Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 04:14 AM EDT

PDB ID	:	3K0C
Title	:	Crystal structure of the phosphorylation-site double mutant S431A/T432E of the KaiC circadian clock protein
Authors	:	Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on	:	2009-09-24
Resolution	:	3.30 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:

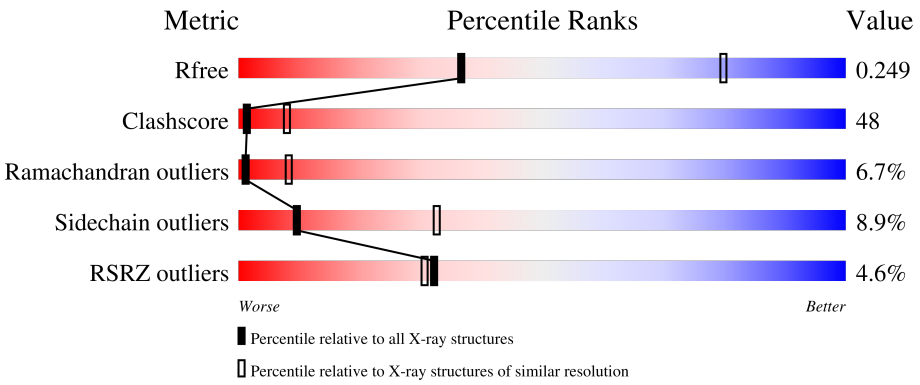
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	8% 33% 57% 6% • •
1	B	519	4% 31% 54% 9% 5%
1	E	519	3% 35% 50% 9% • 5%
1	F	519	5% 31% 55% 10% • •
2	C	519	3% 29% 56% 8% • 6%

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Mol	Chain	Length	Quality of chain
2	D	519	3% 36% 49% 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
1	TPO	A	426	-	-	X	-
1	TPO	B	426	-	-	X	-
1	TPO	F	426	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23919 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	506	3990	2510	701	763	1	15	0	0	0
1	B	491	3875	2440	678	741	1	15	0	0	0
1	E	492	3883	2446	679	742	1	15	0	0	0
1	F	506	3990	2510	701	763	1	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ALA	SER	engineered mutation	UNP Q79PF4
A	432	GLU	THR	engineered mutation	UNP Q79PF4
B	431	ALA	SER	engineered mutation	UNP Q79PF4
B	432	GLU	THR	engineered mutation	UNP Q79PF4
E	431	ALA	SER	engineered mutation	UNP Q79PF4
E	432	GLU	THR	engineered mutation	UNP Q79PF4
F	431	ALA	SER	engineered mutation	UNP Q79PF4
F	432	GLU	THR	engineered mutation	UNP Q79PF4

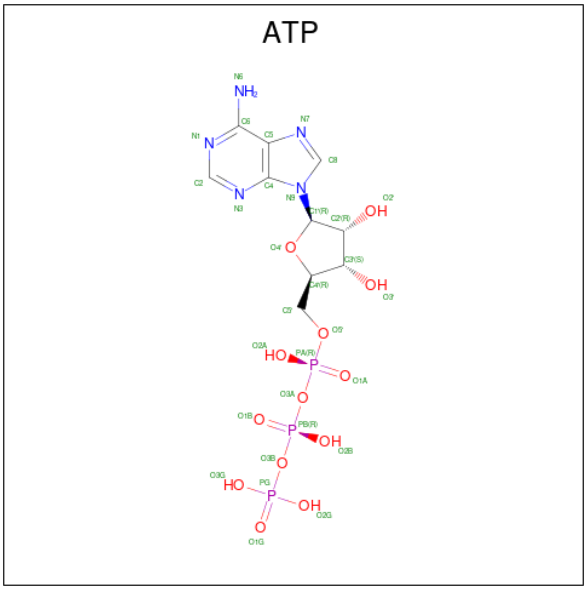
- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	488	3847	2426	674	732	15	0	0	0
2	D	485	3823	2412	671	725	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	431	ALA	SER	engineered mutation	UNP Q79PF4
C	432	GLU	THR	engineered mutation	UNP Q79PF4
D	431	ALA	SER	engineered mutation	UNP Q79PF4
D	432	GLU	THR	engineered mutation	UNP Q79PF4

- Molecule 3 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		
3	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	C	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	C	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	D	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	D	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	E	1	31	10	5	13	3	0	0

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	5	5	5	0	0
			Total	Mg		
4	B	3	3	3	0	0
			Total	Mg		
4	C	4	4	4	0	0
			Total	Mg		
4	D	4	4	4	0	0
			Total	Mg		
4	E	3	3	3	0	0
			Total	Mg		
4	F	3	3	3	0	0

- Molecule 5 is water.

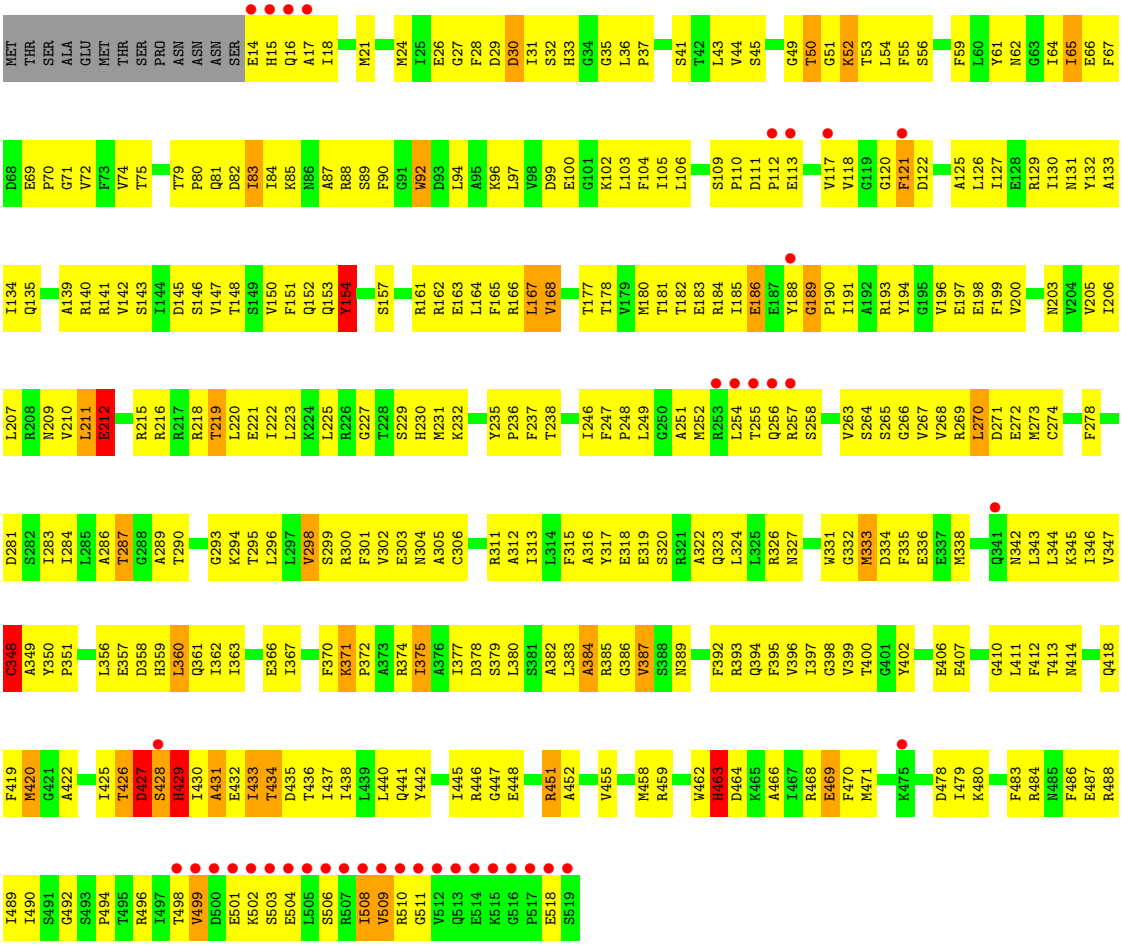
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	12	12	12	0	0
			Total	O		
5	B	18	18	18	0	0
			Total	O		
5	C	22	22	22	0	0
			Total	O		
5	D	31	31	31	0	0
			Total	O		
5	E	13	13	13	0	0
			Total	O		
5	F	21	21	21	0	0

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.

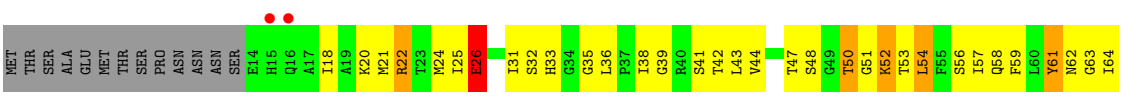
• Molecule 1: Circadian clock protein kinase KaiC

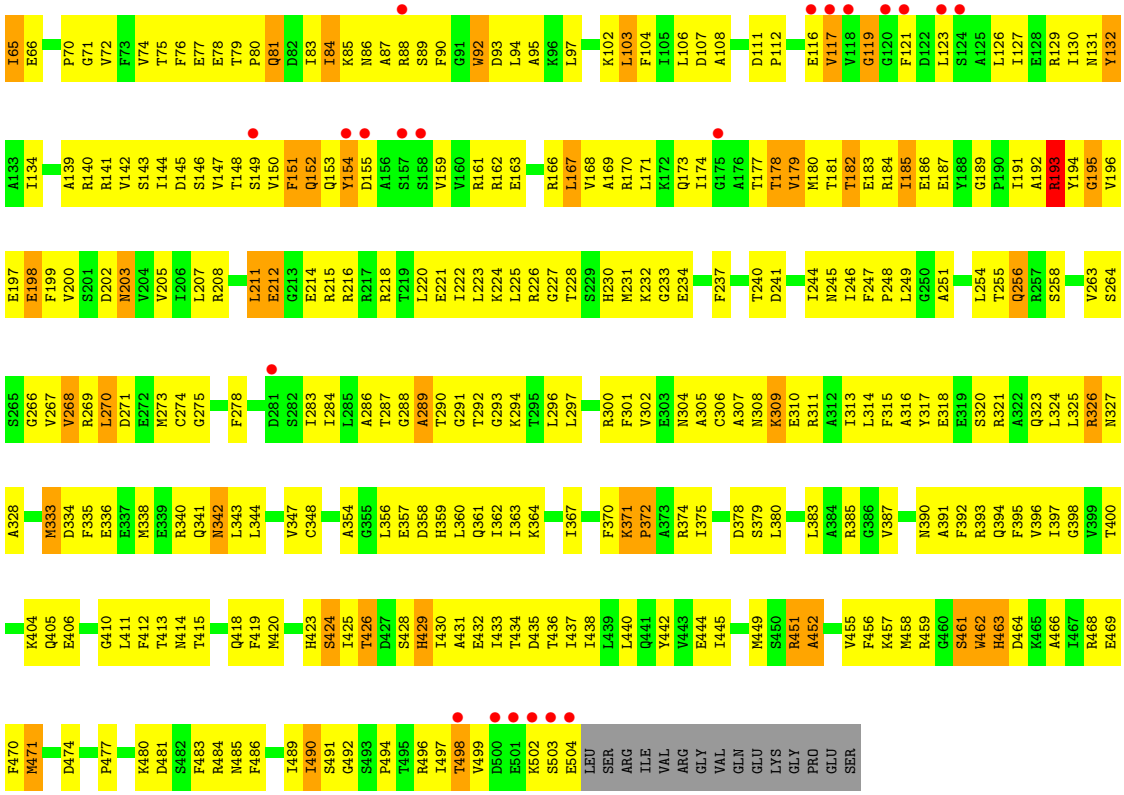
Chain A: 8% 33% 57% 6%



• Molecule 1: Circadian clock protein kinase KaiC

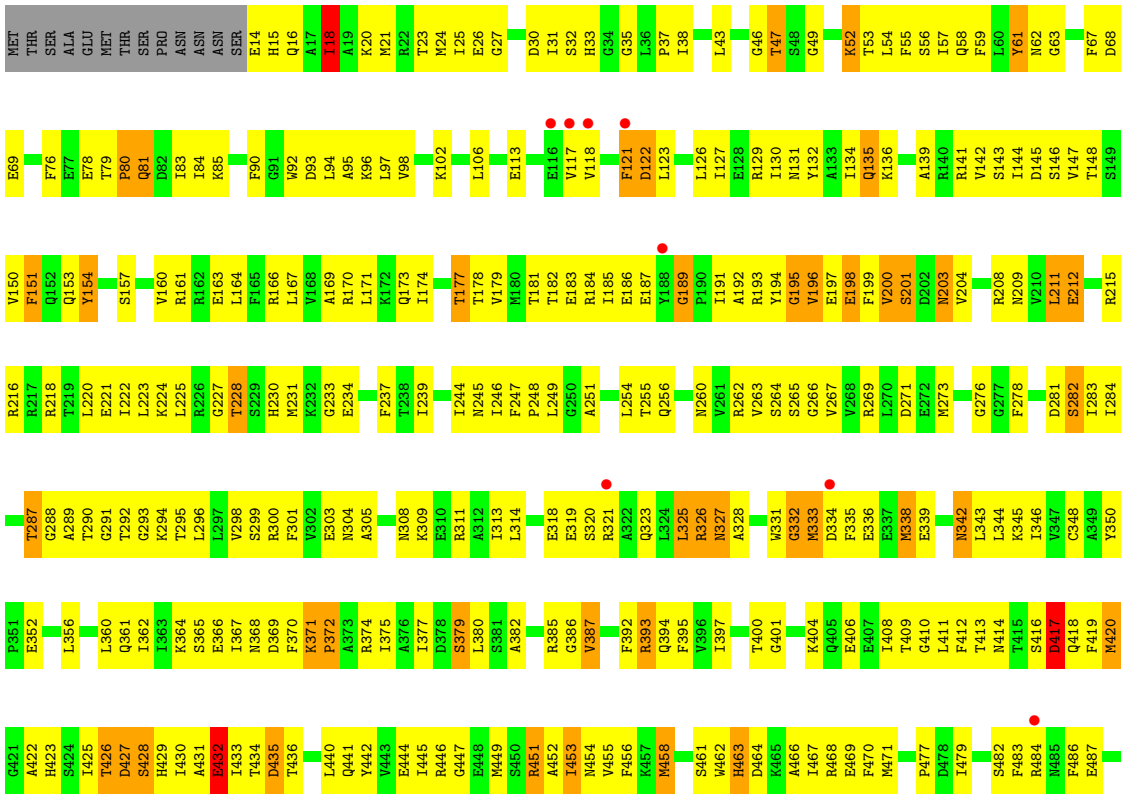
Chain B: 4% 31% 54% 9% 5%

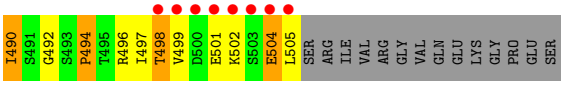




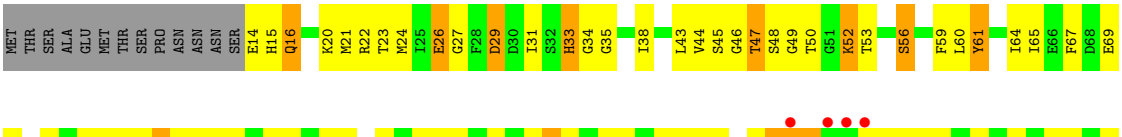
• Molecule 1: Circadian clock protein kinase KaiC

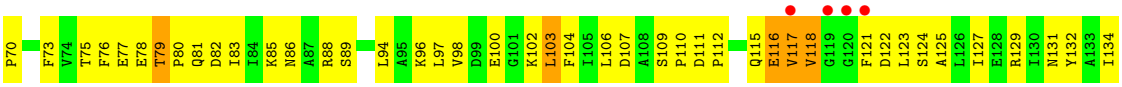
Chain E:

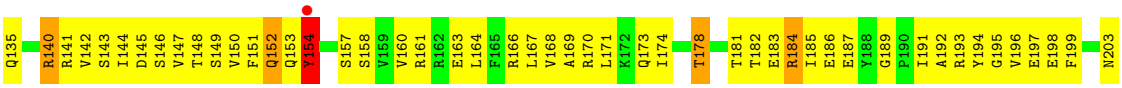


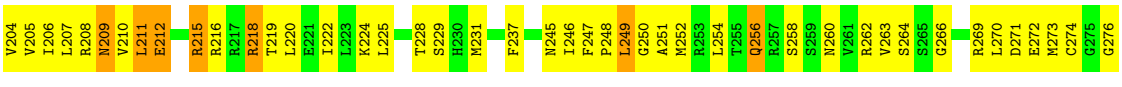


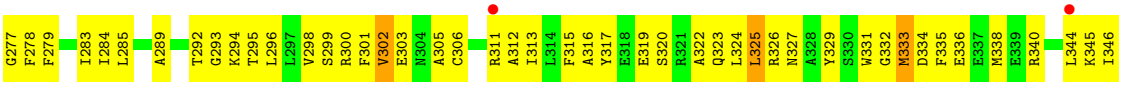
• Molecule 1: Circadian clock protein kinase KaiC

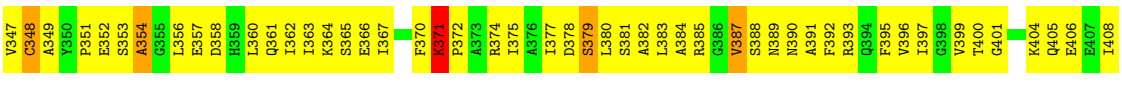


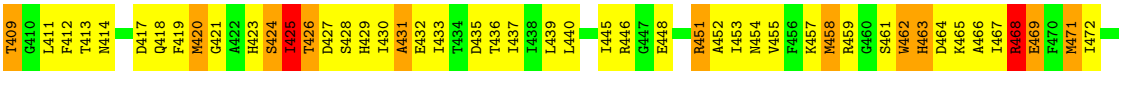


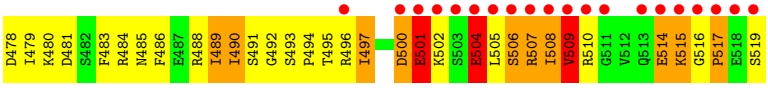




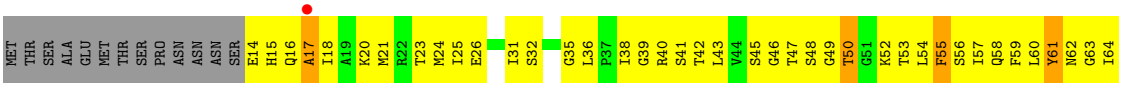


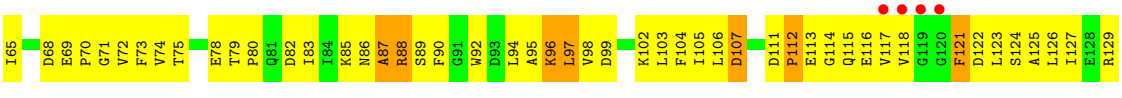


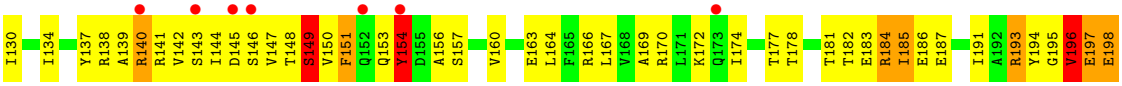


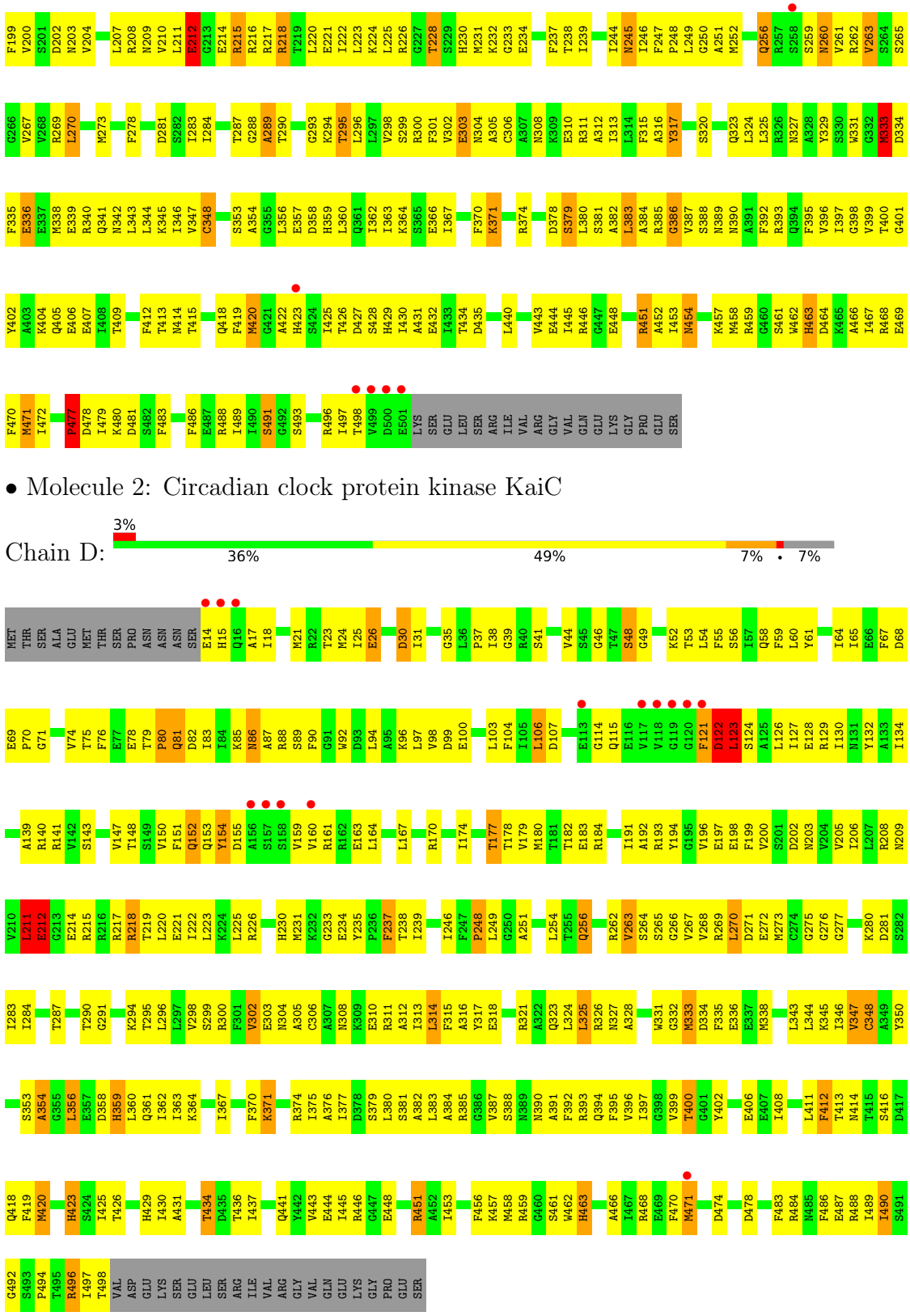


• Molecule 2: Circadian clock protein kinase KaiC









• Molecule 2: Circadian clock protein kinase KaiC

Chain D: 3% 36% 49% 7% • 7%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.28Å 135.03Å 204.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (30.00-3.30) 90.8 (30.07-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.269 0.215 , 0.249	Depositor DCC
R_{free} test set	5141 reflections (9.44%)	wwPDB-VP
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23919	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, TPO, MG

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	0.39	0/4044	0.67	0/5446
1	B	0.37	0/3928	0.64	0/5291
1	E	0.48	0/3936	0.72	2/5302 (0.0%)
1	F	0.45	0/4044	0.71	1/5446 (0.0%)
2	C	0.41	0/3912	0.67	0/5273
2	D	0.45	0/3888	0.70	0/5240
All	All	0.43	0/23752	0.69	3/31998 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	16	GLN	N-CA-C	-5.61	95.85	111.00
1	E	332	GLY	N-CA-C	-5.09	100.38	113.10
1	E	380	LEU	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3990	0	3983	403	0
1	B	3875	0	3861	411	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3883	0	3871	375	0
1	F	3990	0	3982	462	0
2	C	3847	0	3839	418	0
2	D	3823	0	3819	359	0
3	A	62	0	24	6	0
3	B	62	0	24	8	0
3	C	62	0	24	8	0
3	D	62	0	24	5	0
3	E	62	0	24	9	0
3	F	62	0	24	4	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
5	A	12	0	0	1	0
5	B	18	0	0	2	0
5	C	22	0	0	4	0
5	D	31	0	0	6	0
5	E	13	0	0	3	0
5	F	21	0	0	5	0
All	All	23919	0	23499	2276	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 48.

