



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:08 PM UTC

PDB ID : 7DXQ / pdb_00007dxq
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC
Authors : Furuike, Y.; Akiyama, S.
Deposited on : 2021-01-20
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

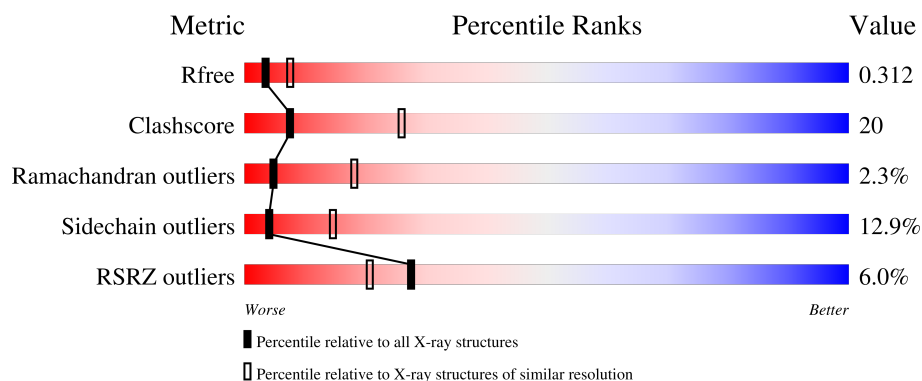
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	519	9% 57% 27% 5% 11%
1	B	519	3% 52% 32% 6% 9%
1	C	519	4% 60% 24% 6% 10%
1	D	519	4% 54% 31% • 11%
1	E	519	6% 57% 27% 5% 10%

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Mol	Chain	Length	Quality of chain
1	F	519	5% 56% 30% • 10%

2 Entry composition [i](#)

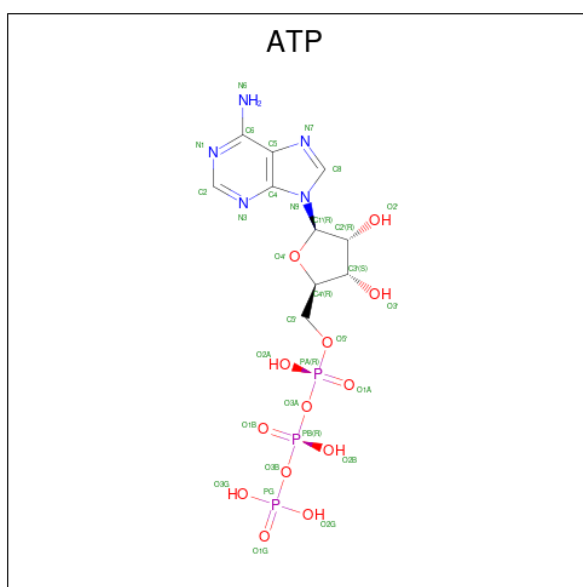
There are 4 unique types of molecules in this entry. The entry contains 21020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	P	S	0	0	0
			3283	2076	564	629	2	12			
1	B	470	Total	C	N	O	P	S	0	1	0
			3560	2256	616	673	2	13			
1	E	465	Total	C	N	O	P	S	0	0	0
			3393	2150	587	642	2	12			
1	F	467	Total	C	N	O	P	S	0	1	0
			3403	2150	587	652	2	12			
1	C	466	Total	C	N	O	P	S	0	0	0
			3474	2202	600	657	2	13			
1	D	462	Total	C	N	O	P	S	0	2	0
			3425	2177	589	645	2	12			

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



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

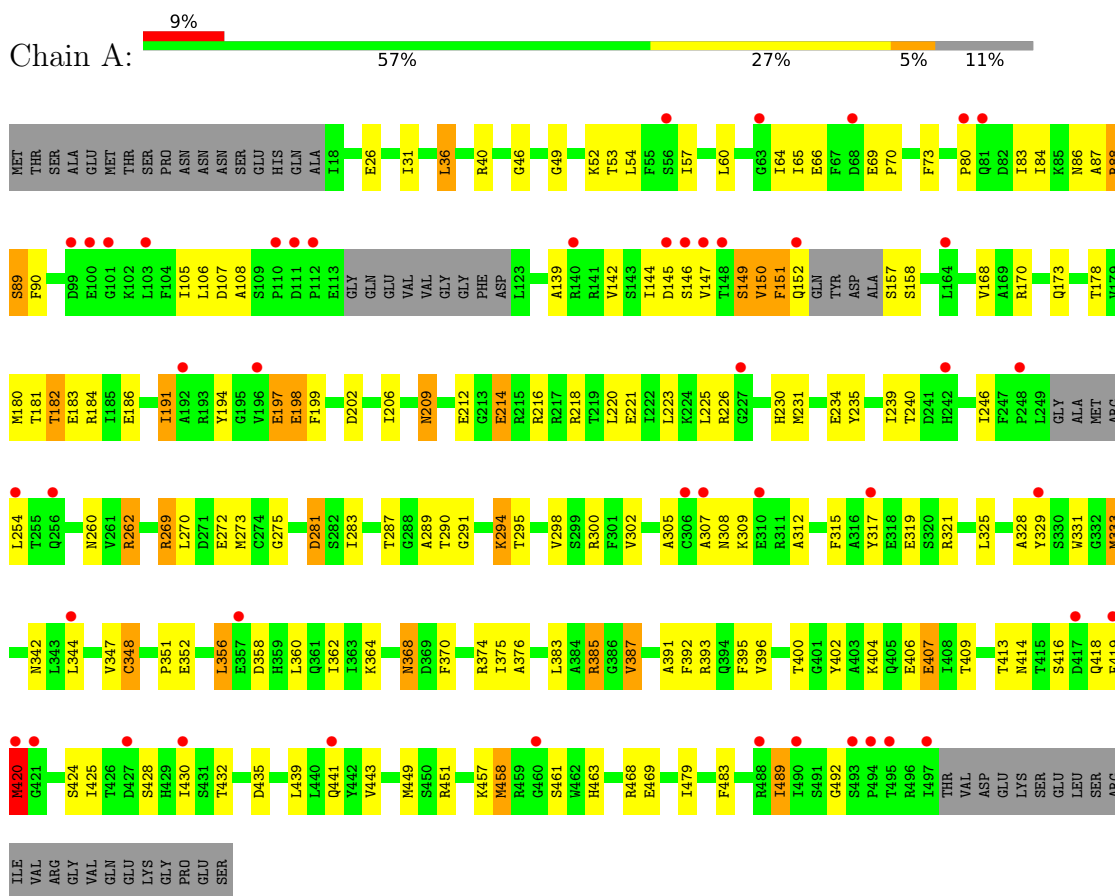
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	31	Total 31	O 31	0	0
4	E	11	Total 11	O 11	0	0
4	F	7	Total 7	O 7	0	0
4	C	15	Total 15	O 15	0	0
4	D	16	Total 16	O 16	0	0

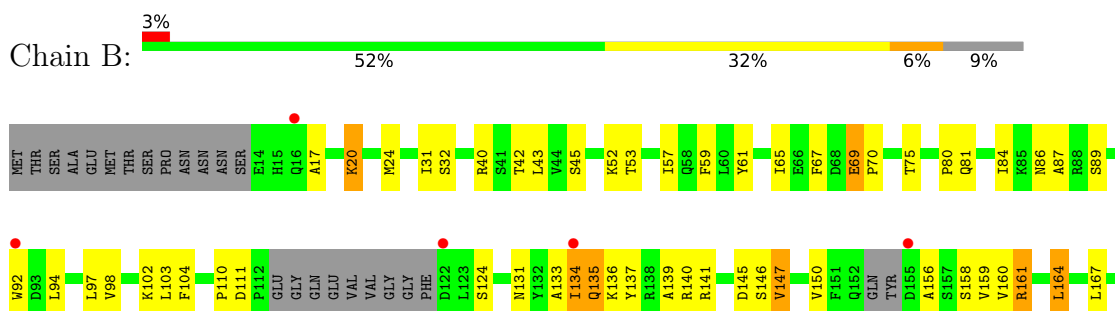
3 Residue-property plots

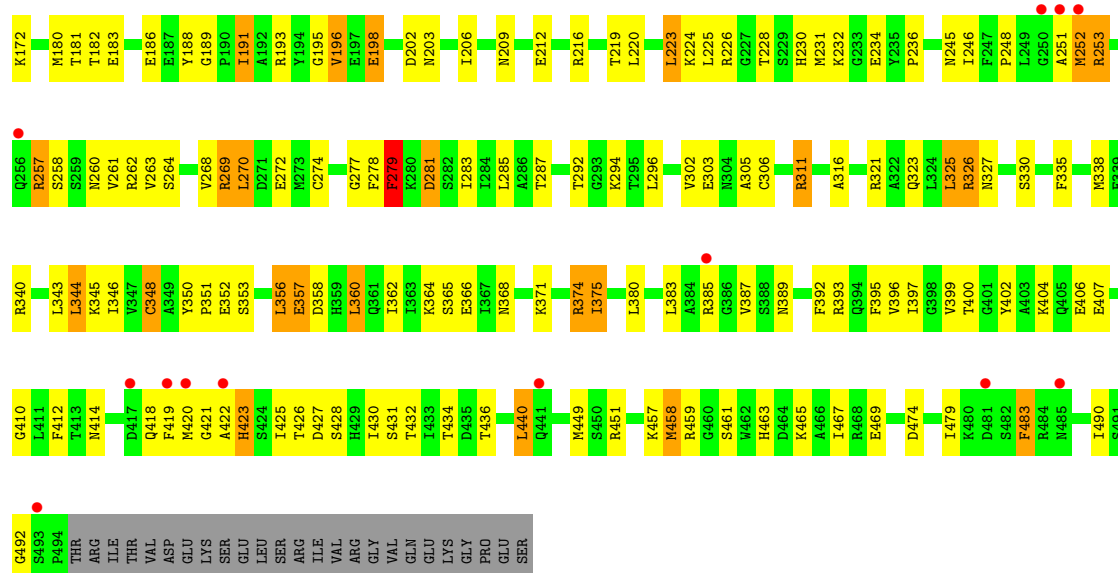
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

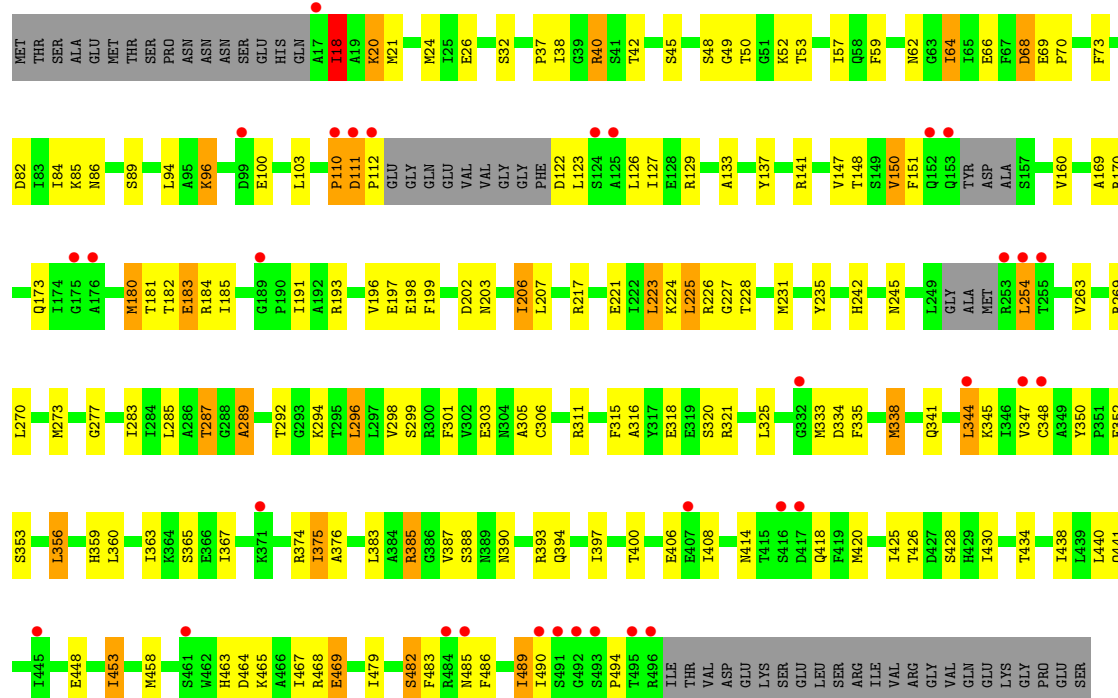


• Molecule 1: Circadian clock protein kinase KaiC



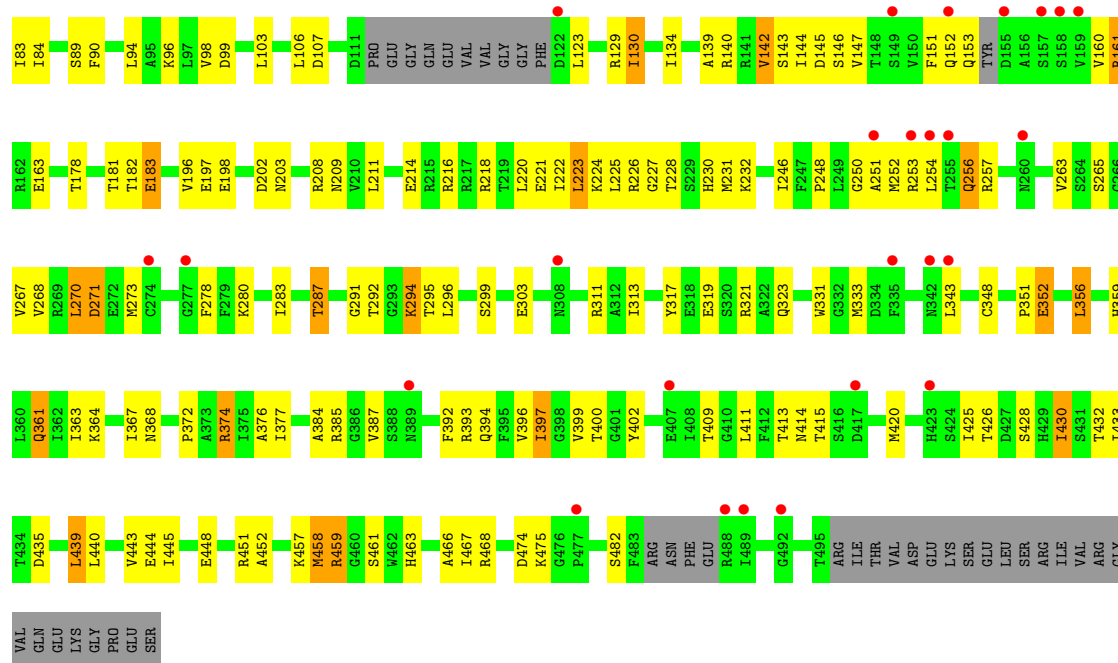


• Molecule 1: Circadian clock protein kinase KaiC

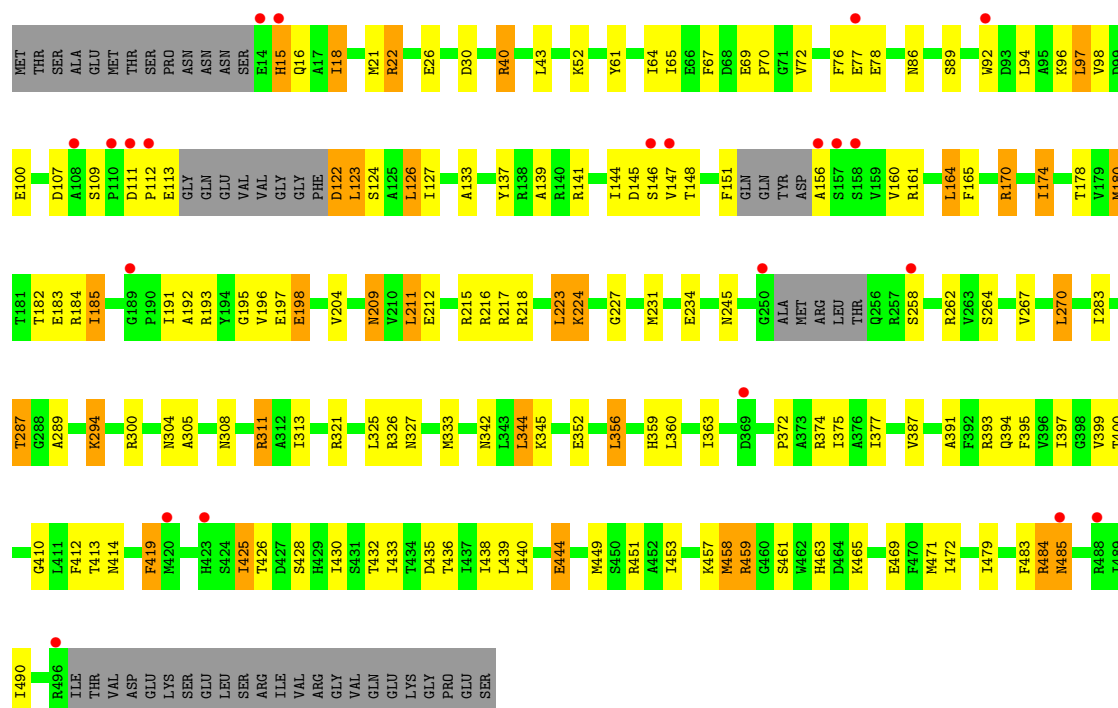


• Molecule 1: Circadian clock protein kinase KaiC



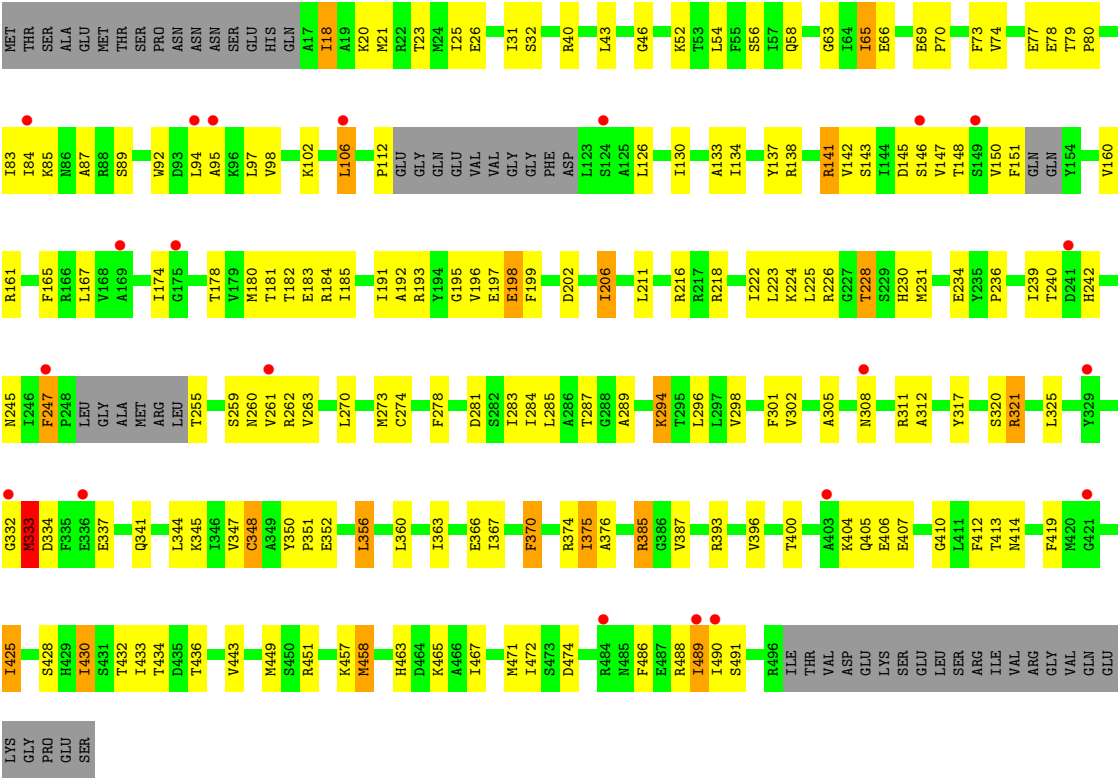


• Molecule 1: Circadian clock protein kinase KaiC



• Molecule 1: Circadian clock protein kinase KaiC





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.41Å 159.87Å 207.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.80 29.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.4 (29.96-2.80) 87.4 (29.96-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.250 , 0.318 0.248 , 0.312	Depositor DCC
R_{free} test set	3284 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	21020	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	0/3315	1.44	0/4510
1	B	0.98	0/3600	1.40	1/4870 (0.0%)
1	C	0.99	0/3508	1.40	0/4750
1	D	1.00	0/3467	1.43	0/4702
1	E	1.00	0/3426	1.43	1/4647 (0.0%)
1	F	1.01	0/3439	1.44	0/4669
All	All	1.00	0/20755	1.42	2/28148 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	GLY	CA-C-O	-5.43	118.23	122.52
1	E	277	GLY	CA-C-O	-5.12	118.18	122.33

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	3283	0	2951	143	0
1	B	3560	0	3445	166	0
1	C	3474	0	3343	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3425	0	3262	147	0
1	E	3393	0	3166	148	0
1	F	3403	0	3162	155	0
2	A	62	0	24	7	0
2	B	62	0	24	5	0
2	C	62	0	24	6	0
2	D	62	0	24	1	0
2	E	62	0	24	8	0
2	F	62	0	24	9	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	18	0	0	0	0
4	B	31	0	0	0	0
4	C	15	0	0	0	0
4	D	16	0	0	0	0
4	E	11	0	0	0	0
4	F	7	0	0	0	0
All	All	21020	0	19473	821	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 20.

