:233:GLY:O	2.08	0.54
2:B:311:ARG:HG3	2:B:371:LYS:HZ1	1.71	0.54
2:C:38:ILE:HG22	2:C:39:GLY:N	2.22	0.54
2:D:273:MET:SD	2:D:468:ARG:HD2	2.48	0.54
2:D:362:ILE:O	2:D:365:SER:HB3	2.07	0.54
2:D:449:MET:CE	2:E:467:ILE:HD11	2.37	0.54
2:E:31:ILE:HA	2:E:231:MET:HG3	1.89	0.54
2:E:472:ILE:HD12	2:E:472:ILE:N	2.23	0.54
2:F:231:MET:CE	2:F:251:ALA:HB2	2.36	0.54
1:A:222:ILE:N	1:A:222:ILE:HD12	2.23	0.54
2:B:155:ASP:OD1	2:B:159:VAL:HG11	2.08	0.54
2:B:451:ARG:N	2:B:451:ARG:HD2	2.22	0.54
2:C:63:GLY:HA3	2:C:141:ARG:NH1	2.23	0.54
2:D:471:MET:HE2	2:D:471:MET:O	2.07	0.54
2:E:292:THR:OG1	2:E:440:LEU:HD12	2.07	0.54
2:E:464:ASP:OD2	2:E:466:ALA:HB3	2.08	0.54
2:F:273:MET:CE	2:F:468:ARG:HD2	2.37	0.54
2:B:187:GLU:OE2	2:B:208:ARG:HG2	2.08	0.54
2:C:231:MET:CE	2:C:251:ALA:HB2	2.37	0.54
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.89	0.54
2:D:61:TYR:CE1	2:D:65:ILE:HD11	2.43	0.54
2:E:420:MET:HE1	2:F:490:ILE:HG13	1.90	0.54
2:E:453:ILE:HG23	2:E:453:ILE:O	2.07	0.54
2:D:127:ILE:HD13	2:D:170:ARG:HG3	1.90	0.54
2:D:419:PHE:H	2:D:419:PHE:HD2	1.56	0.54
2:F:220:LEU:HD23	2:F:220:LEU:C	2.28	0.54
2:F:357:GLU:HG3	2:F:358:ASP:N	2.23	0.54
1:A:123:LEU:O	1:A:126:LEU:HB3	2.09	0.54
1:A:161:ARG:NH2	2:F:77:GLU:OE1	2.37	0.54
1:A:358:ASP:O	1:A:362:ILE:HG12	2.07	0.54
2:C:56:SER:HB2	2:C:143:SER:HB3	1.89	0.54
2:C:215:ARG:HE	2:C:215:ARG:CA	2.18	0.54
2:D:41:SER:HB3	2:D:178:THR:HB	1.89	0.54
2:D:431:ALA:C	2:D:433:ILE:H	2.12	0.54
2:D:461:SER:OG	2:D:462:TRP:N	2.36	0.54
2:E:153:GLN:O	2:F:158:SER:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:ARG:O	2:E:387:VAL:HG23	2.08	0.54
2:F:452:ALA:HA	2:F:469:GLU:HA	1.90	0.54
1:A:364:LYS:HA	1:A:367:ILE:HD12	1.91	0.53
1:A:413:THR:HG21	5:A:535:HOH:O	2.07	0.53
2:B:264:SER:HB3	2:B:304:ASN:HD21	1.72	0.53
2:F:39:GLY:O	2:F:172:LYS:HG3	2.08	0.53
2:F:72:VAL:HG21	2:F:134:ILE:HD13	1.90	0.53
2:B:24:MET:HB2	2:B:62:ASN:HD22	1.73	0.53
2:B:211:LEU:HG	2:B:212:GLU:H	1.74	0.53
2:B:433:ILE:HD12	2:B:433:ILE:N	2.23	0.53
2:C:52:LYS:HD2	2:C:182:THR:O	2.08	0.53
2:E:273:MET:O	2:E:463:HIS:HB2	2.08	0.53
2:E:294:LYS:HG2	2:E:413:THR:HG23	1.90	0.53
2:E:323:GLN:HG2	2:E:327:ASN:HD21	1.72	0.53
1:A:192:ALA:O	1:A:194:TYR:N	2.41	0.53
1:A:341:GLN:O	1:A:343:LEU:HG	2.08	0.53
1:A:378:ASP:HA	1:A:413:THR:HB	1.91	0.53
2:B:191:ILE:HB	2:B:198:GLU:HG3	1.90	0.53
2:C:283:ILE:HD12	2:C:283:ILE:N	2.23	0.53
2:C:381:SER:O	2:C:384:ALA:N	2.36	0.53
2:C:431:ALA:O	2:C:432:TPO:CG2	2.43	0.53
2:D:446:ARG:HB3	2:E:484:ARG:HG3	1.90	0.53
2:E:170:ARG:HB3	2:E:170:ARG:NH1	2.24	0.53
2:E:287:THR:HG22	2:E:288:GLY:N	2.23	0.53
2:E:451:ARG:HH11	2:E:472:ILE:CD1	2.22	0.53
2:F:377:ILE:CD1	2:F:399:VAL:HG11	2.38	0.53
1:A:64:ILE:HG23	1:A:102:LYS:HB3	1.90	0.53
2:B:140:ARG:NH1	2:B:140:ARG:CB	2.67	0.53
2:B:311:ARG:HD2	2:B:371:LYS:HE3	1.90	0.53
2:B:344:LEU:HD13	2:B:344:LEU:C	2.29	0.53
2:C:88:ARG:CZ	2:D:15:HIS:HA	2.36	0.53
2:C:220:LEU:HD23	2:C:221:GLU:N	2.23	0.53
2:C:287:THR:CG2	2:C:288:GLY:H	2.17	0.53
2:E:32:SER:OG	2:E:35:GLY:N	2.42	0.53
2:E:294:LYS:HB2	3:E:901:ATP:O1B	2.08	0.53
2:F:93:ASP:OD1	2:F:95:ALA:HB3	2.07	0.53
1:A:459:ARG:NH1	2:F:319:GLU:HG2	2.23	0.53
1:A:466:ALA:HA	2:F:448:GLU:HG2	1.90	0.53
2:B:204:VAL:HG23	2:B:224:LYS:HG2	1.91	0.53
2:B:326:ARG:HG3	2:C:260:ASN:ND2	2.22	0.53
2:D:64:ILE:CD1	2:D:102:LYS:HB3	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:375:ILE:HG22	2:D:377:ILE:HD11	1.91	0.53
2:D:451:ARG:HD2	2:D:451:ARG:N	2.24	0.53
2:E:186:GLU:OE1	2:E:189:GLY:N	2.42	0.53
2:E:264:SER:HB3	2:E:304:ASN:HD21	1.73	0.53
2:F:461:SER:OG	2:F:462:TRP:N	2.41	0.53
1:A:184:ARG:O	1:A:185:ILE:HD13	2.08	0.53
1:A:371:LYS:O	1:A:371:LYS:CD	2.55	0.53
2:C:164:LEU:O	2:C:167:LEU:N	2.42	0.53
2:D:18:ILE:HD12	2:D:18:ILE:N	2.19	0.53
2:D:313:ILE:HD11	2:D:370:PHE:HB3	1.91	0.53
2:F:75:THR:OG1	2:F:78:GLU:O	2.23	0.53
2:F:426:THR:C	2:F:428:SER:H	2.12	0.53
1:A:21:MET:CE	1:A:59:PHE:HZ	2.22	0.53
1:A:52:LYS:N	1:A:207:LEU:HD12	2.23	0.53
1:A:121:PHE:HD1	1:A:122:ASP:N	2.07	0.53
2:C:389:ASN:HD21	2:C:428:SER:CB	2.22	0.53
2:D:284:ILE:HD12	2:D:284:ILE:N	2.24	0.53
2:F:31:ILE:HA	2:F:231:MET:HG3	1.90	0.53
2:F:231:MET:HB3	2:F:235:TYR:OH	2.08	0.53
2:F:280:LYS:NZ	2:F:407:GLU:HB3	2.23	0.53
2:F:287:THR:HA	2:F:414:ASN:O	2.08	0.53
2:F:302:VAL:HG12	2:F:303:GLU:N	2.23	0.53
2:F:430:ILE:HG22	2:F:430:ILE:O	2.08	0.53
1:A:230:HIS:CE1	1:A:232:LYS:HE3	2.43	0.53
2:D:37:PRO:HG2	2:D:203:ASN:OD1	2.09	0.53
2:D:294:LYS:N	3:D:901:ATP:O1B	2.42	0.53
2:D:347:VAL:O	2:D:348:CYS:CB	2.56	0.53
2:F:47:THR:O	2:F:52:LYS:HE2	2.08	0.53
2:F:462:TRP:CE3	2:F:463:HIS:N	2.77	0.53
1:A:14:GLU:CG	1:A:15:HIS:N	2.68	0.53
2:B:88:ARG:NH1	2:B:93:ASP:HA	2.23	0.53
2:C:438:ILE:HD12	2:C:438:ILE:N	2.24	0.53
2:D:44:VAL:HG13	2:D:205:VAL:HG12	1.89	0.53
2:E:268:VAL:O	2:E:271:ASP:HB2	2.08	0.53
2:E:296:LEU:HD13	2:E:331:TRP:CD2	2.43	0.53
2:E:344:LEU:HD22	2:E:345:LYS:N	2.20	0.53
2:F:418:GLN:NE2	2:F:421:GLY:O	2.41	0.53
1:A:485:ASN:HD22	1:A:498:THR:CG2	2.22	0.53
2:B:119:GLY:C	2:B:121:PHE:N	2.61	0.53
2:B:304:ASN:HB3	2:B:374:ARG:HH12	1.74	0.53
2:D:202:ASP:HA	2:D:226:ARG:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:326:ARG:HD3	2:F:258:SER:OG	2.09	0.53
2:F:364:LYS:HE2	2:F:402:TYR:CD1	2.43	0.53
2:B:117:VAL:O	2:B:117:VAL:HG12	2.09	0.52
2:C:182:THR:HG22	2:C:183:GLU:H	1.73	0.52
2:D:262:ARG:NH1	2:D:275:GLY:O	2.42	0.52
2:D:344:LEU:HD13	2:D:344:LEU:C	2.30	0.52
2:D:443:VAL:O	2:D:445:ILE:HD12	2.09	0.52
2:D:463:HIS:ND1	2:D:464:ASP:O	2.37	0.52
2:E:47:THR:HG21	2:E:187:GLU:OE1	2.09	0.52
2:E:52:LYS:HB2	2:E:52:LYS:NZ	2.24	0.52
2:E:84:ILE:HG21	2:E:95:ALA:HB2	1.91	0.52
2:B:121:PHE:H	2:B:121:PHE:HD1	1.58	0.52
2:B:326:ARG:O	2:B:328:ALA:N	2.42	0.52
2:B:379:SER:CA	2:B:413:THR:HB	2.39	0.52
2:C:31:ILE:O	2:C:231:MET:HG3	2.09	0.52
2:C:98:VAL:HA	2:C:103:LEU:O	2.09	0.52
2:D:353:SER:HA	2:E:250:GLY:O	2.08	0.52
2:E:23:THR:O	2:E:24:MET:HB2	2.07	0.52
2:F:323:GLN:HG2	2:F:327:ASN:HD21	1.73	0.52
1:A:203:ASN:CG	1:A:225:LEU:HD23	2.30	0.52
2:C:184:ARG:NH1	2:C:187:GLU:O	2.41	0.52
2:C:202:ASP:CA	2:C:226:ARG:HD2	2.38	0.52
2:C:337:GLU:O	2:C:340:ARG:N	2.42	0.52
2:C:471:MET:HE1	2:C:478:ASP:HB2	1.91	0.52
1:A:432:TPO:C	1:A:434:THR:H	2.22	0.52
2:B:379:SER:HA	2:B:413:THR:HB	1.90	0.52
2:C:28:PHE:O	2:C:31:ILE:N	2.37	0.52
2:C:223:LEU:O	2:C:223:LEU:HD22	2.10	0.52
2:C:340:ARG:C	2:C:342:ASN:H	2.13	0.52
2:C:392:PHE:O	2:C:395:PHE:N	2.43	0.52
2:D:284:ILE:HD12	2:D:284:ILE:H	1.75	0.52
2:E:18:ILE:HD11	2:E:227:GLY:HA3	1.92	0.52
2:F:31:ILE:CD1	2:F:246:ILE:HG21	2.39	0.52
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.45	0.52
1:A:104:PHE:HD2	1:A:133:ALA:HB1	1.75	0.52
2:B:23:THR:N	2:B:29:ASP:OD1	2.28	0.52
2:B:274:CYS:HB3	2:B:458:MET:SD	2.50	0.52
2:D:294:LYS:CB	2:D:413:THR:HG23	2.39	0.52
2:E:30:ASP:O	2:E:31:ILE:C	2.47	0.52
1:A:246:ILE:O	1:A:248:PRO:HD3	2.10	0.52
1:A:258:SER:OG	2:F:326:ARG:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLU:OE1	1:A:407:GLU:CA	2.57	0.52
2:B:46:GLY:CA	2:B:184:ARG:HD3	2.32	0.52
2:B:479:ILE:H	2:B:479:ILE:HD12	1.74	0.52
2:C:194:TYR:O	2:C:195:GLY:C	2.46	0.52
2:D:164:LEU:O	2:D:168:VAL:HG23	2.10	0.52
2:D:184:ARG:NH2	2:D:189:GLY:O	2.42	0.52
2:E:444:GLU:OE1	2:F:489:ILE:HB	2.08	0.52
2:F:122:ASP:OD2	2:F:123:LEU:N	2.43	0.52
1:A:61:TYR:CZ	1:A:65:ILE:HG13	2.44	0.52
2:B:35:GLY:O	2:B:36:LEU:C	2.48	0.52
2:B:246:ILE:O	2:B:248:PRO:HD3	2.09	0.52
2:C:198:GLU:O	2:C:200:VAL:N	2.43	0.52
2:D:49:GLY:O	2:D:218:ARG:NH2	2.43	0.52
2:D:338:MET:HB3	2:D:344:LEU:HB3	1.90	0.52
2:D:418:GLN:HE21	2:D:422:ALA:HA	1.74	0.52
2:B:359:HIS:O	2:B:360:LEU:C	2.48	0.52
2:C:88:ARG:NH2	2:D:15:HIS:ND1	2.58	0.52
2:C:315:PHE:CE2	2:C:363:ILE:HA	2.44	0.52
2:F:106:LEU:CD1	2:F:129:ARG:NH2	2.73	0.52
2:F:345:LYS:NZ	2:F:366:GLU:OE1	2.41	0.52
2:F:515:LYS:HB3	2:F:517:PRO:HD2	1.92	0.52
1:A:182:THR:HG22	1:A:183:GLU:N	2.25	0.52
1:A:317:TYR:HE1	1:A:377:ILE:HG23	1.74	0.52
1:A:436:THR:HG23	1:A:458:MET:HG2	1.92	0.52
2:B:27:GLY:HA3	2:B:246:ILE:O	2.10	0.52
2:C:461:SER:OG	2:C:462:TRP:N	2.43	0.52
2:D:402:TYR:O	2:D:406:GLU:HB2	2.10	0.52
2:E:148:THR:HG21	2:E:183:GLU:HG3	1.90	0.52
2:E:454:ASN:HD21	2:E:456:PHE:HA	1.75	0.52
1:A:20:LYS:HD3	1:A:35:GLY:O	2.10	0.52
1:A:72:VAL:HB	1:A:142:VAL:HG22	1.92	0.52
1:A:452:ALA:HA	1:A:469:GLU:HA	1.92	0.52
1:A:508:ILE:HD12	1:A:510:ARG:N	2.24	0.52
2:B:52:LYS:HE3	3:B:903:ATP:O1B	2.10	0.52
2:B:134:ILE:HG21	2:B:174:ILE:CG2	2.39	0.52
2:D:375:ILE:CG2	2:D:377:ILE:HD11	2.40	0.52
2:D:387:VAL:HG12	2:D:388:SER:N	2.25	0.52
2:E:273:MET:CE	2:E:468:ARG:HD2	2.40	0.52
2:E:310:GLU:HB3	2:E:373:ALA:HB3	1.92	0.52
2:F:213:GLY:C	2:F:215:ARG:H	2.13	0.52
1:A:194:TYR:O	1:A:196:VAL:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HD2	1:A:272:GLU:OE2	2.10	0.51
2:C:360:LEU:HA	2:C:363:ILE:HD12	1.92	0.51
2:D:23:THR:HB	2:D:25:ILE:HD12	1.91	0.51
2:D:52:LYS:HE3	3:D:903:ATP:O1B	2.10	0.51
2:D:152:GLN:CG	2:E:161:ARG:HH11	2.18	0.51
2:E:70:PRO:HB2	2:E:139:ALA:HA	1.92	0.51
2:E:294:LYS:HE3	2:E:415:THR:OG1	2.10	0.51
2:F:126:LEU:O	2:F:129:ARG:HB2	2.10	0.51
2:B:468:ARG:HG2	2:B:468:ARG:NH1	2.25	0.51
2:C:32:SER:HA	2:C:222:ILE:HD13	1.92	0.51
2:C:454:ASN:OD1	2:C:455:VAL:N	2.43	0.51
2:D:284:ILE:HG23	2:D:436:THR:HB	1.90	0.51
2:D:375:ILE:HG22	2:D:377:ILE:HD12	1.90	0.51
1:A:363:ILE:HG22	1:A:367:ILE:CD1	2.39	0.51
2:B:87:ALA:C	2:B:89:SER:N	2.61	0.51
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.92	0.51
2:C:287:THR:HG23	2:C:414:ASN:ND2	2.24	0.51
2:C:444:GLU:HB2	2:C:449:MET:CE	2.41	0.51
2:D:208:ARG:HD2	2:D:234:GLU:OE2	2.11	0.51
2:F:25:ILE:HD12	2:F:58:GLN:HG2	1.92	0.51
1:A:211:LEU:CD1	1:A:212:GLU:H	2.24	0.51
2:B:161:ARG:HB2	2:B:196:VAL:HG11	1.92	0.51
2:C:393:ARG:NH2	2:C:429:HIS:HB2	2.24	0.51
2:D:37:PRO:HD2	2:D:203:ASN:ND2	2.25	0.51
2:D:363:ILE:HG22	2:D:367:ILE:HD13	1.92	0.51
2:D:414:ASN:HD22	2:D:426:THR:HG22	1.75	0.51
2:E:72:VAL:HG21	2:E:134:ILE:HD13	1.92	0.51
2:E:451:ARG:NH1	2:E:472:ILE:HD13	2.25	0.51
1:A:213:GLY:O	1:A:214:GLU:HB2	2.11	0.51
2:B:222:ILE:HD12	2:B:222:ILE:N	2.25	0.51
2:B:311:ARG:HD2	2:B:371:LYS:CE	2.40	0.51
2:C:136:LYS:HG2	2:C:136:LYS:O	2.10	0.51
2:C:331:TRP:NE1	3:C:901:ATP:N7	2.58	0.51
2:C:434:THR:O	2:C:459:ARG:NH2	2.43	0.51
2:D:79:THR:CG2	2:D:82:ASP:OD2	2.59	0.51
2:D:88:ARG:HG2	2:D:88:ARG:NH1	2.23	0.51
2:E:38:ILE:HA	2:E:177:THR:HG23	1.92	0.51
2:F:171:LEU:CD1	2:F:178:THR:HG21	2.40	0.51
3:A:901:ATP:O3'	2:B:457:LYS:HB2	2.10	0.51
2:B:26:GLU:HB3	2:B:245:ASN:OD1	2.11	0.51
2:B:296:LEU:HD21	2:B:477:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:LYS:N	2:B:372:PRO:HD3	2.25	0.51
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.76	0.51
2:C:419:PHE:HD1	2:C:420:MET:HG3	1.75	0.51
2:D:31:ILE:CG2	2:D:231:MET:HB2	2.41	0.51
2:D:271:ASP:OD1	2:D:277:GLY:HA2	2.09	0.51
2:D:291:GLY:O	3:D:901:ATP:H4'	2.11	0.51
2:D:338:MET:HB3	2:D:344:LEU:CB	2.41	0.51
2:E:203:ASN:HB3	2:E:225:LEU:CD2	2.41	0.51
2:F:14:GLU:HG3	2:F:16:GLN:HG3	1.92	0.51
1:A:199:PHE:CZ	2:F:183:GLU:HB2	2.45	0.51
2:B:87:ALA:O	2:B:89:SER:N	2.44	0.51
2:B:148:THR:HA	2:B:151:PHE:HE1	1.76	0.51
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.92	0.51
2:D:237:PHE:HB3	2:D:246:ILE:HD13	1.92	0.51
2:D:451:ARG:HG2	2:D:451:ARG:HH11	1.75	0.51
2:E:147:VAL:O	2:E:150:VAL:HG12	2.11	0.51
1:A:53:THR:O	1:A:56:SER:N	2.43	0.51
1:A:140:ARG:HH11	1:A:140:ARG:CA	2.23	0.51
1:A:266:GLY:O	1:A:300:ARG:HG3	2.11	0.51
2:B:83:ILE:H	2:B:83:ILE:HD12	1.76	0.51
2:B:341:GLN:O	2:B:342:ASN:C	2.49	0.51
2:C:88:ARG:NE	2:D:15:HIS:HA	2.26	0.51
2:C:127:ILE:HD11	2:C:167:LEU:HD13	1.92	0.51
2:C:220:LEU:HD23	2:C:220:LEU:C	2.31	0.51
2:C:431:ALA:C	2:C:432:TPO:HG22	2.29	0.51
2:E:367:ILE:HD12	2:E:375:ILE:HD11	1.93	0.51
2:F:98:VAL:HG22	2:F:103:LEU:HG	1.92	0.51
2:F:335:PHE:HA	2:F:338:MET:HG2	1.93	0.51
1:A:299:SER:C	1:A:301:PHE:H	2.14	0.51
2:B:392:PHE:O	2:B:395:PHE:N	2.44	0.51
2:C:45:SER:CB	2:C:182:THR:HB	2.35	0.51
2:C:86:ASN:O	2:C:89:SER:N	2.43	0.51
2:C:300:ARG:CA	2:C:333:MET:HE1	2.41	0.51
2:C:370:PHE:O	2:C:371:LYS:C	2.49	0.51
2:C:396:VAL:HG11	2:C:430:ILE:HG23	1.92	0.51
2:C:453:ILE:HG21	2:C:479:ILE:HG13	1.93	0.51
2:D:52:LYS:N	3:D:903:ATP:O1B	2.43	0.51
2:D:144:ILE:HD12	2:D:144:ILE:N	2.26	0.51
2:D:420:MET:HA	5:D:540:HOH:O	2.10	0.51
2:E:355:GLY:O	2:E:358:ASP:HB2	2.11	0.51
1:A:360:LEU:O	1:A:364:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:234:GLU:C	2:C:235:TYR:CD1	2.85	0.51
2:D:325:LEU:CD2	2:D:335:PHE:HB2	2.41	0.51
2:D:443:VAL:CG1	2:D:445:ILE:HD11	2.41	0.51
2:E:237:PHE:C	2:E:237:PHE:CD1	2.84	0.51
2:E:292:THR:HB	2:E:440:LEU:HB3	1.93	0.51
2:F:252:MET:CE	2:F:401:GLY:HA3	2.40	0.51
2:B:94:LEU:O	2:B:98:VAL:HG23	2.10	0.50
2:B:170:ARG:O	2:B:173:GLN:HB2	2.12	0.50
2:B:406:GLU:O	2:B:407:GLU:HB2	2.11	0.50
2:B:430:ILE:O	2:B:434:THR:HG22	2.11	0.50
2:D:279:PHE:HE1	2:D:460:GLY:HA3	1.75	0.50
2:E:18:ILE:HD11	2:E:228:THR:N	2.27	0.50
2:F:479:ILE:N	2:F:479:ILE:HD12	2.27	0.50
1:A:164:LEU:O	1:A:168:VAL:HG23	2.11	0.50
1:A:487:GLU:HG3	1:A:497:ILE:HD11	1.94	0.50
2:B:50:THR:HB	2:B:207:LEU:HB3	1.93	0.50
2:B:140:ARG:HH11	2:B:140:ARG:CA	2.24	0.50
2:B:443:VAL:HG12	2:B:445:ILE:HD11	1.92	0.50
2:C:359:HIS:O	2:C:363:ILE:HG13	2.10	0.50
2:D:315:PHE:HB3	2:D:317:TYR:HE1	1.77	0.50
2:D:354:ALA:HB3	2:D:359:HIS:CE1	2.46	0.50
2:D:446:ARG:HB3	2:E:484:ARG:HG2	1.93	0.50
2:E:392:PHE:HE2	2:E:430:ILE:CD1	2.15	0.50
2:B:232:LYS:N	2:B:232:LYS:HD2	2.27	0.50
2:C:437:ILE:HD12	2:C:457:LYS:HG2	1.93	0.50
2:E:203:ASN:HA	2:E:224:LYS:O	2.11	0.50
2:F:79:THR:HG23	2:F:82:ASP:H	1.77	0.50
1:A:161:ARG:HD2	1:A:196:VAL:HG11	1.94	0.50
1:A:162:ARG:HH11	1:A:162:ARG:HG3	1.76	0.50
1:A:211:LEU:CG	1:A:212:GLU:N	2.73	0.50
2:B:363:ILE:N	2:B:363:ILE:HD12	2.26	0.50
2:C:18:ILE:HD12	2:C:18:ILE:N	2.27	0.50
2:C:111:ASP:O	2:C:113:GLU:N	2.40	0.50
2:D:406:GLU:HB3	2:D:408:ILE:HG12	1.93	0.50
2:F:191:ILE:HB	2:F:198:GLU:OE2	2.12	0.50
2:F:487:GLU:HG3	2:F:497:ILE:HD12	1.93	0.50
1:A:182:THR:HG22	1:A:183:GLU:O	2.11	0.50
1:A:468:ARG:NH1	1:A:468:ARG:HG2	2.26	0.50
2:B:451:ARG:O	2:B:452:ALA:HB2	2.11	0.50
2:D:72:VAL:CG2	2:D:134:ILE:HD13	2.41	0.50
2:F:44:VAL:HG13	2:F:205:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:206:ILE:O	2:F:207:LEU:HD23	2.11	0.50
2:B:182:THR:HG21	2:B:192:ALA:HB1	1.93	0.50
2:B:470:PHE:HB3	2:B:479:ILE:HA	1.93	0.50
2:C:234:GLU:O	2:C:235:TYR:CD1	2.65	0.50
2:E:221:GLU:HB3	5:E:530:HOH:O	2.10	0.50
2:F:313:ILE:HD13	2:F:345:LYS:HB3	1.93	0.50
2:F:514:GLU:OE1	2:F:515:LYS:N	2.38	0.50
2:C:123:LEU:HA	2:C:127:ILE:HD11	1.93	0.50
2:C:219:THR:HB	2:C:234:GLU:HG2	1.93	0.50
2:C:321:ARG:HG2	2:C:348:CYS:SG	2.52	0.50
3:C:901:ATP:O2'	2:D:463:HIS:CD2	2.65	0.50
2:D:182:THR:HG21	2:D:192:ALA:CB	2.41	0.50
2:D:197:GLU:OE2	2:D:197:GLU:N	2.22	0.50
2:D:263:VAL:CG1	2:D:374:ARG:HH21	2.19	0.50
2:D:451:ARG:HD2	2:D:451:ARG:H	1.75	0.50
2:E:438:ILE:HG23	2:E:453:ILE:HD11	1.93	0.50
2:F:205:VAL:HG22	2:F:222:ILE:CD1	2.42	0.50
2:F:377:ILE:HD11	2:F:399:VAL:HG11	1.94	0.50
2:F:451:ARG:NH1	2:F:451:ARG:CG	2.75	0.50
1:A:31:ILE:HG22	1:A:231:MET:HB2	1.92	0.50
1:A:490:ILE:O	1:A:490:ILE:HG22	2.12	0.50
2:B:162:ARG:NH1	2:B:162:ARG:HB2	2.27	0.50
2:B:363:ILE:HD12	2:B:363:ILE:H	1.76	0.50
2:C:17:ALA:C	2:C:18:ILE:HD12	2.32	0.50
2:C:471:MET:HE1	2:C:478:ASP:CB	2.42	0.50
2:D:178:THR:CG2	2:D:179:VAL:N	2.74	0.50
2:D:289:ALA:O	2:D:292:THR:OG1	2.29	0.50
2:E:212:GLU:O	2:E:212:GLU:HG2	2.12	0.50
2:F:72:VAL:CG2	2:F:134:ILE:HD13	2.42	0.50
1:A:447:GLY:HA2	2:B:489:ILE:HD12	1.94	0.50
1:A:453:ILE:HD13	1:A:453:ILE:C	2.32	0.50
2:B:218:ARG:HB3	2:B:237:PHE:CZ	2.46	0.50
2:B:222:ILE:CG2	2:B:225:LEU:HG	2.41	0.50
2:C:146:SER:C	2:C:148:THR:H	2.14	0.50
2:D:65:ILE:HD12	2:D:65:ILE:N	2.27	0.50
2:F:115:GLN:CG	2:F:116:GLU:N	2.75	0.50
1:A:444:GLU:O	1:A:445:ILE:HD13	2.12	0.49
2:B:170:ARG:O	2:B:174:ILE:HG13	2.12	0.49
2:B:287:THR:HG21	2:B:425:ILE:O	2.12	0.49
2:C:20:LYS:HE2	2:C:228:THR:OG1	2.12	0.49
2:C:269:ARG:O	2:C:273:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:LEU:HD11	2:C:346:ILE:HD11	1.94	0.49
2:C:393:ARG:O	2:C:397:ILE:HG12	2.12	0.49
2:C:426:THR:HG22	2:C:428:SER:H	1.77	0.49
2:D:224:LYS:O	2:D:225:LEU:HD23	2.12	0.49
2:D:283:ILE:HG13	2:D:400:THR:HG23	1.94	0.49
2:E:314:LEU:HD12	2:E:376:ALA:O	2.12	0.49
2:E:359:HIS:O	2:E:363:ILE:CD1	2.56	0.49
2:F:127:ILE:CD1	2:F:167:LEU:HA	2.42	0.49
2:F:335:PHE:HD2	2:F:338:MET:HG3	1.77	0.49
1:A:21:MET:HE3	1:A:59:PHE:CZ	2.47	0.49
1:A:90:PHE:HB2	1:A:92:TRP:NE1	2.27	0.49
1:A:134:ILE:HD13	1:A:134:ILE:N	2.27	0.49
2:B:194:TYR:HB2	2:B:197:GLU:OE1	2.12	0.49
2:E:98:VAL:HA	2:E:103:LEU:O	2.13	0.49
2:F:269:ARG:HD2	2:F:272:GLU:OE2	2.11	0.49
2:F:316:ALA:O	2:F:348:CYS:HA	2.12	0.49
2:B:203:ASN:HB3	2:B:225:LEU:CD2	2.41	0.49
2:D:21:MET:HE3	2:D:59:PHE:CZ	2.48	0.49
2:D:27:GLY:O	2:D:31:ILE:HG13	2.13	0.49
2:D:167:LEU:O	2:D:168:VAL:C	2.50	0.49
2:D:179:VAL:O	2:D:179:VAL:HG12	2.12	0.49
2:D:313:ILE:HG13	2:D:372:PRO:HG3	1.94	0.49
2:E:430:ILE:O	2:E:430:ILE:HG22	2.11	0.49
3:E:903:ATP:O3'	2:F:224:LYS:HB2	2.12	0.49
2:F:115:GLN:HG3	2:F:116:GLU:N	2.27	0.49
