Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 11:50 PM EDT

PDB ID	:	3JZM
Title	:	Crystal structure of the phosphorylation-site mutant T432A of the KaiC circadian clock protein
Authors	:	Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on	:	2009-09-23
Resolution	:	2.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

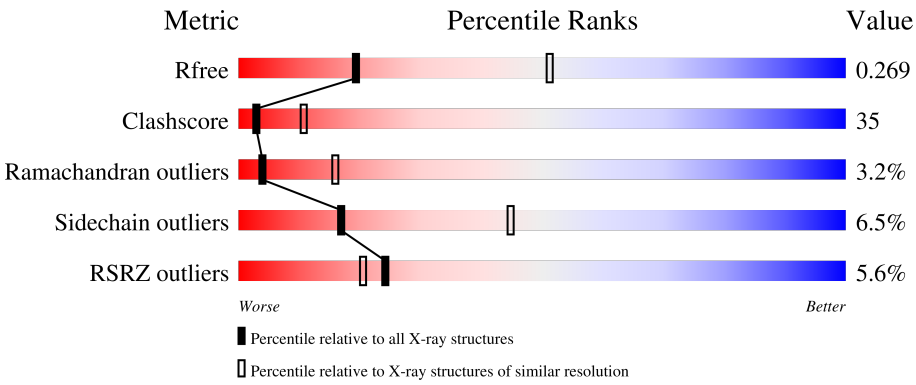
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	6% 45% 43% 5% 7%
1	B	519	7% 44% 45% • 7%
1	C	519	5% 42% 44% 7% 7%
1	D	519	3% 47% 40% 6% • 7%
1	E	519	5% 41% 46% 6% 7%

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Mol	Chain	Length	Quality of chain
1	F	519	4% 39% 47% 7% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	801	-	-	-	X
3	MG	B	701	-	-	-	X
3	MG	B	801	-	-	-	X
3	MG	C	520	-	-	-	X
3	MG	C	801	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23355 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

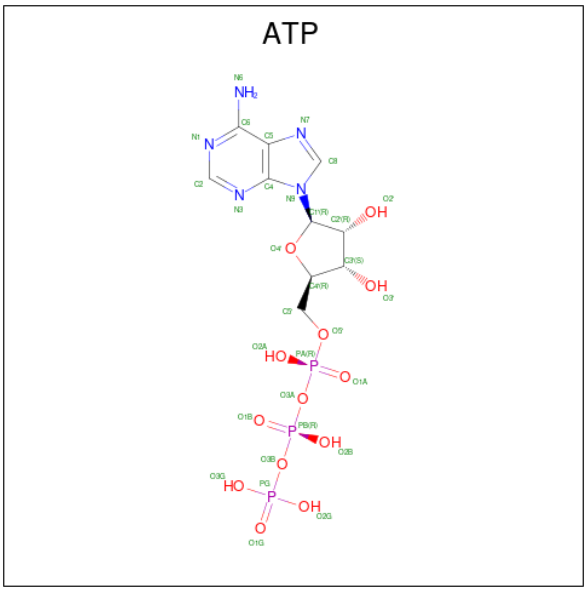
- Molecule 1 is a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	484	3817	2406	670	725	1	15	0	0	0
1	B	484	3817	2406	670	725	1	15	0	0	0
1	C	484	3817	2406	670	725	1	15	0	0	0
1	D	484	3817	2406	670	725	1	15	0	0	0
1	E	484	3817	2406	670	725	1	15	0	0	0
1	F	484	3817	2406	670	725	1	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	ALA	THR	engineered mutation	UNP Q79PF4
B	432	ALA	THR	engineered mutation	UNP Q79PF4
C	432	ALA	THR	engineered mutation	UNP Q79PF4
D	432	ALA	THR	engineered mutation	UNP Q79PF4
E	432	ALA	THR	engineered mutation	UNP Q79PF4
F	432	ALA	THR	engineered mutation	UNP Q79PF4

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

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

- Molecule 4 is water.

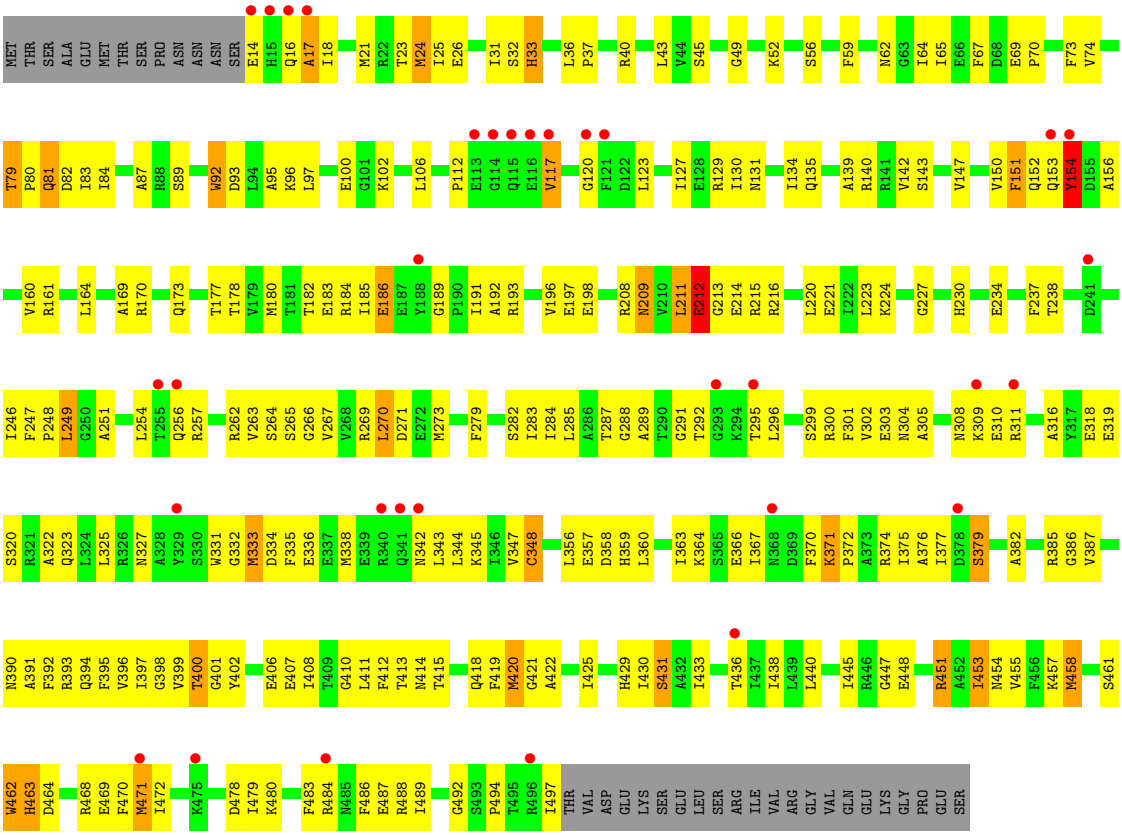
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	7	7	7	0	0
4	B	5	5	5	0	0
4	C	7	7	7	0	0
4	D	12	12	12	0	0
4	E	13	13	13	0	0
4	F	19	19	19	0	0

3 Residue-property plots (i)

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

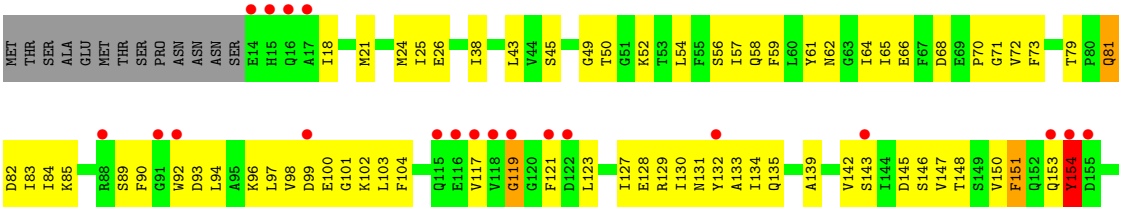
• Molecule 1: Circadian clock protein kinase kaiC

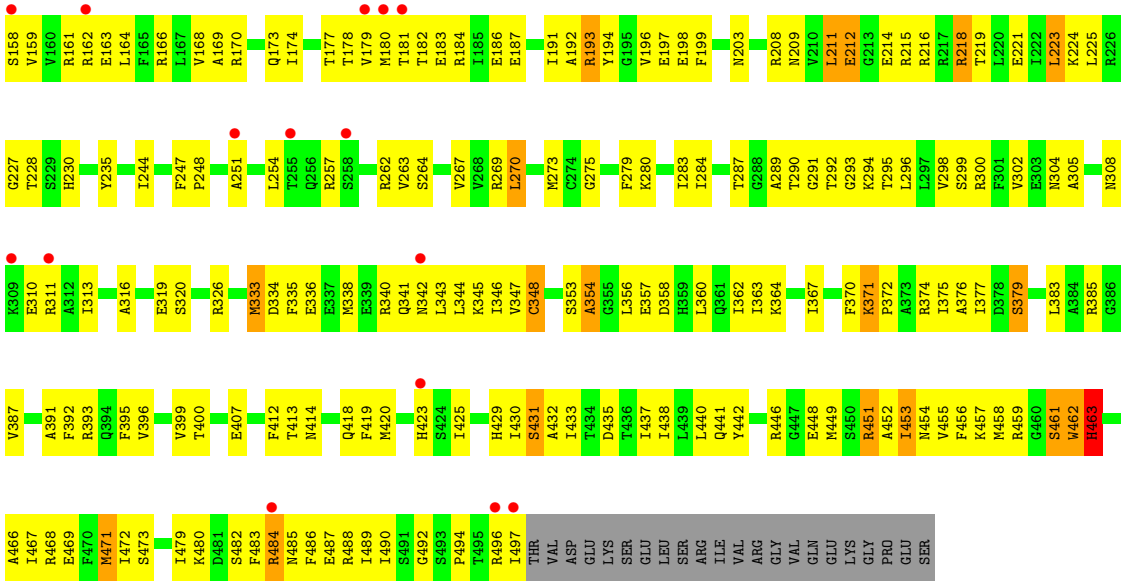
Chain A: 6% 45% 43% 5% 7%



• Molecule 1: Circadian clock protein kinase kaiC

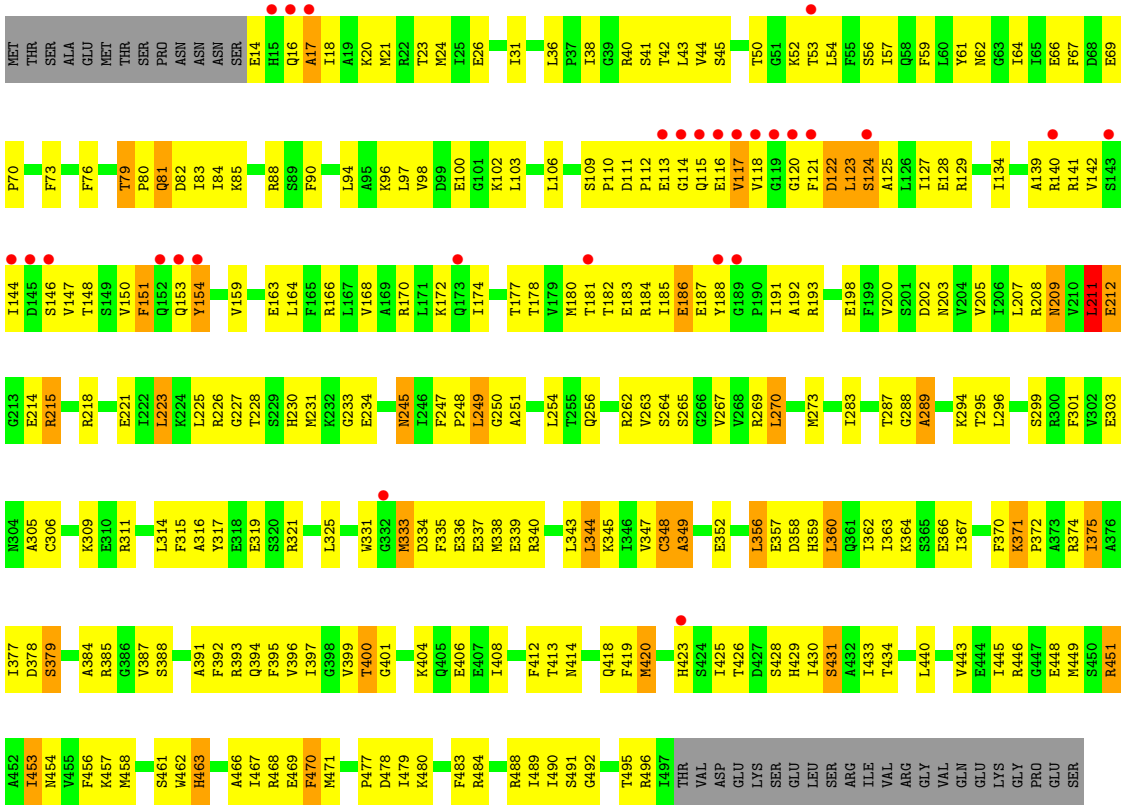
Chain B: 7% 44% 45% • 7%





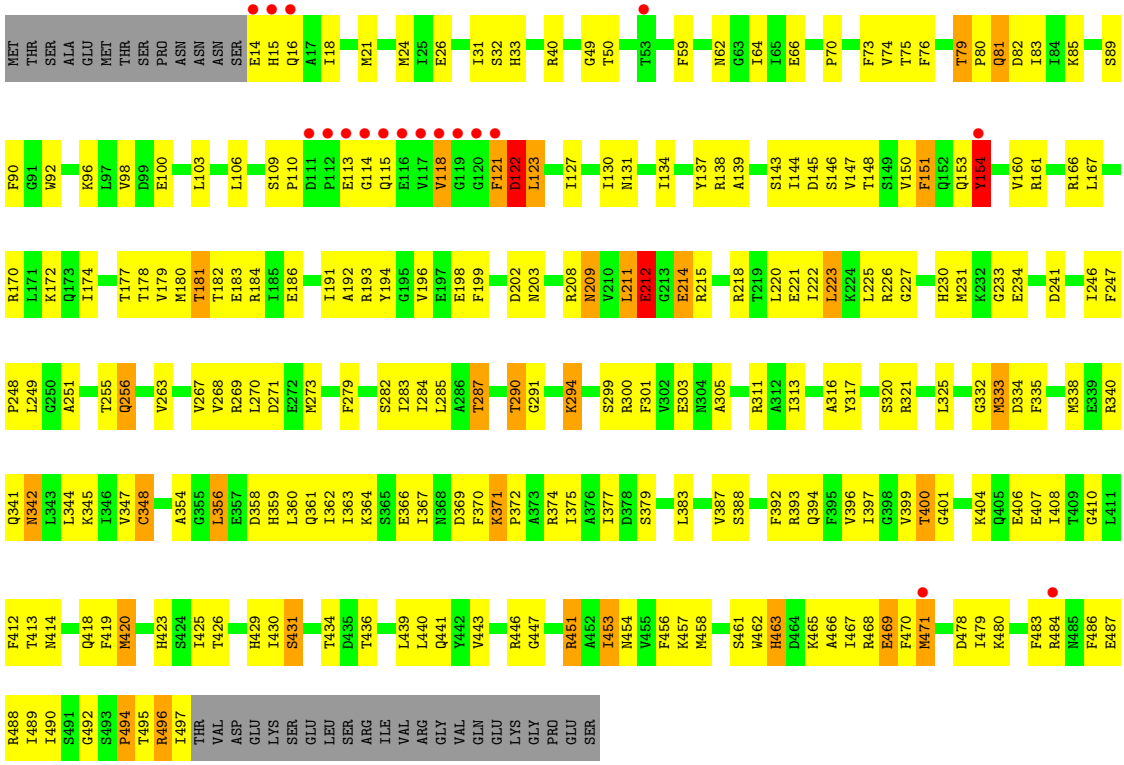
- Molecule 1: Circadian clock protein kinase kaiC

Chain C:



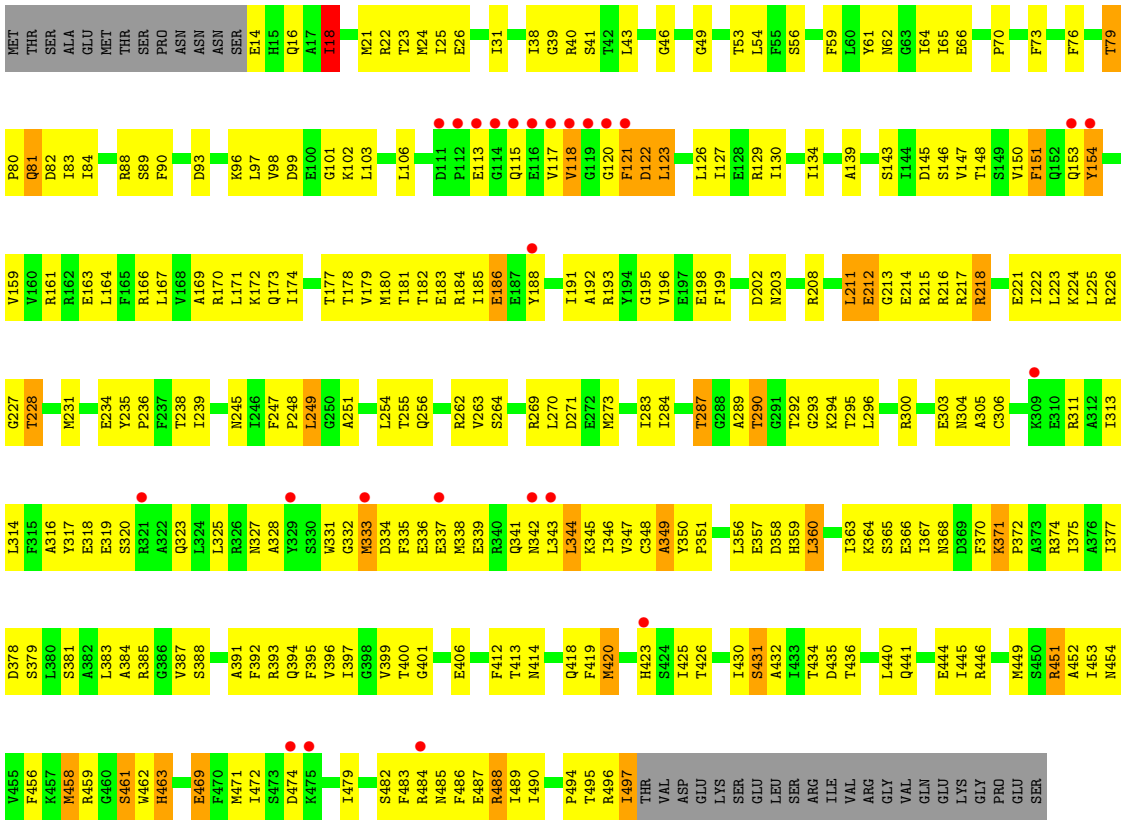
- Molecule 1: Circadian clock protein kinase kaiC

Chain D:



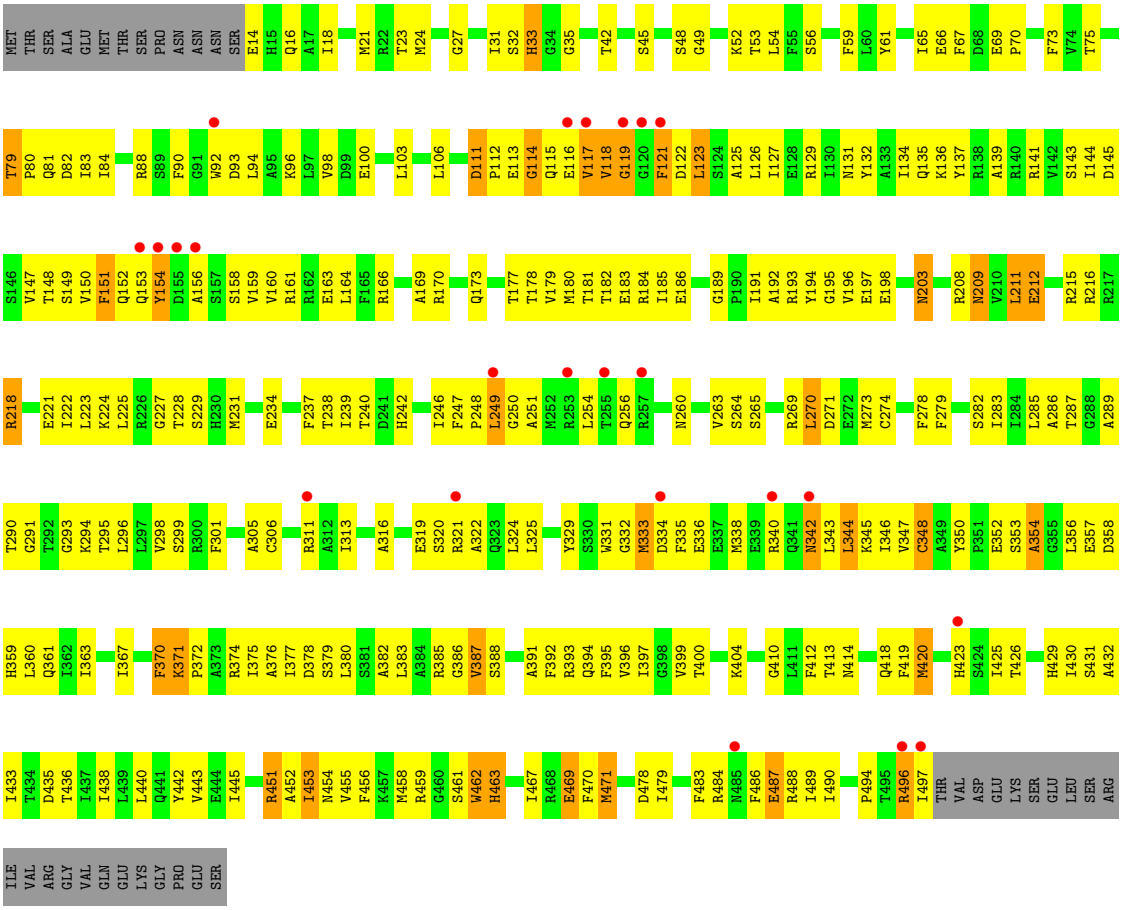
- Molecule 1: Circadian clock protein kinase kaiC

Chain E:



• Molecule 1: Circadian clock protein kinase kaiC

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.37Å 135.11Å 204.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.24 – 2.90 29.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (6.24-2.90) 91.2 (29.66-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.282 0.221 , 0.269	Depositor DCC
R_{free} test set	8295 reflections (9.56%)	wwPDB-VP
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23355	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: ATP, MG, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.40	0/3871	0.66	0/5215
1	B	0.38	0/3871	0.63	0/5215
1	C	0.42	0/3871	0.64	0/5215
1	D	0.47	0/3871	0.68	0/5215
1	E	0.47	0/3871	0.69	2/5215 (0.0%)
1	F	0.44	0/3871	0.67	0/5215
All	All	0.43	0/23226	0.66	2/31290 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	213	GLY	N-CA-C	-5.79	98.62	113.10
1	E	218	ARG	NE-CZ-NH2	-5.28	117.66	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	3817	0	3811	269	0
1	B	3817	0	3810	283	0
1	C	3817	0	3810	287	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3817	0	3811	273	0
1	E	3817	0	3809	288	0
1	F	3817	0	3809	300	0
2	A	62	0	24	5	0
2	B	62	0	24	6	0
2	C	62	0	24	2	0
2	D	62	0	24	6	0
2	E	62	0	24	9	0
2	F	62	0	23	11	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
4	A	7	0	0	2	0
4	B	5	0	0	0	0
4	C	7	0	0	2	0
4	D	12	0	0	0	0
4	E	13	0	0	4	0
4	F	19	0	0	6	0
All	All	23355	0	23003	1609	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (1609) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:VAL:HG12	1:E:374:ARG:HH21	0.99	1.13
1:B:311:ARG:HD2	1:B:371:LYS:HD2	1.29	1.12
1:F:191:ILE:HD12	1:F:198:GLU:HG2	1.35	1.08
1:A:311:ARG:HD2	1:A:371:LYS:HD2	1.34	1.07
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.37	1.05
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.38	1.02
1:A:379:SER:H	1:A:413:THR:HB	1.19	1.01
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.23	1.00
1:A:320:SER:HA	1:B:254:LEU:HG	1.42	0.99
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.28	0.99
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.45	0.98
1:E:263:VAL:HG12	1:E:374:ARG:NH2	1.79	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:LEU:HD13	1:E:166:ARG:HD2	1.43	0.97
1:E:18:ILE:H	1:E:18:ILE:HD13	1.26	0.97
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.28	0.96
1:A:311:ARG:HD2	1:A:371:LYS:CD	1.96	0.96
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.25	0.95
1:C:393:ARG:HH21	1:C:429:HIS:HB2	1.31	0.95
1:B:147:VAL:O	1:B:150:VAL:HG12	1.66	0.95
1:D:287:THR:HG23	1:D:414:ASN:HD22	1.31	0.95
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.50	0.93
1:B:262:ARG:HH22	1:B:461:SER:HB2	1.32	0.93
1:F:147:VAL:O	1:F:150:VAL:HG12	1.68	0.92
1:E:263:VAL:CG1	1:E:374:ARG:HH21	1.84	0.91
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.34	0.90
1:C:344:LEU:HD22	1:C:345:LYS:H	1.36	0.90
1:C:263:VAL:HG12	1:C:374:ARG:HH21	1.35	0.90
1:F:311:ARG:HD2	1:F:371:LYS:HE2	1.53	0.89
1:C:147:VAL:O	1:C:150:VAL:HG12	1.71	0.89
1:D:147:VAL:HG11	1:D:180:MET:HE3	1.53	0.89
1:A:18:ILE:HD12	1:A:227:GLY:HA3	1.54	0.89
1:C:488:ARG:HH22	1:D:488:ARG:HH21	1.18	0.88
1:E:123:LEU:HD22	1:E:127:ILE:HD11	1.55	0.88
1:F:283:ILE:CD1	1:F:400:THR:HG23	2.04	0.88
1:E:311:ARG:HD2	1:E:371:LYS:HD2	1.56	0.88
1:C:287:THR:HG21	1:C:425:ILE:O	1.73	0.88
1:A:436:THR:HG23	1:A:458:MET:HG2	1.56	0.87
1:A:396:VAL:HG11	1:A:430:ILE:CG2	2.04	0.87
1:C:325:LEU:HD23	1:C:335:PHE:HB2	1.56	0.87
1:C:488:ARG:NH2	1:D:488:ARG:HH21	1.70	0.87
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.04	0.87
1:D:191:ILE:HD12	1:D:198:GLU:HG2	1.56	0.87
1:E:18:ILE:HD13	1:E:18:ILE:N	1.89	0.87
1:C:469:GLU:HG3	1:C:480:LYS:HE3	1.53	0.86
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.74	0.86
1:B:393:ARG:HH21	1:B:429:HIS:HB2	1.39	0.86
1:C:287:THR:HG23	1:C:414:ASN:HD22	1.41	0.85
1:F:453:ILE:HD13	1:F:454:ASN:N	1.92	0.85
1:B:45:SER:HB3	1:B:182:THR:HB	1.57	0.84
1:B:263:VAL:HG12	1:B:374:ARG:NH2	1.92	0.84
1:F:263:VAL:HG12	1:F:374:ARG:NH2	1.92	0.84
1:A:396:VAL:HG11	1:A:430:ILE:HG21	1.60	0.84
1:F:191:ILE:HB	1:F:198:GLU:CG	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:HG21	1:A:425:ILE:O	1.78	0.84
1:A:147:VAL:HG11	1:A:180:MET:CE	2.08	0.83
1:E:79:THR:HG22	1:E:82:ASP:H	1.42	0.83
1:A:147:VAL:O	1:A:150:VAL:HG12	1.77	0.83
1:B:18:ILE:HB	1:B:228:THR:CG2	2.08	0.83
1:F:96:LYS:O	1:F:100:GLU:HG3	1.78	0.83
1:E:147:VAL:O	1:E:150:VAL:HG12	1.79	0.83
1:B:453:ILE:HD13	1:B:454:ASN:H	1.43	0.83
1:C:344:LEU:HD22	1:C:345:LYS:N	1.95	0.82
1:D:147:VAL:O	1:D:150:VAL:HG12	1.78	0.82
1:A:117:VAL:HA	1:A:154:TYR:OH	1.80	0.82
1:C:449:MET:HE3	1:D:467:ILE:HD11	1.60	0.82
1:B:311:ARG:HD2	1:B:371:LYS:CD	2.10	0.82
1:E:123:LEU:O	1:E:127:ILE:HG13	1.80	0.81
1:C:495:THR:HA	1:D:487:GLU:OE2	1.81	0.80
1:A:396:VAL:O	1:A:400:THR:HB	1.82	0.80
1:B:43:LEU:HD11	1:B:182:THR:OG1	1.82	0.80
1:E:262:ARG:HH22	1:E:461:SER:HB2	1.46	0.79
1:C:289:ALA:HB2	1:C:419:PHE:HA	1.64	0.79
1:F:283:ILE:HD13	1:F:400:THR:HG23	1.65	0.79
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.63	0.79
1:B:191:ILE:HD12	1:B:198:GLU:HG2	1.65	0.79
1:D:495:THR:HA	1:E:487:GLU:OE2	1.82	0.79
1:C:449:MET:CE	1:D:467:ILE:HD11	2.13	0.79
1:F:379:SER:H	1:F:413:THR:HB	1.46	0.79
1:A:263:VAL:HG12	1:A:374:ARG:NH2	1.98	0.79
1:B:148:THR:HA	1:B:151:PHE:HE1	1.48	0.79
1:A:257:ARG:NH2	1:A:407:GLU:HG2	1.97	0.78
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.65	0.78
1:D:287:THR:HG21	1:D:425:ILE:O	1.83	0.78
1:A:24:MET:CB	1:A:62:ASN:HD22	1.96	0.78
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.65	0.78
1:A:425:ILE:HB	1:A:431:SEP:O1P	1.84	0.78
1:B:262:ARG:NH2	1:B:461:SER:HB2	1.98	0.78
1:B:283:ILE:CD1	1:B:400:THR:HG23	2.13	0.78
1:A:436:THR:HG21	1:A:458:MET:HE3	1.66	0.78
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.63	0.77
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.66	0.77
1:E:379:SER:H	1:E:413:THR:HB	1.50	0.77
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.67	0.77
1:B:287:THR:HG21	1:B:425:ILE:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:HB	1:B:431:SEP:O1P	1.84	0.77
1:D:290:THR:HG22	2:D:901:ATP:O1G	1.84	0.77
1:C:14:GLU:HG3	1:C:16:GLN:H	1.48	0.77
1:D:311:ARG:HD2	1:D:371:LYS:CD	2.14	0.77
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.48	0.77
1:A:392:PHE:HE2	1:A:430:ILE:HD11	1.49	0.77
1:F:396:VAL:O	1:F:400:THR:HB	1.83	0.77
1:E:148:THR:OG1	1:E:182:THR:HG23	1.83	0.77
1:E:431:SEP:O	1:E:434:THR:HG22	1.84	0.77
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.97	0.76
1:E:18:ILE:H	1:E:18:ILE:CD1	1.99	0.76
1:F:184:ARG:HG2	1:F:191:ILE:O	1.86	0.76
1:B:449:MET:HE3	1:C:467:ILE:HD11	1.66	0.76
1:D:287:THR:CG2	1:D:414:ASN:HD22	1.98	0.76
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.68	0.76
1:F:79:THR:HG22	1:F:82:ASP:H	1.50	0.75
1:C:215:ARG:HA	1:C:215:ARG:NE	2.00	0.75
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.14	0.75
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.68	0.75
1:C:263:VAL:HG12	1:C:374:ARG:NH2	2.02	0.75
1:D:191:ILE:HB	1:D:198:GLU:CG	2.17	0.74
1:C:191:ILE:HB	1:C:198:GLU:HG2	1.67	0.74
1:F:489:ILE:HA	1:F:494:PRO:HG3	1.70	0.74
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.23	0.74
1:D:148:THR:CG2	1:D:193:ARG:HD2	2.18	0.74
1:E:446:ARG:HE	1:E:496:ARG:HH22	1.35	0.74
1:A:379:SER:N	1:A:413:THR:HB	2.01	0.74
1:F:287:THR:HG21	1:F:425:ILE:O	1.88	0.74
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.00	0.73
1:B:148:THR:HA	1:B:151:PHE:CE1	2.23	0.73
1:E:348:CYS:HB3	1:F:254:LEU:HD23	1.69	0.73
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.70	0.73
1:F:420:MET:HA	4:F:530:HOH:O	1.86	0.73
1:E:269:ARG:HB3	1:E:479:ILE:HD12	1.70	0.73
1:E:347:VAL:HG21	1:E:366:GLU:OE1	1.89	0.73
1:D:89:SER:HB2	1:E:227:GLY:O	1.88	0.73
1:A:191:ILE:HD12	1:A:198:GLU:HG2	1.71	0.73
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.70	0.73
1:A:316:ALA:O	1:A:348:CYS:HA	1.89	0.73
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.02	0.73
1:A:406:GLU:HB3	1:A:408:ILE:HG13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:THR:HA	4:C:523:HOH:O	1.89	0.72
1:E:320:SER:HA	1:F:254:LEU:HG	1.70	0.72
1:E:489:ILE:HA	1:E:494:PRO:HG3	1.71	0.72
1:F:21:MET:HE1	1:F:59:PHE:HZ	1.54	0.72
1:F:274:CYS:HG	1:F:278:PHE:HE2	1.35	0.72
1:B:451:ARG:HG2	1:B:451:ARG:NH1	1.98	0.72
1:C:396:VAL:HG11	1:C:430:ILE:HG23	1.70	0.72
1:F:185:ILE:HD11	1:F:193:ARG:NH1	2.04	0.72
1:E:311:ARG:HD2	1:E:371:LYS:CD	2.20	0.72
1:F:191:ILE:CD1	1:F:198:GLU:HG2	2.17	0.72
1:A:96:LYS:O	1:A:100:GLU:HG3	1.90	0.72
1:C:121:PHE:O	1:C:125:ALA:HB3	1.89	0.72
1:C:215:ARG:HA	1:C:215:ARG:HE	1.54	0.72
1:D:79:THR:HG22	1:D:82:ASP:H	1.54	0.72
1:A:211:LEU:O	1:A:212:GLU:HB3	1.88	0.72
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.70	0.71
1:B:191:ILE:HB	1:B:198:GLU:CG	2.19	0.71
1:E:159:VAL:O	1:E:163:GLU:HG2	1.89	0.71
1:F:363:ILE:O	1:F:367:ILE:HG13	1.91	0.71
1:B:89:SER:HB2	1:C:227:GLY:O	1.89	0.71
1:C:396:VAL:O	1:C:400:THR:HB	1.90	0.71
1:D:451:ARG:HG2	1:D:451:ARG:HH11	1.53	0.71
1:E:161:ARG:HB2	1:E:196:VAL:HG11	1.72	0.71
1:B:18:ILE:HB	1:B:228:THR:HG23	1.72	0.71
1:A:284:ILE:HB	1:A:411:LEU:HD12	1.71	0.71
1:D:311:ARG:HD2	1:D:371:LYS:HD2	1.71	0.71
1:A:150:VAL:HG13	1:A:151:PHE:N	2.04	0.71
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.56	0.71
1:B:169:ALA:O	1:B:173:GLN:HG3	1.90	0.71
1:E:487:GLU:O	1:E:488:ARG:HB2	1.90	0.71
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.72	0.70
1:D:148:THR:HG21	1:D:193:ARG:HD2	1.73	0.70
1:D:221:GLU:HG3	1:D:233:GLY:O	1.90	0.70
1:A:438:ILE:HG23	1:A:453:ILE:HD11	1.71	0.70
1:E:436:THR:HG23	1:E:458:MET:HG2	1.73	0.70
1:B:469:GLU:HB3	1:B:483:PHE:CZ	2.26	0.70
1:C:379:SER:H	1:C:413:THR:HB	1.56	0.70
1:C:311:ARG:HD2	1:C:371:LYS:CD	2.21	0.70
1:F:371:LYS:HE3	1:F:371:LYS:O	1.91	0.70
1:C:377:ILE:HD11	1:C:399:VAL:HG11	1.72	0.70
1:C:425:ILE:HD11	1:C:456:PHE:CE2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:THR:HG21	1:D:192:ALA:HB1	1.73	0.70
1:D:453:ILE:HG21	1:D:479:ILE:HG12	1.73	0.70
1:A:375:ILE:O	1:A:410:GLY:HA2	1.91	0.70
1:E:18:ILE:HG12	1:E:228:THR:HG23	1.72	0.69
1:D:85:LYS:NZ	1:E:14:GLU:HB3	2.07	0.69
1:E:356:LEU:HD13	1:E:387:VAL:HG21	1.74	0.69
1:E:123:LEU:HD12	1:E:163:GLU:OE2	1.93	0.69
1:F:377:ILE:CD1	1:F:399:VAL:HG11	2.22	0.69
1:A:448:GLU:HG2	1:B:466:ALA:HA	1.75	0.69
1:A:453:ILE:HD13	1:A:454:ASN:N	2.07	0.69
1:C:150:VAL:HG13	1:C:151:PHE:N	2.08	0.69
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.74	0.69
1:A:224:LYS:HE2	1:F:48:SER:OG	1.92	0.69
1:B:299:SER:HB3	1:B:333:MET:HE1	1.74	0.69
1:E:22:ARG:HD3	4:E:531:HOH:O	1.93	0.69
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.57	0.69
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.75	0.69
2:B:901:ATP:H3'	1:C:458:MET:O	1.93	0.69
1:C:191:ILE:HB	1:C:198:GLU:CG	2.23	0.69
1:F:21:MET:O	1:F:35:GLY:HA3	1.93	0.69
1:B:79:THR:HG22	1:B:82:ASP:OD2	1.93	0.69
1:F:24:MET:HG3	1:F:66:GLU:HG3	1.75	0.69
1:D:325:LEU:HD23	1:D:335:PHE:HB2	1.74	0.68
1:D:370:PHE:O	1:D:371:LYS:HD3	1.93	0.68
1:C:142:VAL:O	1:C:178:THR:HA	1.93	0.68
1:B:65:ILE:HG22	1:B:65:ILE:O	1.94	0.68
1:D:267:VAL:CG2	1:D:300:ARG:HG2	2.23	0.68
1:E:14:GLU:HG3	1:E:16:GLN:H	1.57	0.68
1:E:262:ARG:NH2	1:E:461:SER:HB2	2.09	0.68
1:D:161:ARG:HB2	1:D:196:VAL:HG11	1.74	0.68
1:D:263:VAL:HG12	1:D:374:ARG:NH2	2.09	0.68
1:F:247:PHE:HZ	1:F:361:GLN:HG3	1.58	0.68
1:C:325:LEU:HD23	1:C:335:PHE:CB	2.22	0.68
1:D:212:GLU:HG2	1:D:212:GLU:O	1.91	0.68
1:A:299:SER:HB3	1:A:333:MET:HE2	1.75	0.68
1:C:469:GLU:CG	1:C:480:LYS:HE3	2.24	0.68
1:B:448:GLU:HG2	1:C:466:ALA:HA	1.74	0.68
1:F:443:VAL:HG12	1:F:445:ILE:HG13	1.75	0.68
1:F:218:ARG:HD2	4:F:521:HOH:O	1.93	0.67
1:F:325:LEU:HD23	1:F:335:PHE:HB2	1.75	0.67
1:F:377:ILE:HD11	1:F:399:VAL:HG11	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ILE:O	1:B:367:ILE:HG13	1.94	0.67
1:C:221:GLU:HG3	1:C:233:GLY:O	1.93	0.67
1:D:446:ARG:H	1:D:496:ARG:HH12	1.40	0.67
1:A:79:THR:HG22	1:A:82:ASP:H	1.59	0.67
1:F:451:ARG:HG2	1:F:451:ARG:HH11	1.59	0.67
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.76	0.67
1:A:93:ASP:HA	4:A:525:HOH:O	1.93	0.67
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.25	0.67
1:A:393:ARG:HH21	1:A:429:HIS:HB2	1.58	0.67
1:B:453:ILE:HD13	1:B:454:ASN:N	2.09	0.67
1:E:215:ARG:HD3	4:E:528:HOH:O	1.94	0.67
1:F:440:LEU:CD2	1:F:453:ILE:HG12	2.25	0.67
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.08	0.67
1:C:79:THR:HG23	1:C:81:GLN:HG2	1.77	0.67
1:D:256:GLN:HG3	1:D:404:LYS:HD3	1.77	0.67
1:C:431:SEP:O	1:C:434:THR:HG22	1.94	0.67
1:E:40:ARG:HG2	1:E:172:LYS:HE3	1.76	0.67
1:C:363:ILE:O	1:C:367:ILE:HG13	1.94	0.67
1:D:79:THR:HG22	1:D:82:ASP:HB2	1.77	0.67
1:A:43:LEU:HD11	1:A:182:THR:OG1	1.94	0.67
1:B:214:GLU:HB3	1:C:234:GLU:HB2	1.75	0.67
1:C:443:VAL:HG12	1:C:445:ILE:HG13	1.77	0.67
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.94	0.66
1:A:430:ILE:HG23	1:A:433:ILE:HD12	1.76	0.66
1:D:335:PHE:HA	1:D:338:MET:HG3	1.76	0.66
1:E:115:GLN:OE1	1:E:118:VAL:HG21	1.95	0.66
1:A:347:VAL:HG21	1:A:366:GLU:OE1	1.94	0.66
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.60	0.66
1:C:299:SER:C	1:C:333:MET:HE1	2.15	0.66
1:D:114:GLY:O	1:D:115:GLN:HG3	1.96	0.66
1:D:363:ILE:O	1:D:367:ILE:HG13	1.96	0.66
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.31	0.66
1:C:191:ILE:HD12	1:C:198:GLU:HG2	1.78	0.66
1:A:21:MET:HE2	1:A:177:THR:HG21	1.77	0.66
1:F:295:THR:HG21	1:F:319:GLU:OE2	1.96	0.66
1:F:383:LEU:HD13	1:F:395:PHE:CE2	2.31	0.66
1:C:31:ILE:HG23	1:C:231:MET:HB2	1.78	0.66
1:A:363:ILE:O	1:A:367:ILE:HG13	1.96	0.66
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.77	0.65
1:C:317:TYR:HE1	1:C:377:ILE:HG23	1.60	0.65
1:E:393:ARG:O	1:E:397:ILE:HG12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:PHE:HD2	1:E:364:LYS:HZ2	1.45	0.65
1:E:344:LEU:HD11	1:E:346:ILE:HG13	1.79	0.65
1:A:182:THR:HG21	1:A:192:ALA:HB1	1.78	0.65
1:A:392:PHE:CE2	1:A:430:ILE:HD11	2.31	0.65
1:B:45:SER:CB	1:B:182:THR:HB	2.25	0.65
1:B:148:THR:HG21	1:B:193:ARG:HD2	1.78	0.65
1:C:202:ASP:HA	1:C:226:ARG:HD2	1.78	0.65
1:E:49:GLY:HA2	2:E:903:ATP:O2B	1.95	0.65
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.77	0.65
1:B:184:ARG:HG2	1:B:191:ILE:O	1.96	0.65
1:C:471:MET:HG3	1:C:478:ASP:HB3	1.77	0.65
1:E:191:ILE:HB	1:E:198:GLU:CG	2.26	0.65
1:B:123:LEU:O	1:B:127:ILE:HG13	1.96	0.65
1:C:183:GLU:HB2	1:D:199:PHE:CE1	2.31	0.65
1:A:266:GLY:HA3	1:A:300:ARG:O	1.95	0.65
1:C:24:MET:HG3	1:C:66:GLU:HG3	1.78	0.65
1:F:185:ILE:HD11	1:F:193:ARG:HH12	1.61	0.65
1:A:406:GLU:O	1:A:407:GLU:HB2	1.96	0.65
1:B:395:PHE:O	1:B:399:VAL:HG23	1.97	0.65
1:E:347:VAL:HG12	1:E:348:CYS:N	2.10	0.65
1:E:287:THR:HG23	1:E:414:ASN:HB3	1.78	0.65
1:F:122:ASP:OD2	1:F:123:LEU:N	2.30	0.65
1:B:211:LEU:O	1:B:212:GLU:HB3	1.97	0.65
1:B:178:THR:HG22	1:B:179:VAL:N	2.12	0.65
1:D:24:MET:HG3	1:D:66:GLU:HG3	1.79	0.65
1:A:254:LEU:HG	1:F:320:SER:HA	1.80	0.64
1:B:164:LEU:HD11	1:B:197:GLU:HG3	1.79	0.64
1:C:94:LEU:O	1:C:98:VAL:HG23	1.96	0.64
1:D:80:PRO:HD2	1:D:81:GLN:NE2	2.11	0.64
1:F:149:SER:HA	1:F:152:GLN:HB2	1.80	0.64
1:F:396:VAL:HG11	1:F:430:ILE:HG23	1.78	0.64
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.79	0.64
1:F:387:VAL:CG1	1:F:391:ALA:HB3	2.26	0.64
1:B:320:SER:HA	1:C:254:LEU:HG	1.78	0.64
1:D:441:GLN:HE22	1:D:490:ILE:HD13	1.62	0.64
1:A:311:ARG:CD	1:A:371:LYS:HD2	2.21	0.64
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.27	0.64
1:C:211:LEU:O	1:C:212:GLU:HB3	1.96	0.64
1:E:249:LEU:HD12	1:E:394:GLN:OE1	1.98	0.64
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.78	0.64
1:B:273:MET:O	1:B:463:HIS:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ILE:HG21	1:B:97:LEU:HD22	1.79	0.64
1:E:446:ARG:HE	1:E:496:ARG:NH2	1.96	0.64
1:A:18:ILE:CD1	1:A:227:GLY:HA3	2.28	0.64
1:A:191:ILE:HB	1:A:198:GLU:CG	2.27	0.64
1:D:488:ARG:HH12	1:E:488:ARG:HH21	1.44	0.64
1:A:396:VAL:HG21	1:A:430:ILE:HD13	1.80	0.64
1:B:56:SER:HB2	1:B:143:SER:HB3	1.79	0.64
1:B:358:ASP:O	1:B:362:ILE:HG13	1.98	0.64
1:E:316:ALA:O	1:E:348:CYS:HA	1.98	0.64
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.33	0.64
1:D:146:SER:H	1:D:181:THR:HG22	1.62	0.64
1:C:88:ARG:NE	1:D:15:HIS:HA	2.13	0.63
1:D:202:ASP:HA	1:D:226:ARG:HD2	1.81	0.63
1:B:21:MET:HE2	1:B:177:THR:HG21	1.81	0.63
1:B:208:ARG:O	1:B:218:ARG:HA	1.99	0.63
1:C:123:LEU:HD12	1:C:163:GLU:OE2	1.99	0.63
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.80	0.63
1:A:356:LEU:HD11	1:A:387:VAL:HG21	1.81	0.63
1:B:294:LYS:HG2	1:B:413:THR:HG23	1.80	0.63
1:C:311:ARG:HD2	1:C:371:LYS:HD2	1.78	0.63
1:A:14:GLU:HG3	1:A:16:GLN:OE1	1.99	0.63
1:A:486:PHE:HD2	1:A:494:PRO:HB2	1.62	0.63
1:D:151:PHE:C	1:D:153:GLN:H	2.02	0.63
1:C:147:VAL:HG11	1:C:180:MET:HE3	1.81	0.63
1:D:396:VAL:O	1:D:400:THR:HB	1.97	0.63
1:D:471:MET:HG3	1:D:478:ASP:HB3	1.79	0.63
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.80	0.63
1:F:299:SER:HB3	1:F:333:MET:HE2	1.81	0.63
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.79	0.63
1:A:254:LEU:HD23	1:F:348:CYS:HB3	1.81	0.63
1:A:283:ILE:CD1	1:A:400:THR:HG23	2.28	0.63
1:D:294:LYS:HG2	1:D:413:THR:HG23	1.80	0.63
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.64	0.63
1:A:440:LEU:HD23	1:A:453:ILE:HG12	1.81	0.62
1:D:96:LYS:O	1:D:100:GLU:HG3	1.99	0.62
1:D:492:GLY:O	1:D:494:PRO:HD3	1.99	0.62
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.34	0.62
1:A:264:SER:HA	1:A:271:ASP:OD1	1.99	0.62
1:E:169:ALA:O	1:E:173:GLN:HG3	2.00	0.62
1:F:106:LEU:HD11	1:F:129:ARG:CZ	2.29	0.62
1:F:169:ALA:O	1:F:173:GLN:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PHE:CE2	1:A:83:ILE:HD13	2.34	0.62
1:D:14:GLU:CD	1:D:15:HIS:H	2.03	0.62
1:C:316:ALA:O	1:C:348:CYS:HA	2.00	0.62
1:D:446:ARG:N	1:D:496:ARG:HH12	1.97	0.62
1:E:290:THR:HG22	2:E:901:ATP:O1G	2.00	0.62
1:C:203:ASN:HB3	1:C:225:LEU:HD23	1.81	0.62
1:E:150:VAL:HG13	1:E:151:PHE:N	2.14	0.62
1:F:156:ALA:O	1:F:160:VAL:HG23	2.00	0.62
1:F:231:MET:CE	1:F:251:ALA:HB2	2.30	0.62
1:B:56:SER:O	1:B:59:PHE:HB3	2.00	0.62
1:B:147:VAL:HG11	1:B:180:MET:CE	2.29	0.62
1:B:396:VAL:HG11	1:B:430:ILE:HG23	1.81	0.62
1:C:269:ARG:HG2	1:C:479:ILE:HB	1.81	0.62
1:C:453:ILE:HD13	1:C:454:ASN:N	2.14	0.62
1:F:27:GLY:HA3	1:F:246:ILE:HB	1.82	0.62
1:A:89:SER:HB2	1:B:227:GLY:O	2.00	0.62
1:D:269:ARG:HB3	1:D:479:ILE:HD12	1.81	0.62
1:E:79:THR:HG23	1:E:81:GLN:H	1.63	0.62
1:E:385:ARG:HA	1:F:393:ARG:HH12	1.65	0.62
1:F:21:MET:HE2	1:F:177:THR:HG21	1.82	0.62
1:A:18:ILE:HD13	1:A:40:ARG:NH1	2.15	0.61
1:B:130:ILE:O	1:B:134:ILE:HG13	2.01	0.61
1:C:18:ILE:HD12	1:C:227:GLY:HA3	1.82	0.61
1:D:150:VAL:HG13	1:D:151:PHE:N	2.15	0.61
1:B:316:ALA:O	1:B:348:CYS:HA	2.00	0.61
1:C:305:ALA:HB2	1:C:374:ARG:HD2	1.81	0.61
1:D:21:MET:HE1	1:D:177:THR:HB	1.81	0.61
1:D:367:ILE:HG12	1:D:375:ILE:HD11	1.80	0.61
1:F:119:GLY:HA2	1:F:122:ASP:OD1	2.00	0.61
1:B:299:SER:C	1:B:333:MET:HE1	2.21	0.61
1:C:335:PHE:HA	1:C:338:MET:HG3	1.81	0.61
1:E:41:SER:HB3	1:E:178:THR:HB	1.81	0.61
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.82	0.61
1:D:123:LEU:HD12	1:D:166:ARG:HD2	1.82	0.61
1:D:194:TYR:O	1:D:196:VAL:HG23	1.99	0.61
1:B:383:LEU:HD13	1:B:395:PHE:CE2	2.36	0.61
1:F:79:THR:CG2	1:F:81:GLN:HG2	2.31	0.61
1:D:191:ILE:HB	1:D:198:GLU:HG3	1.81	0.61
1:D:358:ASP:O	1:D:362:ILE:HG13	2.01	0.61
1:F:436:THR:OG1	1:F:458:MET:HG2	2.00	0.61
1:A:156:ALA:O	1:A:160:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLN:HB2	1:B:423:HIS:O	2.01	0.61
1:D:267:VAL:HG22	1:D:300:ARG:HG2	1.83	0.61
1:F:370:PHE:O	1:F:371:LYS:HG3	2.00	0.61
1:B:150:VAL:HG13	1:B:151:PHE:N	2.15	0.61
1:C:79:THR:HG22	1:C:82:ASP:OD2	2.00	0.61
1:F:497:ILE:C	1:F:497:ILE:HD12	2.21	0.61
1:F:191:ILE:HD12	1:F:198:GLU:CG	2.22	0.61
1:A:487:GLU:OE1	1:F:496:ARG:HG2	2.01	0.60
1:B:267:VAL:HG12	1:B:270:LEU:H	1.65	0.60
1:B:385:ARG:HG2	1:C:393:ARG:NH1	2.16	0.60
1:C:43:LEU:HD11	1:C:182:THR:OG1	2.01	0.60
1:B:280:LYS:HE2	1:B:407:GLU:O	2.01	0.60
1:D:49:GLY:O	1:D:218:ARG:NH2	2.35	0.60
1:C:182:THR:HG22	1:C:183:GLU:N	2.17	0.60
1:C:446:ARG:HG2	1:C:496:ARG:NH2	2.17	0.60
1:F:31:ILE:HG22	1:F:222:ILE:HD12	1.82	0.60
1:A:247:PHE:HD2	1:A:364:LYS:HZ2	1.49	0.60
1:A:436:THR:CG2	1:A:458:MET:HG2	2.30	0.60
1:D:79:THR:CG2	1:D:82:ASP:H	2.13	0.60
1:D:406:GLU:HB3	1:D:408:ILE:HG13	1.84	0.60
1:E:344:LEU:HD22	1:E:345:LYS:N	2.16	0.60
1:F:53:THR:HG23	1:F:145:ASP:OD1	2.01	0.60
1:F:111:ASP:OD1	1:F:112:PRO:HD2	2.01	0.60
1:A:21:MET:HE1	1:A:59:PHE:HZ	1.67	0.60
1:A:371:LYS:N	1:A:372:PRO:HD3	2.16	0.60
1:B:49:GLY:HA2	2:B:903:ATP:O2B	2.00	0.60
1:C:215:ARG:HE	1:C:215:ARG:CA	2.13	0.60
1:C:263:VAL:CG1	1:C:374:ARG:HH21	2.13	0.60
1:C:393:ARG:O	1:C:397:ILE:HG12	2.01	0.60
1:D:317:TYR:CE2	1:D:383:LEU:HD21	2.36	0.60
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.82	0.60
1:F:353:SER:O	1:F:354:ALA:HB2	2.00	0.60
1:B:379:SER:H	1:B:413:THR:HB	1.66	0.60
1:B:441:GLN:HE22	1:B:490:ILE:HD13	1.66	0.60
1:D:283:ILE:HD12	1:D:400:THR:HG23	1.81	0.60
1:F:311:ARG:CD	1:F:371:LYS:HE2	2.30	0.60
1:A:311:ARG:HA	1:A:343:LEU:O	2.02	0.60
1:B:449:MET:CE	1:C:467:ILE:HD11	2.31	0.60
1:E:218:ARG:HG3	4:E:529:HOH:O	2.02	0.60
1:D:21:MET:HE3	1:D:59:PHE:CZ	2.36	0.60
1:D:284:ILE:HD12	1:D:284:ILE:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.82	0.59
1:B:393:ARG:HH21	1:B:429:HIS:CB	2.13	0.59
1:F:291:GLY:HA3	1:F:442:TYR:OH	2.02	0.59
1:B:452:ALA:HA	1:B:469:GLU:HA	1.83	0.59
1:C:106:LEU:HD11	1:C:129:ARG:NH2	2.17	0.59
1:D:248:PRO:HB2	1:D:251:ALA:HB3	1.84	0.59
1:F:79:THR:HG23	1:F:81:GLN:HG2	1.85	0.59
1:A:461:SER:OG	1:A:462:TRP:N	2.35	0.59
1:E:148:THR:CG2	1:E:193:ARG:HD2	2.32	0.59
1:C:214:GLU:HB3	1:D:234:GLU:HB2	1.85	0.59
1:E:496:ARG:HG3	1:E:497:ILE:H	1.65	0.59
1:C:57:ILE:HD11	1:C:83:ILE:HG23	1.83	0.59
1:D:347:VAL:O	1:D:348:CYS:HB2	2.02	0.59
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.37	0.59
1:A:131:ASN:HD21	1:A:135:GLN:NE2	1.99	0.59
1:B:57:ILE:HD11	1:B:83:ILE:HG23	1.83	0.59
1:B:356:LEU:HD23	1:B:395:PHE:HB2	1.85	0.59
1:B:377:ILE:HD12	1:B:412:PHE:CE2	2.37	0.59
1:C:114:GLY:O	1:C:115:GLN:HB3	2.02	0.59
1:E:193:ARG:NH2	1:F:195:GLY:O	2.28	0.59
1:E:325:LEU:HD23	1:E:335:PHE:CB	2.32	0.59
1:E:79:THR:CG2	1:E:82:ASP:H	2.14	0.59
1:E:147:VAL:HG11	1:E:180:MET:HE2	1.83	0.59
1:F:150:VAL:HG13	1:F:151:PHE:N	2.18	0.59
1:F:393:ARG:O	1:F:397:ILE:HG12	2.03	0.59
1:D:73:PHE:CE2	1:D:83:ILE:HD13	2.38	0.59
1:F:67:PHE:HB2	1:F:69:GLU:HG3	1.84	0.59
1:F:70:PRO:HB2	1:F:139:ALA:HA	1.85	0.59
1:A:191:ILE:CD1	1:A:198:GLU:HG2	2.31	0.59
1:B:273:MET:CE	1:B:468:ARG:HD2	2.32	0.59
1:C:146:SER:H	1:C:181:THR:HB	1.68	0.59
1:C:367:ILE:HG12	1:C:375:ILE:HD11	1.83	0.59
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.84	0.58
1:B:294:LYS:N	2:B:901:ATP:O1B	2.36	0.58
1:C:79:THR:CG2	1:C:81:GLN:HG2	2.33	0.58
1:C:360:LEU:CD2	1:C:364:LYS:HE3	2.33	0.58
1:D:356:LEU:HD21	1:D:387:VAL:HG11	1.83	0.58
1:E:377:ILE:HD12	1:E:412:PHE:HE2	1.66	0.58
1:B:418:GLN:HB2	1:C:423:HIS:O	2.03	0.58
1:D:81:GLN:CD	1:D:81:GLN:H	2.05	0.58
1:D:392:PHE:CE2	1:D:430:ILE:HD11	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ARG:HG2	1:D:451:ARG:NH1	2.18	0.58
1:E:31:ILE:HG22	1:E:222:ILE:HD12	1.85	0.58
1:E:214:GLU:HB3	1:F:234:GLU:HB2	1.84	0.58
1:F:440:LEU:HD21	1:F:453:ILE:HG12	1.84	0.58
1:A:80:PRO:HD2	1:A:81:GLN:NE2	2.18	0.58
1:A:303:GLU:OE2	1:A:333:MET:HB3	2.02	0.58
1:C:273:MET:O	1:C:463:HIS:HA	2.02	0.58
1:C:358:ASP:O	1:C:362:ILE:HG13	2.04	0.58
1:E:485:ASN:HD22	1:E:496:ARG:HD3	1.67	0.58
1:A:445:ILE:HD11	1:A:483:PHE:CE2	2.39	0.58
1:C:265:SER:O	1:C:301:PHE:HA	2.03	0.58
1:D:182:THR:HG21	1:D:192:ALA:CB	2.32	0.58
1:E:191:ILE:HD12	1:E:198:GLU:HG2	1.84	0.58
1:B:283:ILE:HD13	1:B:400:THR:HG23	1.85	0.58
1:C:20:LYS:HE3	1:C:228:THR:HG21	1.85	0.58
1:C:325:LEU:CD2	1:C:335:PHE:HB2	2.31	0.58
1:E:449:MET:HE3	1:F:467:ILE:HD11	1.85	0.58
1:F:392:PHE:HE2	1:F:430:ILE:HD11	1.69	0.58
1:F:425:ILE:HG22	1:F:426:THR:HG23	1.85	0.58
1:B:146:SER:H	1:B:181:THR:HB	1.68	0.58
1:C:147:VAL:HG11	1:C:180:MET:CE	2.33	0.58
1:C:296:LEU:HD13	1:C:331:TRP:CD2	2.39	0.58
1:C:451:ARG:HH11	1:C:451:ARG:HG2	1.67	0.58
1:A:370:PHE:O	1:A:371:LYS:HD3	2.03	0.58
1:B:18:ILE:HB	1:B:228:THR:HG21	1.84	0.58
1:C:321:ARG:HG2	1:C:348:CYS:SG	2.43	0.58
1:F:321:ARG:O	1:F:325:LEU:HD12	2.03	0.58
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.86	0.58
1:F:218:ARG:HB3	4:F:533:HOH:O	2.03	0.58
1:A:191:ILE:HB	1:A:198:GLU:HG2	1.86	0.58
1:B:438:ILE:HG23	1:B:453:ILE:HD11	1.84	0.58
1:C:18:ILE:CD1	1:C:227:GLY:HA3	2.34	0.58
1:D:497:ILE:HD12	1:D:497:ILE:C	2.25	0.58
1:C:225:LEU:HD12	1:C:230:HIS:HB3	1.85	0.57
1:D:439:LEU:HD12	1:D:440:LEU:N	2.19	0.57
1:D:440:LEU:CD2	1:D:453:ILE:HG12	2.34	0.57
1:D:488:ARG:NH1	1:E:488:ARG:HH21	2.02	0.57
1:E:53:THR:HG23	1:E:145:ASP:OD1	2.04	0.57