All (821) 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:F:292:THR:CG2	1:F:440:LEU:HB3	1.86	1.04
1:B:172:LYS:NZ	1:B:202:ASP:OD2	1.92	1.01
1:C:264:SER:O	1:C:374:ARG:NH1	1.95	1.00
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.44	0.99
1:A:157:SER:CB	1:A:194:TYR:HB3	1.92	0.99
1:E:464:ASP:OD2	1:E:468:ARG:NE	1.96	0.98
1:D:301:PHE:O	1:D:374:ARG:NH2	1.97	0.97
1:F:267:VAL:HG11	1:F:270:LEU:CB	1.95	0.96
1:C:52:LYS:NZ	2:C:601:ATP:O3G	2.00	0.94
1:F:292:THR:HG21	1:F:440:LEU:HB3	1.46	0.93
1:C:147:VAL:HG11	1:C:180:MET:CE	1.97	0.93
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:361:GLN:HE21	1:F:361:GLN:HA	1.35	0.92
1:A:86:ASN:OD1	1:B:40:ARG:NH2	2.03	0.90
1:D:80:PRO:O	1:D:84:ILE:HG22	1.71	0.90
1:A:305:ALA:HB2	1:A:374:ARG:HD3	1.55	0.89
1:E:273:MET:CE	1:E:479:ILE:HD13	2.04	0.87
1:F:267:VAL:HG11	1:F:270:LEU:HB2	1.53	0.87
1:E:68:ASP:O	1:E:70:PRO:HD3	1.74	0.87
1:C:147:VAL:HG11	1:C:180:MET:HE2	1.57	0.86
1:B:305:ALA:HB2	1:B:374:ARG:HD3	1.58	0.85
1:D:147:VAL:O	1:D:150:VAL:HG12	1.76	0.84
1:C:438:ILE:HG23	1:C:453:ILE:HD11	1.58	0.84
1:F:89:SER:OG	2:F:601:ATP:N6	2.09	0.84
1:A:294:LYS:HB3	1:A:413:THR:HG23	1.59	0.84
1:E:353:SER:HA	1:F:250:GLY:HA2	1.60	0.83
1:A:88:ARG:O	1:A:90:PHE:N	2.12	0.82
1:E:305:ALA:HB2	1:E:374:ARG:HD3	1.60	0.82
1:D:20:LYS:HE2	1:D:228:THR:HG21	1.62	0.81
1:E:490:ILE:HD11	1:D:449:MET:CE	2.10	0.81
1:D:147:VAL:HG11	1:D:180:MET:HE2	1.62	0.81
1:D:20:LYS:NZ	1:D:32:SER:O	2.12	0.81
1:C:61:TYR:CE1	1:C:92:TRP:HB2	2.15	0.81
1:D:301:PHE:C	1:D:374:ARG:HH21	1.89	0.81
1:B:161:ARG:HG3	1:B:196:VAL:CG1	2.10	0.80
1:C:305:ALA:HB2	1:C:374:ARG:HD3	1.61	0.80
1:B:156:ALA:HB3	1:B:159:VAL:HG23	1.64	0.79
1:B:325:LEU:HD22	1:B:335:PHE:HB2	1.65	0.79
1:E:353:SER:HA	1:F:250:GLY:CA	2.12	0.79
1:D:294:LYS:HG2	1:D:413:THR:HG23	1.65	0.79
1:B:418:GLN:HE21	1:B:421:GLY:HA3	1.48	0.78
2:B:602:ATP:O3G	1:C:457:LYS:NZ	2.15	0.78
1:E:283:ILE:HG13	1:E:400:THR:HG23	1.64	0.78
1:F:161:ARG:HG3	1:F:196:VAL:HG13	1.66	0.78
1:E:110:PRO:HB2	1:E:111:ASP:HA	1.65	0.78
1:B:147:VAL:HG21	1:B:180:MET:HE2	1.65	0.78
1:A:463:HIS:NE2	2:F:602:ATP:O2'	2.18	0.77
1:F:267:VAL:HG11	1:F:270:LEU:HB3	1.67	0.77
1:D:147:VAL:CG1	1:D:180:MET:HE2	2.13	0.77
1:E:273:MET:HE1	1:E:479:ILE:HD13	1.65	0.77
1:C:89:SER:OG	2:C:601:ATP:N6	2.18	0.77
1:A:157:SER:CB	1:A:194:TYR:CB	2.63	0.77
1:E:490:ILE:HD11	1:D:449:MET:HE2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:PHE:CE2	1:F:160:VAL:HG13	2.19	0.76
1:E:206:ILE:HD11	1:E:223:LEU:HG	1.67	0.76
1:B:193:ARG:NH1	1:C:195:GLY:O	2.19	0.76
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.19	0.76
1:B:43:LEU:HD11	1:B:182:THR:OG1	1.86	0.76
1:F:267:VAL:CG1	1:F:270:LEU:HB3	2.16	0.75
1:B:59:PHE:O	1:B:141:ARG:NH1	2.18	0.75
2:A:602:ATP:O2'	1:B:463:HIS:NE2	2.19	0.75
1:F:430:ILE:HD12	1:F:433:ILE:HD12	1.68	0.75
1:C:283:ILE:HG13	1:C:400:THR:HG23	1.67	0.75
1:A:283:ILE:HG13	1:A:400:THR:CG2	2.16	0.75
1:C:484:ARG:N	1:C:485:ASN:CB	2.50	0.75
1:E:50:THR:CG2	1:E:207:LEU:HB3	2.17	0.75
1:C:438:ILE:CG2	1:C:453:ILE:HD11	2.15	0.75
1:F:299:SER:C	1:F:333:MET:HE1	2.12	0.75
1:C:217:ARG:NH2	1:C:394:GLN:OE1	2.19	0.74
1:B:89:SER:HB3	1:C:227:GLY:O	1.87	0.74
1:E:111:ASP:CB	1:E:112:PRO:CD	2.64	0.74
1:C:147:VAL:HG11	1:C:180:MET:HE3	1.70	0.74
2:A:602:ATP:O2'	1:B:463:HIS:CD2	2.41	0.74
1:D:147:VAL:HG11	1:D:180:MET:CE	2.18	0.74
1:F:267:VAL:CG1	1:F:270:LEU:CB	2.65	0.73
1:B:252:MET:HA	1:B:253:ARG:CB	2.17	0.73
1:B:251:ALA:HA	1:B:252:MET:CB	2.18	0.73
1:F:374:ARG:HB3	1:F:409:THR:CG2	2.19	0.73
1:D:356:LEU:CD2	1:D:387:VAL:HG11	2.18	0.73
1:E:110:PRO:HB2	1:E:111:ASP:CA	2.19	0.73
1:F:70:PRO:HB2	1:F:139:ALA:HA	1.72	0.72
1:D:287:THR:HG22	1:D:414:ASN:HB3	1.71	0.72
1:A:393:ARG:NE	1:F:385[B]:ARG:HD2	2.04	0.72
1:C:161:ARG:HG3	1:C:196:VAL:HG13	1.71	0.72
1:D:73:PHE:CE2	1:D:83:ILE:HD13	2.25	0.72
1:C:61:TYR:CZ	1:C:92:TRP:CB	2.74	0.71
1:A:199:PHE:CE1	1:F:183:GLU:HB3	2.26	0.71
1:F:23:THR:HG22	1:F:25:ILE:HG13	1.72	0.71
1:D:58:GLN:HG3	1:D:92:TRP:CH2	2.26	0.70
1:D:31:ILE:HA	1:D:231:MET:HG3	1.72	0.70
1:F:356:LEU:HD21	1:F:387:VAL:HG11	1.74	0.70
1:C:313:ILE:HB	1:C:375:ILE:HD12	1.74	0.69
1:A:150:VAL:HG13	1:A:151:PHE:H	1.57	0.69
1:D:84:ILE:HD11	1:D:95:ALA:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ILE:HG13	1:D:400:THR:HG23	1.74	0.69
1:E:50:THR:CG2	1:E:207:LEU:CB	2.71	0.69
1:F:151:PHE:CD2	1:F:160:VAL:HG13	2.27	0.69
1:F:292:THR:HG22	1:F:440:LEU:HB3	1.74	0.69
1:C:61:TYR:CZ	1:C:92:TRP:HB3	2.28	0.69
1:A:287:THR:HG21	1:A:425:ILE:O	1.93	0.69
1:A:419:PHE:HD1	1:A:420:MET:HE2	1.57	0.69
1:E:50:THR:HG22	1:E:207:LEU:HB3	1.74	0.69
1:B:400:THR:HG22	1:B:412:PHE:HE1	1.56	0.69
1:B:236:PRO:HB2	1:B:357:GLU:CG	2.23	0.68
1:F:374:ARG:HB3	1:F:409:THR:HG23	1.74	0.68
1:D:236:PRO:HG2	1:D:247[B]:PHE:HD2	1.59	0.68
1:E:438:ILE:CG2	1:E:453:ILE:HD11	2.22	0.68
2:E:602:ATP:O2G	1:F:457:LYS:NZ	2.26	0.68
1:D:430:ILE:HG13	1:D:433:ILE:HD12	1.74	0.68
1:B:202:ASP:HA	1:B:226:ARG:HE	1.59	0.68
1:E:273:MET:CE	1:E:479:ILE:HG21	2.24	0.68
1:C:444:GLU:OE2	1:D:489:ILE:HG12	1.94	0.68
1:F:294:LYS:HB3	1:F:413:THR:HG23	1.76	0.68
1:D:31:ILE:HG23	1:D:231:MET:HB2	1.76	0.68
1:B:418:GLN:NE2	1:B:421:GLY:HA3	2.08	0.68
1:A:393:ARG:HD3	1:F:385[B]:ARG:NE	2.09	0.68
1:D:134:ILE:HD12	1:D:174:ILE:HG21	1.76	0.68
1:B:260:ASN:HA	1:B:279:PHE:HE2	1.59	0.67
1:B:263:VAL:CG1	1:B:374:ARG:NH2	2.57	0.67
1:F:209:ASN:O	1:F:216:ARG:NH1	2.26	0.67
1:F:283:ILE:HG13	1:F:400:THR:HG23	1.75	0.67
1:E:86:ASN:OD1	1:F:40:ARG:NH1	2.27	0.67
1:C:311:ARG:HB3	1:C:372:PRO:HA	1.77	0.67
1:C:313:ILE:HB	1:C:375:ILE:CD1	2.23	0.67
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.59	0.67
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.25	0.67
1:A:295:THR:OG1	2:A:602:ATP:O2B	2.13	0.66
1:B:61:TYR:CE1	1:B:92:TRP:HB2	2.30	0.66
1:B:325:LEU:HD22	1:B:335:PHE:CB	2.24	0.66
1:B:385[B]:ARG:HH11	1:B:385[B]:ARG:CG	2.06	0.66
1:E:151:PHE:CE1	1:E:160:VAL:HA	2.30	0.66
1:C:86:ASN:OD1	1:D:40:ARG:NH1	2.26	0.66
1:C:209:ASN:O	1:C:216:ARG:NH1	2.26	0.66
1:C:321:ARG:O	1:C:325:LEU:HG	1.94	0.66
1:A:158:SER:CA	1:F:152:GLN:O	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ARG:NH1	1:C:461:SER:OG	2.28	0.66
1:F:52:LYS:HB3	1:F:181:THR:HG23	1.76	0.66
1:C:43:LEU:HD11	1:C:182:THR:OG1	1.96	0.66
1:E:96:LYS:O	1:E:100:GLU:HG3	1.96	0.65
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.78	0.65
1:C:300:ARG:HD3	1:C:333:MET:HE3	1.77	0.65
1:E:469:GLU:HB3	1:E:483:PHE:CZ	2.31	0.65
1:A:214:GLU:HG3	1:B:234:GLU:HB2	1.78	0.65
1:A:158:SER:CB	1:F:152:GLN:O	2.45	0.65
1:E:254:LEU:HD22	1:D:350:TYR:CE1	2.32	0.65
1:C:161:ARG:HG3	1:C:196:VAL:CG1	2.27	0.65
1:D:167:LEU:HD21	1:D:180:MET:HE1	1.78	0.65
1:E:52:LYS:HB3	1:E:181:THR:HG23	1.78	0.65
1:A:158:SER:HA	1:F:152:GLN:O	1.96	0.65
1:E:292:THR:CG2	1:E:440:LEU:HB3	2.27	0.65
1:D:356:LEU:HD21	1:D:387:VAL:HG11	1.78	0.65
1:A:52:LYS:HB3	1:A:181:THR:HG23	1.79	0.64
2:E:601:ATP:O2G	1:F:226:ARG:NH1	2.31	0.64
1:C:300:ARG:HD3	1:C:333:MET:CE	2.27	0.64
1:C:305:ALA:HB2	1:C:374:ARG:CD	2.27	0.64
1:A:152:GLN:HA	1:B:158:SER:HB2	1.79	0.64
1:A:328:ALA:O	1:A:333:MET:HG2	1.97	0.64
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.63	0.64
1:F:294:LYS:HB3	1:F:413:THR:CG2	2.27	0.64
1:E:393:ARG:O	1:E:397:ILE:HG12	1.98	0.64
1:B:186:GLU:HG3	1:B:189:GLY:N	2.13	0.64
1:D:225:LEU:HB2	1:D:230:HIS:CD2	2.33	0.63
1:E:254:LEU:HD12	1:D:320:SER:HA	1.81	0.63
1:F:46:GLY:N	1:F:52:LYS:HD3	2.14	0.63
1:B:80:PRO:O	1:B:84:ILE:HG13	1.98	0.63
1:C:419:PHE:CE2	1:D:425:ILE:CD1	2.82	0.63
1:C:61:TYR:CZ	1:C:92:TRP:HB2	2.33	0.63
1:B:161:ARG:HG3	1:B:196:VAL:HG11	1.78	0.63
1:D:126:LEU:O	1:D:130:ILE:HG13	1.98	0.63
1:A:147:VAL:HG11	1:A:180:MET:CE	2.29	0.63
1:C:287:THR:HG23	1:C:414:ASN:HD22	1.64	0.62
1:D:298:VAL:O	1:D:302:VAL:HG23	1.98	0.62
1:D:363:ILE:O	1:D:367:ILE:HG13	1.99	0.62
1:F:263:VAL:HG12	1:F:374:ARG:NH2	2.15	0.62
1:A:420:MET:HG3	1:A:492:GLY:HA3	1.81	0.62
1:B:161:ARG:HG3	1:B:196:VAL:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.81	0.62
1:E:344:LEU:HD22	1:E:345:LYS:N	2.15	0.62
2:A:602:ATP:O1G	1:B:459:ARG:NH1	2.33	0.61
1:A:150:VAL:O	1:A:152:GLN:N	2.32	0.61
1:E:320:SER:CB	1:F:256:GLN:HB2	2.30	0.61
1:D:305:ALA:CB	1:D:312:ALA:HB2	2.30	0.61
1:C:191:ILE:CG2	1:C:198:GLU:HG2	2.31	0.61
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.82	0.61
1:A:305:ALA:HB2	1:A:374:ARG:CD	2.28	0.61
1:D:148:THR:HG21	1:D:182:THR:HG23	1.83	0.61
1:F:468:ARG:HA	1:F:482:SER:HA	1.81	0.61
1:E:111:ASP:CB	1:E:112:PRO:HD2	2.31	0.61
1:F:267:VAL:CG1	1:F:270:LEU:HB2	2.27	0.61
1:F:425:ILE:CD1	1:F:439:LEU:CD1	2.79	0.61
1:C:438:ILE:CG2	1:C:453:ILE:CD1	2.79	0.60
1:F:64:ILE:CD1	1:F:103:LEU:HB2	2.30	0.60
1:C:300:ARG:CD	1:C:333:MET:CE	2.79	0.60
1:A:31:ILE:HA	1:A:231:MET:HG3	1.83	0.60
1:A:457:LYS:NZ	2:F:602:ATP:O3G	2.33	0.60
1:A:269:ARG:HG3	1:A:269:ARG:HH11	1.67	0.60
1:A:144:ILE:HD13	1:A:178:THR:CG2	2.32	0.60
1:C:111:ASP:O	1:C:113:GLU:N	2.35	0.60
1:C:211:LEU:O	1:C:215:ARG:O	2.20	0.60
1:E:273:MET:HE1	1:E:479:ILE:HG21	1.83	0.60
1:F:292:THR:HG21	1:F:440:LEU:CB	2.25	0.60
1:C:123:LEU:O	1:C:127:ILE:HG13	2.01	0.60
1:F:352:GLU:OE1	1:F:385[B]:ARG:NH1	2.34	0.59
1:F:356:LEU:CD2	1:F:387:VAL:HG11	2.31	0.59
1:E:123:LEU:O	1:E:127:ILE:N	2.30	0.59
1:E:320:SER:HB2	1:F:256:GLN:HB2	1.85	0.59
1:A:147:VAL:O	1:A:150:VAL:CG1	2.50	0.59
1:E:20:LYS:NZ	1:E:32:SER:O	2.33	0.59
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.84	0.59
1:F:161:ARG:HG3	1:F:196:VAL:CG1	2.32	0.59
1:F:231:MET:HE2	1:F:251:ALA:HB3	1.84	0.59
1:D:63:GLY:HA3	1:D:141:ARG:HD2	1.85	0.59
1:B:209:ASN:O	1:B:216:ARG:NH1	2.33	0.59
1:C:89:SER:HG	2:C:601:ATP:HN61	1.51	0.59
1:E:18:ILE:O	1:E:18:ILE:HG13	2.02	0.59
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.84	0.58
1:B:167:LEU:HD23	1:B:180:MET:HE1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.67	0.58
1:B:43:LEU:CD1	1:B:182:THR:OG1	2.51	0.58
1:F:361:GLN:HA	1:F:361:GLN:NE2	2.12	0.58
1:C:287:THR:HG21	1:C:425:ILE:O	2.02	0.58
1:A:262:ARG:NH2	1:A:275:GLY:O	2.36	0.58
1:B:385[B]:ARG:HH11	1:B:385[B]:ARG:HG2	1.67	0.58
1:B:469:GLU:HB2	1:B:483:PHE:CZ	2.38	0.58
1:C:122:ASP:O	1:C:124:SER:N	2.36	0.58
1:C:344:LEU:HD22	1:C:345:LYS:N	2.18	0.58
1:A:209:ASN:O	1:A:216:ARG:NH1	2.37	0.58
1:E:263:VAL:CG1	1:E:374:ARG:HH22	2.17	0.58
2:E:601:ATP:O1G	1:F:224:LYS:NZ	2.35	0.58
1:F:393:ARG:NH1	1:F:428:SER:O	2.37	0.58
1:D:486:PHE:HB3	1:D:489:ILE:HD12	1.86	0.58
1:A:420:MET:HE3	1:B:490:ILE:HG21	1.84	0.58
1:E:21:MET:HB2	1:E:38:ILE:HD13	1.86	0.58
1:E:448:GLU:HA	1:F:466:ALA:HA	1.85	0.58
1:C:267:VAL:HB	1:C:270:LEU:HB2	1.86	0.58
1:D:145:ASP:CB	1:D:181:THR:HB	2.34	0.58
1:D:347:VAL:HG21	1:D:366:GLU:HG2	1.85	0.58
1:B:131:ASN:O	1:B:134:ILE:HG22	2.03	0.58
1:F:46:GLY:CA	1:F:52:LYS:HD3	2.33	0.58
1:F:393:ARG:O	1:F:397:ILE:HG12	2.03	0.58
1:C:67:PHE:HB2	1:C:69:GLU:HG3	1.85	0.58
1:D:332:GLY:C	1:D:333:MET:HG2	2.27	0.58
1:B:147:VAL:O	1:B:150:VAL:HG12	2.04	0.57
1:E:490:ILE:CD1	1:D:449:MET:CE	2.82	0.57
1:A:49:GLY:HA3	1:B:224:LYS:HB3	1.86	0.57
1:E:110:PRO:CB	1:E:111:ASP:HA	2.32	0.57
1:B:133:ALA:O	1:B:137:TYR:HD1	1.88	0.57
1:B:385[A]:ARG:NE	1:C:432:TPO:O3P	2.34	0.57
1:E:21:MET:SD	1:E:141:ARG:NE	2.77	0.57
1:E:263:VAL:CG1	1:E:374:ARG:NH2	2.68	0.57
1:F:94:LEU:O	1:F:98:VAL:HG23	2.04	0.57
1:C:469:GLU:HB2	1:C:483:PHE:CZ	2.40	0.57
1:B:86:ASN:OD1	1:C:40:ARG:NH2	2.38	0.57
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.34	0.57
1:C:70:PRO:HB2	1:C:139:ALA:HA	1.87	0.57
1:D:151:PHE:CE1	1:D:160:VAL:HG13	2.39	0.57
1:B:67:PHE:HB2	1:B:69:GLU:HG3	1.87	0.57
1:D:489:ILE:N	1:D:489:ILE:HD13	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PHE:CD1	1:A:420:MET:HE2	2.37	0.56
1:B:368:ASN:ND2	1:B:402:TYR:OH	2.34	0.56
1:E:50:THR:HG21	1:E:207:LEU:HB2	1.86	0.56
1:E:425:ILE:HG22	1:E:426:THR:HG23	1.86	0.56
1:C:184:ARG:C	1:C:185:ILE:HD13	2.30	0.56
1:B:306:CYS:CB	1:B:338:MET:HG2	2.35	0.56
1:F:425:ILE:HD12	1:F:439:LEU:CD1	2.35	0.56
1:D:87:ALA:HB1	1:D:94:LEU:HD21	1.86	0.56
1:F:161:ARG:CG	1:F:196:VAL:HG13	2.32	0.56
1:D:148:THR:CG2	1:D:182:THR:HG23	2.35	0.56
1:E:438:ILE:HG23	1:E:453:ILE:HD11	1.86	0.56
1:F:263:VAL:HG21	1:F:280:LYS:HA	1.87	0.56
1:C:156:ALA:O	1:C:160:VAL:HG23	2.06	0.56
1:A:315:PHE:CD2	1:A:347:VAL:HG21	2.40	0.56
1:B:392:PHE:O	1:B:396:VAL:HG23	2.05	0.56
1:C:419:PHE:CE2	1:D:425:ILE:HD12	2.40	0.56
1:D:202:ASP:HA	1:D:226:ARG:HD2	1.87	0.56
1:B:393:ARG:O	1:B:397:ILE:HG12	2.05	0.56
1:B:396:VAL:O	1:B:400:THR:HG23	2.06	0.56
1:E:273:MET:HE3	1:E:479:ILE:HD13	1.86	0.56
1:E:438:ILE:CG2	1:E:453:ILE:CD1	2.83	0.56
1:A:147:VAL:O	1:A:150:VAL:HG12	2.05	0.56
1:A:317:TYR:HB3	1:A:351:PRO:HG3	1.88	0.56
1:E:185:ILE:HD11	1:E:193:ARG:NH1	2.20	0.56
1:D:94:LEU:O	1:D:98:VAL:HG23	2.05	0.56
1:E:254:LEU:HG	1:D:348:CYS:HB3	1.88	0.55
1:B:419:PHE:CD2	1:C:425:ILE:CD1	2.90	0.55
1:A:168:VAL:HG22	1:A:180:MET:SD	2.46	0.55
2:E:602:ATP:O2'	1:F:463:HIS:NE2	2.31	0.55
1:C:435:ASP:HA	1:C:459:ARG:HD2	1.88	0.55
1:D:23:THR:HB	1:D:25:ILE:HD12	1.87	0.55
1:A:458:MET:HE2	1:A:461:SER:HB3	1.89	0.55
1:F:31:ILE:HG22	1:F:222:ILE:HD12	1.89	0.55
1:F:313:ILE:HG13	1:F:372:PRO:HG3	1.89	0.55
1:C:18:ILE:HD12	1:C:18:ILE:H	1.70	0.55
1:D:486:PHE:HB3	1:D:489:ILE:CD1	2.37	0.55
1:A:351:PRO:HB3	1:A:383:LEU:HD23	1.88	0.55
1:F:52:LYS:NZ	2:F:601:ATP:O3G	2.40	0.55
1:D:161:ARG:HB2	1:D:196:VAL:HG11	1.88	0.55
1:A:80:PRO:O	1:A:84:ILE:HG12	2.06	0.55
1:B:268:VAL:O	1:B:272:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:489:ILE:HD13	1:E:494:PRO:HB3	1.88	0.55
1:C:64:ILE:HG21	1:C:97:LEU:CD1	2.36	0.55
1:E:393:ARG:HD3	1:D:385[B]:ARG:NE	2.22	0.55
1:C:484:ARG:CB	1:C:485:ASN:CB	2.84	0.55
1:C:18:ILE:HD12	1:C:18:ILE:N	2.22	0.54
1:C:484:ARG:CA	1:C:485:ASN:CB	2.85	0.54
1:E:21:MET:HB2	1:E:38:ILE:CD1	2.37	0.54
1:D:31:ILE:HG22	1:D:222:ILE:HD12	1.89	0.54
1:B:61:TYR:CZ	1:B:92:TRP:HB3	2.42	0.54
1:E:50:THR:HG22	1:E:207:LEU:CB	2.35	0.54
1:B:147:VAL:CG2	1:B:180:MET:HE2	2.36	0.54
1:E:183:GLU:HG3	1:E:193:ARG:HH21	1.72	0.54
1:B:285:LEU:HB2	1:B:434:THR:HG21	1.89	0.54
1:C:65:ILE:O	1:C:65:ILE:HG22	2.07	0.54
1:B:262:ARG:NH2	1:B:461:SER:HB2	2.23	0.54
1:F:319:GLU:HG2	1:F:323:GLN:HG2	1.90	0.54
1:F:364:LYS:HE3	1:F:402:TYR:CD2	2.43	0.54
1:E:122:ASP:O	1:E:126:LEU:N	2.40	0.54
1:E:151:PHE:HE1	1:E:160:VAL:HA	1.72	0.54
1:F:36:LEU:HD12	1:F:59:PHE:CE1	2.43	0.54
1:D:436:THR:HG23	1:D:458:MET:HG2	1.89	0.54
1:B:303:GLU:HA	1:B:338:MET:HE3	1.90	0.54
1:E:285:LEU:HB2	1:E:434:THR:HG21	1.90	0.54
1:D:56:SER:OG	1:D:143:SER:HB3	2.08	0.54
1:D:283:ILE:HG23	1:D:412:PHE:CE1	2.43	0.54
1:A:144:ILE:HD13	1:A:178:THR:HG21	1.90	0.53
1:E:231:MET:HB3	1:E:235:TYR:OH	2.08	0.53
1:E:303:GLU:HG2	1:E:338:MET:HE1	1.90	0.53
1:D:191:ILE:HD12	1:D:206:ILE:HD11	1.89	0.53
1:E:254:LEU:HD21	1:D:350:TYR:CD1	2.43	0.53
1:F:220:LEU:HD13	1:F:246:ILE:HD11	1.89	0.53
1:A:290:THR:HG21	1:B:431:SEP:HB2	1.90	0.53
1:A:419:PHE:O	1:B:423:HIS:O	2.26	0.53
1:E:273:MET:HE2	1:E:479:ILE:HG21	1.89	0.53
1:F:267:VAL:C	1:F:268:VAL:HG23	2.33	0.53
1:C:26:GLU:CB	1:C:245:ASN:OD1	2.56	0.53
1:B:186:GLU:HG3	1:B:189:GLY:H	1.73	0.53
1:B:385[B]:ARG:CG	1:B:385[B]:ARG:NH1	2.67	0.53
1:E:254:LEU:HD22	1:D:350:TYR:HE1	1.73	0.53
1:E:335:PHE:N	1:E:338:MET:HG3	2.24	0.53
1:F:313:ILE:CD1	1:F:372:PRO:HG3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ILE:HD12	1:C:412:PHE:HE2	1.74	0.53
1:D:305:ALA:HB1	1:D:312:ALA:HB2	1.89	0.53
1:A:146:SER:O	1:A:149:SER:OG	2.26	0.53
1:A:387:VAL:HG12	1:A:391:ALA:HB3	1.91	0.53
1:B:98:VAL:HA	1:B:103:LEU:O	2.09	0.53
1:E:254:LEU:CD2	1:D:350:TYR:CE1	2.91	0.53
1:D:52:LYS:HB3	1:D:181:THR:HG23	1.90	0.53
1:D:65:ILE:HG22	1:D:65:ILE:O	2.09	0.53
1:D:405:GLN:HG3	1:D:406:GLU:N	2.24	0.53
1:B:191:ILE:HB	1:B:198:GLU:HG2	1.90	0.52
1:E:289:ALA:O	1:E:294:LYS:NZ	2.43	0.52
1:E:406:GLU:HB2	1:E:408:ILE:HG13	1.91	0.52
1:A:225:LEU:HB2	1:A:230:HIS:HD2	1.73	0.52
1:A:368:ASN:N	1:A:368:ASN:HD22	2.07	0.52
1:C:483:PHE:C	1:C:485:ASN:CB	2.83	0.52
1:B:220:LEU:HD13	1:B:246:ILE:HD11	1.91	0.52
1:B:350:TYR:HB2	1:B:353:SER:HB3	1.92	0.52
1:E:335:PHE:CA	1:E:338:MET:HG3	2.40	0.52
1:F:75:THR:HG22	1:F:107:ASP:HA	1.92	0.52
1:E:468:ARG:HA	1:E:482:SER:HA	1.91	0.52
1:D:133:ALA:O	1:D:137:TYR:HD1	1.91	0.52
1:D:184:ARG:HG2	1:D:191:ILE:O	2.09	0.52
1:A:430:ILE:HG22	1:A:430:ILE:O	2.10	0.52
1:B:283:ILE:HG12	1:B:404:LYS:HE3	1.91	0.52
1:E:217:ARG:NH1	1:E:394:GLN:OE1	2.42	0.52
1:A:197:GLU:OE2	1:A:197:GLU:N	2.34	0.52
1:E:62:ASN:O	1:E:66:GLU:HB2	2.10	0.52
1:C:191:ILE:HB	1:C:198:GLU:HG2	1.91	0.52
1:A:89:SER:OG	2:A:601:ATP:N6	2.19	0.52
1:B:248:PRO:CB	1:B:251:ALA:HB3	2.38	0.52
2:B:602:ATP:H3'	1:C:458:MET:O	2.09	0.52
1:A:298:VAL:O	1:A:302:VAL:HG23	2.09	0.52
1:F:331:TRP:HZ2	2:F:602:ATP:H5'2	1.75	0.52
1:B:338:MET:HB3	1:B:344:LEU:HB2	1.91	0.52
1:E:42:THR:HG23	1:E:203:ASN:HB2	1.91	0.52
1:C:356:LEU:HG	1:C:395:PHE:HB2	1.91	0.52
1:E:49:GLY:HA3	1:F:224:LYS:HB3	1.92	0.51
1:E:84:ILE:HG23	1:E:94:LEU:HB2	1.91	0.51
1:F:425:ILE:HD13	1:F:439:LEU:HD11	1.92	0.51
2:C:602:ATP:O2G	1:D:457:LYS:NZ	2.42	0.51
1:E:321:ARG:O	1:E:325:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ILE:O	1:F:134:ILE:HG12	2.11	0.51
1:C:94:LEU:O	1:C:98:VAL:HG23	2.10	0.51
1:A:86:ASN:CG	1:B:40:ARG:HH22	2.17	0.51
1:B:449:MET:HE3	1:C:490:ILE:HD11	1.93	0.51
1:C:425:ILE:HG22	1:C:426:THR:HG23	1.93	0.51
1:D:147:VAL:CG1	1:D:180:MET:CE	2.84	0.51
1:A:52:LYS:HD2	1:A:182:THR:O	2.10	0.51
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.93	0.51
1:A:234:GLU:OE2	1:F:211:LEU:HD21	2.10	0.51
1:A:404:LYS:C	1:A:406:GLU:H	2.17	0.51
1:B:236:PRO:HB2	1:B:357:GLU:HG2	1.93	0.51
1:B:262:ARG:HH22	1:B:461:SER:CB	2.22	0.51
1:A:147:VAL:HG11	1:A:180:MET:HE2	1.92	0.51
1:A:347:VAL:O	1:A:348:CYS:HB2	2.09	0.51
1:E:50:THR:CG2	1:E:207:LEU:HB2	2.39	0.51
1:C:359:HIS:O	1:C:363:ILE:HG13	2.09	0.51
1:D:150:VAL:HG13	1:D:151:PHE:CD2	2.45	0.51
1:B:344:LEU:HD22	1:B:345:LYS:N	2.26	0.51
1:E:173:GLN:HE22	1:D:112:PRO:HG2	1.74	0.51
1:B:302:VAL:HG11	1:B:344:LEU:HD21	1.93	0.51
1:F:46:GLY:HA3	1:F:52:LYS:HD3	1.91	0.51
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.92	0.51
1:F:78:GLU:HB3	1:F:83:ILE:HD11	1.93	0.51
1:A:147:VAL:C	1:A:150:VAL:HG12	2.36	0.51
1:B:395:PHE:O	1:B:399:VAL:HG23	2.10	0.51
1:E:59:PHE:O	1:E:141:ARG:NH1	2.40	0.51
1:E:133:ALA:O	1:E:137:TYR:HD1	1.94	0.51
1:A:489:ILE:HD13	1:F:444:GLU:OE2	2.11	0.51
1:E:467:ILE:HD11	1:D:449:MET:HE2	1.92	0.51
1:E:485:ASN:O	1:E:486:PHE:CD2	2.64	0.51
1:D:18:ILE:HD12	1:D:18:ILE:N	2.26	0.51
1:D:167:LEU:CD2	1:D:180:MET:HE1	2.40	0.51
1:E:350:TYR:CZ	1:F:254:LEU:HD13	2.45	0.50