1:A:230:HIS:HE1	1:A:232:LYS:HG3	1.78	0.49
2:B:134:ILE:HG21	2:B:174:ILE:HG21	1.94	0.49
2:C:182:THR:CG2	2:C:183:GLU:N	2.75	0.49
2:D:65:ILE:HD12	2:D:65:ILE:H	1.77	0.49
2:D:321:ARG:HG2	2:D:348:CYS:SG	2.53	0.49
2:D:375:ILE:HG12	2:D:408:ILE:HG21	1.93	0.49
2:D:380:LEU:HD11	2:D:412:PHE:HB3	1.94	0.49
2:E:52:LYS:HB3	2:E:181:THR:CG2	2.42	0.49
2:E:220:LEU:C	2:E:220:LEU:HD23	2.33	0.49
2:F:43:LEU:HD23	2:F:204:VAL:HG13	1.94	0.49
2:F:285:LEU:CB	2:F:437:ILE:HD12	2.36	0.49
1:A:82:ASP:O	1:A:85:LYS:N	2.45	0.49
2:C:357:GLU:HG3	2:C:358:ASP:N	2.28	0.49
2:C:467:ILE:N	2:C:467:ILE:HD12	2.28	0.49
2:E:82:ASP:O	2:E:85:LYS:HB3	2.13	0.49
2:F:454:ASN:HB2	2:F:467:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:O	1:A:70:PRO:O	2.31	0.49
1:A:111:ASP:C	1:A:113:GLU:H	2.15	0.49
1:A:144:ILE:HB	1:A:180:MET:HG2	1.94	0.49
2:B:52:LYS:H	2:B:207:LEU:CD1	2.26	0.49
2:B:54:LEU:HD23	2:B:239:ILE:HD12	1.95	0.49
2:B:423:HIS:O	2:B:424:SER:HB3	2.11	0.49
2:B:443:VAL:HG12	2:B:445:ILE:CD1	2.43	0.49
2:C:54:LEU:HD11	2:C:90:PHE:CE2	2.46	0.49
2:C:219:THR:CG2	2:C:234:GLU:HG2	2.43	0.49
2:C:371:LYS:O	2:C:371:LYS:CD	2.52	0.49
2:C:426:THR:HG22	2:C:427:ASP:N	2.28	0.49
2:D:155:ASP:OD1	2:D:159:VAL:HG11	2.13	0.49
2:D:334:ASP:OD1	2:D:336:GLU:N	2.46	0.49
2:E:342:ASN:O	2:E:343:LEU:HD23	2.12	0.49
2:F:75:THR:HG21	2:F:80:PRO:HG3	1.94	0.49
2:F:313:ILE:HG12	2:F:372:PRO:HG2	1.95	0.49
2:F:313:ILE:HG22	2:F:314:LEU:N	2.28	0.49
1:A:206:ILE:HD11	1:A:223:LEU:HD12	1.95	0.49
1:A:264:SER:HA	1:A:271:ASP:OD1	2.12	0.49
1:A:468:ARG:HG2	1:A:468:ARG:HH11	1.77	0.49
2:B:316:ALA:O	2:B:348:CYS:HA	2.12	0.49
2:C:283:ILE:HD11	2:C:404:LYS:CD	2.42	0.49
2:D:145:ASP:O	2:D:146:SER:HB2	2.12	0.49
2:D:490:ILE:C	2:D:492:GLY:N	2.66	0.49
2:E:124:SER:HA	2:E:127:ILE:CD1	2.42	0.49
2:E:451:ARG:HH11	2:E:451:ARG:CG	2.25	0.49
2:F:263:VAL:HG11	2:F:374:ARG:HH21	1.76	0.49
2:F:303:GLU:CD	2:F:333:MET:HB3	2.33	0.49
2:F:353:SER:O	2:F:354:ALA:CB	2.61	0.49
1:A:38:ILE:CG2	1:A:39:GLY:N	2.76	0.49
1:A:148:THR:OG1	1:A:182:THR:HG23	2.13	0.49
1:A:356:LEU:HD23	1:A:395:PHE:HB2	1.93	0.49
1:A:514:GLU:C	1:A:515:LYS:HD2	2.32	0.49
2:B:191:ILE:HG21	2:B:204:VAL:HG11	1.95	0.49
3:B:901:ATP:H3'	2:C:458:MET:O	2.13	0.49
2:C:38:ILE:HG22	2:C:39:GLY:H	1.76	0.49
2:C:206:ILE:HG21	2:C:208:ARG:NH1	2.27	0.49
2:C:296:LEU:CD2	2:C:472:ILE:HG12	2.42	0.49
2:D:372:PRO:HG2	2:D:375:ILE:HD11	1.95	0.49
2:E:145:ASP:O	2:E:146:SER:OG	2.28	0.49
2:E:419:PHE:HE2	2:F:425:ILE:HG13	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:505:LEU:O	2:E:505:LEU:HD12	2.13	0.49
2:D:340:ARG:C	2:D:342:ASN:H	2.16	0.49
2:E:499:VAL:O	2:E:499:VAL:HG12	2.13	0.49
2:F:336:GLU:O	2:F:340:ARG:HG3	2.13	0.49
1:A:145:ASP:HA	1:A:181:THR:HB	1.95	0.49
2:C:121:PHE:O	2:C:125:ALA:HB3	2.13	0.49
2:C:146:SER:HA	2:C:181:THR:O	2.12	0.49
2:C:239:ILE:N	5:C:528:HOH:O	2.43	0.49
2:C:440:LEU:N	2:C:440:LEU:HD23	2.27	0.49
3:E:903:ATP:O3'	2:F:224:LYS:HA	2.13	0.49
2:F:325:LEU:HD23	2:F:335:PHE:HB2	1.95	0.49
2:F:425:ILE:HG21	2:F:439:LEU:HD13	1.95	0.49
1:A:334:ASP:HA	5:A:527:HOH:O	2.12	0.48
2:B:451:ARG:HB3	2:B:470:PHE:CE2	2.47	0.48
2:C:483:PHE:H	2:C:483:PHE:HD1	1.59	0.48
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.41	0.48
2:D:468:ARG:NH1	2:D:468:ARG:HG2	2.28	0.48
2:E:298:VAL:HG13	2:E:376:ALA:HB1	1.95	0.48
2:E:319:GLU:HB2	2:E:324:LEU:HG	1.94	0.48
2:E:352:GLU:OE2	2:E:385:ARG:HD2	2.13	0.48
2:F:82:ASP:HA	2:F:85:LYS:HB3	1.95	0.48
1:A:183:GLU:HB3	2:B:199:PHE:CE1	2.48	0.48
2:B:470:PHE:CB	2:B:479:ILE:HA	2.43	0.48
2:D:41:SER:OG	2:D:168:VAL:HG13	2.13	0.48
2:D:296:LEU:HD13	2:D:331:TRP:CD2	2.47	0.48
2:D:430:ILE:O	2:D:433:ILE:HB	2.13	0.48
2:D:444:GLU:HA	2:D:448:GLU:O	2.13	0.48
2:D:484:ARG:HB3	2:D:484:ARG:HH11	1.77	0.48
2:E:79:THR:HG23	2:E:82:ASP:H	1.78	0.48
2:E:301:PHE:HZ	2:E:409:THR:HG22	1.77	0.48
2:E:320:SER:HA	2:F:254:LEU:HG	1.95	0.48
2:E:371:LYS:O	2:E:372:PRO:O	2.30	0.48
2:E:418:GLN:CB	2:F:423:HIS:O	2.52	0.48
2:F:97:LEU:C	2:F:99:ASP:N	2.67	0.48
2:F:313:ILE:HG12	2:F:372:PRO:HG3	1.95	0.48
1:A:64:ILE:CG2	1:A:102:LYS:HB3	2.44	0.48
1:A:445:ILE:O	1:A:448:GLU:N	2.46	0.48
2:B:194:TYR:O	2:B:196:VAL:HG23	2.13	0.48
2:B:287:THR:OG1	2:B:425:ILE:HG22	2.13	0.48
2:C:406:GLU:O	2:C:408:ILE:HG13	2.13	0.48
2:D:220:LEU:HD13	2:D:246:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:ALA:C	2:D:317:TYR:HD1	2.16	0.48
2:D:354:ALA:HB3	2:D:359:HIS:NE2	2.27	0.48
2:E:221:GLU:CG	2:E:222:ILE:H	2.26	0.48
2:F:486:PHE:HD2	2:F:494:PRO:HB2	1.77	0.48
1:A:390:ASN:OD1	2:F:386:GLY:HA2	2.14	0.48
2:B:148:THR:C	2:B:150:VAL:N	2.66	0.48
2:B:150:VAL:CG1	2:B:151:PHE:N	2.76	0.48
2:B:419:PHE:CD2	2:C:425:ILE:HD12	2.49	0.48
2:C:308:ASN:O	2:C:309:LYS:C	2.51	0.48
2:D:472:ILE:N	2:D:472:ILE:HD12	2.28	0.48
1:A:118:VAL:HG23	1:A:118:VAL:O	2.14	0.48
1:A:218:ARG:O	1:A:236:PRO:HA	2.14	0.48
1:A:264:SER:CB	1:A:304:ASN:HD21	2.27	0.48
2:B:218:ARG:O	2:B:236:PRO:HA	2.14	0.48
2:B:283:ILE:HG12	2:B:400:THR:HG23	1.96	0.48
2:B:336:GLU:O	2:B:340:ARG:HG3	2.13	0.48
2:C:469:GLU:HB3	2:C:483:PHE:CE1	2.48	0.48
2:D:184:ARG:NH1	2:D:187:GLU:O	2.47	0.48
2:F:25:ILE:HD11	2:F:58:GLN:HG2	1.96	0.48
2:F:489:ILE:HA	2:F:494:PRO:HG3	1.95	0.48
1:A:31:ILE:HA	1:A:231:MET:SD	2.54	0.48
1:A:351:PRO:CG	1:A:382:ALA:O	2.61	0.48
1:A:429:HIS:HB3	5:F:524:HOH:O	2.13	0.48
2:B:88:ARG:HH12	2:B:93:ASP:HA	1.78	0.48
2:B:460:GLY:O	2:B:461:SER:O	2.31	0.48
2:C:43:LEU:HD12	2:C:180:MET:O	2.13	0.48
2:C:85:LYS:HZ2	2:D:14:GLU:HB3	1.78	0.48
2:C:145:ASP:HA	2:C:181:THR:HB	1.95	0.48
2:C:223:LEU:HD13	2:C:223:LEU:C	2.33	0.48
2:C:418:GLN:HB2	2:D:423:HIS:O	2.14	0.48
2:D:203:ASN:HB3	2:D:225:LEU:HD22	1.95	0.48
2:D:289:ALA:O	2:D:294:LYS:NZ	2.44	0.48
2:E:451:ARG:NH1	2:E:472:ILE:CD1	2.77	0.48
1:A:270:LEU:O	1:A:273:MET:HB2	2.14	0.48
2:B:167:LEU:O	2:B:168:VAL:C	2.52	0.48
2:C:49:GLY:O	2:C:218:ARG:NH2	2.40	0.48
2:C:140:ARG:HH11	2:C:140:ARG:CB	2.26	0.48
2:C:263:VAL:HG12	2:C:374:ARG:NH2	2.28	0.48
2:C:285:LEU:HD23	2:C:434:THR:HG21	1.96	0.48
2:D:123:LEU:CD1	2:D:127:ILE:HD11	2.40	0.48
2:E:221:GLU:CB	5:E:530:HOH:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ILE:HD11	2:F:167:LEU:HA	1.95	0.48
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.14	0.48
1:A:425:ILE:HG21	1:A:439:LEU:HD22	1.96	0.48
2:B:193:ARG:HH11	2:B:193:ARG:CG	2.20	0.48
2:C:223:LEU:HD13	2:C:224:LYS:CB	2.39	0.48
2:C:300:ARG:HA	2:C:333:MET:HE3	1.96	0.48
2:D:194:TYR:O	2:D:195:GLY:C	2.50	0.48
2:D:306:CYS:SG	2:D:343:LEU:HB3	2.53	0.48
2:E:332:GLY:C	2:E:333:MET:HG2	2.33	0.48
2:F:147:VAL:CG2	2:F:148:THR:N	2.77	0.48
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.14	0.48
1:A:430:ILE:H	1:A:430:ILE:HD12	1.78	0.48
2:B:454:ASN:CB	2:B:467:ILE:HD13	2.41	0.48
2:C:75:THR:HG23	2:C:75:THR:O	2.14	0.48
2:C:294:LYS:CG	2:C:413:THR:HG23	2.38	0.48
2:D:18:ILE:HD13	2:D:228:THR:HG22	1.96	0.48
2:D:75:THR:OG1	2:D:78:GLU:O	2.29	0.48
2:E:291:GLY:CA	2:E:442:TYR:OH	2.61	0.48
2:F:24:MET:HE2	2:F:66:GLU:OE2	2.14	0.48
2:F:294:LYS:HB2	3:F:901:ATP:O1B	2.14	0.48
2:F:347:VAL:O	2:F:348:CYS:CB	2.62	0.48
2:F:455:VAL:O	2:F:463:HIS:CE1	2.67	0.48
1:A:52:LYS:CD	1:A:182:THR:O	2.62	0.48
1:A:130:ILE:O	1:A:134:ILE:CD1	2.60	0.48
1:A:289:ALA:HB2	1:A:419:PHE:HA	1.96	0.48
1:A:488:ARG:NE	2:F:488:ARG:NH1	2.58	0.48
1:A:504:GLU:C	1:A:506:SER:H	2.16	0.48
2:B:119:GLY:O	2:B:121:PHE:N	2.47	0.48
2:B:285:LEU:HD23	2:B:437:ILE:HD12	1.95	0.48
2:C:340:ARG:O	2:C:342:ASN:N	2.47	0.48
2:C:356:LEU:O	2:C:357:GLU:C	2.52	0.48
2:D:24:MET:CE	2:D:66:GLU:HG3	2.44	0.48
2:D:47:THR:O	2:D:50:THR:CG2	2.53	0.48
2:E:56:SER:HB2	2:E:143:SER:HB3	1.95	0.48
2:F:187:GLU:OE2	2:F:208:ARG:HA	2.13	0.48
1:A:183:GLU:HB2	2:B:199:PHE:CZ	2.49	0.47
2:B:18:ILE:HB	2:B:228:THR:HG21	1.94	0.47
2:B:31:ILE:CG2	2:B:222:ILE:HD13	2.44	0.47
2:B:207:LEU:CD2	2:B:220:LEU:HD12	2.44	0.47
2:C:106:LEU:CD2	2:C:130:ILE:HG12	2.44	0.47
2:C:156:ALA:O	2:C:160:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:211:LEU:HD12	2:C:215:ARG:O	2.13	0.47
2:E:46:GLY:HA2	2:E:184:ARG:HD3	1.96	0.47
2:E:294:LYS:H	2:E:294:LYS:HD3	1.79	0.47
2:E:504:GLU:CG	2:E:505:LEU:H	2.21	0.47
2:F:185:ILE:HD13	2:F:185:ILE:N	2.29	0.47
2:B:79:THR:OG1	2:B:81:GLN:HG2	2.14	0.47
2:B:90:PHE:HA	2:B:241:ASP:O	2.15	0.47
2:B:193:ARG:NH2	2:C:195:GLY:O	2.47	0.47
2:C:117:VAL:O	2:C:117:VAL:HG12	2.14	0.47
2:C:312:ALA:N	2:C:343:LEU:O	2.44	0.47
2:D:43:LEU:CD2	2:D:197:GLU:HB3	2.44	0.47
2:D:235:TYR:CD2	2:D:248:PRO:HA	2.49	0.47
2:D:273:MET:O	2:D:463:HIS:HA	2.14	0.47
2:D:313:ILE:HG12	2:D:345:LYS:HB3	1.96	0.47
2:E:41:SER:HA	2:E:178:THR:O	2.14	0.47
2:E:470:PHE:HE1	2:E:472:ILE:CD1	2.26	0.47
2:F:332:GLY:O	2:F:333:MET:O	2.31	0.47
2:F:367:ILE:O	2:F:367:ILE:HG22	2.14	0.47
2:F:486:PHE:HE2	2:F:496:ARG:NH1	2.03	0.47
1:A:52:LYS:HE3	3:A:903:ATP:O1B	2.14	0.47
1:A:309:LYS:HA	1:A:343:LEU:HD13	1.96	0.47
1:A:344:LEU:HD11	1:A:346:ILE:HD11	1.96	0.47
2:B:150:VAL:O	2:B:153:GLN:HG3	2.14	0.47
2:D:316:ALA:C	2:D:317:TYR:CD1	2.88	0.47
2:E:88:ARG:CG	2:E:88:ARG:HH11	2.27	0.47
2:F:382:ALA:O	2:F:385:ARG:HG3	2.15	0.47
1:A:150:VAL:HG13	1:A:151:PHE:CD2	2.49	0.47
1:A:254:LEU:HD13	2:F:350:TYR:CZ	2.50	0.47
1:A:319:GLU:OE1	1:A:327:ASN:ND2	2.47	0.47
2:C:245:ASN:C	2:C:245:ASN:HD22	2.17	0.47
2:D:82:ASP:O	2:D:83:ILE:C	2.52	0.47
2:D:287:THR:HG22	2:D:288:GLY:N	2.30	0.47
2:E:383:LEU:HD12	2:E:395:PHE:CE2	2.49	0.47
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.14	0.47
2:B:461:SER:OG	2:B:462:TRP:N	2.47	0.47
2:C:191:ILE:HD12	2:C:191:ILE:N	2.24	0.47
2:C:314:LEU:HB3	2:C:346:ILE:HD13	1.96	0.47
2:D:123:LEU:HG	2:D:163:GLU:OE2	2.14	0.47
2:D:237:PHE:CB	2:D:246:ILE:HD13	2.43	0.47
2:F:275:GLY:HA3	2:F:461:SER:OG	2.14	0.47
1:A:428:SER:OG	1:A:430:ILE:HD11	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ASN:HD22	1:A:498:THR:HG22	1.80	0.47
2:B:204:VAL:HG12	2:B:206:ILE:HD11	1.96	0.47
2:D:31:ILE:HG23	2:D:231:MET:HB2	1.95	0.47
2:D:240:THR:O	2:D:243:GLY:N	2.44	0.47
2:D:313:ILE:CD1	2:D:372:PRO:HG3	2.44	0.47
2:D:388:SER:OG	2:D:391:ALA:HB2	2.14	0.47
2:D:445:ILE:HD11	2:D:483:PHE:HE2	1.79	0.47
2:E:356:LEU:CD1	2:E:356:LEU:H	2.27	0.47
2:F:378:ASP:O	2:F:379:SER:CB	2.63	0.47
2:F:514:GLU:O	2:F:515:LYS:HB2	2.14	0.47
1:A:98:VAL:CG2	1:A:105:ILE:HD13	2.44	0.47
1:A:162:ARG:HG3	1:A:162:ARG:NH1	2.28	0.47
1:A:192:ALA:O	1:A:193:ARG:C	2.52	0.47
1:A:193:ARG:HH21	2:B:199:PHE:HE2	1.62	0.47
1:A:354:ALA:HB1	1:A:358:ASP:HB2	1.97	0.47
2:B:286:ALA:HA	2:B:438:ILE:O	2.15	0.47
2:B:357:GLU:CG	2:B:358:ASP:H	2.28	0.47
2:C:20:LYS:C	2:C:38:ILE:HD11	2.35	0.47
2:C:311:ARG:HB3	2:C:370:PHE:CE2	2.50	0.47
2:D:43:LEU:HD21	2:D:197:GLU:HB2	1.96	0.47
2:D:82:ASP:O	2:D:85:LYS:N	2.48	0.47
2:D:121:PHE:N	2:D:121:PHE:CD1	2.82	0.47
2:D:126:LEU:O	2:D:126:LEU:HG	2.14	0.47
2:D:219:THR:HA	2:D:235:TYR:O	2.15	0.47
2:D:315:PHE:HD2	2:D:347:VAL:HG21	1.75	0.47
2:D:399:VAL:O	2:D:400:THR:C	2.52	0.47
2:E:334:ASP:OD1	2:E:336:GLU:HB2	2.15	0.47
2:E:335:PHE:HA	2:E:338:MET:HG3	1.96	0.47
2:E:417:ASP:OD1	2:F:429:HIS:ND1	2.48	0.47
2:F:237:PHE:HE1	2:F:239:ILE:HG13	1.80	0.47
2:F:315:PHE:CD2	2:F:363:ILE:HG13	2.50	0.47
2:F:332:GLY:C	2:F:333:MET:HG2	2.35	0.47
2:F:487:GLU:O	2:F:489:ILE:N	2.48	0.47
1:A:458:MET:HB2	1:A:463:HIS:CD2	2.44	0.47
2:D:43:LEU:HD21	2:D:197:GLU:HB3	1.95	0.47
2:D:211:LEU:O	2:D:215:ARG:O	2.33	0.47
2:E:194:TYR:O	2:E:195:GLY:C	2.53	0.47
2:E:269:ARG:HH22	2:E:468:ARG:NH2	2.13	0.47
2:F:18:ILE:HG21	2:F:37:PRO:HB3	1.97	0.47
2:F:379:SER:O	2:F:382:ALA:HB3	2.15	0.47
2:F:387:VAL:HG13	2:F:388:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HD23	1:A:220:LEU:C	2.34	0.47
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.96	0.47
2:B:72:VAL:HG21	2:B:134:ILE:HD13	1.97	0.47
2:C:257:ARG:HB3	2:C:407:GLU:OE1	2.15	0.47
2:C:315:PHE:HA	2:C:347:VAL:HB	1.97	0.47
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.96	0.47
2:D:449:MET:HE3	2:E:490:ILE:HD11	1.96	0.47
2:E:202:ASP:HB2	2:E:203:ASN:ND2	2.29	0.47
2:E:268:VAL:HA	2:E:271:ASP:HB2	1.97	0.47
2:F:194:TYR:CD1	2:F:194:TYR:N	2.81	0.47
2:B:350:TYR:CZ	2:C:254:LEU:HD13	2.50	0.47
2:C:60:LEU:CD1	2:C:73:PHE:HB2	2.45	0.47
2:C:90:PHE:N	2:C:90:PHE:CD1	2.83	0.47
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.45	0.47
2:C:483:PHE:N	2:C:483:PHE:CD1	2.83	0.47
2:D:98:VAL:HA	2:D:103:LEU:O	2.14	0.47
2:D:182:THR:CG2	2:D:183:GLU:N	2.76	0.47
2:E:427:ASP:O	2:E:428:SER:HB3	2.15	0.47
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.97	0.46
1:A:347:VAL:HG21	1:A:366:GLU:HG2	1.97	0.46
2:C:363:ILE:O	2:C:364:LYS:C	2.54	0.46
2:C:411:LEU:HD12	2:C:412:PHE:H	1.80	0.46
2:C:426:THR:HG22	2:C:427:ASP:H	1.79	0.46
2:D:99:ASP:C	2:D:101:GLY:H	2.18	0.46
2:D:319:GLU:HG2	2:E:459:ARG:NH1	2.30	0.46
2:E:294:LYS:N	3:E:901:ATP:O1B	2.48	0.46
2:E:304:ASN:HB3	2:E:374:ARG:HH12	1.79	0.46
2:E:315:PHE:CE2	2:E:363:ILE:HG13	2.50	0.46
2:F:268:VAL:O	2:F:271:ASP:HB2	2.15	0.46
2:F:387:VAL:CG1	2:F:388:SER:N	2.78	0.46
2:F:472:ILE:HD12	3:F:901:ATP:C1'	2.45	0.46
1:A:214:GLU:HB3	2:B:234:GLU:HB2	1.97	0.46
2:B:64:ILE:HD11	2:B:70:PRO:CA	2.44	0.46
2:D:18:ILE:HD13	2:D:228:THR:HG23	1.97	0.46
2:D:21:MET:HE3	2:D:59:PHE:HZ	1.79	0.46
2:D:154:TYR:O	2:D:154:TYR:CD1	2.68	0.46
2:E:118:VAL:HG12	2:E:122:ASP:OD2	2.15	0.46
2:E:386:GLY:O	2:E:387:VAL:C	2.54	0.46
2:F:31:ILE:O	2:F:230:HIS:HB2	2.16	0.46
2:F:118:VAL:O	2:F:118:VAL:HG13	2.15	0.46
2:F:209:ASN:HD21	2:F:216:ARG:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:218:ARG:HG3	2:F:237:PHE:O	2.14	0.46
2:F:344:LEU:CD1	2:F:346:ILE:HG13	2.44	0.46
2:F:516:GLY:N	2:F:517:PRO:CD	2.77	0.46
2:B:20:LYS:NZ	2:B:32:SER:O	2.43	0.46
2:B:52:LYS:HB2	3:B:903:ATP:O1B	2.14	0.46
2:C:51:GLY:O	2:C:54:LEU:HB3	2.16	0.46
2:C:68:ASP:OD1	2:C:68:ASP:O	2.33	0.46
2:D:90:PHE:CD1	2:D:90:PHE:N	2.82	0.46
2:D:293:GLY:HA2	3:D:901:ATP:O1A	2.15	0.46
2:D:393:ARG:NH2	5:D:537:HOH:O	2.47	0.46
2:D:437:ILE:HD12	2:D:457:LYS:HG2	1.97	0.46
2:E:211:LEU:HG	2:E:212:GLU:N	2.30	0.46
2:E:430:ILE:O	2:E:431:ALA:C	2.53	0.46
2:E:441:GLN:HE22	2:E:490:ILE:HD13	1.80	0.46
1:A:154:TYR:O	1:A:154:TYR:HD1	1.98	0.46
1:A:451:ARG:NH2	3:A:901:ATP:O2'	2.48	0.46
1:A:488:ARG:CD	2:F:488:ARG:HH12	2.29	0.46
2:B:436:THR:HA	2:B:457:LYS:O	2.15	0.46
2:D:247:PHE:CD1	2:D:247:PHE:N	2.83	0.46
2:D:412:PHE:N	2:D:412:PHE:CD1	2.83	0.46
2:F:21:MET:CE	2:F:177:THR:CB	2.93	0.46
2:F:344:LEU:HD11	2:F:346:ILE:CG1	2.46	0.46
2:F:426:THR:HB	2:F:429:HIS:H	1.80	0.46
1:A:200:VAL:O	1:A:200:VAL:HG12	2.15	0.46
1:A:383:LEU:C	1:A:385:ARG:H	2.19	0.46
2:B:151:PHE:C	2:B:153:GLN:H	2.19	0.46
2:B:245:ASN:ND2	2:B:247:PHE:CZ	2.84	0.46
2:B:280:LYS:O	2:B:409:THR:OG1	2.25	0.46
2:B:469:GLU:HG2	2:B:481:ASP:O	2.16	0.46
2:C:260:ASN:O	2:C:261:VAL:O	2.33	0.46
2:C:313:ILE:HD11	2:C:370:PHE:CB	2.43	0.46
2:C:396:VAL:HG21	2:C:430:ILE:HD12	1.96	0.46
2:C:438:ILE:HD12	2:C:438:ILE:H	1.80	0.46
2:D:134:ILE:HD11	2:D:142:VAL:CG2	2.46	0.46
2:E:160:VAL:HG11	2:E:194:TYR:CD1	2.49	0.46
2:E:186:GLU:OE2	2:E:187:GLU:N	2.48	0.46
2:E:311:ARG:HD3	2:E:370:PHE:CE1	2.50	0.46
2:E:358:ASP:O	2:E:362:ILE:HG12	2.15	0.46
2:F:76:PHE:O	2:F:109:SER:HA	2.16	0.46
2:F:94:LEU:O	2:F:95:ALA:C	2.53	0.46
2:F:453:ILE:HG12	2:F:454:ASN:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLY:O	2:F:89:SER:CB	2.59	0.46
1:A:395:PHE:CE2	1:A:399:VAL:HG21	2.51	0.46
2:B:160:VAL:HG21	2:B:194:TYR:CE1	2.50	0.46
2:C:28:PHE:CA	2:C:246:ILE:HD12	2.46	0.46
2:C:183:GLU:HB2	2:D:199:PHE:CZ	2.50	0.46
2:D:81:GLN:CD	2:D:81:GLN:N	2.64	0.46
2:D:454:ASN:HB2	2:D:467:ILE:HA	1.97	0.46
2:E:164:LEU:HD11	2:E:197:GLU:CG	2.23	0.46
2:E:221:GLU:O	2:E:222:ILE:HD13	2.15	0.46
2:E:468:ARG:HG2	2:E:468:ARG:HH11	1.79	0.46
2:F:163:GLU:HA	2:F:163:GLU:OE2	2.16	0.46
2:F:418:GLN:HG3	2:F:418:GLN:O	2.16	0.46
2:F:426:THR:HB	2:F:429:HIS:HA	1.97	0.46
2:F:431:ALA:HA	2:F:434:THR:CG2	2.46	0.46
2:F:515:LYS:C	2:F:517:PRO:HD2	2.36	0.46
2:B:37:PRO:HD2	2:B:203:ASN:ND2	2.31	0.46
2:B:287:THR:HB	2:B:425:ILE:CG2	2.46	0.46
2:C:52:LYS:N	3:C:903:ATP:O1B	2.48	0.46
2:C:295:THR:HG22	2:C:331:TRP:CZ3	2.51	0.46
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.56	0.46
2:C:311:ARG:HD2	2:C:371:LYS:HE3	1.98	0.46
1:A:61:TYR:C	1:A:63:GLY:N	2.69	0.46
1:A:298:VAL:O	1:A:301:PHE:HB3	2.16	0.46
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.46	0.46
2:B:326:ARG:HD3	2:C:259:SER:O	2.16	0.46
2:C:193:ARG:HH21	2:D:199:PHE:HE2	1.62	0.46
2:D:363:ILE:O	2:D:367:ILE:HD13	2.16	0.46
2:E:265:SER:CB	2:E:278:PHE:CZ	2.99	0.46
2:E:419:PHE:O	2:E:420:MET:O	2.33	0.46
2:F:396:VAL:HG11	2:F:430:ILE:CG2	2.45	0.46
2:F:471:MET:CE	2:F:473:SER:HB3	2.46	0.46
1:A:211:LEU:HD12	1:A:212:GLU:H	1.81	0.46
1:A:489:ILE:O	1:A:491:SER:N	2.48	0.46
2:B:52:LYS:HE3	3:B:903:ATP:PB	2.56	0.46
2:B:245:ASN:ND2	2:B:247:PHE:CE1	2.84	0.46
2:C:21:MET:HE3	2:C:141:ARG:NE	2.30	0.46
2:C:80:PRO:O	2:C:84:ILE:HG12	2.16	0.46
2:C:326:ARG:O	2:C:329:TYR:N	2.49	0.46
2:D:484:ARG:CB	2:D:484:ARG:NH1	2.79	0.46
3:D:901:ATP:O2'	2:E:463:HIS:NE2	2.44	0.46
2:E:31:ILE:HA	2:E:231:MET:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:LYS:HZ3	2:E:366:GLU:HG3	1.78	0.46