All (2276) 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:A:425:ILE:O	1:A:426:TPO:HG22	1.25	1.24
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.26	1.14
1:B:300:ARG:HA	1:B:333:MET:HE1	1.16	1.14
1:A:299:SER:HB3	1:A:333:MET:HE1	1.33	1.10
2:D:379:SER:H	2:D:413:THR:HB	0.97	1.09
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.30	1.07
1:F:426:TPO:CG2	1:F:430:ILE:H	1.66	1.07
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.38	1.06
1:F:191:ILE:HG13	1:F:206:ILE:HD11	1.35	1.04
1:A:379:SER:H	1:A:413:THR:HB	1.19	1.04
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.18	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:ILE:HG12	2:C:58:GLN:HE21	1.24	1.03
2:C:45:SER:HB3	2:C:182:THR:HB	1.41	1.03
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.39	1.02
1:A:211:LEU:O	1:A:212:GLU:HB3	1.58	1.02
1:A:425:ILE:O	1:A:426:TPO:CG2	2.08	1.01
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.42	1.01
1:A:380:LEU:HD11	1:A:412:PHE:CD2	1.96	1.00
2:C:215:ARG:HA	2:C:215:ARG:HE	1.26	1.00
2:D:379:SER:N	2:D:413:THR:HB	1.76	1.00
1:F:426:TPO:HG21	1:F:430:ILE:N	1.77	1.00
1:E:18:ILE:HD11	1:E:227:GLY:HA3	1.43	0.98
1:F:426:TPO:HG21	1:F:430:ILE:H	1.26	0.98
1:B:25:ILE:HG12	1:B:58:GLN:HE21	1.27	0.97
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.29	0.97
1:F:127:ILE:HD11	1:F:167:LEU:HA	1.44	0.97
1:A:14:GLU:HG3	1:A:15:HIS:H	1.30	0.96
1:F:283:ILE:HG23	1:F:412:PHE:HE1	1.31	0.96
1:E:320:SER:HA	1:F:254:LEU:HG	1.47	0.96
1:B:147:VAL:HG11	1:B:180:MET:HE2	1.48	0.95
1:B:273:MET:O	1:B:463:HIS:HA	1.66	0.95
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.46	0.95
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.49	0.94
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.46	0.94
2:C:70:PRO:HB2	2:C:139:ALA:HA	1.51	0.93
1:F:486:PHE:HE2	1:F:496:ARG:HH11	1.10	0.92
1:B:25:ILE:HG23	1:B:58:GLN:HE22	1.32	0.92
1:F:299:SER:HB3	1:F:333:MET:HE1	1.51	0.92
1:E:356:LEU:HD11	1:E:387:VAL:HG21	1.52	0.92
1:E:426:TPO:HG21	1:E:431:ALA:H	1.34	0.91
1:A:380:LEU:HD11	1:A:412:PHE:HD2	1.36	0.90
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.54	0.89
1:B:300:ARG:CA	1:B:333:MET:HE1	2.01	0.88
1:F:515:LYS:HG3	1:F:516:GLY:H	1.39	0.88
1:B:221:GLU:HG3	1:B:233:GLY:O	1.74	0.88
1:E:266:GLY:HA2	1:E:304:ASN:HD22	1.37	0.88
1:E:344:LEU:HD22	1:E:345:LYS:H	1.36	0.88
1:A:350:TYR:CZ	1:B:254:LEU:HD13	2.09	0.88
1:E:426:TPO:HG21	1:E:431:ALA:N	1.89	0.88
1:A:265:SER:O	1:A:301:PHE:HA	1.73	0.88
1:A:429:HIS:HB3	5:F:522:HOH:O	1.73	0.87
2:D:148:THR:HG21	2:D:193:ARG:HD2	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:VAL:HG12	1:E:374:ARG:NH2	1.89	0.87
1:A:441:GLN:HE22	1:A:490:ILE:HD13	1.38	0.87
2:C:261:VAL:HG12	2:C:262:ARG:H	1.39	0.86
1:A:266:GLY:HA3	1:A:300:ARG:O	1.76	0.86
1:B:146:SER:H	1:B:181:THR:HB	1.39	0.86
1:B:497:ILE:HD12	1:B:498:THR:N	1.91	0.86
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.58	0.85
1:B:218:ARG:HD3	1:B:237:PHE:CE1	2.10	0.85
1:B:426:TPO:O1P	1:B:429:HIS:HA	1.77	0.85
1:A:147:VAL:O	1:A:150:VAL:HG12	1.75	0.85
1:F:312:ALA:HA	1:F:372:PRO:HB3	1.58	0.85
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.42	0.85
1:A:263:VAL:CG1	1:A:374:ARG:HH21	1.90	0.84
2:C:220:LEU:HD13	2:C:246:ILE:HD11	1.59	0.84
2:C:451:ARG:HG2	2:C:451:ARG:HH11	1.41	0.84
1:F:313:ILE:HG13	1:F:372:PRO:HG2	1.58	0.84
2:D:147:VAL:HG11	2:D:180:MET:HE3	1.58	0.84
1:F:500:ASP:O	1:F:501:GLU:HB3	1.75	0.84
1:F:171:LEU:HD13	1:F:178:THR:HG21	1.58	0.84
1:B:140:ARG:HB3	1:B:140:ARG:NH1	1.92	0.84
1:E:379:SER:H	1:E:413:THR:HB	1.43	0.84
1:F:170:ARG:HH12	1:F:174:ILE:HG12	1.42	0.83
1:A:264:SER:HA	1:A:271:ASP:OD1	1.78	0.83
1:F:142:VAL:HB	1:F:178:THR:HG23	1.61	0.82
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.13	0.82
1:A:323:GLN:HG2	1:A:327:ASN:HD21	1.42	0.82
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.60	0.82
1:E:294:LYS:HB2	3:E:901:ATP:O1B	1.79	0.82
2:C:182:THR:HG22	2:C:183:GLU:H	1.45	0.82
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.44	0.82
1:A:65:ILE:O	1:A:66:GLU:HG2	1.79	0.82
1:A:211:LEU:HG	1:A:212:GLU:H	1.43	0.82
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.93	0.82
1:A:451:ARG:HD2	1:A:451:ARG:N	1.95	0.81
2:D:52:LYS:HB2	5:D:550:HOH:O	1.80	0.81
2:D:18:ILE:H	2:D:18:ILE:HD12	1.42	0.81
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.59	0.81
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.63	0.81
1:E:418:GLN:HB2	1:F:423:HIS:O	1.81	0.81
2:C:45:SER:CB	2:C:182:THR:HB	2.11	0.81
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:431:ALA:O	2:C:434:THR:HG22	1.79	0.81
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.62	0.81
2:C:287:THR:HG21	2:C:425:ILE:O	1.81	0.81
2:D:436:THR:HG23	2:D:458:MET:HG2	1.62	0.81
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.46	0.81
2:C:409:THR:HA	5:C:539:HOH:O	1.80	0.81
3:B:901:ATP:H3'	2:C:458:MET:O	1.82	0.80
2:C:344:LEU:HD22	2:C:345:LYS:H	1.46	0.80
1:A:72:VAL:HB	1:A:142:VAL:HG22	1.64	0.80
1:B:300:ARG:HA	1:B:333:MET:CE	2.08	0.80
1:E:14:GLU:HG3	1:E:16:GLN:H	1.47	0.80
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.63	0.80
1:E:283:ILE:HG13	1:E:400:THR:HG23	1.63	0.80
1:E:293:GLY:HA2	3:E:901:ATP:O1A	1.81	0.80
1:B:25:ILE:HG23	1:B:58:GLN:NE2	1.97	0.79
2:C:384:ALA:HB2	2:C:392:PHE:CE1	2.16	0.79
2:D:31:ILE:HA	2:D:231:MET:SD	2.23	0.79
2:C:446:ARG:HG2	2:C:496:ARG:NH2	1.97	0.79
2:D:419:PHE:CE2	1:E:425:ILE:HG13	2.16	0.79
1:A:446:ARG:HA	1:A:496:ARG:NH2	1.98	0.79
1:F:303:GLU:OE2	1:F:333:MET:HB3	1.82	0.79
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.12	0.79
1:F:344:LEU:HD22	1:F:345:LYS:H	1.47	0.79
2:C:315:PHE:CE2	2:C:363:ILE:HA	2.19	0.78
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.63	0.78
1:E:263:VAL:CG1	1:E:374:ARG:HH21	1.95	0.78
5:D:538:HOH:O	1:E:432:GLU:HG2	1.84	0.78
1:F:377:ILE:HD11	1:F:399:VAL:HG11	1.66	0.78
1:F:383:LEU:HD13	1:F:395:PHE:CE2	2.18	0.78
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.65	0.78
2:D:347:VAL:HG12	2:D:348:CYS:N	1.98	0.78
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.49	0.78
2:D:294:LYS:O	2:D:298:VAL:HG23	1.83	0.78
1:E:382:ALA:O	1:E:385:ARG:HG3	1.84	0.78
1:F:393:ARG:O	1:F:397:ILE:HG12	1.84	0.77
2:D:170:ARG:O	2:D:174:ILE:HG12	1.84	0.77
2:D:267:VAL:CG2	2:D:300:ARG:HG2	2.14	0.77
1:A:14:GLU:CG	1:A:15:HIS:H	1.97	0.77
2:C:72:VAL:HG22	2:C:104:PHE:HB3	1.65	0.77
1:B:492:GLY:O	1:B:494:PRO:HD3	1.83	0.77
2:C:42:THR:HA	2:C:203:ASN:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:ILE:CD1	1:E:372:PRO:HG2	2.15	0.77
1:E:445:ILE:HG22	1:E:446:ARG:HD2	1.67	0.77
1:E:497:ILE:HG22	1:E:498:THR:H	1.48	0.77
2:C:371:LYS:O	2:C:371:LYS:HD2	1.84	0.77
1:E:464:ASP:OD2	1:E:466:ALA:HB3	1.83	0.77
1:B:116:GLU:HG2	1:B:117:VAL:H	1.50	0.77
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.67	0.77
2:D:212:GLU:HG2	2:D:212:GLU:O	1.84	0.77
1:A:64:ILE:HD11	1:A:103:LEU:HB2	1.65	0.77
2:C:182:THR:HG22	2:C:183:GLU:N	2.00	0.77
2:D:377:ILE:HG22	2:D:377:ILE:O	1.84	0.77
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.00	0.76
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.20	0.76
1:E:24:MET:HA	1:E:24:MET:HE3	1.65	0.76
1:A:16:GLN:O	1:F:88:ARG:HD2	1.85	0.76
1:B:25:ILE:HG12	1:B:58:GLN:NE2	1.99	0.76
1:E:326:ARG:HD3	1:F:258:SER:OG	1.85	0.76
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.68	0.76
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.16	0.76
1:E:294:LYS:HB3	1:E:413:THR:HG23	1.67	0.76
1:E:504:GLU:HG2	1:E:505:LEU:H	1.51	0.76
1:A:320:SER:HA	1:B:254:LEU:HG	1.68	0.75
2:C:245:ASN:C	2:C:245:ASN:HD22	1.88	0.75
2:C:422:ALA:HB1	5:C:536:HOH:O	1.86	0.75
2:D:214:GLU:HB3	1:E:234:GLU:HB2	1.67	0.75
1:F:344:LEU:HD22	1:F:345:LYS:N	2.00	0.75
2:D:371:LYS:HD2	2:D:371:LYS:O	1.85	0.75
1:F:381:SER:HB3	1:F:414:ASN:OD1	1.87	0.75
1:A:425:ILE:C	1:A:426:TPO:O1P	2.24	0.75
1:E:323:GLN:HE21	1:F:459:ARG:HD3	1.50	0.75
1:E:191:ILE:HB	1:E:198:GLU:CG	2.16	0.75
1:B:191:ILE:HB	1:B:198:GLU:CG	2.16	0.75
1:A:323:GLN:HG2	1:A:327:ASN:ND2	2.01	0.75
2:C:261:VAL:HG12	2:C:262:ARG:N	2.01	0.75
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.69	0.75
1:A:386:GLY:HA2	1:B:390:ASN:OD1	1.86	0.75
1:B:52:LYS:H	1:B:207:LEU:HD12	1.51	0.74
1:A:207:LEU:HD21	1:A:220:LEU:HD12	1.70	0.74
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.51	0.74
1:B:56:SER:O	1:B:59:PHE:HB3	1.87	0.74
1:E:148:THR:OG1	1:E:182:THR:HG23	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.17	0.74
1:B:358:ASP:O	1:B:362:ILE:HG12	1.88	0.74
1:B:50:THR:HB	1:B:207:LEU:HB3	1.68	0.74
1:B:426:TPO:O1P	1:B:429:HIS:CA	2.35	0.74
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.69	0.74
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.53	0.74
1:E:461:SER:OG	1:E:462:TRP:N	2.19	0.74
1:A:50:THR:HG22	1:A:209:ASN:HB2	1.70	0.74
1:E:20:LYS:HE3	1:E:228:THR:HG21	1.70	0.74
1:B:263:VAL:HG12	1:B:374:ARG:NH2	2.03	0.73
1:B:379:SER:H	1:B:413:THR:HB	1.53	0.73
1:E:304:ASN:HB3	1:E:374:ARG:HH12	1.53	0.73
1:A:425:ILE:C	1:A:426:TPO:HG22	2.07	0.73
2:C:140:ARG:HB3	2:C:140:ARG:NH1	2.01	0.73
1:F:20:LYS:HE2	1:F:228:THR:HG21	1.69	0.73
1:B:214:GLU:HB3	2:C:234:GLU:HB2	1.70	0.73
2:D:221:GLU:HG3	2:D:233:GLY:O	1.88	0.73
2:D:304:ASN:HB3	2:D:374:ARG:HH12	1.51	0.73
2:D:220:LEU:HD23	2:D:221:GLU:N	2.02	0.73
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.68	0.73
1:B:196:VAL:O	1:B:200:VAL:HG23	1.89	0.73
1:B:316:ALA:HA	1:B:378:ASP:HB3	1.70	0.73
2:D:497:ILE:HD12	2:D:497:ILE:O	1.89	0.73
2:C:232:LYS:HD2	2:C:232:LYS:N	2.02	0.73
2:C:296:LEU:HD21	2:C:477:PRO:HB3	1.70	0.73
1:B:458:MET:HB2	1:B:463:HIS:HD2	1.54	0.73
1:B:21:MET:HB2	1:B:38:ILE:HG12	1.71	0.72
1:F:514:GLU:CD	1:F:515:LYS:H	1.92	0.72
2:C:446:ARG:HG2	2:C:496:ARG:CZ	2.18	0.72
2:C:215:ARG:HA	2:C:215:ARG:NE	2.03	0.72
1:B:195:GLY:HA2	1:B:198:GLU:OE2	1.88	0.72
1:F:383:LEU:HD13	1:F:395:PHE:HE2	1.53	0.72
1:B:318:GLU:OE2	2:C:432:GLU:HB3	1.90	0.72
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.04	0.72
1:F:336:GLU:HB3	1:F:340:ARG:NH2	2.04	0.72
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.53	0.72
2:D:18:ILE:HD12	2:D:18:ILE:N	2.04	0.72
1:F:79:THR:HG23	1:F:81:GLN:H	1.54	0.72
1:B:503:SER:O	1:B:504:GLU:HB2	1.88	0.72
2:D:114:GLY:O	2:D:115:GLN:HG3	1.89	0.72
1:E:134:ILE:HG23	1:E:139:ALA:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:THR:CG2	1:A:458:MET:HG2	2.19	0.72
1:B:140:ARG:HB3	1:B:140:ARG:HH11	1.54	0.72
1:B:184:ARG:HD2	1:B:191:ILE:O	1.89	0.72
1:B:451:ARG:HH11	1:B:451:ARG:HG2	1.54	0.72
1:E:123:LEU:HD13	1:E:163:GLU:OE2	1.90	0.71
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.72	0.71
1:A:258:SER:OG	1:F:326:ARG:HD3	1.89	0.71
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.25	0.71
1:A:84:ILE:HG23	1:A:94:LEU:HB2	1.73	0.71
2:C:300:ARG:N	2:C:333:MET:HE1	2.06	0.71
1:E:436:THR:HG23	1:E:458:MET:HG2	1.72	0.71
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.72	0.71
1:F:497:ILE:O	1:F:497:ILE:HG13	1.88	0.71
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.91	0.71
1:A:447:GLY:HA2	1:B:489:ILE:CD1	2.20	0.71
1:F:191:ILE:HG13	1:F:206:ILE:CD1	2.18	0.71
1:B:84:ILE:HA	1:B:94:LEU:HD12	1.72	0.71
1:B:169:ALA:O	1:B:173:GLN:HG3	1.91	0.71
2:D:67:PHE:HB3	2:D:69:GLU:HG3	1.72	0.71
1:E:344:LEU:HD22	1:E:345:LYS:N	2.06	0.71
1:B:183:GLU:HB2	2:C:199:PHE:CE1	2.25	0.70
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.55	0.70
2:C:146:SER:H	2:C:181:THR:HB	1.55	0.70
2:D:64:ILE:HG21	2:D:97:LEU:HD13	1.71	0.70
1:F:148:THR:HG21	1:F:193:ARG:HD2	1.73	0.70
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.56	0.70
1:A:126:LEU:O	1:A:130:ILE:HG13	1.92	0.70
1:A:379:SER:N	1:A:413:THR:HB	2.02	0.70
1:B:191:ILE:HB	1:B:198:GLU:CD	2.12	0.70
2:C:483:PHE:HB2	2:C:489:ILE:HD13	1.74	0.70
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.73	0.70
2:C:293:GLY:HA2	3:C:901:ATP:O1A	1.90	0.70
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.22	0.70
1:B:341:GLN:O	1:B:343:LEU:HG	1.92	0.70
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.06	0.70
1:F:106:LEU:HD11	1:F:129:ARG:CZ	2.22	0.70
1:A:44:VAL:HG22	1:A:205:VAL:HB	1.72	0.69
1:B:379:SER:HA	1:B:413:THR:O	1.92	0.69
2:D:287:THR:HG21	2:D:425:ILE:O	1.92	0.69
2:C:41:SER:HB3	2:C:178:THR:HB	1.73	0.69
1:A:148:THR:OG1	1:A:182:THR:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:220:LEU:HD13	2:C:246:ILE:CD1	2.21	0.69
1:A:79:THR:HG23	1:A:80:PRO:HD2	1.74	0.69
1:A:438:ILE:HD11	1:A:455:VAL:HG22	1.74	0.69
1:F:325:LEU:HD23	1:F:335:PHE:HB2	1.74	0.69
1:B:75:THR:O	1:B:108:ALA:HB3	1.92	0.69
2:D:21:MET:HE3	2:D:59:PHE:HZ	1.57	0.69
1:F:78:GLU:HB3	1:F:83:ILE:HD11	1.75	0.69
1:A:65:ILE:O	1:A:65:ILE:HG22	1.92	0.69
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.05	0.69
2:C:50:THR:HG21	2:C:207:LEU:C	2.13	0.69
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.23	0.69
1:F:336:GLU:HB3	1:F:340:ARG:HH21	1.57	0.69
1:A:43:LEU:HD11	1:A:182:THR:OG1	1.92	0.69
1:A:488:ARG:HE	1:F:488:ARG:HH12	1.41	0.69
2:C:269:ARG:O	2:C:273:MET:HG3	1.91	0.69
2:D:354:ALA:HB3	2:D:359:HIS:NE2	2.06	0.69
1:B:161:ARG:NH2	1:B:199:PHE:HB2	2.07	0.69
1:A:487:GLU:OE1	1:F:495:THR:HA	1.92	0.69
1:B:426:TPO:O1P	1:B:430:ILE:N	2.26	0.69
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.57	0.69
2:D:64:ILE:HG22	2:D:65:ILE:HD13	1.75	0.69
1:B:56:SER:HB2	1:B:143:SER:HB3	1.75	0.68
2:C:451:ARG:HG2	2:C:451:ARG:NH1	2.08	0.68
1:F:49:GLY:O	1:F:218:ARG:NH2	2.26	0.68
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.56	0.68
1:B:194:TYR:O	1:B:196:VAL:HG23	1.93	0.68
2:C:214:GLU:OE2	2:D:217:ARG:NH1	2.26	0.68
2:D:56:SER:HB2	2:D:143:SER:HB3	1.75	0.68
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.58	0.68
1:A:210:VAL:HG12	1:A:211:LEU:O	1.93	0.68
1:B:130:ILE:O	1:B:134:ILE:HG13	1.92	0.68
2:D:387:VAL:HG12	2:D:388:SER:N	2.08	0.68
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.23	0.68
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.75	0.68
1:E:462:TRP:O	1:E:463:HIS:O	2.11	0.68
1:A:371:LYS:O	1:A:371:LYS:HD2	1.92	0.68
2:C:52:LYS:HD2	2:C:182:THR:O	1.93	0.68
2:D:347:VAL:O	2:D:348:CYS:HB2	1.94	0.68
1:F:266:GLY:HA3	1:F:300:ARG:HG3	1.76	0.68
1:F:426:TPO:O1P	1:F:431:ALA:HB3	1.94	0.68
1:F:516:GLY:N	1:F:517:PRO:HD2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASP:OD1	1:B:159:VAL:HG11	1.93	0.68
2:C:308:ASN:O	2:C:310:GLU:HG3	1.92	0.68
2:C:488:ARG:HH22	2:D:488:ARG:HH21	1.41	0.68
1:E:147:VAL:O	1:E:150:VAL:HG12	1.94	0.68
1:E:281:ASP:O	1:E:282:SER:HB3	1.91	0.68
1:B:293:GLY:HA2	3:B:901:ATP:O1A	1.93	0.68
2:C:50:THR:HB	2:C:207:LEU:HB3	1.74	0.68
1:B:184:ARG:HH22	1:B:187:GLU:C	1.98	0.68
1:E:221:GLU:HG3	1:E:233:GLY:O	1.94	0.68
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.73	0.68
2:C:214:GLU:HB3	2:D:234:GLU:HB2	1.76	0.68
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.58	0.68
2:D:152:GLN:HG3	1:E:161:ARG:NH1	2.09	0.68
2:C:164:LEU:HD11	2:C:197:GLU:HG3	1.76	0.68
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.75	0.67
1:B:315:PHE:CE2	1:B:347:VAL:HG21	2.29	0.67
1:E:319:GLU:O	1:F:254:LEU:HD21	1.94	0.67
1:F:47:THR:HG22	1:F:50:THR:CG2	2.24	0.67
1:F:79:THR:HG22	1:F:82:ASP:H	1.58	0.67
1:F:44:VAL:HG22	1:F:205:VAL:HB	1.76	0.67
1:F:170:ARG:HH22	1:F:174:ILE:HD11	1.57	0.67
1:F:353:SER:O	1:F:354:ALA:HB2	1.93	0.67
1:F:464:ASP:OD2	1:F:466:ALA:HB3	1.94	0.67
2:D:88:ARG:HD3	1:E:15:HIS:O	1.94	0.67
2:D:496:ARG:HG2	1:E:487:GLU:OE1	1.94	0.67
1:E:21:MET:HE1	1:E:141:ARG:HG2	1.76	0.67
1:E:131:ASN:O	1:E:135:GLN:HB2	1.93	0.67
3:E:901:ATP:H3'	1:F:458:MET:O	1.94	0.67
1:B:326:ARG:HG3	2:C:260:ASN:ND2	2.10	0.67
2:D:220:LEU:HD13	2:D:246:ILE:CD1	2.25	0.67
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.59	0.67
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.76	0.67
2:C:488:ARG:NH2	2:D:488:ARG:HH21	1.93	0.67
1:A:348:CYS:SG	1:B:254:LEU:HD23	2.35	0.67
2:D:89:SER:HB2	1:E:227:GLY:O	1.95	0.67
1:E:304:ASN:HB3	1:E:374:ARG:NH1	2.10	0.67
1:B:129:ARG:O	1:B:132:TYR:HB3	1.95	0.67
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.77	0.67
1:B:81:GLN:HE21	1:B:81:GLN:H	1.42	0.67
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.77	0.67
1:E:309:LYS:HA	1:E:343:LEU:HD13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:ILE:HG23	2:C:58:GLN:NE2	2.09	0.66
2:D:332:GLY:O	2:D:333:MET:HG2	1.94	0.66
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.76	0.66
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.78	0.66
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.59	0.66
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.59	0.66
1:E:289:ALA:CB	1:E:419:PHE:HA	2.25	0.66
1:F:338:MET:HB3	1:F:344:LEU:HB3	1.78	0.66
2:D:267:VAL:HG23	2:D:300:ARG:HG2	1.76	0.66
1:A:14:GLU:HG3	1:A:15:HIS:N	2.08	0.66
1:A:274:CYS:HG	1:A:278:PHE:HE2	1.39	0.66
1:B:246:ILE:O	1:B:248:PRO:HD3	1.95	0.66
2:C:70:PRO:HD2	2:C:140:ARG:HG2	1.78	0.66
1:E:431:ALA:O	1:E:434:THR:HG22	1.94	0.66
1:B:304:ASN:HB3	1:B:374:ARG:HH12	1.61	0.66
1:E:94:LEU:O	1:E:98:VAL:HG23	1.96	0.66
1:F:260:ASN:HA	1:F:279:PHE:HE2	1.61	0.66
2:C:21:MET:HB2	2:C:38:ILE:HG13	1.78	0.66
3:C:903:ATP:HO2'	2:D:230:HIS:CE1	2.12	0.66
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.76	0.66
1:E:194:TYR:O	1:E:196:VAL:N	2.29	0.66
1:F:197:GLU:OE2	1:F:197:GLU:N	2.25	0.66
1:E:305:ALA:HB2	1:E:374:ARG:CD	2.18	0.66
1:F:96:LYS:O	1:F:100:GLU:HG3	1.96	0.66
1:A:45:SER:CB	1:A:182:THR:HB	2.26	0.66
1:B:334:ASP:OD1	1:B:336:GLU:HB2	1.96	0.66
2:D:178:THR:HG22	2:D:179:VAL:N	2.11	0.66
2:D:221:GLU:HG3	2:D:233:GLY:C	2.16	0.66
2:D:344:LEU:HD13	2:D:344:LEU:C	2.16	0.66
1:E:313:ILE:HG22	1:E:314:LEU:N	2.10	0.66
1:F:299:SER:CB	1:F:333:MET:HE1	2.25	0.66
1:F:313:ILE:CG1	1:F:372:PRO:HG2	2.26	0.66
1:F:263:VAL:HG12	1:F:374:ARG:NH2	2.12	0.65
1:A:431:ALA:O	1:A:434:THR:HB	1.97	0.65
1:B:178:THR:HG22	1:B:179:VAL:H	1.60	0.65
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.31	0.65
1:E:504:GLU:HG2	1:E:505:LEU:N	2.10	0.65
1:F:118:VAL:HG22	1:F:122:ASP:OD1	1.96	0.65
1:A:191:ILE:N	1:A:191:ILE:HD12	2.11	0.65
2:C:221:GLU:HG3	2:C:233:GLY:O	1.96	0.65
1:A:14:GLU:HG3	1:A:16:GLN:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLY:O	1:F:89:SER:HB2	1.96	0.65
2:C:202:ASP:HA	2:C:226:ARG:HD2	1.77	0.65
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.24	0.65
1:F:144:ILE:HD13	1:F:167:LEU:HD21	1.79	0.65
1:F:377:ILE:CD1	1:F:399:VAL:HG11	2.26	0.65
2:C:52:LYS:N	3:C:903:ATP:O1B	2.29	0.65
1:E:446:ARG:HH21	1:E:496:ARG:HH22	1.45	0.65
1:E:225:LEU:HB2	1:E:230:HIS:HD2	1.61	0.65
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.31	0.65
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.79	0.65
1:E:123:LEU:O	1:E:127:ILE:HG13	1.96	0.65
1:E:142:VAL:HB	1:E:178:THR:HG23	1.77	0.65
1:F:370:PHE:HD2	1:F:372:PRO:HG3	1.61	0.65
1:A:161:ARG:HD2	1:A:196:VAL:HG13	1.79	0.65
1:E:452:ALA:HA	1:E:469:GLU:HA	1.78	0.65
1:F:313:ILE:HG13	1:F:372:PRO:CG	2.26	0.65
1:F:509:VAL:HG12	1:F:510:ARG:H	1.61	0.65
1:A:425:ILE:HG23	1:F:419:PHE:CE2	2.30	0.65
1:B:80:PRO:HA	1:B:83:ILE:HD13	1.79	0.65
2:C:444:GLU:OE2	2:D:489:ILE:HG12	1.97	0.65
2:D:436:THR:CG2	2:D:458:MET:HG2	2.27	0.65
2:D:486:PHE:CE2	2:D:496:ARG:HD3	2.32	0.65
1:F:46:GLY:HA2	1:F:184:ARG:HD2	1.79	0.65
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.61	0.65
1:A:426:TPO:O	1:A:427:ASP:HB2	1.97	0.64
1:E:212:GLU:O	1:E:212:GLU:HG2	1.96	0.64
1:A:31:ILE:HA	1:A:231:MET:SD	2.37	0.64
1:F:400:THR:HG21	1:F:433:ILE:CG2	2.27	0.64
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.12	0.64
2:D:194:TYR:O	2:D:196:VAL:HG23	1.96	0.64
1:A:164:LEU:HD11	1:A:197:GLU:HG3	1.79	0.64
1:E:367:ILE:HG12	1:E:375:ILE:HD11	1.79	0.64
1:E:451:ARG:H	1:E:451:ARG:HD2	1.62	0.64
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.33	0.64
1:F:452:ALA:HA	1:F:469:GLU:HA	1.79	0.64
1:A:273:MET:O	1:A:463:HIS:HA	1.97	0.64
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.10	0.64
1:A:327:ASN:HB3	5:A:531:HOH:O	1.96	0.64
1:B:147:VAL:HG11	1:B:180:MET:CE	2.27	0.64
2:D:225:LEU:HB2	2:D:230:HIS:HD2	1.62	0.64
2:D:225:LEU:HD12	2:D:230:HIS:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:MET:HA	1:E:24:MET:CE	2.26	0.64
1:E:393:ARG:O	1:E:397:ILE:HG12	1.96	0.64
1:E:425:ILE:HG22	1:E:425:ILE:O	1.97	0.64
1:A:130:ILE:O	1:A:134:ILE:HG13	1.97	0.64
2:D:267:VAL:HG22	2:D:300:ARG:HG2	1.79	0.64
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.79	0.64
1:A:161:ARG:NH1	1:F:183:GLU:OE2	2.26	0.64
1:B:123:LEU:HD13	1:B:123:LEU:O	1.98	0.64
1:B:191:ILE:HB	1:B:198:GLU:HG3	1.79	0.64
2:C:21:MET:HE1	2:C:141:ARG:HG2	1.79	0.64
1:E:199:PHE:C	1:E:201:SER:H	2.01	0.64
1:E:427:ASP:O	1:E:428:SER:HB3	1.96	0.64
1:A:436:THR:HG23	1:A:458:MET:HG2	1.80	0.64
1:A:488:ARG:HE	1:F:488:ARG:NH1	1.95	0.64
2:C:25:ILE:CG1	2:C:58:GLN:HE21	2.07	0.64
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.79	0.64
1:F:298:VAL:O	1:F:301:PHE:HB3	1.98	0.64
1:B:145:ASP:OD2	1:B:181:THR:HG21	1.98	0.64
2:D:18:ILE:H	2:D:18:ILE:CD1	2.11	0.64
1:A:27:GLY:O	1:A:30:ASP:HB2	1.98	0.63
1:A:356:LEU:HD11	1:A:387:VAL:HG21	1.80	0.63
2:C:17:ALA:C	2:C:18:ILE:HD12	2.19	0.63
1:B:151:PHE:C	1:B:153:GLN:H	2.02	0.63
1:B:426:TPO:O3P	1:B:426:TPO:O	2.16	0.63
1:E:146:SER:H	1:E:181:THR:HB	1.61	0.63
1:E:294:LYS:N	3:E:901:ATP:O1B	2.30	0.63
1:F:458:MET:SD	1:F:461:SER:HB3	2.37	0.63
1:A:41:SER:HA	1:A:178:THR:O	1.98	0.63
1:B:123:LEU:HD12	1:B:166:ARG:HD2	1.80	0.63
1:E:332:GLY:O	1:E:333:MET:HG2	1.99	0.63
2:C:380:LEU:HD11	2:C:412:PHE:HD2	1.63	0.63
1:E:18:ILE:HD11	1:E:227:GLY:CA	2.25	0.63
1:F:293:GLY:HA2	3:F:901:ATP:O1A	1.98	0.63
1:F:317:TYR:HA	1:F:349:ALA:O	1.97	0.63
1:A:166:ARG:HG3	1:F:112:PRO:O	1.97	0.63
1:F:453:ILE:HG12	1:F:454:ASN:H	1.63	0.63
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.62	0.63
2:C:54:LEU:HD23	2:C:244:ILE:HG13	1.81	0.63
2:C:74:VAL:HG22	2:C:106:LEU:HD23	1.80	0.63
1:E:323:GLN:HG2	1:E:327:ASN:HD21	1.63	0.63
1:E:458:MET:SD	1:E:461:SER:HB3	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:TYR:CZ	1:F:65:ILE:HG13	2.34	0.63
1:A:183:GLU:HB2	1:B:199:PHE:CZ	2.34	0.63
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.99	0.63
1:F:461:SER:OG	1:F:462:TRP:N	2.30	0.63
2:D:283:ILE:HG13	2:D:400:THR:HG23	1.79	0.63
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.81	0.63
1:A:231:MET:HB3	1:A:235:TYR:OH	1.99	0.63
1:A:360:LEU:O	1:A:360:LEU:HD22	1.98	0.63
1:B:88:ARG:HG2	1:B:88:ARG:HH11	1.64	0.63
1:B:192:ALA:O	1:B:194:TYR:N	2.32	0.63
2:C:344:LEU:HD22	2:C:345:LYS:N	2.13	0.63
2:D:496:ARG:HD2	5:D:546:HOH:O	1.97	0.63
1:F:315:PHE:CE1	1:F:375:ILE:HD11	2.34	0.63
1:A:442:TYR:HE1	1:B:456:PHE:CZ	2.17	0.62
1:F:247:PHE:HB3	1:F:249:LEU:CD2	2.29	0.62
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.81	0.62
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.34	0.62
2:C:299:SER:C	2:C:333:MET:HE1	2.20	0.62
2:D:379:SER:HA	2:D:413:THR:O	1.98	0.62
1:F:80:PRO:HG2	1:F:107:ASP:HB2	1.80	0.62
2:C:211:LEU:O	2:C:212:GLU:HB3	1.99	0.62
2:C:316:ALA:O	2:C:348:CYS:HA	1.98	0.62
1:F:264:SER:O	1:F:374:ARG:NH2	2.31	0.62
1:A:50:THR:CG2	1:A:209:ASN:HB2	2.28	0.62
1:B:18:ILE:HB	1:B:228:THR:CG2	2.30	0.62
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.30	0.62
2:D:60:LEU:HD22	2:D:71:GLY:HA3	1.82	0.62
2:D:79:THR:HG22	2:D:82:ASP:OD2	2.00	0.62
1:E:294:LYS:HB3	1:E:413:THR:CG2	2.30	0.62
1:F:168:VAL:HG12	1:F:169:ALA:N	2.14	0.62
1:F:445:ILE:HG13	1:F:483:PHE:HE2	1.63	0.62
2:D:196:VAL:O	2:D:200:VAL:HG23	1.99	0.62
1:F:147:VAL:O	1:F:150:VAL:HG12	2.00	0.62
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.81	0.62
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.30	0.62
2:C:25:ILE:HG23	2:C:58:GLN:HE22	1.64	0.62
1:A:284:ILE:HD12	1:A:436:THR:HB	1.82	0.62
1:B:469:GLU:HB3	1:B:483:PHE:CZ	2.35	0.62
2:C:137:TYR:O	2:C:138:ARG:HB2	1.98	0.62
2:D:266:GLY:HA3	2:D:300:ARG:O	2.00	0.62
2:D:446:ARG:HB3	1:E:484:ARG:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:ILE:HB	1:E:411:LEU:HD12	1.82	0.62
1:E:301:PHE:HZ	1:E:409:THR:HG22	1.65	0.62
1:A:356:LEU:HD23	1:A:395:PHE:HB2	1.80	0.62
1:B:36:LEU:HD12	1:B:59:PHE:CZ	2.35	0.62
1:B:315:PHE:CD2	1:B:347:VAL:HG21	2.34	0.62
2:C:46:GLY:HA2	2:C:184:ARG:HD2	1.79	0.62
1:E:52:LYS:HB3	1:E:181:THR:HG23	1.80	0.62
1:F:504:GLU:O	1:F:505:LEU:HB2	1.98	0.62
1:A:427:ASP:O	1:A:429:HIS:ND1	2.31	0.61
2:C:121:PHE:O	2:C:125:ALA:HB3	2.00	0.61
2:C:311:ARG:HD2	2:C:371:LYS:HE3	1.81	0.61
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.30	0.61
1:E:311:ARG:HD2	1:E:371:LYS:HE3	1.81	0.61
1:A:400:THR:HG21	1:A:433:ILE:HG22	1.82	0.61
1:B:297:LEU:HD12	1:B:440:LEU:HD11	1.83	0.61
2:C:41:SER:HA	2:C:178:THR:O	2.00	0.61
1:B:220:LEU:HD13	1:B:246:ILE:CD1	2.30	0.61
2:C:87:ALA:C	2:C:89:SER:H	2.04	0.61
2:D:147:VAL:CG2	2:D:148:THR:N	2.63	0.61
1:B:31:ILE:HA	1:B:231:MET:SD	2.41	0.61
2:C:24:MET:HB2	2:C:62:ASN:ND2	2.15	0.61
2:C:461:SER:OG	2:C:462:TRP:N	2.33	0.61
2:D:127:ILE:HG12	2:D:167:LEU:HD13	1.81	0.61
2:D:334:ASP:OD1	2:D:336:GLU:N	2.33	0.61
1:E:27:GLY:O	1:E:30:ASP:HB2	2.01	0.61
2:C:182:THR:CG2	2:C:183:GLU:H	2.11	0.61
2:C:267:VAL:HB	2:C:270:LEU:HB2	1.82	0.61
1:A:79:THR:HB	1:A:82:ASP:OD2	2.01	0.61
1:B:461:SER:OG	1:B:462:TRP:N	2.34	0.61
2:C:98:VAL:HG13	2:C:103:LEU:O	2.01	0.61
2:D:80:PRO:HG2	2:D:107:ASP:HB2	1.82	0.61
2:D:273:MET:SD	2:D:468:ARG:HD2	2.39	0.61
1:E:38:ILE:HA	1:E:177:THR:HG23	1.81	0.61
1:E:184:ARG:HD2	1:E:191:ILE:O	2.01	0.61
1:F:171:LEU:CD1	1:F:178:THR:HG21	2.31	0.61
1:A:24:MET:N	1:A:29:ASP:OD2	2.33	0.61
1:A:508:ILE:H	1:A:508:ILE:HD13	1.65	0.61
1:B:170:ARG:O	1:B:174:ILE:HG12	1.99	0.61