1:F:161:ARG:CG	1:F:196:VAL:CG1	2.89	0.50
1:A:321:ARG:O	1:A:325:LEU:HG	2.12	0.50
1:B:264:SER:O	1:B:374:ARG:NH1	2.43	0.50
1:B:430:ILE:O	1:B:430:ILE:HG22	2.11	0.50
1:B:358:ASP:O	1:B:362:ILE:HG12	2.11	0.50
1:F:368:ASN:ND2	1:F:402:TYR:OH	2.45	0.50
1:A:364:LYS:O	1:A:368:ASN:ND2	2.44	0.50
1:B:134:ILE:HG23	1:B:135:GLN:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:MET:N	1:C:465:LYS:O	2.42	0.50
1:E:292:THR:HG21	1:E:440:LEU:CB	2.41	0.50
1:C:15:HIS:HA	1:C:16:GLN:CB	2.42	0.50
1:B:311:ARG:NH1	1:B:371:LYS:O	2.44	0.50
1:E:64:ILE:O	1:E:68:ASP:N	2.37	0.50
1:C:419:PHE:H	1:C:419:PHE:HD2	1.59	0.50
1:A:419:PHE:N	1:B:423:HIS:O	2.44	0.50
1:B:191:ILE:CG2	1:B:198:GLU:HG2	2.42	0.50
1:B:269:ARG:HB3	1:B:479:ILE:HD12	1.93	0.50
1:E:150:VAL:HG22	1:E:150:VAL:O	2.11	0.50
1:F:265:SER:HB3	1:F:278:PHE:CE1	2.46	0.50
1:D:259:SER:OG	1:D:261:VAL:HG23	2.11	0.50
1:A:225:LEU:HB2	1:A:230:HIS:CD2	2.47	0.50
1:A:262:ARG:NH2	1:A:461:SER:OG	2.32	0.50
1:A:358:ASP:O	1:A:362:ILE:HG12	2.12	0.50
1:E:335:PHE:H	1:E:338:MET:HG3	1.76	0.50
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.94	0.50
1:A:106:LEU:HD12	1:A:107:ASP:O	2.11	0.50
1:B:160:VAL:O	1:B:164:LEU:HB2	2.11	0.50
1:C:185:ILE:HD13	1:C:185:ILE:N	2.27	0.50
1:B:419:PHE:CD2	1:C:425:ILE:HD12	2.46	0.49
1:C:440:LEU:HD21	1:C:453:ILE:HD13	1.94	0.49
1:B:385[A]:ARG:HD2	1:C:393:ARG:CD	2.43	0.49
1:F:303:GLU:CB	1:F:333:MET:HE3	2.42	0.49
1:C:289:ALA:HB2	1:C:419:PHE:HA	1.93	0.49
1:A:315:PHE:CE2	1:A:347:VAL:HG21	2.47	0.49
1:A:396:VAL:HG11	1:A:430:ILE:HG21	1.94	0.49
1:B:425:ILE:HG22	1:B:426:THR:HG23	1.93	0.49
1:E:292:THR:HG21	1:E:440:LEU:HB3	1.93	0.49
1:C:191:ILE:HG21	1:C:198:GLU:HG2	1.92	0.49
1:B:183:GLU:OE2	1:C:161:ARG:NH1	2.45	0.49
1:E:254:LEU:CD2	1:E:254:LEU:N	2.76	0.49
1:F:273:MET:O	1:F:463:HIS:HA	2.13	0.49
1:A:283:ILE:CG1	1:A:400:THR:HG23	2.30	0.49
1:B:67:PHE:HB2	1:B:69:GLU:CG	2.43	0.49
1:E:52:LYS:HB3	1:E:181:THR:CG2	2.41	0.49
1:E:254:LEU:CD2	1:D:350:TYR:CD1	2.96	0.49
1:D:393:ARG:NH1	1:D:428:SER:O	2.43	0.49
1:B:203:ASN:HB3	1:B:225:LEU:CD2	2.42	0.49
1:E:24:MET:HB2	1:E:62:ASN:HB3	1.94	0.49
1:E:50:THR:HG21	1:E:207:LEU:CB	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:PRO:HB2	1:E:111:ASP:C	2.37	0.49
1:C:375:ILE:HG22	1:C:410:GLY:HA2	1.95	0.49
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.43	0.49
1:F:452:ALA:HB1	1:F:467:ILE:HG22	1.95	0.49
1:C:377:ILE:HD12	1:C:412:PHE:CE2	2.48	0.49
1:D:289:ALA:HB2	1:D:419:PHE:HA	1.95	0.49
1:A:305:ALA:CB	1:A:374:ARG:HD3	2.37	0.49
1:D:311:ARG:CZ	1:D:370:PHE:O	2.61	0.49
1:A:145:ASP:HA	1:A:146:SER:HA	1.60	0.48
1:E:306:CYS:SG	1:E:338:MET:HB3	2.52	0.48
1:F:52:LYS:HD2	1:F:181:THR:HG23	1.94	0.48
1:A:83:ILE:O	1:A:87:ALA:HB2	2.12	0.48
1:E:344:LEU:HD22	1:E:345:LYS:H	1.78	0.48
1:B:274:CYS:HB3	1:B:458:MET:SD	2.53	0.48
2:C:601:ATP:O1G	1:D:224:LYS:NZ	2.41	0.48
1:B:45:SER:HB3	1:B:182:THR:HB	1.94	0.48
1:C:147:VAL:O	1:C:151:PHE:CE1	2.66	0.48
1:D:191:ILE:HB	1:D:198:GLU:HG2	1.94	0.48
1:E:347:VAL:O	1:E:348:CYS:HB2	2.13	0.48
1:D:236:PRO:HG2	1:D:247[B]:PHE:CD2	2.44	0.48
1:D:375:ILE:HG22	1:D:410:GLY:HA2	1.95	0.48
1:A:419:PHE:CD2	1:B:423:HIS:O	2.67	0.48
1:F:397:ILE:HD13	1:F:433:ILE:HD13	1.96	0.48
1:D:240:THR:C	1:D:242:HIS:H	2.22	0.48
1:A:31:ILE:HD13	1:A:235:TYR:CD1	2.49	0.48
1:A:298:VAL:HG13	1:A:376:ALA:HB1	1.95	0.48
1:A:432:TPO:O3P	1:F:385[B]:ARG:HD3	2.14	0.48
1:B:186:GLU:HG3	1:B:188:TYR:H	1.78	0.48
1:E:199:PHE:CE1	1:D:183:GLU:HB3	2.49	0.48
1:F:18:ILE:HG12	1:F:228:THR:HG23	1.95	0.48
1:F:292:THR:CG2	1:F:440:LEU:CB	2.76	0.48
1:C:283:ILE:HD12	1:C:412:PHE:HE1	1.77	0.48
1:C:377:ILE:CD1	1:C:412:PHE:HE2	2.27	0.48
1:A:432:TPO:CG2	1:F:415:THR:HG21	2.44	0.48
1:B:104:PHE:HD2	1:B:133:ALA:HB1	1.79	0.48
1:E:469:GLU:CB	1:E:483:PHE:CZ	2.97	0.48
1:C:126:LEU:HD12	1:C:126:LEU:O	2.13	0.48
1:B:134:ILE:HD13	1:B:134:ILE:C	2.38	0.48
1:F:458:MET:HE2	1:F:461:SER:HB3	1.95	0.48
1:B:61:TYR:CZ	1:B:65:ILE:HG13	2.49	0.48
1:E:292:THR:HG22	1:E:440:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:HA	1:A:226:ARG:HD2	1.95	0.47
1:E:37:PRO:HB2	1:E:40:ARG:HG3	1.95	0.47
1:E:363:ILE:O	1:E:367:ILE:HG13	2.14	0.47
1:C:430:ILE:HA	1:C:433:ILE:HD12	1.97	0.47
1:D:70:PRO:HA	1:D:102:LYS:O	2.14	0.47
1:F:367:ILE:HG23	1:F:372:PRO:HD2	1.96	0.47
1:A:449:MET:HE2	1:A:449:MET:HA	1.94	0.47
1:E:169:ALA:HB1	1:D:112:PRO:HG3	1.96	0.47
1:F:425:ILE:CD1	1:F:439:LEU:HD11	2.45	0.47
1:A:269:ARG:O	1:A:269:ARG:HD3	2.14	0.47
1:B:316:ALA:O	1:B:348:CYS:HA	2.14	0.47
1:E:298:VAL:HG13	1:E:376:ALA:HB1	1.97	0.47
1:F:425:ILE:HG22	1:F:426:THR:HG23	1.96	0.47
1:D:337:GLU:OE2	1:D:341:GLN:HG3	2.15	0.47
1:B:375:ILE:HG23	1:B:410:GLY:HA2	1.96	0.47
1:C:449:MET:HE2	1:D:467:ILE:HD11	1.95	0.47
1:A:269:ARG:O	1:A:272:GLU:N	2.47	0.47
1:A:281:ASP:CG	1:A:407:GLU:HG3	2.40	0.47
1:B:219:THR:HB	1:B:234:GLU:HB3	1.97	0.47
1:E:48:SER:HB3	1:F:223:LEU:CD1	2.45	0.47
1:E:263:VAL:HG12	1:E:374:ARG:HH22	1.78	0.47
1:E:301:PHE:O	1:E:374:ARG:NH1	2.44	0.47
1:C:182:THR:HG21	1:C:192:ALA:HB1	1.97	0.47
1:C:483:PHE:O	1:C:484:ARG:C	2.57	0.47
1:D:94:LEU:N	1:D:94:LEU:HD22	2.29	0.47
1:C:15:HIS:CA	1:C:16:GLN:CB	2.93	0.47
1:A:170:ARG:HA	1:A:173:GLN:NE2	2.29	0.47
1:A:307:ALA:C	1:A:309:LYS:H	2.23	0.47
1:A:64:ILE:HG12	1:A:69:GLU:O	2.15	0.47
1:A:385:ARG:HG3	1:B:393:ARG:CZ	2.44	0.47
1:A:468:ARG:HB3	1:A:479:ILE:CG2	2.45	0.47
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.45	0.47
1:E:318:GLU:HG2	1:F:432:TPO:O2P	2.15	0.47
1:B:292:THR:HB	1:B:440:LEU:HB3	1.97	0.46
1:B:458:MET:HE2	1:B:461:SER:HB3	1.97	0.46
1:F:361:GLN:HE21	1:F:361:GLN:CA	2.11	0.46
1:A:191:ILE:HG13	1:A:206:ILE:HD11	1.96	0.46
1:D:321:ARG:O	1:D:325:LEU:HG	2.15	0.46
1:B:131:ASN:HA	1:B:134:ILE:HG22	1.96	0.46
1:B:263:VAL:HG12	1:B:374:ARG:NH2	2.30	0.46
1:E:335:PHE:HA	1:E:338:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:SER:HB2	1:F:143:SER:HB2	1.96	0.46
1:C:294:LYS:HG2	1:C:413:THR:HG23	1.98	0.46
1:D:396:VAL:HG11	1:D:430:ILE:HG12	1.97	0.46
1:B:84:ILE:HG23	1:B:94:LEU:HB2	1.97	0.46
1:E:184:ARG:C	1:E:185:ILE:HD13	2.41	0.46
1:C:64:ILE:HG21	1:C:97:LEU:HD12	1.97	0.46
1:B:131:ASN:C	1:B:134:ILE:HG22	2.40	0.46
1:C:72:VAL:HG23	1:C:139:ALA:CB	2.46	0.46
1:C:183:GLU:HB3	1:D:199:PHE:CZ	2.50	0.46
1:C:451:ARG:NH2	2:C:602:ATP:O2'	2.49	0.46
1:A:64:ILE:C	1:A:66:GLU:H	2.23	0.46
1:A:144:ILE:CD1	1:A:178:THR:CG2	2.94	0.46
1:F:377:ILE:HD11	1:F:399:VAL:HG11	1.97	0.46
1:D:263:VAL:CG1	1:D:374:ARG:HH11	2.29	0.46
1:A:84:ILE:HD11	1:A:105:ILE:CD1	2.46	0.46
1:A:302:VAL:CG1	1:A:344:LEU:HD13	2.46	0.46
1:F:54:LEU:HD13	1:F:90:PHE:CZ	2.50	0.46
1:C:223:LEU:HD23	1:C:223:LEU:HA	1.84	0.46
1:A:65:ILE:HG22	1:A:65:ILE:O	2.16	0.46
1:A:312:ALA:O	1:A:344:LEU:HA	2.15	0.46
1:A:469:GLU:HB2	1:A:483:PHE:CE1	2.51	0.46
1:A:53:THR:OG1	2:A:601:ATP:O2B	2.21	0.45
1:A:150:VAL:HG13	1:A:151:PHE:N	2.29	0.45
1:A:404:LYS:O	1:A:407:GLU:OE2	2.34	0.45
1:B:285:LEU:HA	1:B:412:PHE:O	2.15	0.45
1:B:436:THR:HG23	1:B:458:MET:HG2	1.98	0.45
1:E:147:VAL:HG11	1:E:180:MET:HG2	1.97	0.45
1:F:359:HIS:O	1:F:363:ILE:HG13	2.16	0.45
1:F:376:ALA:HA	1:F:411:LEU:O	2.16	0.45
1:C:326:ARG:NH2	1:C:327:ASN:OD1	2.49	0.45
1:B:257:ARG:NH2	1:B:258:SER:O	2.49	0.45
1:B:326:ARG:HG3	1:B:327:ASN:N	2.30	0.45
1:F:84:ILE:HG12	1:F:94:LEU:HB2	1.98	0.45
1:D:285:LEU:HB2	1:D:434:THR:HG21	1.98	0.45
1:B:45:SER:HA	1:B:182:THR:O	2.17	0.45
1:B:270:LEU:HD23	1:B:270:LEU:HA	1.82	0.45
1:D:21:MET:HG3	1:D:141:ARG:NH2	2.30	0.45
1:D:191:ILE:HD12	1:D:206:ILE:CD1	2.47	0.45
1:A:84:ILE:HD11	1:A:105:ILE:HD12	1.98	0.45
1:B:385[A]:ARG:HD2	1:C:393:ARG:HD3	1.98	0.45
2:A:601:ATP:O2'	1:B:230:HIS:NE2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:HG2	1:B:479:ILE:CB	2.33	0.45
1:E:111:ASP:CB	1:E:112:PRO:HD3	2.45	0.45
1:E:191:ILE:N	1:E:191:ILE:HD12	2.32	0.45
1:E:199:PHE:CZ	1:D:183:GLU:HB3	2.51	0.45
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.98	0.45
2:B:602:ATP:O2'	1:C:463:HIS:NE2	2.50	0.45
1:F:414:ASN:ND2	1:F:426:THR:HG22	2.32	0.45
1:D:332:GLY:O	1:D:333:MET:O	2.35	0.45
1:A:294:LYS:HB3	1:A:413:THR:CG2	2.37	0.45
1:B:61:TYR:CZ	1:B:92:TRP:CB	2.99	0.45
1:F:445:ILE:O	1:F:448:GLU:HB2	2.16	0.45
1:C:156:ALA:C	1:C:160:VAL:HG23	2.41	0.45
1:C:165:PHE:CD2	1:C:165:PHE:C	2.93	0.45
1:C:387:VAL:HG12	1:C:391:ALA:HB3	1.99	0.45
1:D:106:LEU:HD12	1:D:106:LEU:C	2.41	0.45
1:B:195:GLY:HA2	1:B:198:GLU:OE1	2.17	0.45
1:B:70:PRO:HA	1:B:102:LYS:O	2.16	0.45
1:F:79:THR:O	1:F:83:ILE:HG12	2.17	0.45
1:F:311:ARG:HA	1:F:343:LEU:O	2.16	0.45
1:D:87:ALA:HB3	1:D:94:LEU:HD23	1.99	0.45
1:A:291:GLY:O	1:A:451:ARG:NH1	2.50	0.44
1:A:400:THR:C	1:A:402:TYR:H	2.25	0.44
1:B:206:ILE:HD11	1:B:223:LEU:HG	1.99	0.44
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.98	0.44
1:C:191:ILE:CB	1:C:198:GLU:HG2	2.47	0.44
1:C:313:ILE:HB	1:C:375:ILE:HD11	1.97	0.44
1:D:430:ILE:HG23	1:D:430:ILE:O	2.17	0.44
1:A:468:ARG:HB3	1:A:479:ILE:HG22	1.99	0.44
1:E:299:SER:O	1:E:303:GLU:HB2	2.18	0.44
1:C:133:ALA:O	1:C:137:TYR:HD1	2.00	0.44
1:D:490:ILE:HG13	1:D:491:SER:N	2.32	0.44
1:A:393:ARG:HD3	1:F:385[B]:ARG:HE	1.80	0.44
1:B:262:ARG:NH2	1:B:461:SER:CB	2.79	0.44
1:E:89:SER:CB	1:F:227:GLY:O	2.65	0.44
1:F:374:ARG:HB3	1:F:409:THR:HG22	1.96	0.44
1:C:22:ARG:O	1:C:141:ARG:NH2	2.49	0.44
1:D:21:MET:CG	1:D:141:ARG:NH2	2.80	0.44
1:A:70:PRO:HB2	1:A:139:ALA:HA	2.00	0.44
1:E:52:LYS:HD3	2:E:601:ATP:O2B	2.18	0.44
1:F:107:ASP:O	1:F:129:ARG:NH2	2.50	0.44
1:D:43:LEU:HD11	1:D:182:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ALA:CB	1:D:94:LEU:HD21	2.47	0.44
1:D:145:ASP:HA	1:D:146:SER:HA	1.59	0.44
1:A:329:TYR:C	1:A:331:TRP:H	2.25	0.44
1:B:311:ARG:HA	1:B:343:LEU:O	2.17	0.44
1:A:54:LEU:CD2	1:A:239:ILE:HG23	2.48	0.44
1:A:199:PHE:CE1	1:F:48:SER:HB2	2.52	0.44
1:B:53:THR:O	1:B:57:ILE:HG12	2.18	0.44
1:B:111:ASP:OD1	1:B:111:ASP:N	2.51	0.44
1:E:463:HIS:NE2	2:D:602:ATP:O2'	2.46	0.44
1:C:300:ARG:HG2	1:C:333:MET:HE1	2.00	0.44
1:A:393:ARG:NH1	1:A:428:SER:O	2.50	0.44
1:B:396:VAL:HG11	1:B:430:ILE:HG21	1.98	0.44
1:E:45:SER:HB3	1:E:182:THR:CG2	2.48	0.44
1:C:472:ILE:N	1:C:472:ILE:HD12	2.33	0.44
1:A:273:MET:O	1:A:463:HIS:HA	2.17	0.44
1:F:161:ARG:HA	1:F:196:VAL:HG11	1.99	0.44
1:D:211:LEU:HD13	1:D:216:ARG:NE	2.33	0.44
1:D:225:LEU:HD23	1:D:225:LEU:HA	1.86	0.44
1:B:136:LYS:HG2	1:B:137:TYR:CE1	2.53	0.44
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.53	0.44
1:F:451:ARG:NH2	2:F:602:ATP:O2'	2.51	0.44
1:C:262:ARG:HG2	1:C:262:ARG:HH21	1.82	0.44
1:D:46:GLY:HA2	1:D:184:ARG:HD3	1.99	0.44
1:D:195:GLY:HA2	1:D:198:GLU:OE1	2.18	0.44
1:A:393:ARG:NH2	1:F:385[B]:ARG:HG2	2.33	0.43
1:A:420:MET:HE2	1:A:420:MET:HB2	1.81	0.43
1:C:484:ARG:CB	1:C:485:ASN:CA	2.96	0.43
1:A:319:GLU:HG2	1:B:459:ARG:HH21	1.84	0.43
1:B:281:ASP:OD2	1:B:407:GLU:HB3	2.18	0.43
1:D:21:MET:HE3	1:D:21:MET:HB2	1.82	0.43
1:F:225:LEU:HD12	1:F:230:HIS:HB3	2.00	0.43
1:C:148:THR:CB	1:C:183:GLU:HG3	2.48	0.43
1:D:296:LEU:HD22	1:D:472:ILE:HD13	1.99	0.43
1:F:435:ASP:HA	1:F:459:ARG:HD3	2.00	0.43
1:C:76:PHE:O	1:C:109:SER:HA	2.18	0.43
1:D:142:VAL:O	1:D:178:THR:HA	2.19	0.43
1:D:147:VAL:O	1:D:150:VAL:CG1	2.58	0.43
1:A:449:MET:HE3	1:B:467:ILE:HD11	2.00	0.43
1:B:45:SER:CB	1:B:182:THR:HB	2.49	0.43
1:E:197:GLU:OE2	1:E:197:GLU:N	2.43	0.43
1:E:393:ARG:CD	1:D:385[B]:ARG:HD3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ARG:CB	1:C:196:VAL:HG11	2.49	0.43
1:E:296:LEU:HD12	1:E:296:LEU:O	2.19	0.43
1:F:24:MET:HE2	1:F:67:PHE:CZ	2.53	0.43
1:B:186:GLU:CG	1:B:189:GLY:N	2.79	0.43
1:B:306:CYS:HB3	1:B:338:MET:HG2	1.99	0.43
1:E:184:ARG:HG2	1:E:191:ILE:O	2.18	0.43
1:E:383:LEU:C	1:E:385:ARG:H	2.25	0.43
2:E:602:ATP:O3'	1:F:457:LYS:HB2	2.18	0.43
1:F:25:ILE:HG12	1:F:58:GLN:HG2	2.00	0.43
1:F:42:THR:HG23	1:F:203:ASN:HB2	2.01	0.43
1:F:425:ILE:CD1	1:F:439:LEU:HD13	2.49	0.43
1:F:430:ILE:HD12	1:F:430:ILE:HA	1.80	0.43
1:A:230:HIS:NE2	2:F:601:ATP:O2'	2.45	0.43
1:A:392:PHE:O	1:A:395:PHE:HB3	2.18	0.43
1:A:416:SER:C	1:A:418:GLN:H	2.26	0.43
1:B:52:LYS:HB3	1:B:181:THR:HG23	1.99	0.43
2:B:601:ATP:O2G	1:C:224:LYS:NZ	2.40	0.43
1:E:269:ARG:HB3	1:E:479:ILE:HD12	2.00	0.43
1:F:295:THR:OG1	2:F:602:ATP:O1B	2.36	0.43
1:D:298:VAL:HG13	1:D:376:ALA:HB1	2.00	0.43
1:F:313:ILE:CG1	1:F:372:PRO:HG3	2.49	0.43
1:D:393:ARG:HA	1:D:430:ILE:HD11	2.01	0.43
1:B:356:LEU:HD12	1:B:356:LEU:HA	1.85	0.43
1:E:147:VAL:O	1:E:151:PHE:CD2	2.72	0.43
1:F:294:LYS:HB3	1:F:413:THR:HG21	2.01	0.43
1:F:363:ILE:O	1:F:367:ILE:HG13	2.19	0.43
1:D:87:ALA:CB	1:D:94:LEU:CD2	2.97	0.43
1:B:131:ASN:O	1:B:135:GLN:HG2	2.19	0.42
1:B:145:ASP:HA	1:B:146:SER:HA	1.75	0.42
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.84	0.42
1:C:86:ASN:CG	1:D:40:ARG:HH12	2.21	0.42
1:A:57:ILE:HD11	1:A:73:PHE:CE1	2.54	0.42
1:A:269:ARG:HD3	1:A:269:ARG:C	2.43	0.42
1:B:260:ASN:HA	1:B:279:PHE:CE2	2.45	0.42
1:E:305:ALA:HB2	1:E:374:ARG:CD	2.41	0.42
1:C:174:ILE:N	1:C:174:ILE:HD13	2.33	0.42
1:E:57:ILE:HD13	1:E:73:PHE:CE1	2.54	0.42
1:D:21:MET:HG3	1:D:141:ARG:HH21	1.84	0.42
1:D:97:LEU:N	1:D:97:LEU:HD23	2.34	0.42
1:B:59:PHE:CZ	1:B:141:ARG:HG2	2.55	0.42
1:B:321:ARG:NH1	1:B:346:ILE:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:LEU:CD2	1:E:335:PHE:HB3	2.50	0.42
1:C:164:LEU:HD12	1:C:197:GLU:HA	2.00	0.42
1:C:267:VAL:HG11	1:C:479:ILE:CD1	2.50	0.42
1:D:134:ILE:O	1:D:138:ARG:N	2.52	0.42
1:D:273:MET:O	1:D:463:HIS:HA	2.20	0.42
1:E:296:LEU:HD12	1:E:296:LEU:C	2.45	0.42
1:E:316:ALA:O	1:E:348:CYS:HA	2.20	0.42
1:F:292:THR:HG22	1:F:440:LEU:HD23	2.01	0.42
1:F:321:ARG:N	1:F:348:CYS:SG	2.93	0.42
1:D:191:ILE:CD1	1:D:206:ILE:HD11	2.50	0.42
1:A:60:LEU:O	1:A:64:ILE:HG13	2.20	0.42
1:A:404:LYS:NZ	1:A:435:ASP:OD2	2.53	0.42
1:D:145:ASP:HB3	1:D:181:THR:HB	2.02	0.42
1:D:334:ASP:OD1	1:D:337:GLU:HB2	2.20	0.42
1:C:77:GLU:HA	1:D:165:PHE:CE2	2.55	0.42
1:A:458:MET:HB2	1:A:463:HIS:CD2	2.54	0.42
1:B:156:ALA:HB3	1:B:159:VAL:CG2	2.44	0.42
2:E:602:ATP:HO2'	1:F:463:HIS:CD2	2.32	0.42
1:F:53:THR:OG1	2:F:601:ATP:O1B	2.38	0.42
1:F:313:ILE:HD11	1:F:372:PRO:HG3	2.02	0.42
1:D:301:PHE:HA	1:D:374:ARG:NH2	2.35	0.42
1:F:397:ILE:CD1	1:F:433:ILE:HD13	2.49	0.42
1:C:204:VAL:HG23	1:C:224:LYS:HE2	2.01	0.42
1:A:191:ILE:N	1:A:191:ILE:CD1	2.82	0.42
1:F:75:THR:CG2	1:F:107:ASP:HA	2.49	0.42
1:C:127:ILE:HG21	1:C:170:ARG:HD3	2.01	0.42
1:A:220:LEU:HD13	1:A:246:ILE:HD13	2.02	0.41
1:A:329:TYR:C	1:A:331:TRP:N	2.78	0.41
1:B:70:PRO:HB2	1:B:139:ALA:HA	2.02	0.41
1:F:75:THR:OG1	1:F:78:GLU:O	2.24	0.41
1:C:96:LYS:O	1:C:100:GLU:HG3	2.19	0.41
1:C:393:ARG:O	1:C:397:ILE:HG12	2.19	0.41
1:C:436:THR:HG23	1:C:458:MET:HG2	2.01	0.41
1:B:20:LYS:NZ	1:B:32:SER:O	2.36	0.41
1:F:145:ASP:HA	1:F:146:SER:HA	1.73	0.41
1:D:74:VAL:HG13	1:D:106:LEU:HG	2.01	0.41
1:D:317:TYR:HB3	1:D:351:PRO:HG3	2.01	0.41
1:F:263:VAL:CG2	1:F:280:LYS:HA	2.50	0.41
1:C:145:ASP:HA	1:C:146:SER:HA	1.67	0.41
1:D:58:GLN:HG3	1:D:92:TRP:HH2	1.81	0.41
1:D:147:VAL:HG23	1:D:148:THR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ALA:HB2	1:D:374:ARG:HD3	2.02	0.41
1:B:145:ASP:HA	1:B:181:THR:HB	2.01	0.41
1:B:360:LEU:HD22	1:B:364:LYS:HE3	2.01	0.41
1:E:53:THR:OG1	2:E:601:ATP:O1B	2.39	0.41
1:F:142:VAL:O	1:F:178:THR:HA	2.19	0.41
1:A:46:GLY:HA2	1:A:184:ARG:HD3	2.02	0.41
1:B:330:SER:O	1:B:474:ASP:HA	2.21	0.41
1:B:385[B]:ARG:NH1	1:B:385[B]:ARG:HG3	2.36	0.41
1:F:254:LEU:HD12	1:F:254:LEU:HA	1.84	0.41
1:F:291:GLY:O	1:F:451:ARG:NH1	2.53	0.41
1:F:299:SER:O	1:F:333:MET:HE1	2.20	0.41
1:F:317:TYR:HB3	1:F:351:PRO:HG3	2.03	0.41
1:C:262:ARG:HH21	1:C:262:ARG:CG	2.33	0.41
1:C:356:LEU:HD12	1:C:356:LEU:HA	1.88	0.41
1:D:274:CYS:HG	1:D:278:PHE:HE2	1.59	0.41
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.94	0.41
1:B:351:PRO:HB3	1:B:383:LEU:HD23	2.02	0.41
1:E:315:PHE:HE1	1:E:375:ILE:HD11	1.85	0.41
1:E:359:HIS:O	1:E:363:ILE:HG13	2.20	0.41
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.83	0.41
1:C:304:ASN:O	1:C:308:ASN:ND2	2.49	0.41
1:B:104:PHE:CD2	1:B:133:ALA:HB1	2.55	0.41
1:E:315:PHE:CE2	1:E:347:VAL:HG21	2.55	0.41
1:E:387:VAL:HG12	1:E:388:SER:O	2.20	0.41
1:C:377:ILE:HD11	1:C:399:VAL:HG11	2.03	0.41
1:D:262:ARG:NH1	1:D:274:CYS:O	2.53	0.41
1:A:191:ILE:HB	1:A:198:GLU:HG2	2.02	0.41
1:E:227:GLY:O	1:D:89:SER:HB2	2.20	0.41
1:F:271:ASP:OD1	1:F:271:ASP:N	2.50	0.41
1:D:84:ILE:CD1	1:D:95:ALA:HB2	2.45	0.41
1:D:192:ALA:HB1	1:D:197:GLU:CD	2.46	0.41
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.86	0.41
1:B:133:ALA:O	1:B:137:TYR:CD1	2.71	0.41
1:B:261:VAL:HG12	1:B:262:ARG:N	2.36	0.41
1:B:420:MET:HG2	1:B:492:GLY:HA3	2.03	0.41
1:F:220:LEU:HD13	1:F:246:ILE:CD1	2.50	0.41
1:F:263:VAL:N	1:F:278:PHE:O	2.41	0.41
1:F:384:ALA:HB2	1:F:392:PHE:CZ	2.56	0.41
1:C:64:ILE:CG2	1:C:97:LEU:CD1	2.99	0.41
1:C:161:ARG:HB2	1:C:196:VAL:HG11	2.03	0.41
1:D:191:ILE:CD1	1:D:206:ILE:CD1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LEU:HD12	1:D:211:LEU:HA	1.93	0.41
1:A:425:ILE:N	1:A:425:ILE:HD12	2.36	0.41
1:B:31:ILE:HG23	1:B:231:MET:HB2	2.02	0.41
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.90	0.41
2:B:602:ATP:O3'	1:C:457:LYS:HB2	2.21	0.41
1:E:82:ASP:O	1:E:86:ASN:CG	2.64	0.41
1:E:224:LYS:HE3	1:E:226:ARG:HD2	2.02	0.41
1:E:292:THR:CG2	1:E:440:LEU:CB	2.98	0.41
1:D:218:ARG:HG2	1:D:218:ARG:HH21	1.85	0.41
1:A:393:ARG:CZ	1:F:385[B]:ARG:HG2	2.51	0.40
1:B:191:ILE:CB	1:B:198:GLU:HG2	2.51	0.40
1:B:389:ASN:HD21	1:B:428:SER:HA	1.86	0.40
1:D:54:LEU:HD21	1:D:239:ILE:HG23	2.03	0.40
1:B:42:THR:HG23	1:B:203:ASN:HB2	2.03	0.40
1:B:97:LEU:N	1:B:97:LEU:HD23	2.36	0.40
1:B:236:PRO:HB2	1:B:357:GLU:HG3	2.01	0.40
1:E:48:SER:HB3	1:F:223:LEU:HD12	2.02	0.40
1:A:191:ILE:CG2	1:A:198:GLU:HG2	2.51	0.40
1:C:209:ASN:HD22	1:C:209:ASN:HA	1.59	0.40
1:A:142:VAL:HG12	1:A:144:ILE:HD12	2.03	0.40
1:A:269:ARG:NH2	1:A:468:ARG:NH1	2.70	0.40
1:E:18:ILE:HG22	1:D:85:LYS:HG3	2.02	0.40
1:C:107:ASP:OD1	1:C:109:SER:OG	2.37	0.40
1:C:144:ILE:O	1:C:180:MET:HA	2.22	0.40
1:D:18:ILE:N	1:D:18:ILE:CD1	2.84	0.40
1:B:87:ALA:HB1	1:B:92:TRP:CD1	2.56	0.40
1:E:151:PHE:CD1	1:E:160:VAL:HG22	2.56	0.40
1:F:52:LYS:HB3	1:F:181:THR:CG2	2.50	0.40
1:F:396:VAL:HG11	1:F:430:ILE:HG13	2.03	0.40
1:D:294:LYS:HB2	1:D:294:LYS:HE2	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/519 (87%)	379 (84%)	61 (14%)	13 (3%)	3	13
1	B	463/519 (89%)	418 (90%)	35 (8%)	10 (2%)	5	19
1	C	456/519 (88%)	411 (90%)	38 (8%)	7 (2%)	8	28
1	D	454/519 (88%)	416 (92%)	30 (7%)	8 (2%)	6	23
1	E	455/519 (88%)	398 (88%)	46 (10%)	11 (2%)	4	17
1	F	458/519 (88%)	397 (87%)	48 (10%)	13 (3%)	4	14
All	All	2739/3114 (88%)	2419 (88%)	258 (9%)	62 (2%)	5	18