2:E:418:GLN:HG3	2:E:418:GLN:O	2.15	0.46
2:E:420:MET:CE	2:F:490:ILE:HG13	2.45	0.46
2:F:79:THR:O	2:F:79:THR:CG2	2.64	0.46
2:F:273:MET:O	2:F:463:HIS:HB2	2.16	0.46
2:F:445:ILE:HG12	2:F:483:PHE:HE2	1.81	0.46
2:F:484:ARG:NH1	2:F:484:ARG:CB	2.78	0.46
1:A:375:ILE:HB	1:A:408:ILE:HG21	1.98	0.46
1:A:379:SER:O	1:A:382:ALA:HB3	2.15	0.46
1:A:441:GLN:HE22	1:A:490:ILE:CD1	2.26	0.46
1:A:457:LYS:HB3	2:F:291:GLY:HA3	1.97	0.46
2:B:279:PHE:O	2:B:280:LYS:C	2.54	0.46
2:C:163:GLU:OE2	2:C:163:GLU:HA	2.16	0.46
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.81	0.46
2:C:300:ARG:HA	2:C:333:MET:HE1	1.98	0.46
2:D:151:PHE:C	2:D:153:GLN:N	2.67	0.46
2:D:462:TRP:CE3	2:D:463:HIS:N	2.84	0.46
2:D:470:PHE:CE1	2:D:472:ILE:HD11	2.51	0.46
2:E:203:ASN:HB3	2:E:225:LEU:HD22	1.98	0.46
2:E:262:ARG:HH12	2:E:461:SER:HB2	1.81	0.46
2:E:441:GLN:HG3	2:E:452:ALA:HB3	1.97	0.46
2:F:468:ARG:NH1	2:F:468:ARG:HG2	2.30	0.46
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.30	0.45
1:A:435:ASP:OD1	2:F:323:GLN:NE2	2.46	0.45
2:B:479:ILE:HD12	2:B:479:ILE:N	2.31	0.45
2:B:486:PHE:CE2	2:B:496:ARG:HB2	2.51	0.45
2:C:110:PRO:HB2	2:D:165:PHE:HE2	1.81	0.45
2:C:451:ARG:NH1	2:C:472:ILE:HD12	2.31	0.45
2:D:88:ARG:NE	2:E:15:HIS:HA	2.31	0.45
2:D:291:GLY:N	3:D:901:ATP:O1G	2.49	0.45
2:D:384:ALA:HB2	2:D:392:PHE:CE2	2.51	0.45
2:E:22:ARG:HE	2:E:22:ARG:HB3	1.29	0.45
2:E:74:VAL:HG12	2:E:76:PHE:CE1	2.51	0.45
2:E:145:ASP:C	2:E:146:SER:OG	2.54	0.45
2:E:313:ILE:CD1	2:E:372:PRO:HG2	2.46	0.45
2:F:504:GLU:HA	2:F:507:ARG:HE	1.81	0.45
2:C:197:GLU:OE2	2:C:197:GLU:N	2.29	0.45
2:C:312:ALA:O	2:C:344:LEU:HA	2.16	0.45
2:D:284:ILE:HD12	2:D:410:GLY:O	2.16	0.45
2:E:386:GLY:O	2:E:387:VAL:O	2.33	0.45
2:F:462:TRP:O	2:F:463:HIS:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:HB3	1:A:140:ARG:HB2	1.99	0.45
1:A:89:SER:CB	2:B:227:GLY:O	2.64	0.45
2:B:54:LEU:CD2	2:B:244:ILE:HG13	2.47	0.45
2:B:294:LYS:CB	2:B:413:THR:HG23	2.44	0.45
2:C:63:GLY:CA	2:C:141:ARG:NH1	2.80	0.45
2:C:88:ARG:HG2	2:C:88:ARG:HH11	1.81	0.45
2:C:326:ARG:O	2:C:328:ALA:N	2.49	0.45
2:D:38:ILE:HA	2:D:177:THR:HG21	1.98	0.45
2:E:240:THR:C	2:E:242:HIS:H	2.20	0.45
2:E:483:PHE:O	2:E:485:ASN:N	2.49	0.45
2:F:193:ARG:C	2:F:195:GLY:H	2.19	0.45
1:A:153:GLN:O	1:A:154:TYR:HB3	2.17	0.45
1:A:215:ARG:NH2	2:B:234:GLU:O	2.50	0.45
2:B:88:ARG:HG2	2:B:88:ARG:NH1	2.32	0.45
2:B:88:ARG:HH12	2:B:93:ASP:CB	2.29	0.45
2:B:334:ASP:OD1	2:B:336:GLU:HB2	2.17	0.45
2:C:44:VAL:O	2:C:44:VAL:HG12	2.15	0.45
2:C:303:GLU:OE1	2:C:304:ASN:N	2.49	0.45
2:C:317:TYR:CE1	2:C:377:ILE:HG23	2.51	0.45
2:C:335:PHE:HA	2:C:338:MET:CG	2.47	0.45
2:D:57:ILE:HG12	2:D:73:PHE:CE1	2.52	0.45
2:E:350:TYR:CE1	2:F:254:LEU:HD13	2.51	0.45
2:F:280:LYS:HZ3	2:F:407:GLU:HB3	1.79	0.45
1:A:230:HIS:CE1	1:A:232:LYS:HG3	2.52	0.45
1:A:254:LEU:HG	2:F:320:SER:HA	1.99	0.45
2:B:214:GLU:OE1	2:C:217:ARG:NH1	2.49	0.45
2:B:227:GLY:O	2:B:228:THR:HG23	2.16	0.45
2:B:285:LEU:HD12	2:B:412:PHE:O	2.17	0.45
5:B:539:HOH:O	2:C:460:GLY:C	2.55	0.45
2:C:87:ALA:C	2:C:89:SER:N	2.70	0.45
2:C:123:LEU:HD11	2:C:163:GLU:HA	1.97	0.45
2:D:497:ILE:HG13	2:D:497:ILE:O	2.17	0.45
2:E:36:LEU:HD23	2:E:36:LEU:HA	1.71	0.45
2:E:280:LYS:HE2	2:E:407:GLU:HB3	1.97	0.45
2:E:287:THR:CG2	2:E:288:GLY:N	2.79	0.45
2:E:313:ILE:CG1	2:E:372:PRO:CG	2.87	0.45
2:F:418:GLN:HE21	2:F:421:GLY:C	2.20	0.45
2:B:25:ILE:HG23	2:B:58:GLN:HE22	1.81	0.45
2:B:273:MET:O	2:B:464:ASP:N	2.48	0.45
2:C:191:ILE:H	2:C:191:ILE:CD1	2.25	0.45
2:C:287:THR:CG2	2:C:414:ASN:HB3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:LEU:HD11	2:D:197:GLU:HG3	1.97	0.45
2:D:286:ALA:O	2:D:294:LYS:CG	2.63	0.45
2:D:306:CYS:SG	2:D:343:LEU:CB	3.05	0.45
2:F:21:MET:CE	2:F:177:THR:CG2	2.93	0.45
2:F:84:ILE:HD11	2:F:98:VAL:HG21	1.98	0.45
2:F:273:MET:SD	2:F:468:ARG:HD2	2.55	0.45
2:F:509:VAL:HG12	2:F:510:ARG:N	2.26	0.45
2:F:515:LYS:CB	2:F:517:PRO:HD2	2.47	0.45
1:A:123:LEU:O	1:A:123:LEU:HD13	2.16	0.45
1:A:487:GLU:CD	1:A:497:ILE:HD13	2.37	0.45
2:B:166:ARG:O	2:B:170:ARG:HG2	2.16	0.45
2:B:296:LEU:HD21	2:B:477:PRO:CD	2.45	0.45
2:B:356:LEU:CD2	2:B:392:PHE:HA	2.46	0.45
2:C:103:LEU:HD12	2:C:104:PHE:N	2.30	0.45
2:C:150:VAL:CG1	2:C:151:PHE:N	2.79	0.45
2:D:488:ARG:HB3	2:D:491:SER:HB3	1.97	0.45
2:F:23:THR:OG1	2:F:29:ASP:OD1	2.32	0.45
2:F:508:ILE:O	2:F:508:ILE:HG22	2.17	0.45
1:A:61:TYR:C	1:A:63:GLY:H	2.19	0.45
1:A:299:SER:C	1:A:301:PHE:N	2.71	0.45
2:B:45:SER:OG	2:B:184:ARG:HD2	2.17	0.45
2:B:244:ILE:HG22	2:B:245:ASN:N	2.32	0.45
2:B:437:ILE:O	2:B:437:ILE:HG22	2.17	0.45
2:C:164:LEU:HB3	2:C:200:VAL:HG11	1.98	0.45
2:C:471:MET:H	2:C:471:MET:HG3	1.56	0.45
2:D:316:ALA:HB3	2:D:348:CYS:SG	2.57	0.45
2:D:473:SER:O	2:D:476:GLY:N	2.50	0.45
2:E:197:GLU:O	2:E:199:PHE:N	2.49	0.45
2:E:451:ARG:NH1	2:E:451:ARG:CG	2.79	0.45
2:F:36:LEU:HA	2:F:37:PRO:HD3	1.81	0.45
2:F:312:ALA:HA	2:F:374:ARG:O	2.16	0.45
2:F:451:ARG:HD2	2:F:451:ARG:N	2.32	0.45
1:A:471:MET:HG2	1:A:478:ASP:HB3	1.95	0.45
2:B:200:VAL:O	2:B:200:VAL:HG12	2.17	0.45
2:B:319:GLU:HG3	5:B:521:HOH:O	2.17	0.45
2:C:144:ILE:HG22	2:C:147:VAL:HG12	1.98	0.45
2:C:281:ASP:O	2:C:282:SER:HB3	2.15	0.45
2:C:296:LEU:O	2:C:299:SER:HB2	2.17	0.45
2:D:72:VAL:HB	2:D:142:VAL:HG22	1.98	0.45
2:D:433:ILE:HD12	2:D:433:ILE:N	2.32	0.45
2:E:171:LEU:O	2:E:174:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:264:SER:O	2:E:374:ARG:NH2	2.50	0.45
2:E:318:GLU:OE2	2:E:379:SER:CB	2.61	0.45
2:F:64:ILE:HD12	2:F:102:LYS:HB3	1.99	0.45
2:F:504:GLU:HA	2:F:507:ARG:HG3	1.99	0.45
2:F:504:GLU:HB2	2:F:505:LEU:H	1.46	0.45
1:A:23:THR:O	1:A:25:ILE:HD12	2.17	0.45
1:A:86:ASN:O	1:A:87:ALA:C	2.56	0.45
1:A:211:LEU:HD21	2:B:188:TYR:HE2	1.81	0.45
2:B:147:VAL:CG2	2:B:148:THR:N	2.80	0.45
2:B:216:ARG:CG	2:C:233:GLY:HA2	2.41	0.45
2:C:54:LEU:CD1	2:C:90:PHE:CZ	2.98	0.45
2:C:435:ASP:HA	2:C:459:ARG:HD2	1.99	0.45
2:D:284:ILE:HA	2:D:436:THR:O	2.17	0.45
2:F:53:THR:OG1	2:F:145:ASP:OD2	2.35	0.45
2:F:283:ILE:HG13	2:F:400:THR:HG23	1.99	0.45
2:F:344:LEU:C	2:F:344:LEU:HD13	2.38	0.45
2:F:380:LEU:O	2:F:383:LEU:N	2.46	0.45
1:A:251:ALA:O	1:A:252:MET:C	2.56	0.44
1:A:265:SER:O	1:A:300:ARG:O	2.35	0.44
1:A:509:VAL:O	1:A:511:GLY:N	2.50	0.44
2:B:90:PHE:HB2	2:B:92:TRP:CE2	2.52	0.44
2:B:334:ASP:O	2:B:338:MET:HG2	2.17	0.44
2:C:90:PHE:HB2	2:C:92:TRP:CE2	2.51	0.44
2:C:123:LEU:HA	2:C:127:ILE:CD1	2.47	0.44
2:C:134:ILE:CG2	2:C:139:ALA:HB3	2.30	0.44
2:C:174:ILE:HG22	2:C:174:ILE:O	2.17	0.44
2:C:482:SER:C	2:C:484:ARG:H	2.20	0.44
2:D:430:ILE:CA	2:D:433:ILE:HD13	2.45	0.44
2:E:338:MET:HB3	2:E:344:LEU:HB2	1.99	0.44
2:F:142:VAL:HB	2:F:178:THR:HG22	1.94	0.44
2:F:371:LYS:HD2	2:F:371:LYS:C	2.37	0.44
1:A:451:ARG:NH1	1:A:472:ILE:CD1	2.78	0.44
2:B:324:LEU:HD23	2:B:324:LEU:HA	1.81	0.44
2:C:64:ILE:CG2	2:C:102:LYS:HB3	2.47	0.44
2:C:217:ARG:O	2:C:217:ARG:CG	2.65	0.44
2:C:389:ASN:O	2:C:392:PHE:N	2.50	0.44
2:E:96:LYS:O	2:E:99:ASP:N	2.50	0.44
2:E:323:GLN:HG2	2:E:327:ASN:ND2	2.32	0.44
1:A:219:THR:HA	1:A:235:TYR:O	2.17	0.44
1:A:332:GLY:O	1:A:333:MET:C	2.56	0.44
2:B:64:ILE:HG22	2:B:65:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:SER:O	2:C:128:GLU:HG2	2.17	0.44
2:D:164:LEU:HB3	2:D:200:VAL:HG11	1.99	0.44
2:E:61:TYR:O	2:E:62:ASN:C	2.56	0.44
2:E:264:SER:CB	2:E:304:ASN:HD21	2.30	0.44
2:F:286:ALA:HA	2:F:438:ILE:O	2.18	0.44
2:F:298:VAL:HA	2:F:411:LEU:CD2	2.47	0.44
2:F:321:ARG:HG2	2:F:348:CYS:HB3	1.99	0.44
1:A:31:ILE:CG2	1:A:231:MET:HB2	2.47	0.44
2:B:240:THR:HG21	2:B:361:GLN:HE22	1.82	0.44
2:B:296:LEU:O	2:B:299:SER:N	2.50	0.44
2:C:463:HIS:ND1	2:C:463:HIS:C	2.69	0.44
2:D:222:ILE:O	2:D:222:ILE:HG22	2.17	0.44
2:E:356:LEU:HD21	2:E:392:PHE:HA	1.98	0.44
2:E:397:ILE:O	2:E:398:GLY:C	2.55	0.44
2:E:451:ARG:HG2	2:E:451:ARG:NH1	2.30	0.44
2:F:203:ASN:CB	2:F:225:LEU:HD23	2.47	0.44
2:F:517:PRO:HG2	2:F:518:GLU:H	1.82	0.44
1:A:222:ILE:O	1:A:222:ILE:HG22	2.18	0.44
2:B:21:MET:CG	2:B:141:ARG:HH21	2.31	0.44
2:B:161:ARG:NH2	2:B:199:PHE:HB2	2.32	0.44
2:C:50:THR:HG21	2:C:207:LEU:O	2.16	0.44
2:D:288:GLY:O	2:D:415:THR:HA	2.17	0.44
2:D:390:ASN:O	2:D:391:ALA:C	2.55	0.44
2:D:446:ARG:H	2:D:496:ARG:NH1	2.06	0.44
3:D:903:ATP:O3'	2:E:224:LYS:HB2	2.17	0.44
2:E:118:VAL:HG12	2:E:118:VAL:O	2.18	0.44
2:E:451:ARG:HD3	2:E:472:ILE:CD1	2.48	0.44
3:E:903:ATP:O2'	2:F:230:HIS:NE2	2.48	0.44
2:F:31:ILE:HG23	2:F:231:MET:HB2	1.99	0.44
2:F:170:ARG:HB3	2:F:170:ARG:CZ	2.47	0.44
1:A:104:PHE:CD2	1:A:133:ALA:HB1	2.53	0.44
1:A:134:ILE:HG23	1:A:139:ALA:HB3	1.98	0.44
1:A:351:PRO:C	1:A:353:SER:H	2.21	0.44
1:A:414:ASN:HD21	1:A:426:TPO:HA	1.79	0.44
1:A:425:ILE:O	1:A:426:TPO:HG22	2.18	0.44
2:B:396:VAL:HG21	2:B:430:ILE:HD12	2.00	0.44
2:C:295:THR:HG22	2:C:296:LEU:N	2.32	0.44
2:D:388:SER:OG	2:D:391:ALA:CB	2.66	0.44
2:E:85:LYS:O	2:E:88:ARG:N	2.48	0.44
2:E:356:LEU:HD12	2:E:356:LEU:N	2.32	0.44
2:E:436:THR:CG2	2:E:458:MET:HE2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:ILE:HG23	2:F:58:GLN:NE2	2.32	0.44
2:F:218:ARG:HE	2:F:218:ARG:HB3	1.55	0.44
1:A:51:GLY:HA3	1:A:207:LEU:CD1	2.42	0.44
1:A:284:ILE:HB	1:A:411:LEU:HD12	2.00	0.44
2:B:323:GLN:HA	2:C:258:SER:OG	2.18	0.44
2:D:89:SER:CB	2:E:227:GLY:O	2.65	0.44
2:F:73:PHE:HE2	2:F:83:ILE:HG12	1.83	0.44
2:F:299:SER:O	2:F:333:MET:HE3	2.18	0.44
2:F:344:LEU:HD22	2:F:345:LYS:H	1.81	0.44
2:F:379:SER:HA	2:F:413:THR:O	2.18	0.44
2:F:501:GLU:HG3	2:F:502:LYS:N	2.32	0.44
1:A:136:LYS:HD3	1:A:137:TYR:CE1	2.53	0.44
2:B:53:THR:O	2:B:57:ILE:HG12	2.17	0.44
2:B:313:ILE:HG22	2:B:314:LEU:N	2.33	0.44
2:B:326:ARG:C	2:B:328:ALA:N	2.71	0.44
2:B:428:SER:O	2:B:429:HIS:HB2	2.17	0.44
2:B:451:ARG:HH11	2:B:451:ARG:CG	2.25	0.44
2:C:340:ARG:C	2:C:342:ASN:N	2.71	0.44
2:D:235:TYR:HD2	2:D:248:PRO:HA	1.83	0.44
2:E:47:THR:HG23	5:E:525:HOH:O	2.18	0.44
2:E:94:LEU:HB3	2:E:103:LEU:HD21	1.99	0.44
2:F:256:GLN:H	2:F:256:GLN:HG2	1.50	0.44
2:F:296:LEU:O	2:F:297:LEU:C	2.55	0.44
1:A:65:ILE:O	1:A:65:ILE:CG2	2.60	0.44
1:A:191:ILE:HB	1:A:198:GLU:CG	2.48	0.44
1:A:463:HIS:CE1	1:A:465:LYS:NZ	2.86	0.44
2:C:48:SER:O	2:D:223:LEU:HD21	2.18	0.44
2:C:425:ILE:HD12	2:C:425:ILE:H	1.83	0.44
2:D:222:ILE:CG2	2:D:230:HIS:CD2	3.00	0.44
2:E:24:MET:HB2	2:E:62:ASN:HB3	2.00	0.44
2:E:60:LEU:HD12	2:E:73:PHE:HD1	1.82	0.44
2:E:125:ALA:O	2:E:129:ARG:HG3	2.18	0.44
2:E:335:PHE:O	2:E:338:MET:N	2.51	0.44
2:E:357:GLU:HG3	2:E:358:ASP:N	2.33	0.44
2:F:264:SER:OG	2:F:265:SER:N	2.51	0.44
2:F:293:GLY:O	2:F:294:LYS:C	2.55	0.44
2:F:445:ILE:O	2:F:446:ARG:HB2	2.17	0.44
2:F:472:ILE:HD12	3:F:901:ATP:O4'	2.18	0.44
1:A:64:ILE:HD12	1:A:102:LYS:O	2.17	0.43
1:A:157:SER:OG	1:A:158:SER:N	2.51	0.43
1:A:439:LEU:HD12	1:A:440:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ASP:O	2:B:146:SER:OG	2.31	0.43
2:B:326:ARG:C	2:B:328:ALA:H	2.21	0.43
2:C:116:GLU:O	2:C:117:VAL:HB	2.17	0.43
2:C:386:GLY:HA2	2:D:390:ASN:OD1	2.18	0.43
2:C:435:ASP:O	2:C:457:LYS:HE3	2.17	0.43
2:D:323:GLN:HE21	2:D:327:ASN:HD21	1.64	0.43
2:E:378:ASP:O	2:E:379:SER:CB	2.66	0.43
2:F:25:ILE:O	2:F:27:GLY:N	2.51	0.43
1:A:335:PHE:O	1:A:338:MET:N	2.51	0.43
1:A:357:GLU:HG3	1:A:358:ASP:N	2.33	0.43
1:A:437:ILE:HB	1:A:456:PHE:HB3	1.99	0.43
1:A:518:GLU:HB2	1:A:519:SER:H	1.48	0.43
2:B:157:SER:OG	2:B:158:SER:N	2.51	0.43
2:B:295:THR:HG21	2:B:319:GLU:OE2	2.18	0.43
2:B:304:ASN:HB3	2:B:374:ARG:NH1	2.32	0.43
2:C:45:SER:HA	2:C:182:THR:O	2.18	0.43
2:C:320:SER:HB3	2:D:256:GLN:HG2	2.01	0.43
2:C:387:VAL:HG12	2:C:391:ALA:HB3	1.99	0.43
2:D:200:VAL:O	2:D:200:VAL:HG12	2.18	0.43
2:D:408:ILE:HG22	2:D:409:THR:N	2.33	0.43
2:E:52:LYS:HB3	2:E:181:THR:HG23	1.99	0.43
2:E:443:VAL:HB	2:E:445:ILE:CD1	2.48	0.43
1:A:44:VAL:O	1:A:181:THR:HA	2.18	0.43
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.44	0.43
1:A:267:VAL:HG11	1:A:270:LEU:HB2	1.99	0.43
1:A:461:SER:OG	1:A:462:TRP:N	2.51	0.43
2:B:21:MET:HG2	2:B:141:ARG:HH21	1.82	0.43
2:B:451:ARG:HG2	2:B:451:ARG:NH1	2.27	0.43
2:B:492:GLY:C	2:B:494:PRO:HD3	2.38	0.43
2:C:182:THR:CG2	2:C:183:GLU:H	2.31	0.43
2:D:105:ILE:N	2:D:105:ILE:HD12	2.34	0.43
2:D:238:THR:HG23	2:D:358:ASP:OD1	2.17	0.43
2:E:313:ILE:HG22	2:E:314:LEU:N	2.32	0.43
2:E:363:ILE:N	2:E:363:ILE:HD12	2.33	0.43
1:A:370:PHE:C	1:A:372:PRO:HD3	2.38	0.43
1:A:419:PHE:O	1:A:420:MET:O	2.36	0.43
2:B:162:ARG:CB	2:B:162:ARG:HH11	2.32	0.43
2:B:218:ARG:HB3	2:B:237:PHE:CE2	2.53	0.43
2:B:471:MET:HB3	2:B:480:LYS:HZ1	1.83	0.43
2:C:219:THR:HA	2:C:235:TYR:O	2.18	0.43
2:C:356:LEU:CD1	2:C:356:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:430:ILE:O	2:D:433:ILE:HD13	2.17	0.43
2:E:160:VAL:HG21	2:E:194:TYR:CG	2.53	0.43
2:E:318:GLU:CD	2:E:379:SER:HB2	2.37	0.43
2:E:446:ARG:HE	2:E:496:ARG:NH2	2.16	0.43
2:F:435:ASP:OD1	2:F:459:ARG:NH1	2.51	0.43
2:B:453:ILE:HD13	2:B:453:ILE:C	2.39	0.43
2:C:127:ILE:CD1	2:C:167:LEU:HD13	2.48	0.43
2:C:219:THR:HG22	2:C:235:TYR:C	2.38	0.43
2:E:43:LEU:HD23	2:E:204:VAL:CG1	2.34	0.43
2:E:323:GLN:HE21	2:F:459:ARG:HD3	1.84	0.43
2:E:323:GLN:NE2	2:F:459:ARG:HD3	2.33	0.43
2:E:329:TYR:O	2:E:332:GLY:N	2.45	0.43
2:F:316:ALA:HB2	2:F:324:LEU:HD11	2.01	0.43
2:F:322:ALA:O	2:F:325:LEU:HB2	2.19	0.43
1:A:109:SER:HA	1:A:110:PRO:HD3	1.81	0.43
2:B:289:ALA:HB1	2:B:419:PHE:HB3	2.00	0.43
2:B:309:LYS:HA	2:B:343:LEU:HD13	2.01	0.43
2:C:225:LEU:HD23	2:C:225:LEU:HA	1.85	0.43
2:C:296:LEU:HA	2:C:331:TRP:CZ3	2.53	0.43
2:D:174:ILE:O	2:D:176:ALA:N	2.52	0.43
2:D:214:GLU:O	2:D:215:ARG:NE	2.49	0.43
2:E:264:SER:HB3	2:E:304:ASN:ND2	2.33	0.43
2:E:425:ILE:HD12	2:E:439:LEU:CD1	2.44	0.43
2:F:70:PRO:HA	2:F:102:LYS:O	2.18	0.43
1:A:82:ASP:O	1:A:84:ILE:N	2.52	0.43
1:A:496:ARG:HH11	2:B:497:ILE:HD13	1.83	0.43
2:B:50:THR:HB	2:B:207:LEU:HB2	1.99	0.43
2:B:385:ARG:NH1	2:C:397:ILE:HD11	2.34	0.43
2:C:129:ARG:O	2:C:132:TYR:HB3	2.18	0.43
2:C:303:GLU:OE1	2:C:303:GLU:C	2.57	0.43
2:D:367:ILE:HG22	2:D:368:ASN:N	2.33	0.43
2:F:47:THR:CG2	2:F:48:SER:N	2.81	0.43
2:F:182:THR:HG22	2:F:183:GLU:O	2.19	0.43
2:F:431:ALA:HA	2:F:434:THR:HG22	2.00	0.43
1:A:18:ILE:HG21	1:A:37:PRO:HB3	2.00	0.43
1:A:449:MET:HA	1:A:449:MET:CE	2.48	0.43
2:B:36:LEU:HD22	2:B:42:THR:OG1	2.18	0.43
2:B:206:ILE:HD12	2:B:206:ILE:N	2.34	0.43
2:B:267:VAL:HG23	2:B:300:ARG:HG2	2.00	0.43
2:B:436:THR:HG23	2:B:458:MET:HG2	2.00	0.43
2:B:439:LEU:HD12	2:B:440:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:ASN:O	2:C:87:ALA:C	2.56	0.43
2:C:149:SER:HB3	2:D:161:ARG:NH2	2.33	0.43
2:C:313:ILE:HG22	2:C:315:PHE:CE1	2.54	0.43
2:D:42:THR:N	2:D:178:THR:O	2.49	0.43
2:D:453:ILE:CG1	2:D:454:ASN:N	2.82	0.43
2:E:148:THR:HG23	2:E:193:ARG:HD2	1.99	0.43
2:E:380:LEU:HD21	2:E:412:PHE:HD2	1.84	0.43
2:E:469:GLU:HB3	2:E:483:PHE:CE1	2.54	0.43
2:F:115:GLN:OE1	2:F:116:GLU:O	2.37	0.43
2:F:211:LEU:O	2:F:212:GLU:CD	2.57	0.43
2:F:311:ARG:HG3	2:F:371:LYS:HZ1	1.83	0.43
2:F:328:ALA:O	2:F:332:GLY:O	2.37	0.43
2:F:387:VAL:HG11	2:F:392:PHE:HB2	2.00	0.43
1:A:125:ALA:O	1:A:129:ARG:HG3	2.18	0.43
1:A:420:MET:HG2	1:A:492:GLY:HA3	2.01	0.43
2:B:52:LYS:HE3	2:B:52:LYS:HB2	1.84	0.43
2:C:363:ILE:O	2:C:365:SER:N	2.52	0.43
2:D:45:SER:HB2	2:D:182:THR:HB	2.00	0.43
2:D:443:VAL:HG21	2:D:489:ILE:HG22	2.01	0.43
2:E:60:LEU:CD1	2:E:73:PHE:HD1	2.32	0.43
2:E:65:ILE:HD12	2:E:65:ILE:N	2.33	0.43
2:E:94:LEU:O	2:E:95:ALA:C	2.58	0.43
2:E:345:LYS:CE	2:E:366:GLU:HG3	2.49	0.43
2:E:433:ILE:HD12	2:E:433:ILE:N	2.33	0.43
2:F:20:LYS:HB3	2:F:35:GLY:O	2.19	0.43
1:A:27:GLY:O	1:A:31:ILE:HG13	2.19	0.43
1:A:106:LEU:C	1:A:106:LEU:HD12	2.39	0.43
1:A:334:ASP:OD1	1:A:337:GLU:N	2.45	0.43
1:A:344:LEU:HD11	1:A:346:ILE:CD1	2.49	0.43
2:B:153:GLN:O	2:B:154:TYR:HB3	2.18	0.43
2:B:301:PHE:O	2:B:374:ARG:NH1	2.49	0.43
2:C:52:LYS:HB2	2:C:52:LYS:HE3	1.80	0.43
2:C:326:ARG:C	2:C:328:ALA:N	2.70	0.43
2:C:381:SER:O	2:C:382:ALA:C	2.57	0.43
2:D:38:ILE:CG2	2:D:39:GLY:N	2.82	0.43
2:E:21:MET:SD	2:E:38:ILE:HD13	2.59	0.43
2:F:497:ILE:O	2:F:497:ILE:CG1	2.67	0.43
2:F:505:LEU:O	2:F:506:SER:HB3	2.18	0.43
1:A:234:GLU:O	1:A:235:TYR:CD1	2.72	0.42
2:C:83:ILE:O	2:C:83:ILE:HG22	2.17	0.42
2:C:292:THR:HB	2:C:440:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:348:CYS:O	2:C:349:ALA:HB2	2.19	0.42
2:D:164:LEU:CD1	2:D:197:GLU:HG3	2.49	0.42
2:D:170:ARG:HH12	2:D:174:ILE:HD11	1.84	0.42
2:D:420:MET:HB3	2:D:492:GLY:HA3	2.01	0.42
2:D:441:GLN:HB2	5:D:540:HOH:O	2.18	0.42
2:E:246:ILE:HG22	2:E:247:PHE:N	2.34	0.42
2:E:315:PHE:HB3	2:E:317:TYR:CE1	2.54	0.42
2:F:65:ILE:O	2:F:66:GLU:HG2	2.19	0.42
2:F:440:LEU:HD21	2:F:453:ILE:HD12	2.01	0.42
2:F:445:ILE:HD12	2:F:445:ILE:N	2.34	0.42
1:A:442:TYR:HE1	2:B:456:PHE:CZ	2.37	0.42
2:B:370:PHE:C	2:B:372:PRO:HD3	2.40	0.42
2:C:295:THR:HG22	2:C:331:TRP:CH2	2.53	0.42
2:D:21:MET:CE	2:D:177:THR:HB	2.49	0.42
2:D:271:ASP:O	2:D:276:GLY:N	2.52	0.42
2:D:462:TRP:CH2	2:D:464:ASP:HA	2.54	0.42
2:E:184:ARG:HD2	2:E:191:ILE:O	2.18	0.42
2:E:426:THR:HG21	2:E:431:ALA:H	1.83	0.42
2:E:486:PHE:HA	2:E:495:THR:O	2.19	0.42
2:F:18:ILE:HD12	2:F:40:ARG:HH12	1.83	0.42
2:F:37:PRO:O	2:F:40:ARG:HB2	2.19	0.42
2:F:285:LEU:CD2	2:F:437:ILE:HD12	2.44	0.42
2:F:471:MET:HE2	2:F:471:MET:O	2.19	0.42