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.68	0.57
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.85	0.57
1:F:182:THR:HG21	1:F:192:ALA:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:MET:CB	1:B:62:ASN:HD22	2.17	0.57
1:B:483:PHE:HB3	1:B:486:PHE:CD1	2.37	0.57
1:C:85:LYS:NZ	1:D:14:GLU:HB3	2.19	0.57
1:D:203:ASN:HB3	1:D:225:LEU:HD23	1.86	0.57
1:D:392:PHE:O	1:D:396:VAL:HG23	2.04	0.57
1:F:115:GLN:HG3	1:F:116:GLU:H	1.68	0.57
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.69	0.57
1:A:69:GLU:HB3	1:A:140:ARG:HB2	1.87	0.57
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.70	0.57
1:C:24:MET:CB	1:C:62:ASN:HD22	2.17	0.57
1:A:323:GLN:HG2	1:A:327:ASN:HD21	1.68	0.57
1:A:323:GLN:HG2	1:A:327:ASN:ND2	2.19	0.57
1:D:367:ILE:O	1:D:372:PRO:HD3	2.04	0.57
1:E:186:GLU:OE1	1:E:188:TYR:N	2.35	0.57
1:E:387:VAL:HG12	1:E:391:ALA:HB3	1.85	0.57
1:F:21:MET:HE1	1:F:59:PHE:CZ	2.37	0.57
1:D:364:LYS:O	1:D:367:ILE:HB	2.04	0.57
1:B:392:PHE:HE2	1:B:430:ILE:HD11	1.70	0.57
1:E:24:MET:HB2	1:E:62:ASN:HD22	1.68	0.57
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.35	0.57
1:E:496:ARG:HG3	1:E:497:ILE:N	2.19	0.57
1:B:316:ALA:HB3	1:B:348:CYS:SG	2.45	0.57
1:A:484:ARG:NH1	1:A:484:ARG:HB3	2.19	0.57
1:C:359:HIS:O	1:C:363:ILE:HG13	2.04	0.57
1:C:396:VAL:HG11	1:C:430:ILE:CG2	2.34	0.57
1:E:461:SER:OG	1:E:462:TRP:N	2.37	0.57
1:B:123:LEU:O	1:B:123:LEU:HD13	2.04	0.57
1:B:211:LEU:O	1:B:215:ARG:O	2.23	0.57
1:B:433:ILE:HG22	1:B:433:ILE:O	2.05	0.57
1:D:269:ARG:HG2	1:D:479:ILE:HB	1.85	0.57
1:D:316:ALA:O	1:D:348:CYS:HA	2.04	0.57
1:B:267:VAL:HG23	1:B:300:ARG:HG2	1.87	0.56
1:B:471:MET:HE3	1:B:473:SER:N	2.20	0.56
1:D:305:ALA:HB2	1:D:374:ARG:HD2	1.86	0.56
1:E:359:HIS:O	1:E:363:ILE:HG13	2.05	0.56
1:F:116:GLU:OE1	1:F:117:VAL:HG23	2.05	0.56
1:F:239:ILE:HB	4:F:531:HOH:O	2.04	0.56
1:A:150:VAL:CG1	1:A:151:PHE:N	2.67	0.56
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.87	0.56
1:A:377:ILE:HD11	1:A:399:VAL:HG11	1.86	0.56
1:A:451:ARG:NH1	1:A:472:ILE:HD12	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:THR:CG2	1:D:81:GLN:HG2	2.34	0.56
1:D:420:MET:HE2	1:D:492:GLY:HA3	1.87	0.56
1:F:14:GLU:HG2	4:F:537:HOH:O	2.04	0.56
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.70	0.56
1:B:50:THR:HG22	1:B:209:ASN:HB2	1.88	0.56
1:B:308:ASN:O	1:B:310:GLU:HG3	2.05	0.56
1:C:123:LEU:HD13	1:C:166:ARG:HD2	1.87	0.56
1:C:347:VAL:HG21	1:C:366:GLU:OE1	2.05	0.56
1:C:393:ARG:NH2	1:C:429:HIS:HB2	2.11	0.56
1:D:263:VAL:HG12	1:D:374:ARG:HH21	1.70	0.56
1:D:287:THR:HG23	1:D:414:ASN:ND2	2.13	0.56
1:D:425:ILE:HD11	1:D:456:PHE:CE2	2.41	0.56
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.36	0.56
1:F:115:GLN:HG3	1:F:116:GLU:N	2.20	0.56
1:F:396:VAL:HG11	1:F:430:ILE:CG2	2.36	0.56
1:A:147:VAL:HG11	1:A:180:MET:HE2	1.84	0.56
1:C:21:MET:HE2	1:C:177:THR:HG21	1.88	0.56
1:C:295:THR:HG23	1:C:378:ASP:OD2	2.05	0.56
1:D:193:ARG:NH2	1:E:195:GLY:O	2.32	0.56
1:E:148:THR:HG21	1:E:183:GLU:CG	2.36	0.56
1:F:122:ASP:O	1:F:126:LEU:N	2.30	0.56
1:A:396:VAL:HG11	1:A:430:ILE:HG23	1.84	0.56
1:B:164:LEU:O	1:B:168:VAL:HG23	2.05	0.56
1:C:148:THR:OG1	1:C:182:THR:HG23	2.06	0.56
1:C:187:GLU:O	1:C:208:ARG:HD3	2.06	0.56
1:F:49:GLY:HA2	2:F:903:ATP:O2B	2.06	0.56
1:A:130:ILE:O	1:A:134:ILE:HG13	2.05	0.56
1:F:115:GLN:CG	1:F:116:GLU:H	2.17	0.56
1:F:313:ILE:CD1	1:F:372:PRO:HG2	2.36	0.56
1:B:344:LEU:HD22	1:B:345:LYS:N	2.21	0.56
1:C:370:PHE:O	1:C:371:LYS:HD3	2.06	0.56
1:F:435:ASP:HA	1:F:459:ARG:HD2	1.86	0.56
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.88	0.56
1:A:471:MET:HG3	1:A:478:ASP:HB3	1.88	0.56
1:B:293:GLY:O	1:B:296:LEU:HB3	2.05	0.56
1:C:211:LEU:HD12	1:C:215:ARG:O	2.05	0.56
1:F:334:ASP:O	1:F:338:MET:HG2	2.06	0.56
1:A:21:MET:CE	1:A:59:PHE:HZ	2.18	0.56
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.88	0.56
1:A:364:LYS:HG2	1:A:402:TYR:CE2	2.41	0.56
1:B:123:LEU:HD12	1:B:166:ARG:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ILE:CD1	1:C:399:VAL:HG11	2.35	0.56
1:D:85:LYS:HZ3	1:E:14:GLU:HB3	1.69	0.56
1:E:311:ARG:HA	1:E:343:LEU:O	2.06	0.56
1:A:347:VAL:O	1:A:348:CYS:HB2	2.05	0.55
1:A:488:ARG:NE	1:F:488:ARG:HH12	2.05	0.55
1:C:150:VAL:CG1	1:C:151:PHE:N	2.69	0.55
1:D:161:ARG:HD2	1:D:196:VAL:HG13	1.88	0.55
1:F:357:GLU:HG3	1:F:358:ASP:N	2.21	0.55
1:B:62:ASN:O	1:B:66:GLU:HB2	2.06	0.55
1:D:483:PHE:HB2	1:D:489:ILE:HD13	1.88	0.55
1:E:148:THR:HG21	1:E:183:GLU:HG3	1.87	0.55
1:A:348:CYS:HB3	1:B:254:LEU:HD23	1.87	0.55
1:E:264:SER:O	1:E:374:ARG:NH2	2.40	0.55
1:E:313:ILE:CD1	1:E:372:PRO:HG2	2.36	0.55
1:A:70:PRO:HA	1:A:102:LYS:O	2.06	0.55
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.22	0.55
1:B:131:ASN:O	1:B:135:GLN:HG3	2.06	0.55
1:D:75:THR:HG23	1:D:75:THR:O	2.07	0.55
1:F:191:ILE:HB	1:F:198:GLU:CD	2.26	0.55
1:F:387:VAL:HG13	1:F:391:ALA:HB3	1.87	0.55
1:A:49:GLY:HA2	2:A:903:ATP:O2B	2.06	0.55
1:A:230:HIS:CD2	2:F:903:ATP:O2'	2.59	0.55
1:C:144:ILE:HG21	1:C:147:VAL:HG12	1.88	0.55
1:E:357:GLU:HG3	1:E:358:ASP:N	2.21	0.55
1:F:294:LYS:N	2:F:901:ATP:O1B	2.40	0.55
1:F:357:GLU:HG3	1:F:358:ASP:H	1.71	0.55
1:C:406:GLU:HB3	1:C:408:ILE:HG13	1.88	0.55
1:E:185:ILE:HD11	1:E:193:ARG:HH12	1.72	0.55
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.71	0.55
1:B:471:MET:HB3	1:B:480:LYS:NZ	2.21	0.55
1:C:85:LYS:HZ1	1:D:14:GLU:HB3	1.72	0.55
1:D:426:THR:OG1	1:D:431:SEP:O3P	2.23	0.55
1:A:87:ALA:O	1:A:92:TRP:HB2	2.06	0.55
1:B:340:ARG:C	1:B:342:ASN:H	2.10	0.55
1:C:267:VAL:HB	1:C:270:LEU:HB2	1.89	0.55
1:D:332:GLY:O	1:D:333:MET:O	2.25	0.55
1:F:249:LEU:HD12	1:F:394:GLN:CD	2.27	0.55
1:D:321:ARG:HG2	1:D:348:CYS:SG	2.47	0.55
1:D:393:ARG:O	1:D:397:ILE:HG12	2.06	0.55
2:E:901:ATP:H3'	1:F:458:MET:O	2.07	0.55
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.87	0.55
1:A:45:SER:HB3	1:A:182:THR:HB	1.89	0.55
1:B:393:ARG:NH2	1:B:429:HIS:HB2	2.17	0.55
1:A:184:ARG:HD3	4:A:524:HOH:O	2.08	0.54
1:A:220:LEU:C	1:A:220:LEU:HD23	2.27	0.54
1:B:150:VAL:O	1:B:153:GLN:HG3	2.06	0.54
1:C:311:ARG:HA	1:C:343:LEU:O	2.07	0.54
1:D:178:THR:HG22	1:D:179:VAL:N	2.22	0.54
1:D:221:GLU:HG3	1:D:233:GLY:C	2.26	0.54
1:F:79:THR:HG23	1:F:81:GLN:H	1.72	0.54
1:B:191:ILE:HB	1:B:198:GLU:HG3	1.88	0.54
1:C:360:LEU:HD21	1:C:364:LYS:HE3	1.90	0.54
1:F:191:ILE:HB	1:F:198:GLU:HG3	1.85	0.54
1:B:71:GLY:O	1:B:103:LEU:HD12	2.08	0.54
1:C:67:PHE:HB2	1:C:69:GLU:HG3	1.88	0.54
1:F:344:LEU:HD22	1:F:345:LYS:N	2.22	0.54
1:B:448:GLU:HG2	1:C:466:ALA:CA	2.37	0.54
1:C:41:SER:HA	1:C:178:THR:O	2.07	0.54
1:D:18:ILE:HD13	1:D:40:ARG:NH1	2.22	0.54
1:D:294:LYS:HB2	2:D:901:ATP:O1B	2.08	0.54
1:F:247:PHE:HZ	1:F:361:GLN:CG	2.19	0.54
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.71	0.54
1:B:377:ILE:HD12	1:B:412:PHE:HE2	1.71	0.54
1:B:437:ILE:CD1	1:B:457:LYS:HE2	2.37	0.54
1:C:146:SER:HA	1:C:181:THR:O	2.06	0.54
1:C:185:ILE:HD11	1:C:193:ARG:HH12	1.73	0.54
1:F:170:ARG:HD2	1:F:173:GLN:OE1	2.07	0.54
1:A:84:ILE:HG21	1:A:95:ALA:HB2	1.89	0.54
1:B:283:ILE:HD12	1:B:400:THR:HG23	1.90	0.54
1:C:334:ASP:O	1:C:338:MET:HG2	2.08	0.54
1:C:448:GLU:HG2	1:D:466:ALA:HA	1.90	0.54
1:D:379:SER:H	1:D:413:THR:HB	1.72	0.54
1:E:56:SER:HB2	1:E:143:SER:HB2	1.89	0.54
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.90	0.54
1:D:76:PHE:O	1:D:109:SER:HA	2.08	0.54
1:E:147:VAL:HG11	1:E:180:MET:CE	2.37	0.54
1:E:284:ILE:N	1:E:284:ILE:HD12	2.22	0.54
1:E:294:LYS:N	2:E:901:ATP:O1B	2.40	0.54
1:D:377:ILE:HD12	1:D:412:PHE:CE2	2.42	0.54
1:F:347:VAL:O	1:F:348:CYS:HB2	2.07	0.54
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:VAL:HG12	1:B:391:ALA:HB3	1.90	0.54
1:B:461:SER:OG	1:B:462:TRP:N	2.41	0.54
1:F:461:SER:OG	1:F:462:TRP:N	2.39	0.54
1:C:371:LYS:HD3	1:C:371:LYS:O	2.08	0.53
1:C:440:LEU:CD2	1:C:453:ILE:HG12	2.38	0.53
1:E:449:MET:HE3	1:F:490:ILE:HD11	1.90	0.53
1:A:357:GLU:HG3	1:A:358:ASP:N	2.24	0.53
1:D:356:LEU:CD2	1:D:387:VAL:HG11	2.37	0.53
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.89	0.53
1:E:381:SER:O	1:E:384:ALA:HB3	2.08	0.53
1:F:370:PHE:C	1:F:371:LYS:HG3	2.29	0.53
1:B:73:PHE:CE2	1:B:83:ILE:HD13	2.43	0.53
1:B:164:LEU:CD1	1:B:197:GLU:HG3	2.38	0.53
1:C:45:SER:HB2	1:C:182:THR:HB	1.90	0.53
1:E:150:VAL:CG1	1:E:151:PHE:N	2.71	0.53
1:E:306:CYS:SG	1:E:344:LEU:HB2	2.48	0.53
1:B:438:ILE:CG2	1:B:453:ILE:HD11	2.38	0.53
1:D:285:LEU:HD12	1:D:412:PHE:O	2.07	0.53
1:E:295:THR:HG21	1:E:319:GLU:OE2	2.07	0.53
1:F:131:ASN:HD21	1:F:135:GLN:NE2	2.05	0.53
1:F:144:ILE:CG2	1:F:147:VAL:HG12	2.39	0.53
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.43	0.53
1:A:186:GLU:HB3	1:A:189:GLY:HA3	1.90	0.53
1:A:344:LEU:HD22	1:A:345:LYS:N	2.24	0.53
1:C:247:PHE:HD2	1:C:364:LYS:HZ2	1.56	0.53
1:C:70:PRO:HA	1:C:102:LYS:O	2.08	0.53
1:C:116:GLU:O	1:C:117:VAL:HB	2.08	0.53
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.38	0.53
1:F:21:MET:HE3	1:F:59:PHE:CE1	2.44	0.53
1:A:364:LYS:HG2	1:A:402:TYR:CD2	2.43	0.53
1:A:436:THR:CG2	1:A:458:MET:HE3	2.38	0.53
1:C:23:THR:O	1:C:24:MET:HB2	2.08	0.53
1:C:45:SER:CB	1:C:182:THR:HB	2.39	0.53
1:F:248:PRO:O	1:F:250:GLY:N	2.42	0.53
1:A:256:GLN:O	1:F:322:ALA:HB3	2.09	0.53
1:A:387:VAL:HG12	1:A:391:ALA:HB3	1.89	0.53
1:A:440:LEU:CD2	1:A:453:ILE:HG12	2.39	0.53
1:B:57:ILE:HD11	1:B:83:ILE:CG2	2.38	0.53
1:B:455:VAL:HG11	1:B:463:HIS:HB2	1.90	0.53
1:C:462:TRP:O	1:C:463:HIS:O	2.27	0.53
1:D:150:VAL:O	1:D:153:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:VAL:HG23	1:D:300:ARG:HG2	1.90	0.53
1:D:447:GLY:HA2	1:E:489:ILE:HD12	1.90	0.53
1:E:89:SER:HB2	1:F:227:GLY:O	2.08	0.53
1:F:21:MET:CE	1:F:59:PHE:CZ	2.91	0.53
1:F:283:ILE:HD11	1:F:404:LYS:HG3	1.91	0.53
1:A:79:THR:HG23	1:A:81:GLN:HE21	1.73	0.53
1:D:317:TYR:CD2	1:D:383:LEU:HD21	2.43	0.53
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.91	0.53
1:C:81:GLN:CD	1:C:81:GLN:H	2.12	0.53
1:C:299:SER:O	1:C:333:MET:HE1	2.09	0.53
1:F:371:LYS:N	1:F:372:PRO:HD3	2.24	0.53
1:B:99:ASP:C	1:B:101:GLY:H	2.10	0.52
1:B:212:GLU:O	1:B:212:GLU:HG2	2.08	0.52
1:C:185:ILE:HD11	1:C:193:ARG:NH1	2.25	0.52
1:C:446:ARG:HG2	1:C:496:ARG:CZ	2.38	0.52
1:E:80:PRO:O	1:E:84:ILE:HG13	2.09	0.52
1:C:81:GLN:H	1:C:81:GLN:NE2	2.07	0.52
1:C:397:ILE:HD13	1:C:433:ILE:HD13	1.90	0.52
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.42	0.52
1:E:363:ILE:O	1:E:367:ILE:HG13	2.10	0.52
1:F:56:SER:HB2	1:F:143:SER:HB2	1.90	0.52
1:C:420:MET:HE2	1:C:492:GLY:HA3	1.91	0.52
1:E:123:LEU:CD1	1:E:166:ARG:HD2	2.29	0.52
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.91	0.52
1:A:80:PRO:HD2	1:A:81:GLN:HE21	1.73	0.52
1:A:451:ARG:HG2	1:A:451:ARG:NH1	2.24	0.52
1:C:159:VAL:O	1:C:163:GLU:HG2	2.09	0.52
1:E:81:GLN:H	1:E:81:GLN:CD	2.11	0.52
1:F:94:LEU:O	1:F:98:VAL:HG23	2.10	0.52
1:F:113:GLU:O	1:F:114:GLY:O	2.27	0.52
1:F:129:ARG:O	1:F:132:TYR:HB3	2.09	0.52
1:D:335:PHE:HA	1:D:338:MET:CG	2.40	0.52
1:E:367:ILE:HG12	1:E:375:ILE:HD11	1.90	0.52
1:F:382:ALA:O	1:F:385:ARG:HG3	2.09	0.52
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.75	0.52
1:D:392:PHE:HE2	1:D:430:ILE:HD11	1.74	0.52
1:E:21:MET:HE3	1:E:59:PHE:CE1	2.45	0.52
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.92	0.52
1:F:329:TYR:HA	1:F:332:GLY:O	2.10	0.52
1:F:425:ILE:HD11	1:F:456:PHE:CE2	2.44	0.52
1:B:85:LYS:HE3	1:C:17:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HG23	1:C:139:ALA:HB3	1.92	0.52
1:D:396:VAL:HG11	1:D:430:ILE:CG2	2.39	0.52
1:E:344:LEU:C	1:E:344:LEU:HD13	2.30	0.52
1:F:316:ALA:O	1:F:348:CYS:HA	2.10	0.52
1:F:393:ARG:HH21	1:F:429:HIS:HB2	1.74	0.52
1:B:117:VAL:HG12	1:B:117:VAL:O	2.10	0.52
1:B:492:GLY:C	1:B:494:PRO:HD3	2.30	0.52
1:C:122:ASP:O	1:C:123:LEU:C	2.47	0.52
1:C:215:ARG:NE	1:C:215:ARG:CA	2.70	0.52
1:C:392:PHE:CE2	1:C:430:ILE:HD11	2.45	0.52
1:C:469:GLU:HB3	1:C:483:PHE:CZ	2.44	0.52
1:A:359:HIS:O	1:A:363:ILE:HG13	2.10	0.52
1:A:382:ALA:O	1:A:385:ARG:HG3	2.10	0.52
1:B:170:ARG:O	1:B:174:ILE:HG13	2.10	0.52
1:D:130:ILE:O	1:D:134:ILE:HG13	2.09	0.52
1:E:365:SER:HA	1:E:368:ASN:HD22	1.75	0.52
1:B:18:ILE:CB	1:B:228:THR:HG23	2.40	0.52
1:B:370:PHE:O	1:B:371:LYS:HD3	2.10	0.52
1:B:451:ARG:HD2	1:B:451:ARG:N	2.25	0.52
2:B:901:ATP:O3'	1:C:457:LYS:HB2	2.09	0.52
1:D:488:ARG:HH12	1:E:488:ARG:NH2	2.08	0.52
1:E:293:GLY:HA2	2:E:901:ATP:O1A	2.10	0.52
1:F:21:MET:HG2	1:F:141:ARG:NH2	2.25	0.52
1:B:73:PHE:HE2	1:B:83:ILE:HD13	1.74	0.51
1:B:353:SER:O	1:B:354:ALA:HB2	2.10	0.51
1:C:111:ASP:OD2	1:C:113:GLU:HG2	2.09	0.51
1:C:356:LEU:CD2	1:C:387:VAL:HG11	2.40	0.51
1:D:143:SER:HA	1:D:179:VAL:O	2.10	0.51
1:D:347:VAL:HG21	1:D:366:GLU:OE1	2.10	0.51
1:E:335:PHE:O	1:E:339:GLU:HG3	2.10	0.51
1:F:340:ARG:C	1:F:342:ASN:H	2.13	0.51
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.75	0.51
1:C:127:ILE:HD13	1:C:170:ARG:HG3	1.92	0.51
1:F:23:THR:O	1:F:24:MET:HB2	2.10	0.51
1:F:264:SER:O	1:F:374:ARG:NH2	2.43	0.51
1:A:150:VAL:HG13	1:A:151:PHE:H	1.71	0.51
1:C:262:ARG:NH2	1:C:461:SER:HB2	2.25	0.51
1:E:81:GLN:CD	1:E:81:GLN:N	2.63	0.51
1:F:159:VAL:O	1:F:163:GLU:HG2	2.11	0.51
1:B:49:GLY:O	1:B:218:ARG:NH2	2.43	0.51
1:D:495:THR:O	1:D:495:THR:HG22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:GLN:CD	1:F:81:GLN:N	2.63	0.51
1:A:291:GLY:O	2:A:901:ATP:H4'	2.09	0.51
1:C:120:GLY:C	1:C:122:ASP:H	2.14	0.51
1:D:338:MET:HB3	1:D:344:LEU:HB3	1.93	0.51
1:D:375:ILE:O	1:D:410:GLY:HA2	2.10	0.51
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.92	0.51
1:F:73:PHE:CE2	1:F:83:ILE:HD13	2.44	0.51
1:B:85:LYS:HZ3	1:C:14:GLU:HB3	1.76	0.51
1:C:262:ARG:HH22	1:C:461:SER:HB2	1.76	0.51
1:D:303:GLU:OE2	1:D:333:MET:HB3	2.10	0.51
1:E:24:MET:CB	1:E:62:ASN:HD22	2.23	0.51
1:E:462:TRP:O	1:E:463:HIS:CD2	2.64	0.51
1:D:50:THR:HG22	1:D:209:ASN:HB2	1.91	0.51
1:D:354:ALA:HB3	1:D:359:HIS:CE1	2.45	0.51
1:D:471:MET:O	1:D:471:MET:HE2	2.10	0.51
1:D:487:GLU:OE1	1:D:497:ILE:HG21	2.11	0.51
1:E:14:GLU:HG3	1:E:16:GLN:HB2	1.92	0.51
1:E:444:GLU:HB2	1:E:449:MET:HE1	1.93	0.51
1:B:25:ILE:HG12	1:B:58:GLN:NE2	2.26	0.51
1:C:117:VAL:HG12	1:C:117:VAL:O	2.11	0.51
1:D:334:ASP:O	1:D:338:MET:HG2	2.11	0.51
1:D:344:LEU:HD22	1:D:345:LYS:N	2.25	0.51
1:D:469:GLU:HG3	1:D:480:LYS:HE3	1.93	0.51
1:F:357:GLU:CG	1:F:358:ASP:H	2.24	0.51
1:A:21:MET:CE	1:A:59:PHE:CZ	2.94	0.51
1:B:371:LYS:HD3	1:B:371:LYS:O	2.11	0.51
1:C:18:ILE:HB	1:C:228:THR:HG23	1.93	0.51
1:C:44:VAL:HG22	1:C:205:VAL:HB	1.92	0.51
1:C:64:ILE:CD1	1:C:103:LEU:HB2	2.40	0.51
1:A:152:GLN:NE2	1:A:193:ARG:HD3	2.25	0.51
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.93	0.51
1:B:449:MET:HE1	1:C:490:ILE:HD11	1.93	0.51
1:C:88:ARG:HG2	1:C:88:ARG:HH11	1.75	0.51
1:F:359:HIS:O	1:F:363:ILE:HG13	2.11	0.51
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.41	0.50
1:C:377:ILE:HD12	1:C:412:PHE:CE2	2.46	0.50
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.46	0.50
1:B:334:ASP:OD1	1:B:336:GLU:HB2	2.11	0.50
1:F:123:LEU:HD12	1:F:166:ARG:HD2	1.92	0.50
1:F:486:PHE:CE2	1:F:496:ARG:HD2	2.46	0.50
1:B:150:VAL:CG1	1:B:151:PHE:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ILE:CG2	1:C:147:VAL:HG12	2.41	0.50
1:D:431:SEP:O	1:D:434:THR:HG22	2.11	0.50
1:E:371:LYS:O	1:E:371:LYS:HD3	2.11	0.50
1:E:396:VAL:O	1:E:400:THR:HB	2.11	0.50
1:B:367:ILE:HG12	1:B:375:ILE:HD11	1.92	0.50
1:E:357:GLU:HG3	1:E:358:ASP:H	1.76	0.50
1:F:451:ARG:HD2	1:F:451:ARG:N	2.26	0.50
1:B:392:PHE:CE2	1:B:430:ILE:HD11	2.46	0.50
1:B:487:GLU:O	1:B:488:ARG:HB2	2.12	0.50
1:D:412:PHE:CD1	1:D:412:PHE:N	2.79	0.50
1:E:73:PHE:CE2	1:E:83:ILE:HD13	2.46	0.50
1:A:21:MET:HE3	1:A:59:PHE:CE1	2.47	0.50
1:A:334:ASP:OD1	1:A:336:GLU:HB2	2.12	0.50
1:C:151:PHE:C	1:C:153:GLN:H	2.12	0.50
1:C:387:VAL:HG13	1:C:391:ALA:HB3	1.93	0.50
1:E:41:SER:CB	1:E:178:THR:HB	2.41	0.50
1:E:385:ARG:HA	1:F:393:ARG:NH1	2.25	0.50
1:B:159:VAL:O	1:B:163:GLU:HG2	2.11	0.50
1:B:371:LYS:N	1:B:372:PRO:HD3	2.27	0.50
1:E:143:SER:HA	1:E:179:VAL:O	2.11	0.50
1:A:471:MET:HE2	1:A:478:ASP:HB3	1.92	0.50
1:B:129:ARG:O	1:B:132:TYR:HB3	2.12	0.50
1:B:178:THR:CG2	1:B:179:VAL:N	2.75	0.50
1:C:96:LYS:O	1:C:100:GLU:HG3	2.12	0.50
1:D:284:ILE:HD12	1:D:284:ILE:N	2.26	0.50
1:D:294:LYS:N	2:D:901:ATP:O1B	2.42	0.50
1:D:320:SER:HA	1:E:254:LEU:HG	1.94	0.50
1:F:400:THR:HG21	1:F:433:ILE:CG2	2.42	0.50
1:C:150:VAL:CG1	1:C:151:PHE:H	2.25	0.50
1:D:451:ARG:HB3	1:D:470:PHE:CE2	2.47	0.50
1:A:150:VAL:CG1	1:A:151:PHE:H	2.24	0.49
1:B:462:TRP:O	1:B:463:HIS:O	2.29	0.49
1:B:497:ILE:HD12	1:B:497:ILE:C	2.32	0.49
1:C:385:ARG:HA	1:D:393:ARG:HH12	1.76	0.49
1:F:293:GLY:HA2	2:F:901:ATP:O1A	2.12	0.49
1:D:283:ILE:CD1	1:D:400:THR:HG23	2.43	0.49
1:D:468:ARG:HG2	1:D:468:ARG:HH11	1.77	0.49
1:D:495:THR:HG23	1:E:487:GLU:OE2	2.13	0.49
1:E:444:GLU:OE1	1:F:490:ILE:HG12	2.12	0.49
1:A:56:SER:HB2	1:A:143:SER:HB2	1.94	0.49
1:B:84:ILE:HG23	1:B:94:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:LEU:HD21	1:C:387:VAL:HG11	1.94	0.49
1:F:123:LEU:O	1:F:127:ILE:HG13	2.12	0.49
1:F:285:LEU:HD12	1:F:286:ALA:N	2.26	0.49
1:A:131:ASN:ND2	1:A:135:GLN:NE2	2.59	0.49
1:A:451:ARG:HD2	1:A:451:ARG:N	2.28	0.49
1:B:430:ILE:O	1:B:433:ILE:HB	2.12	0.49
1:C:191:ILE:HD13	1:C:223:LEU:HD12	1.95	0.49
1:D:182:THR:HG22	1:D:183:GLU:N	2.26	0.49
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.95	0.49
1:F:49:GLY:CA	2:F:903:ATP:O2B	2.60	0.49
1:F:231:MET:HE3	1:F:251:ALA:HB2	1.94	0.49
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.92	0.49
1:B:127:ILE:HG22	1:B:127:ILE:O	2.13	0.49
1:B:145:ASP:HA	1:B:181:THR:HB	1.93	0.49
1:C:184:ARG:HG2	1:C:191:ILE:O	2.12	0.49
1:C:488:ARG:HH22	1:D:488:ARG:NH2	1.98	0.49
1:D:64:ILE:CD1	1:D:103:LEU:HB2	2.42	0.49
1:D:279:PHE:HB2	1:D:282:SER:HB3	1.94	0.49
1:D:311:ARG:HD2	1:D:371:LYS:HD3	1.94	0.49
1:D:371:LYS:HD3	1:D:371:LYS:O	2.13	0.49
1:D:486:PHE:CE2	1:D:496:ARG:HB3	2.47	0.49
1:E:452:ALA:HA	1:E:469:GLU:HA	1.93	0.49
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.77	0.49
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.42	0.49
1:E:318:GLU:OE2	1:F:432:ALA:HB1	2.12	0.49
1:F:52:LYS:N	2:F:903:ATP:O1B	2.43	0.49
1:F:144:ILE:HG22	1:F:147:VAL:HG12	1.95	0.49
1:A:127:ILE:HD13	1:A:170:ARG:HG3	1.95	0.49
1:A:230:HIS:NE2	2:F:903:ATP:O2'	2.45	0.49
1:C:214:GLU:O	1:C:215:ARG:NH2	2.42	0.49
1:D:79:THR:HG22	1:D:82:ASP:CB	2.42	0.49
1:E:46:GLY:HA2	1:E:184:ARG:HD3	1.94	0.49
1:E:484:ARG:NH1	1:E:484:ARG:HB3	2.26	0.49
1:A:211:LEU:O	1:A:212:GLU:CB	2.61	0.49
1:A:285:LEU:HA	1:A:412:PHE:O	2.13	0.49
1:C:301:PHE:O	1:C:374:ARG:NH1	2.46	0.49
1:C:325:LEU:CD2	1:C:335:PHE:CB	2.90	0.49
1:F:21:MET:CE	1:F:59:PHE:HZ	2.22	0.49
1:F:131:ASN:ND2	1:F:135:GLN:NE2	2.60	0.49
1:F:336:GLU:HB3	1:F:340:ARG:NH2	2.28	0.49
1:B:211:LEU:HA	1:B:216:ARG:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ASN:OD1	1:D:225:LEU:HA	2.13	0.49
1:A:338:MET:HB3	1:A:344:LEU:HB3	1.95	0.49
1:C:337:GLU:OE1	1:C:340:ARG:NH1	2.45	0.49
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.47	0.49
1:E:292:THR:HB	1:E:440:LEU:HB3	1.94	0.49
1:F:240:THR:C	1:F:242:HIS:H	2.15	0.49
1:F:486:PHE:HE2	1:F:496:ARG:CD	2.25	0.49
1:D:64:ILE:HD11	1:D:103:LEU:HB2	1.94	0.48
1:D:79:THR:HG23	1:D:81:GLN:HG2	1.95	0.48
1:D:151:PHE:C	1:D:153:GLN:N	2.67	0.48
1:E:170:ARG:O	1:E:174:ILE:HG13	2.13	0.48
1:F:453:ILE:HD13	1:F:454:ASN:H	1.75	0.48
1:A:273:MET:O	1:A:464:ASP:N	2.38	0.48
1:C:150:VAL:O	1:C:153:GLN:HG3	2.13	0.48
1:C:392:PHE:HE2	1:C:430:ILE:HD11	1.79	0.48
1:C:419:PHE:O	1:C:420:MET:HB2	2.13	0.48
1:E:43:LEU:HD11	1:E:182:THR:OG1	2.13	0.48
1:E:348:CYS:O	1:E:349:ALA:HB2	2.14	0.48
1:F:484:ARG:HB3	1:F:484:ARG:NH1	2.28	0.48
1:D:269:ARG:NH1	1:D:269:ARG:HG3	2.27	0.48
1:D:299:SER:HB3	1:D:333:MET:HE1	1.95	0.48
1:D:340:ARG:C	1:D:342:ASN:H	2.16	0.48
1:E:396:VAL:HG11	1:E:430:ILE:CG2	2.44	0.48
1:E:425:ILE:HD11	1:E:456:PHE:CE2	2.48	0.48
1:F:194:TYR:O	1:F:196:VAL:HG23	2.13	0.48
1:F:311:ARG:HA	1:F:343:LEU:O	2.11	0.48
1:B:65:ILE:O	1:B:65:ILE:CG2	2.60	0.48
1:B:194:TYR:O	1:B:196:VAL:HG23	2.14	0.48
1:B:425:ILE:HD11	1:B:456:PHE:CE2	2.48	0.48
1:B:451:ARG:NH1	1:B:451:ARG:CG	2.67	0.48
1:D:98:VAL:HA	1:D:103:LEU:O	2.13	0.48
1:F:154:TYR:HD1	1:F:154:TYR:O	1.97	0.48
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.43	0.48
1:A:269:ARG:HG2	1:A:479:ILE:HB	1.95	0.48
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.46	0.48
1:B:441:GLN:NE2	1:B:490:ILE:HD13	2.28	0.48
1:C:214:GLU:C	1:C:215:ARG:HE	2.17	0.48
1:D:182:THR:CG2	1:D:183:GLU:N	2.75	0.48
1:E:248:PRO:HB2	1:E:251:ALA:CB	2.43	0.48
1:E:295:THR:HG23	1:E:378:ASP:OD2	2.13	0.48
1:A:45:SER:CB	1:A:182:THR:HB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:HG23	1:A:81:GLN:H	1.77	0.48
1:A:283:ILE:HD11	1:A:400:THR:HG23	1.93	0.48
1:A:316:ALA:HB3	1:A:348:CYS:SG	2.54	0.48
1:C:400:THR:HG22	1:C:401:GLY:N	2.28	0.48
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.29	0.48
1:F:118:VAL:HG12	1:F:153:GLN:HE22	1.78	0.48
1:F:484:ARG:HB3	1:F:484:ARG:HH11	1.78	0.48
1:A:131:ASN:HD21	1:A:135:GLN:HE22	1.61	0.48
1:B:90:PHE:HB2	1:B:92:TRP:NE1	2.29	0.48
1:B:430:ILE:O	1:B:433:ILE:N	2.36	0.48
1:D:74:VAL:HG22	1:D:106:LEU:HD23	1.96	0.48
1:D:483:PHE:HB2	1:D:489:ILE:CD1	2.44	0.48
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.47	0.48
1:B:354:ALA:HB1	1:B:358:ASP:HB2	1.96	0.48
1:B:492:GLY:O	1:B:494:PRO:HD3	2.14	0.48
1:C:54:LEU:HD13	1:C:90:PHE:CZ	2.49	0.48
1:E:53:THR:HG1	2:E:903:ATP:PG	2.37	0.48
1:E:392:PHE:HE2	1:E:430:ILE:HD11	1.78	0.48
1:B:446:ARG:HE	1:B:496:ARG:HH12	1.61	0.48
1:C:311:ARG:HB3	1:C:370:PHE:CE2	2.49	0.48
1:E:334:ASP:OD1	1:E:336:GLU:HB2	2.14	0.48
1:F:247:PHE:CZ	1:F:361:GLN:HG3	2.44	0.48
1:C:248:PRO:HB2	1:C:251:ALA:HB3	1.96	0.48
1:C:348:CYS:O	1:C:349:ALA:HB2	2.13	0.48
1:C:418:GLN:HB2	1:D:423:HIS:O	2.13	0.48
1:E:88:ARG:HH11	1:E:88:ARG:HG2	1.79	0.48
1:E:364:LYS:O	1:E:368:ASN:ND2	2.47	0.48
1:A:142:VAL:O	1:A:178:THR:HA	2.14	0.47
1:B:267:VAL:CG1	1:B:270:LEU:HB2	2.44	0.47
1:B:347:VAL:O	1:B:348:CYS:HB2	2.14	0.47
1:B:441:GLN:HE22	1:B:490:ILE:HA	1.79	0.47
1:E:287:THR:HG21	1:E:425:ILE:O	2.14	0.47
1:F:144:ILE:HB	1:F:180:MET:HG2	1.95	0.47
1:B:54:LEU:CD2	1:B:244:ILE:HG13	2.44	0.47
1:C:387:VAL:CG1	1:C:391:ALA:HB3	2.44	0.47
1:C:440:LEU:HD21	1:C:453:ILE:HG12	1.96	0.47
1:E:247:PHE:HD2	1:E:364:LYS:NZ	2.10	0.47
1:E:334:ASP:OD1	1:E:336:GLU:N	2.47	0.47
1:F:134:ILE:HA	1:F:139:ALA:HB3	1.97	0.47
1:B:93:ASP:OD2	1:B:96:LYS:HB2	2.14	0.47
1:C:80:PRO:O	1:C:84:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ILE:HG22	1:C:426:THR:HG23	1.95	0.47
1:D:249:LEU:HD12	1:D:394:GLN:OE1	2.14	0.47
1:F:313:ILE:HD11	1:F:372:PRO:HG2	1.96	0.47
1:C:24:MET:HB2	1:C:62:ASN:HD22	1.77	0.47
1:C:150:VAL:HG13	1:C:151:PHE:H	1.75	0.47
1:D:90:PHE:HA	1:D:241:ASP:O	2.15	0.47
1:A:64:ILE:HG21	1:A:97:LEU:HD22	1.95	0.47
1:A:458:MET:O	2:F:901:ATP:H3'	2.14	0.47
1:B:216:ARG:NE	1:C:221:GLU:OE1	2.32	0.47
1:C:352:GLU:OE2	1:C:385:ARG:HD2	2.15	0.47
1:D:131:ASN:OD1	1:D:174:ILE:HD13	2.14	0.47
1:D:393:ARG:HH21	1:D:429:HIS:HB2	1.79	0.47
1:F:340:ARG:C	1:F:342:ASN:N	2.68	0.47
1:A:21:MET:HE3	1:A:59:PHE:CZ	2.49	0.47
1:A:169:ALA:O	1:A:173:GLN:HG3	2.15	0.47
1:A:299:SER:O	1:A:333:MET:HE1	2.14	0.47
1:B:440:LEU:CD2	1:B:453:ILE:HG12	2.44	0.47
1:C:264:SER:O	1:C:374:ARG:NH2	2.47	0.47
1:D:191:ILE:HD12	1:D:198:GLU:CG	2.37	0.47
1:D:215:ARG:NH2	1:E:234:GLU:O	2.47	0.47
1:D:486:PHE:CE2	1:D:496:ARG:HD3	2.50	0.47
1:A:24:MET:HB2	1:A:62:ASN:ND2	2.15	0.47
1:A:73:PHE:HE2	1:A:83:ILE:HD13	1.78	0.47
1:A:211:LEU:HD13	1:A:216:ARG:NE	2.29	0.47
1:A:224:LYS:HB2	2:F:903:ATP:H3'	1.97	0.47
1:B:182:THR:HG21	1:B:192:ALA:CB	2.43	0.47
1:B:182:THR:HG22	1:B:183:GLU:N	2.30	0.47
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.97	0.47
1:C:76:PHE:O	1:C:109:SER:HA	2.15	0.47
1:C:357:GLU:HG3	1:C:358:ASP:N	2.30	0.47
1:D:268:VAL:O	1:D:271:ASP:HB2	2.15	0.47
1:E:99:ASP:C	1:E:101:GLY:H	2.18	0.47
1:F:61:TYR:CE2	1:F:65:ILE:HG13	2.49	0.47
1:F:117:VAL:HA	1:F:154:TYR:OH	2.14	0.47
1:F:238:THR:HG22	1:F:239:ILE:N	2.29	0.47
1:F:357:GLU:CG	1:F:358:ASP:N	2.78	0.47
1:F:387:VAL:HG12	1:F:388:SER:O	2.14	0.47
1:A:308:ASN:O	1:A:310:GLU:HG3	2.15	0.47
1:B:191:ILE:HD12	1:B:198:GLU:CG	2.42	0.47
1:C:148:THR:CG2	1:C:193:ARG:HD2	2.45	0.47
1:E:24:MET:HG3	1:E:66:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ASP:HA	1:B:459:ARG:HD2	1.97	0.47
1:C:248:PRO:O	1:C:250:GLY:N	2.48	0.47
1:E:357:GLU:CD	4:E:529:HOH:O	2.53	0.47
1:E:383:LEU:HD13	1:E:395:PHE:CE2	2.50	0.47
1:F:178:THR:HG22	1:F:179:VAL:N	2.30	0.47
1:C:315:PHE:CZ	1:C:363:ILE:HG23	2.50	0.47
1:D:462:TRP:O	1:D:463:HIS:CG	2.68	0.47
1:E:148:THR:HG21	1:E:193:ARG:HD2	1.97	0.47
1:F:203:ASN:CB	1:F:225:LEU:HD23	2.26	0.47
1:A:311:ARG:HD2	1:A:371:LYS:HD3	1.93	0.46
1:C:471:MET:CG	1:C:478:ASP:HB3	2.42	0.46
1:D:40:ARG:HG2	1:D:172:LYS:HE3	1.97	0.46
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.97	0.46
1:E:392:PHE:O	1:E:395:PHE:HB3	2.15	0.46
1:F:238:THR:HB	1:F:361:GLN:HE22	1.80	0.46
1:F:264:SER:HA	1:F:271:ASP:OD1	2.15	0.46