2:C:347:VAL:O	2:C:348:CYS:HB2	1.99	0.61
2:D:23:THR:HB	2:D:25:ILE:HG13	1.82	0.61
2:D:375:ILE:HG13	2:D:408:ILE:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:HB2	1:A:182:THR:HB	1.83	0.61
1:B:187:GLU:OE2	1:B:208:ARG:HA	2.01	0.61
2:D:218:ARG:HG3	2:D:237:PHE:O	2.00	0.61
1:F:115:GLN:CG	1:F:116:GLU:H	2.13	0.61
1:F:363:ILE:O	1:F:367:ILE:HG13	2.00	0.61
2:D:123:LEU:O	2:D:127:ILE:HG13	2.00	0.61
1:E:469:GLU:HB3	1:E:483:PHE:CE1	2.36	0.61
1:F:313:ILE:CD1	1:F:372:PRO:HG2	2.31	0.61
1:B:112:PRO:O	2:C:166:ARG:HG3	2.01	0.61
2:C:170:ARG:O	2:C:174:ILE:HG12	2.01	0.61
1:E:31:ILE:HA	1:E:231:MET:HG3	1.83	0.61
1:E:93:ASP:OD1	1:E:95:ALA:HB3	2.01	0.61
1:F:484:ARG:HB3	1:F:484:ARG:HH11	1.66	0.61
2:C:283:ILE:HG13	2:C:400:THR:HG23	1.81	0.60
2:C:315:PHE:HA	2:C:347:VAL:HB	1.83	0.60
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.66	0.60
1:F:64:ILE:HG22	1:F:65:ILE:HD13	1.82	0.60
1:B:326:ARG:HD3	2:C:259:SER:O	2.01	0.60
2:C:488:ARG:O	2:C:491:SER:HB3	2.01	0.60
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.36	0.60
1:F:194:TYR:O	1:F:196:VAL:HG23	2.00	0.60
1:A:191:ILE:HB	1:A:198:GLU:CG	2.31	0.60
1:A:418:GLN:HB2	1:B:423:HIS:O	2.02	0.60
1:B:414:ASN:ND2	1:B:426:TPO:HG23	2.17	0.60
1:E:170:ARG:O	1:E:174:ILE:HG12	2.01	0.60
1:A:79:THR:HG22	1:A:81:GLN:HG2	1.83	0.60
2:C:315:PHE:HE2	2:C:363:ILE:HA	1.62	0.60
1:A:32:SER:OG	1:A:35:GLY:N	2.34	0.60
1:A:52:LYS:HD2	1:A:181:THR:HG23	1.84	0.60
1:B:202:ASP:HA	1:B:226:ARG:HD2	1.82	0.60
1:B:311:ARG:HD2	1:B:371:LYS:HE3	1.84	0.60
2:C:48:SER:HB2	2:D:199:PHE:CE1	2.36	0.60
2:D:48:SER:HA	5:D:526:HOH:O	2.01	0.60
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.36	0.60
2:C:156:ALA:O	2:C:160:VAL:HG23	2.01	0.60
2:C:70:PRO:HG2	2:C:138:ARG:O	2.02	0.60
2:D:380:LEU:N	2:D:413:THR:O	2.32	0.60
1:E:455:VAL:HG11	1:E:463:HIS:HB2	1.82	0.60
1:F:269:ARG:O	1:F:272:GLU:HB2	2.01	0.60
1:A:273:MET:O	1:A:464:ASP:N	2.30	0.60
2:C:393:ARG:NH2	2:C:429:HIS:HB2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:GLN:H	2:D:81:GLN:CD	2.05	0.60
2:D:163:GLU:HA	2:D:163:GLU:OE2	2.01	0.60
1:E:52:LYS:HB3	1:E:181:THR:CG2	2.31	0.60
1:F:247:PHE:HB3	1:F:249:LEU:HD21	1.81	0.60
1:F:451:ARG:HG2	1:F:451:ARG:HH11	1.67	0.60
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.32	0.60
2:C:389:ASN:HD21	2:C:428:SER:HB2	1.67	0.60
1:E:283:ILE:HD12	1:E:412:PHE:HE1	1.66	0.60
1:F:248:PRO:C	1:F:250:GLY:H	2.06	0.60
1:F:260:ASN:HA	1:F:279:PHE:CE2	2.36	0.60
1:B:294:LYS:HB3	1:B:413:THR:HG23	1.83	0.60
1:E:153:GLN:C	1:F:158:SER:HB2	2.22	0.60
1:F:197:GLU:H	1:F:197:GLU:CD	2.03	0.60
1:F:329:TYR:HA	1:F:332:GLY:O	2.01	0.60
1:A:230:HIS:CE1	1:A:232:LYS:HG3	2.37	0.59
1:B:62:ASN:O	1:B:66:GLU:HB2	2.02	0.59
1:E:392:PHE:O	1:E:395:PHE:N	2.35	0.59
1:F:53:THR:OG1	1:F:145:ASP:OD1	2.20	0.59
1:A:147:VAL:HG11	1:A:180:MET:CE	2.32	0.59
2:C:464:ASP:OD1	2:C:466:ALA:N	2.35	0.59
2:C:386:GLY:HA2	2:D:390:ASN:HD21	1.66	0.59
1:A:446:ARG:HA	1:A:496:ARG:HH22	1.67	0.59
1:E:164:LEU:HD11	1:E:197:GLU:HG3	1.85	0.59
1:F:47:THR:CG2	1:F:50:THR:CG2	2.80	0.59
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.82	0.59
1:A:448:GLU:HG2	1:B:466:ALA:HB2	1.84	0.59
1:B:31:ILE:HG23	1:B:231:MET:HB2	1.85	0.59
1:B:52:LYS:O	1:B:53:THR:C	2.41	0.59
2:C:358:ASP:O	2:C:362:ILE:HG12	2.02	0.59
1:E:153:GLN:O	1:F:158:SER:HB2	2.02	0.59
1:F:78:GLU:CB	1:F:83:ILE:HD11	2.32	0.59
1:F:82:ASP:HA	1:F:85:LYS:HB3	1.84	0.59
1:B:221:GLU:HG2	1:B:222:ILE:N	2.15	0.59
1:B:415:THR:HB	2:C:432:GLU:OE2	2.02	0.59
1:B:490:ILE:HG22	1:B:491:SER:N	2.18	0.59
2:D:152:GLN:HG3	1:E:161:ARG:HH11	1.67	0.59
1:E:467:ILE:O	1:E:467:ILE:HG22	2.02	0.59
1:F:311:ARG:HD2	1:F:371:LYS:CE	2.33	0.59
1:A:469:GLU:HG3	1:A:470:PHE:N	2.18	0.59
1:B:123:LEU:O	1:B:127:ILE:HG13	2.02	0.59
2:D:155:ASP:OD1	2:D:159:VAL:HG11	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:VAL:HG21	1:E:477:PRO:HG3	1.85	0.59
1:B:50:THR:HB	1:B:207:LEU:CB	2.33	0.59
2:D:81:GLN:H	2:D:81:GLN:NE2	2.01	0.59
2:D:262:ARG:NH1	2:D:275:GLY:O	2.36	0.59
1:E:501:GLU:O	1:E:502:LYS:HG3	2.03	0.59
1:F:501:GLU:HG3	1:F:502:LYS:N	2.17	0.59
1:A:211:LEU:CG	1:A:212:GLU:H	2.08	0.59
1:B:148:THR:C	1:B:150:VAL:H	2.07	0.59
1:B:363:ILE:O	1:B:367:ILE:HG13	2.03	0.59
1:E:419:PHE:CE2	1:F:425:ILE:HG13	2.37	0.59
1:F:453:ILE:HG12	1:F:454:ASN:N	2.18	0.59
1:A:18:ILE:N	1:A:18:ILE:HD12	2.18	0.58
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.84	0.58
1:F:315:PHE:CE2	1:F:347:VAL:HG21	2.38	0.58
1:B:36:LEU:HD12	1:B:59:PHE:CE1	2.38	0.58
1:B:140:ARG:HH11	1:B:140:ARG:CB	2.15	0.58
1:B:185:ILE:HD13	1:B:185:ILE:N	2.19	0.58
2:D:86:ASN:O	2:D:88:ARG:N	2.36	0.58
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.67	0.58
1:E:184:ARG:NH2	1:E:187:GLU:O	2.36	0.58
1:E:342:ASN:O	1:E:343:LEU:HD23	2.02	0.58
1:E:385:ARG:HA	1:F:393:ARG:NH1	2.19	0.58
1:F:187:GLU:OE2	1:F:208:ARG:HA	2.03	0.58
1:B:193:ARG:NH2	2:C:196:VAL:HG23	2.19	0.58
2:C:220:LEU:HD23	2:C:221:GLU:N	2.17	0.58
2:C:379:SER:H	2:C:413:THR:HB	1.68	0.58
1:E:344:LEU:HD13	1:E:345:LYS:N	2.19	0.58
1:F:150:VAL:HG13	1:F:151:PHE:N	2.17	0.58
1:F:220:LEU:HD23	1:F:220:LEU:C	2.23	0.58
1:F:294:LYS:HB3	1:F:413:THR:HG23	1.83	0.58
1:F:370:PHE:C	1:F:372:PRO:HD3	2.23	0.58
1:A:286:ALA:HA	1:A:438:ILE:O	2.03	0.58
2:D:150:VAL:O	2:D:153:GLN:HG3	2.02	0.58
1:E:21:MET:HE3	1:E:141:ARG:NE	2.18	0.58
1:E:81:GLN:NE2	1:E:81:GLN:H	2.02	0.58
1:A:348:CYS:SG	1:B:254:LEU:CD2	2.91	0.58
2:C:185:ILE:HD13	2:C:185:ILE:N	2.19	0.58
1:E:420:MET:SD	1:F:490:ILE:HG13	2.44	0.58
1:F:191:ILE:HB	1:F:198:GLU:CG	2.32	0.58
1:A:85:LYS:HE3	1:B:18:ILE:HD13	1.85	0.58
1:B:150:VAL:O	1:B:153:GLN:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.69	0.58
1:B:341:GLN:O	1:B:342:ASN:C	2.41	0.58
2:C:106:LEU:CD2	2:C:130:ILE:HG12	2.34	0.58
2:C:311:ARG:HD3	2:C:370:PHE:O	2.04	0.58
1:E:492:GLY:O	1:E:494:PRO:HD3	2.03	0.58
1:A:254:LEU:HG	1:F:320:SER:HA	1.86	0.58
2:C:493:SER:OG	2:D:488:ARG:HG2	2.04	0.58
1:E:311:ARG:HD2	1:E:371:LYS:CE	2.33	0.58
2:C:344:LEU:HD11	2:C:346:ILE:HG13	1.85	0.58
2:D:83:ILE:H	2:D:83:ILE:HD12	1.67	0.58
1:E:126:LEU:O	1:E:130:ILE:HG13	2.04	0.58
1:F:248:PRO:O	1:F:250:GLY:N	2.36	0.58
1:A:360:LEU:HD21	1:A:398:GLY:O	2.03	0.58
1:B:31:ILE:O	1:B:231:MET:HG3	2.04	0.58
1:B:462:TRP:O	1:B:463:HIS:O	2.21	0.58
2:D:21:MET:HE2	2:D:177:THR:HG21	1.86	0.58
2:D:21:MET:O	2:D:35:GLY:HA3	2.03	0.58
2:D:182:THR:HG22	2:D:183:GLU:N	2.18	0.58
2:D:312:ALA:O	2:D:344:LEU:HD22	2.04	0.58
2:D:318:GLU:OE2	1:E:432:GLU:HB3	2.03	0.58
2:D:367:ILE:HD11	2:D:375:ILE:CD1	2.34	0.58
1:E:33:HIS:HD2	1:E:230:HIS:HA	1.69	0.58
1:E:200:VAL:O	1:E:200:VAL:HG12	2.04	0.58
1:E:323:GLN:HG2	1:E:327:ASN:ND2	2.19	0.58
1:F:231:MET:CE	1:F:251:ALA:HB2	2.34	0.58
1:B:24:MET:CB	1:B:62:ASN:HD22	2.17	0.58
2:C:38:ILE:H	2:C:38:ILE:HD12	1.68	0.58
2:C:486:PHE:CE2	2:C:496:ARG:HG2	2.39	0.58
1:F:353:SER:O	1:F:354:ALA:CB	2.51	0.58
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.69	0.58
1:B:81:GLN:H	1:B:81:GLN:NE2	2.01	0.57
2:C:147:VAL:O	2:C:150:VAL:HG12	2.04	0.57
2:C:265:SER:O	2:C:301:PHE:HA	2.04	0.57
2:D:147:VAL:HG11	2:D:180:MET:CE	2.32	0.57
1:A:316:ALA:O	1:A:348:CYS:HA	2.04	0.57
2:C:38:ILE:HG22	2:C:39:GLY:N	2.18	0.57
2:D:151:PHE:C	2:D:153:GLN:H	2.07	0.57
1:F:406:GLU:O	1:F:408:ILE:HG13	2.04	0.57
1:A:274:CYS:SG	1:A:278:PHE:HE2	2.27	0.57
1:B:147:VAL:O	1:B:150:VAL:HG12	2.03	0.57
2:C:493:SER:OG	2:D:488:ARG:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:294:LYS:N	3:D:901:ATP:O1B	2.36	0.57
1:A:152:GLN:HG3	1:B:161:ARG:HH11	1.70	0.57
1:A:284:ILE:CD1	1:A:436:THR:HB	2.34	0.57
2:C:71:GLY:O	2:C:104:PHE:N	2.37	0.57
1:E:291:GLY:C	1:E:442:TYR:OH	2.42	0.57
2:C:182:THR:CG2	2:C:183:GLU:N	2.68	0.57
2:C:298:VAL:O	2:C:301:PHE:HB3	2.04	0.57
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.34	0.57
2:C:497:ILE:HD12	2:C:497:ILE:O	2.04	0.57
2:D:305:ALA:O	2:D:310:GLU:O	2.22	0.57
2:D:332:GLY:O	2:D:333:MET:O	2.22	0.57
1:E:132:TYR:HE2	1:E:136:LYS:HD2	1.69	0.57
1:A:27:GLY:O	1:A:30:ASP:N	2.33	0.57
2:C:70:PRO:HB2	2:C:139:ALA:CA	2.30	0.57
2:D:225:LEU:HB2	2:D:230:HIS:CD2	2.40	0.57
1:F:311:ARG:HD2	1:F:371:LYS:HE3	1.86	0.57
1:B:191:ILE:HD12	1:B:191:ILE:N	2.20	0.57
1:B:436:THR:HA	1:B:457:LYS:O	2.04	0.57
2:C:294:LYS:O	2:C:298:VAL:HG23	2.04	0.57
2:C:296:LEU:CD2	2:C:477:PRO:HB3	2.35	0.57
2:C:389:ASN:O	2:C:392:PHE:N	2.38	0.57
2:D:31:ILE:HA	2:D:231:MET:CG	2.35	0.57
2:D:214:GLU:HG2	1:E:234:GLU:OE1	2.04	0.57
1:E:23:THR:O	1:E:24:MET:HB2	2.04	0.57
1:F:435:ASP:OD1	1:F:459:ARG:NH1	2.37	0.57
1:A:70:PRO:HA	1:A:102:LYS:O	2.04	0.57
1:A:191:ILE:HD13	1:A:198:GLU:OE2	2.04	0.57
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.40	0.57
2:C:149:SER:HB3	2:D:161:ARG:NH2	2.19	0.57
2:D:249:LEU:HD12	2:D:394:GLN:OE1	2.04	0.57
2:D:295:THR:HA	2:D:298:VAL:CG2	2.35	0.57
1:F:52:LYS:HB3	1:F:181:THR:HG23	1.86	0.57
1:F:344:LEU:C	1:F:344:LEU:HD13	2.25	0.57
1:F:379:SER:OG	1:F:382:ALA:HB2	2.04	0.57
1:F:515:LYS:HG3	1:F:516:GLY:N	2.14	0.57
1:B:126:LEU:HD12	1:B:129:ARG:HD3	1.87	0.57
1:B:431:ALA:HA	1:B:434:THR:HG22	1.86	0.57
2:C:212:GLU:O	2:C:212:GLU:HG2	2.04	0.57
2:C:323:GLN:NE2	2:D:459:ARG:HD3	2.20	0.57
1:F:446:ARG:H	1:F:496:ARG:NH2	2.03	0.57
2:D:353:SER:O	2:D:354:ALA:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:THR:CG2	1:E:414:ASN:HD22	2.18	0.57
1:E:445:ILE:HG22	1:E:445:ILE:O	2.04	0.57
1:F:435:ASP:HA	1:F:459:ARG:HD2	1.87	0.57
1:A:458:MET:O	3:F:901:ATP:H3'	2.05	0.56
1:B:435:ASP:HA	1:B:459:ARG:HD2	1.87	0.56
2:C:231:MET:CE	2:C:251:ALA:HB2	2.35	0.56
2:D:151:PHE:O	2:D:153:GLN:N	2.32	0.56
1:E:283:ILE:HD12	1:E:412:PHE:CE1	2.40	0.56
1:A:299:SER:CB	1:A:333:MET:HE1	2.22	0.56
1:B:36:LEU:HD22	1:B:42:THR:HG21	1.86	0.56
1:B:294:LYS:N	3:B:901:ATP:O1B	2.38	0.56
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.70	0.56
2:C:357:GLU:HG3	2:C:358:ASP:N	2.20	0.56
1:E:273:MET:SD	1:E:479:ILE:HD13	2.45	0.56
1:F:103:LEU:C	1:F:103:LEU:HD12	2.26	0.56
1:F:305:ALA:HB2	1:F:374:ARG:CD	2.28	0.56
1:A:188:TYR:HE2	1:F:211:LEU:HD23	1.69	0.56
1:A:298:VAL:HG23	1:A:411:LEU:HD23	1.88	0.56
2:C:24:MET:CB	2:C:62:ASN:HD22	2.16	0.56
2:C:425:ILE:HD12	2:C:425:ILE:H	1.70	0.56
2:D:96:LYS:O	2:D:100:GLU:HG3	2.05	0.56
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.86	0.56
2:D:382:ALA:O	2:D:385:ARG:HG3	2.04	0.56
2:D:461:SER:OG	2:D:462:TRP:N	2.39	0.56
1:E:266:GLY:HA3	1:E:300:ARG:HG3	1.86	0.56
1:E:364:LYS:O	1:E:368:ASN:ND2	2.38	0.56
1:E:444:GLU:OE1	1:F:489:ILE:HB	2.05	0.56
1:E:451:ARG:HD2	1:E:451:ARG:N	2.20	0.56
1:F:379:SER:H	1:F:413:THR:HB	1.70	0.56
1:A:191:ILE:HB	1:A:198:GLU:HG2	1.87	0.56
1:B:308:ASN:O	1:B:310:GLU:HG3	2.05	0.56
1:B:379:SER:N	1:B:413:THR:HB	2.21	0.56
2:C:488:ARG:HH22	2:D:488:ARG:NH2	2.03	0.56
1:B:192:ALA:HB3	1:B:197:GLU:OE2	2.05	0.56
2:C:404:LYS:C	2:C:406:GLU:H	2.09	0.56
2:D:170:ARG:HH12	2:D:174:ILE:HD11	1.70	0.56
1:F:45:SER:HB3	1:F:182:THR:HB	1.87	0.56
1:A:509:VAL:O	1:A:511:GLY:N	2.37	0.56
2:C:150:VAL:HG13	2:C:151:PHE:N	2.20	0.56
2:C:191:ILE:HD12	2:C:191:ILE:H	1.70	0.56
1:F:111:ASP:OD1	1:F:112:PRO:HD2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:TPO:C	1:F:428:SER:H	2.19	0.56
1:A:14:GLU:CG	1:A:15:HIS:N	2.66	0.56
1:B:117:VAL:O	1:B:117:VAL:HG12	2.06	0.56
1:B:150:VAL:HG13	1:B:151:PHE:N	2.20	0.56
1:B:150:VAL:CG1	1:B:151:PHE:N	2.69	0.56
1:B:334:ASP:O	1:B:338:MET:HG2	2.06	0.56
1:B:347:VAL:O	1:B:348:CYS:HB2	2.06	0.56
2:C:315:PHE:HB3	2:C:317:TYR:HE1	1.69	0.56
1:E:146:SER:HA	1:E:181:THR:O	2.06	0.56
1:A:471:MET:CG	1:A:478:ASP:HB3	2.35	0.56
1:B:130:ILE:HG22	1:B:134:ILE:HD11	1.86	0.56
2:C:261:VAL:CG1	2:C:262:ARG:H	2.16	0.56
1:E:379:SER:N	1:E:413:THR:HB	2.19	0.56
1:F:192:ALA:HB3	1:F:197:GLU:OE2	2.06	0.56
1:A:64:ILE:CD1	1:A:103:LEU:HB2	2.34	0.56
1:B:64:ILE:HG21	1:B:97:LEU:HD13	1.86	0.56
1:B:123:LEU:HG	1:B:163:GLU:HB3	1.87	0.56
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.46	0.56
2:D:346:ILE:CG2	2:D:347:VAL:N	2.68	0.56
1:E:221:GLU:HG2	1:E:222:ILE:N	2.19	0.56
1:E:371:LYS:HD2	1:E:371:LYS:O	2.05	0.56
1:A:219:THR:HA	1:A:235:TYR:O	2.06	0.56
1:B:502:LYS:HG3	1:B:504:GLU:O	2.06	0.56
2:C:20:LYS:C	2:C:38:ILE:HD11	2.27	0.56
2:D:468:ARG:HG2	2:D:468:ARG:HH11	1.71	0.56
1:F:484:ARG:HB3	1:F:484:ARG:NH1	2.19	0.56
1:A:254:LEU:HD23	1:F:348:CYS:SG	2.46	0.55
1:A:318:GLU:OE2	1:B:432:GLU:HB3	2.05	0.55
2:C:471:MET:SD	2:C:478:ASP:HB3	2.46	0.55
2:D:294:LYS:H	2:D:294:LYS:HD3	1.71	0.55
2:D:350:TYR:CE1	1:E:254:LEU:HD13	2.42	0.55
1:F:362:ILE:O	1:F:365:SER:HB3	2.06	0.55
1:F:396:VAL:HG11	1:F:430:ILE:HD12	1.88	0.55
1:F:439:LEU:HD23	1:F:454:ASN:HD22	1.71	0.55
1:F:514:GLU:O	1:F:515:LYS:HB2	2.05	0.55
1:B:237:PHE:HB2	1:B:246:ILE:HG12	1.88	0.55
1:B:325:LEU:O	1:B:328:ALA:HB3	2.06	0.55
1:B:486:PHE:CE2	1:B:496:ARG:HB2	2.41	0.55
1:E:311:ARG:HD3	1:E:370:PHE:CE1	2.40	0.55
1:E:417:ASP:OD2	1:F:429:HIS:CE1	2.60	0.55
1:F:191:ILE:HB	1:F:198:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.46	0.55
1:F:514:GLU:O	1:F:515:LYS:CB	2.53	0.55
1:A:344:LEU:HD13	1:A:344:LEU:C	2.26	0.55
1:A:426:TPO:CG2	1:A:426:TPO:O3P	2.55	0.55
1:E:167:LEU:HG	1:E:171:LEU:HD12	1.89	0.55
1:A:199:PHE:CZ	1:F:183:GLU:HB2	2.41	0.55
1:A:483:PHE:HB2	1:A:489:ILE:CD1	2.36	0.55
2:C:63:GLY:HA3	2:C:141:ARG:CZ	2.36	0.55
2:C:71:GLY:O	2:C:103:LEU:HA	2.05	0.55
2:C:191:ILE:HD12	2:C:191:ILE:N	2.21	0.55
1:F:45:SER:CB	1:F:182:THR:HB	2.37	0.55
1:F:408:ILE:HG22	1:F:408:ILE:O	2.06	0.55
2:C:142:VAL:O	2:C:178:THR:HA	2.07	0.55
2:C:311:ARG:HA	2:C:343:LEU:O	2.06	0.55
2:D:334:ASP:O	2:D:338:MET:HG2	2.07	0.55
2:D:358:ASP:O	2:D:361:GLN:N	2.40	0.55
1:F:323:GLN:HG2	1:F:327:ASN:HD21	1.71	0.55
1:F:515:LYS:HB3	1:F:517:PRO:HD2	1.89	0.55
1:A:317:TYR:HA	1:A:349:ALA:O	2.06	0.55
1:A:350:TYR:OH	1:B:254:LEU:HD13	2.07	0.55
1:A:362:ILE:O	1:A:366:GLU:HB2	2.07	0.55
1:A:414:ASN:ND2	1:A:426:TPO:HA	2.21	0.55
2:D:220:LEU:HD13	2:D:246:ILE:HD11	1.89	0.55
1:E:170:ARG:HD2	1:E:173:GLN:OE1	2.07	0.55
1:A:52:LYS:HB3	1:A:181:THR:HG23	1.88	0.55
1:B:383:LEU:HD13	1:B:395:PHE:CE2	2.42	0.55
2:C:261:VAL:O	2:C:262:ARG:HG2	2.07	0.55
2:C:262:ARG:NH2	2:C:461:SER:HB2	2.22	0.55
2:D:347:VAL:CG1	2:D:348:CYS:N	2.70	0.55
2:D:354:ALA:HB3	2:D:359:HIS:CE1	2.40	0.55
1:B:284:ILE:CD1	1:B:436:THR:HB	2.37	0.55
2:C:94:LEU:O	2:C:98:VAL:HG23	2.06	0.55
2:C:217:ARG:HG3	2:C:217:ARG:O	2.06	0.55
1:E:441:GLN:HE22	1:E:490:ILE:HA	1.71	0.55
1:F:508:ILE:H	1:F:508:ILE:HD12	1.71	0.55
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.22	0.55
2:C:31:ILE:HG23	2:C:231:MET:HB2	1.89	0.55
2:C:252:MET:HE3	2:C:397:ILE:HG22	1.89	0.55
2:D:23:THR:O	2:D:24:MET:HB2	2.07	0.55
2:D:387:VAL:CG1	2:D:388:SER:N	2.68	0.55
1:E:417:ASP:O	1:F:424:SER:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.72	0.55
1:B:291:GLY:HA3	1:B:442:TYR:OH	2.06	0.55
1:F:203:ASN:OD1	1:F:225:LEU:HA	2.06	0.55
1:A:211:LEU:O	1:A:212:GLU:CB	2.44	0.54
1:A:483:PHE:HB2	1:A:489:ILE:HD11	1.88	0.54
1:B:284:ILE:HD12	1:B:436:THR:HB	1.88	0.54
2:D:147:VAL:O	2:D:150:VAL:HG12	2.07	0.54
2:D:315:PHE:HB3	2:D:317:TYR:HE1	1.72	0.54
1:A:363:ILE:O	1:A:367:ILE:HG13	2.07	0.54
1:A:379:SER:O	1:A:382:ALA:HB3	2.08	0.54
1:A:419:PHE:CD2	1:B:425:ILE:HD12	2.43	0.54
1:B:167:LEU:O	1:B:170:ARG:N	2.40	0.54
2:C:379:SER:HA	2:C:413:THR:O	2.07	0.54
1:E:54:LEU:HD13	1:E:90:PHE:CE1	2.42	0.54
1:E:203:ASN:CB	1:E:225:LEU:HD23	2.29	0.54
1:E:451:ARG:HH11	1:E:451:ARG:CG	2.18	0.54
1:F:183:GLU:HG3	1:F:193:ARG:HE	1.72	0.54
1:F:471:MET:HE2	1:F:471:MET:O	2.07	0.54
1:A:442:TYR:CE1	1:B:456:PHE:CZ	2.95	0.54
1:A:501:GLU:O	1:A:503:SER:N	2.39	0.54
2:C:354:ALA:HB1	2:C:358:ASP:HB2	1.90	0.54
2:D:399:VAL:O	2:D:400:THR:C	2.45	0.54
1:E:294:LYS:CB	1:E:413:THR:HG23	2.37	0.54
1:F:397:ILE:CD1	1:F:433:ILE:HG12	2.38	0.54
1:A:87:ALA:HB1	1:A:92:TRP:CD1	2.42	0.54
1:A:389:ASN:ND2	1:A:428:SER:HB2	2.23	0.54
1:B:51:GLY:O	1:B:54:LEU:HB3	2.08	0.54
2:C:418:GLN:HB2	2:D:423:HIS:O	2.07	0.54
2:D:94:LEU:O	2:D:98:VAL:HG23	2.07	0.54
1:E:132:TYR:CE2	1:E:136:LYS:HD2	2.42	0.54
1:E:290:THR:HG21	1:F:431:ALA:HB1	1.88	0.54
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.88	0.54
2:D:31:ILE:HA	2:D:231:MET:HG3	1.89	0.54
1:E:499:VAL:O	1:E:499:VAL:HG12	2.07	0.54
1:F:418:GLN:NE2	1:F:421:GLY:O	2.40	0.54
1:A:218:ARG:O	1:A:236:PRO:HA	2.07	0.54
1:B:121:PHE:H	1:B:121:PHE:HD1	1.54	0.54
1:B:451:ARG:N	1:B:451:ARG:HD2	2.23	0.54
2:C:72:VAL:HG13	2:C:104:PHE:HD2	1.72	0.54
2:C:426:THR:HG22	2:C:427:ASP:N	2.23	0.54
2:C:462:TRP:O	2:C:463:HIS:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:273:MET:CE	2:D:468:ARG:HD2	2.37	0.54
1:F:436:THR:HG23	1:F:458:MET:HG2	1.89	0.54
3:A:903:ATP:O3'	1:B:224:LYS:HA	2.07	0.54
1:B:131:ASN:HA	1:B:134:ILE:HD12	1.90	0.54
1:B:193:ARG:NH2	2:C:195:GLY:O	2.41	0.54
1:B:293:GLY:O	1:B:296:LEU:HB3	2.08	0.54
2:C:95:ALA:O	2:C:99:ASP:HB2	2.08	0.54
2:D:313:ILE:HG12	2:D:345:LYS:HB3	1.89	0.54
1:F:78:GLU:HB3	1:F:83:ILE:CD1	2.38	0.54
1:F:426:TPO:HG21	1:F:429:HIS:CA	2.38	0.54
1:B:48:SER:OG	2:C:224:LYS:HD3	2.07	0.54
2:D:347:VAL:HG12	2:D:348:CYS:H	1.71	0.54
1:E:106:LEU:HD11	1:E:129:ARG:CZ	2.38	0.54
1:A:426:TPO:O3P	1:A:426:TPO:HG21	2.08	0.54
1:A:429:HIS:CD2	1:F:417:ASP:CG	2.81	0.54
1:B:25:ILE:CG1	1:B:58:GLN:HE21	2.12	0.54
2:C:87:ALA:O	2:C:89:SER:N	2.40	0.54
1:E:169:ALA:O	1:E:173:GLN:HG3	2.06	0.54
1:E:447:GLY:HA2	1:F:467:ILE:HD12	1.90	0.54
1:F:21:MET:HE3	1:F:59:PHE:CE1	2.43	0.54
1:F:163:GLU:HA	1:F:163:GLU:OE2	2.07	0.54
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.37	0.54
2:D:486:PHE:HE2	2:D:496:ARG:HD3	1.70	0.54
1:A:272:GLU:O	1:A:462:TRP:HZ3	1.91	0.53
1:B:287:THR:HG21	1:B:425:ILE:O	2.08	0.53
2:C:20:LYS:HE3	2:C:228:THR:HG21	1.91	0.53
2:C:144:ILE:HG22	2:C:147:VAL:HG12	1.89	0.53
2:D:49:GLY:HA2	1:E:224:LYS:HB3	1.90	0.53
2:D:178:THR:CG2	2:D:179:VAL:N	2.71	0.53
1:E:318:GLU:OE2	1:F:432:GLU:OE1	2.26	0.53
1:E:435:ASP:N	1:E:435:ASP:OD1	2.41	0.53
1:F:170:ARG:HD2	1:F:173:GLN:OE1	2.08	0.53
1:F:504:GLU:HA	1:F:507:ARG:HG3	1.89	0.53
2:C:21:MET:HE3	2:C:141:ARG:CZ	2.39	0.53
2:C:38:ILE:HG23	2:C:177:THR:OG1	2.08	0.53
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.89	0.53
2:C:471:MET:HE2	2:C:478:ASP:H	1.72	0.53
2:D:370:PHE:O	2:D:371:LYS:HG3	2.08	0.53
1:E:504:GLU:CG	1:E:505:LEU:H	2.14	0.53
1:F:64:ILE:HG21	1:F:97:LEU:HD13	1.90	0.53
1:F:256:GLN:HB3	1:F:405:GLN:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:PHE:CE2	1:F:496:ARG:HD2	2.43	0.53
1:A:89:SER:HB2	1:B:227:GLY:O	2.08	0.53
1:A:315:PHE:HE1	1:A:375:ILE:HG12	1.74	0.53
2:C:54:LEU:O	2:C:57:ILE:N	2.42	0.53
1:E:67:PHE:O	1:E:69:GLU:HG3	2.09	0.53
1:F:453:ILE:CG1	1:F:454:ASN:H	2.21	0.53
1:A:459:ARG:NH1	1:F:319:GLU:HG2	2.23	0.53
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.91	0.53
2:C:218:ARG:HD2	5:C:526:HOH:O	2.08	0.53
2:C:310:GLU:O	2:C:343:LEU:HB3	2.08	0.53
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.39	0.53
1:E:194:TYR:O	1:E:196:VAL:HB	2.09	0.53
1:E:497:ILE:HG22	1:E:498:THR:N	2.21	0.53
1:F:52:LYS:HB3	1:F:181:THR:CG2	2.39	0.53
1:B:247:PHE:HZ	1:B:361:GLN:HG3	1.74	0.53
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.74	0.53
2:C:38:ILE:HG22	2:C:39:GLY:H	1.73	0.53
2:D:264:SER:HA	2:D:271:ASP:OD1	2.08	0.53
1:F:316:ALA:HB2	1:F:324:LEU:HD11	1.89	0.53
1:F:437:ILE:HD12	1:F:457:LYS:HG2	1.90	0.53
1:A:24:MET:CB	1:A:62:ASN:HD22	2.21	0.53
1:A:188:TYR:HE2	1:F:211:LEU:CD2	2.22	0.53
2:C:248:PRO:O	2:C:250:GLY:N	2.42	0.53
2:C:386:GLY:CA	2:D:390:ASN:HD21	2.21	0.53
2:D:44:VAL:HG22	2:D:205:VAL:CB	2.39	0.53
2:D:443:VAL:HG13	2:D:494:PRO:HG2	1.89	0.53
1:E:406:GLU:O	1:E:408:ILE:HG13	2.09	0.53
1:F:44:VAL:O	1:F:181:THR:HA	2.08	0.53
1:F:47:THR:HG22	1:F:50:THR:HG22	1.89	0.53
1:F:262:ARG:HD2	1:F:276:GLY:O	2.08	0.53
2:C:23:THR:O	2:C:24:MET:HB2	2.08	0.53
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.90	0.53
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.90	0.53
1:B:286:ALA:HA	1:B:438:ILE:O	2.09	0.53
2:C:170:ARG:HB3	2:C:170:ARG:NH1	2.24	0.53
2:C:248:PRO:O	2:C:251:ALA:N	2.42	0.53
1:E:220:LEU:HD13	1:E:246:ILE:HD11	1.91	0.53
1:E:262:ARG:HD2	1:E:276:GLY:O	2.09	0.53
1:F:118:VAL:O	1:F:118:VAL:HG13	2.08	0.53
1:F:147:VAL:HG23	1:F:148:THR:N	2.24	0.53
1:A:375:ILE:O	1:A:410:GLY:HA2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:VAL:HG21	1:A:430:ILE:HD12	1.91	0.53
1:B:43:LEU:HD12	1:B:180:MET:HB2	1.92	0.53
2:C:71:GLY:N	2:C:102:LYS:O	2.41	0.53
2:D:451:ARG:H	2:D:451:ARG:HD2	1.74	0.53
1:F:451:ARG:HD2	1:F:451:ARG:N	2.24	0.53
1:B:50:THR:HG21	1:B:207:LEU:O	2.09	0.52
2:C:151:PHE:C	2:C:153:GLN:H	2.12	0.52
2:C:334:ASP:O	2:C:338:MET:HG2	2.09	0.52
2:C:426:THR:HG22	2:C:428:SER:H	1.73	0.52
2:D:52:LYS:HE3	5:D:550:HOH:O	2.07	0.52
2:D:468:ARG:HG2	2:D:468:ARG:NH1	2.23	0.52
1:E:303:GLU:OE2	1:E:333:MET:HB3	2.09	0.52
1:E:313:ILE:HD12	1:E:372:PRO:HG2	1.90	0.52
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.90	0.52
1:A:162:ARG:O	1:A:165:PHE:HB3	2.09	0.52
1:A:251:ALA:O	1:A:252:MET:C	2.47	0.52
1:A:257:ARG:NH2	1:A:407:GLU:HG2	2.23	0.52
1:A:379:SER:HA	1:A:413:THR:O	2.09	0.52
2:C:50:THR:HG21	2:C:207:LEU:O	2.08	0.52
2:C:464:ASP:OD1	2:C:464:ASP:C	2.47	0.52
1:E:451:ARG:HG2	1:E:470:PHE:CE1	2.45	0.52
1:E:497:ILE:O	1:E:498:THR:OG1	2.21	0.52
1:F:73:PHE:HE2	1:F:75:THR:HB	1.74	0.52
1:F:127:ILE:CD1	1:F:167:LEU:HD12	2.39	0.52
1:F:131:ASN:O	1:F:135:GLN:HB2	2.09	0.52
1:F:514:GLU:OE1	1:F:515:LYS:N	2.42	0.52
1:A:296:LEU:HD13	1:A:331:TRP:CE2	2.45	0.52
1:B:316:ALA:O	1:B:348:CYS:HA	2.09	0.52
2:C:469:GLU:HG3	2:C:480:LYS:HE3	1.92	0.52
1:E:47:THR:HG23	5:E:527:HOH:O	2.09	0.52
1:E:416:SER:C	1:E:418:GLN:H	2.12	0.52
1:F:94:LEU:O	1:F:98:VAL:HG23	2.10	0.52
1:F:127:ILE:HD13	1:F:167:LEU:HD12	1.91	0.52
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.90	0.52
1:A:436:THR:OG1	1:A:458:MET:HG2	2.08	0.52
1:B:385:ARG:NH1	2:C:397:ILE:HD11	2.24	0.52
2:C:123:LEU:CD2	2:C:167:LEU:HB2	2.40	0.52
2:C:323:GLN:HE22	2:D:459:ARG:HD3	1.75	0.52
2:D:74:VAL:HA	2:D:106:LEU:HB3	1.91	0.52
2:D:296:LEU:HD12	2:D:296:LEU:O	2.08	0.52
1:E:266:GLY:HA2	1:E:304:ASN:ND2	2.15	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:436:THR:CG2	1:F:458:MET:HG2	2.39	0.52
1:B:497:ILE:HD12	1:B:498:THR:H	1.71	0.52
2:C:98:VAL:HA	2:C:103:LEU:O	2.10	0.52
2:C:296:LEU:HD13	2:C:331:TRP:CE2	2.44	0.52
2:C:395:PHE:O	2:C:399:VAL:HG23	2.09	0.52
2:D:183:GLU:HB2	1:E:199:PHE:CE1	2.44	0.52
1:E:313:ILE:CG1	1:E:372:PRO:HG2	2.39	0.52
1:F:115:GLN:CG	1:F:116:GLU:N	2.72	0.52
1:F:150:VAL:CG1	1:F:151:PHE:N	2.72	0.52
1:F:270:LEU:O	1:F:273:MET:N	2.42	0.52
1:F:289:ALA:O	1:F:292:THR:HG23	2.09	0.52
1:F:418:GLN:HE21	1:F:421:GLY:C	2.13	0.52
1:A:344:LEU:HD13	1:A:345:LYS:N	2.25	0.52
1:B:74:VAL:HG13	1:B:106:LEU:HG	1.90	0.52
2:C:14:GLU:OE2	2:C:16:GLN:HB2	2.10	0.52
2:C:42:THR:HG23	2:C:203:ASN:CB	2.40	0.52
2:D:313:ILE:HG21	2:D:315:PHE:CZ	2.44	0.52
1:E:346:ILE:HG22	1:E:348:CYS:SG	2.49	0.52
1:A:199:PHE:CE1	1:F:183:GLU:HB2	2.44	0.52
1:A:371:LYS:N	1:A:372:PRO:HD3	2.24	0.52
1:B:320:SER:HB3	2:C:256:GLN:HG2	1.91	0.52
2:C:174:ILE:HG22	2:C:174:ILE:O	2.10	0.52
2:C:363:ILE:O	2:C:367:ILE:HG13	2.10	0.52
1:A:44:VAL:HA	1:A:205:VAL:O	2.10	0.52
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.45	0.52
1:B:152:GLN:NE2	1:B:194:TYR:OH	2.43	0.52
2:C:357:GLU:CG	2:C:358:ASP:N	2.73	0.52
1:E:255:THR:HG22	1:E:255:THR:O	2.08	0.52
1:A:148:THR:HG1	1:A:182:THR:HG23	1.75	0.52
1:B:326:ARG:C	1:B:328:ALA:H	2.12	0.52
2:C:53:THR:HG23	2:C:145:ASP:OD1	2.10	0.52
2:C:313:ILE:HG12	2:C:345:LYS:HB3	1.90	0.52
2:D:206:ILE:HD11	2:D:223:LEU:HD12	1.92	0.52
2:D:371:LYS:O	2:D:371:LYS:CD	2.56	0.52
1:E:339:GLU:HG2	1:E:344:LEU:HD12	1.91	0.52
1:A:31:ILE:HG23	1:A:231:MET:HB2	1.92	0.52
1:A:147:VAL:HG11	1:A:180:MET:HE2	1.92	0.52
1:A:230:HIS:HE1	1:A:232:LYS:HG3	1.74	0.52
1:A:385:ARG:HG2	1:B:393:ARG:CZ	2.40	0.52
1:B:404:LYS:C	1:B:406:GLU:H	2.14	0.52
2:C:56:SER:O	2:C:59:PHE:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:VAL:HG13	2:C:104:PHE:CD2	2.44	0.52
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.90	0.52
2:C:387:VAL:HG12	2:C:388:SER:O	2.10	0.52
2:D:219:THR:HA	2:D:235:TYR:O	2.10	0.52
1:E:21:MET:O	1:E:35:GLY:HA3	2.10	0.52
1:E:313:ILE:HG13	1:E:372:PRO:HG2	1.88	0.52
1:E:325:LEU:HD21	1:E:336:GLU:H	1.75	0.52
1:F:47:THR:N	1:F:50:THR:HG21	2.25	0.52
1:F:379:SER:O	1:F:382:ALA:HB3	2.10	0.52
1:B:83:ILE:H	1:B:83:ILE:HD12	1.76	0.51
2:C:140:ARG:HH11	2:C:140:ARG:CB	2.20	0.51
1:E:43:LEU:HD23	1:E:204:VAL:HG13	1.92	0.51
1:B:148:THR:O	1:B:150:VAL:N	2.42	0.51
2:C:50:THR:HB	2:C:207:LEU:CB	2.39	0.51
2:C:320:SER:HB3	2:D:256:GLN:HG2	1.92	0.51
2:C:419:PHE:O	2:C:420:MET:HB2	2.10	0.51
1:E:199:PHE:O	1:E:201:SER:N	2.44	0.51
1:F:80:PRO:CG	1:F:107:ASP:HB2	2.40	0.51
1:F:274:CYS:HG	1:F:278:PHE:HE2	1.57	0.51
1:F:302:VAL:HG12	1:F:303:GLU:N	2.25	0.51
1:B:220:LEU:HD13	1:B:246:ILE:HD11	1.91	0.51
1:B:418:GLN:HB2	2:C:423:HIS:O	2.10	0.51
2:C:32:SER:HB3	2:C:222:ILE:HD11	1.92	0.51
2:C:60:LEU:O	2:C:61:TYR:C	2.47	0.51
1:F:20:LYS:HB3	1:F:35:GLY:O	2.09	0.51
1:F:20:LYS:CE	1:F:228:THR:HG21	2.39	0.51
1:B:53:THR:HB	3:B:903:ATP:PA	2.50	0.51
2:C:261:VAL:CG1	2:C:262:ARG:N	2.73	0.51
1:E:444:GLU:O	1:E:494:PRO:HD2	2.11	0.51
1:A:317:TYR:CD2	1:A:349:ALA:O	2.63	0.51
1:B:65:ILE:O	1:B:65:ILE:HG22	2.10	0.51
1:B:194:TYR:O	1:B:196:VAL:N	2.44	0.51
1:B:321:ARG:NH1	5:B:535:HOH:O	2.44	0.51
1:B:486:PHE:HE2	1:B:496:ARG:HB2	1.75	0.51
2:C:359:HIS:O	2:C:363:ILE:HG13	2.10	0.51
2:D:21:MET:HE3	2:D:59:PHE:CZ	2.41	0.51
2:D:164:LEU:CD1	2:D:197:GLU:HG3	2.41	0.51
1:E:56:SER:HB2	1:E:143:SER:HB3	1.91	0.51
1:E:321:ARG:HG2	1:E:348:CYS:SG	2.51	0.51
1:F:207:LEU:HD21	1:F:220:LEU:HD12	1.91	0.51