2:F:503:SER:O	2:F:504:GLU:C	2.57	0.42
1:A:444:GLU:HB2	1:A:449:MET:HE1	2.01	0.42
2:B:216:ARG:NE	2:C:221:GLU:OE1	2.47	0.42
2:B:303:GLU:O	2:B:306:CYS:HB2	2.20	0.42
2:C:150:VAL:HG13	2:C:151:PHE:H	1.84	0.42
2:E:18:ILE:HD12	2:E:228:THR:HG23	2.01	0.42
2:F:247:PHE:HB3	2:F:249:LEU:CD2	2.49	0.42
2:F:331:TRP:HH2	3:F:901:ATP:O2A	2.02	0.42
2:F:357:GLU:HG3	2:F:358:ASP:H	1.84	0.42
2:F:505:LEU:O	2:F:506:SER:CB	2.67	0.42
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.44	0.42
1:A:203:ASN:HB3	1:A:225:LEU:HD23	2.01	0.42
1:A:220:LEU:HD13	1:A:246:ILE:CD1	2.49	0.42
1:A:299:SER:O	1:A:301:PHE:N	2.52	0.42
1:A:498:THR:O	1:A:499:VAL:C	2.56	0.42
2:B:51:GLY:O	2:B:54:LEU:N	2.52	0.42
2:B:255:THR:HG22	2:B:255:THR:O	2.19	0.42
2:C:20:LYS:HA	2:C:38:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:LYS:HB3	2:C:181:THR:HG23	2.00	0.42
2:C:187:GLU:O	2:C:208:ARG:HD3	2.19	0.42
2:D:299:SER:HB3	2:D:335:PHE:HZ	1.84	0.42
2:E:248:PRO:O	2:E:249:LEU:C	2.56	0.42
2:F:204:VAL:HG23	2:F:224:LYS:HG2	2.01	0.42
2:F:220:LEU:HD13	2:F:246:ILE:HD11	2.00	0.42
2:F:468:ARG:HG2	2:F:468:ARG:HH11	1.84	0.42
1:A:52:LYS:HB2	1:A:52:LYS:HE3	1.87	0.42
1:A:85:LYS:O	1:A:88:ARG:HB2	2.19	0.42
1:A:426:TPO:O	1:A:427:ASP:HB2	2.19	0.42
2:B:26:GLU:OE1	2:B:27:GLY:N	2.53	0.42
2:B:281:ASP:O	2:B:282:SER:HB3	2.20	0.42
2:B:356:LEU:H	2:B:356:LEU:HD12	1.77	0.42
2:C:24:MET:CE	2:C:66:GLU:HG3	2.50	0.42
2:C:64:ILE:H	2:C:64:ILE:HD12	1.84	0.42
2:C:248:PRO:C	2:C:250:GLY:N	2.71	0.42
2:C:380:LEU:HD23	2:C:380:LEU:HA	1.87	0.42
2:D:52:LYS:CE	5:D:547:HOH:O	2.67	0.42
2:D:74:VAL:HG13	2:D:106:LEU:HG	2.01	0.42
2:D:311:ARG:CD	2:D:371:LYS:HE3	2.10	0.42
2:E:80:PRO:HD2	2:E:81:GLN:NE2	2.34	0.42
2:E:451:ARG:HG2	2:E:472:ILE:HD11	2.01	0.42
2:F:79:THR:HG23	2:F:79:THR:O	2.19	0.42
2:F:150:VAL:CG1	2:F:151:PHE:N	2.83	0.42
2:F:269:ARG:NH2	2:F:468:ARG:NH2	2.68	0.42
2:F:278:PHE:CZ	2:F:438:ILE:HD11	2.55	0.42
1:A:267:VAL:HG12	1:A:270:LEU:HB2	1.98	0.42
1:A:501:GLU:C	1:A:503:SER:H	2.22	0.42
2:B:65:ILE:O	2:B:65:ILE:HG22	2.20	0.42
2:B:90:PHE:HB2	2:B:92:TRP:CZ2	2.55	0.42
2:B:215:ARG:NE	2:B:215:ARG:HA	2.34	0.42
2:B:294:LYS:N	3:B:901:ATP:O1B	2.52	0.42
2:B:296:LEU:HD22	2:B:472:ILE:HD12	2.01	0.42
2:C:21:MET:HB2	2:C:38:ILE:CG1	2.50	0.42
2:C:111:ASP:OD2	2:C:113:GLU:CG	2.68	0.42
2:D:41:SER:CB	2:D:178:THR:HB	2.49	0.42
2:D:353:SER:O	2:D:354:ALA:HB2	2.19	0.42
2:E:169:ALA:O	2:E:172:LYS:HB3	2.19	0.42
2:F:191:ILE:HG23	2:F:206:ILE:CD1	2.50	0.42
1:A:24:MET:HB2	1:A:62:ASN:HB3	2.00	0.42
1:A:123:LEU:HD13	1:A:123:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:LYS:O	2:B:371:LYS:HD3	2.20	0.42
2:B:502:LYS:HG3	2:B:504:GLU:O	2.20	0.42
2:C:24:MET:HE2	2:C:66:GLU:HG3	2.01	0.42
2:C:274:CYS:HB3	2:C:458:MET:SD	2.59	0.42
2:C:377:ILE:HD11	2:C:399:VAL:HG11	2.01	0.42
2:C:496:ARG:HG3	2:D:487:GLU:OE1	2.20	0.42
2:D:261:VAL:HG12	2:D:262:ARG:N	2.35	0.42
2:D:440:LEU:HD22	2:D:470:PHE:CE2	2.55	0.42
3:D:901:ATP:O2G	2:E:459:ARG:NH2	2.50	0.42
2:E:161:ARG:CA	2:E:196:VAL:HG11	2.49	0.42
2:E:451:ARG:N	2:E:451:ARG:HD2	2.34	0.42
1:A:25:ILE:O	1:A:25:ILE:HG22	2.19	0.42
1:A:248:PRO:O	1:A:250:GLY:N	2.53	0.42
2:B:221:GLU:HG2	2:B:222:ILE:N	2.34	0.42
2:B:296:LEU:CD2	2:B:477:PRO:HB3	2.49	0.42
2:B:340:ARG:C	2:B:342:ASN:H	2.23	0.42
2:B:356:LEU:H	2:B:356:LEU:HD13	1.84	0.42
2:C:52:LYS:H	2:C:52:LYS:HG3	1.60	0.42
2:C:218:ARG:HD2	5:C:528:HOH:O	2.19	0.42
2:C:431:ALA:HA	2:C:434:THR:HG22	2.01	0.42
2:D:65:ILE:O	2:D:65:ILE:HG22	2.19	0.42
2:E:195:GLY:HA2	2:E:198:GLU:OE1	2.20	0.42
2:F:289:ALA:HB2	2:F:419:PHE:HA	2.02	0.42
1:A:32:SER:OG	1:A:35:GLY:HA2	2.20	0.42
1:A:209:ASN:ND2	1:A:216:ARG:HB3	2.35	0.42
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.85	0.42
1:A:397:ILE:HD11	1:A:433:ILE:HD13	2.02	0.42
1:A:462:TRP:CE3	1:A:463:HIS:N	2.87	0.42
2:B:14:GLU:OE2	2:B:16:GLN:HB2	2.19	0.42
2:C:60:LEU:O	2:C:61:TYR:C	2.56	0.42
2:C:82:ASP:C	2:C:84:ILE:N	2.72	0.42
2:C:90:PHE:HA	2:C:241:ASP:O	2.20	0.42
2:C:111:ASP:C	2:C:113:GLU:H	2.23	0.42
2:C:306:CYS:CB	2:C:338:MET:SD	3.07	0.42
2:C:313:ILE:HD12	2:C:372:PRO:CG	2.50	0.42
2:D:18:ILE:H	2:D:18:ILE:CD1	2.28	0.42
2:D:263:VAL:CG2	2:D:280:LYS:HA	2.50	0.42
2:D:468:ARG:HG2	2:D:468:ARG:HH11	1.83	0.42
2:D:483:PHE:N	2:D:483:PHE:CD1	2.88	0.42
2:E:197:GLU:C	2:E:199:PHE:N	2.73	0.42
2:E:262:ARG:NH1	2:E:461:SER:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:318:GLU:CG	2:F:432:TPO:O3P	2.63	0.42
2:E:370:PHE:O	2:E:371:LYS:HG3	2.20	0.42
2:F:240:THR:C	2:F:242:HIS:H	2.23	0.42
2:F:466:ALA:C	2:F:467:ILE:HD13	2.41	0.42
2:F:509:VAL:CG1	2:F:510:ARG:H	2.21	0.42
1:A:21:MET:HE3	1:A:59:PHE:HZ	1.83	0.42
1:A:36:LEU:HD12	1:A:59:PHE:CZ	2.55	0.42
1:A:134:ILE:CD1	1:A:134:ILE:N	2.83	0.42
1:A:389:ASN:ND2	1:A:428:SER:HB2	2.35	0.42
1:A:392:PHE:O	1:A:393:ARG:C	2.58	0.42
1:A:448:GLU:HG2	2:B:466:ALA:HA	2.01	0.42
2:B:48:SER:OG	2:C:224:LYS:HD3	2.20	0.42
2:B:261:VAL:HG12	2:B:262:ARG:N	2.34	0.42
2:B:455:VAL:HG11	2:B:463:HIS:CB	2.48	0.42
2:C:60:LEU:O	2:C:64:ILE:HD13	2.19	0.42
2:C:300:ARG:NH2	2:C:477:PRO:HD2	2.35	0.42
2:D:291:GLY:O	2:D:293:GLY:N	2.52	0.42
2:E:132:TYR:C	2:E:132:TYR:CD2	2.93	0.42
2:E:245:ASN:ND2	2:E:247:PHE:CE2	2.88	0.42
2:E:306:CYS:HB2	2:E:338:MET:SD	2.59	0.42
2:E:313:ILE:CG1	2:E:372:PRO:HG3	2.37	0.42
2:F:116:GLU:O	2:F:117:VAL:CB	2.67	0.42
2:F:222:ILE:CG2	2:F:225:LEU:HG	2.50	0.42
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.70	0.41
1:A:183:GLU:H	1:A:183:GLU:HG2	1.62	0.41
1:A:234:GLU:C	1:A:235:TYR:CD1	2.93	0.41
1:A:480:LYS:HB3	1:A:481:ASP:H	1.64	0.41
2:B:72:VAL:HB	2:B:142:VAL:HG13	2.02	0.41
2:B:83:ILE:HD12	2:B:83:ILE:N	2.35	0.41
2:B:287:THR:CG2	2:B:288:GLY:N	2.81	0.41
2:B:383:LEU:C	2:B:385:ARG:H	2.22	0.41
2:B:383:LEU:HD13	2:B:395:PHE:CE2	2.55	0.41
2:B:418:GLN:O	2:B:422:ALA:HB2	2.19	0.41
2:C:305:ALA:HB2	2:C:374:ARG:HH11	1.85	0.41
2:C:312:ALA:O	2:C:344:LEU:CD2	2.68	0.41
2:D:299:SER:HB2	2:D:333:MET:HE1	2.02	0.41
2:E:18:ILE:HD12	2:E:228:THR:OG1	2.20	0.41
2:E:97:LEU:O	2:E:103:LEU:N	2.49	0.41
2:E:356:LEU:H	2:E:356:LEU:HD12	1.85	0.41
2:E:364:LYS:O	2:E:368:ASN:ND2	2.53	0.41
2:E:380:LEU:HD21	2:E:412:PHE:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:443:VAL:CG1	2:E:494:PRO:HG2	2.50	0.41
2:F:380:LEU:HD23	2:F:380:LEU:HA	1.83	0.41
1:A:84:ILE:HA	1:A:94:LEU:HD12	2.02	0.41
1:A:144:ILE:HG22	1:A:147:VAL:HG12	2.02	0.41
1:A:211:LEU:HD12	1:A:212:GLU:N	2.35	0.41
1:A:344:LEU:HD13	1:A:345:LYS:N	2.35	0.41
1:A:383:LEU:O	1:A:385:ARG:N	2.53	0.41
1:A:489:ILE:C	1:A:491:SER:H	2.23	0.41
2:B:31:ILE:HG21	2:B:222:ILE:HD13	2.02	0.41
2:C:64:ILE:HD11	2:C:71:GLY:HA3	2.01	0.41
2:C:79:THR:OG1	2:C:81:GLN:HG2	2.20	0.41
2:C:106:LEU:HD23	2:C:130:ILE:HG12	2.02	0.41
2:C:370:PHE:O	2:C:370:PHE:CD2	2.73	0.41
2:D:38:ILE:CA	2:D:177:THR:HG23	2.44	0.41
2:D:47:THR:HG22	2:D:184:ARG:HB2	2.02	0.41
2:D:291:GLY:C	2:D:293:GLY:N	2.73	0.41
2:E:285:LEU:HG	2:E:286:ALA:N	2.35	0.41
2:E:435:ASP:O	2:E:459:ARG:HG3	2.20	0.41
2:F:97:LEU:C	2:F:99:ASP:H	2.23	0.41
2:F:486:PHE:CE2	2:F:496:ARG:CD	3.02	0.41
1:A:19:ALA:O	1:A:38:ILE:HG13	2.21	0.41
1:A:158:SER:O	1:A:159:VAL:C	2.59	0.41
1:A:405:GLN:HG3	1:A:406:GLU:N	2.34	0.41
1:A:436:THR:HA	1:A:457:LYS:O	2.20	0.41
2:B:32:SER:OG	2:B:35:GLY:N	2.54	0.41
2:B:140:ARG:HB3	2:B:140:ARG:CZ	2.48	0.41
2:B:211:LEU:HD12	2:B:211:LEU:HA	1.89	0.41
2:B:247:PHE:HD2	2:B:364:LYS:NZ	2.17	0.41
2:B:371:LYS:O	2:B:371:LYS:CD	2.69	0.41
2:B:419:PHE:HD2	2:C:425:ILE:HD12	1.85	0.41
2:C:44:VAL:HG22	2:C:205:VAL:HB	2.03	0.41
2:C:142:VAL:O	2:C:178:THR:HA	2.21	0.41
2:C:439:LEU:C	2:C:440:LEU:HD23	2.41	0.41
2:D:58:GLN:OE1	2:D:243:GLY:HA3	2.21	0.41
2:E:80:PRO:HB2	2:E:81:GLN:NE2	2.35	0.41
2:E:94:LEU:HB3	2:E:103:LEU:HD23	2.01	0.41
1:A:209:ASN:HD21	1:A:216:ARG:HB3	1.85	0.41
1:A:266:GLY:C	1:A:300:ARG:HG3	2.41	0.41
1:A:502:LYS:HG3	1:A:502:LYS:O	2.21	0.41
2:B:263:VAL:HG12	2:B:374:ARG:NH2	2.35	0.41
2:C:146:SER:C	2:C:148:THR:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:122:ASP:HB3	2:D:123:LEU:H	1.49	0.41
2:D:144:ILE:HG22	2:D:147:VAL:HG12	2.02	0.41
2:D:211:LEU:O	2:D:212:GLU:CG	2.59	0.41
2:D:355:GLY:O	2:D:358:ASP:HB2	2.20	0.41
3:D:903:ATP:O1G	2:E:224:LYS:NZ	2.54	0.41
2:E:54:LEU:HD23	2:E:239:ILE:HG12	2.02	0.41
2:E:145:ASP:C	2:E:146:SER:HG	2.20	0.41
2:E:313:ILE:CG1	2:E:372:PRO:HG2	2.49	0.41
2:E:481:ASP:O	2:E:482:SER:O	2.38	0.41
2:F:49:GLY:HA2	3:F:903:ATP:O2B	2.21	0.41
2:F:116:GLU:O	2:F:117:VAL:HB	2.19	0.41
2:F:329:TYR:O	2:F:332:GLY:N	2.43	0.41
2:F:360:LEU:O	2:F:360:LEU:HD22	2.21	0.41
2:F:418:GLN:O	2:F:422:ALA:HB2	2.20	0.41
2:F:489:ILE:O	2:F:491:SER:N	2.54	0.41
1:A:196:VAL:O	1:A:198:GLU:N	2.53	0.41
1:A:383:LEU:C	1:A:385:ARG:N	2.74	0.41
1:A:439:LEU:O	1:A:453:ILE:HA	2.19	0.41
2:B:75:THR:O	2:B:108:ALA:HB3	2.20	0.41
2:B:496:ARG:CG	2:B:498:THR:HG23	2.43	0.41
2:C:28:PHE:CE1	2:C:55:PHE:HZ	2.39	0.41
2:C:54:LEU:HD12	2:C:54:LEU:HA	1.83	0.41
2:C:126:LEU:O	2:C:129:ARG:N	2.53	0.41
2:C:278:PHE:N	2:C:278:PHE:CD2	2.87	0.41
2:C:338:MET:HB3	2:C:344:LEU:HB3	2.03	0.41
2:C:444:GLU:OE2	2:D:489:ILE:HG12	2.20	0.41
2:D:191:ILE:HB	2:D:198:GLU:CD	2.40	0.41
2:E:85:LYS:HE3	2:F:18:ILE:HD13	2.02	0.41
2:E:199:PHE:C	2:E:201:SER:H	2.22	0.41
2:E:375:ILE:HD13	2:E:375:ILE:HA	1.85	0.41
2:E:392:PHE:CE2	2:E:430:ILE:CD1	2.95	0.41
2:E:470:PHE:CD1	2:E:470:PHE:C	2.94	0.41
2:F:111:ASP:HA	2:F:112:PRO:HD3	1.83	0.41
2:F:165:PHE:O	2:F:166:ARG:C	2.57	0.41
2:F:187:GLU:HG3	2:F:208:ARG:HB3	2.02	0.41
2:F:294:LYS:HZ2	2:F:415:THR:HG23	1.84	0.41
2:F:325:LEU:CD2	2:F:335:PHE:HB2	2.50	0.41
1:A:84:ILE:HG23	1:A:94:LEU:HB2	2.01	0.41
1:A:189:GLY:O	1:A:190:PRO:C	2.59	0.41
1:A:347:VAL:CG2	1:A:366:GLU:HG2	2.50	0.41
1:A:458:MET:SD	1:A:461:SER:HB3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:HD13	2:B:90:PHE:CE1	2.55	0.41
2:B:196:VAL:C	2:B:198:GLU:N	2.72	0.41
2:B:385:ARG:NH2	2:C:432:TPO:O2P	2.53	0.41
2:C:192:ALA:HB3	2:C:197:GLU:HB2	2.01	0.41
2:D:484:ARG:HB3	2:D:484:ARG:NH1	2.35	0.41
2:F:144:ILE:CG2	2:F:147:VAL:HG12	2.50	0.41
2:F:225:LEU:HD23	2:F:225:LEU:HA	1.83	0.41
2:F:245:ASN:HB3	2:F:361:GLN:HE22	1.85	0.41
2:F:246:ILE:CG2	2:F:247:PHE:N	2.84	0.41
2:F:443:VAL:HB	2:F:445:ILE:CD1	2.50	0.41
2:F:500:ASP:O	2:F:501:GLU:CB	2.56	0.41
1:A:69:GLU:O	1:A:70:PRO:C	2.59	0.41
1:A:90:PHE:CD1	1:A:90:PHE:N	2.89	0.41
1:A:170:ARG:O	1:A:174:ILE:HG12	2.20	0.41
1:A:191:ILE:HD12	1:A:206:ILE:HD11	2.02	0.41
1:A:262:ARG:HA	1:A:278:PHE:O	2.20	0.41
1:A:266:GLY:O	1:A:300:ARG:CG	2.68	0.41
2:B:144:ILE:CG2	2:B:147:VAL:HG12	2.51	0.41
2:B:356:LEU:HD11	2:B:387:VAL:HG21	2.03	0.41
2:B:455:VAL:CG1	2:B:463:HIS:HB2	2.51	0.41
2:B:484:ARG:HB2	5:B:528:HOH:O	2.19	0.41
2:C:32:SER:HB3	2:C:222:ILE:HD11	2.02	0.41
2:C:43:LEU:N	2:C:203:ASN:O	2.47	0.41
2:C:311:ARG:NE	2:C:371:LYS:HE3	2.35	0.41
2:C:317:TYR:HE1	2:C:377:ILE:HG23	1.85	0.41
2:C:438:ILE:CG2	2:C:453:ILE:HD11	2.51	0.41
2:D:181:THR:CG2	5:D:547:HOH:O	2.68	0.41
2:D:288:GLY:HA2	2:D:440:LEU:O	2.20	0.41
2:D:294:LYS:HB2	2:D:294:LYS:HE2	1.85	0.41
2:D:299:SER:HB3	2:D:335:PHE:CZ	2.55	0.41
2:E:87:ALA:O	2:E:89:SER:N	2.53	0.41
2:E:197:GLU:C	2:E:199:PHE:H	2.24	0.41
2:E:205:VAL:HG13	2:E:222:ILE:HD13	2.01	0.41
2:E:352:GLU:OE1	2:F:397:ILE:HD13	2.21	0.41
2:E:360:LEU:HD13	2:E:360:LEU:C	2.40	0.41
2:F:431:ALA:C	2:F:434:THR:HG22	2.41	0.41
1:A:35:GLY:O	1:A:36:LEU:C	2.59	0.41
1:A:37:PRO:HG2	1:A:203:ASN:ND2	2.35	0.41
1:A:182:THR:CG2	1:A:183:GLU:N	2.84	0.41
2:B:116:GLU:HG2	2:B:117:VAL:N	2.29	0.41
2:B:497:ILE:C	2:B:499:VAL:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:PHE:N	2:C:246:ILE:HD12	2.36	0.41
2:C:70:PRO:HD2	2:C:140:ARG:HG2	2.03	0.41
2:C:123:LEU:HD11	2:C:163:GLU:CA	2.51	0.41
2:C:298:VAL:O	2:C:301:PHE:HB3	2.21	0.41
2:C:318:GLU:OE2	2:D:432:TPO:HB	2.21	0.41
2:C:480:LYS:HB2	2:C:480:LYS:HE3	1.69	0.41
2:E:14:GLU:HG3	2:E:16:GLN:N	2.29	0.41
2:E:237:PHE:HB2	2:E:245:ASN:O	2.21	0.41
2:E:497:ILE:O	2:E:498:THR:OG1	2.24	0.41
2:F:324:LEU:HD23	2:F:324:LEU:HA	1.93	0.41
2:F:490:ILE:C	2:F:492:GLY:N	2.74	0.41
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.56	0.41
1:A:79:THR:O	1:A:82:ASP:HB2	2.21	0.41
1:A:210:VAL:CG1	1:A:211:LEU:O	2.67	0.41
1:A:348:CYS:O	1:A:349:ALA:HB2	2.21	0.41
2:B:24:MET:O	2:B:62:ASN:ND2	2.54	0.41
2:B:273:MET:CE	2:B:468:ARG:HD2	2.51	0.41
2:B:379:SER:HA	2:B:413:THR:O	2.21	0.41
2:B:380:LEU:HB3	2:B:392:PHE:HZ	1.86	0.41
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.46	0.41
2:C:487:GLU:N	2:C:497:ILE:HD11	2.36	0.41
2:D:43:LEU:HD11	2:D:182:THR:OG1	2.21	0.41
2:D:150:VAL:CG1	2:D:151:PHE:H	2.34	0.41
2:D:270:LEU:HD21	2:D:438:ILE:HD12	2.02	0.41
2:D:397:ILE:HG13	2:D:397:ILE:H	1.66	0.41
2:E:161:ARG:HB2	2:E:196:VAL:HG11	2.02	0.41
2:E:291:GLY:C	2:E:442:TYR:OH	2.60	0.41
2:E:445:ILE:HG22	2:E:445:ILE:O	2.19	0.41
2:E:489:ILE:HD13	2:E:489:ILE:HA	1.89	0.41
2:F:240:THR:C	2:F:242:HIS:N	2.72	0.41
2:F:272:GLU:O	2:F:274:CYS:N	2.54	0.41
2:F:426:THR:O	2:F:428:SER:N	2.49	0.41
2:F:453:ILE:CG1	2:F:454:ASN:N	2.83	0.41
2:F:471:MET:HE1	2:F:473:SER:HB3	2.03	0.41
1:A:298:VAL:HG12	1:A:299:SER:N	2.36	0.41
1:A:379:SER:HA	1:A:413:THR:O	2.20	0.41
2:B:61:TYR:O	2:B:64:ILE:N	2.53	0.41
2:B:64:ILE:O	2:B:66:GLU:N	2.51	0.41
2:B:472:ILE:HD13	2:B:477:PRO:HA	2.03	0.41
2:B:497:ILE:O	2:B:498:THR:C	2.60	0.41
2:C:221:GLU:CD	2:C:233:GLY:O	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:THR:HG21	2:C:430:ILE:CG1	2.46	0.41
2:D:223:LEU:O	2:D:223:LEU:HD23	2.21	0.41
3:D:901:ATP:O3'	2:E:457:LYS:HB2	2.20	0.41
2:E:317:TYR:CD2	2:E:383:LEU:HD21	2.56	0.41
2:F:296:LEU:HG	2:F:297:LEU:N	2.36	0.41
1:A:395:PHE:CD2	1:A:395:PHE:C	2.94	0.40
1:A:488:ARG:HD3	2:F:488:ARG:HH12	1.86	0.40
2:B:61:TYR:HE1	2:B:92:TRP:HB2	1.85	0.40
2:B:105:ILE:O	2:B:105:ILE:HG22	2.21	0.40
2:B:169:ALA:O	2:B:173:GLN:HG3	2.21	0.40
2:B:283:ILE:C	2:B:284:ILE:HD13	2.42	0.40
2:B:313:ILE:CD1	2:B:372:PRO:HG2	2.51	0.40
2:B:451:ARG:HB3	2:B:452:ALA:H	1.73	0.40
2:C:256:GLN:H	2:C:256:GLN:HG2	1.60	0.40
2:C:312:ALA:O	2:C:344:LEU:HD22	2.21	0.40
2:D:181:THR:HG21	5:D:547:HOH:O	2.21	0.40
2:E:96:LYS:C	2:E:98:VAL:N	2.74	0.40
2:E:132:TYR:C	2:E:132:TYR:HD2	2.25	0.40
2:E:214:GLU:O	2:F:233:GLY:HA3	2.21	0.40
2:E:231:MET:CE	2:E:251:ALA:HB2	2.52	0.40
2:F:117:VAL:O	2:F:118:VAL:HB	2.21	0.40
2:F:215:ARG:NE	2:F:215:ARG:HA	2.33	0.40
2:F:237:PHE:CD1	2:F:237:PHE:C	2.94	0.40
2:F:455:VAL:HG11	2:F:463:HIS:HB2	2.03	0.40
2:F:484:ARG:CB	2:F:484:ARG:CZ	2.99	0.40
2:F:497:ILE:O	2:F:497:ILE:CD1	2.67	0.40
1:A:248:PRO:HB2	1:A:251:ALA:CB	2.50	0.40
1:A:488:ARG:N	2:F:444:GLU:OE2	2.54	0.40
2:B:287:THR:CB	2:B:425:ILE:CG2	2.99	0.40
2:B:471:MET:HB3	2:B:480:LYS:NZ	2.36	0.40
2:C:88:ARG:HG2	2:C:88:ARG:NH1	2.36	0.40
2:C:488:ARG:HG3	2:C:488:ARG:HH11	1.85	0.40
2:D:263:VAL:O	2:D:278:PHE:N	2.54	0.40
2:D:295:THR:N	3:D:901:ATP:O1B	2.47	0.40
2:E:59:PHE:CZ	2:E:141:ARG:HD3	2.57	0.40
2:E:163:GLU:OE2	2:E:163:GLU:HA	2.20	0.40
2:E:492:GLY:C	2:E:494:PRO:HD3	2.41	0.40
2:F:83:ILE:H	2:F:83:ILE:HD12	1.86	0.40
2:F:94:LEU:HD22	2:F:103:LEU:HD22	2.02	0.40
2:F:117:VAL:HG22	5:F:536:HOH:O	2.20	0.40
2:F:213:GLY:C	2:F:215:ARG:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:438:ILE:HG23	2:F:453:ILE:HD11	2.04	0.40
2:F:471:MET:CG	2:F:480:LYS:HE2	2.42	0.40
1:A:261:VAL:O	1:A:279:PHE:HA	2.22	0.40
2:B:18:ILE:N	2:B:18:ILE:CD1	2.83	0.40
2:B:121:PHE:N	2:B:121:PHE:CD1	2.89	0.40
2:B:297:LEU:HD23	2:B:297:LEU:HA	1.79	0.40
2:C:203:ASN:HB3	2:C:225:LEU:CD2	2.51	0.40
2:C:396:VAL:O	2:C:397:ILE:C	2.58	0.40
2:C:418:GLN:HG3	2:C:418:GLN:O	2.21	0.40
2:D:41:SER:HA	2:D:178:THR:HB	2.03	0.40
2:D:491:SER:C	2:D:493:SER:H	2.24	0.40
2:E:249:LEU:HD13	2:E:394:GLN:HG2	2.03	0.40
2:F:79:THR:CG2	2:F:82:ASP:H	2.33	0.40
1:A:230:HIS:O	1:A:232:LYS:HD2	2.22	0.40
1:A:392:PHE:O	1:A:395:PHE:N	2.55	0.40
1:A:489:ILE:C	1:A:491:SER:N	2.75	0.40
2:B:133:ALA:HA	2:B:136:LYS:HB3	2.03	0.40
2:B:156:ALA:O	2:B:157:SER:C	2.59	0.40
2:B:249:LEU:HD13	2:B:394:GLN:HG2	2.03	0.40
2:C:73:PHE:CD1	2:C:143:SER:HB2	2.54	0.40
2:C:483:PHE:HB2	2:C:489:ILE:HD13	2.04	0.40
2:D:161:ARG:CB	2:D:196:VAL:HG11	2.48	0.40
2:E:451:ARG:HB2	2:E:470:PHE:O	2.22	0.40
2:F:296:LEU:HD13	2:F:331:TRP:CD2	2.56	0.40
2:F:372:PRO:O	2:F:408:ILE:HD12	2.22	0.40
2:B:24:MET:HB3	2:B:62:ASN:HD22	1.85	0.40
2:B:164:LEU:HD23	2:B:164:LEU:HA	1.89	0.40
2:B:363:ILE:H	2:B:363:ILE:CD1	2.33	0.40
2:C:161:ARG:HB2	2:C:196:VAL:HG11	2.03	0.40
3:C:903:ATP:HO2'	2:D:230:HIS:CE1	2.40	0.40
2:D:24:MET:HE1	2:D:66:GLU:CD	2.42	0.40
2:D:79:THR:O	2:D:80:PRO:C	2.58	0.40
2:D:147:VAL:CG2	2:D:148:THR:N	2.82	0.40
2:E:301:PHE:O	2:E:374:ARG:NH1	2.54	0.40
2:F:18:ILE:HB	2:F:228:THR:CG2	2.51	0.40
2:F:387:VAL:CG1	2:F:392:PHE:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/519 (97%)	364 (72%)	98 (20%)	40 (8%)	1	4
2	B	488/519 (94%)	368 (75%)	86 (18%)	34 (7%)	1	6
2	C	485/519 (93%)	371 (76%)	80 (16%)	34 (7%)	1	6
2	D	482/519 (93%)	378 (78%)	83 (17%)	21 (4%)	2	15
2	E	489/519 (94%)	374 (76%)	86 (18%)	29 (6%)	1	9
2	F	503/519 (97%)	384 (76%)	75 (15%)	44 (9%)	1	3
All	All	2949/3114 (95%)	2239 (76%)	508 (17%)	202 (7%)	1	6