1:A:447:GLY:HA2	1:B:489:ILE:HD12	1.97	0.46
1:B:81:GLN:H	1:B:81:GLN:NE2	2.12	0.46
1:B:98:VAL:HA	1:B:103:LEU:O	2.14	0.46
1:B:262:ARG:HH22	1:B:461:SER:CB	2.17	0.46
1:D:451:ARG:HD2	1:D:451:ARG:N	2.30	0.46
1:E:23:THR:O	1:E:24:MET:HB2	2.14	0.46
1:E:323:GLN:HG2	1:E:327:ASN:HD21	1.78	0.46
1:A:344:LEU:HD22	1:A:345:LYS:H	1.79	0.46
1:A:390:ASN:OD1	1:F:386:GLY:HA2	2.15	0.46
1:B:104:PHE:HD2	1:B:133:ALA:HB1	1.80	0.46
1:B:161:ARG:HD2	1:B:196:VAL:HG13	1.98	0.46
1:C:62:ASN:O	1:C:66:GLU:HB2	2.16	0.46
1:D:184:ARG:HG2	1:D:191:ILE:O	2.15	0.46
1:E:61:TYR:CE2	1:E:65:ILE:HG13	2.50	0.46
1:E:371:LYS:N	1:E:372:PRO:HD3	2.31	0.46
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.27	0.46
1:F:378:ASP:OD1	1:F:413:THR:HG21	2.15	0.46
1:A:267:VAL:HG22	1:A:300:ARG:HG2	1.97	0.46
1:A:291:GLY:N	2:A:901:ATP:O2B	2.49	0.46
1:B:85:LYS:NZ	1:C:16:GLN:O	2.45	0.46
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.97	0.46
1:C:182:THR:HG21	1:C:192:ALA:HB1	1.97	0.46
1:D:127:ILE:HD11	1:D:167:LEU:HA	1.97	0.46
1:F:18:ILE:HG13	1:F:227:GLY:HA3	1.97	0.46
1:F:451:ARG:HB3	1:F:470:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:THR:HG21	1:D:81:GLN:HG2	1.97	0.46
1:D:256:GLN:N	1:D:256:GLN:OE1	2.48	0.46
1:F:248:PRO:HB2	1:F:251:ALA:CB	2.46	0.46
1:A:264:SER:HB3	1:A:304:ASN:ND2	2.30	0.46
1:B:264:SER:HB3	1:B:304:ASN:HD21	1.81	0.46
1:C:273:MET:CE	1:C:468:ARG:HD2	2.46	0.46
1:D:255:THR:HG22	1:D:255:THR:O	2.16	0.46
1:D:370:PHE:O	1:D:371:LYS:CD	2.63	0.46
1:D:440:LEU:HD21	1:D:453:ILE:HG12	1.98	0.46
1:E:287:THR:CG2	1:E:414:ASN:HD22	2.28	0.46
1:A:16:GLN:O	1:A:17:ALA:O	2.33	0.46
1:A:65:ILE:HG22	1:A:65:ILE:O	2.15	0.46
1:A:220:LEU:HD23	1:A:221:GLU:N	2.31	0.46
1:C:111:ASP:C	1:C:113:GLU:H	2.19	0.46
1:D:325:LEU:HD23	1:D:335:PHE:CB	2.43	0.46
1:D:387:VAL:HG12	1:D:388:SER:O	2.16	0.46
1:F:356:LEU:CD1	1:F:387:VAL:HG21	2.45	0.46
1:F:451:ARG:HG2	1:F:451:ARG:NH1	2.29	0.46
1:A:273:MET:O	1:A:463:HIS:HA	2.15	0.46
1:B:85:LYS:NZ	1:C:14:GLU:HB3	2.31	0.46
1:B:178:THR:HG22	1:B:179:VAL:H	1.81	0.46
1:C:334:ASP:OD1	1:C:336:GLU:HB2	2.15	0.46
1:F:42:THR:HG23	1:F:203:ASN:HB2	1.97	0.46
1:F:94:LEU:HB3	1:F:103:LEU:CD2	2.46	0.46
1:F:150:VAL:O	1:F:153:GLN:HG3	2.16	0.46
1:F:265:SER:O	1:F:301:PHE:HA	2.15	0.46
1:B:90:PHE:HB2	1:B:92:TRP:CD1	2.50	0.46
1:C:53:THR:OG1	2:C:903:ATP:O2G	2.33	0.46
1:C:295:THR:HG21	1:C:319:GLU:OE2	2.16	0.46
1:C:306:CYS:O	1:C:309:LYS:N	2.48	0.46
1:C:371:LYS:N	1:C:372:PRO:HD3	2.30	0.46
1:D:21:MET:HE3	1:D:59:PHE:CE1	2.51	0.46
1:D:439:LEU:HD12	1:D:440:LEU:H	1.81	0.46
1:E:14:GLU:HG3	1:E:16:GLN:N	2.27	0.46
1:E:21:MET:HE1	1:E:177:THR:HB	1.97	0.46
1:F:191:ILE:CB	1:F:198:GLU:CG	2.88	0.46
1:F:209:ASN:HD21	1:F:216:ARG:HB3	1.80	0.46
1:F:469:GLU:HG3	1:F:470:PHE:N	2.30	0.46
1:A:23:THR:C	1:A:25:ILE:H	2.19	0.46
1:C:123:LEU:CD1	1:C:166:ARG:HD2	2.46	0.46
1:C:393:ARG:HH21	1:C:429:HIS:CB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:PHE:N	1:C:483:PHE:CD1	2.84	0.46
1:D:150:VAL:CG1	1:D:151:PHE:N	2.78	0.46
1:D:396:VAL:HG11	1:D:430:ILE:HG23	1.98	0.46
1:F:32:SER:HB3	1:F:222:ILE:CD1	2.46	0.46
1:F:54:LEU:HD13	1:F:90:PHE:CE1	2.51	0.46
1:F:118:VAL:O	1:F:118:VAL:HG22	2.16	0.46
1:A:497:ILE:C	1:A:497:ILE:HD12	2.36	0.45
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.17	0.45
1:C:42:THR:HA	1:C:203:ASN:HB2	1.98	0.45
1:C:50:THR:HB	1:C:207:LEU:HB3	1.98	0.45
1:D:484:ARG:HH11	1:D:484:ARG:HB3	1.80	0.45
1:E:487:GLU:O	1:E:488:ARG:CB	2.64	0.45
1:F:123:LEU:O	1:F:123:LEU:HD13	2.15	0.45
1:F:352:GLU:N	1:F:352:GLU:CD	2.69	0.45
1:A:106:LEU:HD11	1:A:129:ARG:NE	2.31	0.45
1:C:317:TYR:CE1	1:C:377:ILE:HG23	2.47	0.45
1:E:248:PRO:O	1:E:251:ALA:N	2.47	0.45
1:F:338:MET:HB3	1:F:344:LEU:HB3	1.99	0.45
1:F:353:SER:O	1:F:354:ALA:CB	2.65	0.45
1:A:285:LEU:HD12	1:A:412:PHE:O	2.16	0.45
1:A:292:THR:HB	1:A:440:LEU:HB3	1.98	0.45
1:B:68:ASP:OD1	1:B:102:LYS:NZ	2.44	0.45
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.33	0.45
1:C:80:PRO:HD2	1:C:81:GLN:NE2	2.31	0.45
1:C:40:ARG:HG2	1:C:172:LYS:HE3	1.97	0.45
1:C:294:LYS:HB2	2:C:901:ATP:O1B	2.17	0.45
1:C:296:LEU:HD21	1:C:477:PRO:HB3	1.99	0.45
1:D:436:THR:HA	1:D:457:LYS:O	2.17	0.45
1:E:18:ILE:HD11	1:E:227:GLY:O	2.16	0.45
1:E:238:THR:HG22	1:E:239:ILE:N	2.32	0.45
1:E:303:GLU:HB2	1:E:333:MET:CE	2.47	0.45
1:A:213:GLY:C	1:A:215:ARG:H	2.20	0.45
1:B:291:GLY:HA3	1:B:442:TYR:OH	2.16	0.45
1:B:433:ILE:O	1:B:433:ILE:CG2	2.65	0.45
1:B:471:MET:HE3	1:B:472:ILE:C	2.37	0.45
1:D:400:THR:HG22	1:D:401:GLY:N	2.32	0.45
1:E:344:LEU:HD11	1:E:346:ILE:CG1	2.44	0.45
1:E:346:ILE:HG22	1:E:347:VAL:N	2.32	0.45
1:F:21:MET:HE3	1:F:59:PHE:HE1	1.81	0.45
1:A:289:ALA:HB2	1:A:419:PHE:HA	1.98	0.45
1:B:273:MET:C	1:B:275:GLY:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:MET:SD	1:C:141:ARG:NE	2.89	0.45
1:C:118:VAL:O	1:C:118:VAL:HG12	2.16	0.45
1:E:284:ILE:HD12	1:E:284:ILE:H	1.82	0.45
1:F:84:ILE:HA	1:F:94:LEU:HD12	1.98	0.45
1:F:211:LEU:O	1:F:212:GLU:HB3	2.16	0.45
1:F:392:PHE:CE2	1:F:430:ILE:HD11	2.51	0.45
1:A:445:ILE:CD1	1:A:483:PHE:CE2	2.99	0.45
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.52	0.45
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.99	0.45
1:B:490:ILE:HD13	1:B:490:ILE:HA	1.87	0.45
1:D:486:PHE:HE2	1:D:496:ARG:HD3	1.81	0.45
1:E:184:ARG:HG2	1:E:191:ILE:O	2.17	0.45
1:E:287:THR:HG22	1:E:414:ASN:HD22	1.82	0.45
1:E:360:LEU:HD22	1:E:364:LYS:HE3	1.99	0.45
1:F:136:LYS:HD3	1:F:137:TYR:CE1	2.50	0.45
1:A:32:SER:O	1:A:33:HIS:HB2	2.17	0.45
1:A:211:LEU:HD12	1:A:215:ARG:O	2.17	0.45
1:B:344:LEU:HD11	1:B:346:ILE:HG13	1.98	0.45
1:F:106:LEU:CD1	1:F:129:ARG:CZ	2.94	0.45
1:F:121:PHE:O	1:F:125:ALA:N	2.43	0.45
1:C:208:ARG:NH2	1:C:221:GLU:OE2	2.50	0.45
1:D:70:PRO:HB2	1:D:139:ALA:HA	1.99	0.45
1:E:399:VAL:HG11	1:E:412:PHE:HE2	1.82	0.45
1:A:302:VAL:HG13	1:A:344:LEU:HD23	1.99	0.45
1:B:151:PHE:C	1:B:153:GLN:H	2.21	0.45
1:B:247:PHE:HD2	1:B:364:LYS:HZ2	1.65	0.45
1:C:294:LYS:HB2	1:C:294:LYS:HE2	1.79	0.45
1:C:451:ARG:HG2	1:C:451:ARG:NH1	2.30	0.45
1:D:14:GLU:CG	1:D:15:HIS:N	2.80	0.45
1:D:123:LEU:HD22	1:D:123:LEU:HA	1.79	0.45
1:D:291:GLY:CA	2:D:901:ATP:O2B	2.65	0.45
1:E:153:GLN:C	1:F:158:SER:HB2	2.37	0.45
1:E:435:ASP:HA	1:E:459:ARG:HD2	1.99	0.45
2:E:903:ATP:C2	1:F:229:SER:HB3	2.52	0.45
1:F:117:VAL:O	1:F:118:VAL:HB	2.17	0.45
1:F:286:ALA:HA	1:F:438:ILE:O	2.17	0.45
1:F:471:MET:HE2	1:F:471:MET:O	2.17	0.45
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.99	0.44
1:B:211:LEU:O	1:B:212:GLU:CB	2.66	0.44
1:C:461:SER:OG	1:C:462:TRP:N	2.48	0.44
1:D:92:TRP:HE3	1:D:92:TRP:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:HIS:O	1:D:465:LYS:NZ	2.44	0.44
1:E:80:PRO:HD2	1:E:81:GLN:NE2	2.32	0.44
1:E:185:ILE:HD11	1:E:193:ARG:NH1	2.32	0.44
1:B:357:GLU:HG3	1:B:358:ASP:N	2.32	0.44
1:C:211:LEU:O	1:C:212:GLU:CB	2.60	0.44
1:D:15:HIS:O	1:D:16:GLN:HG3	2.17	0.44
1:D:344:LEU:HD13	1:D:344:LEU:C	2.37	0.44
1:E:283:ILE:HD12	1:E:400:THR:HG23	1.98	0.44
1:F:329:TYR:O	1:F:332:GLY:N	2.46	0.44
1:B:18:ILE:CG1	1:B:228:THR:HG23	2.47	0.44
1:B:61:TYR:CZ	1:B:92:TRP:CE3	3.06	0.44
1:B:269:ARG:O	1:B:273:MET:HG3	2.16	0.44
1:C:186:GLU:OE1	1:C:188:TYR:N	2.35	0.44
1:C:387:VAL:HG12	1:C:388:SER:O	2.16	0.44
1:D:203:ASN:HB3	1:D:225:LEU:CD2	2.47	0.44
1:D:208:ARG:NE	1:D:234:GLU:OE2	2.50	0.44
1:E:147:VAL:HG23	1:E:148:THR:N	2.31	0.44
1:E:153:GLN:O	1:F:158:SER:HB2	2.18	0.44
1:F:270:LEU:O	1:F:273:MET:HB2	2.16	0.44
1:A:273:MET:SD	1:A:468:ARG:HD2	2.57	0.44
1:B:64:ILE:HD11	1:B:103:LEU:HB2	1.99	0.44
1:B:335:PHE:HA	1:B:338:MET:HG3	1.99	0.44
1:C:174:ILE:HG22	1:C:174:ILE:O	2.18	0.44
1:D:151:PHE:CZ	1:D:160:VAL:HG13	2.53	0.44
1:D:191:ILE:CD1	1:D:223:LEU:HD12	2.47	0.44
1:E:317:TYR:HB3	1:E:351:PRO:HG3	2.00	0.44
1:E:396:VAL:HG11	1:E:430:ILE:HG23	2.00	0.44
1:E:445:ILE:O	1:E:446:ARG:HB2	2.17	0.44
1:F:148:THR:HG21	1:F:183:GLU:CG	2.47	0.44
1:A:332:GLY:O	1:A:333:MET:C	2.54	0.44
1:A:433:ILE:O	1:A:433:ILE:HG22	2.17	0.44
1:C:124:SER:O	1:C:128:GLU:HG3	2.18	0.44
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.79	0.44
1:D:247:PHE:CZ	1:D:361:GLN:HB2	2.53	0.44
1:D:419:PHE:O	1:D:420:MET:HB2	2.17	0.44
1:E:64:ILE:CG2	1:E:102:LYS:HB3	2.46	0.44
1:E:130:ILE:O	1:E:134:ILE:HG13	2.17	0.44
1:E:350:TYR:CE2	1:F:397:ILE:HG23	2.53	0.44
1:F:294:LYS:HD3	2:F:901:ATP:O1B	2.17	0.44
1:F:380:LEU:HB3	1:F:392:PHE:HZ	1.82	0.44
1:A:36:LEU:HD12	1:A:59:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:NH2	1:A:461:SER:HB2	2.33	0.44
1:A:393:ARG:O	1:A:397:ILE:HG12	2.18	0.44
1:A:400:THR:HG22	1:A:401:GLY:N	2.32	0.44
1:B:153:GLN:O	1:B:154:TYR:HB3	2.17	0.44
1:B:191:ILE:HD11	1:B:223:LEU:CD1	2.46	0.44
1:C:287:THR:HG22	1:C:288:GLY:N	2.32	0.44
1:D:21:MET:HE2	1:D:177:THR:HG21	1.99	0.44
1:D:269:ARG:O	1:D:273:MET:HG3	2.17	0.44
1:E:38:ILE:HG22	1:E:39:GLY:N	2.33	0.44
1:F:344:LEU:HD13	1:F:344:LEU:C	2.37	0.44
1:A:127:ILE:HD13	1:A:170:ARG:CB	2.48	0.44
1:A:371:LYS:HD3	1:A:371:LYS:O	2.17	0.44
1:A:486:PHE:CD2	1:A:494:PRO:HB2	2.47	0.44
1:B:123:LEU:HG	1:B:163:GLU:OE2	2.17	0.44
1:B:334:ASP:OD1	1:B:336:GLU:N	2.51	0.44
1:D:18:ILE:HD12	1:D:227:GLY:HA3	2.00	0.44
1:D:441:GLN:NE2	1:D:490:ILE:HD13	2.31	0.44
1:E:64:ILE:HD12	1:E:97:LEU:HD13	2.00	0.44
1:E:123:LEU:CD1	1:E:163:GLU:OE2	2.64	0.44
1:E:167:LEU:HG	1:E:171:LEU:HD12	1.99	0.44
1:E:334:ASP:O	1:E:338:MET:HG2	2.16	0.44
1:A:21:MET:HE2	1:A:177:THR:CG2	2.47	0.44
1:D:484:ARG:HB3	1:D:484:ARG:NH1	2.32	0.44
1:E:126:LEU:O	1:E:129:ARG:HB2	2.17	0.44
1:E:365:SER:HA	1:E:368:ASN:ND2	2.33	0.44
1:F:452:ALA:HA	1:F:469:GLU:HA	1.99	0.44
1:C:203:ASN:CB	1:C:225:LEU:HD23	2.47	0.44
1:C:397:ILE:CD1	1:C:433:ILE:HD13	2.47	0.44
1:D:453:ILE:HB	1:D:470:PHE:CD2	2.52	0.44
1:E:332:GLY:O	1:E:333:MET:O	2.36	0.44
1:F:164:LEU:HD11	1:F:197:GLU:HG3	2.00	0.44
1:C:214:GLU:HG2	1:D:234:GLU:OE1	2.17	0.43
1:C:311:ARG:HD2	1:C:371:LYS:HD3	1.97	0.43
1:D:367:ILE:HG23	1:D:372:PRO:HD2	2.00	0.43
1:F:118:VAL:CG1	1:F:153:GLN:HE22	2.31	0.43
1:F:164:LEU:CD1	1:F:197:GLU:HG3	2.48	0.43
1:F:344:LEU:HD11	1:F:346:ILE:CG1	2.48	0.43
1:A:18:ILE:CD1	1:A:40:ARG:HH12	2.31	0.43
1:B:356:LEU:HD13	1:B:387:VAL:HG21	1.98	0.43
1:D:21:MET:CE	1:D:59:PHE:CZ	3.01	0.43
1:E:323:GLN:HE21	1:F:459:ARG:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:MET:HB2	1:E:333:MET:HE2	1.78	0.43
2:E:901:ATP:C2	1:F:462:TRP:HA	2.53	0.43
1:F:143:SER:HA	1:F:179:VAL:O	2.18	0.43
1:A:421:GLY:O	1:A:422:ALA:C	2.57	0.43
1:A:457:LYS:HB2	2:F:901:ATP:O3'	2.19	0.43
1:B:295:THR:HG21	1:B:319:GLU:OE2	2.18	0.43
1:B:302:VAL:CG1	1:B:344:LEU:HD23	2.48	0.43
1:C:88:ARG:HG2	1:C:88:ARG:NH1	2.33	0.43
1:C:123:LEU:O	1:C:124:SER:C	2.56	0.43
1:C:283:ILE:HD12	1:C:404:LYS:HE3	1.99	0.43
1:F:150:VAL:CG1	1:F:151:PHE:N	2.81	0.43
1:B:161:ARG:CB	1:B:196:VAL:HG11	2.48	0.43
1:B:187:GLU:OE2	1:B:208:ARG:HA	2.17	0.43
1:B:292:THR:HB	1:B:440:LEU:HB3	2.01	0.43
1:C:248:PRO:C	1:C:250:GLY:H	2.21	0.43
1:D:151:PHE:O	1:D:153:GLN:N	2.47	0.43
1:E:449:MET:CE	1:F:467:ILE:HD11	2.48	0.43
1:E:495:THR:HG23	1:F:487:GLU:OE2	2.19	0.43
1:F:194:TYR:CD1	1:F:194:TYR:N	2.87	0.43
1:A:183:GLU:OE2	1:B:161:ARG:NH2	2.45	0.43
1:A:287:THR:HG23	1:A:414:ASN:ND2	2.12	0.43
1:C:245:ASN:ND2	1:C:247:PHE:CZ	2.86	0.43
1:C:335:PHE:O	1:C:339:GLU:HG3	2.18	0.43
1:D:377:ILE:HD11	1:D:399:VAL:HG11	2.00	0.43
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.58	0.43
1:A:224:LYS:HD3	1:F:49:GLY:CA	2.49	0.43
1:B:219:THR:HA	1:B:235:TYR:O	2.18	0.43
1:E:211:LEU:HD13	1:E:216:ARG:NE	2.34	0.43
1:E:328:ALA:O	1:E:332:GLY:O	2.37	0.43
1:C:102:LYS:HA	1:C:102:LYS:HD3	1.84	0.43
1:C:425:ILE:HD11	1:C:456:PHE:CD2	2.54	0.43
1:D:31:ILE:HA	1:D:231:MET:SD	2.59	0.43
1:D:79:THR:HG22	1:D:82:ASP:N	2.29	0.43
1:D:147:VAL:HG11	1:D:180:MET:CE	2.36	0.43
1:E:31:ILE:HG22	1:E:222:ILE:CD1	2.48	0.43
1:E:217:ARG:HE	1:E:236:PRO:HB3	1.84	0.43
1:F:332:GLY:O	1:F:333:MET:C	2.56	0.43
1:B:298:VAL:HG13	1:B:376:ALA:HB1	2.01	0.43
1:D:269:ARG:HG3	1:D:269:ARG:HH11	1.83	0.43
1:E:163:GLU:OE2	1:E:163:GLU:HA	2.18	0.43
1:E:273:MET:O	1:E:463:HIS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:ARG:HB3	1:E:484:ARG:HH11	1.83	0.43
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.99	0.43
1:A:471:MET:HB3	1:A:480:LYS:NZ	2.34	0.43
1:A:484:ARG:O	1:A:484:ARG:HG2	2.19	0.43
1:C:384:ALA:HB2	1:C:392:PHE:CE1	2.54	0.43
1:D:447:GLY:HA2	1:E:489:ILE:CD1	2.48	0.43
1:A:471:MET:HB3	1:A:480:LYS:HZ1	1.83	0.43
1:C:122:ASP:O	1:C:124:SER:N	2.51	0.43
1:C:249:LEU:HD12	1:C:394:GLN:OE1	2.19	0.43
1:D:92:TRP:HA	1:D:92:TRP:CE3	2.54	0.43
1:D:183:GLU:HB2	1:E:199:PHE:CE1	2.54	0.43
1:D:347:VAL:O	1:D:348:CYS:CB	2.65	0.43
1:D:347:VAL:HG12	1:D:348:CYS:N	2.34	0.43
1:E:425:ILE:HG22	1:E:426:THR:HG23	2.01	0.43
1:F:88:ARG:HG2	1:F:88:ARG:HH11	1.84	0.43
1:A:288:GLY:O	1:A:415:THR:HA	2.19	0.42
1:A:488:ARG:HE	1:F:488:ARG:HH12	1.66	0.42
1:B:267:VAL:HG12	1:B:270:LEU:HB2	2.01	0.42
1:B:292:THR:HB	1:B:440:LEU:CB	2.49	0.42
1:C:61:TYR:CE1	1:C:97:LEU:HD11	2.54	0.42
1:C:66:GLU:HB3	1:C:67:PHE:CE1	2.54	0.42
1:D:214:GLU:HG2	1:E:234:GLU:OE1	2.19	0.42
1:E:21:MET:HE3	1:E:59:PHE:CZ	2.53	0.42
1:E:148:THR:HG23	1:E:193:ARG:HD2	2.01	0.42
1:F:116:GLU:O	1:F:117:VAL:HB	2.19	0.42
1:F:150:VAL:HG13	1:F:151:PHE:H	1.84	0.42
1:F:269:ARG:HB3	1:F:479:ILE:HD12	2.01	0.42
1:F:333:MET:HB2	1:F:333:MET:HE3	1.90	0.42
1:A:65:ILE:O	1:A:65:ILE:CG2	2.67	0.42
1:A:279:PHE:HB2	1:A:282:SER:HB3	2.00	0.42
1:A:309:LYS:HA	1:A:343:LEU:HD13	2.01	0.42
1:B:54:LEU:HD13	1:B:90:PHE:CZ	2.54	0.42
1:B:484:ARG:HB3	1:B:484:ARG:NH1	2.33	0.42
1:C:182:THR:CG2	1:C:183:GLU:N	2.81	0.42
1:C:209:ASN:HD22	1:C:209:ASN:HA	1.63	0.42
1:E:14:GLU:CG	1:E:16:GLN:HB2	2.49	0.42
1:E:191:ILE:HG21	1:E:198:GLU:HG3	2.02	0.42
1:F:240:THR:C	1:F:242:HIS:N	2.72	0.42
1:F:356:LEU:HD13	1:F:387:VAL:HG21	2.01	0.42
1:B:344:LEU:HD22	1:B:345:LYS:H	1.83	0.42
1:D:451:ARG:NH1	1:D:451:ARG:CG	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:TRP:CD2	1:D:463:HIS:N	2.87	0.42
2:D:903:ATP:O3G	2:D:903:ATP:O2A	2.36	0.42
1:E:80:PRO:HD2	1:E:81:GLN:HE22	1.84	0.42
1:E:203:ASN:HA	1:E:224:LYS:O	2.19	0.42
1:E:347:VAL:O	1:E:348:CYS:CB	2.67	0.42
1:F:16:GLN:HE22	1:F:33:HIS:CB	2.32	0.42
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.49	0.42
1:A:420:MET:HG2	1:A:492:GLY:HA3	2.01	0.42
1:B:24:MET:HB2	1:B:62:ASN:HB3	2.01	0.42
1:B:273:MET:HE1	1:B:468:ARG:HD2	2.00	0.42
1:B:284:ILE:N	1:B:284:ILE:HD12	2.34	0.42
1:C:111:ASP:O	1:C:113:GLU:N	2.50	0.42
1:C:208:ARG:O	1:C:218:ARG:HA	2.18	0.42
1:E:400:THR:HG22	1:E:401:GLY:N	2.34	0.42
1:A:93:ASP:OD2	1:A:96:LYS:HB2	2.19	0.42
1:A:266:GLY:C	1:A:300:ARG:HG3	2.39	0.42
1:C:446:ARG:HG2	1:C:496:ARG:NH1	2.35	0.42
1:D:461:SER:OG	1:D:462:TRP:N	2.52	0.42
1:E:106:LEU:CD1	1:E:129:ARG:NH2	2.83	0.42
1:B:311:ARG:HA	1:B:343:LEU:O	2.20	0.42
1:C:36:LEU:HD12	1:C:59:PHE:CE1	2.54	0.42
1:C:451:ARG:HB3	1:C:470:PHE:CE2	2.54	0.42
1:D:109:SER:HA	1:D:110:PRO:HD3	1.89	0.42
1:D:121:PHE:CD1	1:D:121:PHE:N	2.87	0.42
1:D:191:ILE:HD11	1:D:223:LEU:CD1	2.50	0.42
1:D:396:VAL:HG11	1:D:430:ILE:HG21	2.01	0.42
1:E:370:PHE:O	1:E:371:LYS:HD3	2.20	0.42
1:F:73:PHE:HE2	1:F:75:THR:HB	1.84	0.42
1:F:153:GLN:O	1:F:154:TYR:HB3	2.20	0.42
1:F:375:ILE:O	1:F:410:GLY:HA2	2.19	0.42
1:B:25:ILE:HG12	1:B:58:GLN:HE21	1.85	0.42
1:C:148:THR:HA	1:C:151:PHE:CE1	2.55	0.42
1:C:385:ARG:HA	1:D:393:ARG:NH1	2.35	0.42
1:D:62:ASN:O	1:D:66:GLU:HB2	2.20	0.42
1:E:150:VAL:CG1	1:E:151:PHE:H	2.33	0.42
1:E:231:MET:HB3	1:E:235:TYR:OH	2.20	0.42
1:E:335:PHE:HA	1:E:338:MET:HG3	2.02	0.42
1:E:446:ARG:HH21	1:E:496:ARG:NH2	2.17	0.42
1:F:347:VAL:O	1:F:348:CYS:CB	2.67	0.42
2:A:901:ATP:H3'	1:B:458:MET:O	2.20	0.42
1:B:57:ILE:HG22	1:B:58:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ARG:HH21	1:B:496:ARG:NH1	2.18	0.42
1:E:118:VAL:HG12	1:E:118:VAL:O	2.20	0.42
1:E:120:GLY:O	1:E:121:PHE:C	2.58	0.42
1:E:211:LEU:HA	1:E:216:ARG:HD3	2.01	0.42
1:E:211:LEU:O	1:E:212:GLU:HB3	2.19	0.42
1:F:483:PHE:HB3	1:F:486:PHE:CD1	2.55	0.42
1:B:24:MET:HG3	1:B:66:GLU:HG3	2.02	0.42
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.84	0.42
1:B:290:THR:HG22	2:B:901:ATP:O1G	2.20	0.42
1:C:360:LEU:HD22	1:C:364:LYS:HE3	2.00	0.42
1:C:489:ILE:C	1:C:491:SER:N	2.72	0.42
1:D:121:PHE:O	1:D:122:ASP:O	2.38	0.42
1:D:144:ILE:HD12	1:D:180:MET:HG2	2.02	0.42
1:F:191:ILE:CB	1:F:198:GLU:HG3	2.49	0.42
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.85	0.42
1:B:21:MET:CE	1:B:177:THR:HG21	2.50	0.42
1:C:370:PHE:HD2	1:C:372:PRO:HG3	1.83	0.42
1:C:484:ARG:NH1	1:C:484:ARG:HB3	2.34	0.42
1:D:191:ILE:HD11	1:D:223:LEU:HD12	2.02	0.42
1:E:23:THR:HB	1:E:25:ILE:HG13	2.02	0.42
1:E:79:THR:HG23	1:E:81:GLN:N	2.32	0.42
1:E:164:LEU:HD23	1:E:164:LEU:HA	1.79	0.42
1:E:451:ARG:NH1	1:E:472:ILE:HD12	2.35	0.42
1:B:52:LYS:HE3	2:B:903:ATP:O1B	2.19	0.41
1:B:150:VAL:CG1	1:B:151:PHE:H	2.33	0.41
1:C:164:LEU:HB3	1:C:200:VAL:HG11	2.02	0.41
1:C:248:PRO:O	1:C:251:ALA:N	2.41	0.41
1:C:449:MET:HE2	1:D:467:ILE:HD11	1.95	0.41
1:D:146:SER:H	1:D:181:THR:CG2	2.31	0.41
1:E:54:LEU:HD13	1:E:90:PHE:CE1	2.55	0.41
1:E:430:ILE:O	1:E:432:ALA:N	2.53	0.41
1:F:118:VAL:O	1:F:122:ASP:CG	2.58	0.41
1:F:484:ARG:NH1	1:F:484:ARG:CB	2.83	0.41
1:A:24:MET:HB2	1:A:62:ASN:HB3	2.02	0.41
1:A:370:PHE:O	1:A:371:LYS:CD	2.69	0.41
1:C:21:MET:HB2	1:C:38:ILE:HG12	2.01	0.41
1:D:211:LEU:O	1:D:215:ARG:O	2.37	0.41
1:E:387:VAL:HG12	1:E:388:SER:N	2.34	0.41
1:E:431:SEP:C	1:E:434:THR:HG22	2.48	0.41
1:F:93:ASP:HA	4:F:523:HOH:O	2.18	0.41
1:F:191:ILE:HB	1:F:198:GLU:HG2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:HA	1:A:182:THR:O	2.21	0.41
1:A:87:ALA:HB1	1:A:92:TRP:HB2	2.02	0.41
1:A:161:ARG:HD2	1:A:196:VAL:HG13	2.01	0.41
1:A:397:ILE:HG23	1:F:350:TYR:CE2	2.56	0.41
1:B:38:ILE:HA	1:B:177:THR:CG2	2.50	0.41
1:B:211:LEU:HD13	1:B:216:ARG:NE	2.35	0.41
1:B:334:ASP:O	1:B:338:MET:HG2	2.20	0.41
1:C:296:LEU:CD2	1:C:477:PRO:HB3	2.50	0.41
1:D:49:GLY:HA2	2:D:903:ATP:O2B	2.20	0.41
1:D:220:LEU:HD13	1:D:246:ILE:HD11	2.02	0.41
1:E:146:SER:H	1:E:181:THR:HB	1.84	0.41
1:E:392:PHE:CE2	1:E:430:ILE:HD11	2.55	0.41
1:E:419:PHE:O	1:E:420:MET:O	2.39	0.41
2:E:903:ATP:O1G	1:F:224:LYS:NZ	2.54	0.41
1:F:260:ASN:HA	1:F:279:PHE:CE2	2.55	0.41
1:A:249:LEU:CD1	1:A:394:GLN:HG2	2.51	0.41
1:B:257:ARG:NH2	1:B:407:GLU:HG2	2.36	0.41
1:B:453:ILE:CD1	1:B:454:ASN:N	2.82	0.41
1:C:64:ILE:HD11	1:C:103:LEU:HB2	2.01	0.41
1:F:203:ASN:HB3	1:F:225:LEU:CD2	2.27	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.90	0.41
1:B:70:PRO:HA	1:B:102:LYS:O	2.20	0.41
1:B:161:ARG:HB2	1:B:196:VAL:CG1	2.49	0.41
1:B:279:PHE:HE1	1:B:461:SER:H	1.67	0.41
1:C:269:ARG:NE	4:C:526:HOH:O	2.49	0.41
1:D:14:GLU:CG	1:D:15:HIS:H	2.33	0.41
1:D:468:ARG:HG2	1:D:468:ARG:NH1	2.35	0.41
1:E:333:MET:O	1:E:333:MET:HG3	2.21	0.41
1:E:454:ASN:HD21	1:E:456:PHE:HA	1.86	0.41
1:F:298:VAL:HG13	1:F:376:ALA:HB1	2.01	0.41
1:F:344:LEU:CD1	1:F:346:ILE:HG13	2.51	0.41
1:A:192:ALA:HB3	1:A:197:GLU:OE2	2.21	0.41
1:B:89:SER:CB	1:C:227:GLY:O	2.64	0.41
1:B:299:SER:CB	1:B:333:MET:HE1	2.47	0.41
1:B:313:ILE:HG13	1:B:372:PRO:HG3	2.02	0.41
1:B:471:MET:HE2	1:B:471:MET:O	2.21	0.41
1:C:468:ARG:NH1	1:C:468:ARG:HG2	2.36	0.41
1:D:283:ILE:O	1:D:283:ILE:HG22	2.20	0.41
1:D:317:TYR:CZ	1:D:383:LEU:HD11	2.55	0.41
1:D:377:ILE:CD1	1:D:399:VAL:HG11	2.51	0.41
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:GLU:O	1:E:341:GLN:HG3	2.20	0.41
1:E:344:LEU:CD1	1:E:346:ILE:HG13	2.48	0.41
1:F:79:THR:HA	1:F:80:PRO:HD3	1.98	0.41
1:F:151:PHE:C	1:F:153:GLN:H	2.24	0.41
1:F:370:PHE:HD2	1:F:372:PRO:HG3	1.84	0.41
1:F:392:PHE:O	1:F:395:PHE:HB3	2.20	0.41
1:A:89:SER:CB	1:B:227:GLY:O	2.67	0.41
1:A:311:ARG:HG2	1:A:343:LEU:HA	2.02	0.41
1:B:446:ARG:NE	1:B:496:ARG:HH12	2.18	0.41
1:C:41:SER:OG	1:C:168:VAL:HG13	2.21	0.41
1:C:392:PHE:O	1:C:395:PHE:HB3	2.20	0.41
1:D:418:GLN:HB2	1:E:423:HIS:O	2.21	0.41
1:E:146:SER:HA	1:E:181:THR:O	2.21	0.41
1:E:264:SER:HB3	1:E:304:ASN:ND2	2.36	0.41
1:E:300:ARG:HA	1:E:333:MET:HE3	2.03	0.41
1:E:323:GLN:HG2	1:E:327:ASN:ND2	2.36	0.41
1:E:486:PHE:HA	1:E:495:THR:O	2.20	0.41
1:F:316:ALA:CB	1:F:324:LEU:HD11	2.50	0.41
1:A:23:THR:C	1:A:25:ILE:N	2.73	0.41
1:A:265:SER:O	1:A:301:PHE:HA	2.21	0.41
1:A:335:PHE:O	1:A:338:MET:HB2	2.21	0.41
1:D:453:ILE:HD13	1:D:454:ASN:N	2.35	0.41
1:E:106:LEU:HD11	1:E:129:ARG:CZ	2.50	0.41
1:E:122:ASP:HB3	1:E:123:LEU:H	1.67	0.41
1:E:303:GLU:OE2	1:E:333:MET:HB3	2.20	0.41
1:E:379:SER:HA	1:E:413:THR:HG22	2.03	0.41
1:E:469:GLU:CB	1:E:483:PHE:CZ	3.04	0.41
1:F:18:ILE:HB	1:F:228:THR:HG23	2.03	0.41
1:F:211:LEU:HD12	1:F:215:ARG:O	2.20	0.41
1:A:209:ASN:HD22	1:A:209:ASN:HA	1.71	0.41
1:A:284:ILE:CB	1:A:411:LEU:HD12	2.45	0.41
1:A:318:GLU:OE2	1:B:432:ALA:HB1	2.21	0.41
1:B:61:TYR:CE1	1:B:92:TRP:HB3	2.55	0.41
1:B:142:VAL:HG12	1:B:143:SER:N	2.35	0.41
1:B:147:VAL:CG2	1:B:148:THR:N	2.82	0.41
1:D:21:MET:CE	1:D:59:PHE:HZ	2.34	0.41
1:D:32:SER:HB3	1:D:222:ILE:CD1	2.51	0.41
1:D:301:PHE:CZ	1:D:374:ARG:HD3	2.56	0.41
1:D:313:ILE:CD1	1:D:372:PRO:HG3	2.51	0.41
1:D:362:ILE:CG2	1:D:366:GLU:OE2	2.69	0.41
1:E:98:VAL:HA	1:E:103:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:387:VAL:CG1	1:E:391:ALA:HB3	2.51	0.41
1:E:425:ILE:HD11	1:E:456:PHE:CD2	2.56	0.41
1:E:462:TRP:O	1:E:463:HIS:CG	2.74	0.41
1:F:191:ILE:CG2	1:F:198:GLU:HG3	2.51	0.41
1:A:191:ILE:CB	1:A:198:GLU:HG2	2.51	0.41
1:A:334:ASP:O	1:A:338:MET:HG2	2.21	0.41
1:A:486:PHE:HB2	1:A:489:ILE:HD11	2.02	0.41
1:B:85:LYS:CE	1:C:17:ALA:O	2.69	0.41
1:B:294:LYS:HE2	1:B:294:LYS:HB2	1.92	0.41
1:B:483:PHE:O	1:B:485:ASN:N	2.54	0.41
1:C:425:ILE:HD12	1:C:431:SEP:O2P	2.20	0.41
1:E:264:SER:HA	1:E:271:ASP:OD1	2.21	0.41
1:E:418:GLN:HB2	1:F:423:HIS:O	2.21	0.41
1:A:220:LEU:HD13	1:A:246:ILE:CD1	2.51	0.40
1:A:266:GLY:O	1:A:300:ARG:NE	2.52	0.40
1:A:392:PHE:O	1:A:395:PHE:HB3	2.22	0.40
1:A:453:ILE:HB	1:A:470:PHE:CD2	2.56	0.40
1:B:25:ILE:HG23	1:B:58:GLN:HE22	1.85	0.40
1:C:52:LYS:HD3	1:C:182:THR:O	2.20	0.40
1:C:56:SER:OG	1:C:73:PHE:HE1	2.05	0.40
1:C:69:GLU:HB3	1:C:140:ARG:HB2	2.03	0.40
1:C:76:PHE:O	1:C:110:PRO:HD3	2.21	0.40
1:C:120:GLY:C	1:C:122:ASP:N	2.75	0.40
1:C:191:ILE:CB	1:C:198:GLU:HG2	2.44	0.40
1:C:191:ILE:CD1	1:C:198:GLU:HG2	2.49	0.40
1:D:147:VAL:CG2	1:D:148:THR:N	2.84	0.40
1:D:211:LEU:HD12	1:D:215:ARG:O	2.20	0.40
1:A:266:GLY:O	1:A:300:ARG:HG3	2.21	0.40
1:A:376:ALA:HA	1:A:411:LEU:O	2.21	0.40
1:A:453:ILE:HD13	1:A:454:ASN:H	1.83	0.40
1:B:158:SER:O	1:B:162:ARG:HG3	2.21	0.40
1:D:127:ILE:HD13	1:D:170:ARG:HG3	2.03	0.40
1:D:137:TYR:O	1:D:138:ARG:HB2	2.21	0.40
1:D:269:ARG:HB3	1:D:479:ILE:CD1	2.47	0.40
1:D:406:GLU:O	1:D:407:GLU:HB2	2.22	0.40
1:D:443:VAL:CG1	1:D:494:PRO:HG2	2.51	0.40
1:E:212:GLU:O	1:E:212:GLU:HG2	2.18	0.40
1:F:237:PHE:CD1	1:F:237:PHE:C	2.95	0.40
1:F:486:PHE:HE2	1:F:496:ARG:HH11	1.69	0.40
1:A:262:ARG:HH22	1:A:461:SER:HB2	1.86	0.40
1:A:322:ALA:O	1:A:325:LEU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:VAL:HG23	1:B:139:ALA:CB	2.52	0.40
1:B:344:LEU:C	1:B:344:LEU:HD13	2.42	0.40
1:B:371:LYS:HD3	1:B:371:LYS:C	2.42	0.40
1:C:88:ARG:CZ	1:D:15:HIS:HA	2.51	0.40
1:D:303:GLU:O	1:D:303:GLU:HG2	2.22	0.40
1:D:495:THR:O	1:D:497:ILE:HG23	2.21	0.40
1:F:61:TYR:CZ	1:F:92:TRP:CE3	3.09	0.40
1:F:182:THR:CG2	1:F:192:ALA:HB1	2.45	0.40
1:A:151:PHE:C	1:A:153:GLN:H	2.23	0.40
1:A:212:GLU:O	1:A:212:GLU:HG2	2.22	0.40
1:A:471:MET:HE2	1:A:478:ASP:CB	2.51	0.40
1:B:25:ILE:HG23	1:B:58:GLN:NE2	2.36	0.40
1:B:119:GLY:C	1:B:121:PHE:H	2.24	0.40
1:B:145:ASP:O	1:B:146:SER:OG	2.34	0.40
1:B:145:ASP:OD2	1:B:181:THR:HG21	2.22	0.40
1:B:170:ARG:HB3	1:B:170:ARG:NH1	2.37	0.40
1:C:370:PHE:O	1:C:371:LYS:C	2.60	0.40
1:D:118:VAL:O	1:D:118:VAL:HG12	2.21	0.40
1:D:153:GLN:O	1:D:154:TYR:HB3	2.22	0.40
1:E:182:THR:HG21	1:E:192:ALA:HB1	2.03	0.40
1:F:453:ILE:HB	1:F:470:PHE:CD2	2.56	0.40
1:A:52:LYS:HE3	1:A:52:LYS:HB2	1.73	0.40
1:A:234:GLU:O	1:F:215:ARG:NH2	2.55	0.40
1:A:237:PHE:HB3	1:A:246:ILE:HG12	2.04	0.40
2:A:903:ATP:O1G	1:B:224:LYS:NZ	2.55	0.40
1:B:311:ARG:HB3	1:B:370:PHE:CE2	2.57	0.40
1:B:467:ILE:O	1:B:482:SER:HA	2.22	0.40
1:C:24:MET:HB2	1:C:62:ASN:HB3	2.03	0.40
1:C:283:ILE:HD13	1:C:400:THR:HG23	2.03	0.40
1:D:33:HIS:CD2	1:D:230:HIS:HA	2.57	0.40
1:D:340:ARG:O	1:D:342:ASN:N	2.54	0.40
1:E:21:MET:CE	1:E:59:PHE:CZ	3.04	0.40
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.36	0.40
1:E:469:GLU:HB2	1:E:483:PHE:CZ	2.56	0.40
1:F:111:ASP:OD1	1:F:112:PRO:CD	2.69	0.40
1:F:311:ARG:HB3	1:F:370:PHE:CE2	2.57	0.40
1:F:332:GLY:O	1:F:333:MET:O	2.39	0.40
1:F:396:VAL:O	1:F:400:THR:CB	2.63	0.40
1:F:418:GLN:HG3	1:F:418:GLN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/519 (93%)	427 (89%)	36 (8%)	18 (4%)	3	13
1	B	481/519 (93%)	414 (86%)	52 (11%)	15 (3%)	4	16
1	C	481/519 (93%)	428 (89%)	37 (8%)	16 (3%)	4	15
1	D	481/519 (93%)	431 (90%)	38 (8%)	12 (2%)	5	21
1	E	481/519 (93%)	423 (88%)	43 (9%)	15 (3%)	4	16
1	F	481/519 (93%)	429 (89%)	37 (8%)	15 (3%)	4	16
All	All	2886/3114 (93%)	2552 (88%)	243 (8%)	91 (3%)	4	16