1:B:72:VAL:HB	1:B:142:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:PHE:CB	1:B:246:ILE:HG12	2.40	0.51
1:B:360:LEU:C	1:B:360:LEU:HD13	2.31	0.51
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.91	0.51
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.92	0.51
1:E:335:PHE:HA	1:E:338:MET:HG3	1.91	0.51
1:F:273:MET:O	1:F:463:HIS:HB2	2.10	0.51
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.93	0.51
1:B:54:LEU:CD2	1:B:244:ILE:HG13	2.40	0.51
1:B:268:VAL:O	1:B:271:ASP:N	2.44	0.51
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.92	0.51
1:E:25:ILE:HG23	1:E:58:GLN:NE2	2.25	0.51
1:A:94:LEU:HD22	1:A:103:LEU:CD2	2.40	0.51
1:A:164:LEU:HD11	1:A:197:GLU:CG	2.41	0.51
1:B:39:GLY:H	1:B:177:THR:CB	2.24	0.51
1:B:247:PHE:HE2	1:B:364:LYS:HD2	1.76	0.51
1:B:294:LYS:H	1:B:294:LYS:HD3	1.74	0.51
2:C:245:ASN:C	2:C:245:ASN:ND2	2.60	0.51
2:C:295:THR:HG22	2:C:331:TRP:CH2	2.46	0.51
1:F:211:LEU:HD12	1:F:215:ARG:O	2.10	0.51
1:F:334:ASP:OD1	1:F:336:GLU:HB2	2.10	0.51
1:F:430:ILE:O	1:F:432:GLU:N	2.44	0.51
1:A:164:LEU:CD1	1:A:197:GLU:HG3	2.39	0.51
1:B:61:TYR:CE1	1:B:92:TRP:HB2	2.45	0.51
1:B:65:ILE:O	1:B:66:GLU:HG2	2.11	0.51
1:B:145:ASP:HA	1:B:181:THR:HB	1.92	0.51
2:C:90:PHE:N	2:C:90:PHE:CD1	2.78	0.51
2:D:67:PHE:O	2:D:68:ASP:HB3	2.11	0.51
2:D:323:GLN:O	2:D:326:ARG:HB3	2.11	0.51
1:E:97:LEU:N	1:E:97:LEU:HD23	2.25	0.51
1:E:453:ILE:HG22	1:E:470:PHE:HD2	1.76	0.51
1:F:329:TYR:O	1:F:332:GLY:N	2.36	0.51
1:A:483:PHE:N	1:A:483:PHE:CD1	2.79	0.51
2:D:393:ARG:O	2:D:397:ILE:HG12	2.11	0.51
1:E:194:TYR:O	1:E:195:GLY:C	2.49	0.51
1:E:265:SER:HB3	1:E:278:PHE:CZ	2.46	0.51
1:E:292:THR:N	1:E:442:TYR:OH	2.43	0.51
1:F:316:ALA:O	1:F:348:CYS:HA	2.11	0.51
1:A:21:MET:HE1	1:A:59:PHE:HZ	1.74	0.50
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.41	0.50
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.76	0.50
1:B:357:GLU:CG	1:B:358:ASP:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:ILE:H	1:F:38:ILE:HD12	1.76	0.50
1:F:149:SER:O	1:F:152:GLN:HB2	2.11	0.50
1:A:52:LYS:HB2	3:A:903:ATP:O1B	2.11	0.50
1:B:183:GLU:HG3	1:B:193:ARG:HD2	1.94	0.50
1:B:197:GLU:O	1:B:200:VAL:N	2.39	0.50
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.45	0.50
2:C:82:ASP:O	2:C:85:LYS:N	2.44	0.50
2:D:64:ILE:CD1	2:D:97:LEU:HD13	2.41	0.50
2:D:182:THR:CG2	2:D:183:GLU:N	2.74	0.50
1:F:311:ARG:HG3	1:F:371:LYS:NZ	2.26	0.50
1:F:505:LEU:O	1:F:506:SER:HB3	2.11	0.50
1:A:131:ASN:HD21	1:A:135:GLN:NE2	2.09	0.50
1:B:79:THR:O	1:B:83:ILE:HD12	2.11	0.50
2:D:184:ARG:HG2	2:D:191:ILE:O	2.11	0.50
1:E:451:ARG:CG	1:E:451:ARG:NH1	2.72	0.50
1:F:56:SER:O	1:F:59:PHE:HB3	2.11	0.50
1:A:359:HIS:O	1:A:363:ILE:HG13	2.11	0.50
1:B:193:ARG:NH1	5:B:525:HOH:O	2.44	0.50
1:B:248:PRO:O	1:B:251:ALA:N	2.44	0.50
1:B:287:THR:HG22	1:B:288:GLY:N	2.27	0.50
2:D:445:ILE:HA	2:D:496:ARG:HH12	1.75	0.50
2:D:484:ARG:CB	2:D:484:ARG:NH1	2.75	0.50
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.31	0.50
1:F:370:PHE:HB3	1:F:372:PRO:HD3	1.94	0.50
1:F:486:PHE:HB2	1:F:489:ILE:HD11	1.94	0.50
1:F:515:LYS:CB	1:F:517:PRO:HD2	2.41	0.50
2:D:39:GLY:N	2:D:177:THR:HG23	2.25	0.50
2:D:152:GLN:HB3	1:E:161:ARG:HD3	1.93	0.50
1:E:425:ILE:HD12	1:E:456:PHE:CE2	2.45	0.50
1:E:441:GLN:HG3	1:E:441:GLN:O	2.12	0.50
1:F:357:GLU:HG3	1:F:358:ASP:N	2.27	0.50
1:B:53:THR:HA	1:B:145:ASP:OD1	2.11	0.50
1:B:146:SER:N	1:B:181:THR:HB	2.18	0.50
1:B:161:ARG:HH21	1:B:199:PHE:HB2	1.77	0.50
1:B:273:MET:O	1:B:464:ASP:N	2.45	0.50
2:D:486:PHE:HB3	2:D:489:ILE:CD1	2.41	0.50
1:E:445:ILE:HG13	1:E:483:PHE:HE2	1.77	0.50
1:F:59:PHE:CE1	1:F:141:ARG:HD3	2.46	0.50
1:A:52:LYS:O	1:A:55:PHE:N	2.45	0.50
1:A:145:ASP:O	1:A:146:SER:OG	2.26	0.50
1:A:326:ARG:HD3	1:B:258:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:263:VAL:HG12	2:C:374:ARG:HH21	1.77	0.50
1:E:61:TYR:CZ	1:E:92:TRP:CD1	3.00	0.50
1:E:178:THR:HG22	1:E:179:VAL:N	2.27	0.50
1:E:303:GLU:OE1	1:E:333:MET:HE3	2.11	0.50
1:E:323:GLN:CG	1:E:327:ASN:HD21	2.25	0.50
1:F:103:LEU:HD12	1:F:104:PHE:N	2.27	0.50
1:B:232:LYS:H	1:B:232:LYS:HD2	1.77	0.50
1:B:426:TPO:O3P	1:B:426:TPO:C	2.60	0.50
2:C:49:GLY:O	2:C:218:ARG:NH2	2.45	0.50
2:C:54:LEU:O	2:C:56:SER:N	2.44	0.50
2:D:425:ILE:HD11	2:D:456:PHE:CE2	2.47	0.50
2:D:451:ARG:HD2	2:D:451:ARG:N	2.27	0.50
1:E:313:ILE:CG2	1:E:314:LEU:N	2.75	0.50
1:F:471:MET:HE3	1:F:472:ILE:C	2.32	0.50
1:A:82:ASP:O	1:A:83:ILE:C	2.49	0.50
1:A:153:GLN:O	1:A:154:TYR:HB3	2.12	0.50
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.27	0.50
2:C:193:ARG:NH2	2:D:199:PHE:HE2	2.10	0.50
2:D:222:ILE:CG2	2:D:225:LEU:HG	2.42	0.50
2:D:270:LEU:O	2:D:270:LEU:HD23	2.12	0.50
2:D:425:ILE:HG22	2:D:426:THR:HG23	1.94	0.50
1:E:303:GLU:OE2	1:E:333:MET:CB	2.60	0.50
1:E:418:GLN:CB	1:F:423:HIS:O	2.57	0.50
1:F:59:PHE:CZ	1:F:141:ARG:HD3	2.47	0.50
1:F:467:ILE:O	1:F:467:ILE:HG22	2.12	0.50
1:A:183:GLU:OE2	1:B:161:ARG:NH2	2.44	0.49
1:A:294:LYS:HB3	1:A:413:THR:HG23	1.94	0.49
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.12	0.49
1:B:182:THR:HG21	1:B:192:ALA:CB	2.37	0.49
2:C:452:ALA:HA	2:C:469:GLU:HA	1.92	0.49
2:D:103:LEU:HD12	2:D:104:PHE:N	2.26	0.49
1:E:262:ARG:HH12	1:E:461:SER:HB2	1.77	0.49
1:A:426:TPO:O2P	1:A:429:HIS:HA	2.11	0.49
2:C:87:ALA:HB1	2:C:92:TRP:CD1	2.47	0.49
2:D:82:ASP:O	2:D:83:ILE:C	2.49	0.49
2:D:191:ILE:HB	2:D:198:GLU:CG	2.41	0.49
2:D:332:GLY:C	2:D:333:MET:HG2	2.33	0.49
1:F:294:LYS:N	3:F:901:ATP:O1B	2.46	0.49
1:F:360:LEU:HD13	1:F:360:LEU:C	2.32	0.49
1:F:516:GLY:N	1:F:517:PRO:CD	2.74	0.49
2:D:121:PHE:N	2:D:121:PHE:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:412:PHE:N	2:D:412:PHE:CD1	2.79	0.49
2:D:437:ILE:O	2:D:437:ILE:HG22	2.12	0.49
1:E:299:SER:C	1:E:333:MET:HE1	2.33	0.49
1:F:52:LYS:HB2	3:F:903:ATP:O1B	2.13	0.49
1:F:298:VAL:HA	1:F:411:LEU:CD2	2.42	0.49
1:B:284:ILE:N	1:B:410:GLY:O	2.34	0.49
1:E:215:ARG:HD3	5:F:528:HOH:O	2.11	0.49
1:A:191:ILE:N	1:A:191:ILE:CD1	2.76	0.49
2:D:164:LEU:HD11	2:D:197:GLU:HG3	1.95	0.49
2:D:202:ASP:HA	2:D:226:ARG:HD2	1.94	0.49
1:A:87:ALA:HB1	1:A:92:TRP:HD1	1.77	0.49
2:C:217:ARG:O	2:C:217:ARG:CG	2.59	0.49
2:C:295:THR:HB	3:C:901:ATP:O3A	2.12	0.49
2:C:469:GLU:HB3	2:C:483:PHE:CE1	2.47	0.49
1:E:386:GLY:O	1:E:387:VAL:O	2.30	0.49
1:E:433:ILE:HD12	1:E:433:ILE:N	2.28	0.49
1:A:215:ARG:NH2	1:B:234:GLU:O	2.46	0.49
1:A:402:TYR:O	1:A:406:GLU:HB2	2.13	0.49
1:A:430:ILE:O	1:A:431:ALA:C	2.51	0.49
1:B:75:THR:HG21	1:B:78:GLU:O	2.12	0.49
1:B:445:ILE:HD12	1:B:486:PHE:CE1	2.47	0.49
2:C:21:MET:O	2:C:35:GLY:HA3	2.13	0.49
2:C:311:ARG:CD	2:C:371:LYS:HE3	2.43	0.49
2:D:52:LYS:HD2	2:D:182:THR:O	2.13	0.49
2:D:262:ARG:HD2	2:D:276:GLY:O	2.13	0.49
1:E:245:ASN:ND2	1:E:247:PHE:CE2	2.81	0.49
1:E:344:LEU:HD13	1:E:344:LEU:C	2.33	0.49
1:F:27:GLY:O	1:F:31:ILE:HG13	2.12	0.49
2:D:21:MET:CE	2:D:177:THR:HB	2.43	0.49
1:F:426:TPO:HG21	1:F:429:HIS:C	2.30	0.49
1:A:371:LYS:O	1:A:371:LYS:CD	2.59	0.49
2:D:271:ASP:O	2:D:277:GLY:N	2.36	0.49
1:E:148:THR:CG2	1:E:193:ARG:HD2	2.43	0.49
1:E:311:ARG:HD2	1:E:371:LYS:NZ	2.28	0.49
1:F:47:THR:HG23	1:F:48:SER:N	2.27	0.49
1:F:83:ILE:N	1:F:83:ILE:HD12	2.28	0.49
1:F:462:TRP:O	1:F:463:HIS:O	2.31	0.49
1:F:463:HIS:CE1	1:F:465:LYS:HD3	2.48	0.49
1:A:18:ILE:HD11	1:F:86:ASN:HA	1.94	0.49
1:A:61:TYR:CZ	1:A:65:ILE:HG13	2.48	0.49
1:A:64:ILE:HG21	1:A:97:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PHE:HE2	1:F:193:ARG:NH2	2.11	0.49
1:A:356:LEU:HB3	1:A:395:PHE:HD1	1.78	0.49
1:B:52:LYS:H	1:B:207:LEU:CD1	2.24	0.49
1:B:317:TYR:CD2	1:B:383:LEU:HD21	2.48	0.49
2:C:197:GLU:H	2:C:197:GLU:CD	2.13	0.49
2:C:215:ARG:HE	2:C:215:ARG:CA	2.11	0.49
2:C:453:ILE:HG12	2:C:454:ASN:N	2.28	0.49
2:D:130:ILE:O	2:D:134:ILE:HG13	2.12	0.49
2:D:264:SER:OG	2:D:265:SER:N	2.46	0.49
1:E:54:LEU:HD13	1:E:90:PHE:CZ	2.48	0.49
1:F:379:SER:HA	1:F:413:THR:O	2.12	0.49
1:F:486:PHE:HE2	1:F:496:ARG:NH1	1.93	0.49
1:A:207:LEU:CD2	1:A:220:LEU:HD12	2.41	0.48
1:A:357:GLU:HG3	1:A:358:ASP:N	2.28	0.48
1:B:215:ARG:NH2	2:C:234:GLU:O	2.46	0.48
1:B:385:ARG:HD3	2:C:393:ARG:HD3	1.94	0.48
2:C:73:PHE:HD1	2:C:143:SER:HB2	1.78	0.48
2:C:121:PHE:N	2:C:121:PHE:CD1	2.81	0.48
2:C:149:SER:HB3	2:D:161:ARG:CZ	2.43	0.48
2:D:60:LEU:O	2:D:61:TYR:C	2.52	0.48
1:E:295:THR:O	1:E:298:VAL:HB	2.13	0.48
1:F:31:ILE:CD1	1:F:246:ILE:HG21	2.43	0.48
1:F:164:LEU:O	1:F:167:LEU:N	2.46	0.48
1:A:379:SER:OG	1:A:382:ALA:HB2	2.14	0.48
1:A:483:PHE:H	1:A:483:PHE:HD1	1.60	0.48
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.43	0.48
2:D:268:VAL:O	2:D:271:ASP:HB2	2.13	0.48
1:E:167:LEU:O	1:E:171:LEU:HB2	2.12	0.48
1:E:289:ALA:O	1:E:292:THR:HG23	2.13	0.48
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.94	0.48
1:A:448:GLU:HG2	1:B:466:ALA:CB	2.43	0.48
1:B:32:SER:HB3	1:B:222:ILE:HD11	1.95	0.48
1:B:127:ILE:O	1:B:127:ILE:HG22	2.12	0.48
1:B:380:LEU:HB3	1:B:392:PHE:HZ	1.78	0.48
3:C:903:ATP:O2'	2:D:230:HIS:CE1	2.65	0.48
2:D:212:GLU:O	2:D:212:GLU:CG	2.58	0.48
2:D:411:LEU:HD12	2:D:412:PHE:N	2.29	0.48
1:F:20:LYS:HD3	1:F:35:GLY:O	2.13	0.48
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.49	0.48
1:B:387:VAL:HG12	1:B:391:ALA:HB3	1.95	0.48
2:C:396:VAL:HG11	2:C:430:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:314:LEU:O	2:D:314:LEU:HG	2.13	0.48
1:E:32:SER:OG	1:E:35:GLY:N	2.45	0.48
1:E:294:LYS:HG2	1:E:413:THR:HG23	1.93	0.48
1:A:104:PHE:HD2	1:A:133:ALA:HB1	1.79	0.48
1:A:273:MET:HA	1:A:464:ASP:HB2	1.95	0.48
1:B:21:MET:CB	1:B:38:ILE:HG12	2.42	0.48
2:C:123:LEU:HD12	2:C:163:GLU:OE2	2.14	0.48
2:C:184:ARG:NH1	2:C:187:GLU:O	2.47	0.48
2:C:281:ASP:OD1	2:C:407:GLU:HA	2.14	0.48
2:C:384:ALA:HB2	2:C:392:PHE:CZ	2.47	0.48
1:E:265:SER:O	1:E:301:PHE:HA	2.13	0.48
1:F:23:THR:O	1:F:24:MET:HB2	2.13	0.48
1:A:161:ARG:HD3	1:F:152:GLN:HB3	1.95	0.48
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.49	0.48
1:B:25:ILE:CG1	1:B:58:GLN:NE2	2.75	0.48
1:B:146:SER:H	1:B:181:THR:CB	2.17	0.48
1:B:220:LEU:HD13	1:B:246:ILE:HD13	1.96	0.48
2:C:237:PHE:CB	2:C:246:ILE:HA	2.43	0.48
2:C:304:ASN:HB3	2:C:374:ARG:HH12	1.77	0.48
2:D:486:PHE:CB	2:D:489:ILE:HD11	2.43	0.48
1:F:16:GLN:NE2	1:F:33:HIS:HB3	2.27	0.48
1:A:426:TPO:O3P	1:A:431:ALA:HB2	2.14	0.48
1:B:64:ILE:O	1:B:66:GLU:N	2.44	0.48
1:B:197:GLU:CD	1:B:197:GLU:H	2.17	0.48
1:A:366:GLU:HA	1:A:366:GLU:OE2	2.13	0.48
2:C:42:THR:HG23	2:C:203:ASN:HB2	1.95	0.48
2:C:42:THR:HG22	2:C:43:LEU:N	2.28	0.48
2:D:147:VAL:HG23	2:D:148:THR:N	2.29	0.48
1:E:308:ASN:O	1:E:309:LYS:HB2	2.14	0.48
1:E:311:ARG:HB3	1:E:370:PHE:CE2	2.49	0.48
1:F:154:TYR:O	1:F:154:TYR:HD1	1.97	0.48
1:F:273:MET:SD	1:F:468:ARG:HD2	2.53	0.48
1:A:306:CYS:SG	1:A:338:MET:SD	3.12	0.48
1:A:377:ILE:HD11	1:A:399:VAL:HG11	1.96	0.48
2:C:53:THR:HG22	2:C:53:THR:O	2.14	0.48
2:C:123:LEU:O	2:C:127:ILE:HG13	2.14	0.48
2:C:334:ASP:OD1	2:C:336:GLU:HB2	2.14	0.48
2:C:419:PHE:O	2:C:419:PHE:CG	2.67	0.48
2:C:483:PHE:HB2	2:C:489:ILE:CD1	2.43	0.48
2:D:269:ARG:O	2:D:272:GLU:HB2	2.13	0.48
1:F:426:TPO:HG23	1:F:429:HIS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:HB2	1:A:92:TRP:NE1	2.29	0.48
1:A:426:TPO:O	1:A:427:ASP:CB	2.60	0.48
1:A:458:MET:HB2	1:A:463:HIS:HD2	1.78	0.48
1:B:52:LYS:HB2	3:B:903:ATP:O1B	2.14	0.48
1:B:273:MET:O	1:B:463:HIS:CA	2.52	0.48
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.44	0.48
2:D:484:ARG:NH1	2:D:484:ARG:HB2	2.28	0.48
1:F:191:ILE:HB	1:F:198:GLU:CD	2.33	0.48
1:A:220:LEU:HD23	1:A:220:LEU:C	2.34	0.47
1:B:87:ALA:C	1:B:89:SER:H	2.18	0.47
1:B:183:GLU:HB2	2:C:199:PHE:CZ	2.48	0.47
1:B:211:LEU:HD13	1:B:216:ARG:NE	2.28	0.47
1:B:371:LYS:O	1:B:371:LYS:CD	2.62	0.47
1:B:437:ILE:HD12	1:B:457:LYS:HG2	1.96	0.47
2:C:246:ILE:HG22	2:C:247:PHE:N	2.28	0.47
2:C:340:ARG:O	2:C:342:ASN:N	2.47	0.47
2:C:353:SER:O	2:C:354:ALA:HB2	2.14	0.47
2:D:380:LEU:O	2:D:382:ALA:N	2.47	0.47
1:E:31:ILE:HA	1:E:231:MET:CG	2.43	0.47
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.37	0.47
1:E:362:ILE:O	1:E:365:SER:HB3	2.14	0.47
3:E:903:ATP:O3'	1:F:224:LYS:HB2	2.14	0.47
1:B:323:GLN:HG3	1:B:326:ARG:NH2	2.30	0.47
2:C:256:GLN:HG3	2:C:404:LYS:HD3	1.96	0.47
2:C:389:ASN:O	2:C:390:ASN:C	2.52	0.47
1:E:183:GLU:OE2	1:F:161:ARG:NH1	2.40	0.47
1:F:263:VAL:CG1	1:F:374:ARG:NH2	2.69	0.47
1:F:296:LEU:HD13	1:F:331:TRP:CE2	2.49	0.47
1:F:504:GLU:HA	1:F:507:ARG:HE	1.80	0.47
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.79	0.47
1:B:148:THR:HG21	1:B:193:ARG:HD2	1.95	0.47
1:B:269:ARG:O	1:B:273:MET:HG3	2.13	0.47
1:B:304:ASN:HB3	1:B:374:ARG:NH1	2.26	0.47
2:C:344:LEU:HD13	2:C:345:LYS:N	2.28	0.47
2:D:25:ILE:HG23	2:D:58:GLN:NE2	2.29	0.47
2:D:67:PHE:CB	2:D:69:GLU:HG3	2.41	0.47
1:E:199:PHE:C	1:E:201:SER:N	2.66	0.47
2:C:54:LEU:O	2:C:55:PHE:C	2.52	0.47
1:E:160:VAL:HG21	1:E:194:TYR:CD2	2.48	0.47
1:E:446:ARG:HE	1:E:496:ARG:HH22	1.62	0.47
1:A:332:GLY:O	1:A:333:MET:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ARG:NH1	1:F:385:ARG:HA	2.30	0.47
1:B:51:GLY:O	1:B:52:LYS:C	2.53	0.47
1:B:264:SER:HA	1:B:271:ASP:OD1	2.14	0.47
2:C:64:ILE:HG12	2:C:69:GLU:O	2.14	0.47
2:C:340:ARG:C	2:C:342:ASN:N	2.68	0.47
2:D:484:ARG:CB	2:D:484:ARG:HH11	2.28	0.47
1:E:53:THR:O	1:E:54:LEU:C	2.52	0.47
1:E:294:LYS:CB	3:E:901:ATP:O1B	2.57	0.47
1:E:313:ILE:CG1	1:E:372:PRO:CG	2.89	0.47
1:F:79:THR:HG22	1:F:82:ASP:OD2	2.14	0.47
1:F:312:ALA:HA	1:F:374:ARG:O	2.15	0.47
1:B:32:SER:OG	1:B:35:GLY:HA2	2.15	0.47
1:B:148:THR:HA	1:B:151:PHE:CE1	2.49	0.47
1:B:326:ARG:O	1:B:328:ALA:N	2.48	0.47
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.28	0.47
2:C:248:PRO:HB2	2:C:251:ALA:HB3	1.96	0.47
2:D:431:ALA:O	2:D:434:THR:HG23	2.15	0.47
1:E:352:GLU:CD	1:E:352:GLU:H	2.17	0.47
1:E:356:LEU:CD2	1:E:392:PHE:HA	2.44	0.47
1:E:404:LYS:C	1:E:406:GLU:H	2.17	0.47
1:E:446:ARG:HE	1:E:496:ARG:NH2	2.13	0.47
1:F:65:ILE:HD11	1:F:97:LEU:HD11	1.97	0.47
1:F:334:ASP:O	1:F:338:MET:HG2	2.14	0.47
1:F:446:ARG:H	1:F:496:ARG:HH22	1.63	0.47
1:A:211:LEU:CG	1:A:212:GLU:N	2.78	0.47
1:A:420:MET:CE	1:B:490:ILE:HG21	2.45	0.47
1:B:63:GLY:HA3	1:B:141:ARG:HD2	1.97	0.47
1:B:72:VAL:HG23	1:B:139:ALA:CB	2.45	0.47
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.96	0.47
1:B:315:PHE:HE1	1:B:375:ILE:HD11	1.80	0.47
1:B:344:LEU:HD13	1:B:344:LEU:C	2.35	0.47
2:C:197:GLU:OE2	2:C:197:GLU:N	2.26	0.47
2:D:21:MET:HE1	2:D:177:THR:HB	1.96	0.47
2:D:151:PHE:CE1	2:D:160:VAL:HG13	2.50	0.47
2:D:383:LEU:HD13	2:D:395:PHE:CE2	2.49	0.47
1:E:21:MET:HB2	1:E:38:ILE:HG12	1.97	0.47
1:E:31:ILE:HG22	1:E:222:ILE:CD1	2.45	0.47
1:E:371:LYS:O	1:E:371:LYS:CD	2.63	0.47
1:E:469:GLU:HB3	1:E:483:PHE:CZ	2.49	0.47
1:A:104:PHE:CD1	1:A:104:PHE:C	2.86	0.47
1:A:320:SER:O	1:A:324:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLN:CB	1:B:423:HIS:O	2.63	0.47
1:B:119:GLY:C	1:B:121:PHE:H	2.18	0.47
1:B:284:ILE:HG23	1:B:436:THR:HB	1.97	0.47
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.47	0.47
1:F:31:ILE:HD11	1:F:246:ILE:HG21	1.96	0.47
1:A:498:THR:O	1:A:499:VAL:C	2.54	0.47
1:B:240:THR:HG21	1:B:361:GLN:HE22	1.79	0.47
1:B:283:ILE:HD13	1:B:410:GLY:HA3	1.96	0.47
2:D:30:ASP:OD2	2:D:30:ASP:N	2.48	0.47
2:D:44:VAL:HA	2:D:205:VAL:O	2.15	0.47
1:E:58:GLN:HG2	1:E:62:ASN:ND2	2.30	0.47
1:E:183:GLU:H	1:E:183:GLU:HG2	1.56	0.47
1:E:313:ILE:CD1	1:E:372:PRO:CG	2.91	0.47
1:F:76:PHE:O	1:F:109:SER:HA	2.15	0.47
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.97	0.47
1:F:325:LEU:CD2	1:F:335:PHE:HB2	2.44	0.47
1:F:371:LYS:N	1:F:372:PRO:HD3	2.29	0.47
1:A:266:GLY:C	1:A:300:ARG:HG3	2.35	0.47
1:A:273:MET:HE3	1:A:468:ARG:HD2	1.97	0.47
1:A:382:ALA:O	1:A:385:ARG:HG3	2.15	0.47
2:D:106:LEU:HD11	2:D:129:ARG:HH21	1.80	0.47
1:E:61:TYR:C	1:E:63:GLY:N	2.66	0.47
1:E:417:ASP:HB2	1:E:427:ASP:OD2	2.14	0.47
1:F:98:VAL:HA	1:F:103:LEU:O	2.15	0.47
1:F:115:GLN:HG3	1:F:116:GLU:N	2.29	0.47
1:F:315:PHE:HE1	1:F:375:ILE:HD11	1.76	0.47
1:F:486:PHE:HD2	1:F:494:PRO:HB2	1.80	0.47
1:A:229:SER:O	1:A:230:HIS:HB3	2.14	0.46
2:C:191:ILE:H	2:C:191:ILE:CD1	2.28	0.46
2:C:299:SER:C	2:C:333:MET:CE	2.82	0.46
2:D:328:ALA:O	2:D:332:GLY:O	2.34	0.46
1:E:246:ILE:HG22	1:E:247:PHE:N	2.29	0.46
1:E:264:SER:O	1:E:374:ARG:NH2	2.48	0.46
1:F:211:LEU:O	1:F:212:GLU:HB3	2.15	0.46
1:F:484:ARG:NH1	1:F:484:ARG:CB	2.78	0.46
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.45	0.46
1:A:440:LEU:HA	1:A:452:ALA:O	2.15	0.46
1:A:451:ARG:HD2	1:A:451:ARG:H	1.75	0.46
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.97	0.46
1:B:148:THR:C	1:B:150:VAL:N	2.68	0.46
1:B:455:VAL:HG11	1:B:463:HIS:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:ASP:O	2:C:113:GLU:N	2.43	0.46
2:C:315:PHE:CZ	2:C:363:ILE:HG23	2.51	0.46
2:D:316:ALA:O	2:D:348:CYS:HA	2.14	0.46
2:D:445:ILE:O	2:D:446:ARG:HB2	2.15	0.46
1:F:204:VAL:HG23	1:F:224:LYS:HG2	1.98	0.46
1:F:453:ILE:CG1	1:F:454:ASN:N	2.77	0.46
1:A:121:PHE:HD1	1:A:122:ASP:N	2.14	0.46
1:A:162:ARG:HH11	1:A:162:ARG:HG3	1.80	0.46
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.48	0.46
1:B:290:THR:O	1:B:442:TYR:HE1	1.99	0.46
2:D:58:GLN:OE1	2:D:92:TRP:HH2	1.99	0.46
2:D:121:PHE:O	2:D:124:SER:OG	2.26	0.46
1:F:356:LEU:HD13	1:F:387:VAL:HG21	1.98	0.46
1:A:283:ILE:HD12	1:A:412:PHE:CE1	2.51	0.46
1:A:426:TPO:HG21	1:A:431:ALA:H	1.80	0.46
2:D:90:PHE:N	2:D:90:PHE:CD1	2.83	0.46
2:D:436:THR:HA	2:D:457:LYS:O	2.16	0.46
2:D:492:GLY:O	2:D:494:PRO:HD3	2.16	0.46
1:F:29:ASP:O	1:F:34:GLY:N	2.45	0.46
1:F:144:ILE:HG21	1:F:147:VAL:HG12	1.97	0.46
1:A:51:GLY:O	1:A:52:LYS:C	2.54	0.46
1:A:237:PHE:HB3	1:A:246:ILE:HG12	1.96	0.46
2:C:53:THR:HG21	2:C:78:GLU:OE2	2.15	0.46
2:C:123:LEU:HD11	2:C:163:GLU:HA	1.97	0.46
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.97	0.46
2:D:313:ILE:HD11	2:D:370:PHE:HB3	1.96	0.46
1:E:24:MET:HB2	1:E:62:ASN:HB3	1.98	0.46
1:E:27:GLY:HA3	1:E:246:ILE:HB	1.97	0.46
1:E:186:GLU:OE1	1:E:189:GLY:N	2.48	0.46
1:E:211:LEU:CD1	1:E:216:ARG:HG2	2.45	0.46
1:F:20:LYS:C	1:F:38:ILE:CD1	2.84	0.46
1:F:47:THR:HB	5:F:523:HOH:O	2.15	0.46
1:F:146:SER:H	1:F:181:THR:HB	1.79	0.46
1:F:218:ARG:HG3	1:F:237:PHE:O	2.14	0.46
1:F:247:PHE:CE1	1:F:360:LEU:HD12	2.51	0.46
1:A:96:LYS:O	1:A:100:GLU:HG3	2.14	0.46
1:B:44:VAL:HG22	1:B:205:VAL:HG11	1.98	0.46
1:B:371:LYS:N	1:B:372:PRO:HD3	2.30	0.46
1:B:428:SER:O	1:B:429:HIS:HB2	2.15	0.46
2:C:88:ARG:NH2	2:D:15:HIS:ND1	2.64	0.46
2:C:396:VAL:HG11	2:C:430:ILE:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:448:GLU:HA	2:D:466:ALA:HA	1.98	0.46
2:D:37:PRO:HD2	2:D:203:ASN:ND2	2.31	0.46
2:D:324:LEU:C	2:D:326:ARG:H	2.18	0.46
1:E:382:ALA:O	1:E:385:ARG:CG	2.59	0.46
1:A:227:GLY:O	1:F:89:SER:CB	2.64	0.46
2:C:232:LYS:N	2:C:232:LYS:CD	2.76	0.46
2:C:404:LYS:O	2:C:406:GLU:N	2.49	0.46
2:D:49:GLY:O	2:D:218:ARG:NH2	2.48	0.46
2:D:222:ILE:HG21	2:D:225:LEU:HG	1.97	0.46
2:D:346:ILE:HG22	2:D:347:VAL:N	2.29	0.46
1:E:326:ARG:O	1:E:328:ALA:N	2.48	0.46
1:F:231:MET:SD	1:F:251:ALA:HB2	2.55	0.46
1:F:266:GLY:HA3	1:F:300:ARG:O	2.16	0.46
1:F:425:ILE:HG21	1:F:439:LEU:HD13	1.98	0.46
1:F:451:ARG:HG2	1:F:451:ARG:NH1	2.30	0.46
1:A:129:ARG:O	1:A:132:TYR:HB3	2.15	0.46
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.98	0.46
1:A:302:VAL:HG12	1:A:303:GLU:N	2.30	0.46
1:B:65:ILE:HD11	1:B:97:LEU:HD11	1.98	0.46
1:B:194:TYR:C	1:B:196:VAL:N	2.68	0.46
1:B:245:ASN:ND2	1:B:247:PHE:CZ	2.84	0.46
2:D:193:ARG:HG2	2:D:193:ARG:HH11	1.80	0.46
2:D:358:ASP:O	2:D:360:LEU:N	2.49	0.46
2:D:420:MET:HE3	2:D:492:GLY:O	2.15	0.46
1:E:218:ARG:NH1	1:E:239:ILE:HD12	2.31	0.46
1:E:296:LEU:HD13	1:E:331:TRP:CE2	2.51	0.46
1:E:332:GLY:O	1:E:333:MET:O	2.33	0.46
1:E:392:PHE:O	1:E:395:PHE:HB3	2.16	0.46
1:E:446:ARG:NH2	1:E:496:ARG:HH22	2.11	0.46
1:A:332:GLY:O	1:A:333:MET:C	2.54	0.46
1:A:429:HIS:CD2	1:F:417:ASP:OD2	2.68	0.46
1:B:191:ILE:CB	1:B:198:GLU:HG3	2.46	0.46
1:B:211:LEU:O	1:B:212:GLU:HB3	2.15	0.46
2:C:96:LYS:O	2:C:99:ASP:N	2.49	0.46
2:C:311:ARG:HH11	2:C:371:LYS:HG3	1.81	0.46
1:E:377:ILE:O	1:E:377:ILE:HG22	2.14	0.46
1:E:453:ILE:CG2	1:E:470:PHE:HD2	2.28	0.46
1:A:21:MET:CE	1:A:59:PHE:HZ	2.28	0.46
1:A:161:ARG:NH1	1:F:152:GLN:HG3	2.30	0.46
1:A:200:VAL:O	1:A:200:VAL:HG12	2.16	0.46
1:B:18:ILE:HB	1:B:228:THR:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ARG:NH1	1:B:162:ARG:HB2	2.31	0.46
1:B:166:ARG:O	1:B:170:ARG:HG2	2.16	0.46
2:C:469:GLU:CG	2:C:480:LYS:HE3	2.46	0.46
2:D:38:ILE:HG23	2:D:39:GLY:N	2.31	0.46
2:D:396:VAL:HG11	2:D:430:ILE:HG21	1.98	0.46
1:E:191:ILE:HG21	1:E:198:GLU:HG3	1.98	0.46
1:F:367:ILE:HD11	1:F:375:ILE:CD1	2.46	0.46
1:A:396:VAL:O	1:A:397:ILE:C	2.55	0.45
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.98	0.45
2:C:440:LEU:CD2	2:C:453:ILE:HG13	2.46	0.45
1:E:197:GLU:O	1:E:199:PHE:N	2.49	0.45
1:E:367:ILE:O	1:E:367:ILE:HG22	2.16	0.45
1:A:266:GLY:O	1:A:300:ARG:HG3	2.16	0.45
1:A:442:TYR:HE1	1:B:456:PHE:CE2	2.34	0.45
2:C:211:LEU:O	2:C:212:GLU:CB	2.64	0.45
2:C:335:PHE:HA	2:C:338:MET:HG3	1.99	0.45
2:C:435:ASP:HA	2:C:459:ARG:HD2	1.97	0.45
2:D:94:LEU:HD23	2:D:94:LEU:N	2.31	0.45
1:F:298:VAL:HA	1:F:411:LEU:HD23	1.98	0.45
1:F:426:TPO:HG23	1:F:430:ILE:H	1.70	0.45
1:A:188:TYR:CE2	1:F:211:LEU:HD23	2.50	0.45
1:B:93:ASP:OD1	1:B:95:ALA:HB3	2.16	0.45
2:C:64:ILE:HG22	2:C:65:ILE:HD13	1.97	0.45
2:C:123:LEU:HD11	2:C:163:GLU:O	2.16	0.45
2:D:67:PHE:HD1	2:D:141:ARG:NH2	2.14	0.45
2:D:315:PHE:HA	2:D:347:VAL:HB	1.98	0.45
2:D:317:TYR:CD2	2:D:383:LEU:HD21	2.50	0.45
2:D:471:MET:CG	2:D:478:ASP:HB3	2.46	0.45
1:E:118:VAL:O	1:E:118:VAL:HG12	2.17	0.45
1:E:416:SER:O	1:E:418:GLN:N	2.49	0.45
1:F:161:ARG:NH2	1:F:199:PHE:HB2	2.32	0.45
1:F:256:GLN:H	1:F:256:GLN:HG2	1.58	0.45
1:F:294:LYS:O	1:F:295:THR:C	2.54	0.45
1:F:514:GLU:HG2	1:F:519:SER:HB3	1.98	0.45
1:A:61:TYR:CE1	1:A:97:LEU:HD11	2.52	0.45
1:B:71:GLY:O	1:B:103:LEU:HA	2.17	0.45
1:B:151:PHE:O	1:B:153:GLN:N	2.45	0.45
1:B:247:PHE:CE2	1:B:364:LYS:HD2	2.51	0.45
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.97	0.45
2:C:116:GLU:C	2:C:118:VAL:H	2.20	0.45
2:C:191:ILE:HB	2:C:198:GLU:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:220:LEU:HD13	2:D:246:ILE:HD13	1.97	0.45
2:D:406:GLU:HB3	2:D:408:ILE:HG13	1.98	0.45
1:E:350:TYR:CE1	1:F:254:LEU:HD13	2.51	0.45
1:F:170:ARG:HB3	1:F:170:ARG:NH1	2.32	0.45
1:F:367:ILE:O	1:F:367:ILE:HG22	2.16	0.45
1:F:379:SER:CB	1:F:382:ALA:HB2	2.46	0.45
1:F:418:GLN:HG3	1:F:418:GLN:O	2.17	0.45
1:A:28:PHE:H	1:A:246:ILE:HD12	1.82	0.45
1:A:165:PHE:CE2	1:F:110:PRO:HB2	2.52	0.45
1:B:20:LYS:HG2	1:B:35:GLY:O	2.16	0.45
1:B:70:PRO:HA	1:B:102:LYS:O	2.17	0.45
1:B:74:VAL:HB	1:B:144:ILE:HG23	1.98	0.45
1:B:311:ARG:HA	1:B:343:LEU:O	2.17	0.45
1:B:311:ARG:HG2	1:B:343:LEU:HA	1.98	0.45
2:C:87:ALA:C	2:C:89:SER:N	2.70	0.45
2:C:392:PHE:O	2:C:395:PHE:HB3	2.15	0.45
1:F:293:GLY:O	1:F:296:LEU:HB3	2.17	0.45
1:A:254:LEU:HD11	5:F:535:HOH:O	2.15	0.45
1:B:216:ARG:NE	2:C:221:GLU:OE1	2.41	0.45
2:C:126:LEU:O	2:C:129:ARG:N	2.50	0.45
2:C:287:THR:HG22	2:C:288:GLY:N	2.32	0.45
2:C:381:SER:C	2:C:383:LEU:N	2.70	0.45
2:D:358:ASP:O	2:D:359:HIS:C	2.54	0.45
1:E:21:MET:CE	1:E:141:ARG:HG2	2.46	0.45
1:F:73:PHE:C	1:F:73:PHE:CD2	2.90	0.45
1:F:127:ILE:CD1	1:F:167:LEU:HA	2.31	0.45
1:F:170:ARG:HH12	1:F:174:ILE:CG1	2.19	0.45
1:F:430:ILE:O	1:F:430:ILE:HG22	2.16	0.45
1:F:504:GLU:HA	1:F:507:ARG:CG	2.47	0.45
1:A:45:SER:HB3	1:A:182:THR:HB	1.96	0.45
1:A:267:VAL:CG1	1:A:270:LEU:HB2	2.47	0.45
1:B:305:ALA:CB	1:B:374:ARG:HD2	2.29	0.45
1:B:371:LYS:O	1:B:371:LYS:HD2	2.16	0.45
1:B:458:MET:HB2	1:B:463:HIS:CD2	2.43	0.45
2:C:382:ALA:O	2:C:385:ARG:HG3	2.17	0.45
2:D:203:ASN:HB3	2:D:225:LEU:HD23	1.98	0.45
1:E:281:ASP:O	1:E:282:SER:CB	2.63	0.45
1:E:386:GLY:O	1:E:387:VAL:C	2.55	0.45
1:F:384:ALA:HB2	1:F:392:PHE:CE1	2.51	0.45
1:F:420:MET:HE2	1:F:492:GLY:HA3	1.99	0.45
1:A:21:MET:HE2	1:A:177:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PRO:HB3	1:A:105:ILE:HG21	1.99	0.45
1:A:426:TPO:OG1	1:A:427:ASP:N	2.50	0.45
1:B:232:LYS:HD2	1:B:232:LYS:N	2.32	0.45
1:B:274:CYS:HG	1:B:278:PHE:HE2	1.62	0.45
1:B:283:ILE:HD12	1:B:412:PHE:CE1	2.52	0.45
1:B:359:HIS:O	1:B:360:LEU:C	2.56	0.45
2:C:46:GLY:HA2	2:C:184:ARG:CD	2.47	0.45
2:C:312:ALA:N	2:C:343:LEU:O	2.43	0.45
2:D:152:GLN:CB	1:E:161:ARG:HD3	2.45	0.45
1:E:33:HIS:HD2	1:E:230:HIS:CA	2.30	0.45
1:E:84:ILE:O	1:E:85:LYS:C	2.54	0.45
1:E:247:PHE:HZ	1:E:361:GLN:HG3	1.82	0.45
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.98	0.45
1:A:52:LYS:HB3	1:A:181:THR:CG2	2.46	0.45
1:A:290:THR:HG23	1:A:290:THR:O	2.17	0.45
1:A:425:ILE:O	1:A:425:ILE:HG13	2.15	0.45
1:B:216:ARG:HH21	2:C:221:GLU:CD	2.19	0.45
2:C:54:LEU:HD23	2:C:244:ILE:CG1	2.45	0.45
2:C:360:LEU:O	2:C:360:LEU:HD23	2.16	0.45
2:D:52:LYS:N	3:D:903:ATP:O1B	2.47	0.45
2:D:387:VAL:CG1	2:D:388:SER:H	2.29	0.45
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.99	0.45
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.47	0.45
1:A:167:LEU:O	1:A:168:VAL:C	2.56	0.45
1:A:273:MET:O	1:A:463:HIS:CA	2.64	0.45
1:A:293:GLY:HA2	3:A:901:ATP:O1A	2.16	0.45
1:B:335:PHE:O	1:B:336:GLU:C	2.56	0.45
2:C:263:VAL:HG12	2:C:374:ARG:NH2	2.32	0.45
2:D:334:ASP:OD1	2:D:334:ASP:C	2.55	0.45
1:E:52:LYS:O	1:E:55:PHE:HB3	2.16	0.45
1:E:301:PHE:O	1:E:374:ARG:NH1	2.49	0.45
1:E:323:GLN:NE2	1:F:459:ARG:CD	2.78	0.45
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.47	0.45
1:F:252:MET:CE	1:F:401:GLY:HA3	2.46	0.45
1:F:332:GLY:O	1:F:333:MET:O	2.35	0.45
1:F:361:GLN:O	1:F:362:ILE:C	2.56	0.45
1:F:426:TPO:HG21	1:F:429:HIS:HA	1.99	0.45
1:A:140:ARG:HB3	1:A:140:ARG:HH11	1.81	0.44
1:A:247:PHE:O	1:A:249:LEU:N	2.50	0.44
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.81	0.44
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.98	0.44
1:B:326:ARG:C	1:B:328:ALA:N	2.71	0.44
2:C:295:THR:HB	3:C:901:ATP:PA	2.57	0.44