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	A	89	SER
1	B	422	ALA
1	E	111	ASP
1	F	15	HIS
1	F	257	ARG
1	C	123	LEU
1	C	485	ASN
1	D	333	MET
1	A	108	ALA
1	A	150	VAL
1	A	151	PHE
1	A	289	ALA
1	A	424	SER
1	B	253	ARG
1	B	278	PHE
1	B	279	PHE
1	E	26	GLU
1	E	334	ASP
1	C	112	PRO
1	C	193	ARG
1	C	484	ARG
1	D	66	GLU
1	D	308	ASN
1	D	370	PHE
1	A	26	GLU
1	A	197	GLU

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Mol	Chain	Res	Type
1	B	212	GLU
1	E	18	ILE
1	E	110	PRO
1	E	482	SER
1	F	106	LEU
1	F	123	LEU
1	F	214	GLU
1	F	253	ARG
1	F	420	MET
1	F	475	LYS
1	C	15	HIS
1	A	420	MET
1	B	423	HIS
1	E	418	GLN
1	E	420	MET
1	D	26	GLU
1	A	348	CYS
1	A	370	PHE
1	B	110	PRO
1	B	252	MET
1	B	281	ASP
1	E	289	ALA
1	F	197	GLU
1	F	474	ASP
1	C	212	GLU
1	D	77	GLU
1	D	488	ARG
1	A	308	ASN
1	B	17	ALA
1	D	65	ILE
1	E	150	VAL
1	F	147	VAL
1	E	64	ILE
1	F	248	PRO
1	F	130	ILE