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	117	VAL
1	A	154	TYR
1	A	211	LEU
1	A	463	HIS
1	B	154	TYR
1	B	463	HIS
1	C	17	ALA
1	C	117	VAL
1	C	123	LEU
1	C	154	TYR
1	C	333	MET
1	C	463	HIS
1	D	122	ASP
1	D	154	TYR
1	D	333	MET
1	E	122	ASP
1	E	154	TYR
1	E	333	MET
1	F	114	GLY

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Mol	Chain	Res	Type
1	F	118	VAL
1	F	154	TYR
1	F	249	LEU
1	F	333	MET
1	F	463	HIS
1	A	333	MET
1	A	420	MET
1	B	119	GLY
1	B	211	LEU
1	B	420	MET
1	B	461	SER
1	B	484	ARG
1	C	122	ASP
1	C	211	LEU
1	D	214	GLU
1	D	420	MET
1	D	494	PRO
1	E	211	LEU
1	E	420	MET
1	E	463	HIS
1	F	189	GLY
1	F	211	LEU
1	F	354	ALA
1	A	120	GLY
1	A	249	LEU
1	B	326	ARG
1	B	333	MET
1	C	112	PRO
1	C	249	LEU
1	C	289	ALA
1	C	348	CYS
1	C	349	ALA
1	D	113	GLU
1	D	211	LEU
1	D	341	GLN
1	E	123	LEU
1	E	349	ALA
1	E	482	SER
1	E	488	ARG
1	F	117	VAL
1	F	420	MET
1	A	379	SER

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Mol	Chain	Res	Type
1	B	100	GLU
1	B	341	GLN
1	B	379	SER
1	C	420	MET
1	D	212	GLU
1	E	113	GLU
1	F	370	PHE
1	A	212	GLU
1	A	214	GLU
1	A	348	CYS
1	B	193	ARG
1	B	348	CYS
1	B	354	ALA
1	C	124	SER
1	E	117	VAL
1	E	249	LEU
1	F	348	CYS
1	F	387	VAL
1	A	24	MET
1	A	112	PRO
1	C	379	SER
1	D	348	CYS
1	A	386	GLY
1	D	118	VAL
1	E	118	VAL
1	A	185	ILE
1	A	398	GLY
1	E	18	ILE
1	F	119	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/442 (93%)	386 (94%)	24 (6%)	19	49
1	B	410/442 (93%)	393 (96%)	17 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	410/442 (93%)	384 (94%)	26 (6%)	18	46
1	D	410/442 (93%)	378 (92%)	32 (8%)	12	34
1	E	410/442 (93%)	379 (92%)	31 (8%)	13	36
1	F	410/442 (93%)	381 (93%)	29 (7%)	14	40
All	All	2460/2652 (93%)	2301 (94%)	159 (6%)	17	45

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	33	HIS
1	A	79	THR
1	A	81	GLN
1	A	92	TRP
1	A	123	LEU
1	A	151	PHE
1	A	154	TYR
1	A	186	GLU
1	A	209	ASN
1	A	212	GLU
1	A	223	LEU
1	A	238	THR
1	A	270	LEU
1	A	342	ASN
1	A	360	LEU
1	A	371	LYS
1	A	400	THR
1	A	451	ARG
1	A	453	ILE
1	A	458	MET
1	A	462	TRP
1	A	469	GLU
1	A	471	MET
1	B	26	GLU
1	B	81	GLN
1	B	128	GLU
1	B	151	PHE
1	B	154	TYR
1	B	186	GLU
1	B	212	GLU
1	B	218	ARG

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Mol	Chain	Res	Type
1	B	223	LEU
1	B	270	LEU
1	B	360	LEU
1	B	371	LYS
1	B	451	ARG
1	B	453	ILE
1	B	462	TRP
1	B	463	HIS
1	B	471	MET
1	C	26	GLU
1	C	79	THR
1	C	81	GLN
1	C	151	PHE
1	C	154	TYR
1	C	186	GLU
1	C	209	ASN
1	C	211	LEU
1	C	212	GLU
1	C	215	ARG
1	C	223	LEU
1	C	245	ASN
1	C	256	GLN
1	C	270	LEU
1	C	303	GLU
1	C	314	LEU
1	C	344	LEU
1	C	356	LEU
1	C	360	LEU
1	C	371	LYS
1	C	375	ILE
1	C	400	THR
1	C	428	SER
1	C	451	ARG
1	C	453	ILE
1	C	470	PHE
1	D	26	GLU
1	D	79	THR
1	D	81	GLN
1	D	121	PHE
1	D	122	ASP
1	D	123	LEU
1	D	145	ASP

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Mol	Chain	Res	Type
1	D	151	PHE
1	D	154	TYR
1	D	181	THR
1	D	186	GLU
1	D	209	ASN
1	D	212	GLU
1	D	223	LEU
1	D	256	GLN
1	D	270	LEU
1	D	287	THR
1	D	290	THR
1	D	294	LYS
1	D	342	ASN
1	D	356	LEU
1	D	360	LEU
1	D	369	ASP
1	D	371	LYS
1	D	400	THR
1	D	451	ARG
1	D	453	ILE
1	D	458	MET
1	D	463	HIS
1	D	469	GLU
1	D	471	MET
1	D	496	ARG
1	E	18	ILE
1	E	26	GLU
1	E	79	THR
1	E	81	GLN
1	E	121	PHE
1	E	151	PHE
1	E	154	TYR
1	E	186	GLU
1	E	212	GLU
1	E	223	LEU
1	E	228	THR
1	E	245	ASN
1	E	255	THR
1	E	256	GLN
1	E	270	LEU
1	E	287	THR
1	E	290	THR