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	65	ILE
1	A	154	TYR
1	A	193	ARG
1	A	212	GLU
1	A	420	MET
1	A	427	ASP
1	A	431	ALA
1	A	463	HIS
1	A	480	LYS
1	A	499	VAL
1	A	502	LYS
2	B	52	LYS
2	B	65	ILE
2	B	154	TYR
2	B	461	SER
2	B	463	HIS
2	B	494	PRO
2	B	498	THR
2	C	17	ALA

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Mol	Chain	Res	Type
2	C	117	VAL
2	C	154	TYR
2	C	198	GLU
2	C	199	PHE
2	C	249	LEU
2	C	261	VAL
2	C	289	ALA
2	C	333	MET
2	C	463	HIS
2	D	17	ALA
2	D	122	ASP
2	D	152	GLN
2	D	154	TYR
2	D	333	MET
2	E	154	TYR
2	E	333	MET
2	E	372	PRO
2	E	387	VAL
2	E	420	MET
2	E	428	SER
2	E	463	HIS
2	E	482	SER
2	F	26	GLU
2	F	52	LYS
2	F	117	VAL
2	F	118	VAL
2	F	154	TYR
2	F	157	SER
2	F	214	GLU
2	F	333	MET
2	F	387	VAL
2	F	463	HIS
2	F	488	ARG
2	F	504	GLU
2	F	506	SER
2	F	507	ARG
2	F	508	ILE
2	F	515	LYS
1	A	64	ILE
1	A	70	PRO
1	A	187	GLU
1	A	197	GLU