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/442 (67%)	255 (86%)	40 (14%)	3	13
1	B	359/442 (81%)	311 (87%)	48 (13%)	4	13
1	C	347/442 (78%)	306 (88%)	41 (12%)	5	17
1	D	337/442 (76%)	293 (87%)	44 (13%)	4	14
1	E	320/442 (72%)	274 (86%)	46 (14%)	3	11
1	F	324/442 (73%)	286 (88%)	38 (12%)	5	18
All	All	1982/2652 (75%)	1725 (87%)	257 (13%)	4	14

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	40	ARG
1	A	149	SER
1	A	182	THR
1	A	183	GLU
1	A	186	GLU
1	A	191	ILE
1	A	198	GLU
1	A	209	ASN
1	A	212	GLU
1	A	214	GLU
1	A	218	ARG
1	A	221	GLU
1	A	223	LEU
1	A	240	THR
1	A	254	LEU
1	A	260	ASN
1	A	262	ARG
1	A	269	ARG
1	A	270	LEU
1	A	281	ASP
1	A	294	LYS
1	A	300	ARG
1	A	333	MET
1	A	342	ASN
1	A	352	GLU
1	A	356	LEU
1	A	360	LEU

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Mol	Chain	Res	Type
1	A	368	ASN
1	A	375	ILE
1	A	385	ARG
1	A	387	VAL
1	A	407	GLU
1	A	409	THR
1	A	420	MET
1	A	439	LEU
1	A	441	GLN
1	A	443	VAL
1	A	458	MET
1	A	489	ILE
1	B	20	LYS
1	B	24	MET
1	B	69	GLU
1	B	75	THR
1	B	81	GLN
1	B	124	SER
1	B	134	ILE
1	B	135	GLN
1	B	140	ARG
1	B	147	VAL
1	B	161	ARG
1	B	164	LEU
1	B	191	ILE
1	B	196	VAL
1	B	198	GLU
1	B	223	LEU
1	B	228	THR
1	B	232	LYS
1	B	245	ASN
1	B	257	ARG
1	B	269	ARG
1	B	270	LEU
1	B	279	PHE
1	B	294	LYS
1	B	296	LEU
1	B	311	ARG
1	B	323	GLN
1	B	325	LEU
1	B	326	ARG
1	B	340	ARG

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Mol	Chain	Res	Type
1	B	344	LEU
1	B	348	CYS
1	B	352	GLU
1	B	356	LEU
1	B	357	GLU
1	B	360	LEU
1	B	365	SER
1	B	366	GLU
1	B	374	ARG
1	B	375	ILE
1	B	406	GLU
1	B	427	ASP
1	B	440	LEU
1	B	451	ARG
1	B	457	LYS
1	B	458	MET
1	B	465	LYS
1	B	483	PHE
1	E	18	ILE
1	E	20	LYS
1	E	40	ARG
1	E	68	ASP
1	E	69	GLU
1	E	85	LYS
1	E	96	LYS
1	E	103	LEU
1	E	129	ARG
1	E	148	THR
1	E	170	ARG
1	E	180	MET
1	E	183	GLU
1	E	196	VAL
1	E	198	GLU
1	E	206	ILE
1	E	221	GLU
1	E	223	LEU
1	E	225	LEU
1	E	228	THR
1	E	242	HIS
1	E	245	ASN
1	E	254	LEU
1	E	270	LEU

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Mol	Chain	Res	Type
1	E	287	THR
1	E	296	LEU
1	E	311	ARG
1	E	333	MET
1	E	338	MET
1	E	341	GLN
1	E	344	LEU
1	E	352	GLU
1	E	356	LEU
1	E	360	LEU
1	E	365	SER
1	E	375	ILE
1	E	385	ARG
1	E	390	ASN
1	E	428	SER
1	E	430	ILE
1	E	441	GLN
1	E	453	ILE
1	E	458	MET
1	E	465	LYS
1	E	469	GLU
1	E	489	ILE
1	F	22	ARG
1	F	24	MET
1	F	26	GLU
1	F	40	ARG
1	F	45	SER
1	F	69	GLU
1	F	96	LYS
1	F	99	ASP
1	F	140	ARG
1	F	142	VAL
1	F	144	ILE
1	F	153	GLN
1	F	161	ARG
1	F	163	GLU
1	F	182	THR
1	F	183	GLU
1	F	198	GLU
1	F	202	ASP
1	F	218	ARG
1	F	223	LEU