2:C:468:ARG:HA	2:C:481:ASP:O	2.17	0.44
2:D:99:ASP:HA	5:D:545:HOH:O	2.17	0.44
2:D:484:ARG:HH11	2:D:484:ARG:HB3	1.82	0.44
1:E:18:ILE:CD1	1:E:227:GLY:HA3	2.31	0.44
1:E:46:GLY:HA2	1:E:184:ARG:HD3	1.99	0.44
1:E:150:VAL:HG13	1:E:151:PHE:N	2.32	0.44
1:F:61:TYR:O	1:F:64:ILE:HB	2.17	0.44
1:F:351:PRO:HD2	1:F:352:GLU:OE1	2.17	0.44
1:A:154:TYR:O	1:A:154:TYR:HD1	2.00	0.44
1:A:184:ARG:NH2	1:A:186:GLU:O	2.50	0.44
1:A:344:LEU:HD11	1:A:346:ILE:HG13	1.97	0.44
1:A:356:LEU:N	1:A:356:LEU:HD12	2.32	0.44
1:B:393:ARG:O	1:B:397:ILE:HG12	2.17	0.44
1:B:451:ARG:HG2	1:B:451:ARG:NH1	2.27	0.44
2:D:64:ILE:HD12	2:D:97:LEU:HD13	1.99	0.44
1:A:52:LYS:HD3	1:A:182:THR:O	2.17	0.44
1:A:430:ILE:O	1:A:432:GLU:N	2.51	0.44
2:D:140:ARG:HB3	2:D:140:ARG:NH1	2.31	0.44
2:D:402:TYR:O	2:D:406:GLU:HB2	2.18	0.44
1:E:193:ARG:NH2	1:F:195:GLY:O	2.48	0.44
1:E:266:GLY:CA	1:E:300:ARG:HG3	2.47	0.44
1:E:375:ILE:O	1:E:410:GLY:HA2	2.16	0.44
1:F:160:VAL:HG21	1:F:194:TYR:CD2	2.51	0.44
1:B:106:LEU:O	1:B:107:ASP:C	2.55	0.44
2:C:295:THR:HG22	2:C:331:TRP:HH2	1.83	0.44
2:C:315:PHE:HB3	2:C:317:TYR:CE1	2.50	0.44
2:D:64:ILE:HD12	2:D:97:LEU:CD1	2.48	0.44
1:E:211:LEU:HD12	1:E:211:LEU:HA	1.72	0.44
1:F:269:ARG:HG2	1:F:479:ILE:CG2	2.47	0.44
1:F:382:ALA:O	1:F:385:ARG:HG3	2.17	0.44
1:A:56:SER:O	1:A:59:PHE:HB3	2.16	0.44
1:A:351:PRO:CG	1:A:382:ALA:O	2.66	0.44
1:B:182:THR:CG2	1:B:192:ALA:HB1	2.43	0.44
1:B:357:GLU:HG3	1:B:358:ASP:N	2.33	0.44
1:B:418:GLN:HG3	1:B:418:GLN:O	2.17	0.44
1:B:464:ASP:OD2	1:B:468:ARG:NE	2.50	0.44
2:C:72:VAL:HA	2:C:104:PHE:O	2.18	0.44
2:C:220:LEU:HD23	2:C:220:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:ILE:HB	2:D:198:GLU:HG2	1.97	0.44
2:D:302:VAL:HG21	2:D:314:LEU:HB2	1.99	0.44
2:D:315:PHE:CE2	2:D:347:VAL:HG21	2.52	0.44
1:A:82:ASP:O	1:A:85:LYS:N	2.51	0.44
1:A:118:VAL:HG23	1:A:118:VAL:O	2.18	0.44
1:A:189:GLY:O	1:A:190:PRO:C	2.56	0.44
1:A:221:GLU:HG2	1:A:222:ILE:N	2.32	0.44
2:D:272:GLU:O	2:D:275:GLY:N	2.45	0.44
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.52	0.44
3:D:901:ATP:O2'	1:E:463:HIS:NE2	2.46	0.44
1:F:65:ILE:O	1:F:65:ILE:HG22	2.17	0.44
1:F:148:THR:HG21	1:F:183:GLU:CG	2.48	0.44
1:F:303:GLU:CD	1:F:333:MET:HB3	2.38	0.44
1:F:380:LEU:C	1:F:382:ALA:N	2.71	0.44
1:F:486:PHE:CE2	1:F:496:ARG:CD	3.00	0.44
1:A:492:GLY:O	1:A:494:PRO:HD3	2.17	0.44
1:B:86:ASN:HD21	2:C:40:ARG:HH22	1.64	0.44
1:B:237:PHE:C	1:B:237:PHE:CD1	2.90	0.44
1:B:480:LYS:HB3	1:B:481:ASP:H	1.62	0.44
2:C:111:ASP:OD2	2:C:113:GLU:HG2	2.18	0.44
2:C:396:VAL:O	2:C:400:THR:HB	2.17	0.44
1:A:166:ARG:O	1:A:167:LEU:C	2.56	0.44
1:A:194:TYR:O	1:A:196:VAL:HG23	2.18	0.44
1:A:322:ALA:HB3	1:B:256:GLN:O	2.18	0.44
1:A:458:MET:HB2	1:A:463:HIS:CD2	2.53	0.44
1:B:88:ARG:HG2	1:B:88:ARG:NH1	2.31	0.44
1:B:151:PHE:C	1:B:153:GLN:N	2.68	0.44
1:B:171:LEU:HA	1:B:174:ILE:HG12	2.00	0.44
1:B:452:ALA:HA	1:B:469:GLU:HA	2.00	0.44
2:C:21:MET:HB2	2:C:38:ILE:CG1	2.47	0.44
2:D:52:LYS:HB2	2:D:52:LYS:HE3	1.84	0.44
1:E:192:ALA:HB3	1:E:197:GLU:OE2	2.18	0.44
1:E:468:ARG:HG2	1:E:468:ARG:HH11	1.83	0.44
1:F:61:TYR:CE2	1:F:65:ILE:HG13	2.53	0.44
1:F:79:THR:CG2	1:F:82:ASP:H	2.26	0.44
1:A:163:GLU:HA	1:A:163:GLU:OE2	2.18	0.44
1:A:311:ARG:HA	1:A:343:LEU:O	2.18	0.44
1:B:44:VAL:HG22	1:B:205:VAL:CG1	2.47	0.44
1:B:54:LEU:HD13	1:B:90:PHE:CE1	2.53	0.44
2:C:80:PRO:HB3	2:C:105:ILE:HG21	1.99	0.44
2:C:86:ASN:O	2:C:87:ALA:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:VAL:CG1	2:D:151:PHE:N	2.81	0.44
1:E:24:MET:CE	1:E:24:MET:CA	2.92	0.44
1:E:397:ILE:O	1:E:401:GLY:N	2.35	0.44
1:F:20:LYS:C	1:F:38:ILE:HD11	2.39	0.44
1:F:38:ILE:HD12	1:F:38:ILE:N	2.32	0.44
1:F:142:VAL:HB	1:F:178:THR:CG2	2.41	0.44
1:F:380:LEU:C	1:F:382:ALA:H	2.19	0.44
1:B:414:ASN:ND2	1:B:426:TPO:CG2	2.81	0.43
2:C:232:LYS:HD2	2:C:232:LYS:H	1.80	0.43
2:C:294:LYS:HB2	3:C:901:ATP:O1B	2.17	0.43
2:D:52:LYS:CD	2:D:182:THR:O	2.66	0.43
1:E:123:LEU:HD21	1:E:166:ARG:HG2	2.00	0.43
1:E:144:ILE:HD11	1:E:171:LEU:HD11	1.99	0.43
1:E:294:LYS:CG	1:E:413:THR:HG23	2.48	0.43
1:E:386:GLY:HA2	1:F:390:ASN:OD1	2.18	0.43
1:F:116:GLU:O	1:F:117:VAL:CB	2.66	0.43
1:F:154:TYR:O	1:F:154:TYR:CD1	2.71	0.43
1:F:408:ILE:O	1:F:409:THR:C	2.56	0.43
1:B:25:ILE:CG2	1:B:58:GLN:NE2	2.75	0.43
2:C:340:ARG:C	2:C:342:ASN:H	2.21	0.43
2:C:430:ILE:O	2:C:431:ALA:C	2.56	0.43
2:D:21:MET:HE2	2:D:177:THR:CG2	2.48	0.43
2:D:46:GLY:O	2:D:183:GLU:HA	2.18	0.43
1:E:121:PHE:CD1	1:E:121:PHE:N	2.87	0.43
1:F:124:SER:OG	1:F:166:ARG:NH1	2.51	0.43
1:F:507:ARG:O	1:F:508:ILE:O	2.36	0.43
1:B:36:LEU:CD1	1:B:59:PHE:CE1	3.01	0.43
1:B:64:ILE:C	1:B:66:GLU:H	2.21	0.43
1:B:273:MET:C	1:B:275:GLY:H	2.20	0.43
1:B:483:PHE:O	1:B:485:ASN:N	2.51	0.43
2:C:79:THR:HG23	2:C:82:ASP:H	1.84	0.43
2:C:118:VAL:O	2:C:118:VAL:HG12	2.18	0.43
2:C:311:ARG:HD2	2:C:371:LYS:CD	2.49	0.43
2:C:347:VAL:HG12	2:C:348:CYS:N	2.33	0.43
2:D:21:MET:HE2	2:D:177:THR:CB	2.48	0.43
2:D:38:ILE:HA	2:D:177:THR:HG23	2.00	0.43
2:D:161:ARG:CB	2:D:196:VAL:HG11	2.46	0.43
2:D:263:VAL:CG2	2:D:280:LYS:HA	2.48	0.43
1:E:102:LYS:HA	1:E:102:LYS:HD3	1.55	0.43
1:E:150:VAL:CG1	1:E:151:PHE:N	2.81	0.43
1:E:392:PHE:O	1:E:394:GLN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:SER:C	1:E:418:GLN:N	2.71	0.43
1:F:246:ILE:HG22	1:F:247:PHE:N	2.34	0.43
1:A:487:GLU:OE1	1:F:496:ARG:HG2	2.18	0.43
1:B:437:ILE:HB	1:B:456:PHE:HB3	2.00	0.43
2:C:126:LEU:O	2:C:129:ARG:HB2	2.18	0.43
2:C:302:VAL:HG12	2:C:303:GLU:N	2.33	0.43
2:D:78:GLU:HB3	2:D:83:ILE:HD11	2.01	0.43
2:D:223:LEU:HD23	2:D:223:LEU:O	2.18	0.43
1:E:198:GLU:O	1:E:224:LYS:HE2	2.19	0.43
1:F:98:VAL:HG22	1:F:103:LEU:HG	1.99	0.43
1:A:269:ARG:O	1:A:272:GLU:HB2	2.19	0.43
1:A:425:ILE:HD12	1:A:437:ILE:HG21	2.00	0.43
1:A:426:TPO:O1P	1:A:426:TPO:N	2.51	0.43
1:A:451:ARG:HH11	1:A:451:ARG:CG	2.28	0.43
1:B:52:LYS:N	3:B:903:ATP:O1B	2.51	0.43
1:B:419:PHE:CD2	2:C:425:ILE:HD12	2.53	0.43
2:C:31:ILE:HA	2:C:231:MET:SD	2.58	0.43
2:C:64:ILE:O	2:C:68:ASP:HA	2.19	0.43
2:C:70:PRO:CG	2:C:138:ARG:O	2.66	0.43
2:C:329:TYR:CD2	2:C:329:TYR:O	2.71	0.43
2:C:435:ASP:OD1	2:C:459:ARG:NH1	2.51	0.43
2:D:31:ILE:O	2:D:231:MET:HG3	2.18	0.43
2:D:67:PHE:CD1	2:D:141:ARG:NH2	2.86	0.43
2:D:332:GLY:O	2:D:333:MET:CG	2.65	0.43
2:D:338:MET:HB3	2:D:344:LEU:HB3	2.00	0.43
2:D:443:VAL:HG13	2:D:494:PRO:CG	2.49	0.43
2:D:446:ARG:HB3	1:E:484:ARG:CG	2.46	0.43
1:F:21:MET:HE3	1:F:59:PHE:HE1	1.83	0.43
1:F:169:ALA:O	1:F:173:GLN:HG3	2.18	0.43
1:F:212:GLU:O	1:F:212:GLU:OE2	2.37	0.43
1:F:430:ILE:C	1:F:432:GLU:H	2.20	0.43
1:A:299:SER:C	1:A:301:PHE:N	2.71	0.43
1:A:334:ASP:OD1	1:A:336:GLU:HB2	2.18	0.43
1:A:441:GLN:HG3	1:A:441:GLN:O	2.18	0.43
1:B:103:LEU:HD12	1:B:104:PHE:N	2.34	0.43
1:B:291:GLY:O	1:B:293:GLY:N	2.52	0.43
1:B:380:LEU:O	1:B:383:LEU:HB2	2.18	0.43
2:C:194:TYR:HD1	2:C:197:GLU:OE1	2.01	0.43
1:E:446:ARG:O	1:E:447:GLY:C	2.57	0.43
1:F:33:HIS:CD2	1:F:229:SER:OG	2.72	0.43
1:F:191:ILE:CG1	1:F:206:ILE:HD11	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LYS:O	1:A:53:THR:C	2.56	0.43
1:A:71:GLY:O	1:A:103:LEU:HA	2.18	0.43
2:C:127:ILE:HG12	2:C:167:LEU:HD13	2.01	0.43
2:D:151:PHE:C	2:D:153:GLN:N	2.71	0.43
2:D:315:PHE:CE1	2:D:363:ILE:HG23	2.54	0.43
1:E:37:PRO:HG2	1:E:225:LEU:HD22	2.01	0.43
1:E:191:ILE:HB	1:E:198:GLU:HG3	1.98	0.43
1:F:22:ARG:HA	1:F:29:ASP:OD2	2.18	0.43
1:A:109:SER:HA	1:A:110:PRO:HD3	1.80	0.43
1:A:153:GLN:O	1:A:154:TYR:CB	2.66	0.43
1:A:206:ILE:HD11	1:A:223:LEU:CD1	2.49	0.43
1:A:248:PRO:HB2	1:A:251:ALA:CB	2.46	0.43
1:A:358:ASP:O	1:A:361:GLN:N	2.52	0.43
1:B:26:GLU:HB3	1:B:245:ASN:OD1	2.19	0.43
1:B:116:GLU:HG2	1:B:117:VAL:N	2.27	0.43
1:B:145:ASP:HA	1:B:181:THR:CB	2.48	0.43
1:B:451:ARG:HB3	1:B:452:ALA:H	1.69	0.43
2:C:278:PHE:CE1	2:C:284:ILE:HG21	2.54	0.43
2:C:316:ALA:HB2	2:C:324:LEU:HD11	2.01	0.43
2:C:378:ASP:O	2:C:379:SER:HB3	2.19	0.43
2:C:400:THR:O	2:C:402:TYR:N	2.52	0.43
2:D:122:ASP:O	2:D:123:LEU:C	2.57	0.43
2:D:295:THR:HA	2:D:298:VAL:HG23	2.00	0.43
2:D:418:GLN:HB2	1:E:423:HIS:O	2.19	0.43
1:E:61:TYR:O	1:E:63:GLY:N	2.51	0.43
1:E:292:THR:HB	1:E:440:LEU:HB3	2.01	0.43
1:E:360:LEU:HD13	1:E:360:LEU:C	2.39	0.43
1:F:116:GLU:O	1:F:117:VAL:HG23	2.18	0.43
1:F:181:THR:HG22	1:F:182:THR:N	2.34	0.43
1:F:256:GLN:HE21	1:F:404:LYS:HB3	1.82	0.43
1:A:504:GLU:C	1:A:506:SER:H	2.22	0.43
1:B:50:THR:O	1:B:207:LEU:HD13	2.19	0.43
2:C:211:LEU:HA	2:C:216:ARG:HD3	2.00	0.43
2:C:294:LYS:NZ	2:C:415:THR:HG23	2.34	0.43
2:D:79:THR:O	2:D:79:THR:HG23	2.18	0.43
2:D:304:ASN:O	2:D:308:ASN:ND2	2.44	0.43
2:D:384:ALA:HB2	2:D:392:PHE:CE1	2.54	0.43
3:D:901:ATP:H3'	1:E:458:MET:O	2.19	0.43
1:E:430:ILE:O	1:E:431:ALA:C	2.56	0.43
1:F:452:ALA:CB	1:F:469:GLU:HA	2.49	0.43
1:A:379:SER:CB	1:A:382:ALA:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:N	1:A:426:TPO:O1P	2.52	0.43
1:A:447:GLY:HA2	1:B:489:ILE:HD13	2.00	0.43
1:B:240:THR:CG2	1:B:361:GLN:HE22	2.32	0.43
2:C:311:ARG:NE	2:C:371:LYS:HE3	2.34	0.43
2:C:323:GLN:HE21	2:C:327:ASN:HD21	1.66	0.43
1:F:262:ARG:HA	1:F:278:PHE:O	2.18	0.43
1:F:289:ALA:HB2	1:F:419:PHE:HA	2.00	0.43
1:F:364:LYS:O	1:F:365:SER:C	2.55	0.43
1:A:52:LYS:N	3:A:903:ATP:O1B	2.52	0.42
1:B:54:LEU:HD21	1:B:244:ILE:HG13	2.01	0.42
1:B:191:ILE:N	1:B:191:ILE:CD1	2.83	0.42
2:D:443:VAL:CG1	2:D:494:PRO:HG2	2.49	0.42
1:E:191:ILE:CB	1:E:198:GLU:CG	2.93	0.42
1:E:194:TYR:CD1	1:E:194:TYR:N	2.87	0.42
1:F:29:ASP:OD1	1:F:29:ASP:N	2.51	0.42
1:F:222:ILE:HG21	1:F:225:LEU:HG	2.01	0.42
1:F:471:MET:HG2	1:F:480:LYS:HE2	2.01	0.42
1:A:199:PHE:CE2	1:F:193:ARG:NH2	2.86	0.42
1:A:389:ASN:HD21	1:A:428:SER:HB2	1.85	0.42
1:B:22:ARG:O	1:B:141:ARG:NH2	2.52	0.42
1:B:42:THR:O	1:B:179:VAL:HA	2.19	0.42
1:B:335:PHE:HA	1:B:338:MET:CG	2.49	0.42
1:B:359:HIS:O	1:B:361:GLN:N	2.51	0.42
1:B:396:VAL:C	1:B:398:GLY:N	2.73	0.42
2:C:43:LEU:HD11	2:C:182:THR:OG1	2.18	0.42
2:C:170:ARG:HB3	2:C:170:ARG:HH11	1.82	0.42
2:C:208:ARG:HG3	5:C:535:HOH:O	2.18	0.42
2:C:400:THR:HG22	2:C:401:GLY:N	2.34	0.42
2:C:404:LYS:C	2:C:406:GLU:N	2.72	0.42
2:C:483:PHE:CD1	2:C:483:PHE:N	2.87	0.42
2:D:291:GLY:CA	3:D:901:ATP:O2B	2.68	0.42
2:D:451:ARG:HG2	2:D:451:ARG:HH11	1.84	0.42
1:E:356:LEU:HD12	1:E:356:LEU:N	2.34	0.42
1:F:500:ASP:O	1:F:501:GLU:CB	2.54	0.42
1:A:184:ARG:HH22	1:A:188:TYR:CA	2.32	0.42
1:A:299:SER:C	1:A:301:PHE:H	2.22	0.42
1:A:435:ASP:HA	1:A:459:ARG:HD2	2.01	0.42
1:B:179:VAL:O	1:B:179:VAL:HG12	2.20	0.42
1:B:317:TYR:CE2	1:B:383:LEU:HD21	2.54	0.42
1:B:423:HIS:O	1:B:424:SER:HB3	2.19	0.42
1:B:451:ARG:NH1	1:B:451:ARG:CG	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ILE:HA	1:B:490:ILE:HD13	1.82	0.42
2:C:73:PHE:HE2	2:C:83:ILE:HD13	1.83	0.42
2:C:163:GLU:OE2	2:C:163:GLU:HA	2.19	0.42
2:C:185:ILE:N	2:C:185:ILE:CD1	2.81	0.42
2:C:248:PRO:C	2:C:250:GLY:N	2.72	0.42
2:C:263:VAL:CG1	2:C:374:ARG:HH21	2.32	0.42
2:D:81:GLN:CD	2:D:81:GLN:N	2.71	0.42
2:D:305:ALA:CB	2:D:374:ARG:HD2	2.33	0.42
1:E:266:GLY:O	1:E:300:ARG:NE	2.52	0.42
1:E:352:GLU:CD	1:E:352:GLU:N	2.72	0.42
1:F:129:ARG:O	1:F:132:TYR:HB3	2.19	0.42
1:F:294:LYS:HD3	1:F:294:LYS:H	1.84	0.42
1:F:356:LEU:CD1	1:F:387:VAL:HG21	2.49	0.42
1:B:148:THR:HA	1:B:151:PHE:HE1	1.84	0.42
1:B:193:ARG:HG2	1:B:193:ARG:NH1	2.33	0.42
2:C:148:THR:C	2:C:150:VAL:H	2.21	0.42
2:C:202:ASP:CA	2:C:226:ARG:HD2	2.47	0.42
2:C:204:VAL:HG21	2:C:224:LYS:HE2	2.02	0.42
2:C:364:LYS:HE2	2:C:402:TYR:CD1	2.54	0.42
2:C:425:ILE:HD12	2:C:425:ILE:N	2.32	0.42
2:D:361:GLN:O	2:D:364:LYS:N	2.52	0.42
1:E:67:PHE:O	1:E:68:ASP:C	2.58	0.42
1:E:78:GLU:HB2	1:E:83:ILE:HD11	2.02	0.42
1:F:312:ALA:HB2	1:F:374:ARG:HB2	2.00	0.42
1:F:485:ASN:O	1:F:486:PHE:CD1	2.72	0.42
1:A:111:ASP:C	1:A:113:GLU:H	2.22	0.42
1:A:146:SER:H	1:A:181:THR:HB	1.85	0.42
1:B:284:ILE:O	1:B:411:LEU:HA	2.19	0.42
3:B:901:ATP:O3'	2:C:457:LYS:HB2	2.19	0.42
2:D:219:THR:HB	2:D:234:GLU:HB3	2.00	0.42
2:D:380:LEU:O	2:D:383:LEU:N	2.52	0.42
2:D:385:ARG:O	2:D:387:VAL:HG23	2.20	0.42
1:E:121:PHE:O	1:E:122:ASP:C	2.58	0.42
1:F:47:THR:HG22	1:F:50:THR:HG21	2.00	0.42
1:F:271:ASP:OD1	1:F:277:GLY:HA2	2.19	0.42
1:F:360:LEU:HD13	1:F:360:LEU:O	2.19	0.42
1:A:49:GLY:HA2	3:A:903:ATP:O2B	2.20	0.42
1:A:51:GLY:O	1:A:54:LEU:HB3	2.18	0.42
1:A:419:PHE:O	1:A:420:MET:HB2	2.20	0.42
1:B:90:PHE:HA	1:B:241:ASP:O	2.19	0.42
1:B:119:GLY:C	1:B:121:PHE:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ILE:CD1	1:B:494:PRO:HG2	2.50	0.42
2:C:24:MET:CB	2:C:62:ASN:ND2	2.79	0.42
2:C:88:ARG:CZ	2:D:15:HIS:HA	2.49	0.42
2:C:123:LEU:HD13	2:C:166:ARG:HD2	2.02	0.42
2:C:204:VAL:CG2	2:C:224:LYS:HE2	2.49	0.42
2:D:123:LEU:HD11	2:D:167:LEU:HB2	2.00	0.42
1:E:58:GLN:CG	1:E:62:ASN:ND2	2.83	0.42
1:E:298:VAL:O	1:E:301:PHE:HB3	2.20	0.42
1:E:393:ARG:NH2	5:E:524:HOH:O	2.52	0.42
1:F:311:ARG:HG3	1:F:371:LYS:HZ1	1.85	0.42
1:F:389:ASN:O	1:F:392:PHE:N	2.53	0.42
1:A:32:SER:OG	1:A:35:GLY:CA	2.68	0.42
1:A:49:GLY:CA	3:A:903:ATP:O2B	2.68	0.42
1:A:183:GLU:H	1:A:183:GLU:HG2	1.67	0.42
1:A:209:ASN:ND2	1:A:218:ARG:HG3	2.34	0.42
1:A:420:MET:SD	1:B:490:ILE:HG13	2.60	0.42
1:B:50:THR:O	1:B:237:PHE:HZ	2.02	0.42
1:B:278:PHE:CD1	1:B:301:PHE:HE1	2.37	0.42
1:B:392:PHE:C	1:B:394:GLN:N	2.71	0.42
2:C:61:TYR:CD1	2:C:97:LEU:HD11	2.54	0.42
2:C:123:LEU:O	2:C:124:SER:C	2.58	0.42
2:C:146:SER:C	2:C:148:THR:H	2.23	0.42
2:D:38:ILE:HA	2:D:177:THR:CG2	2.50	0.42
2:D:161:ARG:HD2	2:D:196:VAL:HG13	2.02	0.42
2:D:361:GLN:O	2:D:362:ILE:C	2.56	0.42
1:E:269:ARG:HG2	1:E:479:ILE:HB	2.02	0.42
1:F:116:GLU:O	1:F:117:VAL:HB	2.19	0.42
1:F:134:ILE:HD11	1:F:142:VAL:HG21	2.01	0.42
1:A:191:ILE:HD12	1:A:191:ILE:H	1.83	0.42
1:A:306:CYS:CB	1:A:338:MET:SD	3.07	0.42
1:A:380:LEU:O	1:A:392:PHE:HE1	2.03	0.42
1:B:41:SER:O	1:B:203:ASN:ND2	2.53	0.42
1:B:51:GLY:O	1:B:54:LEU:N	2.53	0.42
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.82	0.42
2:C:87:ALA:HB1	2:C:92:TRP:HD1	1.82	0.42
2:C:169:ALA:O	2:C:172:LYS:HB3	2.20	0.42
2:C:299:SER:CB	2:C:333:MET:HE1	2.49	0.42
2:C:378:ASP:O	2:C:379:SER:CB	2.67	0.42
1:E:61:TYR:O	1:E:62:ASN:C	2.58	0.42
1:E:249:LEU:CD1	1:E:394:GLN:HG2	2.50	0.42
1:E:331:TRP:NE1	3:E:901:ATP:N7	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:PHE:CD2	1:F:347:VAL:HG21	2.55	0.42
1:F:387:VAL:HG13	1:F:391:ALA:HB3	2.02	0.42
1:A:94:LEU:O	1:A:97:LEU:N	2.52	0.42
1:A:383:LEU:C	1:A:385:ARG:H	2.23	0.42
1:B:52:LYS:HB2	1:B:52:LYS:HE3	1.81	0.42
1:B:52:LYS:HE3	3:B:903:ATP:O3B	2.20	0.42
1:B:215:ARG:NE	1:B:215:ARG:HA	2.33	0.42
1:B:266:GLY:O	1:B:300:ARG:CG	2.68	0.42
1:B:284:ILE:HB	1:B:411:LEU:HD12	2.01	0.42
1:B:356:LEU:N	1:B:356:LEU:CD1	2.82	0.42
2:C:123:LEU:HD21	2:C:167:LEU:HB2	2.01	0.42
2:C:384:ALA:HB2	2:C:392:PHE:CD1	2.54	0.42
2:D:14:GLU:CD	2:D:15:HIS:H	2.23	0.42
2:D:304:ASN:O	2:D:304:ASN:OD1	2.37	0.42
2:D:344:LEU:C	2:D:344:LEU:CD1	2.86	0.42
1:E:300:ARG:N	1:E:333:MET:HE1	2.35	0.42
1:E:431:ALA:O	1:E:432:GLU:C	2.58	0.42
1:F:140:ARG:HH11	1:F:140:ARG:CB	2.30	0.42
1:A:508:ILE:HD13	1:A:508:ILE:N	2.33	0.42
2:C:73:PHE:CD1	2:C:143:SER:HB2	2.55	0.42
2:C:75:THR:HB	2:C:83:ILE:HD11	2.02	0.42
2:C:191:ILE:HB	2:C:198:GLU:HG2	2.02	0.42
2:C:196:VAL:HG12	2:C:197:GLU:N	2.34	0.42
2:C:445:ILE:O	2:C:445:ILE:HG22	2.19	0.42
2:D:128:GLU:O	2:D:132:TYR:N	2.49	0.42
2:D:317:TYR:HE2	2:D:383:LEU:HD21	1.80	0.42
2:D:396:VAL:HG11	2:D:430:ILE:CG2	2.50	0.42
1:E:49:GLY:HA2	3:E:903:ATP:O2B	2.20	0.42
1:E:288:GLY:O	1:E:294:LYS:NZ	2.48	0.42
1:F:79:THR:HA	1:F:80:PRO:HD3	1.87	0.42
1:F:437:ILE:HD11	1:F:457:LYS:HE2	2.01	0.42
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.81	0.41
1:A:184:ARG:O	1:A:185:ILE:HD13	2.19	0.41
1:A:281:ASP:OD1	1:A:407:GLU:OE1	2.38	0.41
1:A:356:LEU:CD1	1:A:356:LEU:N	2.83	0.41
1:A:445:ILE:HD12	1:A:486:PHE:CE2	2.54	0.41
2:C:316:ALA:HB3	2:C:348:CYS:SG	2.60	0.41
2:C:480:LYS:HE3	2:C:480:LYS:HB2	1.93	0.41
2:D:76:PHE:CZ	2:D:126:LEU:CD2	3.03	0.41
2:D:441:GLN:HE22	2:D:490:ILE:HD12	1.85	0.41
1:E:123:LEU:HD23	1:E:123:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:LEU:HD23	1:F:60:LEU:HA	1.73	0.41
1:F:388:SER:O	1:F:389:ASN:C	2.57	0.41
1:A:264:SER:HB3	1:A:304:ASN:ND2	2.36	0.41
1:A:448:GLU:HA	1:B:466:ALA:HA	2.02	0.41
1:B:76:PHE:HE1	1:B:144:ILE:CG2	2.33	0.41
2:C:60:LEU:O	2:C:62:ASN:N	2.53	0.41
2:C:164:LEU:HB3	2:C:200:VAL:HG11	2.02	0.41
2:D:237:PHE:HE1	2:D:239:ILE:HG13	1.86	0.41
2:D:323:GLN:HG2	2:D:327:ASN:ND2	2.35	0.41
1:E:404:LYS:C	1:E:406:GLU:N	2.73	0.41
1:E:496:ARG:O	1:E:497:ILE:HD13	2.20	0.41
1:F:170:ARG:O	1:F:174:ILE:HG12	2.20	0.41
1:F:377:ILE:HD12	1:F:412:PHE:CD2	2.55	0.41
1:F:426:TPO:CG2	1:F:429:HIS:CA	2.99	0.41
1:A:384:ALA:HB2	1:A:392:PHE:CE1	2.55	0.41
1:B:38:ILE:HA	1:B:177:THR:CG2	2.51	0.41
2:C:245:ASN:ND2	2:C:247:PHE:CZ	2.88	0.41
2:C:344:LEU:HD13	2:C:344:LEU:C	2.40	0.41
2:D:54:LEU:HD13	2:D:90:PHE:CZ	2.55	0.41
2:D:78:GLU:HB3	2:D:83:ILE:CD1	2.50	0.41
1:F:504:GLU:HB2	1:F:505:LEU:H	1.49	0.41
1:A:65:ILE:HD11	1:A:97:LEU:HD21	2.03	0.41
1:B:218:ARG:HD3	1:B:237:PHE:CZ	2.53	0.41
2:C:107:ASP:C	2:C:107:ASP:OD1	2.59	0.41
2:C:166:ARG:O	2:C:166:ARG:HG2	2.19	0.41
2:C:261:VAL:C	2:C:262:ARG:HG2	2.40	0.41
2:C:317:TYR:N	2:C:317:TYR:CD1	2.88	0.41
2:D:76:PHE:HZ	2:D:126:LEU:CD2	2.34	0.41
1:E:54:LEU:CD2	1:E:244:ILE:HG13	2.50	0.41
1:E:283:ILE:HG23	1:E:412:PHE:CE1	2.55	0.41
3:E:903:ATP:O3G	1:F:224:LYS:NZ	2.44	0.41
1:F:61:TYR:O	1:F:64:ILE:N	2.41	0.41
1:F:145:ASP:O	1:F:146:SER:OG	2.30	0.41
1:F:462:TRP:CE3	1:F:463:HIS:N	2.88	0.41
1:A:256:GLN:O	1:F:322:ALA:HB3	2.20	0.41
1:B:425:ILE:HD12	1:B:425:ILE:H	1.85	0.41
2:C:111:ASP:HA	2:C:112:PRO:HD3	1.93	0.41
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.49	0.41
2:C:252:MET:CE	2:C:397:ILE:HG22	2.49	0.41
2:C:335:PHE:O	2:C:339:GLU:HG3	2.20	0.41
1:E:184:ARG:C	1:E:185:ILE:HD13	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:ALA:CA	1:F:372:PRO:HB3	2.40	0.41
1:A:18:ILE:N	1:A:18:ILE:CD1	2.83	0.41
1:A:129:ARG:O	1:A:130:ILE:C	2.59	0.41
1:B:167:LEU:O	1:B:170:ARG:HB2	2.21	0.41
1:B:311:ARG:O	1:B:372:PRO:HA	2.20	0.41
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.94	0.41
2:C:54:LEU:C	2:C:56:SER:N	2.74	0.41
2:C:320:SER:HA	2:D:254:LEU:HG	2.03	0.41
2:D:182:THR:HG21	2:D:192:ALA:CB	2.51	0.41
2:D:306:CYS:C	2:D:308:ASN:N	2.74	0.41
2:D:344:LEU:HD13	2:D:345:LYS:N	2.36	0.41
2:D:486:PHE:CB	2:D:489:ILE:CD1	2.98	0.41
2:D:487:GLU:O	2:D:494:PRO:HA	2.21	0.41
1:E:218:ARG:HG3	1:E:237:PHE:O	2.20	0.41
1:E:334:ASP:HA	5:E:525:HOH:O	2.19	0.41
1:E:348:CYS:HB3	1:F:254:LEU:HD23	2.03	0.41
1:E:470:PHE:CD1	1:E:470:PHE:C	2.94	0.41
1:F:117:VAL:HA	1:F:154:TYR:OH	2.20	0.41
1:F:218:ARG:HB2	1:F:237:PHE:CE2	2.55	0.41
1:F:317:TYR:OH	1:F:363:ILE:HD11	2.20	0.41
1:F:490:ILE:H	1:F:490:ILE:HG12	1.61	0.41
1:A:27:GLY:O	1:A:28:PHE:C	2.58	0.41
1:A:71:GLY:HA2	1:A:141:ARG:O	2.20	0.41
1:A:267:VAL:HG22	1:A:300:ARG:HG2	2.02	0.41
1:A:313:ILE:HD12	1:A:372:PRO:HG2	2.03	0.41
1:B:451:ARG:HB2	1:B:470:PHE:O	2.21	0.41
1:B:503:SER:O	1:B:504:GLU:CB	2.66	0.41
2:C:150:VAL:CG1	2:C:151:PHE:N	2.82	0.41
2:D:53:THR:C	2:D:55:PHE:N	2.73	0.41
2:D:208:ARG:O	2:D:218:ARG:HA	2.21	0.41
1:F:153:GLN:O	1:F:154:TYR:CB	2.69	0.41
1:F:284:ILE:HB	1:F:411:LEU:HA	2.03	0.41
1:F:426:TPO:HG23	1:F:429:HIS:H	1.86	0.41
1:A:79:THR:O	1:A:82:ASP:HB2	2.20	0.41
1:A:125:ALA:O	1:A:129:ARG:HG3	2.20	0.41
1:A:162:ARG:HG3	1:A:162:ARG:NH1	2.36	0.41
1:B:340:ARG:C	1:B:342:ASN:H	2.24	0.41
2:C:64:ILE:HG23	2:C:102:LYS:HB3	2.03	0.41
2:D:303:GLU:C	2:D:305:ALA:H	2.23	0.41
2:D:358:ASP:C	2:D:360:LEU:N	2.74	0.41
1:E:81:GLN:H	1:E:81:GLN:HE21	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:THR:N	5:F:523:HOH:O	2.54	0.41
1:F:67:PHE:CB	1:F:69:GLU:HG3	2.51	0.41
1:F:171:LEU:O	1:F:174:ILE:HB	2.20	0.41
1:F:295:THR:HA	1:F:378:ASP:OD2	2.20	0.41
1:A:96:LYS:HE2	1:A:100:GLU:OE1	2.21	0.41
1:A:147:VAL:HG21	1:A:180:MET:CE	2.50	0.41
1:A:249:LEU:HD13	1:A:394:GLN:HG2	2.02	0.41
1:A:392:PHE:O	1:A:393:ARG:C	2.57	0.41
1:B:57:ILE:C	1:B:59:PHE:N	2.74	0.41
1:B:64:ILE:HG22	1:B:65:ILE:N	2.35	0.41
1:B:195:GLY:HA2	1:B:198:GLU:CD	2.39	0.41
2:C:46:GLY:O	2:C:52:LYS:HD3	2.21	0.41
2:C:153:GLN:O	2:C:154:TYR:HB3	2.21	0.41
2:C:187:GLU:OE2	2:C:208:ARG:HA	2.21	0.41
2:C:289:ALA:HB2	2:C:419:PHE:HA	2.02	0.41
2:C:295:THR:HG22	2:C:296:LEU:N	2.34	0.41
2:C:451:ARG:NH1	2:C:451:ARG:CG	2.74	0.41
2:D:75:THR:HG23	2:D:75:THR:O	2.21	0.41
2:D:208:ARG:NE	2:D:234:GLU:OE2	2.54	0.41
2:D:265:SER:N	2:D:271:ASP:OD1	2.52	0.41
2:D:267:VAL:HG12	2:D:270:LEU:H	1.86	0.41
2:D:306:CYS:C	2:D:308:ASN:H	2.23	0.41
2:D:324:LEU:C	2:D:326:ARG:N	2.74	0.41
2:D:331:TRP:O	2:D:333:MET:HG2	2.20	0.41
2:D:356:LEU:HD23	2:D:391:ALA:O	2.20	0.41
2:D:392:PHE:O	2:D:395:PHE:HB3	2.21	0.41
2:D:486:PHE:HB3	2:D:489:ILE:HD11	2.02	0.41
2:D:496:ARG:NH2	1:E:486:PHE:O	2.54	0.41
1:E:57:ILE:HA	1:E:57:ILE:HD13	1.85	0.41
1:E:80:PRO:HB2	1:E:81:GLN:NE2	2.36	0.41
1:E:362:ILE:O	1:E:365:SER:N	2.51	0.41
1:F:76:PHE:HB2	1:F:146:SER:HG	1.85	0.41
1:F:208:ARG:O	1:F:218:ARG:HA	2.20	0.41
1:F:237:PHE:HA	1:F:245:ASN:O	2.21	0.41
1:F:371:LYS:C	1:F:371:LYS:HD2	2.41	0.41
1:F:425:ILE:N	1:F:425:ILE:HD12	2.36	0.41
1:F:426:TPO:CG2	1:F:429:HIS:N	2.84	0.41
1:F:489:ILE:O	1:F:491:SER:N	2.54	0.41
1:A:150:VAL:HG13	1:A:151:PHE:N	2.35	0.41
1:A:191:ILE:CD1	1:A:191:ILE:H	2.33	0.41
1:A:361:GLN:O	1:A:362:ILE:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:THR:CB	2:C:207:LEU:HB3	2.47	0.41
2:C:239:ILE:HG22	3:C:903:ATP:N3	2.36	0.41
2:D:376:ALA:HA	2:D:411:LEU:O	2.21	0.41
1:E:131:ASN:OD1	1:E:135:GLN:NE2	2.54	0.41
1:F:21:MET:CE	1:F:59:PHE:CZ	3.04	0.41
1:F:191:ILE:N	1:F:191:ILE:CD1	2.84	0.41
1:F:419:PHE:O	1:F:420:MET:O	2.39	0.41
1:A:147:VAL:HG11	1:A:180:MET:HE3	2.02	0.40
1:A:211:LEU:HA	1:A:216:ARG:HD3	2.03	0.40
1:A:441:GLN:NE2	1:A:490:ILE:HD13	2.21	0.40
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.86	0.40
1:B:167:LEU:O	1:B:168:VAL:C	2.59	0.40
1:B:273:MET:HA	1:B:464:ASP:HB2	2.03	0.40
1:B:306:CYS:CB	1:B:338:MET:SD	3.09	0.40
1:B:313:ILE:HG22	1:B:314:LEU:N	2.36	0.40
2:C:42:THR:HG23	2:C:203:ASN:HB3	2.03	0.40
2:D:44:VAL:HG22	2:D:205:VAL:CG1	2.52	0.40
2:D:299:SER:HB3	2:D:333:MET:CE	2.51	0.40
2:D:444:GLU:HA	2:D:448:GLU:O	2.21	0.40
1:E:21:MET:CE	1:E:59:PHE:CZ	3.04	0.40
1:E:145:ASP:O	1:E:146:SER:OG	2.37	0.40
1:E:191:ILE:CB	1:E:198:GLU:HG2	2.42	0.40
1:E:426:TPO:O3P	1:E:429:HIS:HA	2.22	0.40
1:F:70:PRO:HA	1:F:102:LYS:O	2.21	0.40
1:F:117:VAL:O	1:F:118:VAL:HB	2.20	0.40
1:F:170:ARG:CA	1:F:170:ARG:HH11	2.34	0.40
1:F:294:LYS:CB	1:F:413:THR:HG23	2.48	0.40
1:A:69:GLU:HB3	1:A:140:ARG:HB2	2.02	0.40
1:A:121:PHE:CD1	1:A:122:ASP:N	2.89	0.40
1:A:161:ARG:HH11	1:F:152:GLN:HG3	1.86	0.40
1:A:273:MET:HE1	1:A:479:ILE:HG21	2.03	0.40
1:A:312:ALA:O	1:A:344:LEU:HD22	2.21	0.40
1:B:86:ASN:O	1:B:89:SER:N	2.48	0.40
1:B:307:ALA:C	1:B:309:LYS:H	2.24	0.40
1:B:397:ILE:O	1:B:397:ILE:HG22	2.20	0.40
1:B:449:MET:CE	2:C:467:ILE:HD11	2.52	0.40
2:C:48:SER:HB2	2:D:199:PHE:CD1	2.55	0.40
2:C:57:ILE:HD13	2:C:57:ILE:HA	1.94	0.40
2:C:64:ILE:CD1	2:C:103:LEU:HB2	2.52	0.40
2:C:393:ARG:O	2:C:396:VAL:N	2.54	0.40
2:D:225:LEU:CB	2:D:230:HIS:HD2	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:209:ASN:O	1:F:216:ARG:NH1	2.54	0.40
1:F:256:GLN:NE2	1:F:404:LYS:HB3	2.36	0.40
1:F:371:LYS:O	1:F:371:LYS:CD	2.69	0.40
1:F:378:ASP:OD1	1:F:413:THR:HG21	2.21	0.40
1:F:433:ILE:N	1:F:433:ILE:HD12	2.36	0.40
1:A:287:THR:HG23	1:A:414:ASN:HB3	2.03	0.40
1:A:438:ILE:HD13	1:A:455:VAL:HA	2.04	0.40
1:B:356:LEU:HD23	1:B:395:PHE:HB2	2.04	0.40
1:B:449:MET:HE3	2:C:467:ILE:HD11	2.03	0.40
2:C:231:MET:HE3	2:C:251:ALA:HB2	2.03	0.40
2:C:412:PHE:N	2:C:412:PHE:CD1	2.89	0.40
2:C:443:VAL:HG12	2:C:445:ILE:HG12	2.04	0.40
2:D:85:LYS:O	2:D:86:ASN:C	2.60	0.40
1:E:47:THR:O	1:E:52:LYS:HE2	2.21	0.40
1:E:360:LEU:HD13	1:E:360:LEU:O	2.22	0.40
1:E:454:ASN:ND2	1:E:456:PHE:HD1	2.19	0.40
1:F:47:THR:CG2	1:F:50:THR:HG22	2.51	0.40
1:F:248:PRO:C	1:F:250:GLY:N	2.74	0.40
1:F:263:VAL:HG12	1:F:264:SER:H	1.86	0.40
1:F:440:LEU:HD23	1:F:453:ILE:HG13	2.03	0.40
1:A:31:ILE:HD11	1:A:246:ILE:CG2	2.40	0.40
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.86	0.40
1:A:180:MET:HE2	1:A:180:MET:HB3	1.93	0.40
1:A:255:THR:O	1:A:255:THR:HG22	2.22	0.40
1:A:488:ARG:HA	1:F:493:SER:HB2	2.02	0.40
1:B:87:ALA:C	1:B:89:SER:N	2.74	0.40
1:B:266:GLY:O	1:B:300:ARG:HG2	2.20	0.40
1:B:400:THR:HG21	1:B:433:ILE:CG2	2.51	0.40
2:C:106:LEU:O	2:C:106:LEU:HG	2.21	0.40
2:C:370:PHE:O	2:C:371:LYS:HG3	2.21	0.40
2:D:41:SER:HA	2:D:178:THR:O	2.22	0.40
2:D:80:PRO:HA	2:D:83:ILE:HD13	2.03	0.40
2:D:311:ARG:HA	2:D:343:LEU:O	2.20	0.40
2:D:443:VAL:HG11	2:D:483:PHE:CE2	2.57	0.40
1:E:262:ARG:NH1	1:E:461:SER:HB2	2.36	0.40
1:E:311:ARG:HA	1:E:343:LEU:O	2.21	0.40
1:E:356:LEU:CD1	1:E:356:LEU:H	2.35	0.40
1:F:452:ALA:CA	1:F:469:GLU:HA	2.50	0.40
1:A:59:PHE:HD2	1:A:143:SER:OG	2.05	0.40
1:B:39:GLY:N	1:B:177:THR:OG1	2.39	0.40
1:B:255:THR:HG22	1:B:255:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:GLU:O	1:B:494:PRO:HD2	2.22	0.40
2:C:18:ILE:HD12	2:C:18:ILE:N	2.37	0.40
2:C:208:ARG:O	2:C:218:ARG:HA	2.22	0.40
2:C:451:ARG:NH1	2:C:472:ILE:HD12	2.37	0.40
2:D:193:ARG:NH2	1:E:195:GLY:O	2.45	0.40
2:D:211:LEU:HD12	2:D:215:ARG:O	2.22	0.40
2:D:263:VAL:CG1	2:D:374:ARG:HH21	2.34	0.40
1:E:67:PHE:CB	1:E:69:GLU:HG3	2.51	0.40
1:E:160:VAL:O	1:E:161:ARG:C	2.58	0.40
1:F:420:MET:HE2	1:F:492:GLY:CA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	503/519 (97%)	377 (75%)	92 (18%)	34 (7%)	1 8
1	B	488/519 (94%)	365 (75%)	82 (17%)	41 (8%)	1 5
1	E	489/519 (94%)	375 (77%)	79 (16%)	35 (7%)	1 7
1	F	503/519 (97%)	399 (79%)	70 (14%)	34 (7%)	1 8
2	C	486/519 (94%)	373 (77%)	81 (17%)	32 (7%)	1 8
2	D	483/519 (93%)	392 (81%)	69 (14%)	22 (5%)	2 15
All	All	2952/3114 (95%)	2281 (77%)	473 (16%)	198 (7%)	1 8