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Mol	Chain	Res	Type
1	A	249	LEU
1	A	264	SER
1	A	268	VAL
1	A	309	LYS
1	A	333	MET
1	A	342	ASN
1	A	417	ASP
1	A	433	ILE
1	A	510	ARG
2	B	106	LEU
2	B	119	GLY
2	B	193	ARG
2	B	212	GLU
2	B	327	ASN
2	B	420	MET
2	B	424	SER
2	B	452	ALA
2	C	115	GLN
2	C	157	SER
2	C	341	GLN
2	C	400	THR
2	D	195	GLY
2	D	463	HIS
2	E	85	LYS
2	E	117	VAL
2	E	122	ASP
2	E	198	GLU
2	E	211	LEU
2	E	348	CYS
2	E	379	SER
2	E	431	ALA
2	E	484	ARG
2	F	47	THR
2	F	129	ARG
2	F	189	GLY
2	F	289	ALA
2	F	296	LEU
2	F	354	ALA
2	F	379	SER
2	F	420	MET
2	F	489	ILE
2	F	501	GLU

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Mol	Chain	Res	Type
2	F	509	VAL
1	A	17	ALA
1	A	26	GLU
2	B	17	ALA
2	B	132	TYR
2	B	167	LEU
2	B	326	ARG
2	B	370	PHE
2	B	405	GLN
2	B	429	HIS
2	C	88	ARG
2	C	112	PRO
2	C	196	VAL
2	C	327	ASN
2	C	349	ALA
2	C	483	PHE
2	C	484	ARG
2	D	26	GLU
2	D	214	GLU
2	D	348	CYS
2	D	420	MET
2	E	26	GLU
2	E	86	ASN
2	E	189	GLY
2	E	422	ALA
2	F	115	GLN
2	F	294	LYS
1	A	83	ILE
1	A	120	GLY
1	A	384	ALA
1	A	490	ILE
2	B	88	ARG
2	B	157	SER
2	C	123	LEU
2	C	348	CYS
2	C	420	MET
2	D	175	GLY
2	D	292	THR
2	D	365	SER
2	D	378	ASP
2	E	212	GLU
2	E	282	SER

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Mol	Chain	Res	Type
2	E	498	THR
2	E	504	GLU
2	F	194	TYR
2	F	211	LEU
2	F	212	GLU
2	F	273	MET
2	F	297	LEU
2	F	480	LYS
1	A	117	VAL
1	A	300	ARG
1	A	501	GLU
2	B	77	GLU
2	B	211	LEU
2	B	341	GLN
2	B	342	ASN
2	B	348	CYS
2	C	77	GLU
2	C	189	GLY
2	C	211	LEU
2	C	309	LYS
2	D	212	GLU
2	D	341	GLN
2	D	379	SER
2	F	61	TYR
2	F	303	GLU
2	F	468	ARG
2	F	490	ILE
1	A	112	PRO
1	A	157	SER
1	A	189	GLY
2	B	55	PHE
2	B	168	VAL
2	C	28	PHE
2	C	193	ARG
2	C	212	GLU
2	C	401	GLY
2	D	168	VAL
2	D	347	VAL
2	E	426	THR
2	F	370	PHE
2	C	268	VAL
2	D	492	GLY

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Mol	Chain	Res	Type
2	E	425	ILE
2	F	110	PRO
2	B	268	VAL
2	E	227	GLY
2	F	80	PRO
1	A	118	VAL
2	B	117	VAL
2	C	347	VAL
2	E	293	GLY
2	F	347	VAL
1	A	347	VAL
1	A	363	ILE
2	B	489	ILE
2	F	517	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/441 (97%)	397 (92%)	32 (8%)	13	43
2	B	417/442 (94%)	383 (92%)	34 (8%)	11	39
2	C	414/442 (94%)	377 (91%)	37 (9%)	9	35
2	D	411/442 (93%)	367 (89%)	44 (11%)	6	26
2	E	418/442 (95%)	383 (92%)	35 (8%)	11	38
2	F	430/442 (97%)	385 (90%)	45 (10%)	7	27
All	All	2519/2651 (95%)	2292 (91%)	227 (9%)	9	35

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	29	ASP
1	A	30	ASP
1	A	48	SER

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Mol	Chain	Res	Type
1	A	75	THR
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	121	PHE
1	A	134	ILE
1	A	183	GLU
1	A	212	GLU
1	A	223	LEU
1	A	230	HIS
1	A	238	THR
1	A	270	LEU
1	A	287	THR
1	A	298	VAL
1	A	336	GLU
1	A	342	ASN
1	A	360	LEU
1	A	371	LYS
1	A	375	ILE
1	A	406	GLU
1	A	407	GLU
1	A	427	ASP
1	A	434	THR
1	A	451	ARG
1	A	453	ILE
1	A	463	HIS
1	A	469	GLU
1	A	518	GLU
2	B	26	GLU
2	B	33	HIS
2	B	47	THR
2	B	50	THR
2	B	67	PHE
2	B	81	GLN
2	B	92	TRP
2	B	103	LEU
2	B	111	ASP
2	B	140	ARG
2	B	150	VAL
2	B	151	PHE
2	B	154	TYR
2	B	182	THR

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Mol	Chain	Res	Type
2	B	185	ILE
2	B	186	GLU
2	B	193	ARG
2	B	198	GLU
2	B	212	GLU
2	B	223	LEU
2	B	238	THR
2	B	270	LEU
2	B	302	VAL
2	B	333	MET
2	B	371	LYS
2	B	428	SER
2	B	434	THR
2	B	451	ARG
2	B	453	ILE
2	B	462	TRP
2	B	463	HIS
2	B	471	MET
2	B	474	ASP
2	B	490	ILE
2	C	15	HIS
2	C	26	GLU
2	C	50	THR
2	C	99	ASP
2	C	122	ASP
2	C	127	ILE
2	C	149	SER
2	C	151	PHE
2	C	154	TYR
2	C	184	ARG
2	C	186	GLU
2	C	215	ARG
2	C	219	THR
2	C	223	LEU
2	C	238	THR
2	C	245	ASN
2	C	256	GLN
2	C	260	ASN
2	C	263	VAL
2	C	290	THR
2	C	300	ARG
2	C	303	GLU

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Mol	Chain	Res	Type
2	C	333	MET
2	C	336	GLU
2	C	356	LEU
2	C	371	LYS
2	C	375	ILE
2	C	383	LEU
2	C	428	SER
2	C	451	ARG
2	C	453	ILE
2	C	454	ASN
2	C	463	HIS
2	C	471	MET
2	C	474	ASP
2	C	491	SER
2	C	497	ILE
2	D	26	GLU
2	D	30	ASP
2	D	75	THR
2	D	77	GLU
2	D	81	GLN
2	D	106	LEU
2	D	122	ASP
2	D	123	LEU
2	D	154	TYR
2	D	177	THR
2	D	186	GLU
2	D	211	LEU
2	D	212	GLU
2	D	238	THR
2	D	246	ILE
2	D	247	PHE
2	D	256	GLN
2	D	263	VAL
2	D	270	LEU
2	D	274	CYS
2	D	284	ILE
2	D	290	THR
2	D	292	THR
2	D	302	VAL
2	D	321	ARG
2	D	356	LEU
2	D	360	LEU

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Mol	Chain	Res	Type
2	D	366	GLU
2	D	371	LYS
2	D	394	GLN
2	D	399	VAL
2	D	423	HIS
2	D	428	SER
2	D	434	THR
2	D	451	ARG
2	D	463	HIS
2	D	469	GLU
2	D	471	MET
2	D	474	ASP
2	D	489	ILE
2	D	490	ILE
2	D	491	SER
2	D	496	ARG
2	D	498	THR
2	E	18	ILE
2	E	26	GLU
2	E	41	SER
2	E	81	GLN
2	E	113	GLU
2	E	121	PHE
2	E	132	TYR
2	E	135	GLN
2	E	146	SER
2	E	151	PHE
2	E	154	TYR
2	E	161	ARG
2	E	170	ARG
2	E	177	THR
2	E	201	SER
2	E	212	GLU
2	E	217	ARG
2	E	218	ARG
2	E	223	LEU
2	E	228	THR
2	E	238	THR
2	E	240	THR
2	E	256	GLN
2	E	260	ASN
2	E	271	ASP

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Mol	Chain	Res	Type
2	E	325	LEU
2	E	366	GLU
2	E	371	LYS
2	E	387	VAL
2	E	449	MET
2	E	450	SER
2	E	451	ARG
2	E	456	PHE
2	E	458	MET
2	E	471	MET
2	F	15	HIS
2	F	26	GLU
2	F	47	THR
2	F	48	SER
2	F	56	SER
2	F	75	THR
2	F	76	PHE
2	F	77	GLU
2	F	103	LEU
2	F	121	PHE
2	F	140	ARG
2	F	154	TYR
2	F	168	VAL
2	F	178	THR
2	F	183	GLU
2	F	184	ARG
2	F	185	ILE
2	F	186	GLU
2	F	209	ASN
2	F	210	VAL
2	F	212	GLU
2	F	215	ARG
2	F	218	ARG
2	F	256	GLN
2	F	263	VAL
2	F	300	ARG
2	F	302	VAL
2	F	325	LEU
2	F	366	GLU
2	F	371	LYS
2	F	375	ILE
2	F	424	SER

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Mol	Chain	Res	Type
2	F	427	ASP
2	F	451	ARG
2	F	456	PHE
2	F	458	MET
2	F	462	TRP
2	F	469	GLU
2	F	471	MET
2	F	493	SER
2	F	496	ARG
2	F	497	ILE
2	F	501	GLU
2	F	504	GLU
2	F	514	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	62	ASN
1	A	131	ASN
1	A	152	GLN
1	A	209	ASN
1	A	304	ASN
1	A	308	ASN
1	A	327	ASN
1	A	414	ASN
1	A	441	GLN
1	A	454	ASN
1	A	463	HIS
2	B	62	ASN
2	B	81	GLN
2	B	209	ASN
2	B	361	GLN
2	B	394	GLN
2	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	245	ASN
2	C	323	GLN

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Mol	Chain	Res	Type
2	C	359	HIS
2	C	389	ASN
2	C	414	ASN
2	C	418	GLN
2	D	33	HIS
2	D	245	ASN
2	D	323	GLN
2	D	418	GLN
2	D	441	GLN
2	E	15	HIS
2	E	33	HIS
2	E	62	ASN
2	E	81	GLN
2	E	135	GLN
2	E	153	GLN
2	E	209	ASN
2	E	304	ASN
2	E	323	GLN
2	E	361	GLN
2	E	368	ASN
2	E	441	GLN
2	E	454	ASN
2	F	152	GLN
2	F	209	ASN
2	F	245	ASN
2	F	308	ASN
2	F	327	ASN
2	F	418	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	A	432	1	8,10,11	1.64	3 (37%)	10,14,16	2.57	1 (10%)
1	TPO	A	426	1	8,10,11	1.24	1 (12%)	10,14,16	1.32	1 (10%)
2	TPO	C	432	2	8,10,11	3.68	5 (62%)	10,14,16	1.97	4 (40%)
2	TPO	F	432	2	8,10,11	1.87	2 (25%)	10,14,16	2.17	1 (10%)
2	TPO	E	432	2	8,10,11	1.87	2 (25%)	10,14,16	2.44	1 (10%)
2	TPO	D	432	2	8,10,11	1.27	1 (12%)	10,14,16	1.98	1 (10%)
2	TPO	B	432	2	8,10,11	1.19	2 (25%)	10,14,16	2.10	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	-	4/9/11/13	-
1	TPO	A	426	1	-	1/9/11/13	-
2	TPO	C	432	2	-	1/9/11/13	-
2	TPO	F	432	2	-	0/9/11/13	-
2	TPO	E	432	2	-	4/9/11/13	-
2	TPO	D	432	2	-	0/9/11/13	-
2	TPO	B	432	2	-	1/9/11/13	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	432	TPO	P-O2P	6.67	1.80	1.54
2	C	432	TPO	CB-CA	6.23	1.67	1.53
2	F	432	TPO	CG2-CB	-3.90	1.42	1.51
2	E	432	TPO	CG2-CB	-3.74	1.42	1.51
2	C	432	TPO	P-O1P	-2.79	1.41	1.50
2	E	432	TPO	P-O2P	-2.77	1.44	1.54
1	A	432	TPO	P-O2P	-2.69	1.44	1.54
2	C	432	TPO	P-O3P	2.69	1.65	1.54
2	C	432	TPO	CA-N	2.67	1.56	1.47
2	F	432	TPO	P-O2P	-2.47	1.45	1.54
1	A	432	TPO	CG2-CB	-2.31	1.46	1.51
1	A	432	TPO	P-O3P	2.30	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	TPO	CG2-CB	2.23	1.56	1.51
2	B	432	TPO	P-O2P	-2.13	1.46	1.54
2	D	432	TPO	P-O3P	2.05	1.62	1.54
2	B	432	TPO	P-O3P	2.01	1.62	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	TPO	P-OG1-CB	-7.28	101.22	123.21
2	E	432	TPO	P-OG1-CB	-6.69	102.99	123.21
2	F	432	TPO	P-OG1-CB	-5.84	105.56	123.21
2	B	432	TPO	P-OG1-CB	-5.59	106.32	123.21
2	D	432	TPO	P-OG1-CB	-5.36	107.03	123.21
2	C	432	TPO	O3P-P-O2P	-3.48	94.32	107.64
1	A	426	TPO	P-OG1-CB	-3.09	113.88	123.21
2	C	432	TPO	O3P-P-OG1	2.92	119.07	105.99
2	C	432	TPO	O2P-P-OG1	2.43	116.89	105.99
2	C	432	TPO	OG1-P-O1P	-2.24	100.75	109.39
2	B	432	TPO	CG2-CB-CA	-2.21	108.80	113.16