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Mol	Chain	Res	Type
1	F	232	LYS
1	F	252	MET
1	F	256	GLN
1	F	270	LEU
1	F	271	ASP
1	F	287	THR
1	F	294	LYS
1	F	352	GLU
1	F	356	LEU
1	F	361	GLN
1	F	374	ARG
1	F	394	GLN
1	F	397	ILE
1	F	430	ILE
1	F	439	LEU
1	F	443	VAL
1	F	458	MET
1	F	459	ARG
1	C	18	ILE
1	C	21	MET
1	C	22	ARG
1	C	30	ASP
1	C	40	ARG
1	C	78	GLU
1	C	97	LEU
1	C	122	ASP
1	C	126	LEU
1	C	164	LEU
1	C	170	ARG
1	C	174	ILE
1	C	178	THR
1	C	180	MET
1	C	185	ILE
1	C	198	GLU
1	C	209	ASN
1	C	211	LEU
1	C	218	ARG
1	C	223	LEU
1	C	224	LYS
1	C	231	MET
1	C	234	GLU
1	C	258	SER

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Mol	Chain	Res	Type
1	C	270	LEU
1	C	287	THR
1	C	294	LYS
1	C	311	ARG
1	C	342	ASN
1	C	344	LEU
1	C	352	GLU
1	C	356	LEU
1	C	360	LEU
1	C	419	PHE
1	C	425	ILE
1	C	428	SER
1	C	439	LEU
1	C	444	GLU
1	C	458	MET
1	C	459	ARG
1	C	471	MET
1	D	18	ILE
1	D	69	GLU
1	D	78	GLU
1	D	79	THR
1	D	106	LEU
1	D	141	ARG
1	D	185	ILE
1	D	193	ARG
1	D	198	GLU
1	D	206	ILE
1	D	223	LEU
1	D	228	THR
1	D	234	GLU
1	D	245	ASN
1	D	247[A]	PHE
1	D	247[B]	PHE
1	D	255	THR
1	D	260	ASN
1	D	270	LEU
1	D	281	ASP
1	D	284	ILE
1	D	294	LYS
1	D	321	ARG
1	D	333	MET
1	D	344	LEU

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Mol	Chain	Res	Type
1	D	345	LYS
1	D	348	CYS
1	D	352	GLU
1	D	356	LEU
1	D	360	LEU
1	D	375	ILE
1	D	385[A]	ARG
1	D	385[B]	ARG
1	D	404	LYS
1	D	407	GLU
1	D	425	ILE
1	D	430	ILE
1	D	443	VAL
1	D	451	ARG
1	D	458	MET
1	D	465	LYS
1	D	471	MET
1	D	474	ASP
1	D	489	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	209	ASN
1	A	260	ASN
1	A	323	GLN
1	A	368	ASN
1	A	414	ASN
1	B	209	ASN
1	B	245	ASN
1	B	260	ASN
1	B	414	ASN
1	B	418	GLN
1	E	173	GLN
1	E	203	ASN
1	E	209	ASN
1	E	256	GLN
1	E	414	ASN
1	E	429	HIS
1	F	131	ASN
1	F	203	ASN

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Mol	Chain	Res	Type
1	F	341	GLN
1	F	361	GLN
1	F	368	ASN
1	F	389	ASN
1	F	414	ASN
1	F	418	GLN
1	C	131	ASN
1	C	209	ASN
1	C	304	ASN
1	C	414	ASN
1	C	429	HIS
1	D	209	ASN
1	D	304	ASN
1	D	368	ASN
1	D	414	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	432	1	8,10,11	0.83	0	10,14,16	0.85	0
1	SEP	B	431	1	8,9,10	0.64	0	7,12,14	0.62	0
1	TPO	B	432	1	8,10,11	0.85	0	10,14,16	0.88	1 (10%)
1	SEP	F	431	1	8,9,10	0.63	0	7,12,14	0.77	0
1	TPO	A	432	1	8,10,11	0.71	0	10,14,16	0.88	0
1	SEP	D	431	1	8,9,10	0.61	0	7,12,14	0.69	0
1	SEP	A	431	1	8,9,10	0.61	0	7,12,14	0.67	0
1	TPO	D	432	1	8,10,11	0.86	0	10,14,16	0.90	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	C	431	1	8,9,10	0.63	0	7,12,14	0.62	0
1	TPO	C	432	1	8,10,11	0.77	0	10,14,16	0.88	0
1	SEP	E	431	1	8,9,10	0.61	0	7,12,14	0.69	0
1	TPO	F	432	1	8,10,11	0.85	0	10,14,16	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	E	432	1	-	0/9/11/13	-
1	SEP	B	431	1	-	2/6/8/10	-
1	TPO	B	432	1	-	1/9/11/13	-
1	SEP	F	431	1	-	2/6/8/10	-
1	TPO	A	432	1	-	1/9/11/13	-
1	SEP	D	431	1	-	1/6/8/10	-
1	SEP	A	431	1	-	1/6/8/10	-
1	TPO	D	432	1	-	2/9/11/13	-
1	SEP	C	431	1	-	1/6/8/10	-
1	TPO	C	432	1	-	0/9/11/13	-
1	SEP	E	431	1	-	1/6/8/10	-
1	TPO	F	432	1	-	0/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	TPO	O-C-CA	-2.02	119.58	124.77
1	D	432	TPO	O-C-CA	-2.01	119.59	124.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	431	SEP	N-CA-CB-OG
1	B	431	SEP	CB-OG-P-O1P
1	E	431	SEP	N-CA-CB-OG
1	F	431	SEP	N-CA-CB-OG
1	F	431	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	C	431	SEP	N-CA-CB-OG
1	D	431	SEP	N-CA-CB-OG
1	B	431	SEP	CB-OG-P-O3P
1	A	432	TPO	O-C-CA-CB
1	D	432	TPO	O-C-CA-CB
1	B	432	TPO	N-CA-CB-CG2
1	D	432	TPO	N-CA-CB-CG2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	431	SEP	1	0
1	A	432	TPO	2	0
1	C	432	TPO	1	0
1	F	432	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	F	601	3	32,33,33	0.53	0	48,52,52	0.68	0
2	ATP	A	602	3	32,33,33	0.53	0	48,52,52	0.75	1 (2%)
2	ATP	A	601	3	32,33,33	0.52	0	48,52,52	0.62	0
2	ATP	B	601	3	32,33,33	0.52	0	48,52,52	0.72	1 (2%)
2	ATP	D	601	3	32,33,33	0.49	0	48,52,52	0.65	0
2	ATP	C	601	3	32,33,33	0.51	0	48,52,52	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	F	602	3	32,33,33	0.52	0	48,52,52	0.57	0
2	ATP	E	601	3	32,33,33	0.53	0	48,52,52	0.70	1 (2%)
2	ATP	D	602	3	32,33,33	0.54	0	48,52,52	0.59	0
2	ATP	C	602	3	32,33,33	0.56	0	48,52,52	0.66	0
2	ATP	E	602	3	32,33,33	0.55	0	48,52,52	0.67	0
2	ATP	B	602	3	32,33,33	0.53	0	48,52,52	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	F	601	3	-	5/22/38/38	0/3/3/3
2	ATP	A	602	3	-	6/22/38/38	0/3/3/3
2	ATP	A	601	3	-	5/22/38/38	0/3/3/3
2	ATP	B	601	3	-	7/22/38/38	0/3/3/3
2	ATP	D	601	3	-	6/22/38/38	0/3/3/3
2	ATP	C	601	3	-	3/22/38/38	0/3/3/3
2	ATP	F	602	3	-	6/22/38/38	0/3/3/3
2	ATP	E	601	3	-	0/22/38/38	0/3/3/3
2	ATP	D	602	3	-	2/22/38/38	0/3/3/3
2	ATP	C	602	3	-	2/22/38/38	0/3/3/3
2	ATP	E	602	3	-	1/22/38/38	0/3/3/3
2	ATP	B	602	3	-	1/22/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	ATP	C3'-C2'-C1'	2.46	106.12	101.46
2	B	601	ATP	C3'-C2'-C1'	2.15	105.54	101.46
2	E	601	ATP	C3'-C2'-C1'	2.04	105.33	101.46

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O2A
2	A	601	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	C5'-O5'-PA-O2A
2	B	601	ATP	C5'-O5'-PA-O3A
2	F	601	ATP	C5'-O5'-PA-O1A
2	F	601	ATP	C5'-O5'-PA-O2A
2	F	601	ATP	C5'-O5'-PA-O3A
2	F	601	ATP	O4'-C4'-C5'-O5'
2	F	602	ATP	C5'-O5'-PA-O1A
2	F	602	ATP	C5'-O5'-PA-O3A
2	C	601	ATP	C5'-O5'-PA-O2A
2	D	601	ATP	C5'-O5'-PA-O1A
2	D	601	ATP	C5'-O5'-PA-O2A
2	D	601	ATP	C5'-O5'-PA-O3A
2	F	601	ATP	C3'-C4'-C5'-O5'
2	F	602	ATP	C3'-C4'-C5'-O5'
2	B	601	ATP	C3'-C4'-C5'-O5'
2	C	601	ATP	C3'-C4'-C5'-O5'
2	A	602	ATP	O4'-C4'-C5'-O5'
2	A	602	ATP	C3'-C4'-C5'-O5'
2	F	602	ATP	O4'-C4'-C5'-O5'
2	A	601	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	O4'-C4'-C5'-O5'
2	C	601	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	PA-O3A-PB-O1B
2	C	602	ATP	PA-O3A-PB-O2B
2	D	601	ATP	PA-O3A-PB-O1B
2	A	602	ATP	C5'-O5'-PA-O1A
2	F	602	ATP	C5'-O5'-PA-O2A
2	A	601	ATP	PA-O3A-PB-O2B
2	D	602	ATP	PG-O3B-PB-O1B
2	A	602	ATP	PB-O3A-PA-O1A
2	B	601	ATP	PA-O3A-PB-O2B
2	E	602	ATP	PA-O3A-PB-O2B
2	C	602	ATP	PA-O3A-PB-O1B
2	D	601	ATP	PA-O3A-PB-O2B
2	D	601	ATP	O4'-C4'-C5'-O5'
2	A	602	ATP	PB-O3A-PA-O2A
2	B	602	ATP	PA-O3A-PB-O2B
2	F	602	ATP	PG-O3B-PB-O2B

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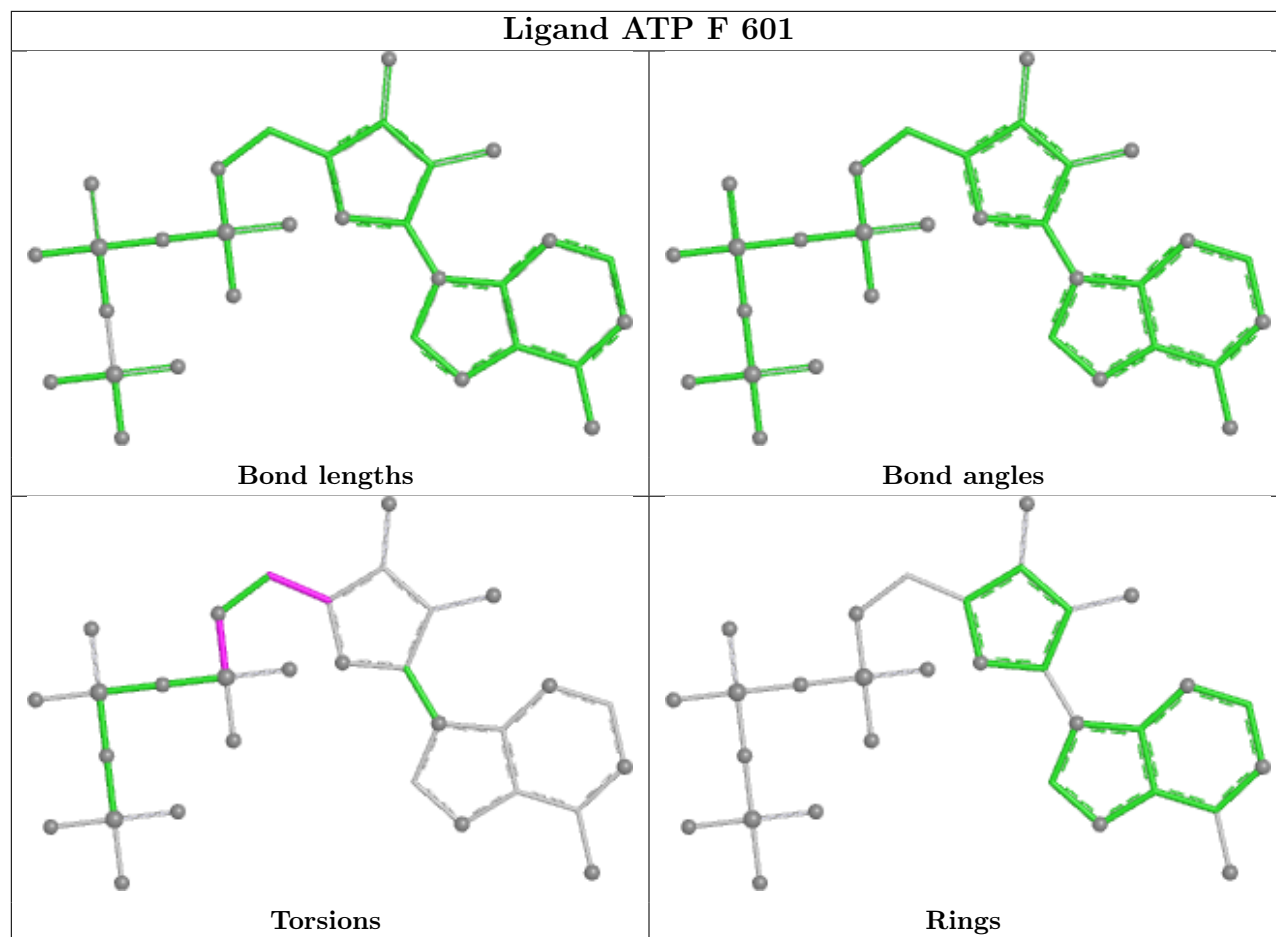
Mol	Chain	Res	Type	Atoms
2	D	602	ATP	PG-O3B-PB-O2B

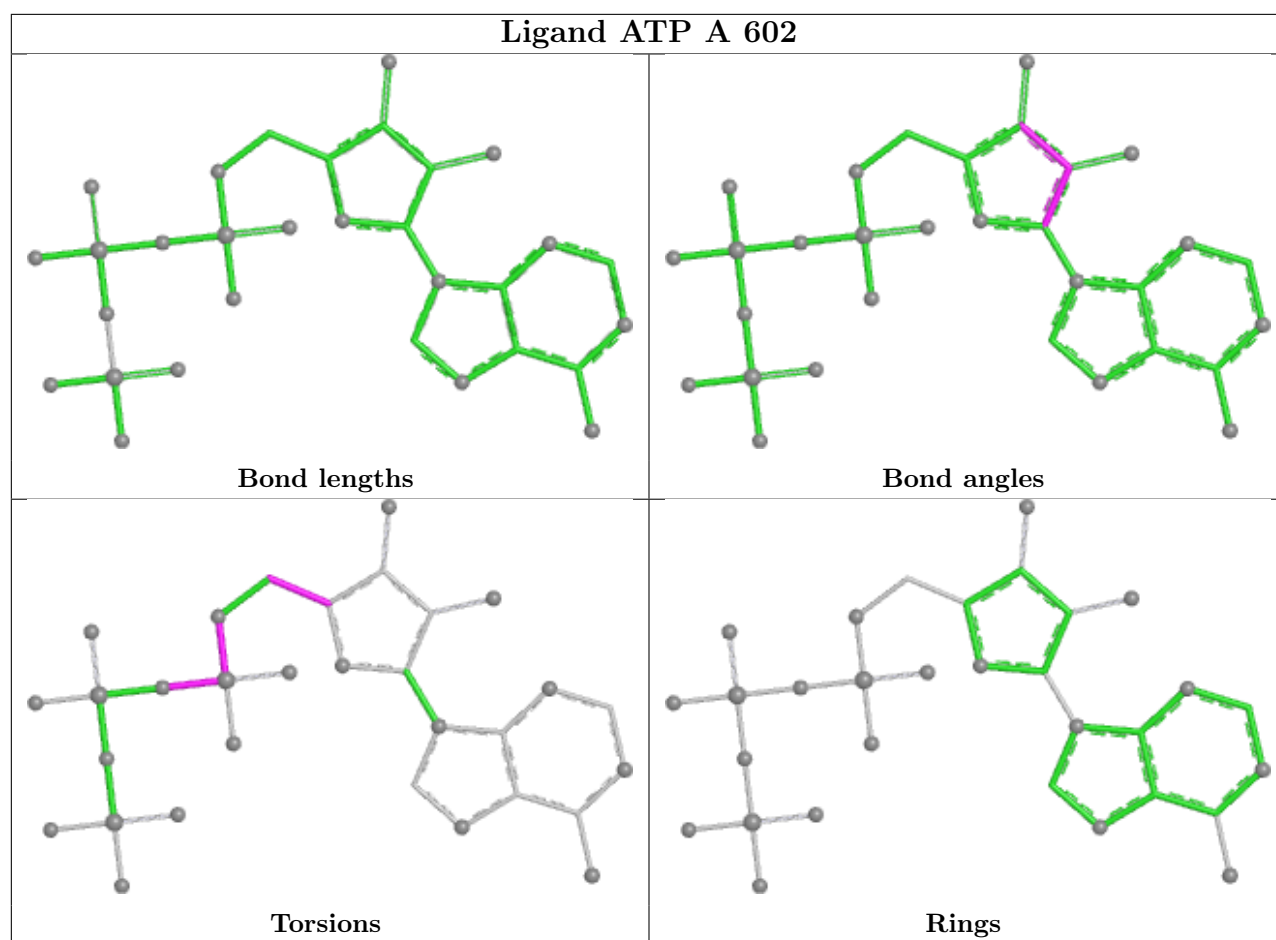
There are no ring outliers.