All (198) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	65	ILE

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Mol	Chain	Res	Type
1	A	154	TYR
1	A	212	GLU
1	A	333	MET
1	A	427	ASP
1	A	499	VAL
1	A	502	LYS
1	A	510	ARG
1	B	52	LYS
1	B	65	ILE
1	B	154	TYR
1	B	193	ARG
1	B	461	SER
1	B	463	HIS
2	C	17	ALA
2	C	88	ARG
2	C	117	VAL
2	C	154	TYR
2	C	333	MET
2	C	463	HIS
2	D	87	ALA
2	D	122	ASP
2	D	154	TYR
2	D	333	MET
1	E	122	ASP
1	E	154	TYR
1	E	157	SER
1	E	195	GLY
1	E	333	MET
1	E	372	PRO
1	E	387	VAL
1	E	428	SER
1	E	463	HIS
1	F	26	GLU
1	F	117	VAL
1	F	118	VAL
1	F	154	TYR
1	F	249	LEU
1	F	333	MET
1	F	354	ALA
1	F	431	ALA
1	F	463	HIS
1	F	504	GLU

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Mol	Chain	Res	Type
1	F	506	SER
1	F	507	ARG
1	F	508	ILE
1	F	515	LYS
1	A	17	ALA
1	A	167	LEU
1	A	189	GLY
1	A	387	VAL
1	A	420	MET
1	A	429	HIS
1	A	431	ALA
1	A	463	HIS
1	B	26	GLU
1	B	119	GLY
1	B	132	TYR
1	B	149	SER
1	B	249	LEU
1	B	292	THR
1	B	342	ASN
1	B	370	PHE
1	B	372	PRO
1	B	420	MET
1	B	484	ARG
2	C	47	THR
2	C	115	GLN
2	C	149	SER
2	C	193	ARG
2	C	249	LEU
2	C	405	GLN
2	D	17	ALA
2	D	152	GLN
2	D	211	LEU
2	D	381	SER
2	D	400	THR
1	E	117	VAL
1	E	198	GLU
1	E	200	VAL
1	E	282	SER
1	E	327	ASN
1	E	393	ARG
1	E	417	ASP
1	E	420	MET

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Mol	Chain	Res	Type
1	E	422	ALA
1	E	427	ASP
1	E	494	PRO
1	E	498	THR
1	E	504	GLU
1	F	47	THR
1	F	189	GLY
1	F	420	MET
1	F	501	GLU
1	A	157	SER
1	A	422	ALA
1	A	480	LYS
1	B	22	ARG
1	B	61	TYR
1	B	211	LEU
1	B	327	ASN
1	B	354	ALA
1	B	424	SER
1	B	429	HIS
2	C	55	PHE
2	C	61	TYR
2	C	96	LYS
2	C	97	LEU
2	C	107	ASP
2	C	112	PRO
2	C	114	GLY
2	C	157	SER
2	C	341	GLN
2	C	398	GLY
2	D	86	ASN
2	D	123	LEU
2	D	420	MET
1	E	211	LEU
1	E	326	ARG
1	E	342	ASN
1	E	432	GLU
1	F	52	LYS
1	F	490	ILE
1	A	347	VAL
1	A	384	ALA
1	A	428	SER
1	B	167	LEU

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Mol	Chain	Res	Type
1	B	189	GLY
1	B	326	ARG
1	B	405	GLN
1	B	452	ALA
1	B	498	THR
2	C	197	GLU
2	C	289	ALA
2	C	477	PRO
2	D	325	LEU
2	D	429	HIS
1	E	18	ILE
1	E	47	THR
1	E	52	LYS
1	E	379	SER
1	E	482	SER
1	E	490	ILE
1	F	61	TYR
1	F	116	GLU
1	F	379	SER
1	F	468	ARG
1	A	120	GLY
1	A	211	LEU
1	A	289	ALA
1	B	54	LEU
1	B	152	GLN
1	B	198	GLU
1	B	268	VAL
1	B	289	ALA
1	B	309	LYS
2	C	212	GLU
2	C	379	SER
2	C	386	GLY
2	D	26	GLU
2	D	212	GLU
2	D	348	CYS
2	D	463	HIS
1	E	61	TYR
1	F	157	SER
1	F	211	LEU
1	F	500	ASP
1	F	517	PRO
1	A	112	PRO

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Mol	Chain	Res	Type
1	A	117	VAL
1	A	268	VAL
1	A	348	CYS
1	B	85	LYS
2	C	87	ALA
2	C	348	CYS
2	C	420	MET
2	D	248	PRO
2	D	354	ALA
2	D	359	HIS
1	F	152	GLN
1	F	409	THR
1	B	84	ILE
1	B	117	VAL
1	B	195	GLY
1	F	425	ILE
1	F	489	ILE
1	F	509	VAL
1	A	509	VAL
2	C	196	VAL
2	D	347	VAL
1	E	80	PRO
1	A	168	VAL
1	B	179	VAL
1	F	371	LYS
1	A	433	ILE
1	A	83	ILE
1	E	189	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	430/442 (97%)	400 (93%)	30 (7%)	15 43
1	B	417/442 (94%)	387 (93%)	30 (7%)	14 41
1	E	418/442 (95%)	385 (92%)	33 (8%)	12 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	430/442 (97%)	383 (89%)	47 (11%)	6	24
2	C	415/443 (94%)	371 (89%)	44 (11%)	6	25
2	D	412/443 (93%)	372 (90%)	40 (10%)	8	29
All	All	2522/2654 (95%)	2298 (91%)	224 (9%)	9	32

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	30	ASP
1	A	33	HIS
1	A	50	THR
1	A	75	THR
1	A	92	TRP
1	A	99	ASP
1	A	121	PHE
1	A	154	TYR
1	A	186	GLU
1	A	212	GLU
1	A	219	THR
1	A	238	THR
1	A	270	LEU
1	A	287	THR
1	A	298	VAL
1	A	335	PHE
1	A	342	ASN
1	A	348	CYS
1	A	360	LEU
1	A	371	LYS
1	A	375	ILE
1	A	427	ASP
1	A	429	HIS
1	A	434	THR
1	A	451	ARG
1	A	463	HIS
1	A	469	GLU
1	A	508	ILE
1	A	518	GLU
1	B	26	GLU
1	B	33	HIS
1	B	47	THR

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Mol	Chain	Res	Type
1	B	50	THR
1	B	77	GLU
1	B	81	GLN
1	B	92	TRP
1	B	103	LEU
1	B	111	ASP
1	B	151	PHE
1	B	154	TYR
1	B	178	THR
1	B	182	THR
1	B	185	ILE
1	B	186	GLU
1	B	193	ARG
1	B	203	ASN
1	B	212	GLU
1	B	223	LEU
1	B	256	GLN
1	B	270	LEU
1	B	302	VAL
1	B	333	MET
1	B	371	LYS
1	B	451	ARG
1	B	462	TRP
1	B	471	MET
1	B	474	ASP
1	B	490	ILE
1	B	499	VAL
2	C	15	HIS
2	C	26	GLU
2	C	50	THR
2	C	121	PHE
2	C	122	ASP
2	C	140	ARG
2	C	149	SER
2	C	151	PHE
2	C	154	TYR
2	C	184	ARG
2	C	185	ILE
2	C	186	GLU
2	C	196	VAL
2	C	198	GLU
2	C	209	ASN

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Mol	Chain	Res	Type
2	C	210	VAL
2	C	212	GLU
2	C	215	ARG
2	C	218	ARG
2	C	223	LEU
2	C	228	THR
2	C	238	THR
2	C	245	ASN
2	C	256	GLN
2	C	260	ASN
2	C	263	VAL
2	C	270	LEU
2	C	290	THR
2	C	295	THR
2	C	303	GLU
2	C	317	TYR
2	C	333	MET
2	C	336	GLU
2	C	356	LEU
2	C	366	GLU
2	C	371	LYS
2	C	383	LEU
2	C	451	ARG
2	C	454	ASN
2	C	470	PHE
2	C	471	MET
2	C	477	PRO
2	C	491	SER
2	C	498	THR
2	D	26	GLU
2	D	30	ASP
2	D	48	SER
2	D	80	PRO
2	D	81	GLN
2	D	106	LEU
2	D	121	PHE
2	D	122	ASP
2	D	123	LEU
2	D	154	TYR
2	D	177	THR
2	D	209	ASN
2	D	211	LEU

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Mol	Chain	Res	Type
2	D	212	GLU
2	D	218	ARG
2	D	237	PHE
2	D	238	THR
2	D	256	GLN
2	D	263	VAL
2	D	270	LEU
2	D	281	ASP
2	D	284	ILE
2	D	290	THR
2	D	302	VAL
2	D	314	LEU
2	D	321	ARG
2	D	356	LEU
2	D	371	LYS
2	D	412	PHE
2	D	416	SER
2	D	423	HIS
2	D	434	THR
2	D	451	ARG
2	D	453	ILE
2	D	463	HIS
2	D	471	MET
2	D	474	ASP
2	D	490	ILE
2	D	496	ARG
2	D	498	THR
1	E	18	ILE
1	E	26	GLU
1	E	81	GLN
1	E	113	GLU
1	E	121	PHE
1	E	135	GLN
1	E	151	PHE
1	E	154	TYR
1	E	177	THR
1	E	196	VAL
1	E	201	SER
1	E	203	ASN
1	E	209	ASN
1	E	212	GLU
1	E	223	LEU

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Mol	Chain	Res	Type
1	E	228	THR
1	E	256	GLN
1	E	260	ASN
1	E	271	ASP
1	E	287	THR
1	E	325	LEU
1	E	338	MET
1	E	366	GLU
1	E	369	ASP
1	E	371	LYS
1	E	417	ASP
1	E	432	GLU
1	E	435	ASP
1	E	449	MET
1	E	451	ARG
1	E	453	ILE
1	E	458	MET
1	E	471	MET
1	F	15	HIS
1	F	26	GLU
1	F	29	ASP
1	F	33	HIS
1	F	43	LEU
1	F	56	SER
1	F	77	GLU
1	F	79	THR
1	F	103	LEU
1	F	121	PHE
1	F	123	LEU
1	F	140	ARG
1	F	143	SER
1	F	154	TYR
1	F	178	THR
1	F	184	ARG
1	F	185	ILE
1	F	186	GLU
1	F	209	ASN
1	F	210	VAL
1	F	212	GLU
1	F	215	ARG
1	F	218	ARG
1	F	219	THR

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Mol	Chain	Res	Type
1	F	256	GLN
1	F	285	LEU
1	F	302	VAL
1	F	325	LEU
1	F	348	CYS
1	F	366	GLU
1	F	371	LYS
1	F	387	VAL
1	F	424	SER
1	F	425	ILE
1	F	427	ASP
1	F	451	ARG
1	F	458	MET
1	F	462	TRP
1	F	468	ARG
1	F	469	GLU
1	F	471	MET
1	F	481	ASP
1	F	497	ILE
1	F	501	GLU
1	F	504	GLU
1	F	509	VAL
1	F	514	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	33	HIS
1	A	62	ASN
1	A	135	GLN
1	A	152	GLN
1	A	209	ASN
1	A	327	ASN
1	A	414	ASN
1	A	441	GLN
1	B	58	GLN
1	B	62	ASN
1	B	81	GLN
1	B	152	GLN
1	B	203	ASN
1	B	209	ASN

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Mol	Chain	Res	Type
1	B	361	GLN
2	C	33	HIS
2	C	58	GLN
2	C	62	ASN
2	C	152	GLN
2	C	209	ASN
2	C	245	ASN
2	C	260	ASN
2	C	323	GLN
2	C	389	ASN
2	C	414	ASN
2	C	418	GLN
2	D	33	HIS
2	D	81	GLN
2	D	209	ASN
2	D	323	GLN
2	D	414	ASN
2	D	441	GLN
1	E	33	HIS
1	E	62	ASN
1	E	81	GLN
1	E	135	GLN
1	E	153	GLN
1	E	209	ASN
1	E	256	GLN
1	E	304	ASN
1	E	323	GLN
1	E	368	ASN
1	E	414	ASN
1	E	441	GLN
1	E	454	ASN
1	F	16	GLN
1	F	33	HIS
1	F	153	GLN
1	F	209	ASN
1	F	256	GLN
1	F	327	ASN
1	F	418	GLN
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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	E	426	1	8,10,11	0.92	0	10,14,16	1.72	2 (20%)
1	TPO	B	426	1	8,10,11	1.54	2 (25%)	10,14,16	2.40	3 (30%)
1	TPO	A	426	1	8,10,11	1.06	1 (12%)	10,14,16	0.87	0
1	TPO	F	426	1	8,10,11	1.46	1 (12%)	10,14,16	2.31	5 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	E	426	1	-	3/9/11/13	-
1	TPO	B	426	1	-	4/9/11/13	-
1	TPO	A	426	1	-	2/9/11/13	-
1	TPO	F	426	1	-	2/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	426	TPO	CG2-CB	3.16	1.59	1.51
1	F	426	TPO	CB-CA	3.05	1.60	1.53
1	A	426	TPO	P-OG1	-2.12	1.55	1.59
1	B	426	TPO	P-O1P	-2.03	1.44	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	426	TPO	P-OG1-CB	-5.53	106.50	123.21
1	B	426	TPO	CG2-CB-CA	-3.92	105.42	113.16
1	E	426	TPO	P-OG1-CB	-3.53	112.55	123.21
1	F	426	TPO	CG2-CB-CA	-3.52	106.22	113.16
1	F	426	TPO	O2P-P-O1P	-3.46	97.14	110.68
1	E	426	TPO	CG2-CB-CA	-3.46	106.34	113.16
1	F	426	TPO	P-OG1-CB	-3.19	113.57	123.21
1	F	426	TPO	O2P-P-OG1	2.92	119.09	105.99
1	F	426	TPO	O3P-P-O2P	2.67	117.85	107.64
1	B	426	TPO	O2P-P-OG1	2.48	117.13	105.99

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	426	TPO	3	0
1	B	426	TPO	7	0
1	A	426	TPO	15	0
1	F	426	TPO	13	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	E	903	4	26,33,33	1.17	1 (3%)	31,52,52	1.74	6 (19%)
3	ATP	A	903	4	26,33,33	1.28	4 (15%)	31,52,52	1.73	4 (12%)
3	ATP	F	903	4	26,33,33	1.37	4 (15%)	31,52,52	1.77	6 (19%)
3	ATP	B	903	4	26,33,33	1.31	4 (15%)	31,52,52	1.81	6 (19%)
3	ATP	E	901	4	26,33,33	1.31	2 (7%)	31,52,52	1.81	8 (25%)
3	ATP	C	903	4	26,33,33	1.33	4 (15%)	31,52,52	1.86	5 (16%)
3	ATP	D	901	4	26,33,33	1.42	3 (11%)	31,52,52	1.71	6 (19%)
3	ATP	A	901	4	26,33,33	1.32	3 (11%)	31,52,52	1.81	7 (22%)
3	ATP	F	901	4	26,33,33	1.33	3 (11%)	31,52,52	1.75	5 (16%)
3	ATP	B	901	4	26,33,33	1.17	3 (11%)	31,52,52	1.69	3 (9%)
3	ATP	C	901	4	26,33,33	1.33	3 (11%)	31,52,52	1.79	7 (22%)
3	ATP	D	903	4	26,33,33	1.37	4 (15%)	31,52,52	1.76	5 (16%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	F	901	4	-	6/18/38/38	0/3/3/3
3	ATP	B	901	4	-	5/18/38/38	0/3/3/3
3	ATP	C	901	4	-	8/18/38/38	0/3/3/3
3	ATP	D	903	4	-	7/18/38/38	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	ATP	C2-N3	4.31	1.39	1.32
3	F	903	ATP	C2-N3	4.29	1.39	1.32
3	C	901	ATP	C2-N3	4.24	1.38	1.32
3	A	901	ATP	C2-N3	4.23	1.38	1.32
3	F	901	ATP	C2-N3	4.14	1.38	1.32
3	B	903	ATP	C2-N3	4.12	1.38	1.32
3	E	901	ATP	C2-N3	4.02	1.38	1.32
3	D	903	ATP	C2-N3	3.99	1.38	1.32
3	C	903	ATP	C2-N3	3.97	1.38	1.32
3	A	903	ATP	C2-N3	3.87	1.38	1.32
3	E	903	ATP	C2-N3	3.65	1.38	1.32
3	B	901	ATP	C2-N3	3.19	1.37	1.32
3	D	903	ATP	C4-N3	2.95	1.39	1.35
3	F	901	ATP	O4'-C1'	2.89	1.45	1.41
3	A	901	ATP	O4'-C1'	2.87	1.45	1.41
3	B	903	ATP	O4'-C1'	2.85	1.45	1.41
3	C	903	ATP	C2'-C1'	-2.74	1.49	1.53
3	D	903	ATP	C2'-C1'	-2.63	1.49	1.53
3	D	901	ATP	C2-N1	2.53	1.38	1.33
3	F	903	ATP	C2'-C1'	-2.46	1.50	1.53
3	B	901	ATP	O4'-C1'	2.43	1.44	1.41
3	F	901	ATP	C2-N1	2.39	1.38	1.33
3	F	903	ATP	C2-N1	2.39	1.38	1.33
3	A	903	ATP	C2-N1	2.37	1.38	1.33
3	F	903	ATP	O4'-C1'	2.32	1.44	1.41
3	A	903	ATP	C2'-C1'	-2.31	1.50	1.53
3	B	903	ATP	C2-N1	2.24	1.38	1.33
3	B	903	ATP	C4-N3	2.21	1.38	1.35
3	A	903	ATP	O4'-C1'	2.19	1.44	1.41
3	D	901	ATP	C2'-C1'	-2.19	1.50	1.53
3	A	901	ATP	C2-N1	2.19	1.38	1.33
3	C	901	ATP	O4'-C1'	2.17	1.44	1.41
3	C	903	ATP	O4'-C1'	2.17	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	ATP	C2-N1	2.15	1.37	1.33
3	E	901	ATP	O4'-C1'	2.13	1.44	1.41
3	D	903	ATP	C2-N1	2.12	1.37	1.33
3	C	903	ATP	C2-N1	2.10	1.37	1.33
3	C	901	ATP	C2'-C1'	-2.07	1.50	1.53

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	901	ATP	N3-C2-N1	-5.56	119.98	128.68
3	E	901	ATP	N3-C2-N1	-5.56	119.99	128.68
3	D	903	ATP	N3-C2-N1	-5.55	120.01	128.68
3	E	903	ATP	N3-C2-N1	-5.51	120.06	128.68
3	B	903	ATP	N3-C2-N1	-5.50	120.08	128.68
3	B	901	ATP	N3-C2-N1	-5.49	120.10	128.68
3	C	903	ATP	N3-C2-N1	-5.45	120.15	128.68
3	C	901	ATP	N3-C2-N1	-5.36	120.30	128.68
3	F	901	ATP	N3-C2-N1	-5.36	120.31	128.68
3	A	903	ATP	N3-C2-N1	-5.28	120.42	128.68
3	F	903	ATP	N3-C2-N1	-5.26	120.45	128.68
3	A	901	ATP	N3-C2-N1	-5.16	120.62	128.68
3	B	903	ATP	C4-C5-N7	-4.42	104.79	109.40
3	C	903	ATP	C4-C5-N7	-4.33	104.88	109.40
3	D	903	ATP	C4-C5-N7	-4.28	104.94	109.40
3	B	903	ATP	C5-C6-N6	4.24	126.79	120.35
3	F	901	ATP	C4-C5-N7	-4.24	104.98	109.40
3	C	903	ATP	C5-C6-N6	4.23	126.78	120.35
3	C	901	ATP	C4-C5-N7	-4.21	105.01	109.40
3	F	903	ATP	C5-C6-N6	4.19	126.71	120.35
3	B	901	ATP	C5-C6-N6	4.17	126.69	120.35
3	A	901	ATP	C5-C6-N6	4.16	126.68	120.35
3	A	901	ATP	C4-C5-N7	-4.15	105.08	109.40
3	B	901	ATP	C4-C5-N7	-4.11	105.11	109.40
3	F	903	ATP	C4-C5-N7	-4.09	105.14	109.40
3	E	903	ATP	C4-C5-N7	-4.06	105.17	109.40
3	F	901	ATP	C5-C6-N6	4.02	126.47	120.35
3	C	901	ATP	C5-C6-N6	4.02	126.47	120.35
3	E	901	ATP	C4-C5-N7	-3.98	105.25	109.40
3	A	903	ATP	C4-C5-N7	-3.91	105.32	109.40
3	D	903	ATP	C5-C6-N6	3.83	126.18	120.35
3	E	903	ATP	C5-C6-N6	3.78	126.10	120.35
3	A	903	ATP	C5-C6-N6	3.76	126.06	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	901	ATP	C5-C6-N6	3.73	126.03	120.35
3	D	901	ATP	C4-C5-N7	-3.67	105.58	109.40
3	D	901	ATP	C5-C6-N6	3.39	125.51	120.35
3	D	903	ATP	PB-O3B-PG	-3.07	122.28	132.83
3	A	901	ATP	C3'-C2'-C1'	2.59	104.87	100.98
3	E	901	ATP	O2'-C2'-C3'	2.58	120.18	111.82
3	E	903	ATP	PB-O3B-PG	-2.56	124.05	132.83
3	C	903	ATP	C3'-C2'-C1'	2.55	104.82	100.98
3	D	901	ATP	C3'-C2'-C1'	2.49	104.72	100.98
3	F	903	ATP	N6-C6-N1	-2.46	113.47	118.57
3	A	901	ATP	PB-O3B-PG	-2.43	124.48	132.83
3	E	901	ATP	O2G-PG-O3B	2.41	112.72	104.64
3	B	903	ATP	N6-C6-N1	-2.41	113.57	118.57
3	B	903	ATP	PB-O3B-PG	-2.36	124.72	132.83
3	A	903	ATP	O2'-C2'-C3'	2.34	119.40	111.82
3	C	903	ATP	N6-C6-N1	-2.30	113.81	118.57
3	E	901	ATP	C3'-C2'-C1'	2.29	104.43	100.98
3	F	901	ATP	O2'-C2'-C3'	2.29	119.23	111.82
3	F	903	ATP	C2'-C3'-C4'	2.26	107.04	102.64
3	A	901	ATP	N6-C6-N1	-2.25	113.91	118.57
3	C	901	ATP	N6-C6-N1	-2.24	113.92	118.57
3	D	903	ATP	N6-C6-N1	-2.22	113.96	118.57
3	C	901	ATP	C3'-C2'-C1'	2.19	104.28	100.98
3	F	903	ATP	O2G-PG-O3B	2.16	111.87	104.64
3	C	901	ATP	C2'-C3'-C4'	2.13	106.78	102.64
3	F	901	ATP	N6-C6-N1	-2.12	114.17	118.57
3	A	901	ATP	C2'-C3'-C4'	2.12	106.77	102.64
3	D	901	ATP	C2'-C3'-C4'	2.10	106.73	102.64
3	D	901	ATP	O2G-PG-O3B	2.10	111.67	104.64
3	E	903	ATP	N6-C6-N1	-2.09	114.24	118.57
3	B	903	ATP	O2'-C2'-C3'	2.07	118.53	111.82
3	E	901	ATP	N6-C6-N1	-2.07	114.28	118.57
3	E	901	ATP	C2'-C3'-C4'	2.03	106.59	102.64
3	C	901	ATP	O2'-C2'-C3'	2.03	118.38	111.82
3	E	903	ATP	O2G-PG-O3B	2.02	111.42	104.64

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	A	901	ATP	C3'-C4'-C5'-O5'
3	A	903	ATP	PB-O3B-PG-O3G
3	A	903	ATP	C3'-C4'-C5'-O5'
3	B	901	ATP	C5'-O5'-PA-O1A
3	B	901	ATP	C3'-C4'-C5'-O5'
3	B	903	ATP	PB-O3B-PG-O3G
3	B	903	ATP	O4'-C4'-C5'-O5'
3	B	903	ATP	C3'-C4'-C5'-O5'
3	C	901	ATP	PB-O3B-PG-O2G
3	C	901	ATP	PB-O3B-PG-O3G
3	C	901	ATP	C5'-O5'-PA-O3A
3	C	901	ATP	O4'-C4'-C5'-O5'
3	C	901	ATP	C3'-C4'-C5'-O5'
3	C	903	ATP	PB-O3B-PG-O3G
3	C	903	ATP	C5'-O5'-PA-O1A
3	C	903	ATP	C3'-C4'-C5'-O5'
3	D	901	ATP	C5'-O5'-PA-O3A
3	D	901	ATP	C3'-C4'-C5'-O5'
3	D	903	ATP	O4'-C4'-C5'-O5'
3	D	903	ATP	C3'-C4'-C5'-O5'
3	E	901	ATP	PB-O3B-PG-O3G
3	E	901	ATP	PB-O3A-PA-O5'
3	E	901	ATP	C5'-O5'-PA-O3A
3	E	901	ATP	C3'-C4'-C5'-O5'
3	E	903	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	C5'-O5'-PA-O3A
3	F	901	ATP	C3'-C4'-C5'-O5'
3	F	903	ATP	PB-O3B-PG-O3G
3	F	903	ATP	C5'-O5'-PA-O1A
3	F	903	ATP	O4'-C4'-C5'-O5'
3	F	903	ATP	C3'-C4'-C5'-O5'
3	A	901	ATP	O4'-C4'-C5'-O5'
3	B	901	ATP	O4'-C4'-C5'-O5'
3	C	903	ATP	O4'-C4'-C5'-O5'
3	D	901	ATP	O4'-C4'-C5'-O5'
3	E	903	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	O4'-C4'-C5'-O5'
3	F	901	ATP	O4'-C4'-C5'-O5'
3	A	903	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	PB-O3A-PA-O5'
3	A	903	ATP	PB-O3A-PA-O5'
3	B	901	ATP	PB-O3A-PA-O5'

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

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Mol	Chain	Res	Type	Atoms
3	E	901	ATP	PB-O3B-PG-O1G

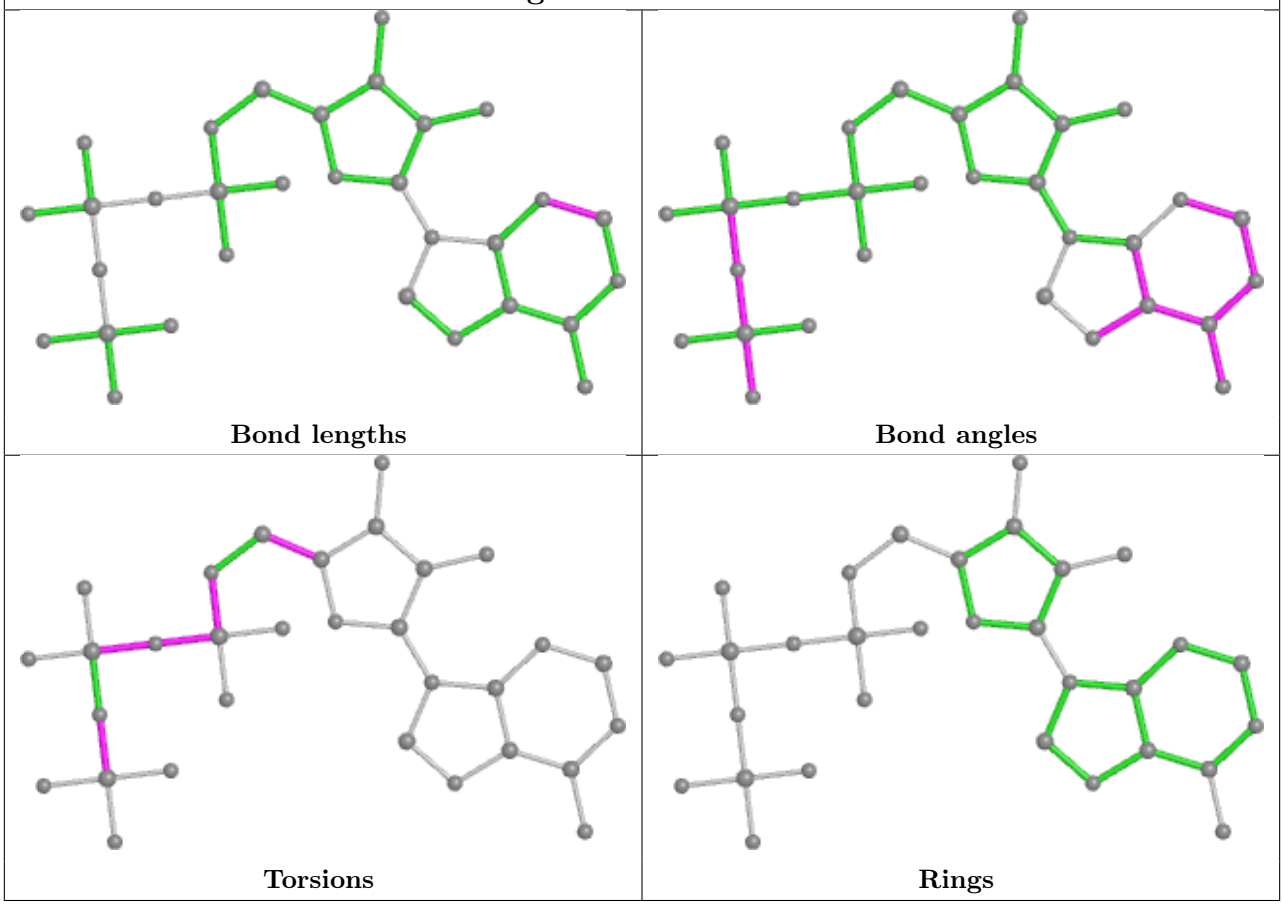
There are no ring outliers.