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Mol	Chain	Res	Type
1	E	314	LEU
1	E	342	ASN
1	E	344	LEU
1	E	360	LEU
1	E	371	LYS
1	E	406	GLU
1	E	451	ARG
1	E	453	ILE
1	E	458	MET
1	E	461	SER
1	E	469	GLU
1	E	471	MET
1	E	474	ASP
1	E	497	ILE
1	F	33	HIS
1	F	45	SER
1	F	79	THR
1	F	111	ASP
1	F	121	PHE
1	F	123	LEU
1	F	151	PHE
1	F	181	THR
1	F	186	GLU
1	F	203	ASN
1	F	209	ASN
1	F	212	GLU
1	F	218	ARG
1	F	223	LEU
1	F	256	GLN
1	F	270	LEU
1	F	282	SER
1	F	290	THR
1	F	342	ASN
1	F	344	LEU
1	F	360	LEU
1	F	371	LYS
1	F	451	ARG
1	F	453	ILE
1	F	462	TRP
1	F	469	GLU
1	F	471	MET
1	F	487	GLU

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Mol	Chain	Res	Type
1	F	496	ARG

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

Mol	Chain	Res	Type
1	A	33	HIS
1	A	62	ASN
1	A	81	GLN
1	A	135	GLN
1	A	152	GLN
1	A	209	ASN
1	A	323	GLN
1	A	361	GLN
1	A	368	ASN
1	A	414	ASN
1	B	15	HIS
1	B	33	HIS
1	B	62	ASN
1	B	81	GLN
1	B	209	ASN
1	B	361	GLN
1	B	368	ASN
1	B	414	ASN
1	B	441	GLN
1	C	33	HIS
1	C	62	ASN
1	C	81	GLN
1	C	209	ASN
1	C	245	ASN
1	C	323	GLN
1	C	368	ASN
1	C	389	ASN
1	C	414	ASN
1	C	418	GLN
1	C	454	ASN
1	D	33	HIS
1	D	81	GLN
1	D	209	ASN
1	D	368	ASN
1	D	414	ASN
1	D	441	GLN
1	E	33	HIS

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Mol	Chain	Res	Type
1	E	62	ASN
1	E	81	GLN
1	E	209	ASN
1	E	245	ASN
1	E	327	ASN
1	E	368	ASN
1	E	414	ASN
1	E	441	GLN
1	E	454	ASN
1	F	16	GLN
1	F	81	GLN
1	F	135	GLN
1	F	153	GLN
1	F	209	ASN
1	F	361	GLN
1	F	368	ASN
1	F	414	ASN
1	F	454	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	D	431	1	8,9,10	1.54	1 (12%)	8,12,14	1.39	2 (25%)
1	SEP	A	431	1	8,9,10	1.56	1 (12%)	8,12,14	1.73	2 (25%)
1	SEP	F	431	1	8,9,10	1.61	1 (12%)	8,12,14	1.80	2 (25%)
1	SEP	B	431	1	8,9,10	1.58	1 (12%)	8,12,14	1.65	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	C	431	1	8,9,10	1.65	1 (12%)	8,12,14	3.42	2 (25%)
1	SEP	E	431	1	8,9,10	1.53	1 (12%)	8,12,14	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	D	431	1	-	1/5/8/10	-
1	SEP	A	431	1	-	1/5/8/10	-
1	SEP	F	431	1	-	0/5/8/10	-
1	SEP	B	431	1	-	1/5/8/10	-
1	SEP	C	431	1	-	1/5/8/10	-
1	SEP	E	431	1	-	1/5/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	431	SEP	P-O1P	3.44	1.61	1.50
1	B	431	SEP	P-O1P	3.38	1.61	1.50
1	D	431	SEP	P-O1P	3.38	1.61	1.50
1	F	431	SEP	P-O1P	3.37	1.61	1.50
1	A	431	SEP	P-O1P	3.36	1.61	1.50
1	E	431	SEP	P-O1P	3.34	1.61	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	431	SEP	OG-CB-CA	7.49	115.43	108.14
1	C	431	SEP	P-OG-CB	-5.65	102.72	118.30
1	F	431	SEP	P-OG-CB	-3.75	107.97	118.30
1	A	431	SEP	OG-CB-CA	3.44	111.50	108.14
1	B	431	SEP	P-OG-CB	-3.11	109.72	118.30
1	B	431	SEP	OG-CB-CA	2.92	110.99	108.14
1	A	431	SEP	P-OG-CB	-2.84	110.48	118.30
1	F	431	SEP	OG-CB-CA	2.81	110.88	108.14
1	D	431	SEP	P-OG-CB	-2.41	111.64	118.30
1	D	431	SEP	OG-CB-CA	2.32	110.40	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	431	SEP	N-CA-CB-OG
1	B	431	SEP	N-CA-CB-OG
1	C	431	SEP	N-CA-CB-OG
1	E	431	SEP	N-CA-CB-OG
1	D	431	SEP	CB-OG-P-O2P

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	431	SEP	2	0
1	A	431	SEP	1	0
1	B	431	SEP	1	0
1	C	431	SEP	2	0
1	E	431	SEP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 18 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	$\#\|Z\| > 2$
2	ATP	E	903	3	26,33,33	1.42	3 (11%)	31,52,52	1.95	7 (22%)
2	ATP	C	903	3	26,33,33	1.23	2 (7%)	31,52,52	1.68	4 (12%)
2	ATP	B	903	3	26,33,33	1.37	3 (11%)	31,52,52	1.72	5 (16%)
2	ATP	B	901	3	26,33,33	1.27	3 (11%)	31,52,52	1.70	6 (19%)
2	ATP	E	901	3	26,33,33	1.44	4 (15%)	31,52,52	1.75	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	D	903	3	26,33,33	1.33	3 (11%)	31,52,52	1.88	6 (19%)
2	ATP	F	903	3	26,33,33	1.67	6 (23%)	31,52,52	1.71	4 (12%)
2	ATP	C	901	3	26,33,33	1.44	4 (15%)	31,52,52	1.68	5 (16%)
2	ATP	A	903	3	26,33,33	1.30	2 (7%)	31,52,52	1.78	6 (19%)
2	ATP	D	901	3	26,33,33	1.37	4 (15%)	31,52,52	1.80	7 (22%)
2	ATP	A	901	3	26,33,33	1.41	4 (15%)	31,52,52	1.81	6 (19%)
2	ATP	F	901	3	26,33,33	1.39	5 (19%)	31,52,52	1.84	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	ATP	C2-N3	4.73	1.39	1.32
2	E	901	ATP	C2-N3	4.59	1.39	1.32
2	E	903	ATP	C2-N3	4.42	1.39	1.32
2	B	903	ATP	C2-N3	4.17	1.38	1.32
2	A	901	ATP	C2-N3	4.15	1.38	1.32
2	F	901	ATP	C2-N3	4.09	1.38	1.32
2	F	903	ATP	C2-N3	4.08	1.38	1.32
2	A	903	ATP	C2-N3	4.05	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	903	ATP	PG-O1G	3.98	1.63	1.50
2	D	903	ATP	C2-N3	3.80	1.38	1.32
2	C	903	ATP	C2-N3	3.79	1.38	1.32
2	B	901	ATP	C2-N3	3.65	1.38	1.32
2	D	901	ATP	C2-N3	3.65	1.38	1.32
2	F	901	ATP	O4'-C1'	3.16	1.45	1.41
2	D	903	ATP	C2'-C1'	-3.02	1.49	1.53
2	D	901	ATP	C2'-C1'	-2.99	1.49	1.53
2	F	903	ATP	O2'-C2'	-2.87	1.36	1.43
2	F	903	ATP	C2'-C1'	-2.71	1.49	1.53
2	E	901	ATP	C4-N3	2.68	1.39	1.35
2	E	901	ATP	O4'-C1'	2.65	1.44	1.41
2	B	901	ATP	O4'-C1'	2.53	1.44	1.41
2	B	903	ATP	O4'-C1'	2.49	1.44	1.41
2	A	901	ATP	O4'-C1'	2.47	1.44	1.41
2	D	903	ATP	O2'-C2'	-2.45	1.37	1.43
2	E	903	ATP	C2'-C1'	-2.43	1.50	1.53
2	F	901	ATP	C2-N1	2.36	1.38	1.33
2	A	901	ATP	C2'-C1'	-2.36	1.50	1.53
2	A	901	ATP	C2-N1	2.34	1.38	1.33
2	C	901	ATP	C2-N1	2.29	1.38	1.33
2	C	901	ATP	O4'-C1'	2.27	1.44	1.41
2	F	901	ATP	C4-N3	2.23	1.38	1.35
2	E	903	ATP	O4'-C4'	-2.22	1.40	1.45
2	D	901	ATP	O4'-C1'	2.20	1.44	1.41
2	E	901	ATP	C2-N1	2.15	1.37	1.33
2	F	903	ATP	PB-O1B	-2.15	1.43	1.50
2	B	903	ATP	C2-N1	2.14	1.37	1.33
2	F	903	ATP	C2-N1	2.12	1.37	1.33
2	C	903	ATP	C2'-C1'	-2.10	1.50	1.53
2	F	901	ATP	C2'-C1'	-2.09	1.50	1.53
2	C	901	ATP	C2'-C1'	-2.07	1.50	1.53
2	D	901	ATP	C2-N1	2.06	1.37	1.33
2	A	903	ATP	C2-N1	2.05	1.37	1.33
2	B	901	ATP	C2'-C1'	-2.01	1.50	1.53

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	903	ATP	N3-C2-N1	-5.98	119.34	128.68
2	F	903	ATP	N3-C2-N1	-5.80	119.62	128.68
2	B	901	ATP	N3-C2-N1	-5.73	119.72	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	903	ATP	N3-C2-N1	-5.54	120.02	128.68
2	F	901	ATP	N3-C2-N1	-5.50	120.08	128.68
2	D	901	ATP	N3-C2-N1	-5.50	120.08	128.68
2	C	903	ATP	N3-C2-N1	-5.44	120.18	128.68
2	B	903	ATP	N3-C2-N1	-5.43	120.19	128.68
2	E	901	ATP	N3-C2-N1	-5.32	120.36	128.68
2	A	903	ATP	N3-C2-N1	-5.28	120.43	128.68
2	A	901	ATP	N3-C2-N1	-5.26	120.45	128.68
2	C	901	ATP	N3-C2-N1	-5.21	120.54	128.68
2	E	903	ATP	C4-C5-N7	-4.56	104.65	109.40
2	E	901	ATP	C4-C5-N7	-4.20	105.02	109.40
2	D	901	ATP	C4-C5-N7	-4.19	105.03	109.40
2	F	901	ATP	C4-C5-N7	-4.18	105.05	109.40
2	D	903	ATP	C4-C5-N7	-4.16	105.07	109.40
2	C	901	ATP	C4-C5-N7	-4.09	105.14	109.40
2	B	903	ATP	C4-C5-N7	-4.07	105.16	109.40
2	C	903	ATP	C4-C5-N7	-4.03	105.20	109.40
2	A	901	ATP	C4-C5-N7	-4.02	105.21	109.40
2	A	901	ATP	C5-C6-N6	4.01	126.44	120.35
2	D	901	ATP	C5-C6-N6	3.98	126.40	120.35
2	C	903	ATP	C5-C6-N6	3.98	126.39	120.35
2	E	903	ATP	C5-C6-N6	3.93	126.33	120.35
2	A	903	ATP	C4-C5-N7	-3.88	105.36	109.40
2	D	903	ATP	C5-C6-N6	3.86	126.22	120.35
2	B	903	ATP	C5-C6-N6	3.83	126.18	120.35
2	F	901	ATP	C5-C6-N6	3.82	126.15	120.35
2	B	901	ATP	C4-C5-N7	-3.81	105.43	109.40
2	A	903	ATP	C5-C6-N6	3.73	126.03	120.35
2	F	903	ATP	C4-C5-N7	-3.69	105.56	109.40
2	B	901	ATP	C5-C6-N6	3.67	125.93	120.35
2	C	901	ATP	C5-C6-N6	3.54	125.73	120.35
2	E	901	ATP	C5-C6-N6	3.48	125.64	120.35
2	D	903	ATP	PB-O3B-PG	-3.48	120.89	132.83
2	A	903	ATP	O2G-PG-O3B	3.44	116.17	104.64
2	F	903	ATP	C5-C6-N6	3.22	125.25	120.35
2	E	903	ATP	PB-O3B-PG	-3.07	122.29	132.83
2	A	901	ATP	O2G-PG-O3B	3.07	114.93	104.64
2	F	901	ATP	O2G-PG-O3B	3.03	114.80	104.64
2	E	903	ATP	O2G-PG-O3B	3.02	114.75	104.64
2	D	901	ATP	O2G-PG-O3B	2.97	114.60	104.64
2	E	903	ATP	C3'-C2'-C1'	2.82	105.23	100.98
2	D	903	ATP	O2G-PG-O3B	2.78	113.96	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	903	ATP	PB-O3B-PG	-2.78	123.30	132.83
2	E	901	ATP	C3'-C2'-C1'	2.72	105.07	100.98
2	C	901	ATP	C3'-C2'-C1'	2.64	104.95	100.98
2	F	903	ATP	O2G-PG-O3B	2.59	113.32	104.64
2	F	901	ATP	O2'-C2'-C3'	2.55	120.08	111.82
2	A	901	ATP	C3'-C2'-C1'	2.54	104.80	100.98
2	B	903	ATP	PB-O3B-PG	-2.43	124.50	132.83
2	E	901	ATP	O2G-PG-O3B	2.43	112.78	104.64
2	E	903	ATP	N6-C6-N1	-2.37	113.65	118.57
2	C	903	ATP	N6-C6-N1	-2.36	113.67	118.57
2	B	901	ATP	O2'-C2'-C3'	2.32	119.33	111.82
2	A	901	ATP	N6-C6-N1	-2.21	113.98	118.57
2	D	903	ATP	N6-C6-N1	-2.16	114.08	118.57
2	C	901	ATP	O2G-PG-O3B	2.16	111.88	104.64
2	D	901	ATP	N6-C6-N1	-2.15	114.11	118.57
2	B	901	ATP	O2G-PG-O3B	2.13	111.79	104.64
2	F	901	ATP	N6-C6-N1	-2.11	114.19	118.57
2	B	903	ATP	N6-C6-N1	-2.11	114.19	118.57
2	B	901	ATP	N6-C6-N1	-2.11	114.19	118.57
2	D	901	ATP	O2'-C2'-C3'	2.04	118.41	111.82
2	A	903	ATP	N6-C6-N1	-2.02	114.39	118.57
2	F	901	ATP	PB-O3B-PG	-2.01	125.91	132.83
2	D	901	ATP	C3'-C2'-C1'	2.00	104.00	100.98

There are no chirality outliers.

All (95) torsion outliers are listed below:

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

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

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

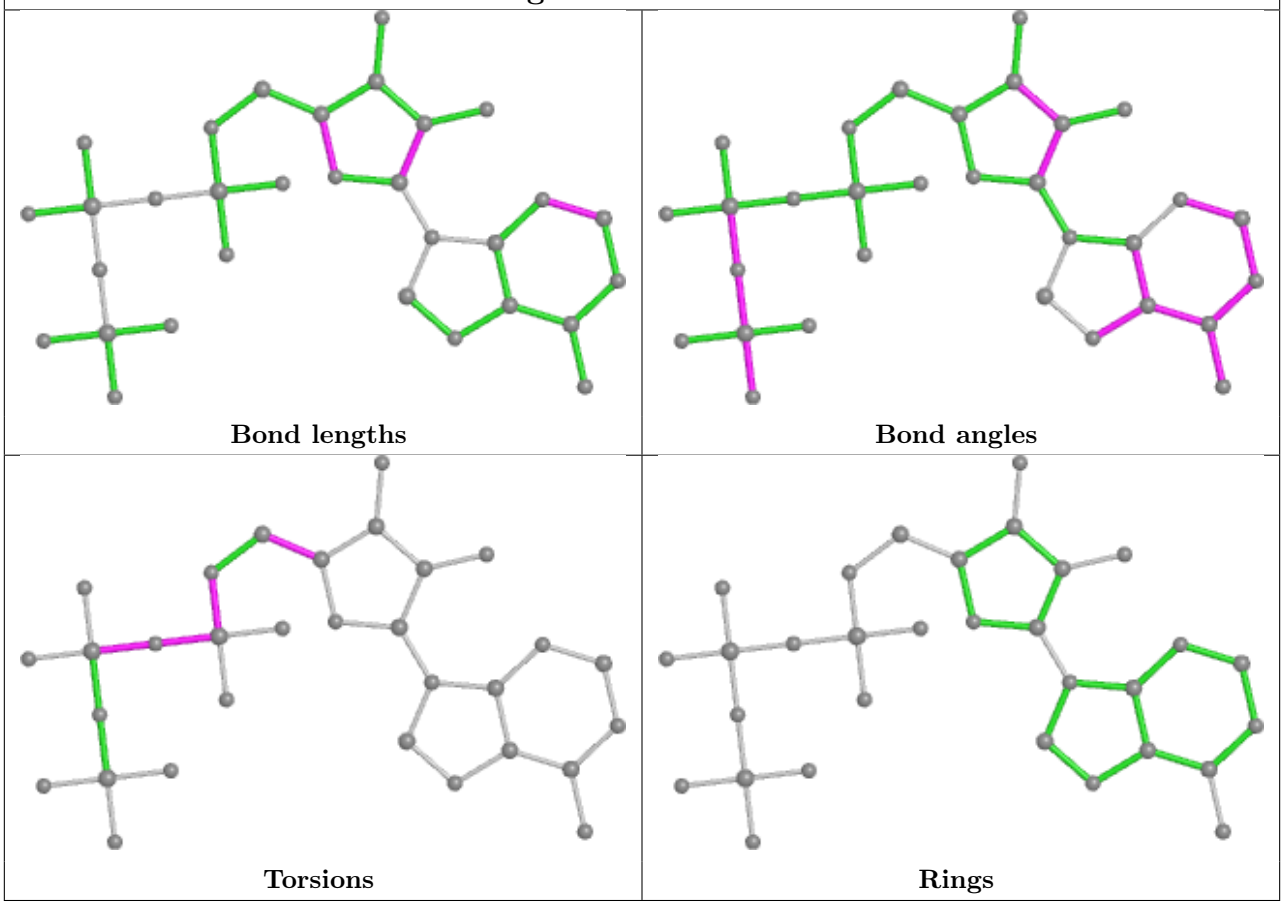
There are no ring outliers.

12 monomers are involved in 39 short contacts:

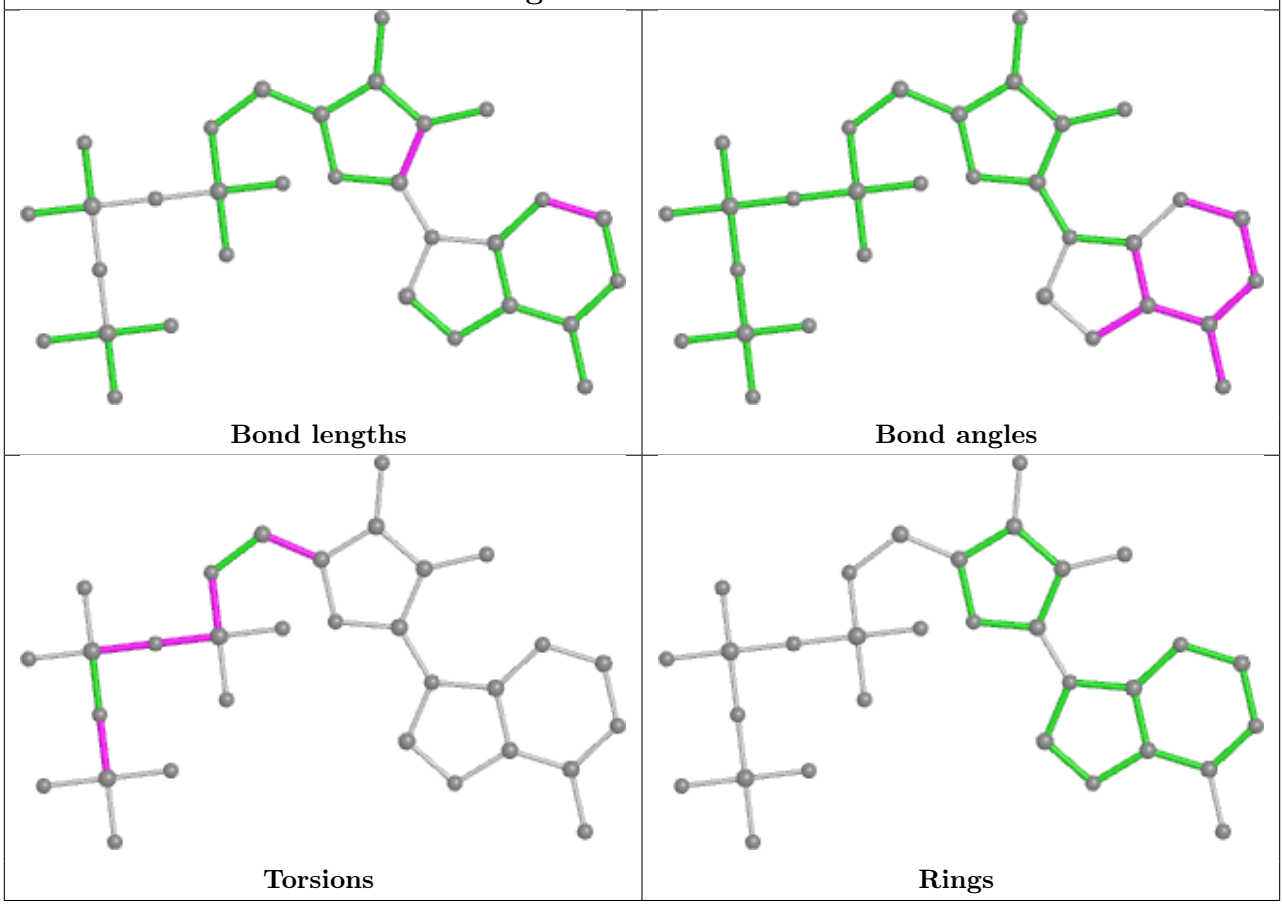
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	903	ATP	4	0
2	C	903	ATP	1	0
2	B	903	ATP	2	0
2	B	901	ATP	4	0
2	E	901	ATP	5	0
2	D	903	ATP	2	0
2	F	903	ATP	6	0
2	C	901	ATP	1	0
2	A	903	ATP	2	0
2	D	901	ATP	4	0
2	A	901	ATP	3	0
2	F	901	ATP	5	0

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 then 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.