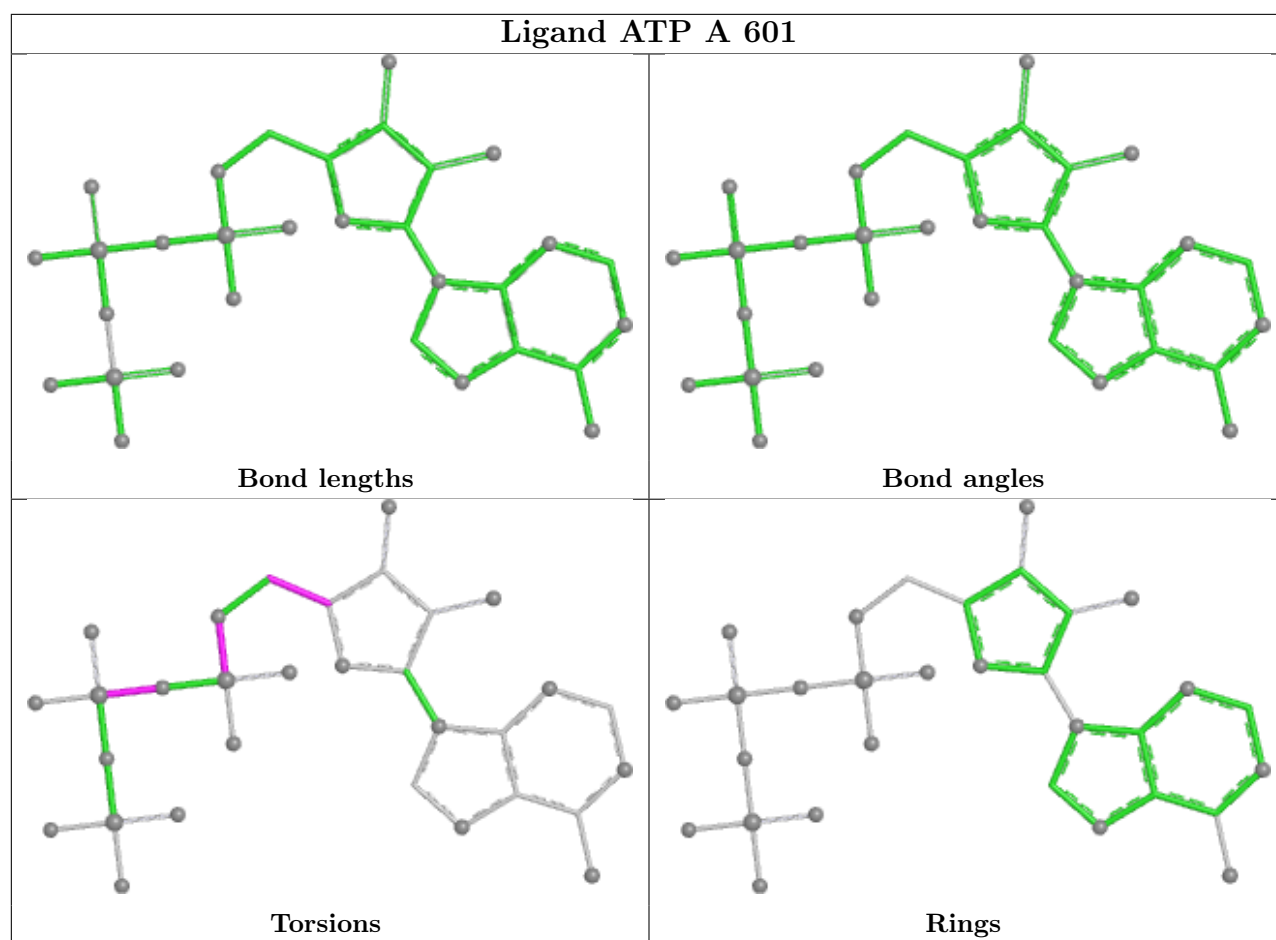
11 monomers are involved in 36 short contacts:

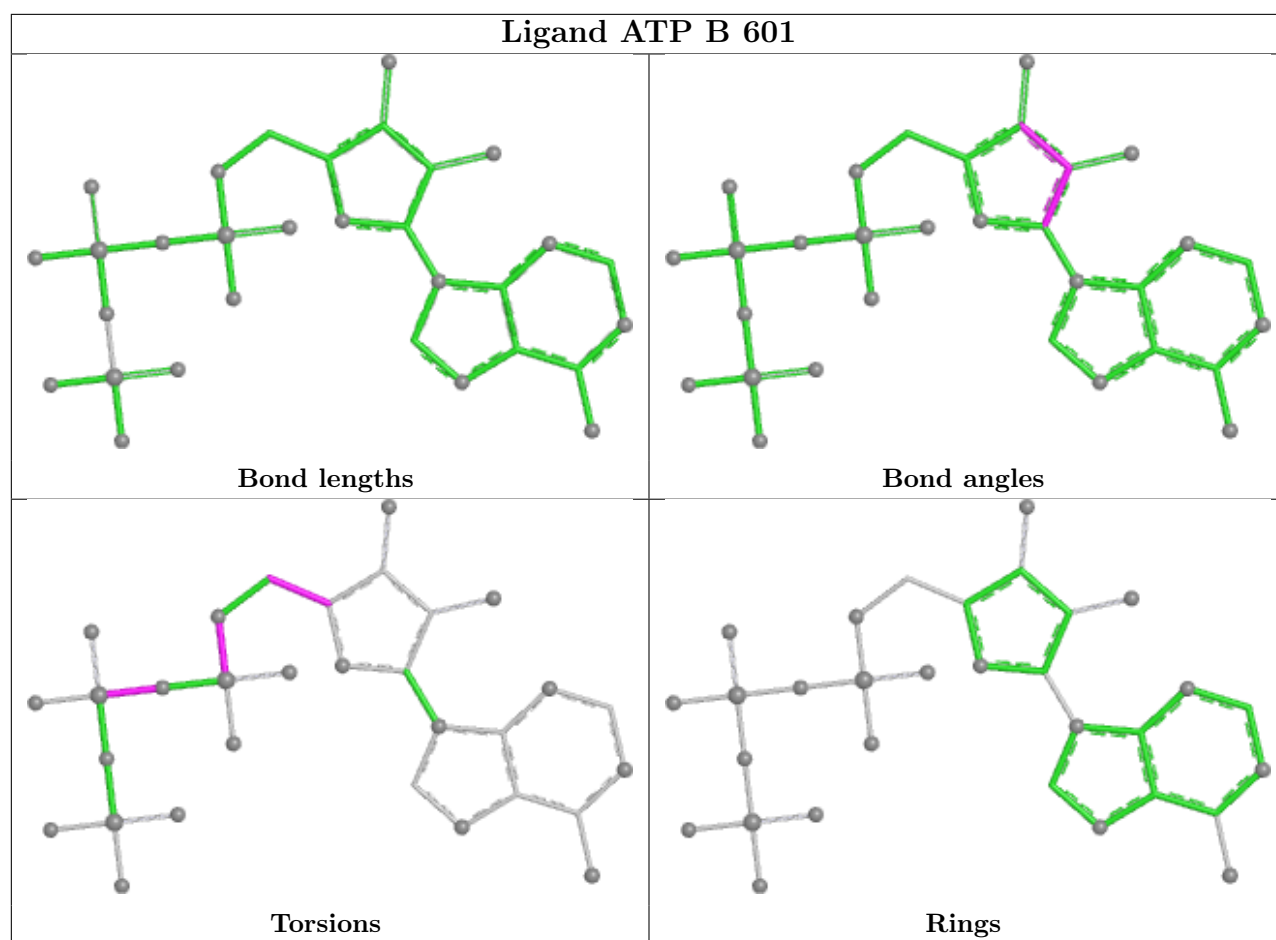
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	ATP	4	0
2	A	602	ATP	4	0
2	A	601	ATP	3	0
2	B	601	ATP	1	0
2	C	601	ATP	4	0
2	F	602	ATP	5	0
2	E	601	ATP	4	0
2	D	602	ATP	1	0
2	C	602	ATP	2	0
2	E	602	ATP	4	0
2	B	602	ATP	4	0

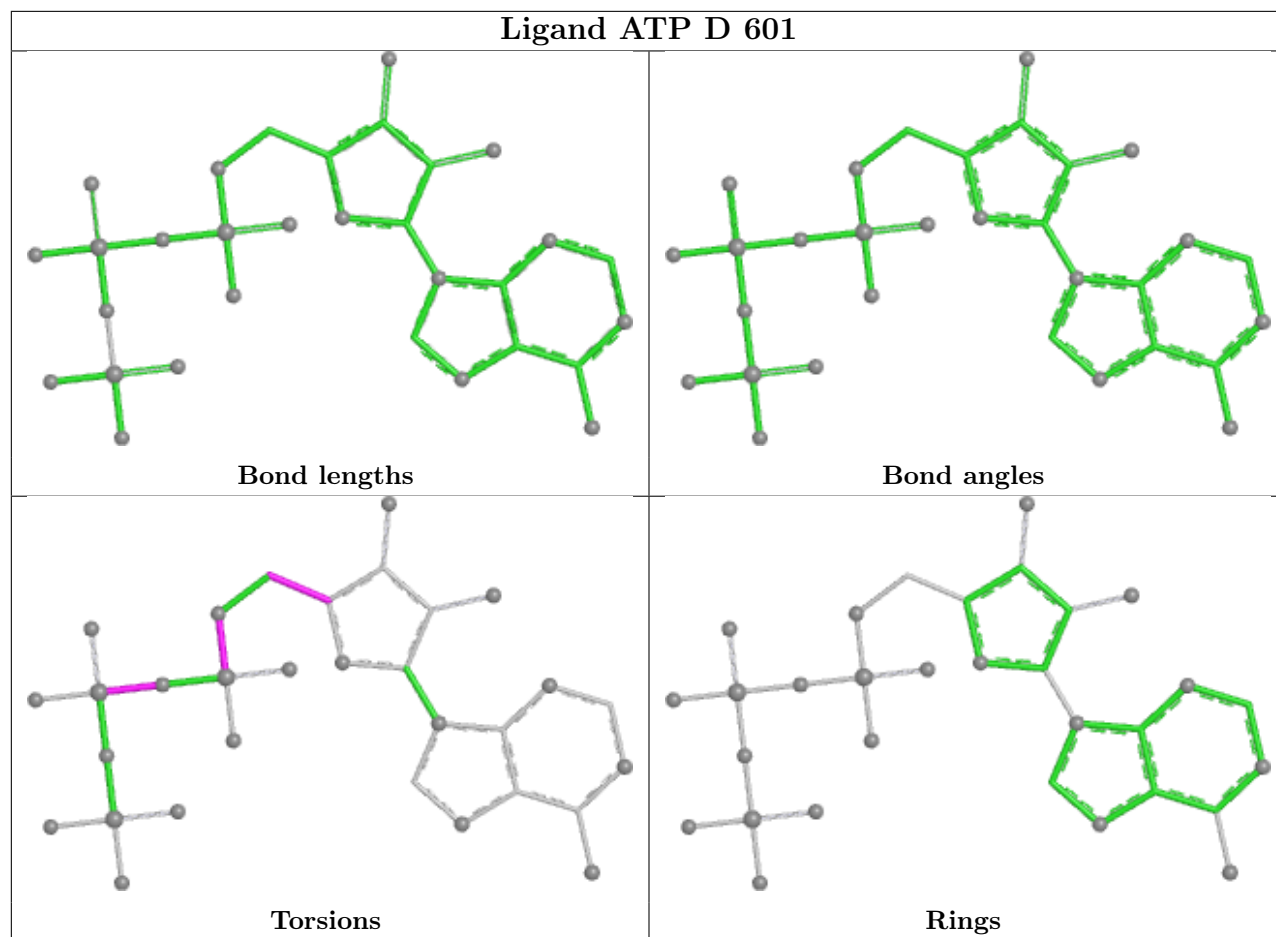
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