12 monomers are involved in 40 short contacts:

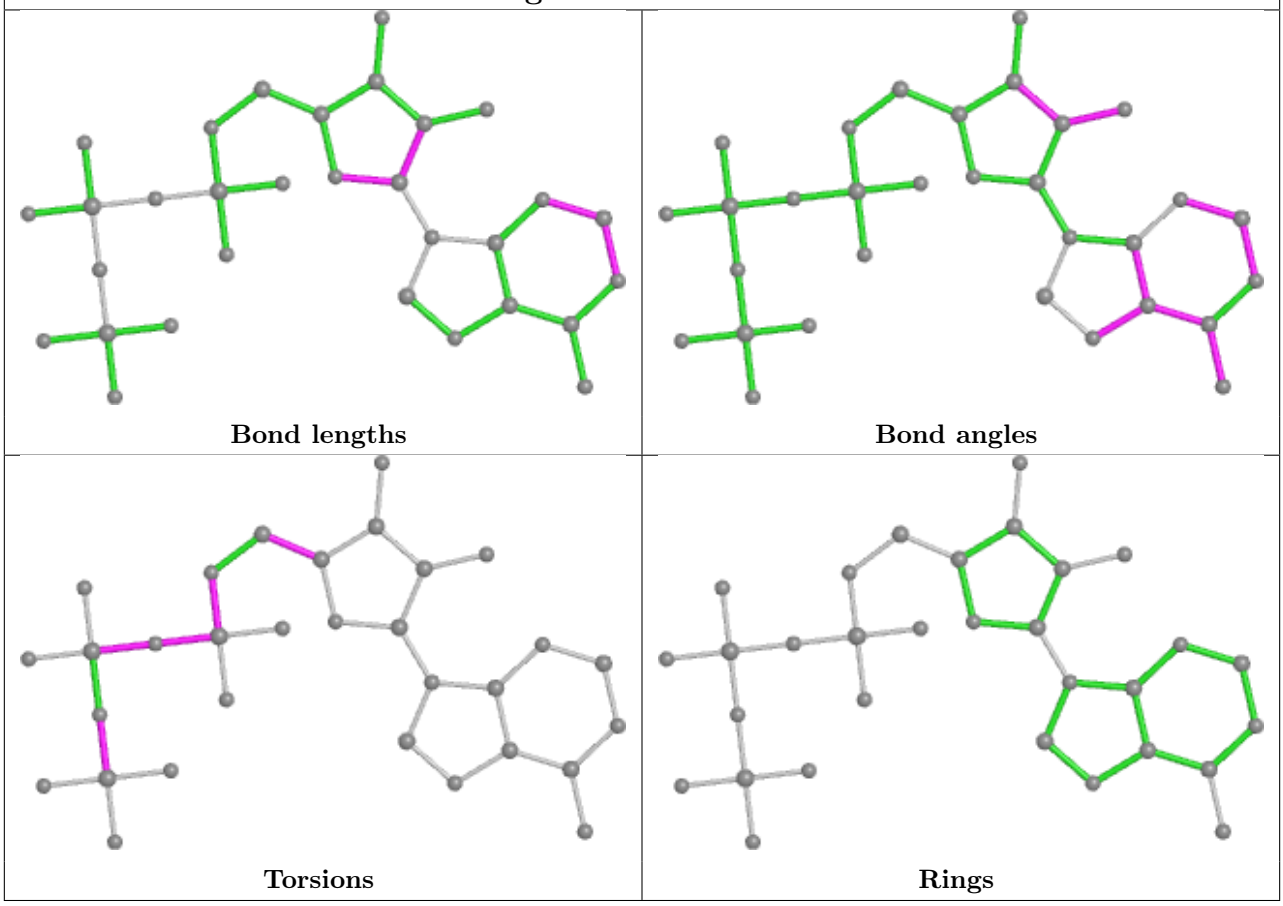
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	903	ATP	3	0
3	A	903	ATP	5	0
3	F	903	ATP	1	0
3	B	903	ATP	4	0
3	E	901	ATP	6	0
3	C	903	ATP	4	0
3	D	901	ATP	4	0
3	A	901	ATP	1	0
3	F	901	ATP	3	0
3	B	901	ATP	4	0
3	C	901	ATP	4	0
3	D	903	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

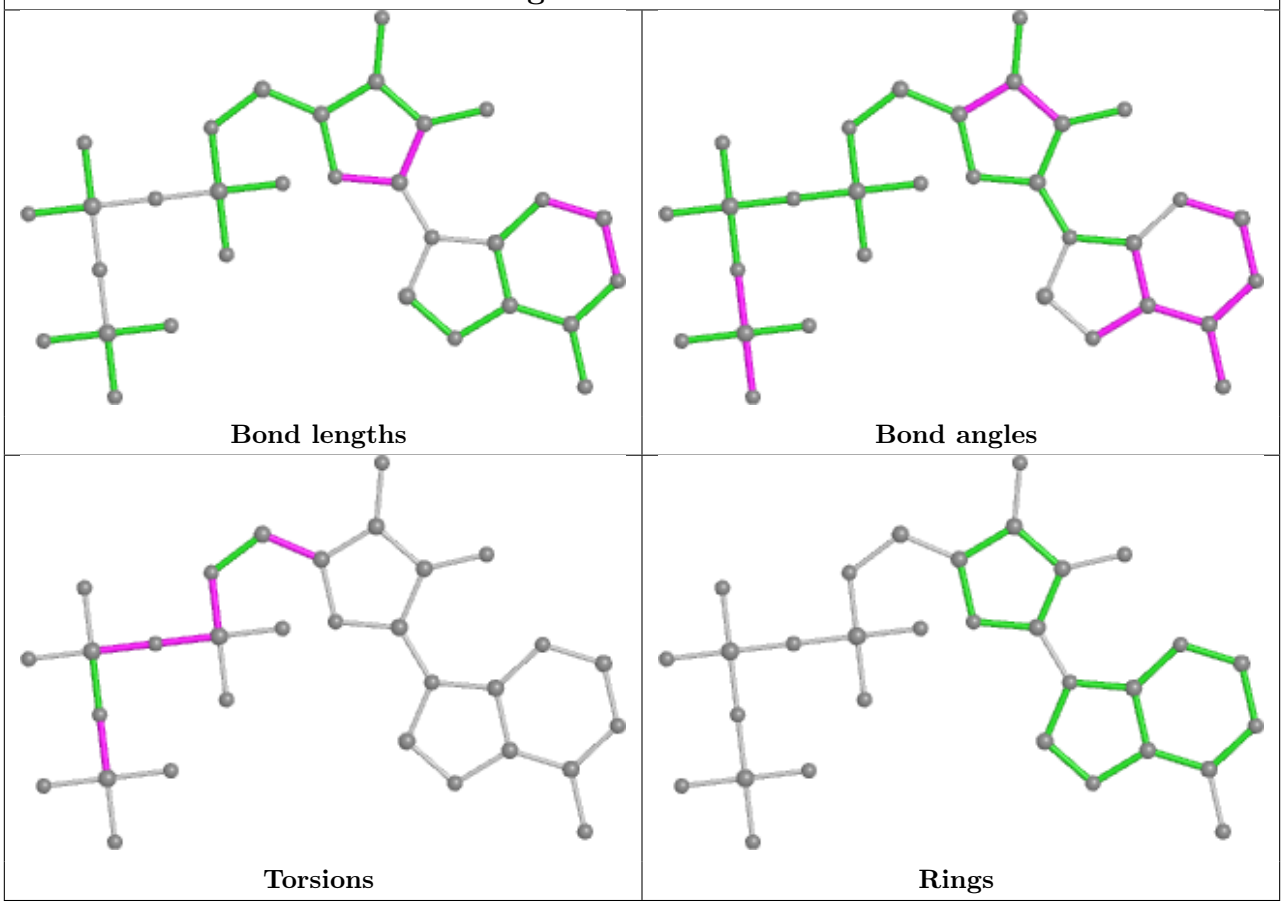
Ligand ATP E 903



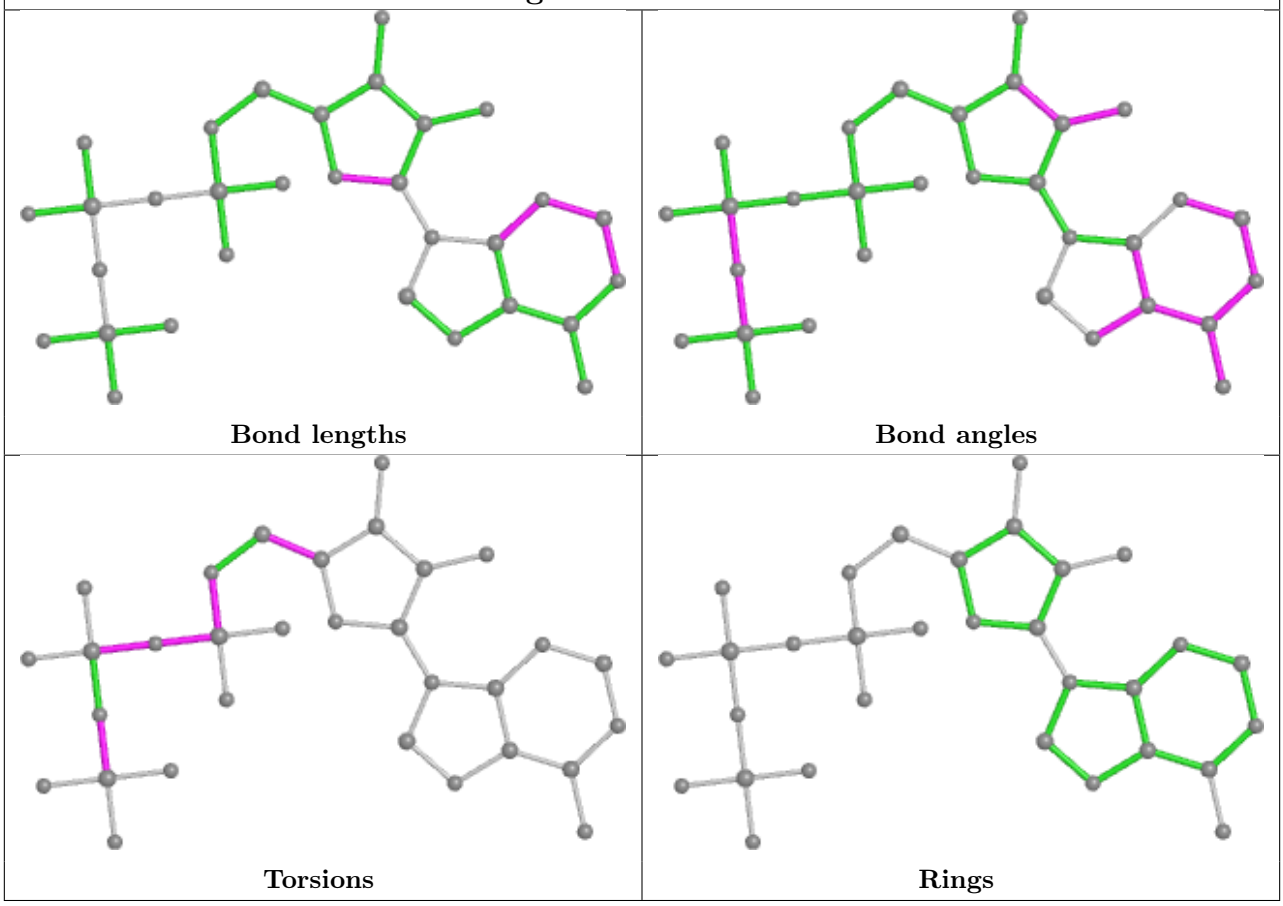
Ligand ATP A 903



Ligand ATP F 903



Ligand ATP B 903



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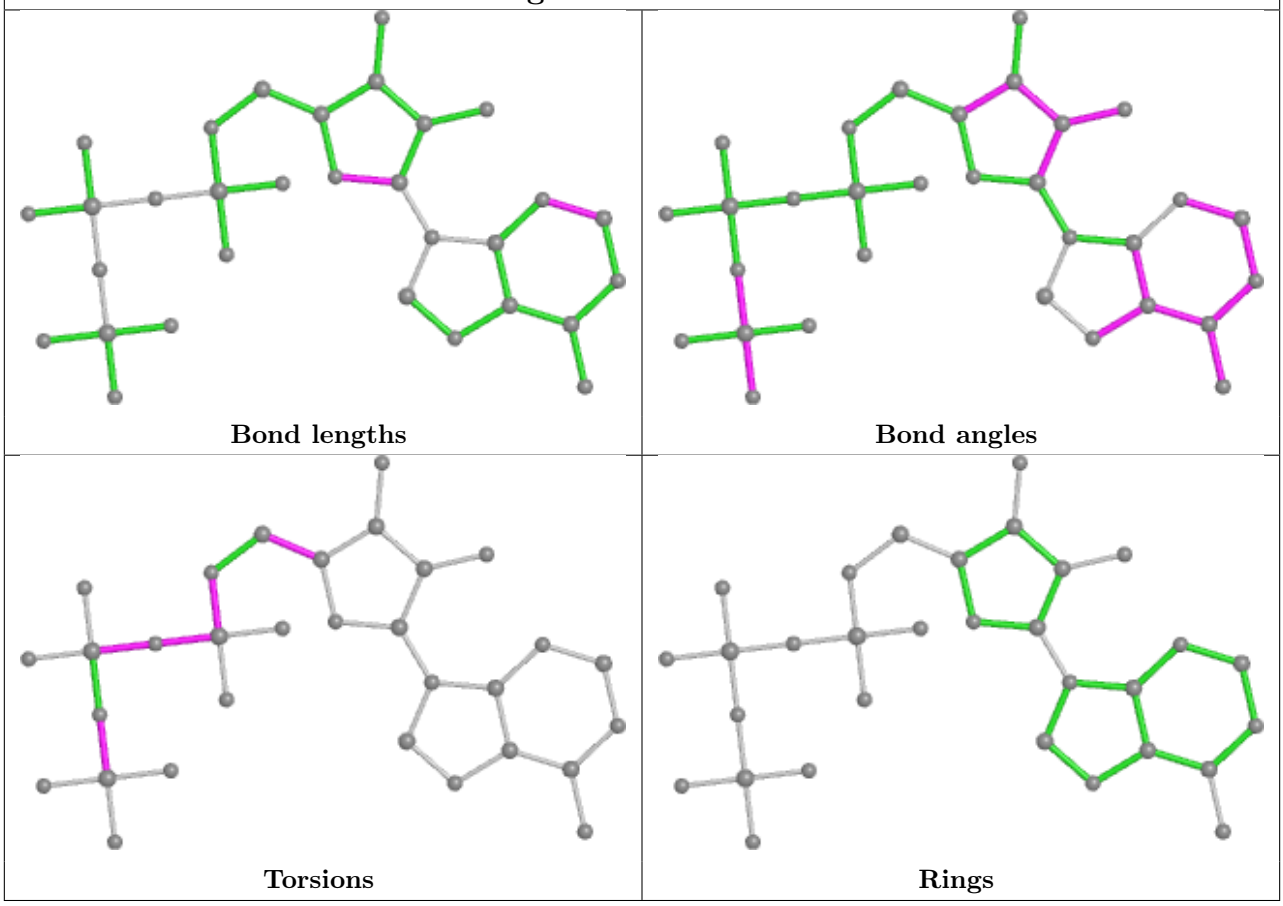

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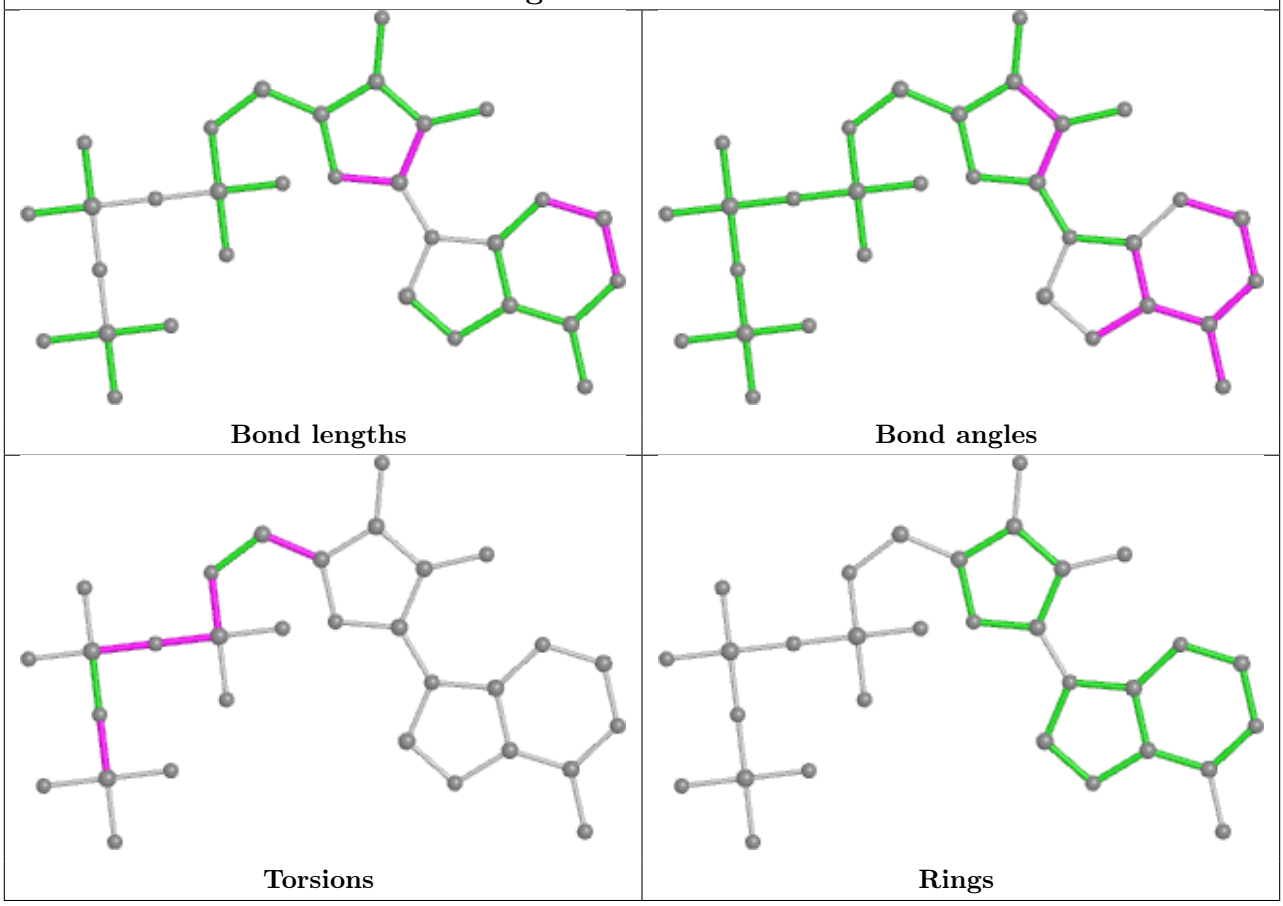

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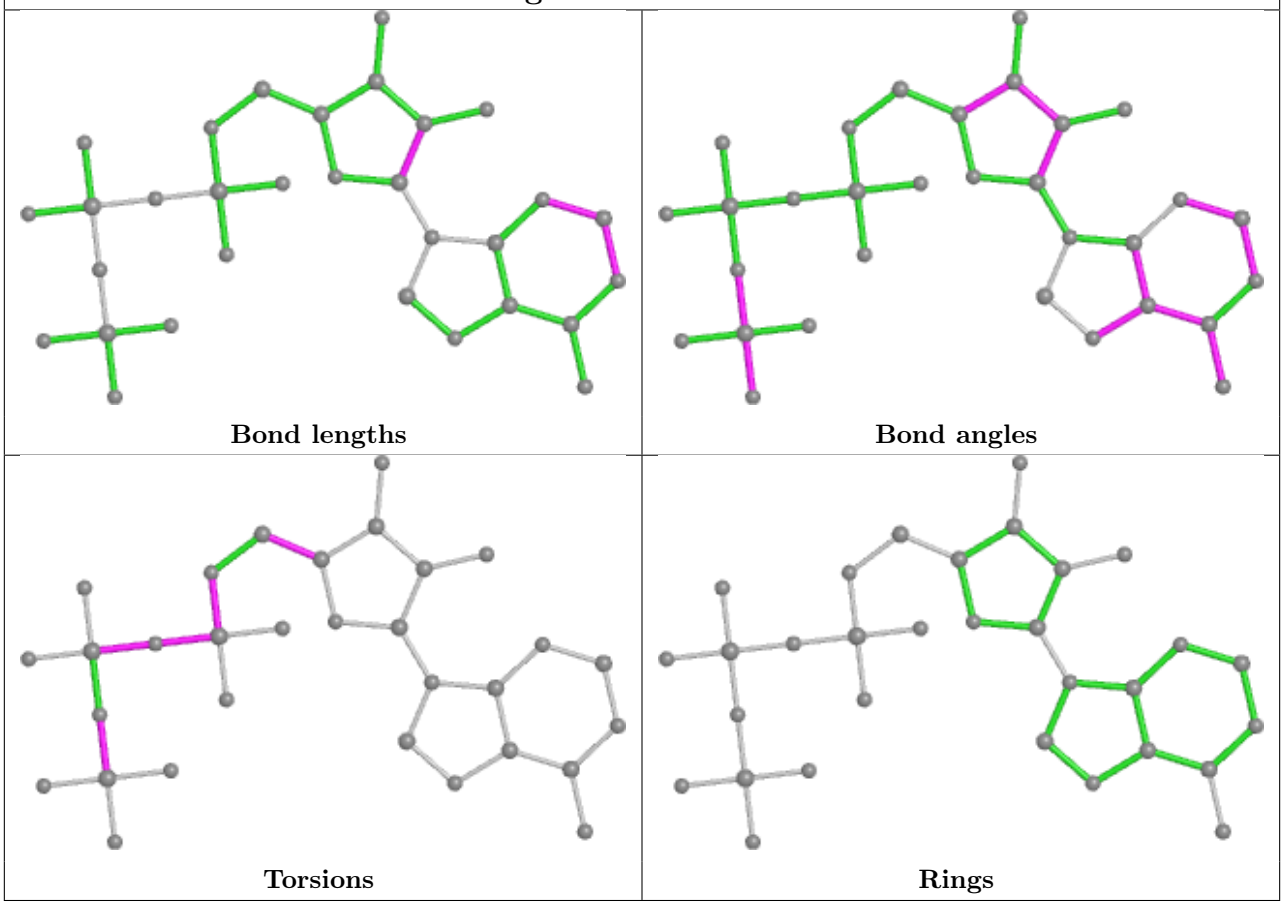

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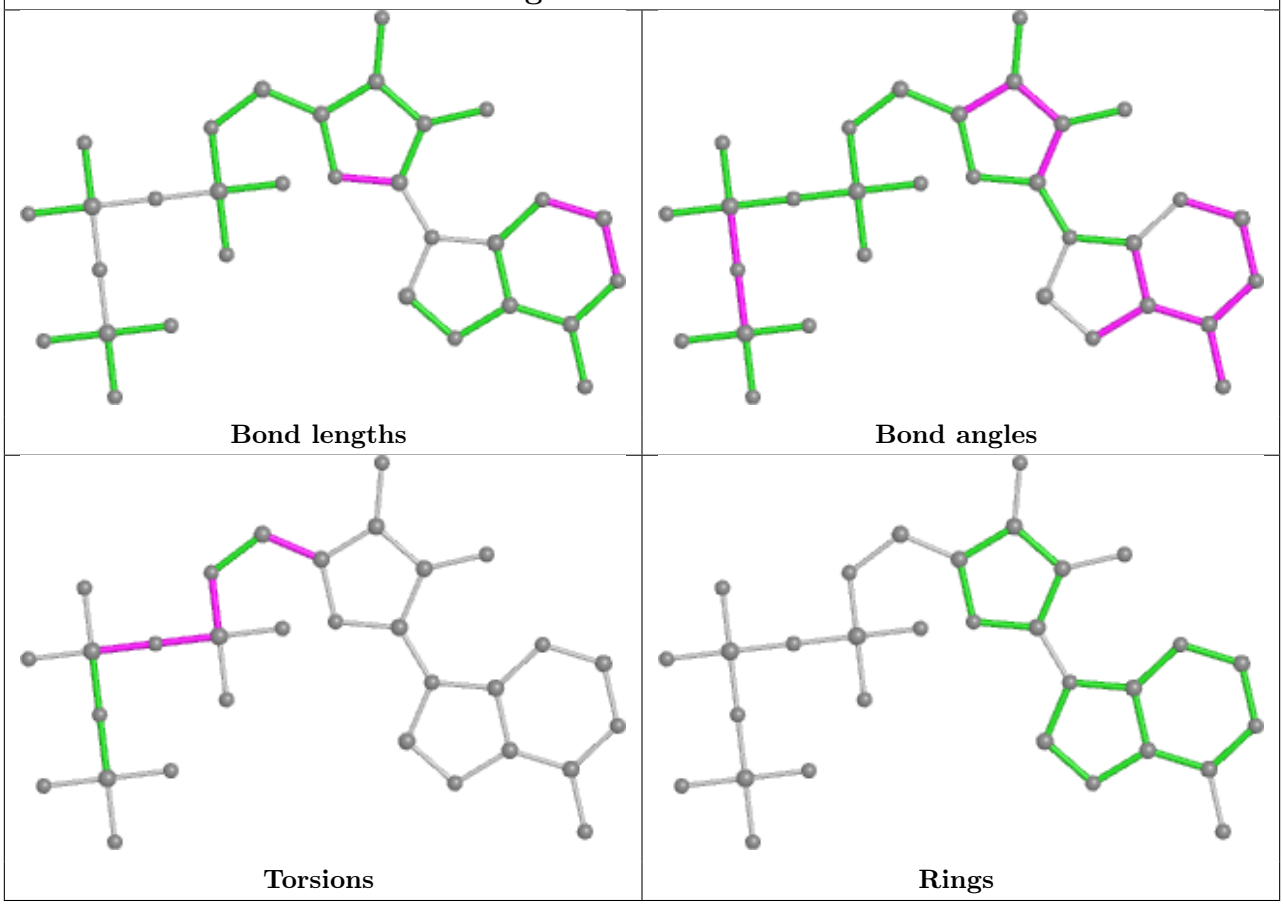

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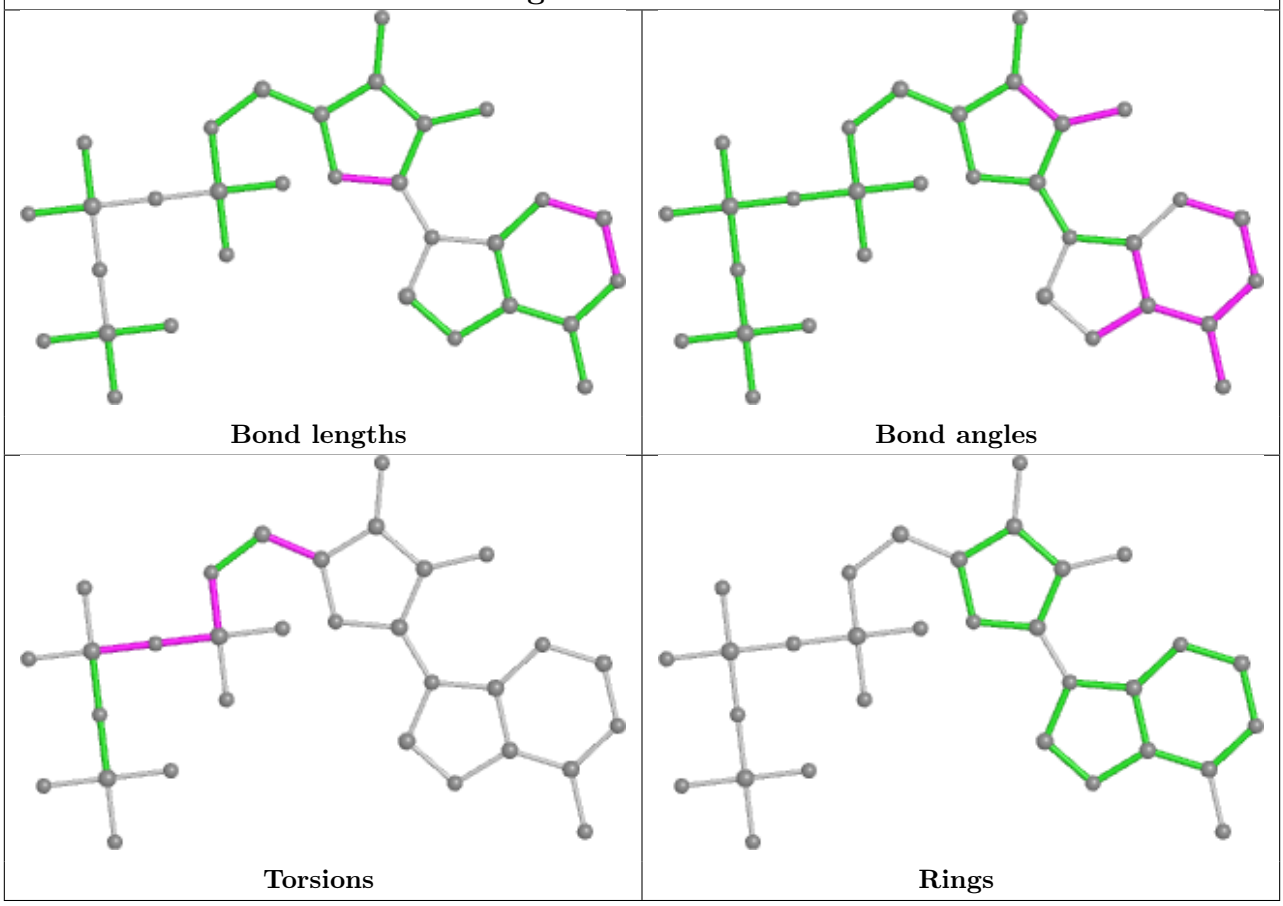

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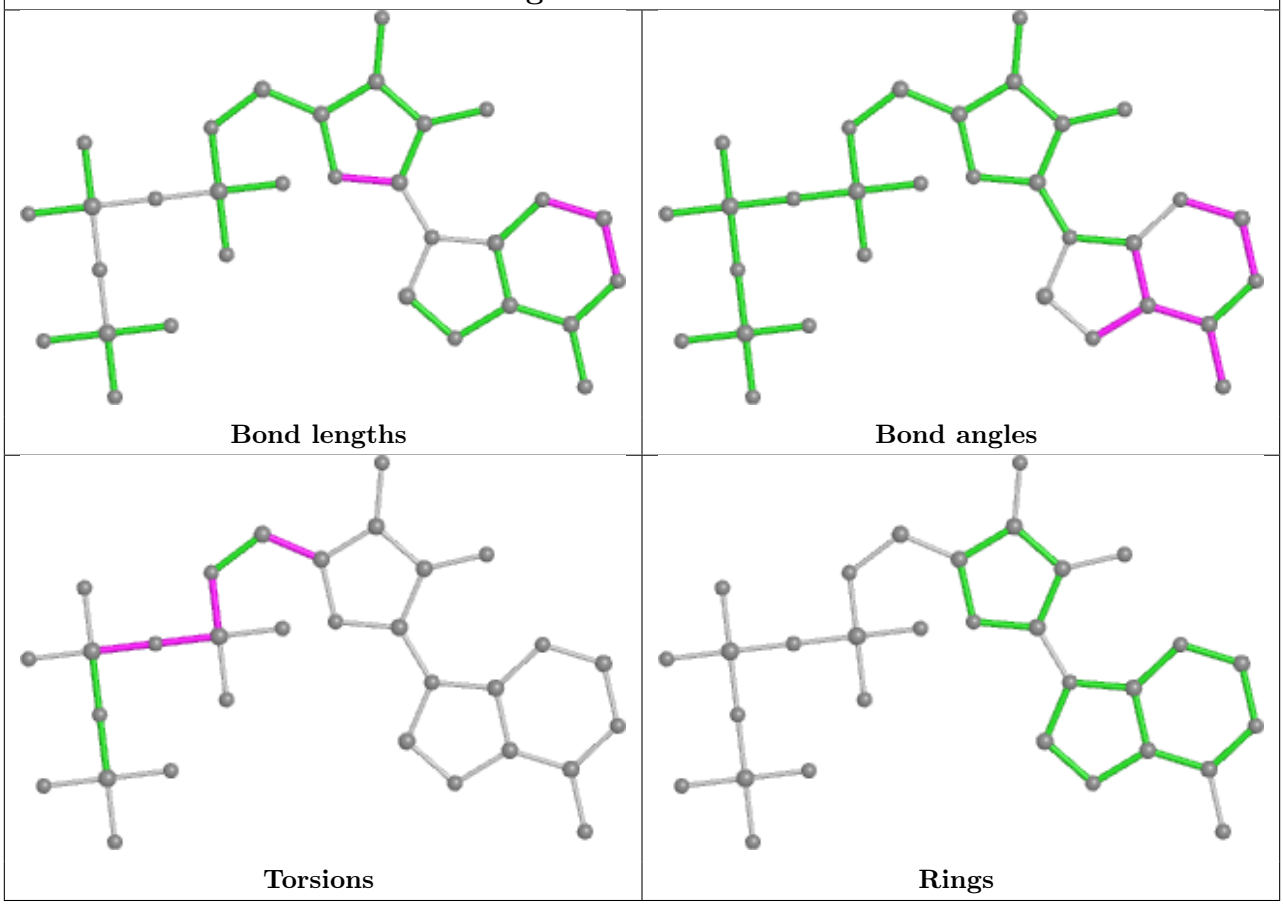

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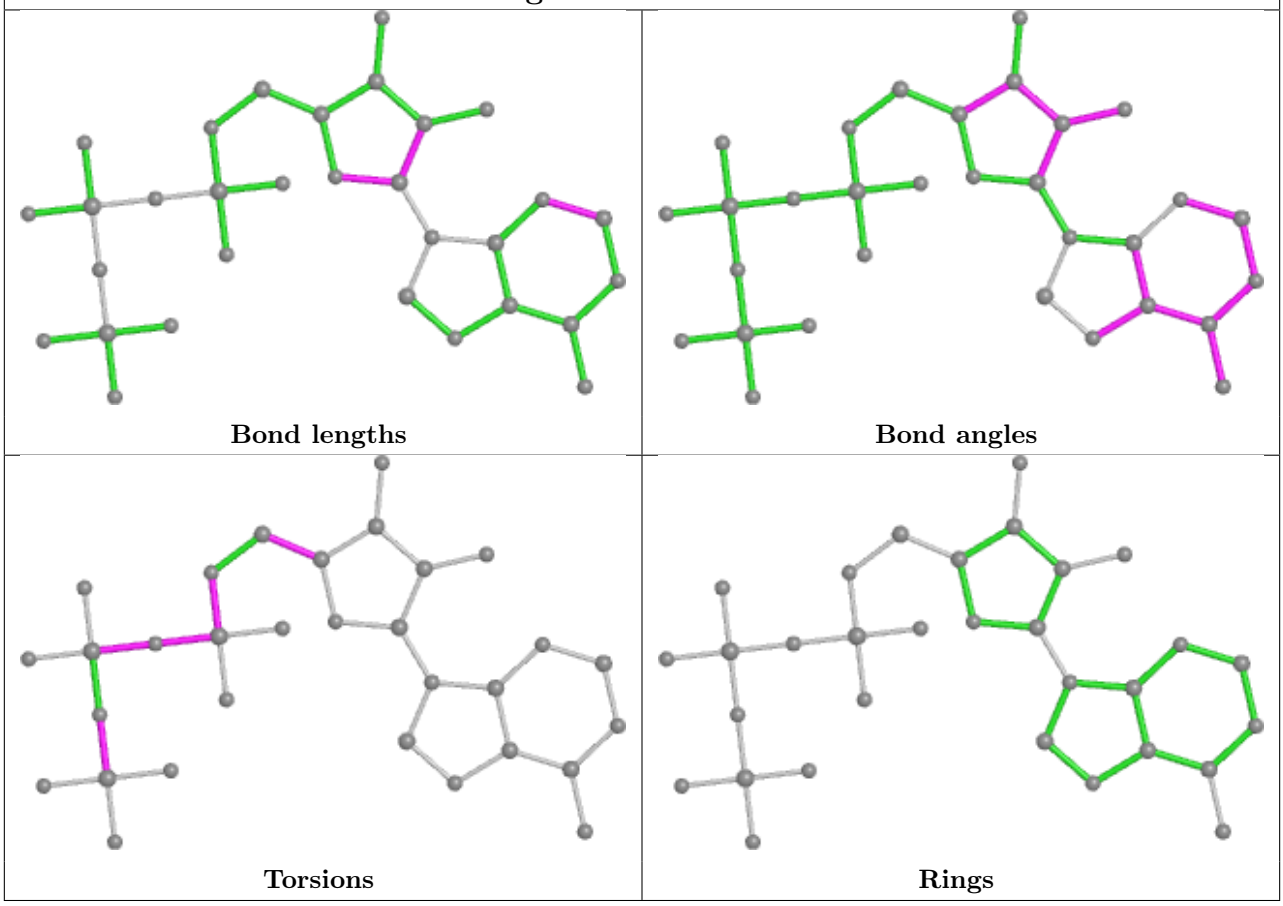