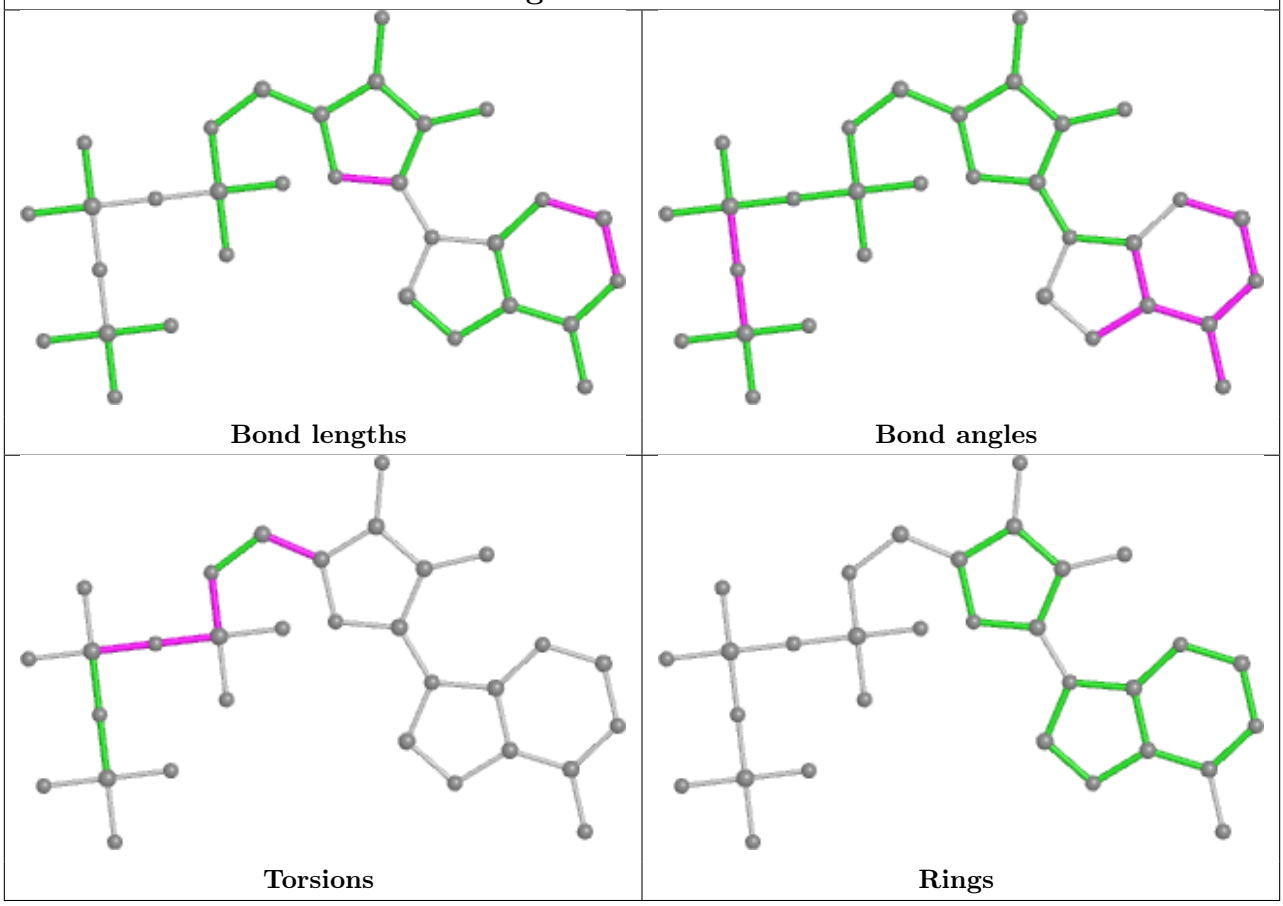
Ligand ATP E 903



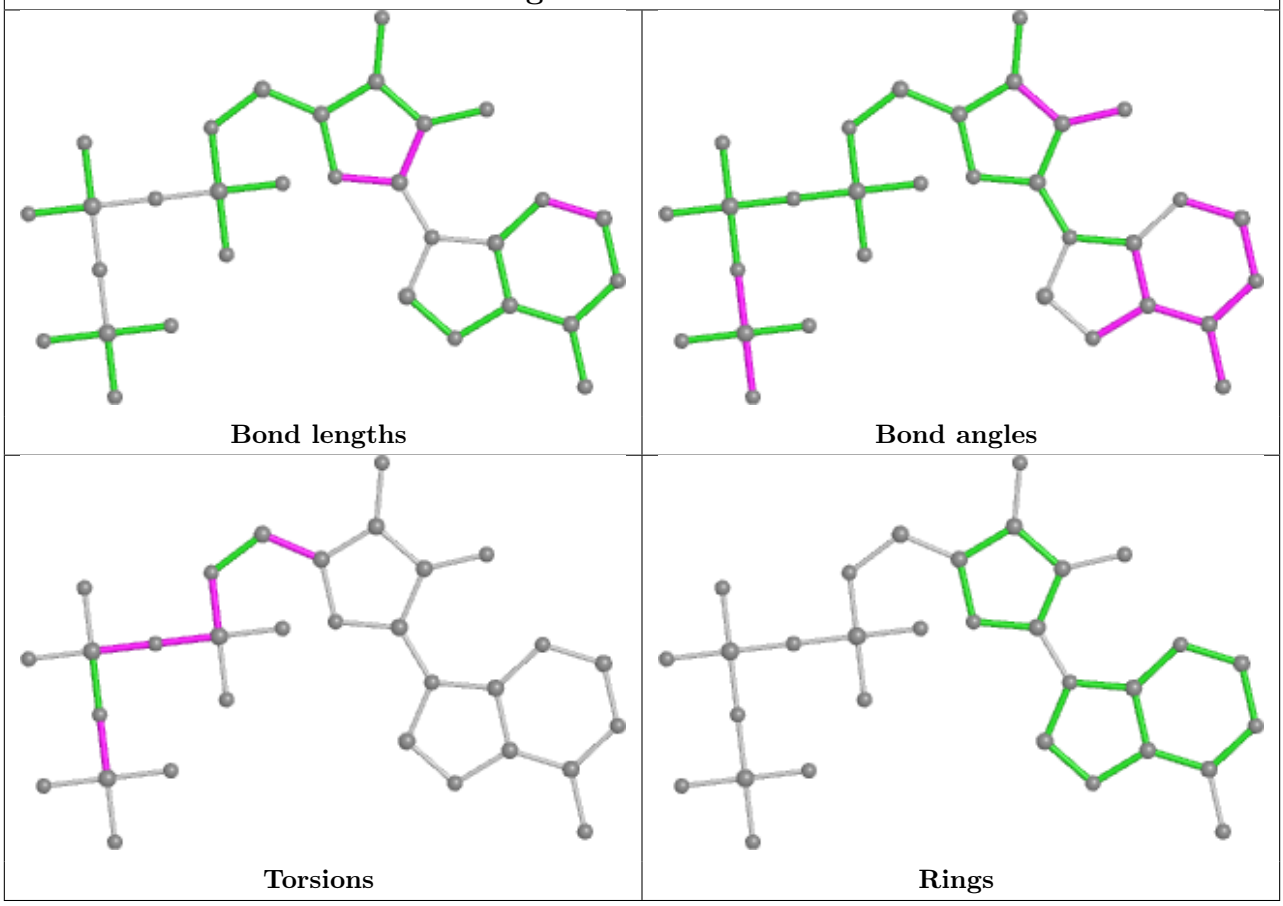
Ligand ATP C 903



Ligand ATP B 903



Ligand ATP B 901



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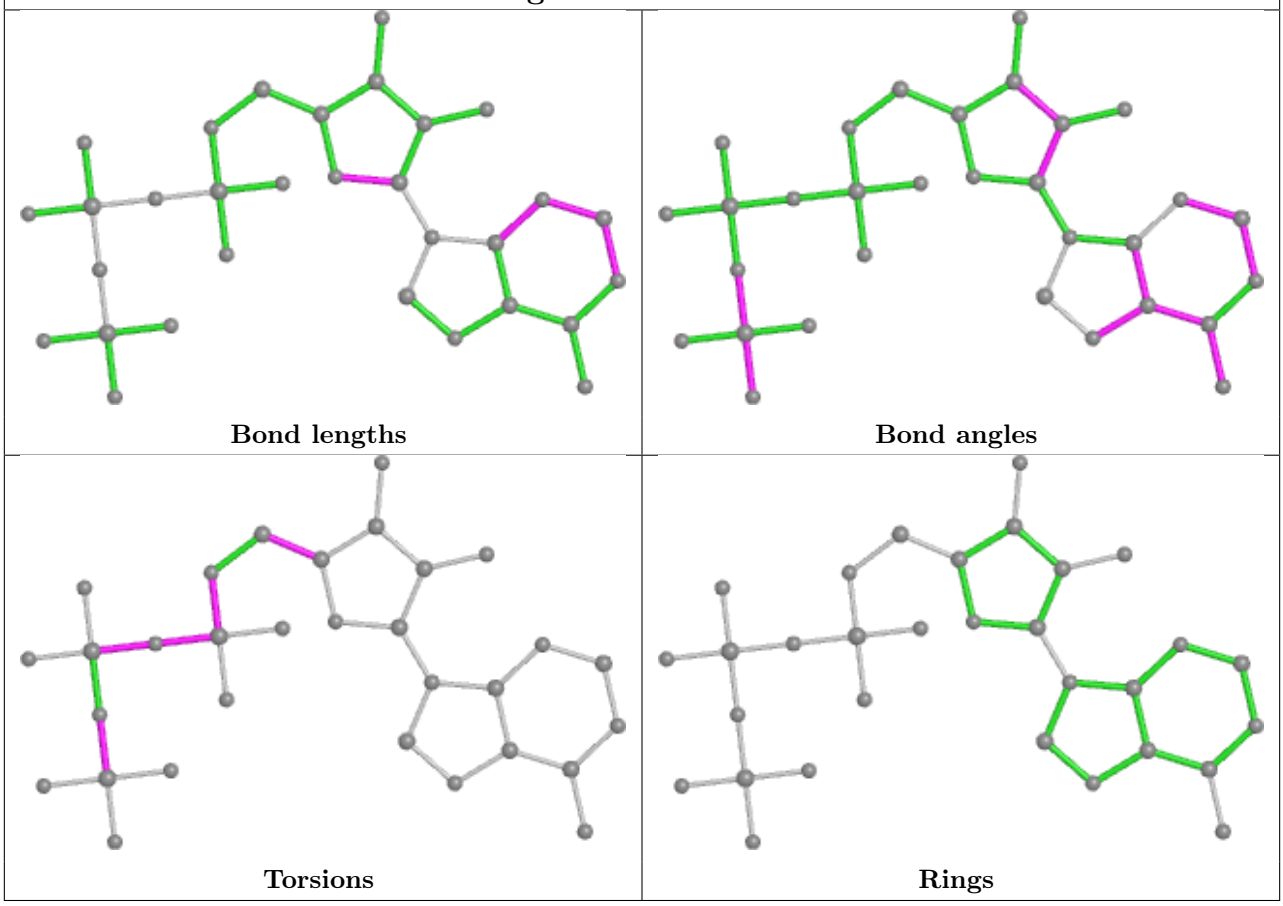
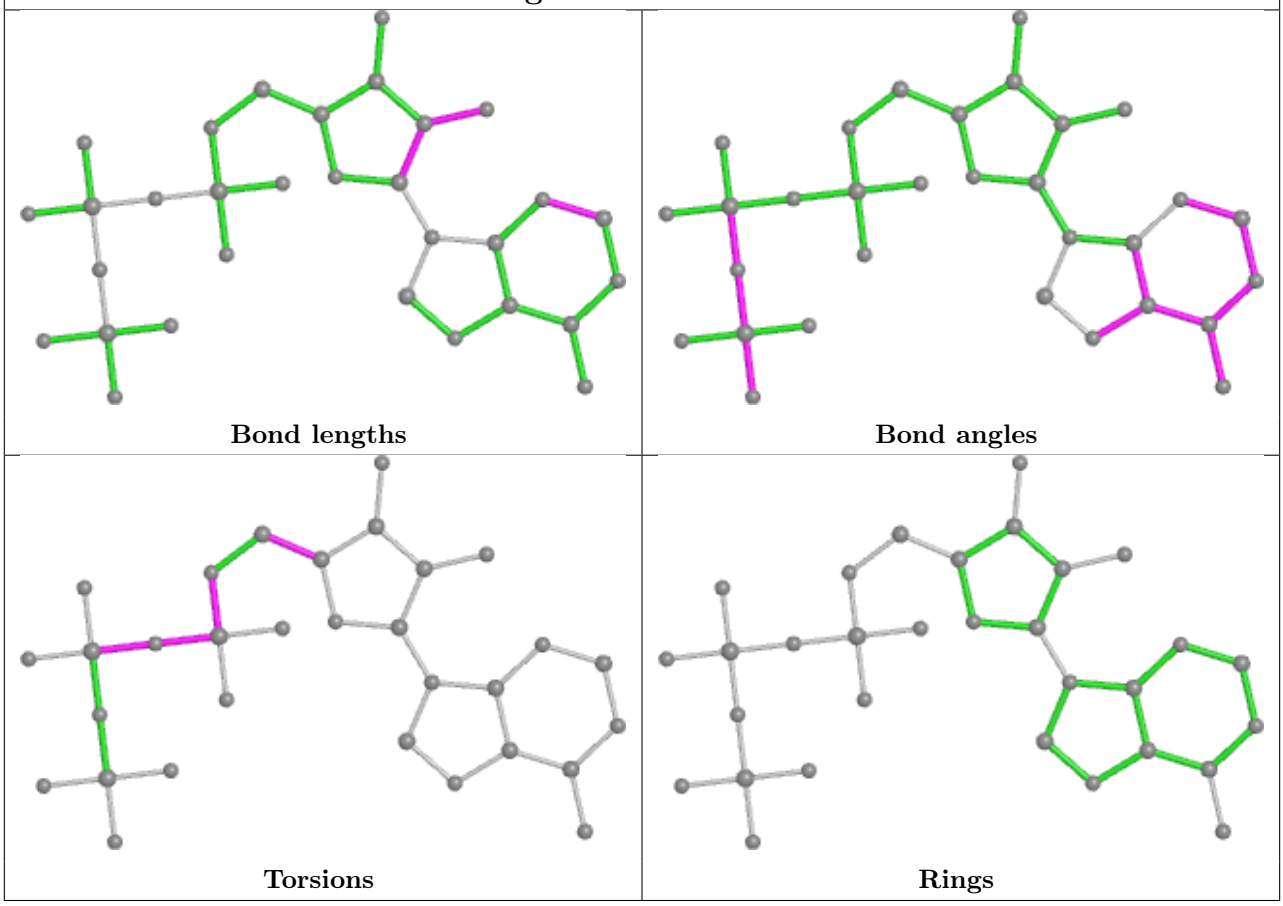


Ligand ATP D 903



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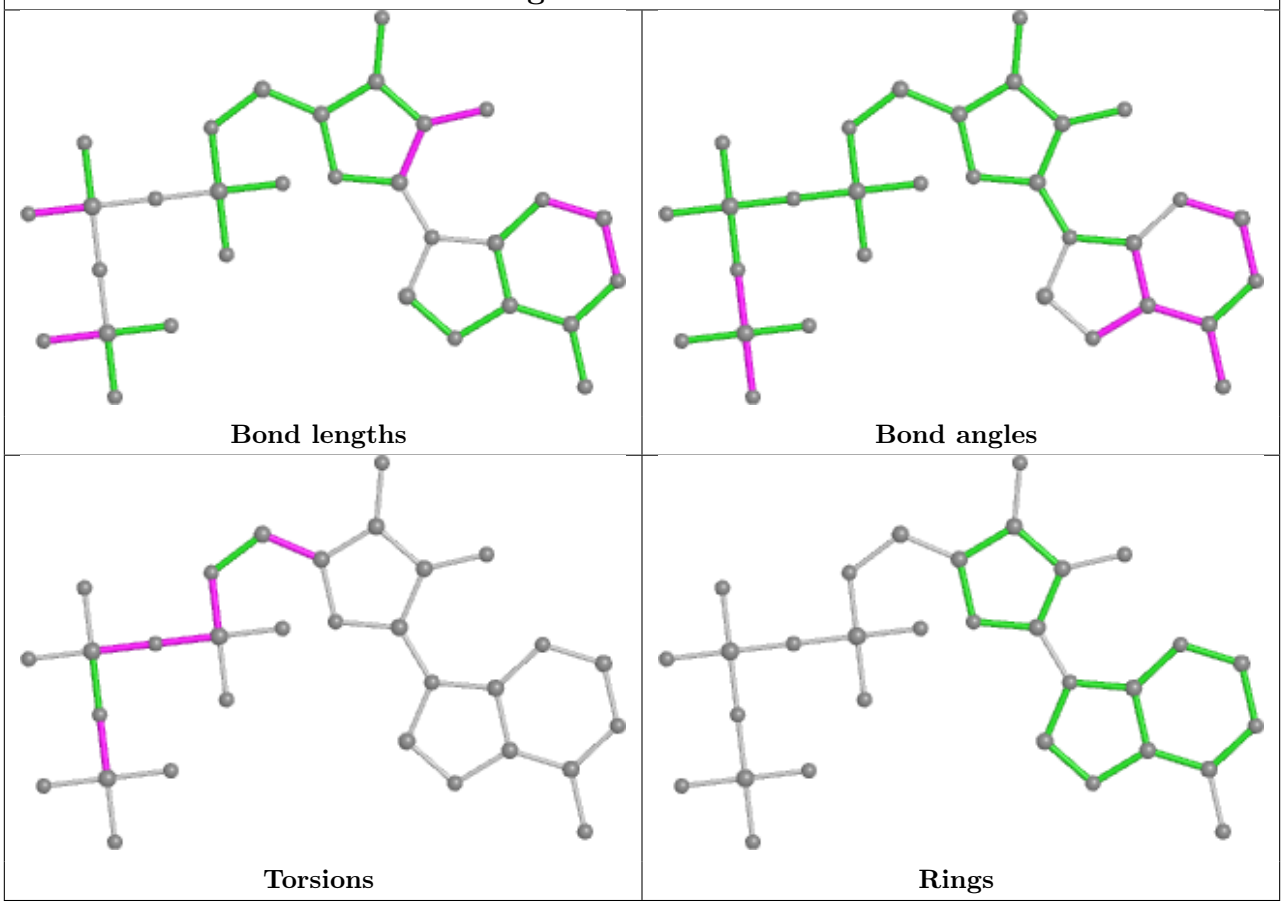

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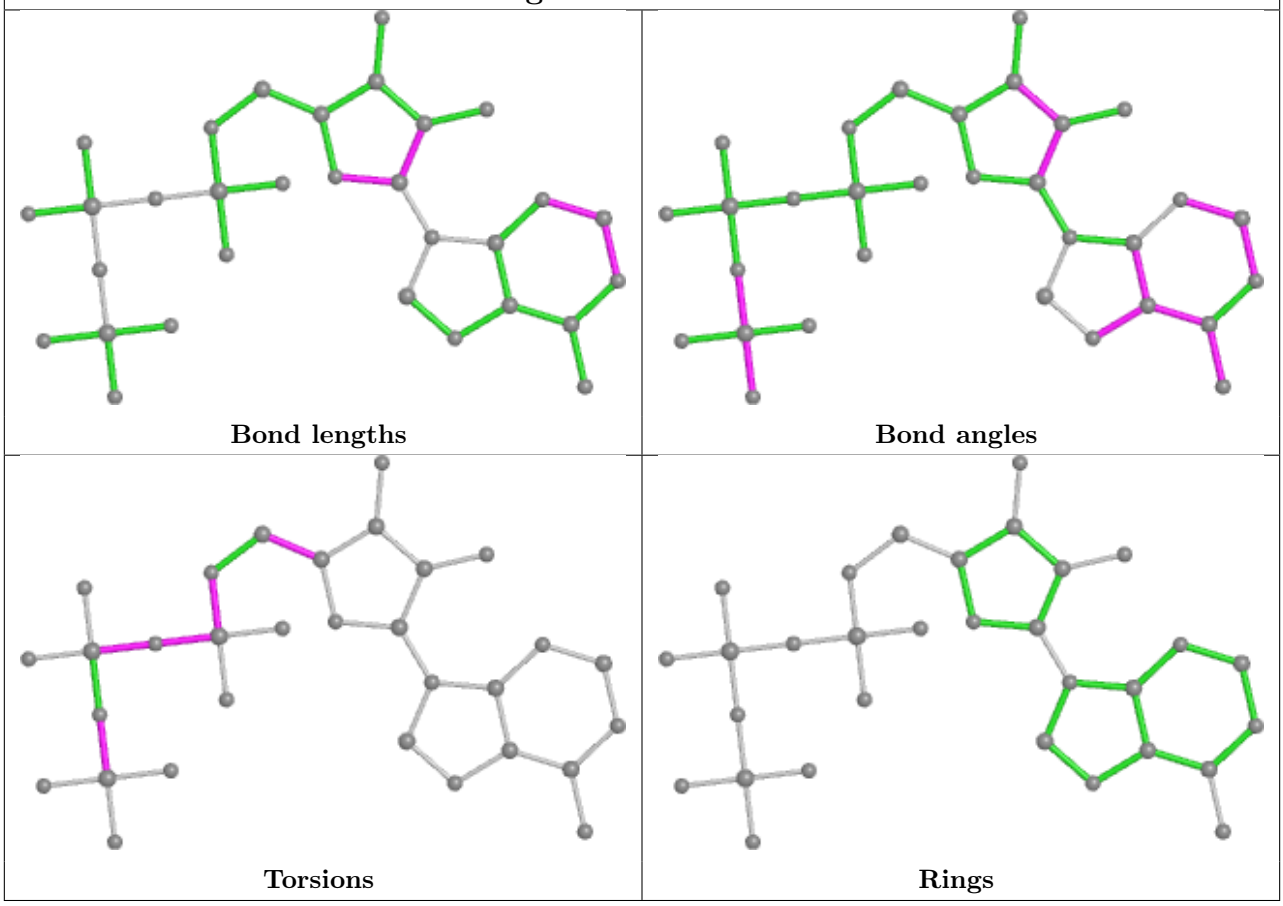

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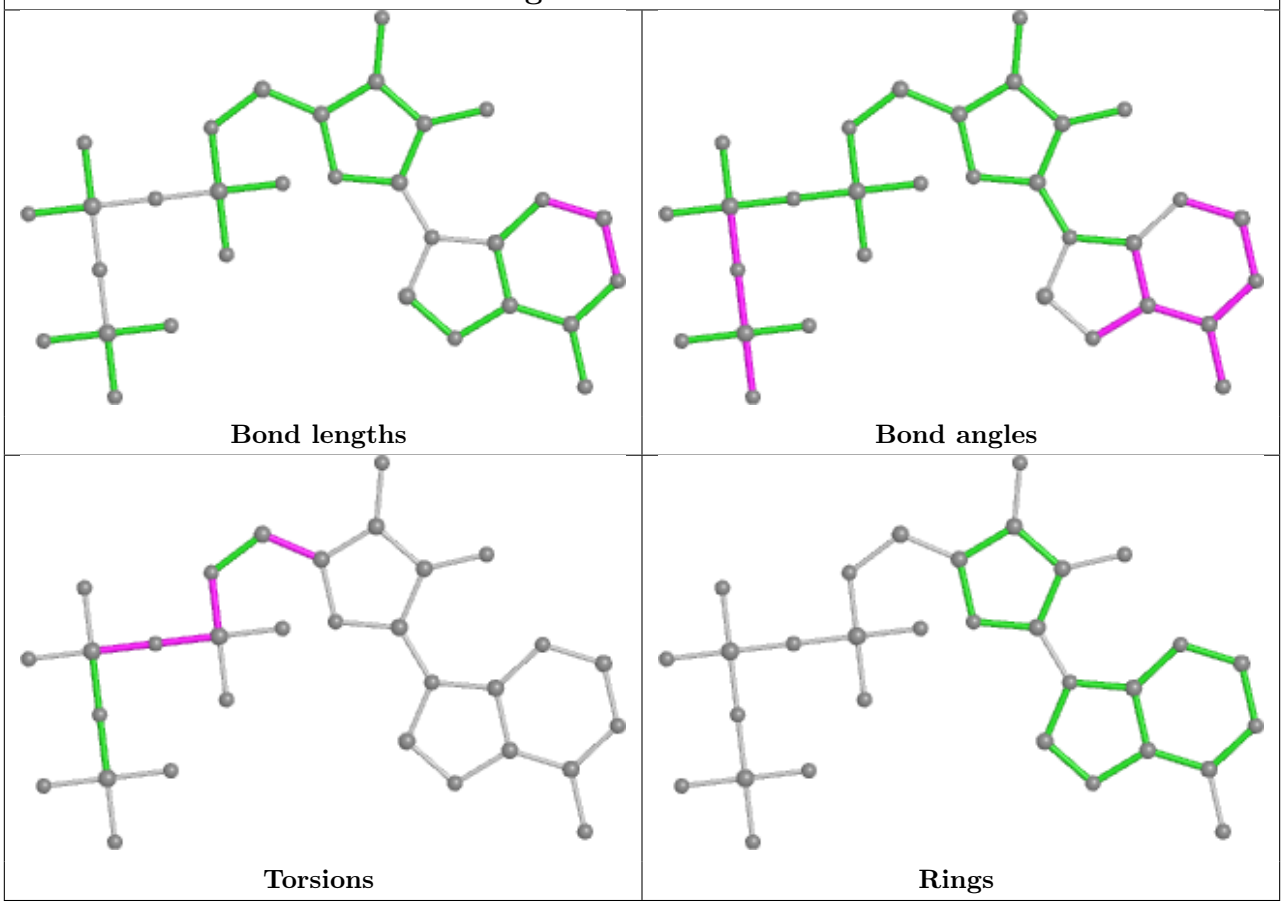

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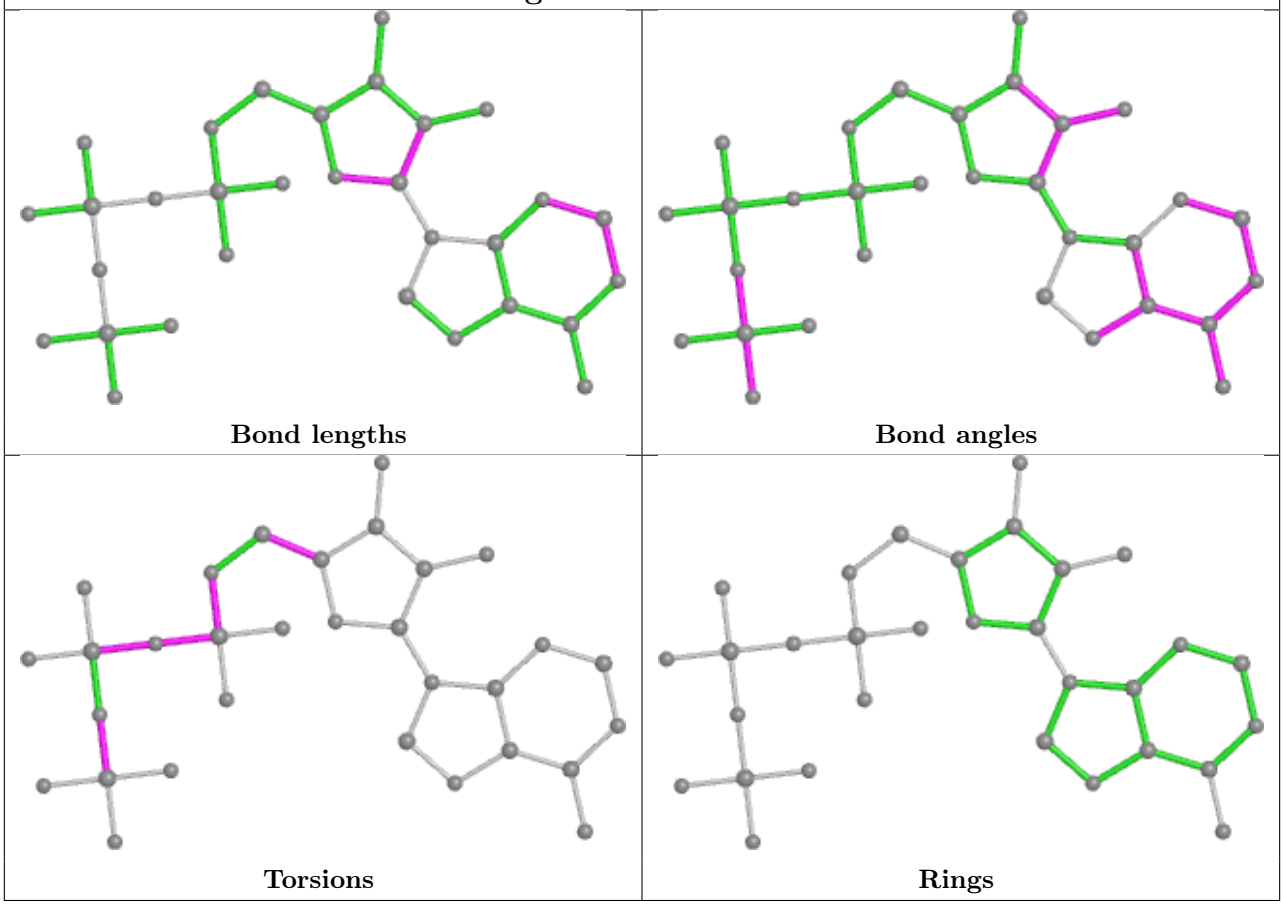

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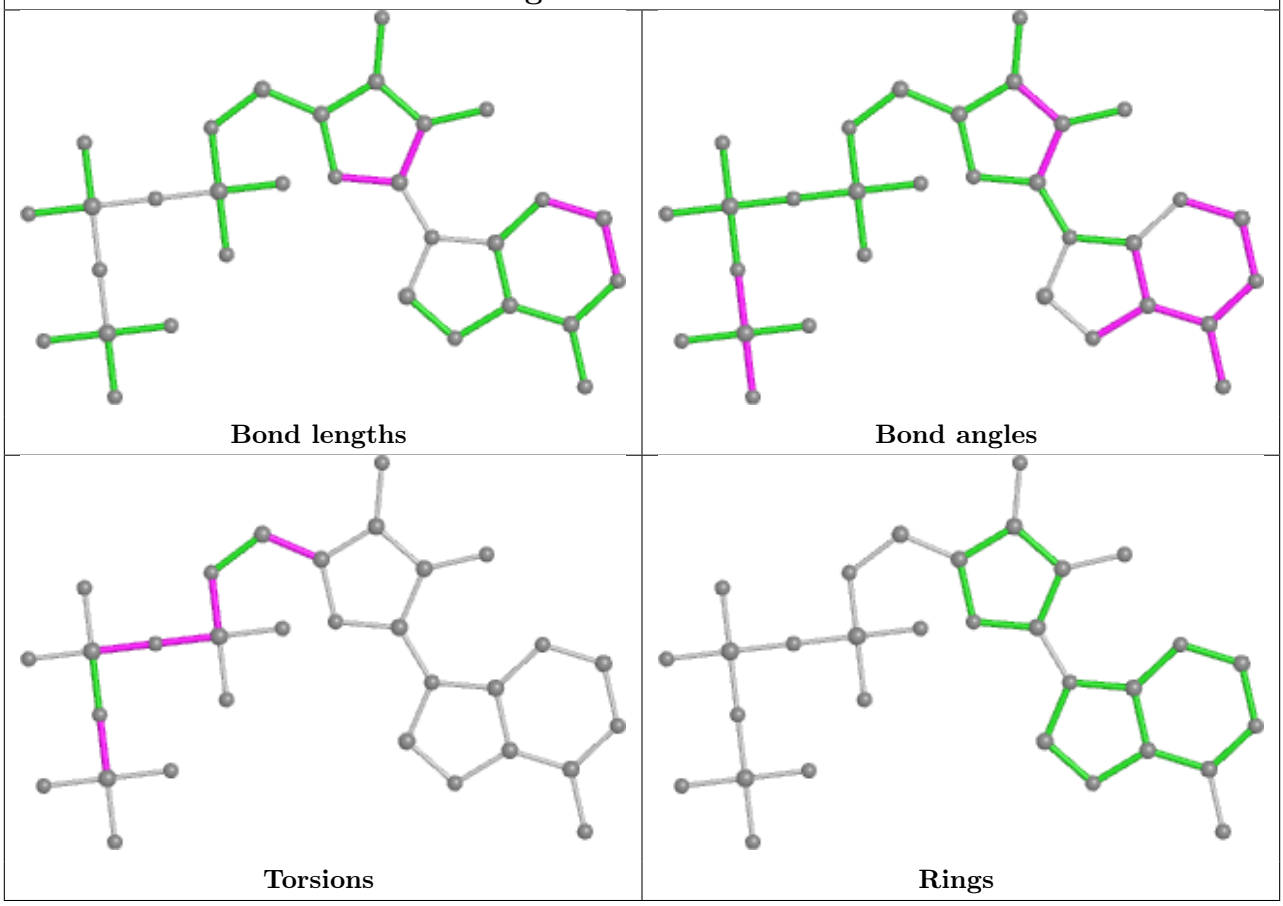

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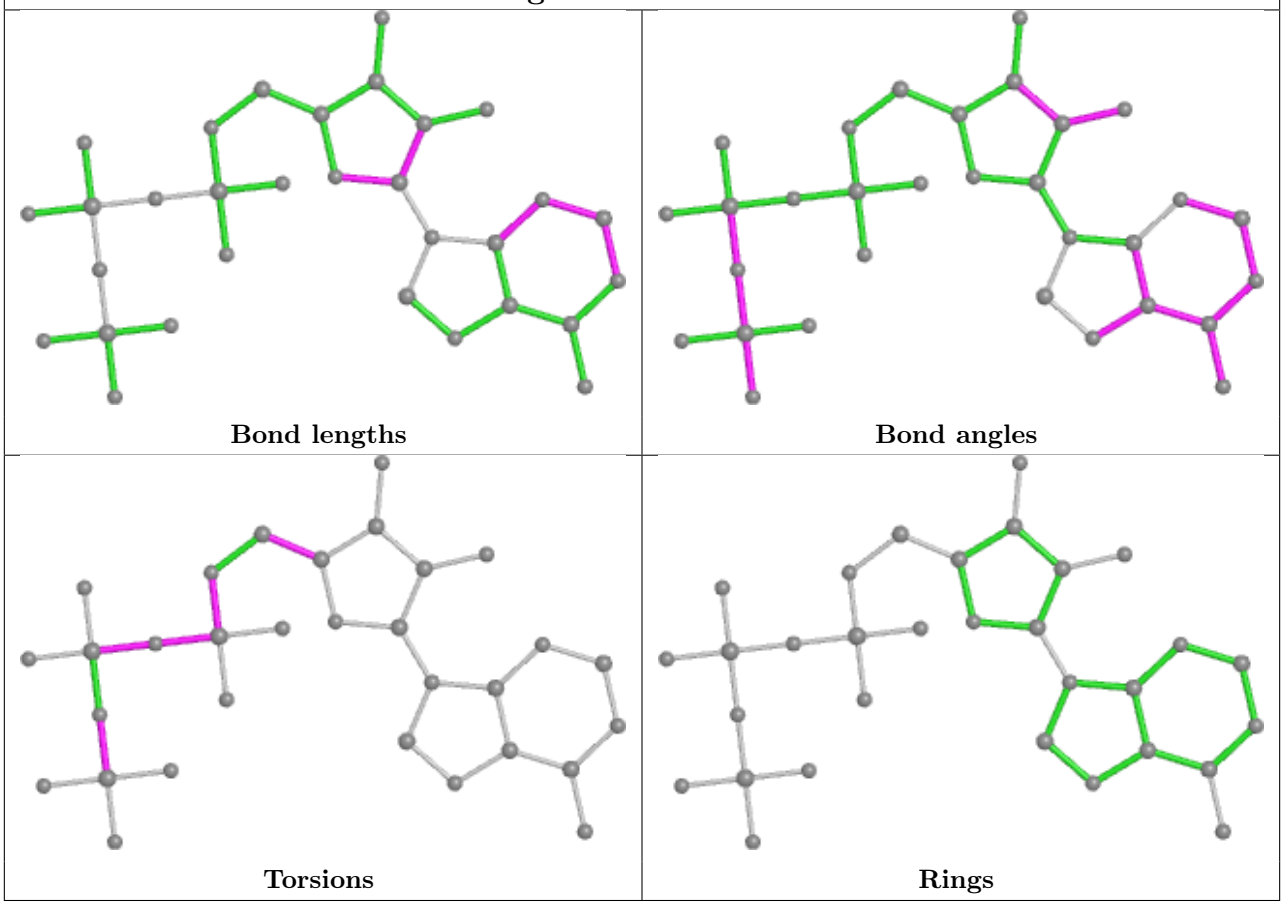