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 21 short contacts:

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	E	901	4	26,33,33	1.28	2 (7%)	31,52,52	1.80	6 (19%)
3	ATP	C	903	4	26,33,33	1.15	2 (7%)	31,52,52	1.82	5 (16%)
3	ATP	F	901	4	26,33,33	1.31	3 (11%)	31,52,52	1.85	6 (19%)
3	ATP	B	901	4	26,33,33	1.29	3 (11%)	31,52,52	1.73	5 (16%)
3	ATP	D	903	4	26,33,33	1.24	2 (7%)	31,52,52	1.80	6 (19%)
3	ATP	A	903	4	26,33,33	1.27	2 (7%)	31,52,52	1.63	4 (12%)
3	ATP	D	901	4	26,33,33	1.45	4 (15%)	31,52,52	1.71	4 (12%)
3	ATP	C	901	4	26,33,33	1.41	4 (15%)	31,52,52	1.76	7 (22%)
3	ATP	E	903	4	26,33,33	1.20	1 (3%)	31,52,52	1.85	8 (25%)
3	ATP	A	901	4	26,33,33	1.30	3 (11%)	31,52,52	1.71	4 (12%)
3	ATP	B	903	4	26,33,33	1.30	2 (7%)	31,52,52	1.80	7 (22%)
3	ATP	F	903	4	26,33,33	1.37	3 (11%)	31,52,52	1.70	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	901	4	-	6/18/38/38	0/3/3/3
3	ATP	C	903	4	-	6/18/38/38	0/3/3/3
3	ATP	F	901	4	-	6/18/38/38	0/3/3/3
3	ATP	B	901	4	-	7/18/38/38	0/3/3/3
3	ATP	D	903	4	-	9/18/38/38	0/3/3/3
3	ATP	A	903	4	-	8/18/38/38	0/3/3/3
3	ATP	D	901	4	-	6/18/38/38	0/3/3/3
3	ATP	C	901	4	-	10/18/38/38	0/3/3/3
3	ATP	E	903	4	-	7/18/38/38	0/3/3/3
3	ATP	A	901	4	-	6/18/38/38	0/3/3/3
3	ATP	B	903	4	-	9/18/38/38	0/3/3/3
3	ATP	F	903	4	-	8/18/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	901	ATP	C2-N3	4.42	1.39	1.32
3	C	901	ATP	C2-N3	4.39	1.39	1.32
3	F	903	ATP	C2-N3	4.37	1.39	1.32
3	D	901	ATP	C2-N3	4.16	1.38	1.32
3	F	901	ATP	C2-N3	4.15	1.38	1.32
3	B	903	ATP	C2-N3	4.04	1.38	1.32
3	A	901	ATP	C2-N3	3.88	1.38	1.32
3	D	903	ATP	C2-N3	3.83	1.38	1.32
3	B	901	ATP	C2-N3	3.73	1.38	1.32
3	A	903	ATP	C2-N3	3.54	1.37	1.32
3	E	903	ATP	C2-N3	3.53	1.37	1.32
3	C	903	ATP	C2-N3	3.45	1.37	1.32
3	A	903	ATP	O4'-C1'	3.25	1.45	1.41
3	B	903	ATP	O4'-C1'	3.13	1.45	1.41
3	B	901	ATP	O4'-C1'	2.64	1.44	1.41
3	C	901	ATP	C2'-C1'	-2.62	1.49	1.53
3	A	901	ATP	O4'-C1'	2.58	1.44	1.41
3	D	901	ATP	C2-N1	2.51	1.38	1.33
3	B	901	ATP	C2'-C1'	-2.46	1.50	1.53
3	D	901	ATP	O4'-C1'	2.40	1.44	1.41
3	C	901	ATP	O4'-C4'	-2.39	1.39	1.45
3	F	903	ATP	C2'-C1'	-2.36	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	903	ATP	C2-N1	2.25	1.38	1.33
3	C	903	ATP	C2'-C1'	-2.20	1.50	1.53
3	F	901	ATP	O4'-C1'	2.18	1.44	1.41
3	E	901	ATP	C2-N1	2.18	1.38	1.33
3	D	903	ATP	C4-N3	2.17	1.38	1.35
3	C	901	ATP	C2-N1	2.14	1.37	1.33
3	F	901	ATP	C2-N1	2.11	1.37	1.33
3	D	901	ATP	C4-N3	2.10	1.38	1.35
3	A	901	ATP	C2-N1	2.05	1.37	1.33

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	903	ATP	N3-C2-N1	-5.70	119.76	128.68
3	F	901	ATP	N3-C2-N1	-5.64	119.86	128.68
3	D	901	ATP	N3-C2-N1	-5.60	119.92	128.68
3	C	903	ATP	N3-C2-N1	-5.54	120.03	128.68
3	B	901	ATP	N3-C2-N1	-5.52	120.05	128.68
3	E	901	ATP	N3-C2-N1	-5.49	120.09	128.68
3	F	903	ATP	N3-C2-N1	-5.44	120.18	128.68
3	E	903	ATP	N3-C2-N1	-5.41	120.23	128.68
3	A	901	ATP	N3-C2-N1	-5.37	120.28	128.68
3	A	903	ATP	N3-C2-N1	-5.36	120.29	128.68
3	C	901	ATP	N3-C2-N1	-5.35	120.31	128.68
3	B	903	ATP	N3-C2-N1	-5.35	120.31	128.68
3	C	901	ATP	C4-C5-N7	-4.45	104.77	109.40
3	F	903	ATP	C4-C5-N7	-4.34	104.87	109.40
3	A	901	ATP	C4-C5-N7	-4.31	104.91	109.40
3	B	901	ATP	C4-C5-N7	-4.28	104.94	109.40
3	E	901	ATP	C4-C5-N7	-4.27	104.95	109.40
3	B	903	ATP	C4-C5-N7	-4.25	104.97	109.40
3	F	901	ATP	C4-C5-N7	-4.23	104.99	109.40
3	E	903	ATP	C5-C6-N6	4.22	126.77	120.35
3	B	901	ATP	C5-C6-N6	4.19	126.71	120.35
3	C	903	ATP	C4-C5-N7	-4.06	105.17	109.40
3	F	901	ATP	C5-C6-N6	4.06	126.52	120.35
3	C	903	ATP	C5-C6-N6	4.05	126.51	120.35
3	B	903	ATP	C5-C6-N6	4.03	126.47	120.35
3	D	903	ATP	C4-C5-N7	-3.95	105.28	109.40
3	E	903	ATP	C4-C5-N7	-3.88	105.36	109.40
3	F	903	ATP	C5-C6-N6	3.87	126.24	120.35
3	E	901	ATP	C5-C6-N6	3.87	126.23	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	ATP	C5-C6-N6	3.85	126.20	120.35
3	A	903	ATP	C4-C5-N7	-3.84	105.39	109.40
3	D	901	ATP	C4-C5-N7	-3.81	105.42	109.40
3	A	901	ATP	C5-C6-N6	3.79	126.12	120.35
3	D	903	ATP	C5-C6-N6	3.62	125.86	120.35
3	D	901	ATP	C5-C6-N6	3.50	125.67	120.35
3	A	903	ATP	C5-C6-N6	3.43	125.57	120.35
3	C	903	ATP	C3'-C2'-C1'	2.93	105.39	100.98
3	E	903	ATP	PB-O3B-PG	-2.89	122.93	132.83
3	E	903	ATP	C3'-C2'-C1'	2.79	105.19	100.98
3	D	901	ATP	C3'-C2'-C1'	2.59	104.88	100.98
3	E	901	ATP	C3'-C2'-C1'	2.59	104.87	100.98
3	D	903	ATP	PB-O3B-PG	-2.39	124.63	132.83
3	F	901	ATP	C3'-C2'-C1'	2.37	104.55	100.98
3	B	903	ATP	C3'-C2'-C1'	2.37	104.54	100.98
3	E	903	ATP	N6-C6-N1	-2.33	113.75	118.57
3	C	903	ATP	N6-C6-N1	-2.29	113.81	118.57
3	C	901	ATP	O2'-C2'-C3'	2.28	119.20	111.82
3	F	903	ATP	O2G-PG-O3B	2.27	112.26	104.64
3	D	903	ATP	N6-C6-N1	-2.26	113.89	118.57
3	E	901	ATP	N6-C6-N1	-2.23	113.94	118.57
3	B	903	ATP	N6-C6-N1	-2.23	113.95	118.57
3	D	903	ATP	C3'-C2'-C1'	2.21	104.31	100.98
3	B	901	ATP	N6-C6-N1	-2.21	114.00	118.57
3	B	903	ATP	O2'-C2'-C3'	2.19	118.92	111.82
3	B	903	ATP	O2G-PG-O3B	2.19	111.97	104.64
3	C	901	ATP	C3'-C2'-C1'	2.18	104.26	100.98
3	F	901	ATP	O2'-C2'-C3'	2.17	118.85	111.82
3	C	901	ATP	O2G-PG-O3B	2.15	111.86	104.64
3	F	901	ATP	PB-O3B-PG	-2.15	125.44	132.83
3	A	903	ATP	O2G-PG-O3B	2.13	111.78	104.64
3	A	901	ATP	N6-C6-N1	-2.06	114.30	118.57
3	E	901	ATP	O2'-C2'-C3'	2.06	118.48	111.82
3	B	901	ATP	O2'-C2'-C3'	2.05	118.45	111.82
3	F	903	ATP	N6-C6-N1	-2.03	114.37	118.57
3	C	901	ATP	N6-C6-N1	-2.02	114.39	118.57
3	E	903	ATP	C2'-C3'-C4'	2.02	106.56	102.64
3	E	903	ATP	O2G-PG-O3B	2.02	111.40	104.64

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	C3'-C4'-C5'-O5'
3	A	903	ATP	PB-O3B-PG-O3G
3	A	903	ATP	C5'-O5'-PA-O1A
3	A	903	ATP	C3'-C4'-C5'-O5'
3	B	901	ATP	C5'-O5'-PA-O1A
3	B	901	ATP	C3'-C4'-C5'-O5'
3	B	903	ATP	PB-O3B-PG-O3G
3	B	903	ATP	O4'-C4'-C5'-O5'
3	B	903	ATP	C3'-C4'-C5'-O5'
3	C	901	ATP	C5'-O5'-PA-O2A
3	C	901	ATP	C5'-O5'-PA-O3A
3	C	901	ATP	C3'-C4'-C5'-O5'
3	C	903	ATP	PB-O3B-PG-O3G
3	C	903	ATP	PB-O3A-PA-O5'
3	C	903	ATP	C5'-O5'-PA-O1A
3	C	903	ATP	O4'-C4'-C5'-O5'
3	C	903	ATP	C3'-C4'-C5'-O5'
3	D	901	ATP	C5'-O5'-PA-O3A
3	D	901	ATP	C3'-C4'-C5'-O5'
3	D	903	ATP	PB-O3B-PG-O3G
3	D	903	ATP	O4'-C4'-C5'-O5'
3	D	903	ATP	C3'-C4'-C5'-O5'
3	E	901	ATP	C5'-O5'-PA-O3A
3	E	901	ATP	C3'-C4'-C5'-O5'
3	E	903	ATP	C5'-O5'-PA-O1A
3	E	903	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	C5'-O5'-PA-O1A
3	F	901	ATP	C3'-C4'-C5'-O5'
3	F	903	ATP	C5'-O5'-PA-O1A
3	F	903	ATP	C5'-O5'-PA-O3A
3	F	903	ATP	O4'-C4'-C5'-O5'
3	F	903	ATP	C3'-C4'-C5'-O5'
3	A	901	ATP	O4'-C4'-C5'-O5'
3	B	901	ATP	O4'-C4'-C5'-O5'
3	C	901	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	O4'-C4'-C5'-O5'
3	E	903	ATP	O4'-C4'-C5'-O5'
3	F	901	ATP	O4'-C4'-C5'-O5'
3	D	901	ATP	O4'-C4'-C5'-O5'
3	A	903	ATP	O4'-C4'-C5'-O5'
3	F	903	ATP	PB-O3B-PG-O1G
3	B	903	ATP	PB-O3A-PA-O1A

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

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Mol	Chain	Res	Type	Atoms
3	F	903	ATP	PB-O3A-PA-O2A
3	B	903	ATP	C5'-O5'-PA-O1A
3	D	903	ATP	C5'-O5'-PA-O1A

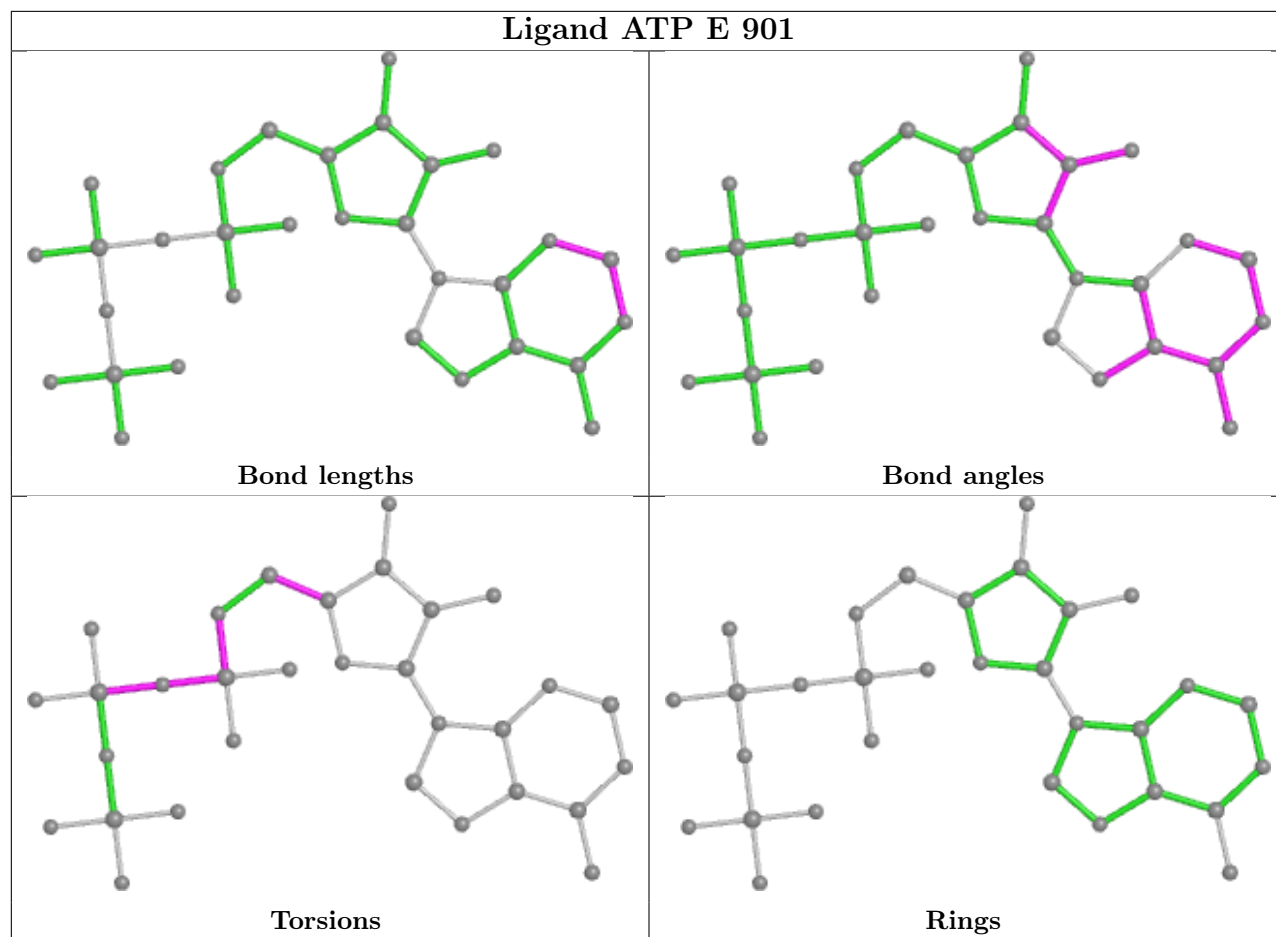
There are no ring outliers.

12 monomers are involved in 47 short contacts:

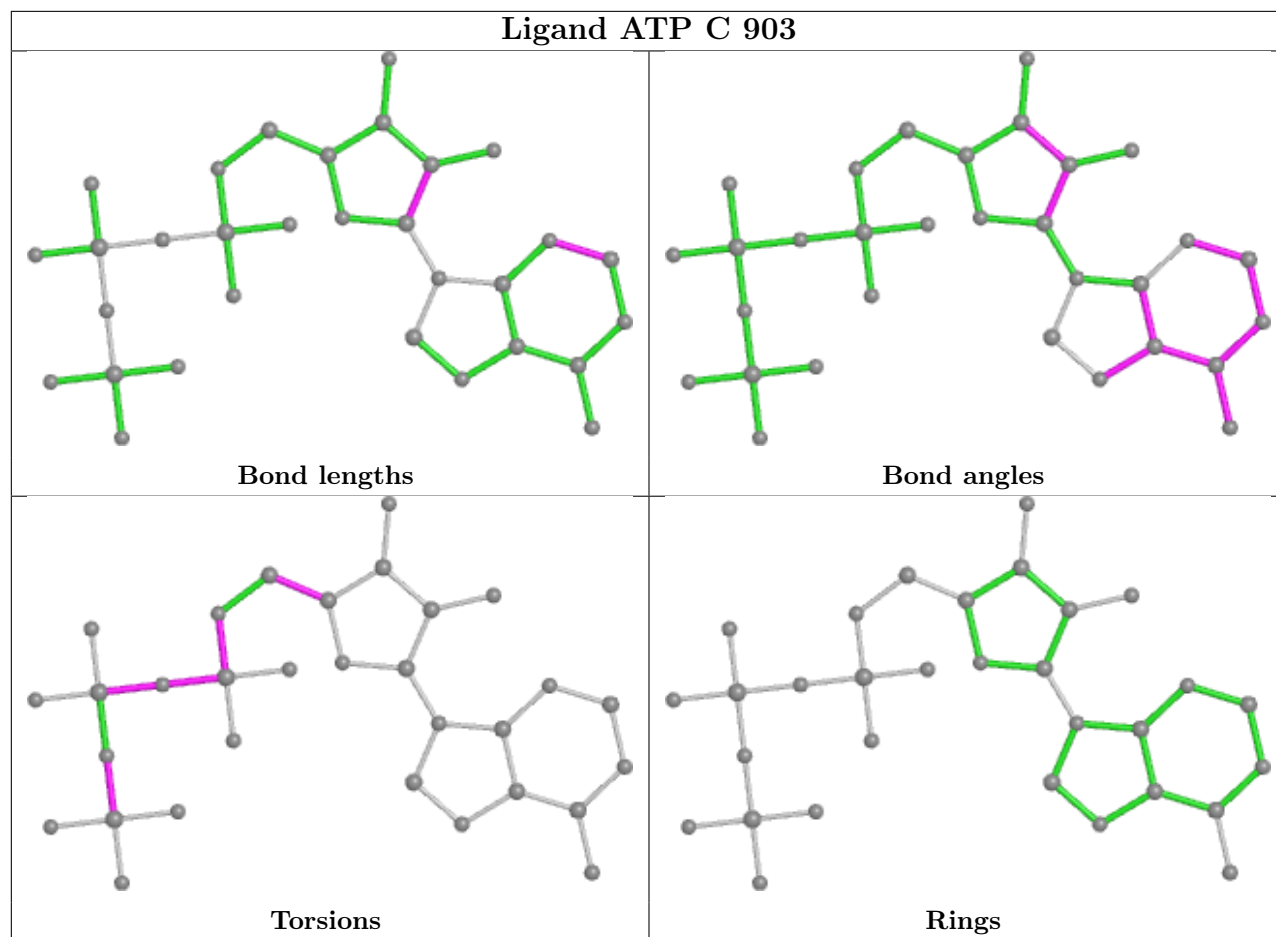
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	901	ATP	3	0
3	C	903	ATP	2	0
3	F	901	ATP	4	0
3	B	901	ATP	4	0
3	D	903	ATP	5	0
3	A	903	ATP	3	0
3	D	901	ATP	8	0
3	C	901	ATP	3	0
3	E	903	ATP	3	0
3	A	901	ATP	5	0
3	B	903	ATP	4	0
3	F	903	ATP	3	0