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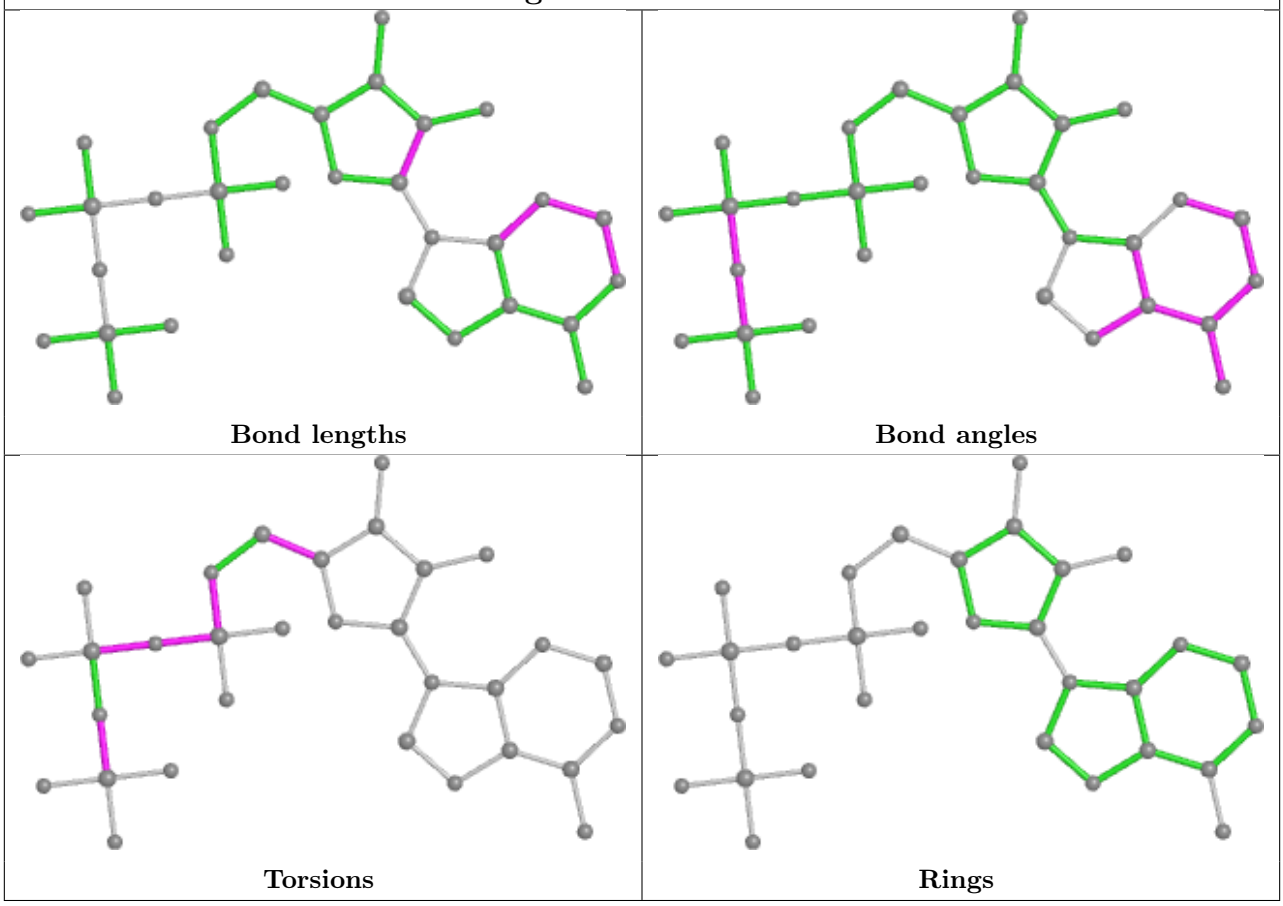

5.7 Other polymers (i)

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	505/519 (97%)	0.28	39 (7%)	13	12	20, 75, 128, 156	0
1	B	490/519 (94%)	0.14	23 (4%)	31	29	31, 78, 130, 168	0
1	E	491/519 (94%)	-0.16	16 (3%)	46	44	2, 47, 110, 149	0
1	F	505/519 (97%)	-0.01	27 (5%)	26	24	2, 57, 123, 139	0
2	C	488/519 (94%)	-0.03	18 (3%)	41	38	8, 62, 129, 167	0
2	D	485/519 (93%)	-0.26	14 (2%)	51	50	5, 42, 100, 152	0
All	All	2964/3114 (95%)	-0.00	137 (4%)	32	30	2, 62, 126, 168	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	517	PRO	8.2
1	A	518	GLU	7.4
1	E	505	LEU	6.9
1	A	513	GLN	6.5
1	A	517	PRO	6.5
1	F	516	GLY	6.4
1	F	518	GLU	6.3
2	D	157	SER	6.0
1	B	117	VAL	5.8
1	A	500	ASP	5.7
1	A	508	ILE	5.5
1	A	515	LYS	5.5
1	E	503	SER	5.3
1	B	504	GLU	5.3
1	B	500	ASP	5.1
1	B	118	VAL	5.1
1	A	514	GLU	5.1
1	E	500	ASP	5.0
1	A	516	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
2	C	120	GLY	4.8
1	F	509	VAL	4.7
2	C	119	GLY	4.7
1	F	503	SER	4.7
1	A	506	SER	4.7
2	C	501	GLU	4.6
1	B	503	SER	4.5
1	F	506	SER	4.4
2	D	117	VAL	4.3
1	A	253	ARG	4.3
1	F	504	GLU	4.3
2	C	500	ASP	4.3
1	A	428	SER	4.2
1	E	501	GLU	4.2
1	E	504	GLU	4.1
2	D	16	GLN	4.1
1	F	519	SER	4.0
1	A	507	ARG	4.0
1	B	498	THR	4.0
1	F	514	GLU	3.9
1	A	519	SER	3.9
1	F	500	ASP	3.9
1	B	121	PHE	3.9
1	A	498	THR	3.9
1	F	507	ARG	3.8
1	B	116	GLU	3.8
1	A	16	GLN	3.8
1	A	509	VAL	3.8
2	C	499	VAL	3.8
1	A	511	GLY	3.7
1	F	508	ILE	3.7
1	F	515	LYS	3.7
2	D	158	SER	3.6
1	A	501	GLU	3.5
1	A	503	SER	3.5
2	D	156	ALA	3.4
2	D	113	GLU	3.3
2	D	118	VAL	3.3
2	C	173	GLN	3.3
1	F	511	GLY	3.3
1	A	257	ARG	3.2
1	A	499	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	143	SER	3.2
1	F	154	TYR	3.2
1	F	513	GLN	3.1
1	F	501	GLU	3.1
2	D	15	HIS	3.1
2	D	471	MET	3.1
1	F	121	PHE	3.1
1	A	14	GLU	3.1
1	B	502	LYS	3.0
2	C	117	VAL	3.0
1	A	475	LYS	3.0
1	A	502	LYS	3.0
1	B	501	GLU	3.0
2	D	120	GLY	2.9
2	C	498	THR	2.9
1	A	512	VAL	2.9
1	E	117	VAL	2.9
2	C	17	ALA	2.9
1	B	157	SER	2.9
2	D	14	GLU	2.8
1	A	17	ALA	2.8
1	E	499	VAL	2.8
1	B	124	SER	2.8
1	A	510	ARG	2.8
1	A	255	THR	2.8
2	C	140	ARG	2.7
2	C	118	VAL	2.7
2	C	154	TYR	2.7
2	D	119	GLY	2.7
1	F	117	VAL	2.7
2	D	121	PHE	2.7
1	A	121	PHE	2.6
1	A	256	GLN	2.6
1	F	502	LYS	2.6
1	E	188	TYR	2.6
1	F	119	GLY	2.6
1	F	120	GLY	2.6
1	F	505	LEU	2.6
1	E	502	LYS	2.6
1	F	510	ARG	2.6
1	B	15	HIS	2.5
1	F	344	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	423	HIS	2.5
2	C	145	ASP	2.4
2	C	146	SER	2.4
1	E	121	PHE	2.3
2	D	160	VAL	2.3
1	B	175	GLY	2.3
1	E	118	VAL	2.3
1	B	158	SER	2.3
1	F	311	ARG	2.3
1	E	498	THR	2.3
2	C	152	GLN	2.3
1	A	117	VAL	2.3
1	B	120	GLY	2.2
1	A	505	LEU	2.2
1	A	504	GLU	2.2
1	B	16	GLN	2.2
1	F	496	ARG	2.2
1	E	116	GLU	2.2
1	B	155	ASP	2.2
1	A	113	GLU	2.2
1	B	281	ASP	2.2
1	A	341	GLN	2.2
1	E	484	ARG	2.2
1	A	254	LEU	2.1
2	C	258	SER	2.1
1	A	112	PRO	2.1
1	E	321	ARG	2.1
1	E	334	ASP	2.1
1	B	149	SER	2.1
1	B	88	ARG	2.1
1	B	154	TYR	2.1
1	B	123	LEU	2.1
1	A	15	HIS	2.0
1	A	188	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	F	426	11/12	0.72	0.35	67,68,79,81	0
1	TPO	E	426	11/12	0.79	0.34	75,89,101,102	0
1	TPO	B	426	11/12	0.83	0.27	79,85,91,92	0
1	TPO	A	426	11/12	0.84	0.28	74,77,78,78	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
4	MG	A	701	1/1	0.82	0.80	70,70,70,70	0
4	MG	F	702	1/1	0.88	0.33	62,62,62,62	0
3	ATP	A	903	31/31	0.89	0.24	57,64,69,70	0
3	ATP	B	903	31/31	0.89	0.23	65,69,75,76	0
4	MG	B	701	1/1	0.90	0.47	49,49,49,49	0
3	ATP	A	901	31/31	0.90	0.29	65,80,87,88	0
3	ATP	F	901	31/31	0.91	0.25	53,79,88,88	0
3	ATP	E	901	31/31	0.91	0.25	35,63,67,68	0
4	MG	F	802	1/1	0.92	0.36	21,21,21,21	0
3	ATP	B	901	31/31	0.93	0.20	42,47,53,54	0
3	ATP	C	903	31/31	0.93	0.20	36,41,67,68	0
3	ATP	D	903	31/31	0.93	0.20	15,19,42,44	0
4	MG	E	520	1/1	0.94	0.44	23,23,23,23	0
3	ATP	F	903	31/31	0.94	0.20	31,36,40,40	0
4	MG	C	701	1/1	0.94	0.58	69,69,69,69	0
4	MG	D	702	1/1	0.95	0.57	70,70,70,70	0
3	ATP	E	903	31/31	0.95	0.19	16,24,41,42	0
4	MG	E	702	1/1	0.95	0.33	70,70,70,70	0
3	ATP	C	901	31/31	0.95	0.20	24,28,38,40	0
3	ATP	D	901	31/31	0.95	0.23	38,43,54,55	0
4	MG	B	801	1/1	0.96	0.20	10,10,10,10	0
4	MG	D	801	1/1	0.96	0.38	72,72,72,72	0
4	MG	F	701	1/1	0.96	0.46	29,29,29,29	0
4	MG	A	520	1/1	0.96	0.45	58,58,58,58	0
4	MG	D	701	1/1	0.96	0.37	67,67,67,67	0

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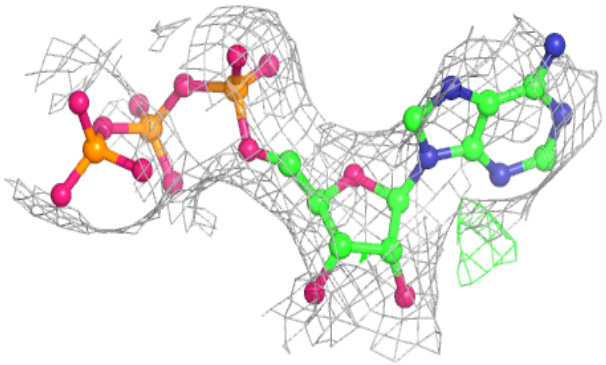
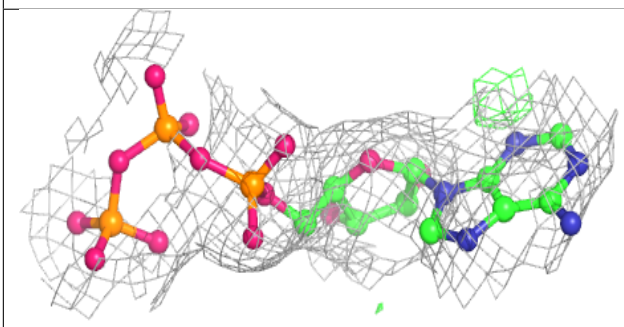
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	702	1/1	0.97	0.38	67,67,67,67	0
4	MG	B	802	1/1	0.97	0.24	61,61,61,61	0
4	MG	D	802	1/1	0.97	0.24	1,1,1,1	0
4	MG	A	702	1/1	0.97	0.28	76,76,76,76	0
4	MG	A	801	1/1	0.97	0.34	31,31,31,31	0
4	MG	A	802	1/1	0.98	0.48	77,77,77,77	0
4	MG	E	801	1/1	0.98	0.24	1,1,1,1	0
4	MG	C	801	1/1	0.98	0.30	6,6,6,6	0
4	MG	C	802	1/1	0.99	0.32	19,19,19,19	0

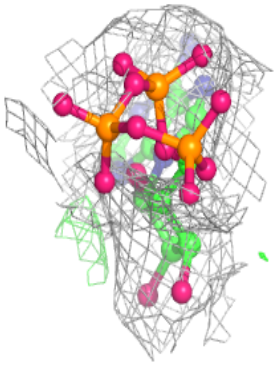
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP 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)

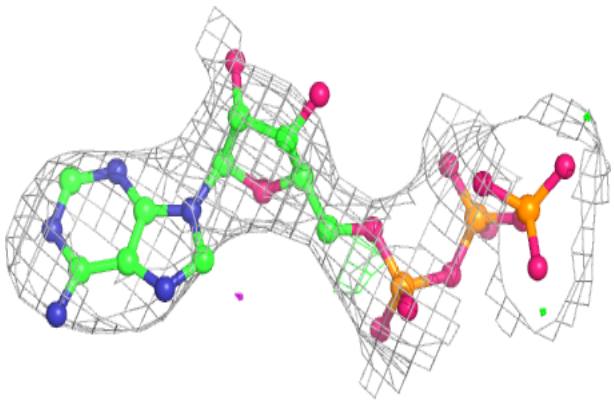


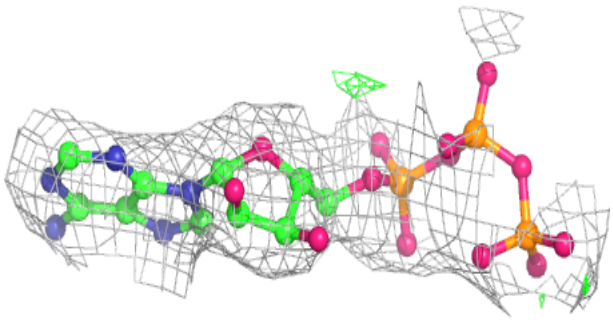


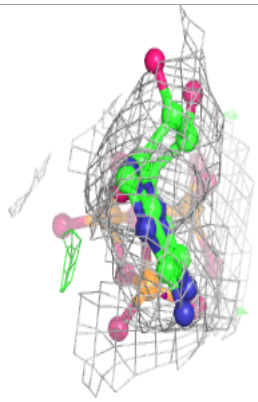


Electron density around ATP B 903:

$2mF_o$-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 A 901:

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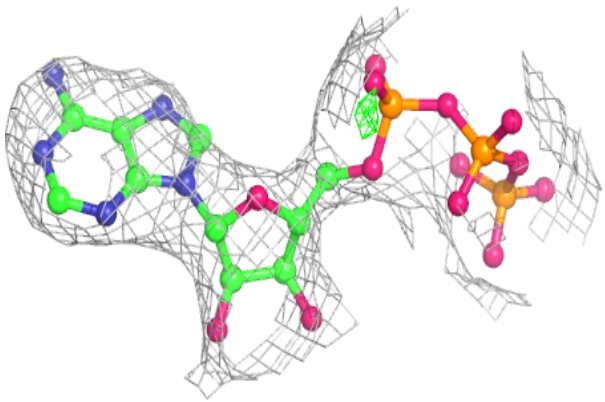
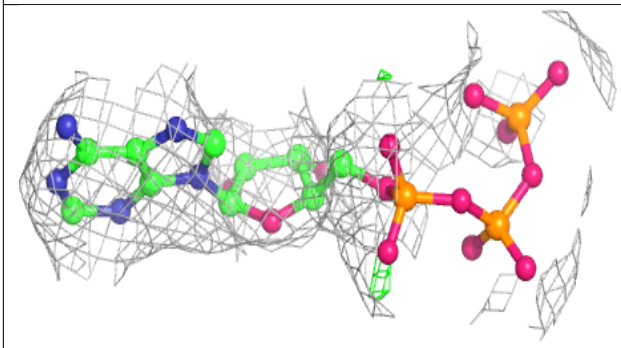
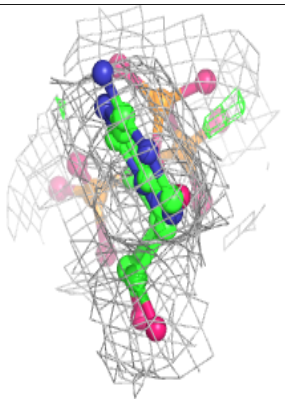
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

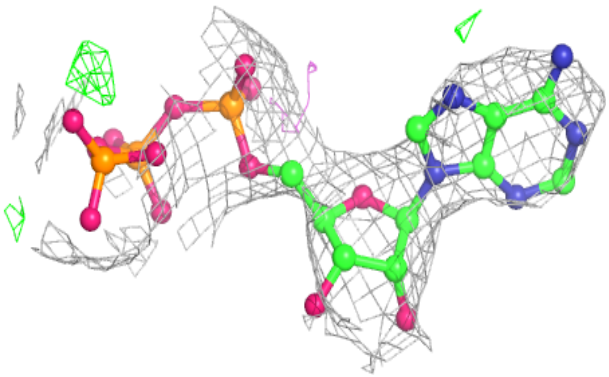


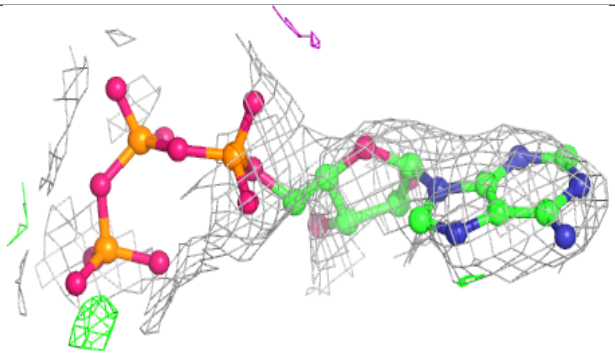




Electron density around ATP F 901:

$2mF_o$-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 E 901:

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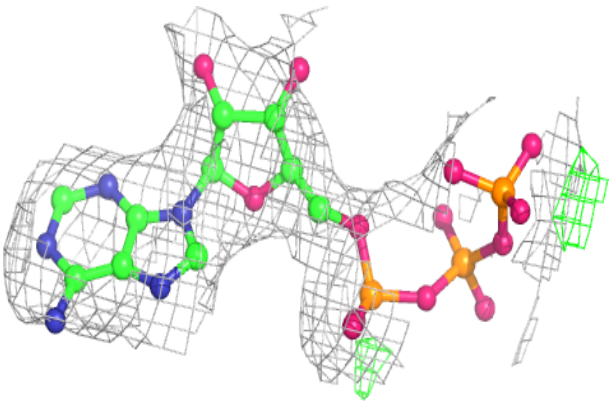
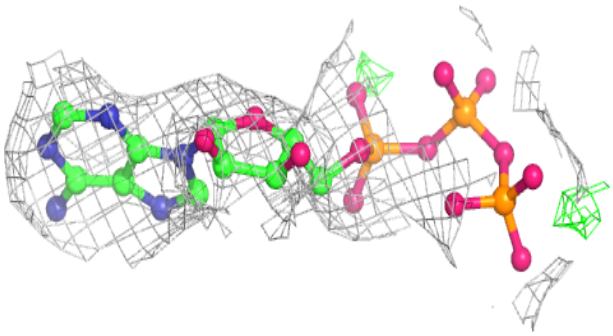
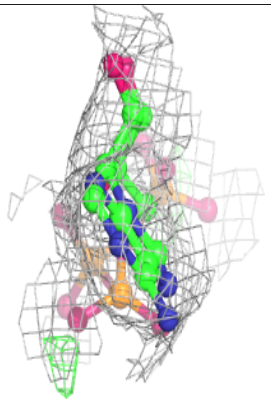
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

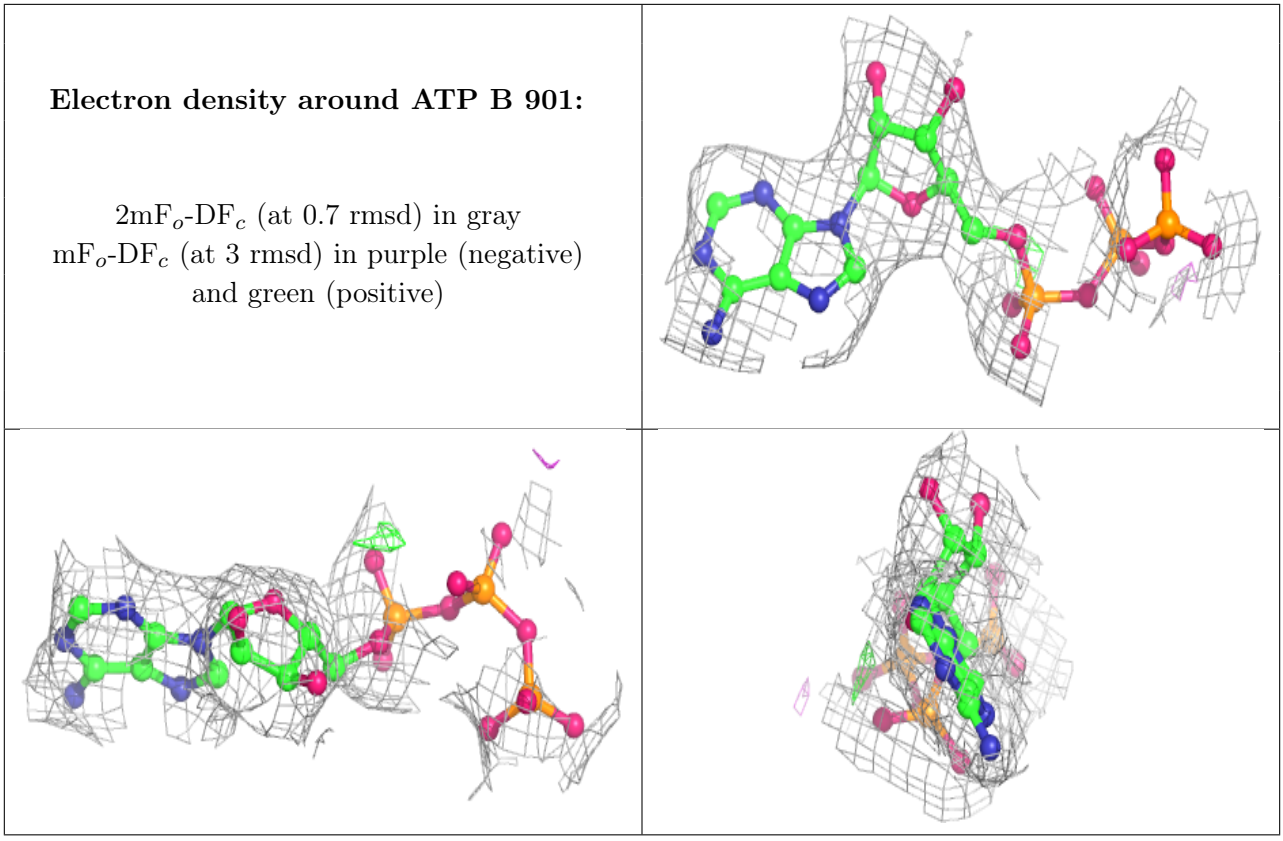






Electron density around ATP B 901:

$2mF_o$-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 903:

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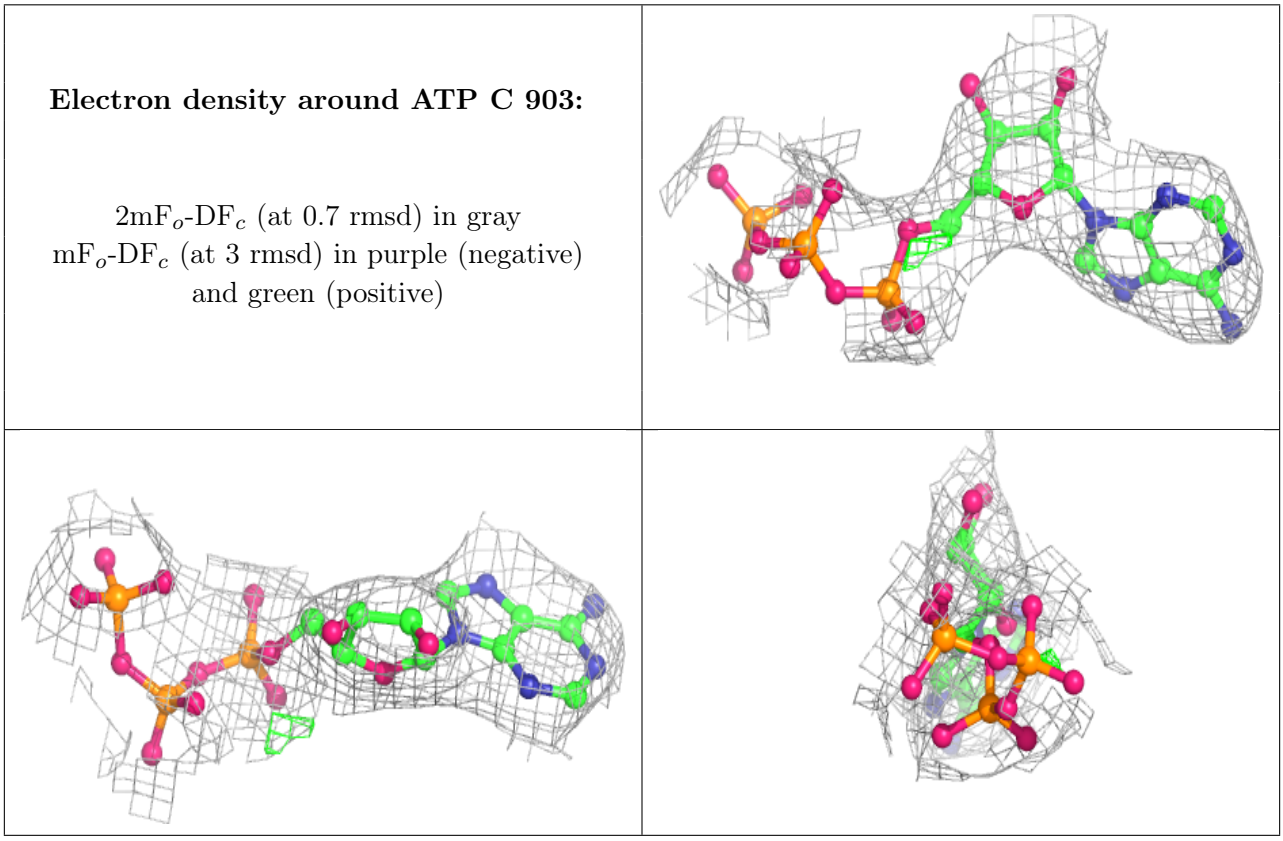
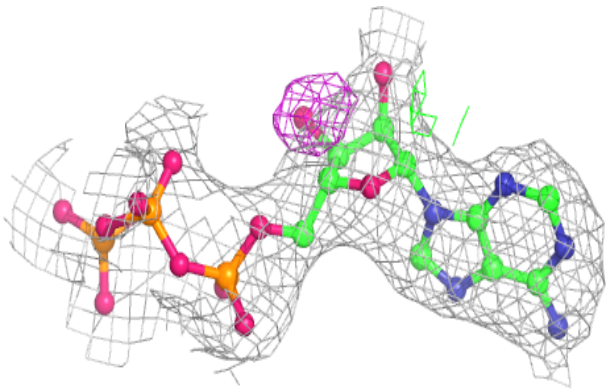
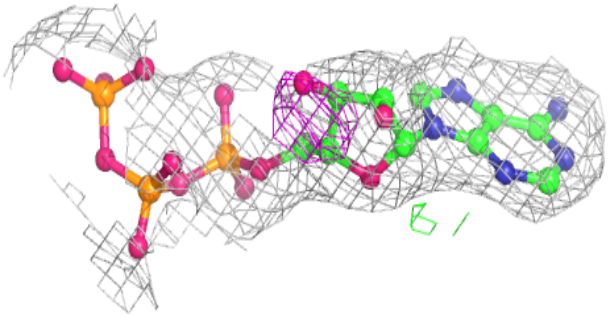
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

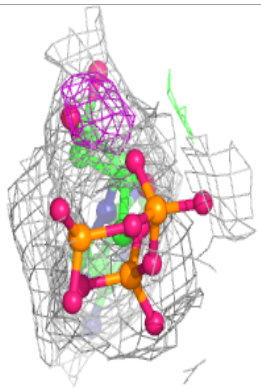


Electron density around ATP D 903:

$2mF_o$-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 F 903:

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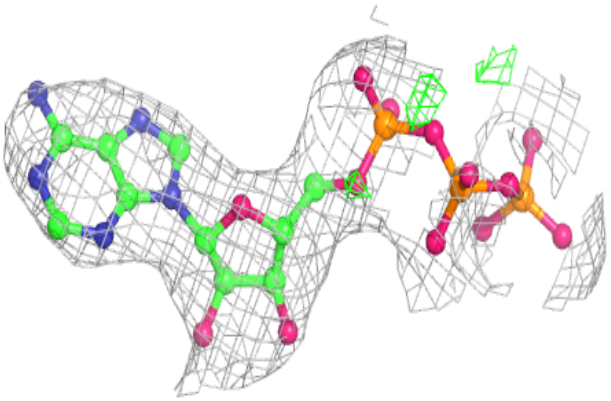
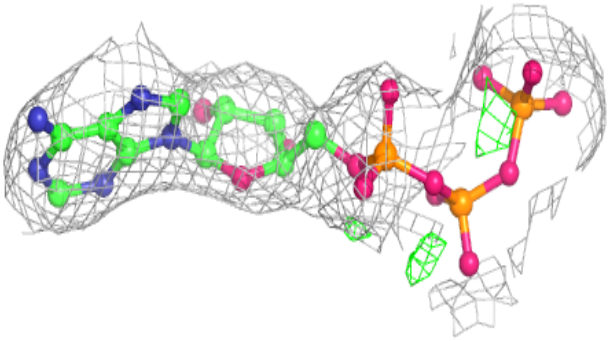
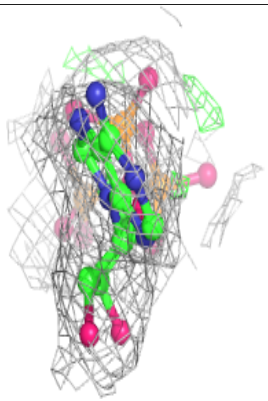
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around ATP E 903:

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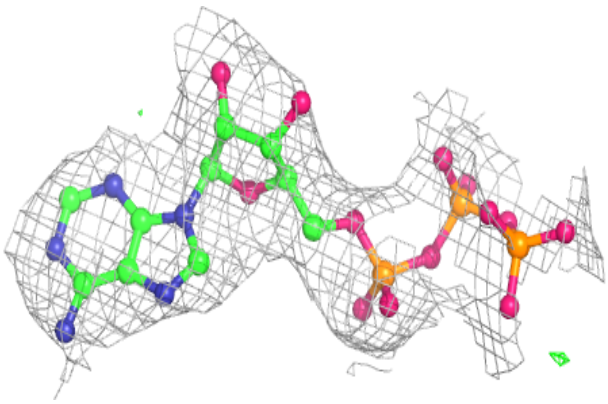
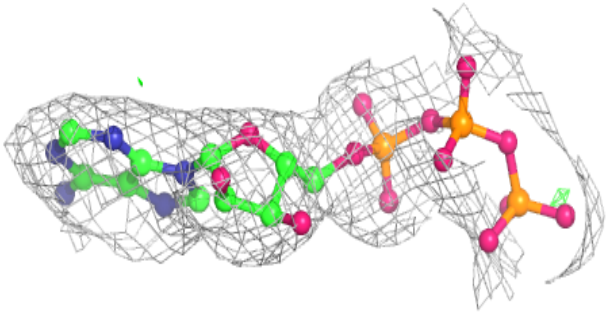
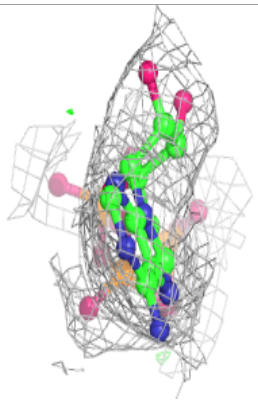
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around ATP C 901:

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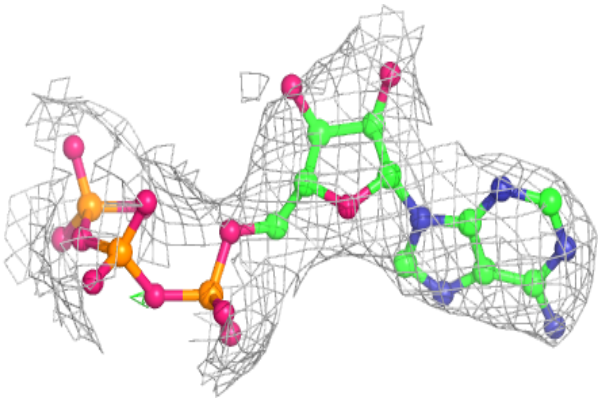
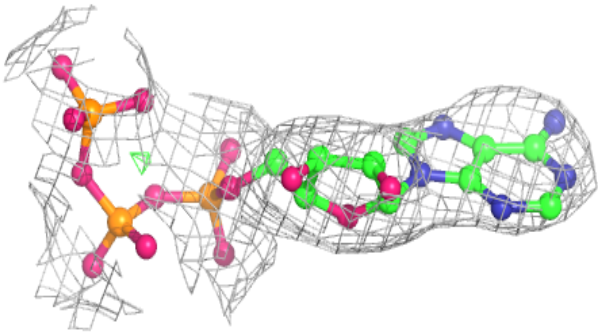
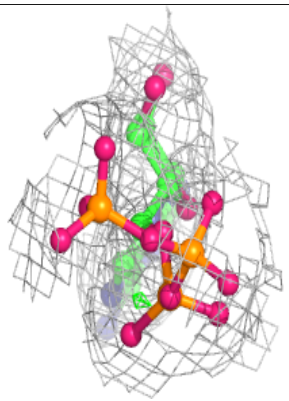
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

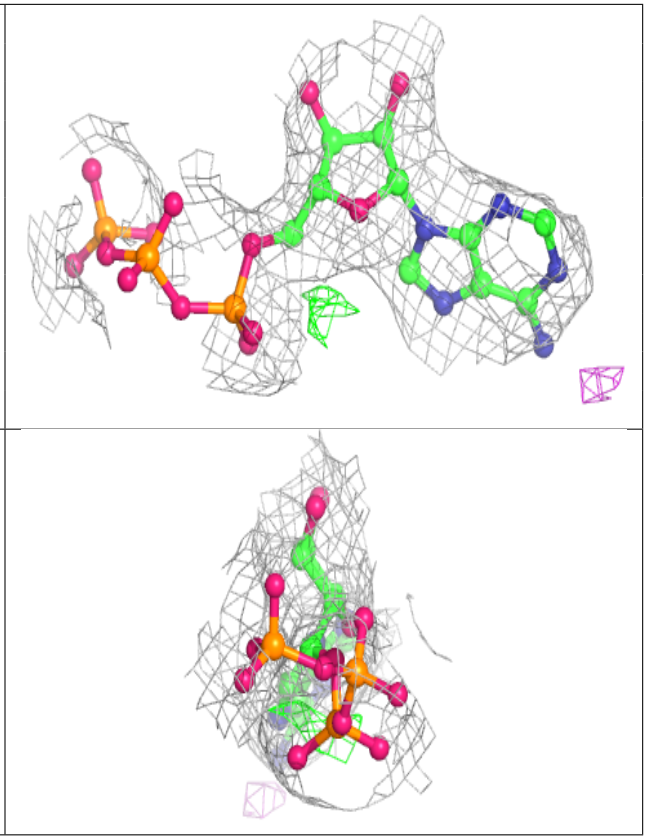






Electron density around ATP D 901:

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



6.5 Other polymers (i)

There are no such residues in this entry.