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	483/519 (93%)	0.27	32 (6%)	18	14	34, 74, 118, 149	0
1	B	483/519 (93%)	0.37	35 (7%)	15	11	46, 78, 120, 159	0
1	C	483/519 (93%)	0.16	28 (5%)	23	19	33, 67, 116, 160	0
1	D	483/519 (93%)	-0.08	18 (3%)	41	37	25, 54, 101, 148	0
1	E	483/519 (93%)	0.02	25 (5%)	27	23	18, 57, 97, 147	0
1	F	483/519 (93%)	0.06	23 (4%)	30	27	24, 65, 106, 143	0
All	All	2898/3114 (93%)	0.13	161 (5%)	24	20	18, 66, 114, 160	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	120	GLY	11.4
1	C	118	VAL	9.0
1	B	116	GLU	8.7
1	F	154	TYR	7.9
1	B	117	VAL	7.8
1	B	121	PHE	7.7
1	A	120	GLY	6.9
1	C	119	GLY	6.7
1	A	154	TYR	6.5
1	A	121	PHE	6.1
1	B	118	VAL	6.1
1	B	154	TYR	5.9
1	E	117	VAL	5.8
1	E	154	TYR	5.4
1	D	15	HIS	5.4
1	E	120	GLY	5.3
1	D	117	VAL	5.3
1	C	117	VAL	5.0
1	A	153	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	118	VAL	4.9
1	A	475	LYS	4.8
1	D	116	GLU	4.7
1	D	115	GLN	4.7
1	B	16	GLN	4.6
1	B	14	GLU	4.5
1	D	120	GLY	4.4
1	D	154	TYR	4.4
1	D	113	GLU	4.4
1	C	423	HIS	4.3
1	B	115	GLN	4.3
1	E	118	VAL	4.3
1	F	117	VAL	4.2
1	B	122	ASP	4.2
1	A	114	GLY	4.2
1	B	88	ARG	4.2
1	B	132	TYR	4.2
1	D	119	GLY	4.1
1	A	115	GLN	4.0
1	A	341	GLN	4.0
1	C	16	GLN	3.9
1	D	16	GLN	3.9
1	A	16	GLN	3.9
1	C	116	GLU	3.9
1	E	113	GLU	3.9
1	C	152	GLN	3.9
1	C	154	TYR	3.8
1	C	121	PHE	3.7
1	E	115	GLN	3.6
1	C	115	GLN	3.6
1	D	121	PHE	3.5
1	F	497	ILE	3.5
1	C	153	GLN	3.4
1	F	119	GLY	3.4
1	F	485	ASN	3.4
1	A	309	LYS	3.3
1	A	496	ARG	3.3
1	E	423	HIS	3.3
1	E	116	GLU	3.3
1	B	162	ARG	3.3
1	A	342	ASN	3.3
1	B	497	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	121	PHE	3.3
1	A	340	ARG	3.3
1	A	116	GLU	3.2
1	E	121	PHE	3.2
1	C	145	ASP	3.2
1	B	15	HIS	3.2
1	F	496	ARG	3.1
1	E	153	GLN	3.1
1	A	255	THR	3.1
1	F	155	ASP	3.1
1	B	119	GLY	3.1
1	F	257	ARG	3.0
1	D	484	ARG	3.0
1	D	471	MET	3.0
1	D	114	GLY	3.0
1	B	423	HIS	3.0
1	C	114	GLY	2.9
1	C	181	THR	2.9
1	F	156	ALA	2.9
1	A	378	ASP	2.9
1	E	112	PRO	2.9
1	E	119	GLY	2.9
1	F	153	GLN	2.8
1	E	114	GLY	2.8
1	C	173	GLN	2.8
1	C	17	ALA	2.8
1	B	342	ASN	2.7
1	B	153	GLN	2.7
1	A	117	VAL	2.7
1	D	112	PRO	2.7
1	A	471	MET	2.6
1	F	255	THR	2.6
1	F	321	ARG	2.6
1	A	14	GLU	2.6
1	C	53	THR	2.6
1	B	181	THR	2.6
1	A	113	GLU	2.6
1	B	17	ALA	2.6
1	E	188	TYR	2.6
1	E	321	ARG	2.5
1	F	253	ARG	2.5
1	B	180	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	255	THR	2.5
1	F	423	HIS	2.5
1	A	329	TYR	2.5
1	C	143	SER	2.5
1	B	258	SER	2.5
1	A	256	GLN	2.5
1	E	309	LYS	2.5
1	E	329	TYR	2.5
1	B	155	ASP	2.4
1	E	474	ASP	2.4
1	B	309	LYS	2.4
1	C	188	TYR	2.4
1	E	484	ARG	2.4
1	F	334	ASP	2.4
1	B	484	ARG	2.4
1	E	337	GLU	2.4
1	B	158	SER	2.4
1	C	15	HIS	2.4
1	B	143	SER	2.4
1	A	15	HIS	2.3
1	E	111	ASP	2.3
1	F	311	ARG	2.3
1	C	144	ILE	2.3
1	B	496	ARG	2.3
1	C	113	GLU	2.3
1	F	120	GLY	2.3
1	C	124	SER	2.3
1	B	92	TRP	2.2
1	E	475	LYS	2.2
1	F	92	TRP	2.2
1	F	340	ARG	2.2
1	C	140	ARG	2.2
1	B	91	GLY	2.2
1	A	188	TYR	2.2
1	D	14	GLU	2.2
1	A	241	ASP	2.2
1	A	436	THR	2.2
1	B	179	VAL	2.2
1	C	146	SER	2.2
1	F	342	ASN	2.1
1	E	333	MET	2.1
1	C	332	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	249	LEU	2.1
1	F	116	GLU	2.1
1	B	251	ALA	2.1
1	E	343	LEU	2.1
1	E	342	ASN	2.1
1	A	295	THR	2.1
1	A	368	ASN	2.1
1	C	189	GLY	2.1
1	D	53	THR	2.0
1	B	99	ASP	2.0
1	B	311	ARG	2.0
1	D	111	ASP	2.0
1	A	311	ARG	2.0
1	A	17	ALA	2.0
1	A	293	GLY	2.0
1	A	484	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	C	431	10/11	0.74	0.30	79,84,100,100	0
1	SEP	E	431	10/11	0.83	0.23	57,65,81,82	0
1	SEP	D	431	10/11	0.84	0.24	69,77,94,96	0
1	SEP	B	431	10/11	0.85	0.23	81,88,100,102	0
1	SEP	F	431	10/11	0.86	0.22	74,79,89,90	0
1	SEP	A	431	10/11	0.89	0.18	78,83,94,95	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

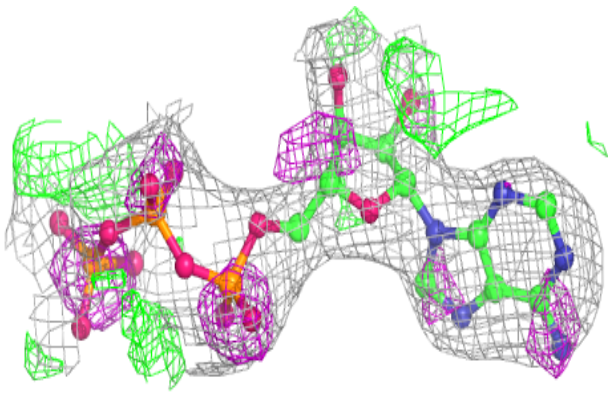
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

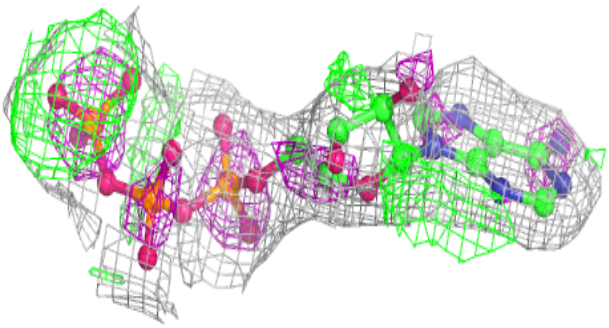
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	527	1/1	0.29	0.33	29,29,29,29	0
3	MG	F	801	1/1	0.50	0.38	31,31,31,31	0
3	MG	C	801	1/1	0.56	0.51	56,56,56,56	0
3	MG	A	801	1/1	0.57	0.56	64,64,64,64	0
3	MG	B	801	1/1	0.61	0.51	69,69,69,69	0
3	MG	C	520	1/1	0.67	0.41	99,99,99,99	0
3	MG	B	701	1/1	0.70	0.52	84,84,84,84	0
3	MG	D	802	1/1	0.76	0.37	35,35,35,35	0
3	MG	D	701	1/1	0.80	0.85	61,61,61,61	0
3	MG	A	701	1/1	0.84	0.38	85,85,85,85	0
3	MG	F	802	1/1	0.86	0.56	91,91,91,91	0
3	MG	E	801	1/1	0.87	0.45	73,73,73,73	0
3	MG	F	701	1/1	0.87	0.60	54,54,54,54	0
2	ATP	C	903	31/31	0.87	0.20	32,33,49,53	0
3	MG	D	702	1/1	0.87	0.29	75,75,75,75	0
2	ATP	A	901	31/31	0.89	0.27	70,82,84,85	0
2	ATP	F	901	31/31	0.89	0.25	70,79,84,85	0
2	ATP	A	903	31/31	0.90	0.19	28,47,55,55	0
3	MG	A	802	1/1	0.90	0.25	75,75,75,75	0
2	ATP	B	903	31/31	0.90	0.17	57,66,69,69	0
2	ATP	D	903	31/31	0.91	0.16	10,17,27,30	0
2	ATP	E	901	31/31	0.91	0.23	63,70,77,77	0
3	MG	E	701	1/1	0.92	0.48	49,49,49,49	0
2	ATP	B	901	31/31	0.92	0.23	69,73,77,78	0
3	MG	F	702	1/1	0.93	0.30	80,80,80,80	0
2	ATP	C	901	31/31	0.94	0.17	41,44,53,56	0
3	MG	E	702	1/1	0.94	0.37	85,85,85,85	0
2	ATP	F	903	31/31	0.94	0.14	10,12,19,19	0
2	ATP	D	901	31/31	0.95	0.21	50,59,61,63	0
2	ATP	E	903	31/31	0.95	0.14	9,13,21,25	0

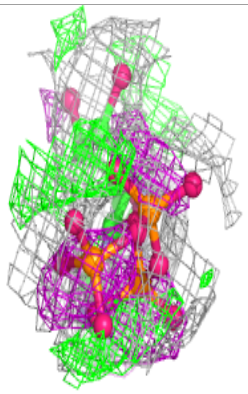
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP 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)

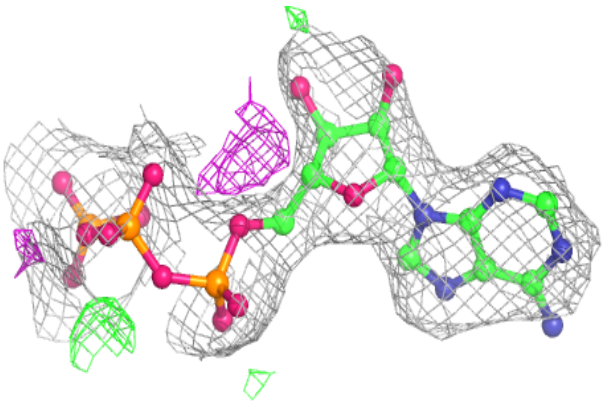


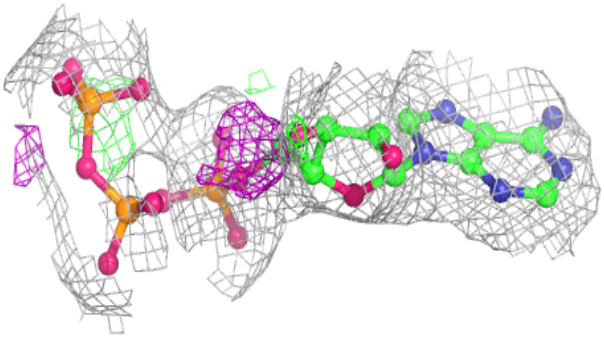


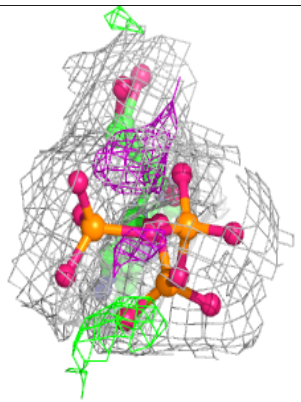


Electron density around ATP A 901:

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

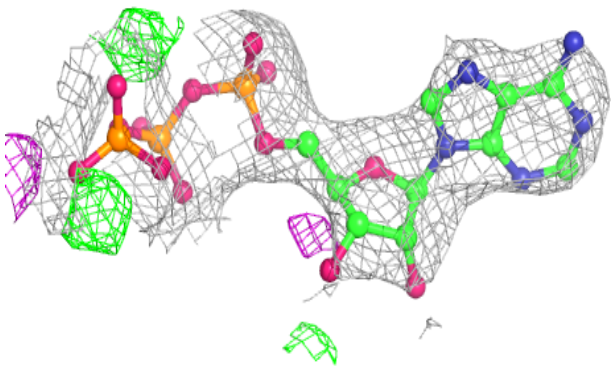


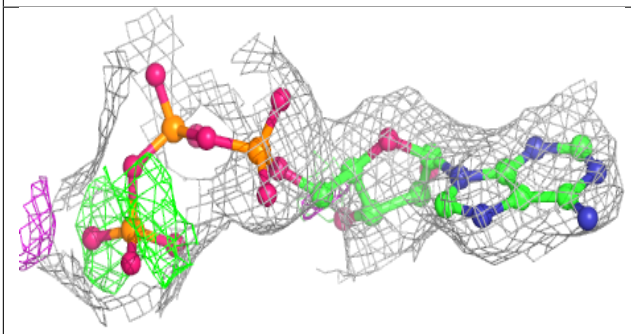


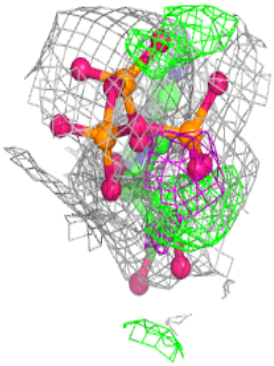


Electron density around ATP F 901:

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

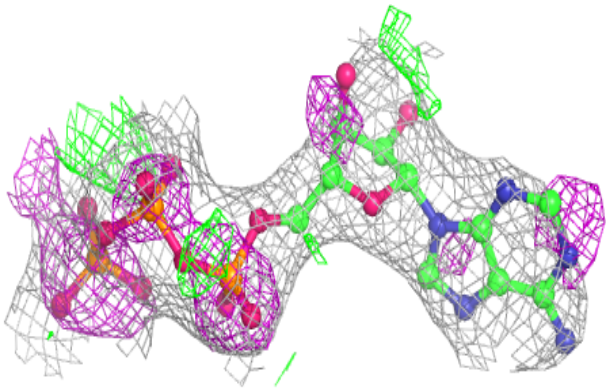


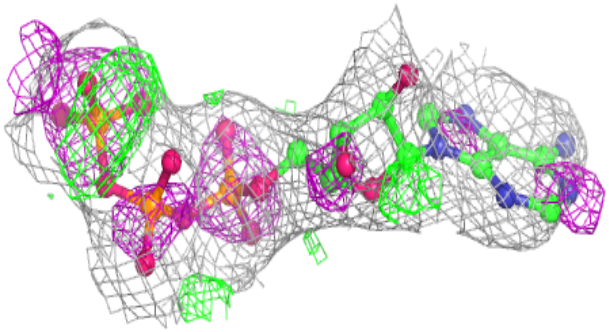


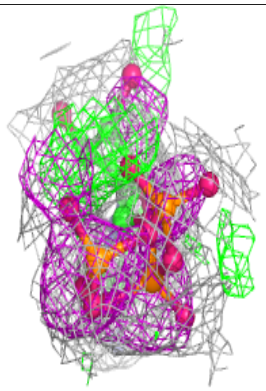


Electron density around ATP A 903:

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

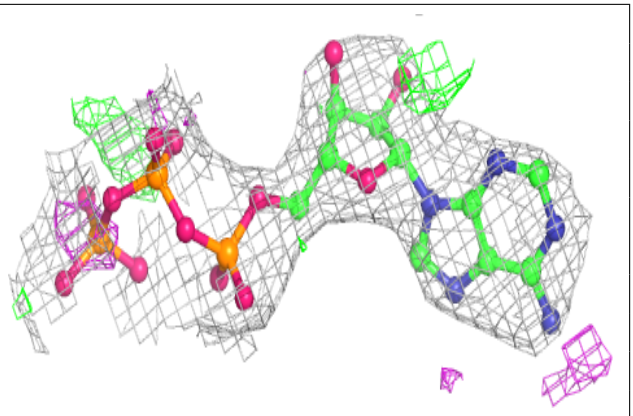


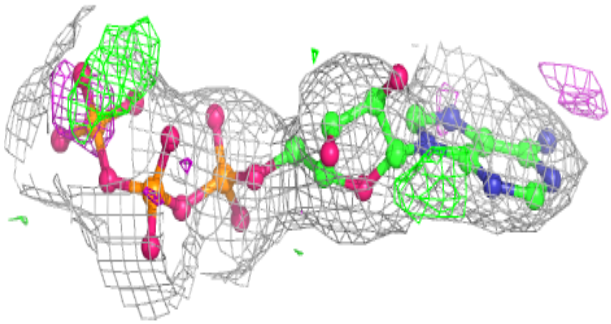


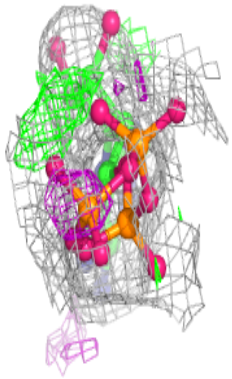


Electron density around ATP B 903:

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

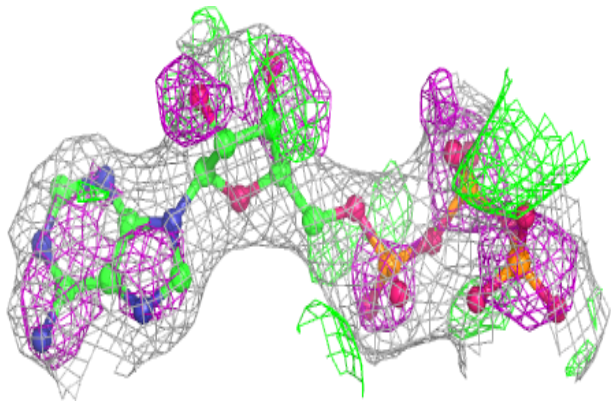


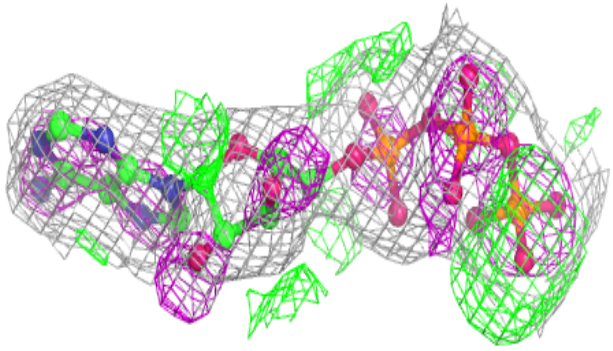


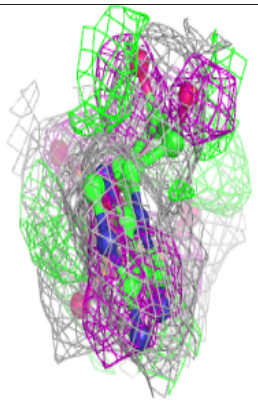


Electron density around ATP D 903:

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

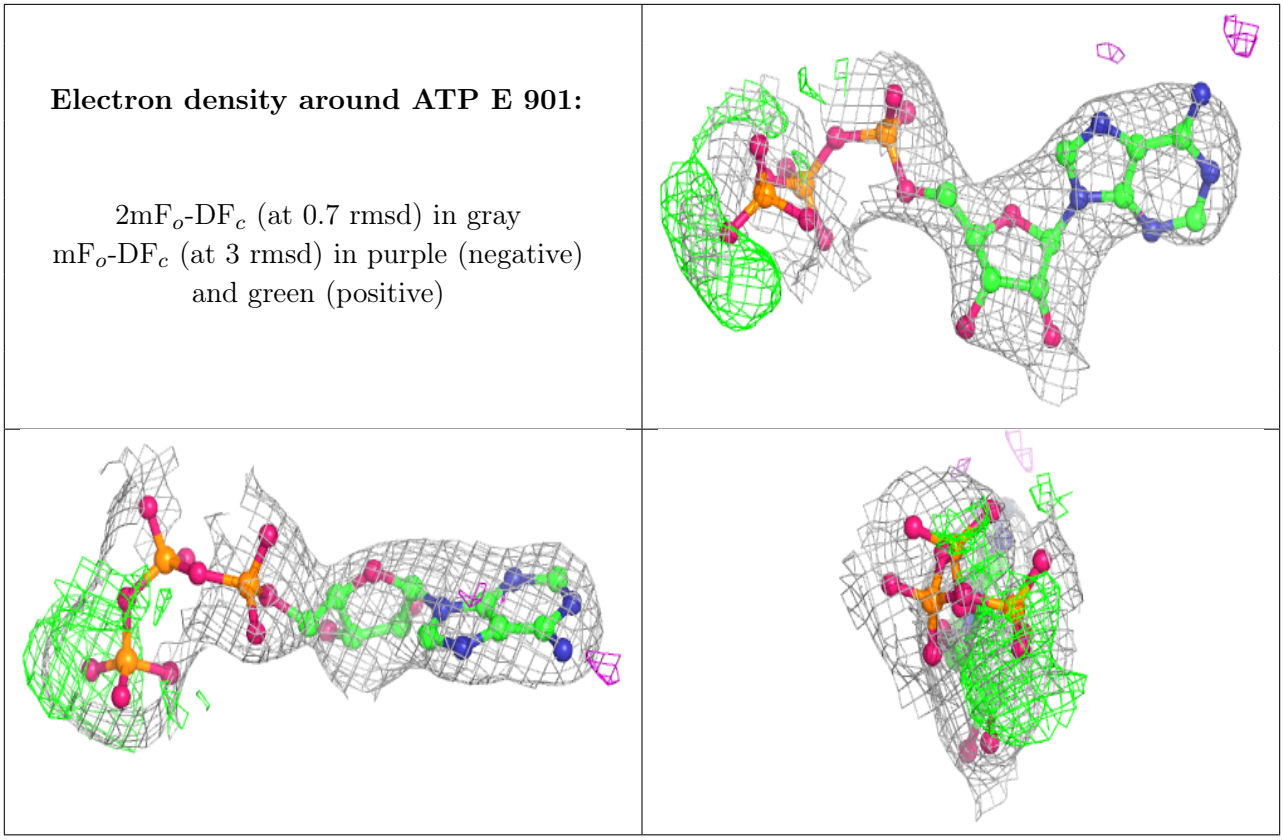






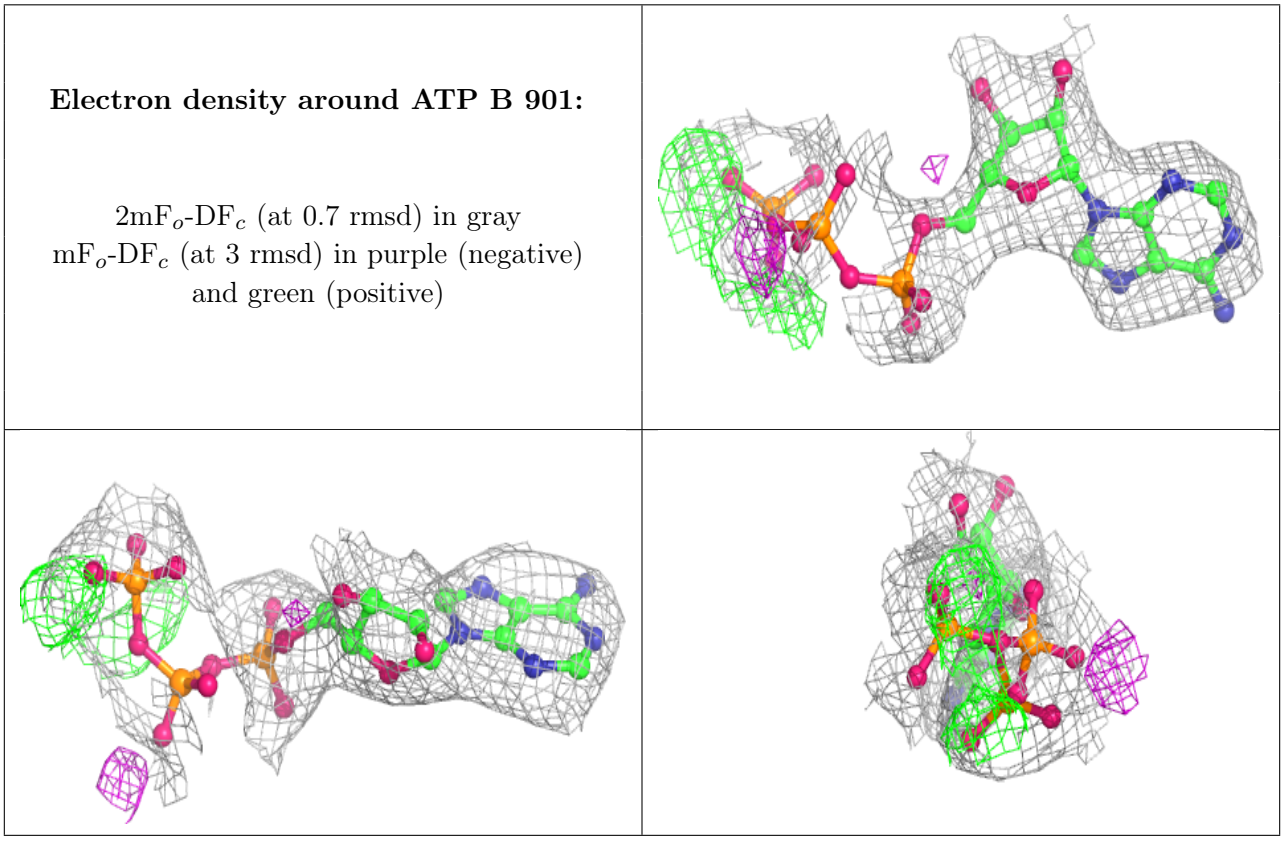
Electron density around ATP E 901:

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



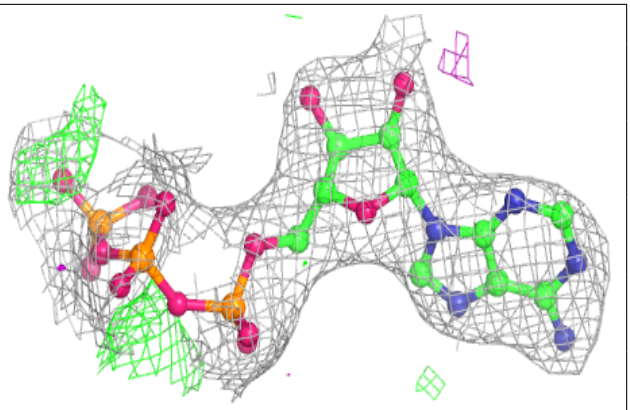
Electron density around ATP B 901:

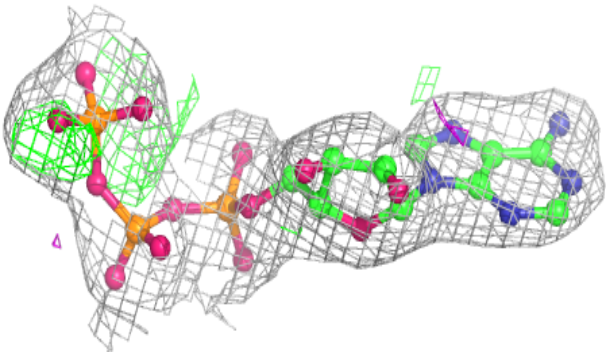
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

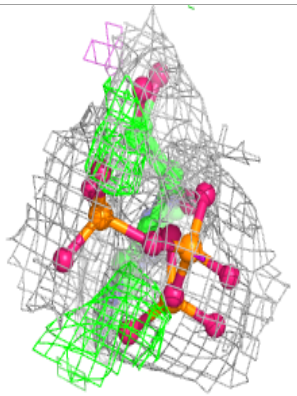


Electron density around ATP C 901:

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

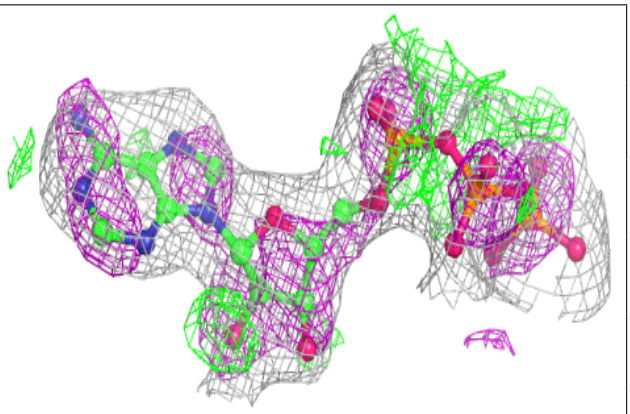


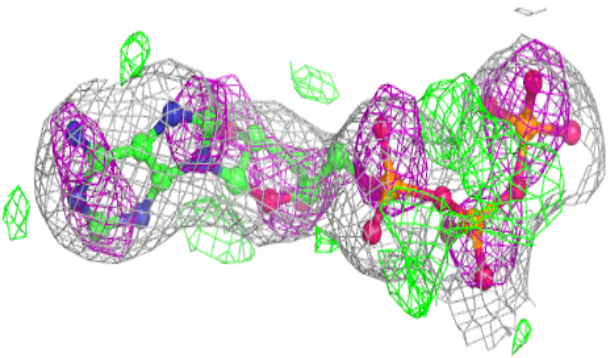


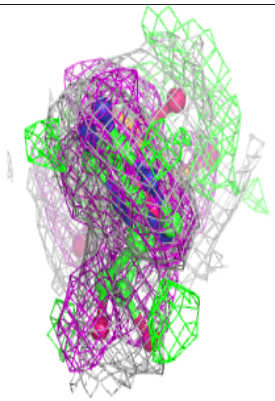


Electron density around ATP F 903:

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

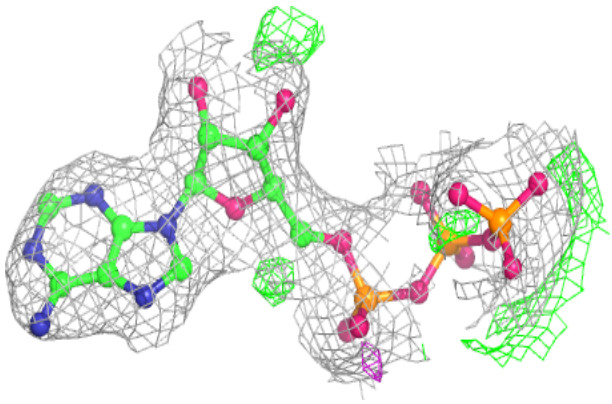


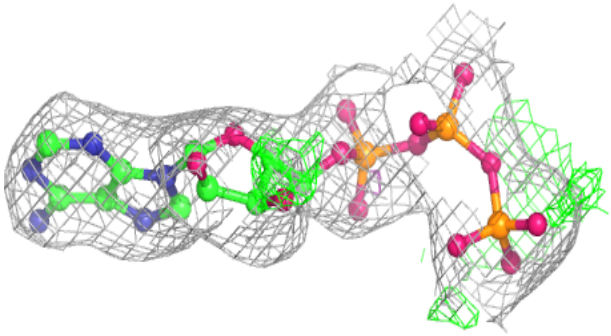


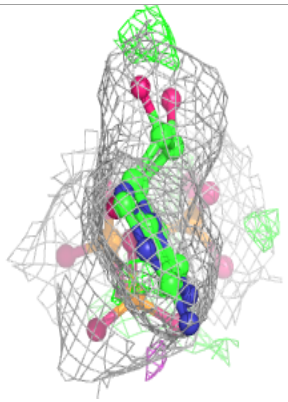


Electron density around ATP D 901:

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

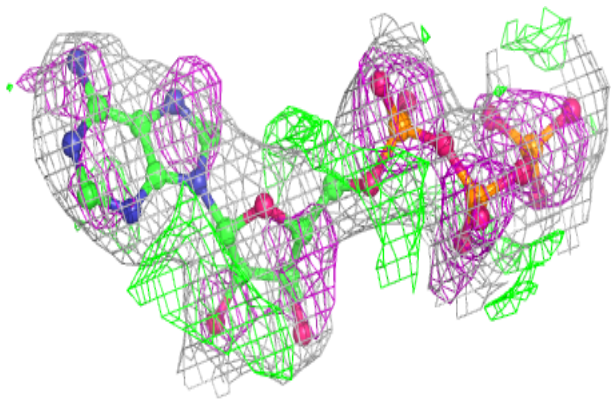


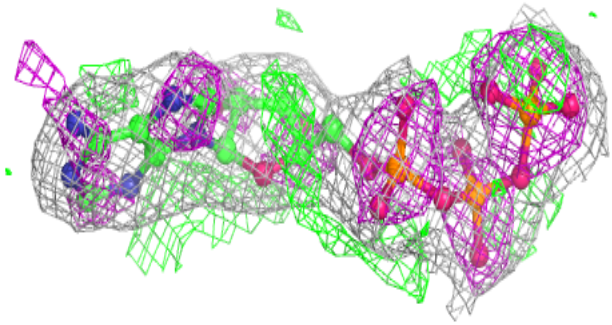


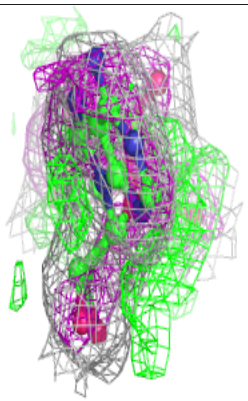


Electron density around ATP E 903:

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







6.5 Other polymers (i)

There are no such residues in this entry.