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

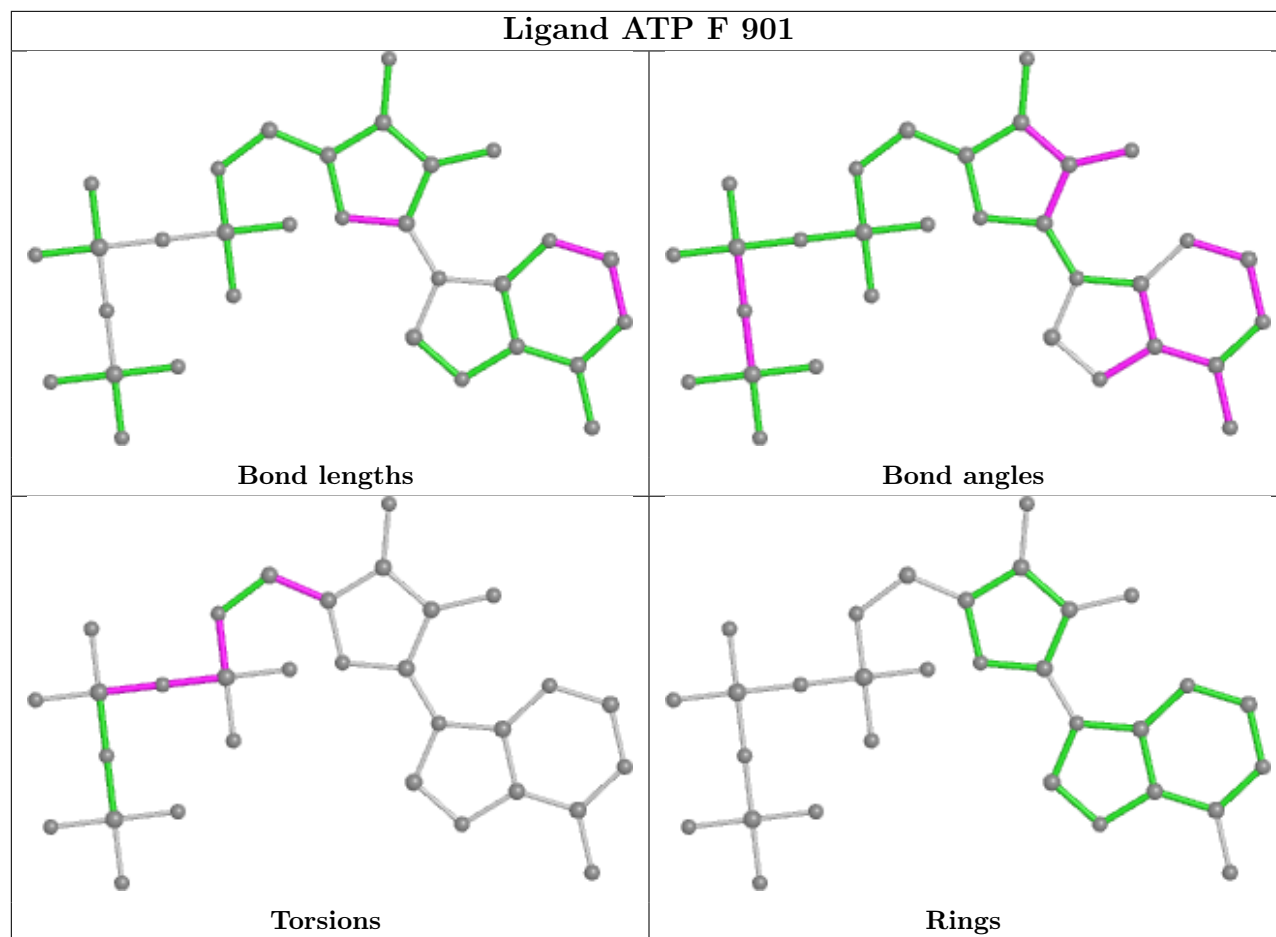
Ligand ATP E 901



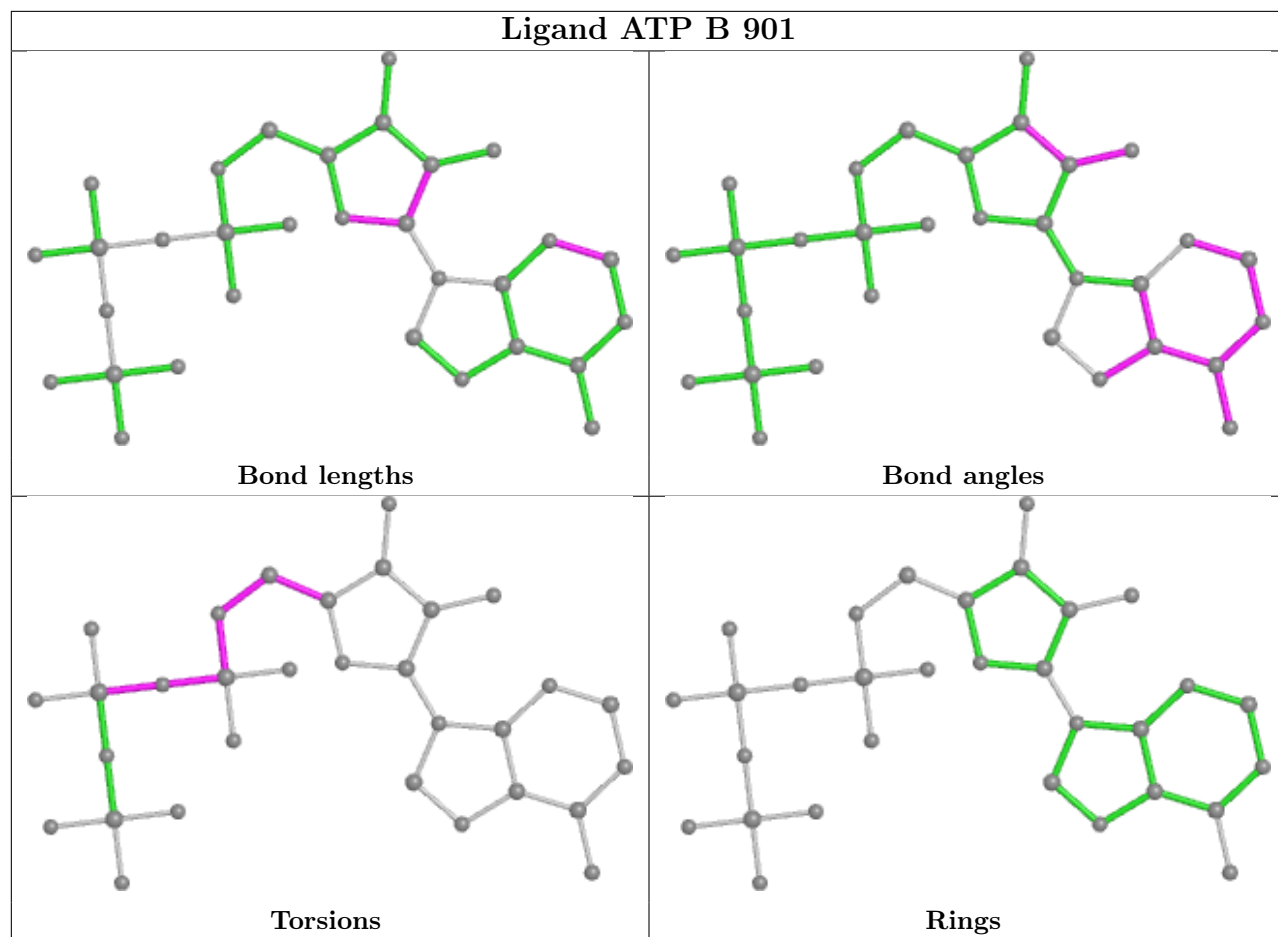
Ligand ATP C 903

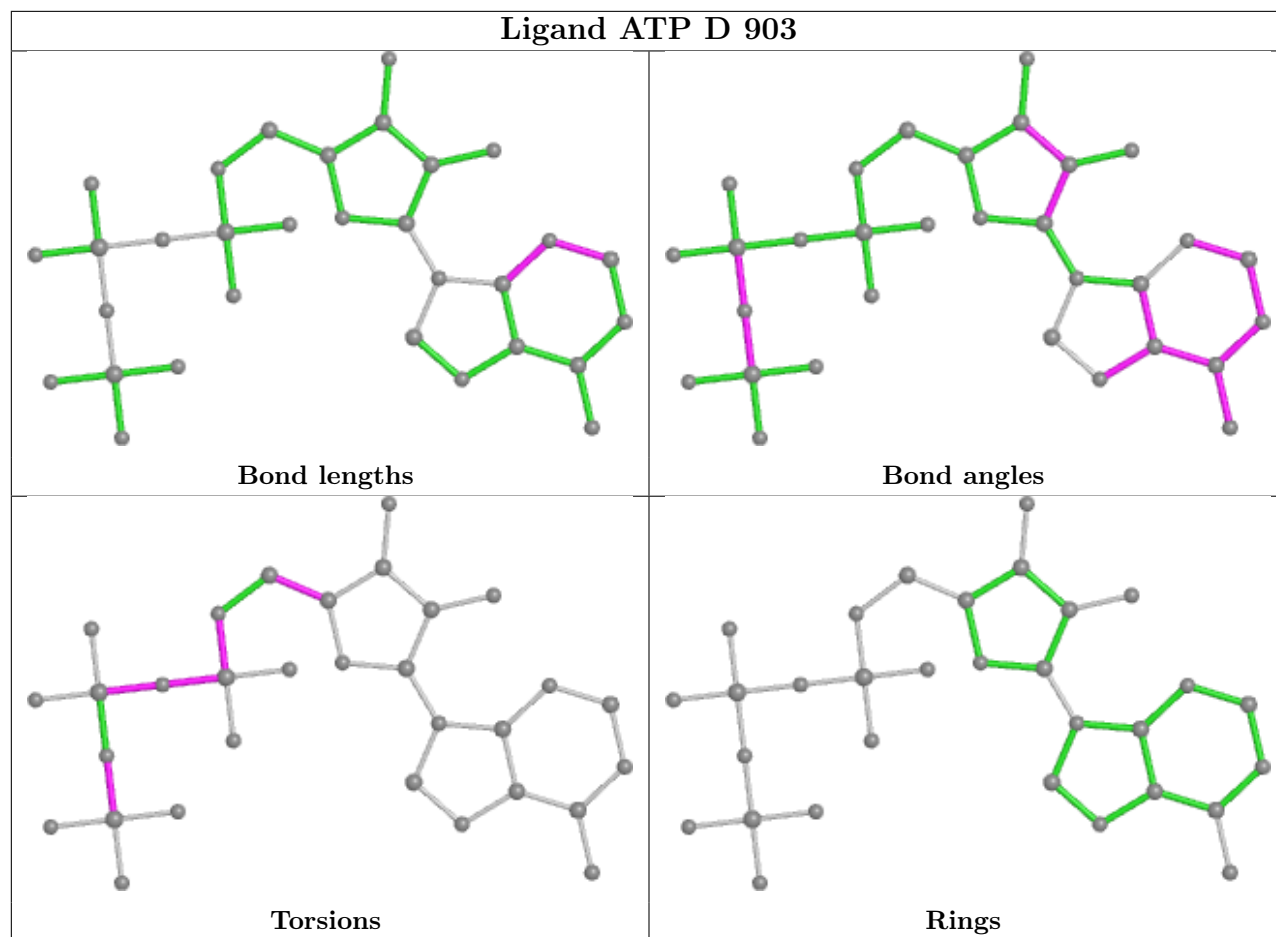


Ligand ATP F 901

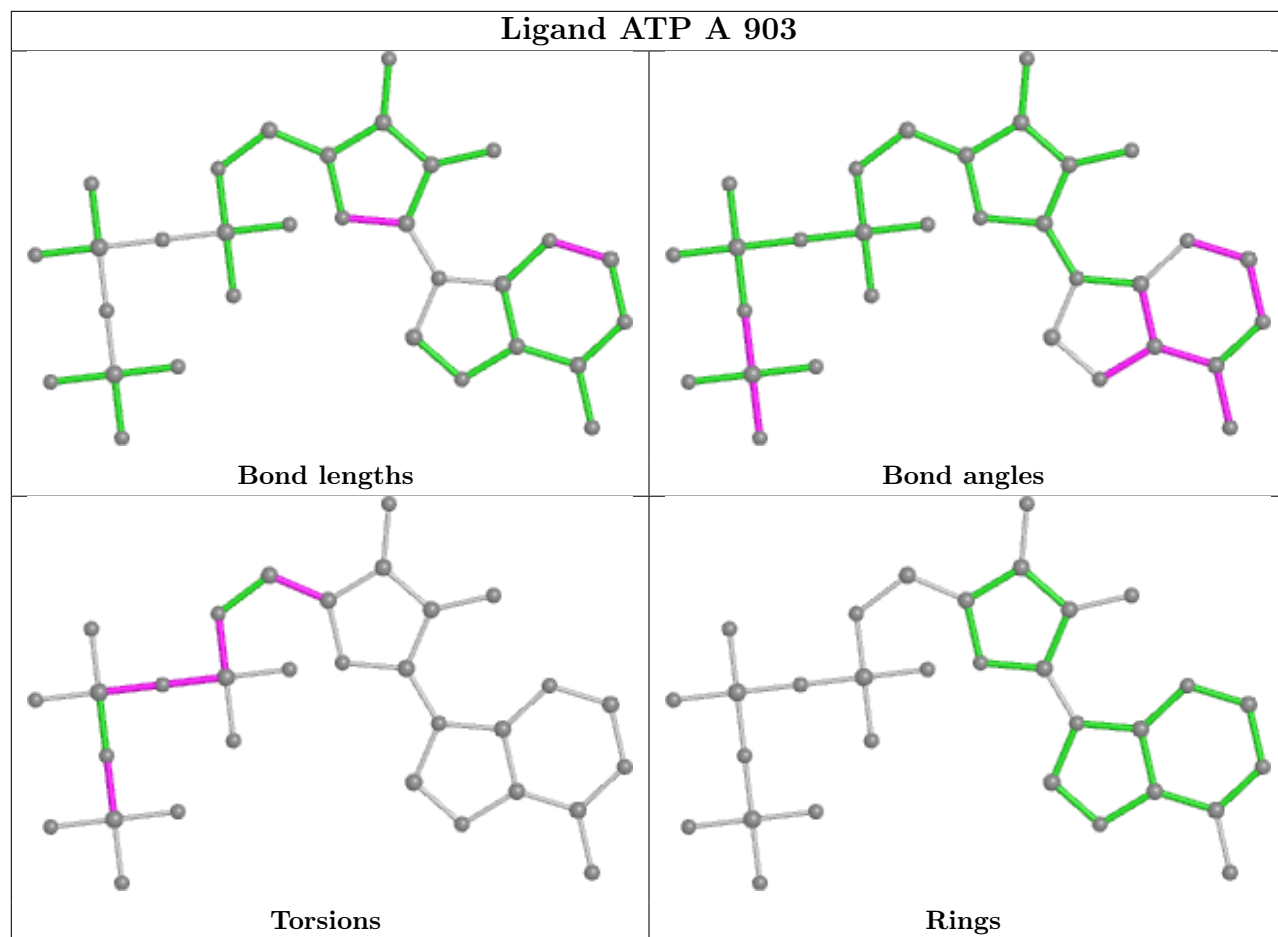


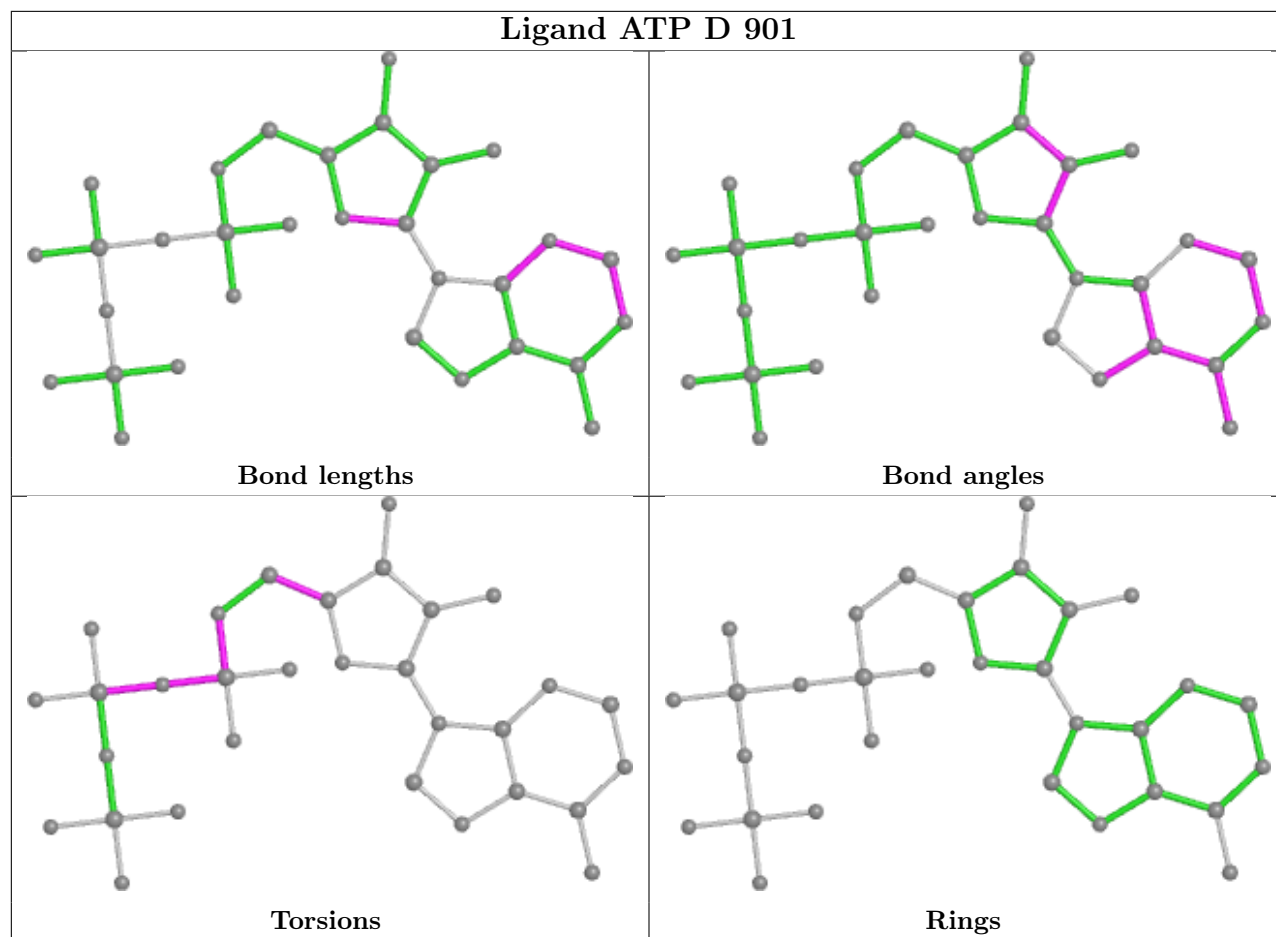
Ligand ATP B 901

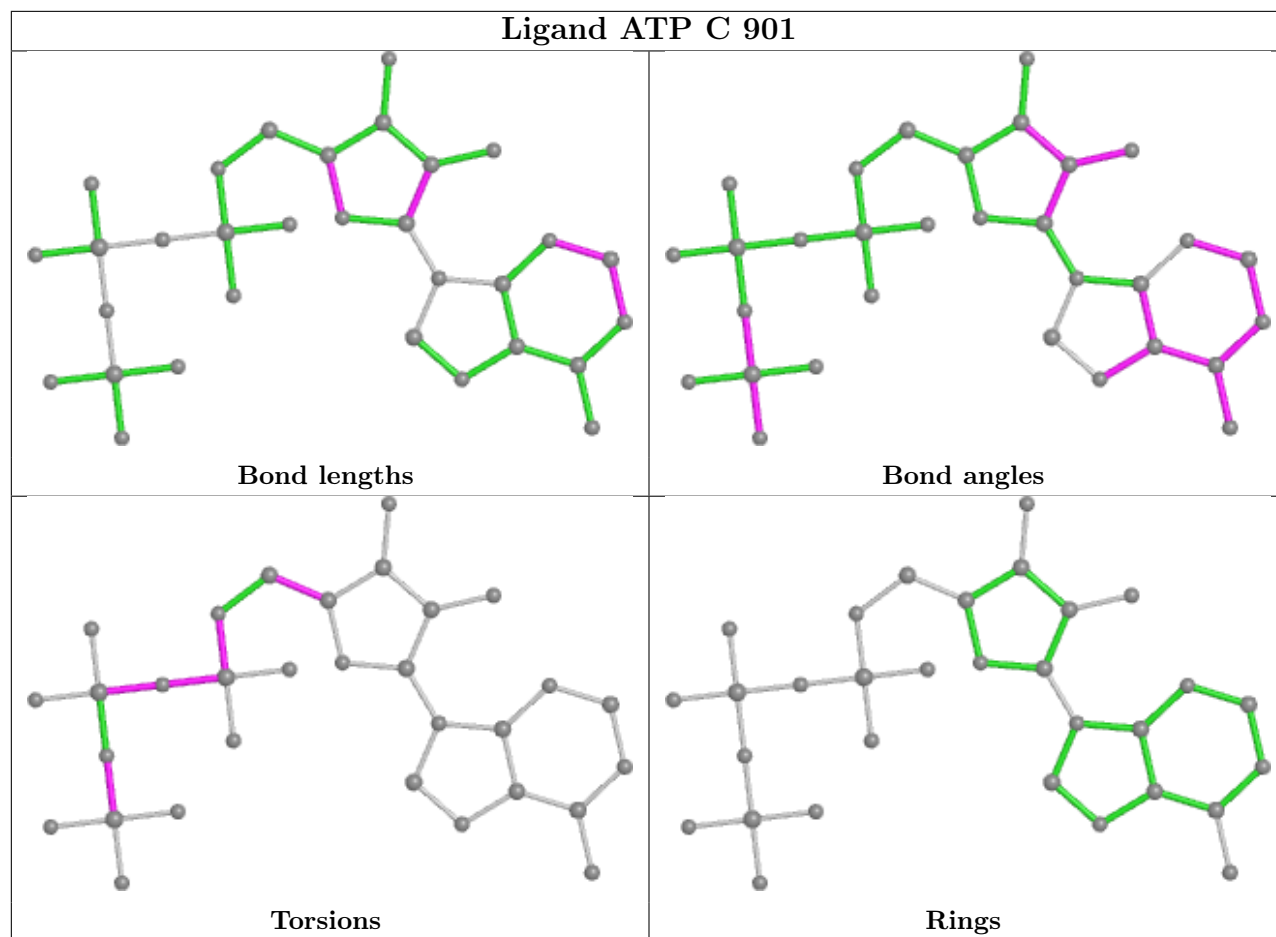




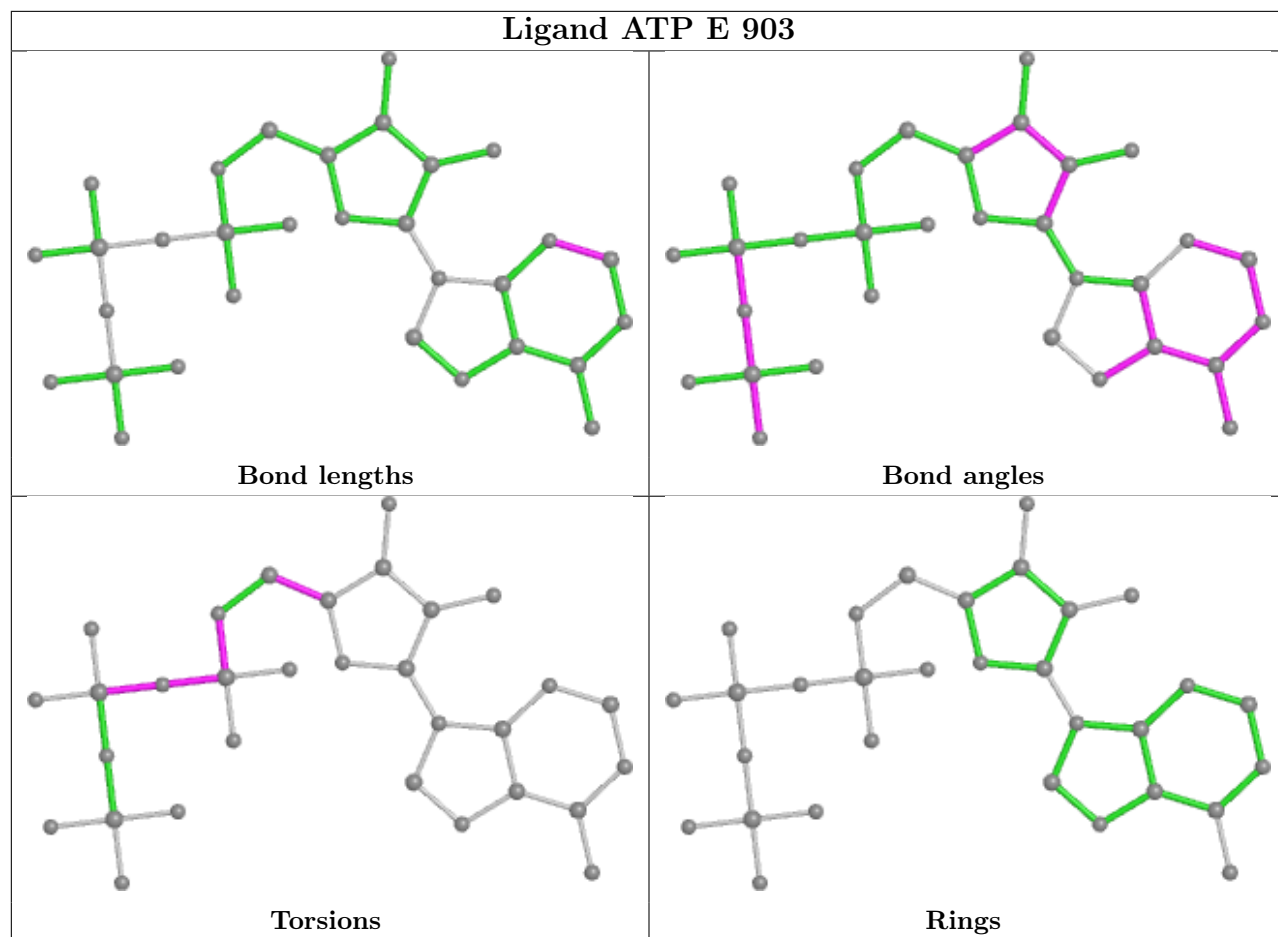
Ligand ATP A 903

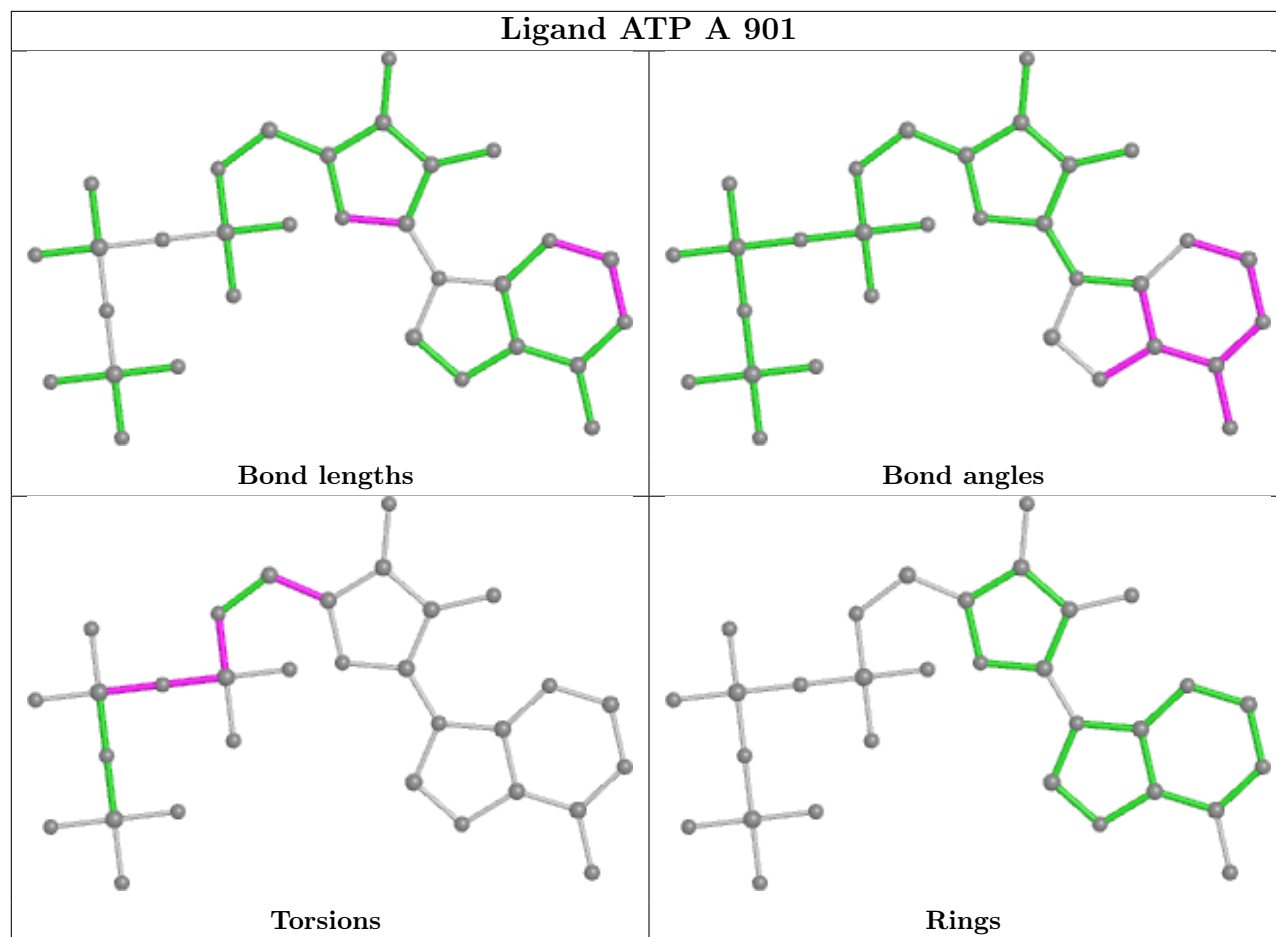




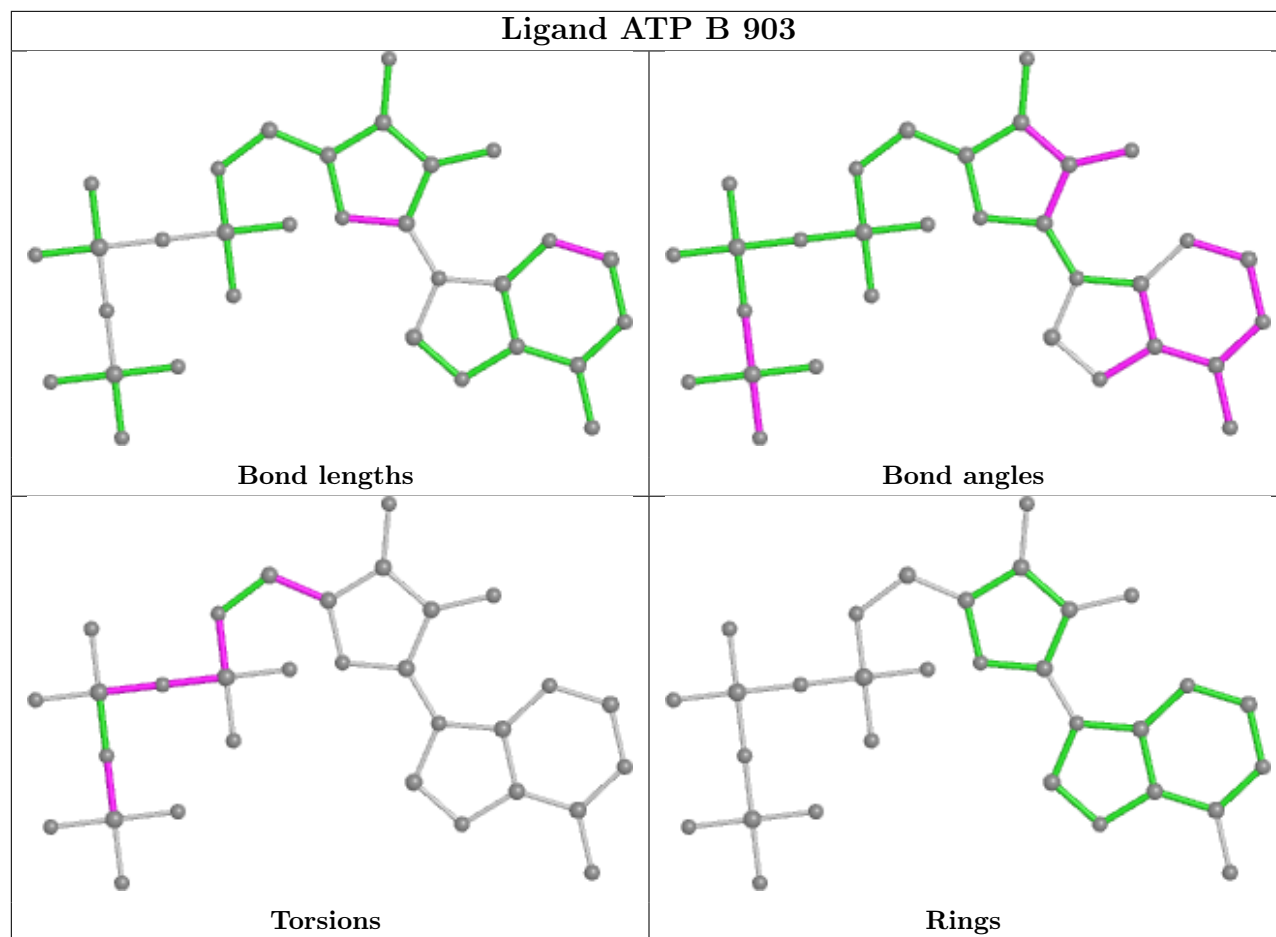


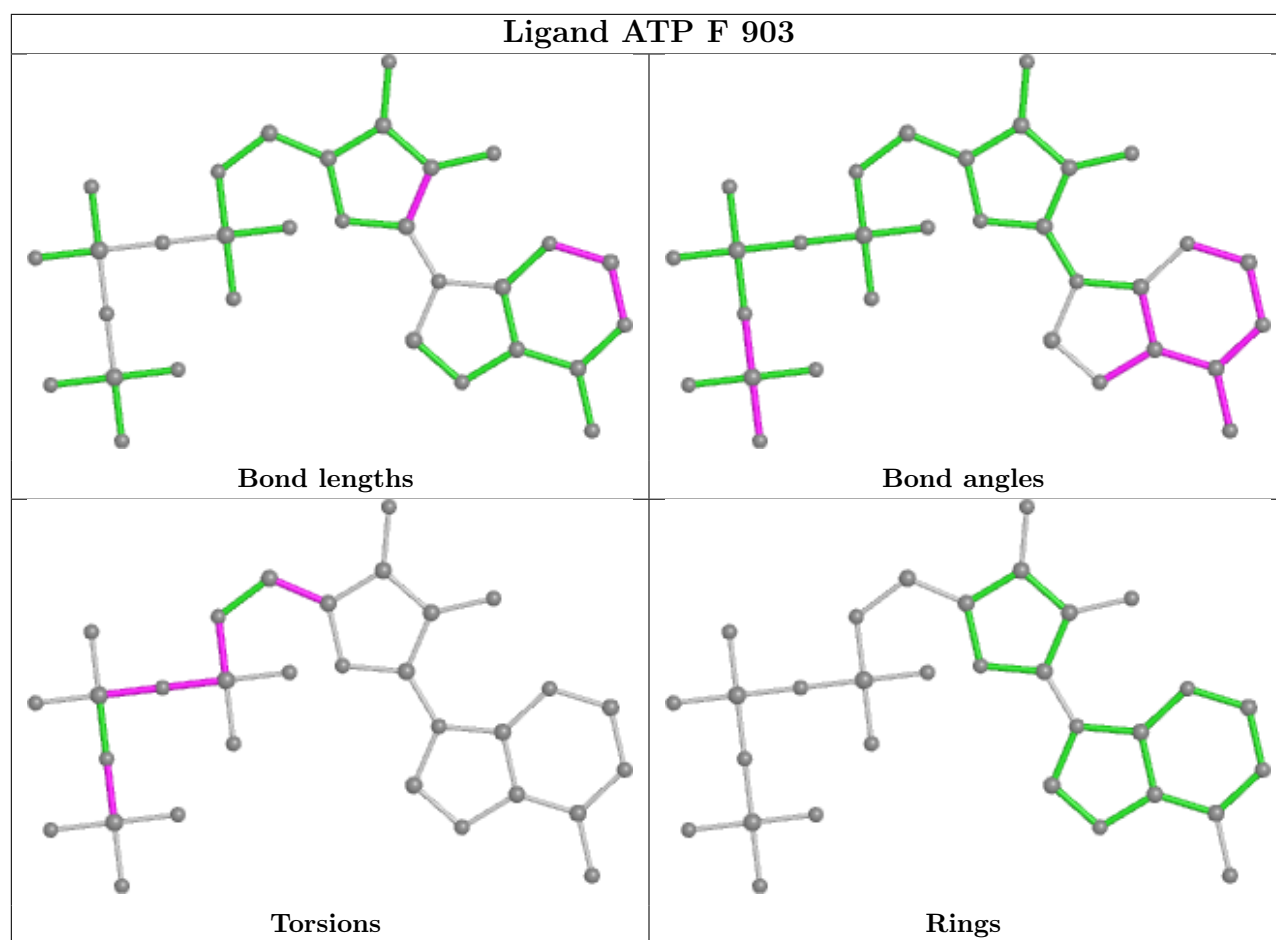
Ligand ATP E 903





Ligand ATP B 903





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

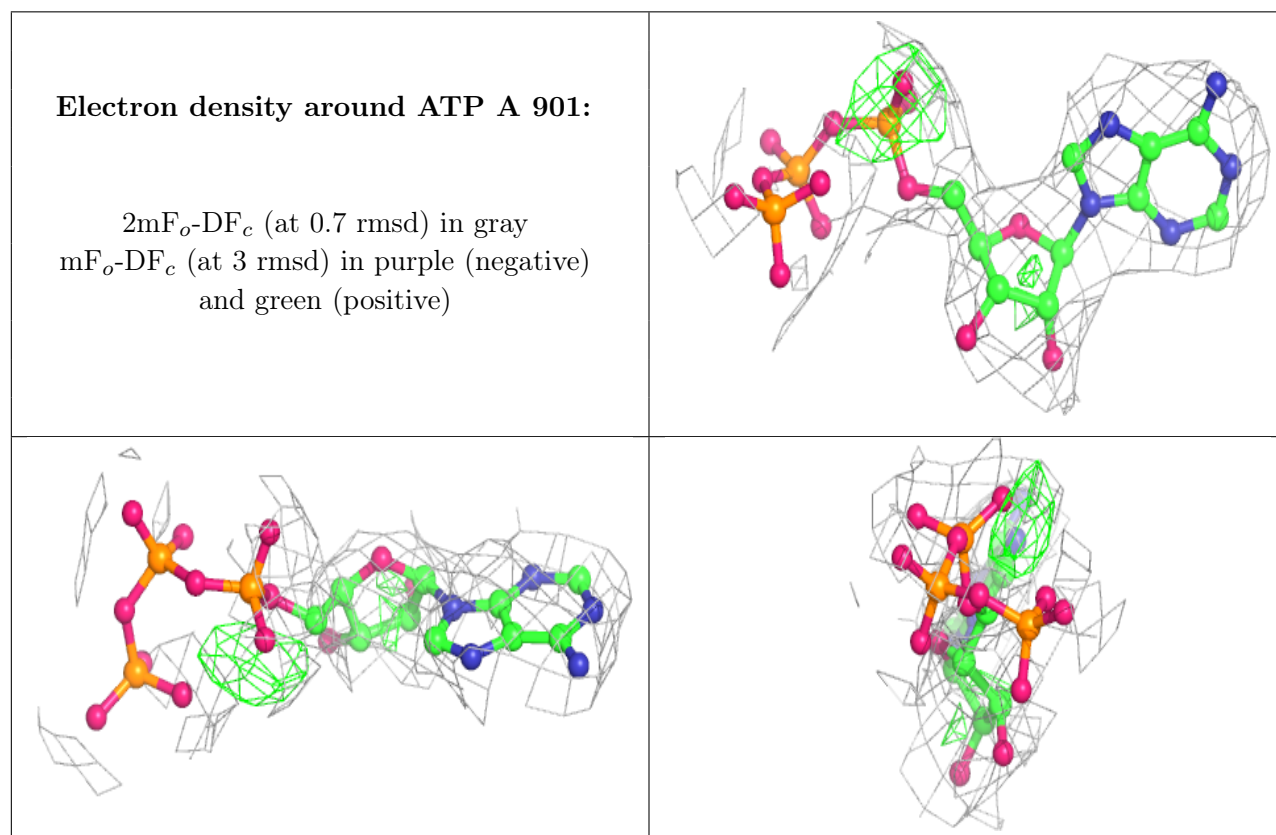
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

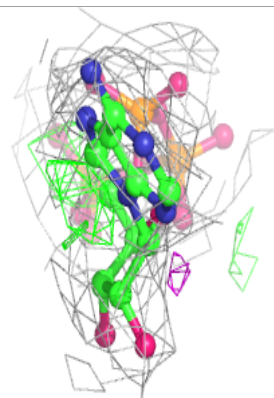
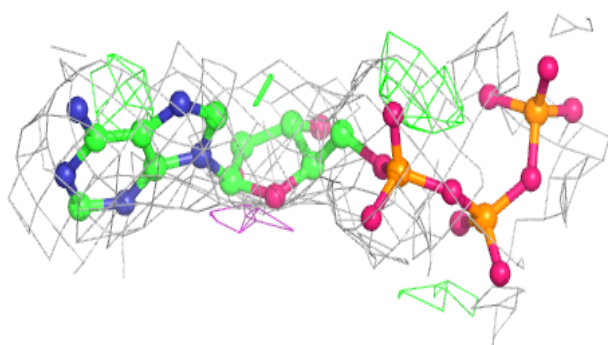
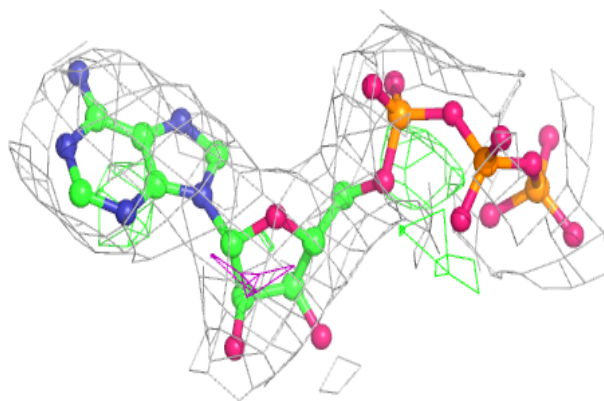
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

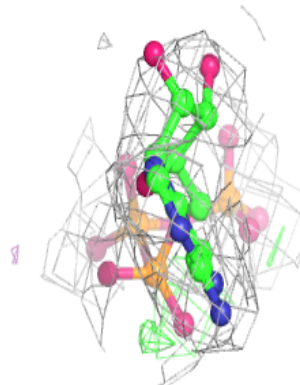
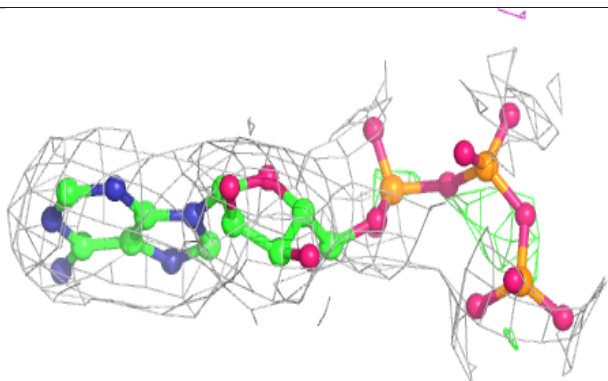
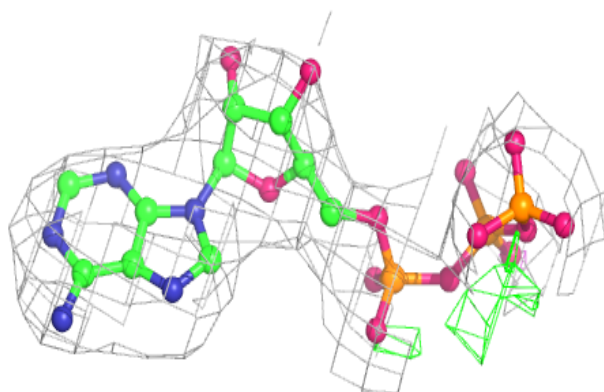


Electron density around ATP A 903:

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

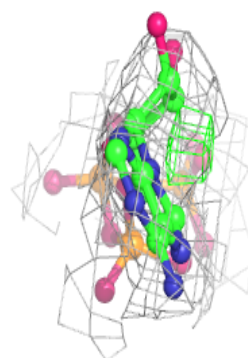
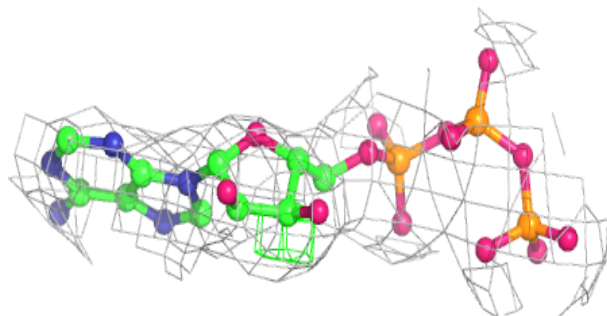
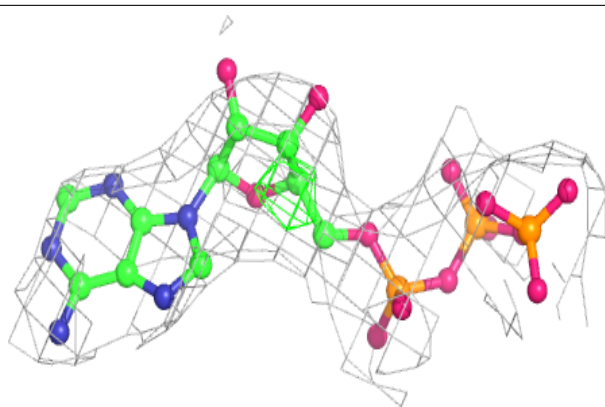
**Electron density around ATP B 901:**

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

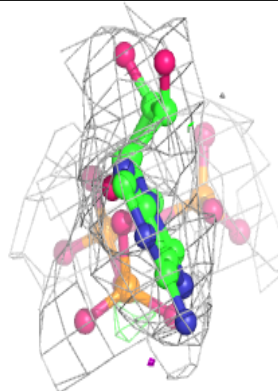
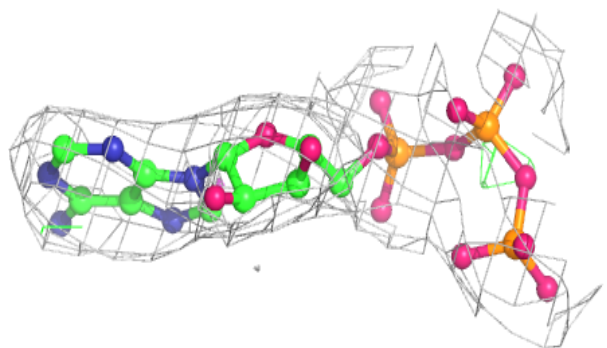
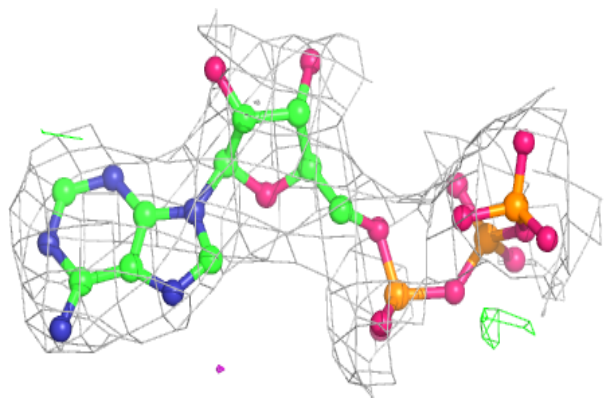


Electron density around ATP B 903:

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

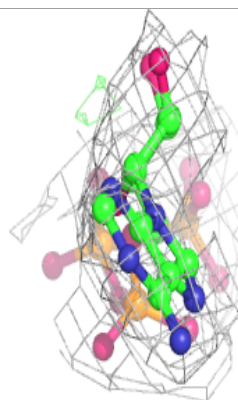
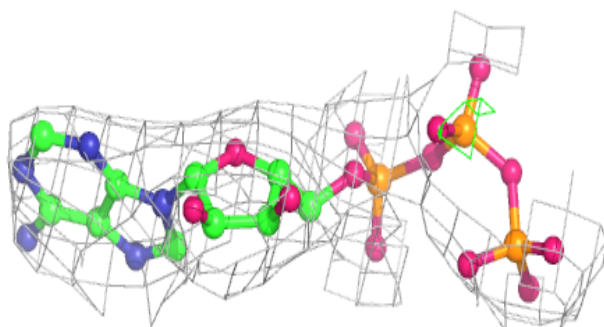
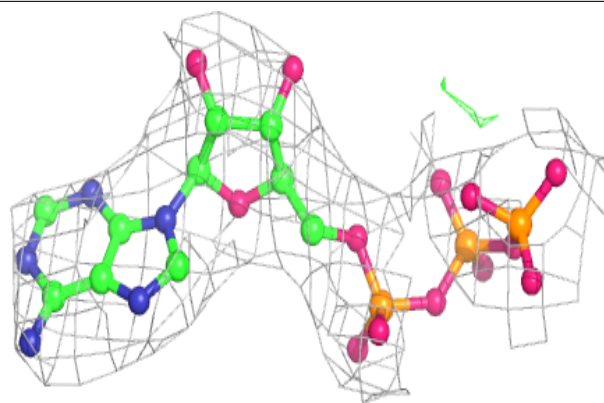
**Electron density around ATP C 901:**

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

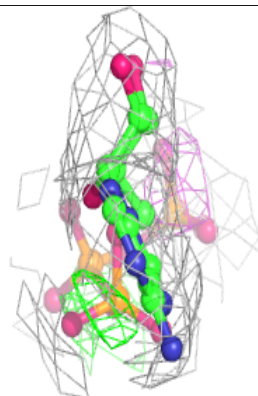
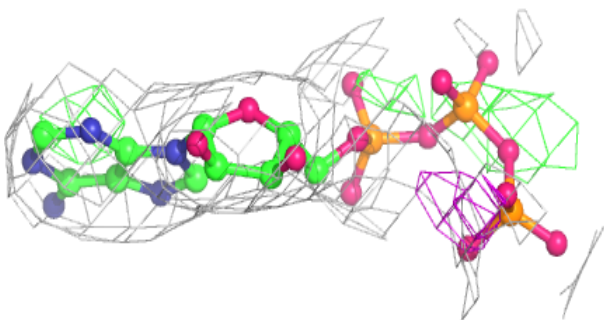
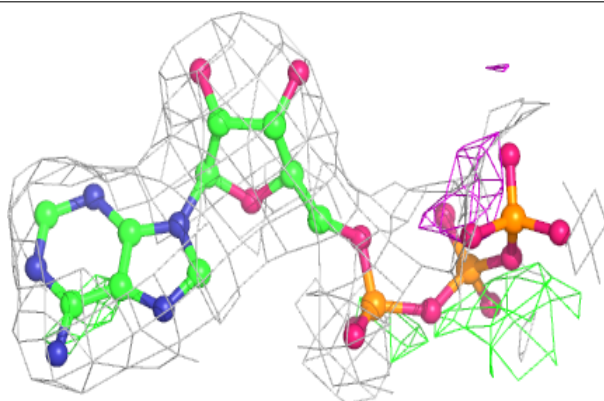


Electron density around ATP C 903:

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

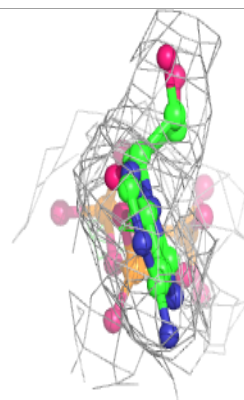
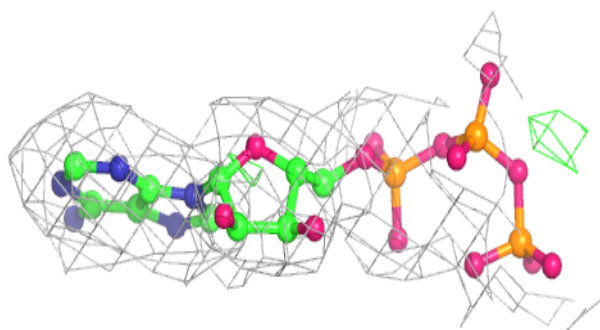
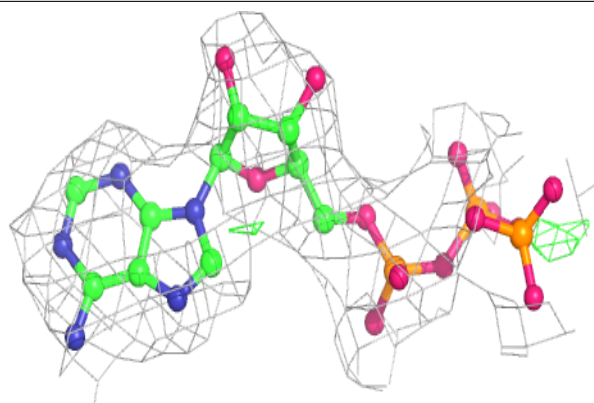
**Electron density around ATP D 901:**

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

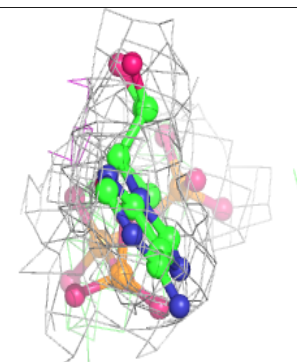
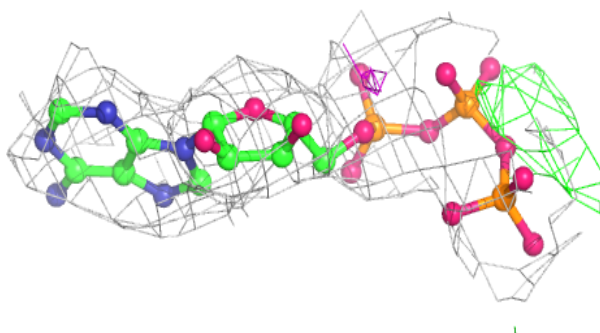
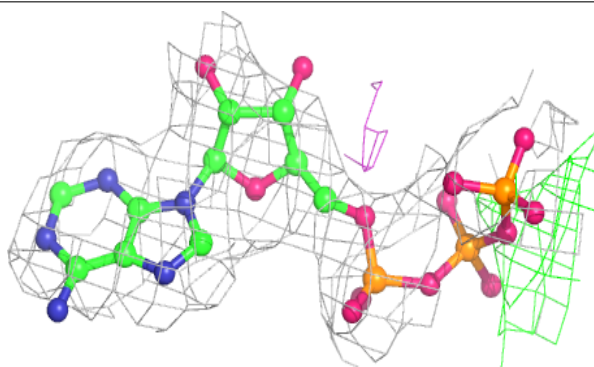


Electron density around ATP D 903:

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

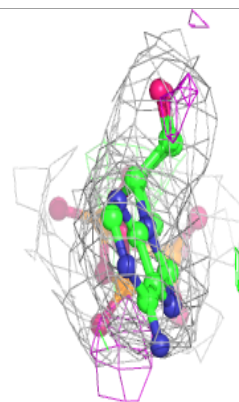
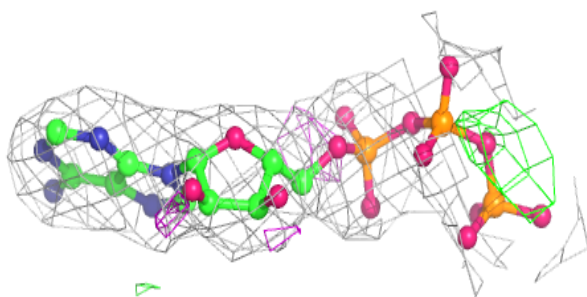
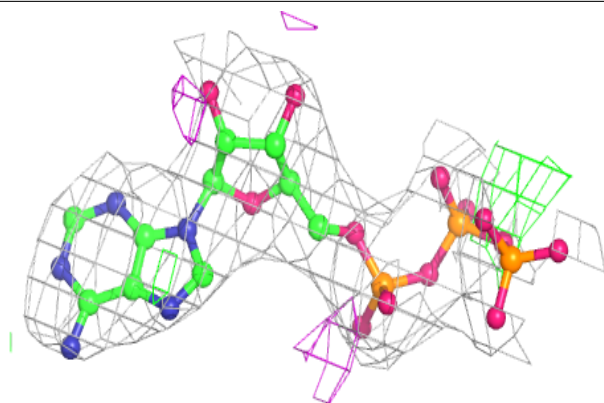
**Electron density around ATP E 901:**

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

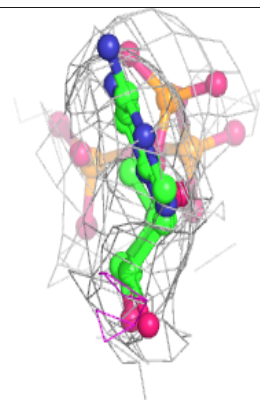
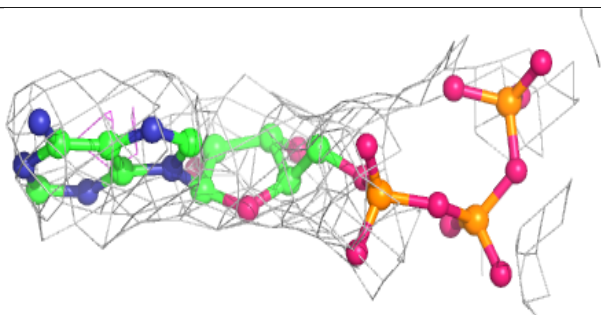
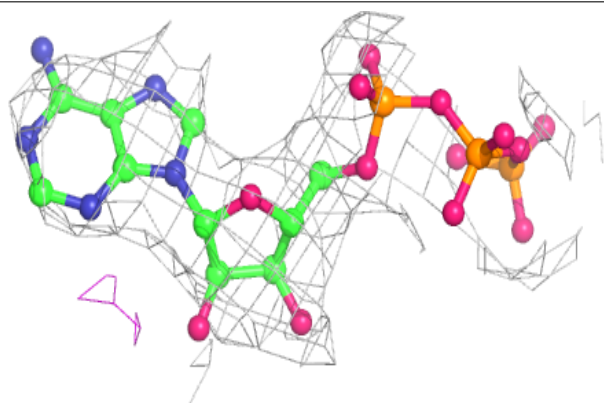


Electron density around ATP E 903:

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

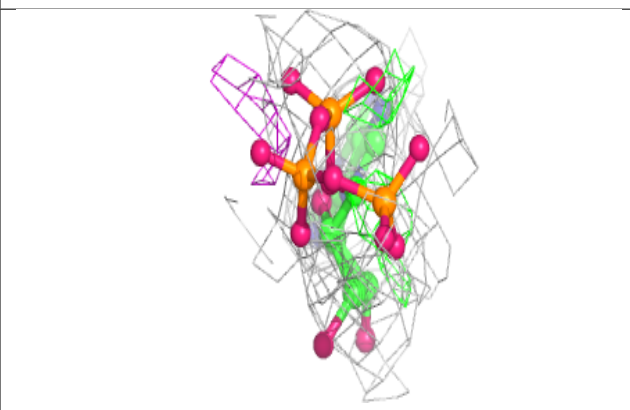
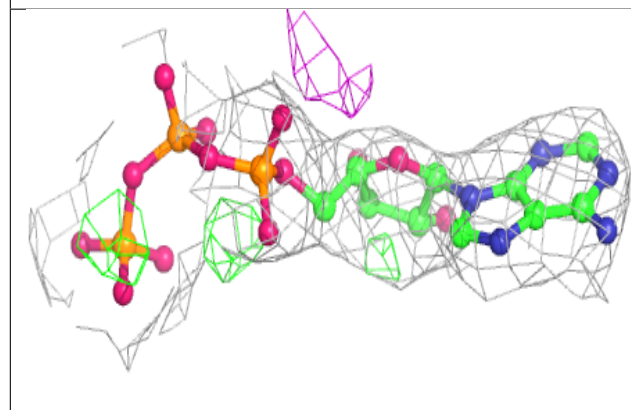
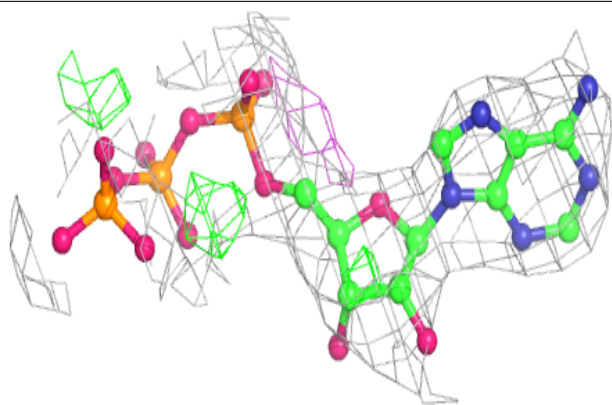
**Electron density around ATP F 901:**

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



Electron density around ATP F 903:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.