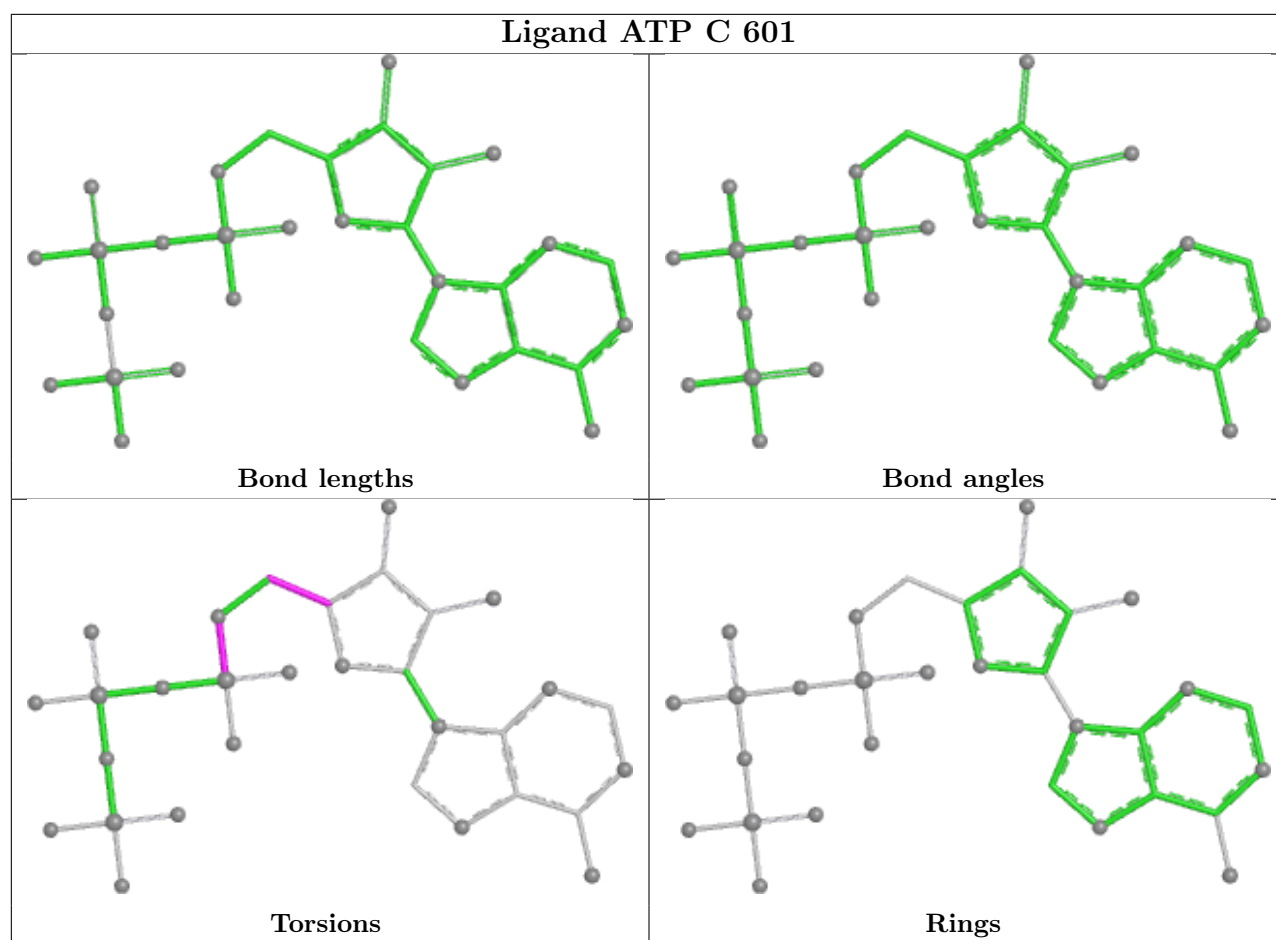




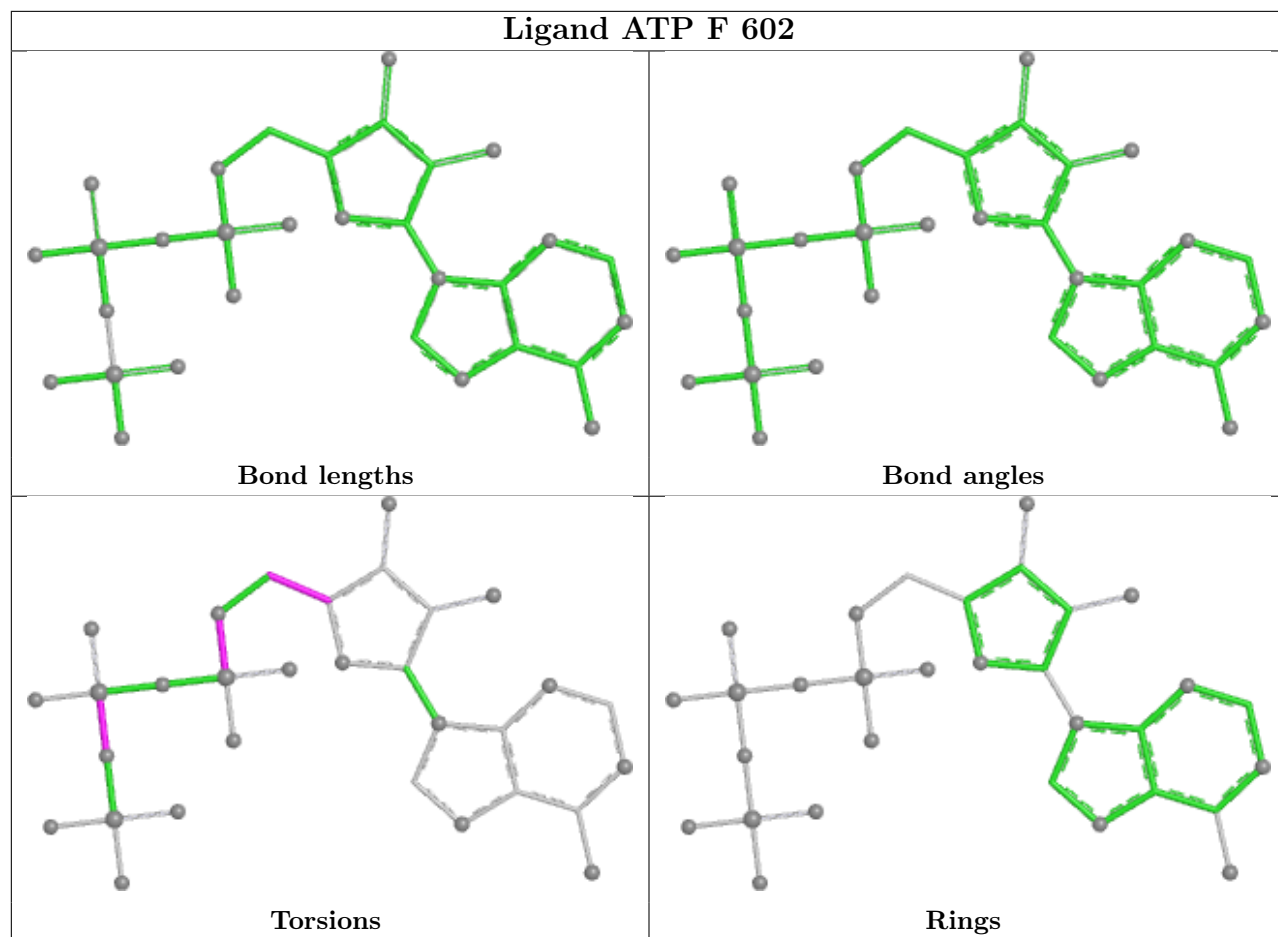




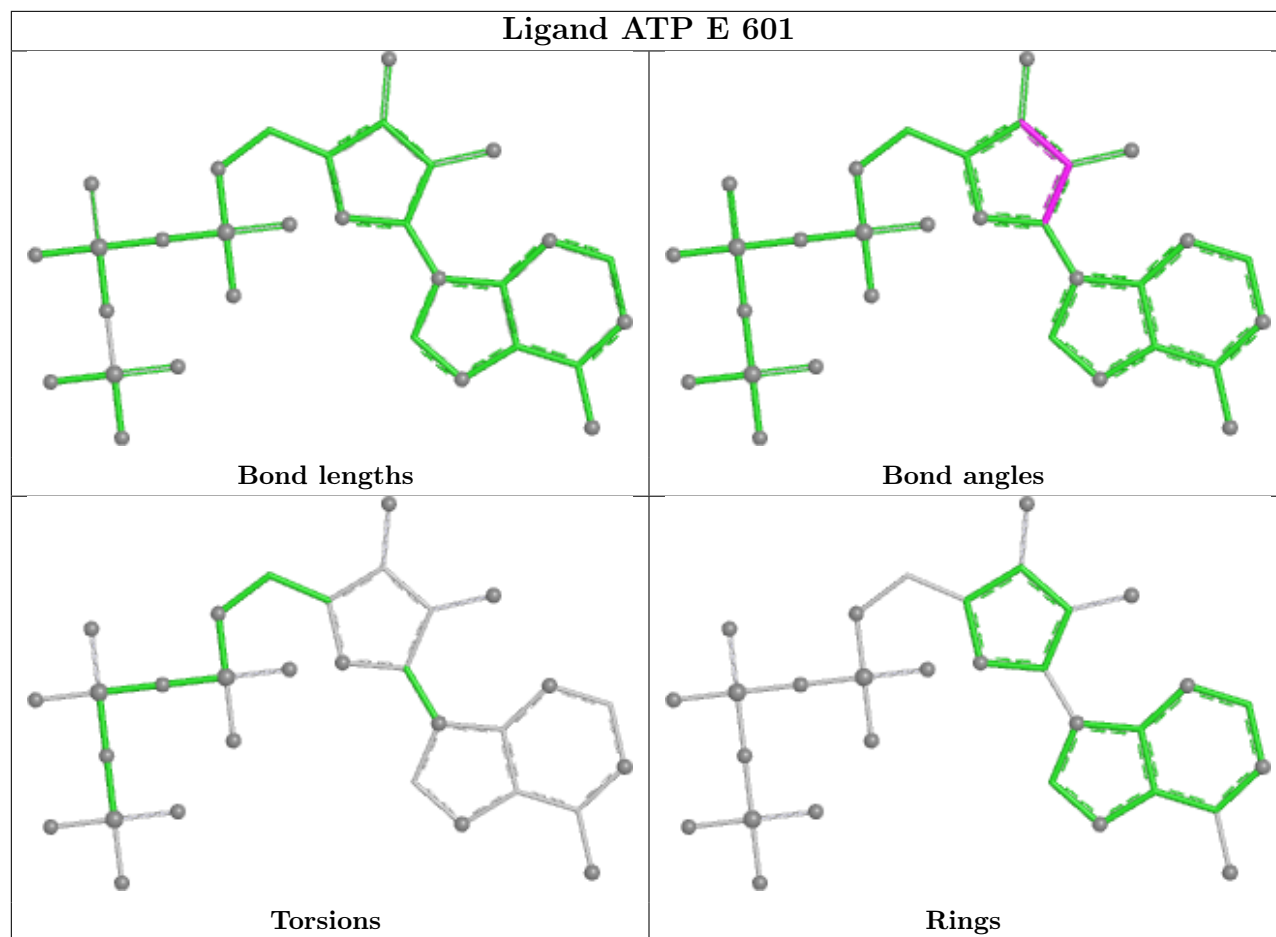


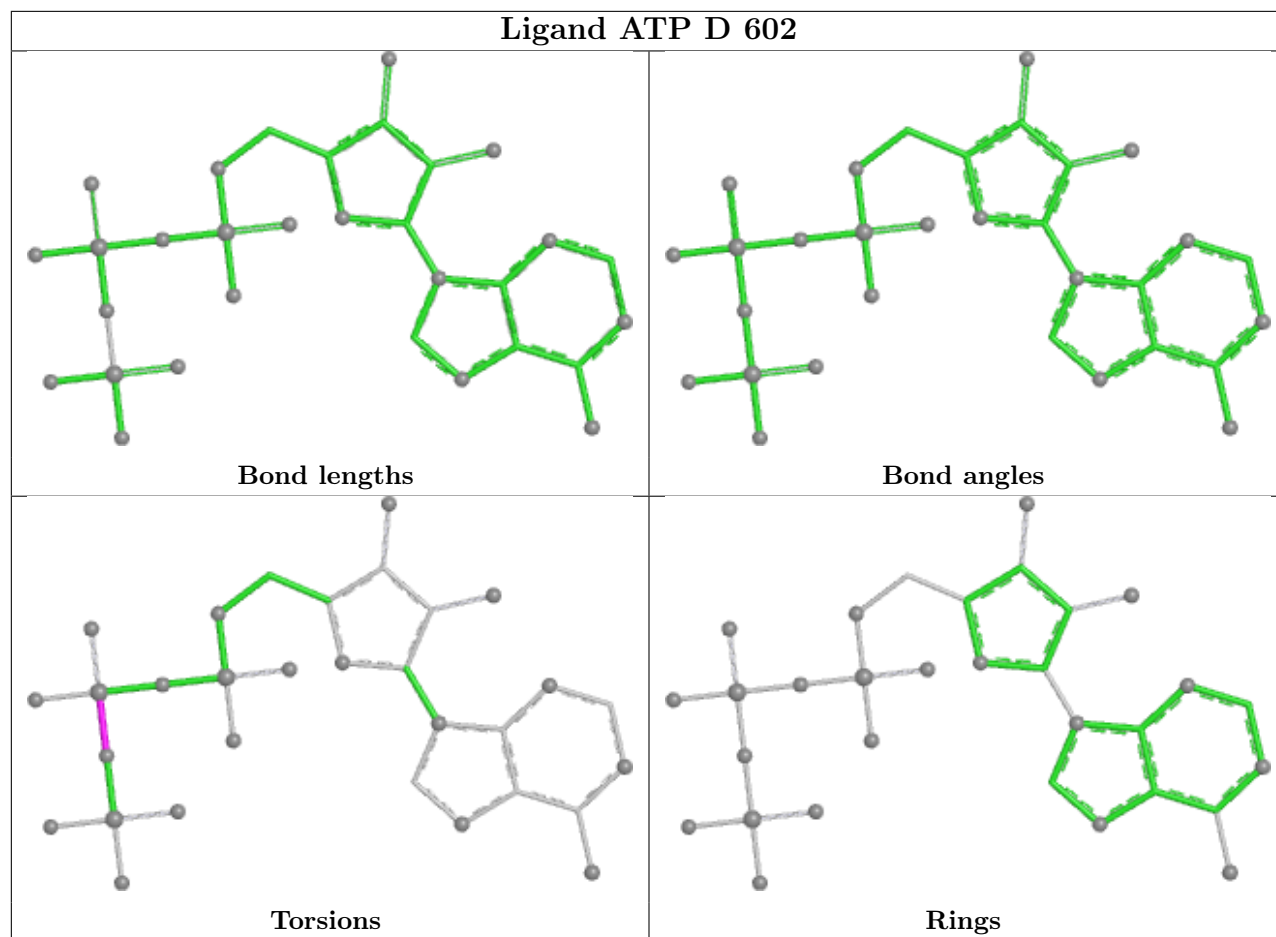


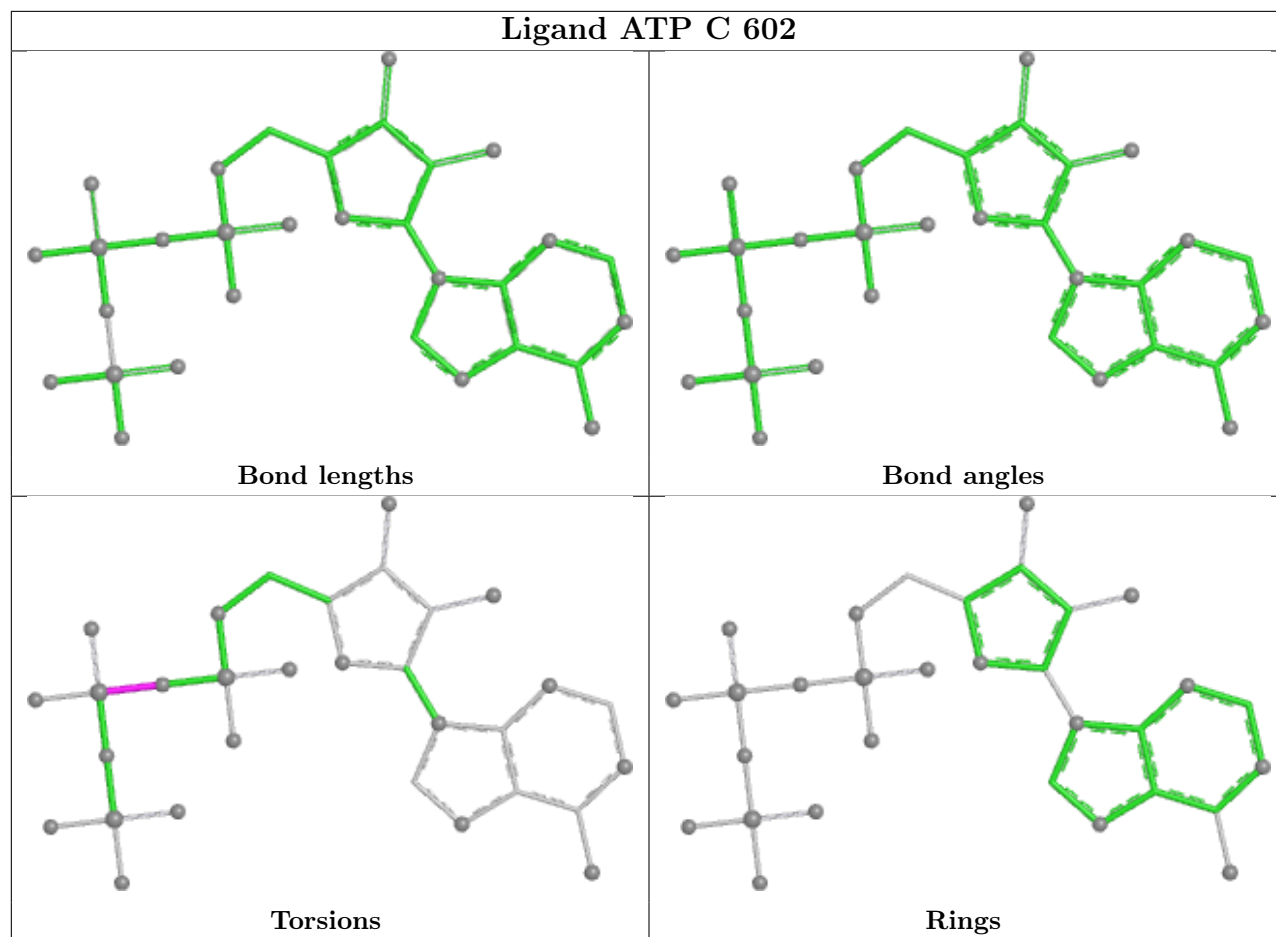
Ligand ATP F 602



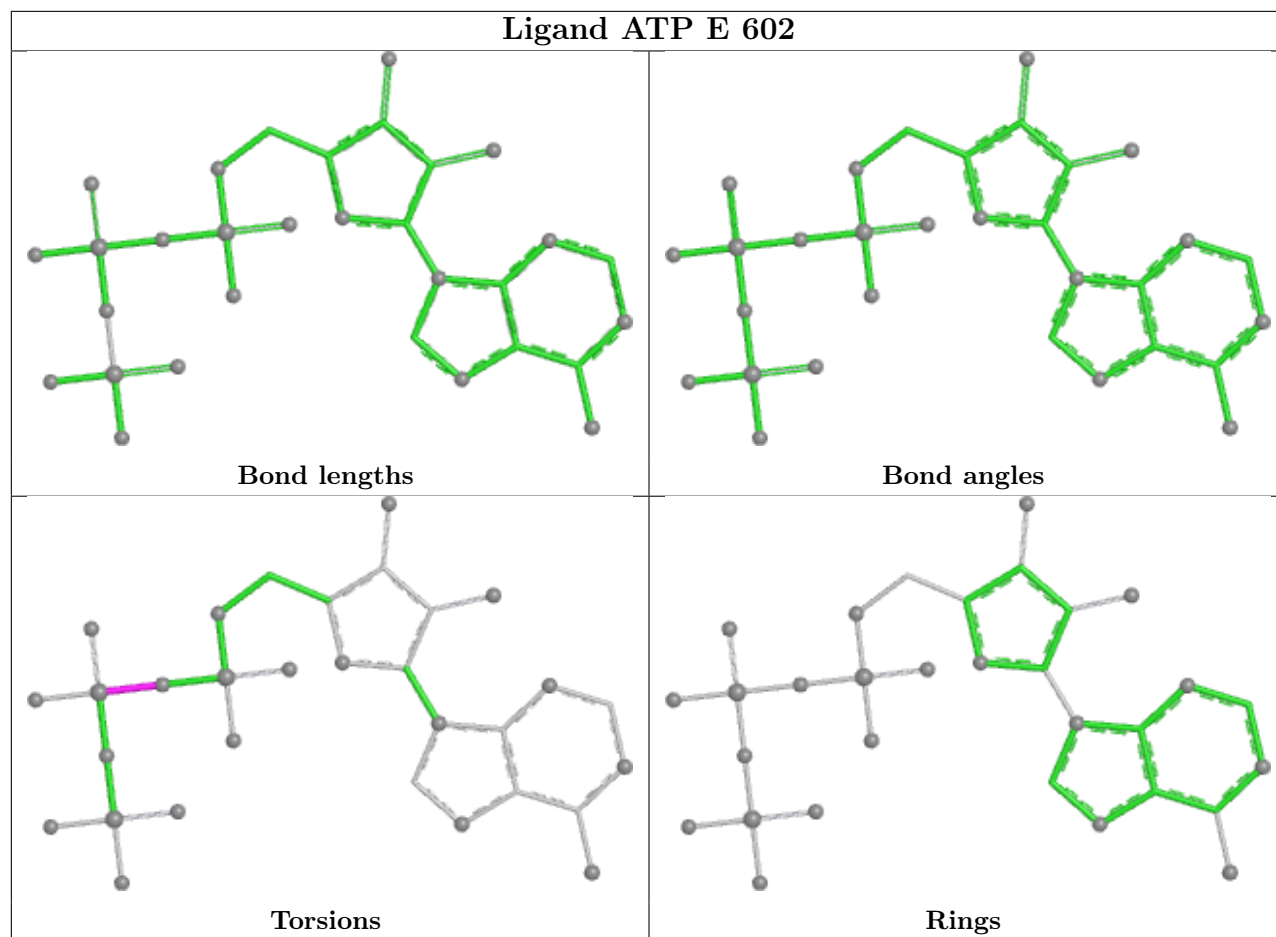
Ligand ATP E 601

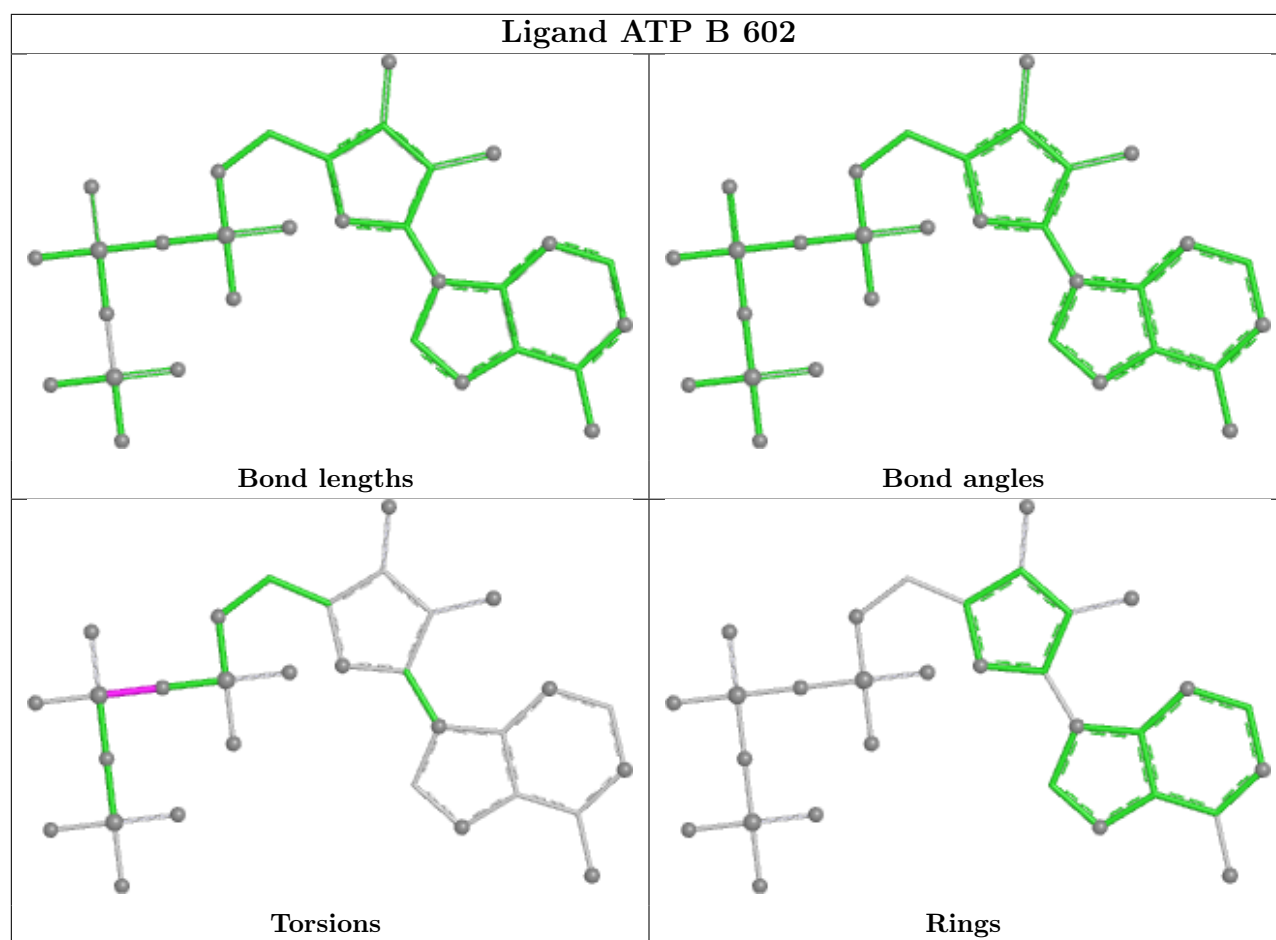






Ligand ATP E 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	461/519 (88%)	0.94	47 (10%) 12 9	25, 55, 78, 95	0
1	B	468/519 (90%)	0.49	18 (3%) 44 35	17, 38, 71, 88	1 (0%)
1	C	464/519 (89%)	0.48	22 (4%) 36 29	17, 38, 65, 105	0
1	D	460/519 (88%)	0.64	21 (4%) 37 29	19, 47, 67, 89	2 (0%)
1	E	463/519 (89%)	0.74	33 (7%) 22 16	22, 47, 76, 97	0
1	F	465/519 (89%)	0.74	27 (5%) 29 22	21, 50, 75, 92	1 (0%)
All	All	2781/3114 (89%)	0.67	168 (6%) 27 21	17, 45, 73, 105	4 (0%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	GLY	4.8
1	E	484	ARG	4.2
1	D	175	GLY	4.2
1	D	247[A]	PHE	3.8
1	E	152	GLN	3.8
1	E	254	LEU	3.8
1	C	189	GLY	3.8
1	C	15	HIS	3.7
1	A	145	ASP	3.7
1	F	389	ASN	3.6
1	F	254	LEU	3.4
1	A	306	CYS	3.4
1	A	256	GLN	3.3
1	B	16	GLN	3.3
1	A	101	GLY	3.3
1	A	417	ASP	3.2
1	F	251	ALA	3.2
1	A	488	ARG	3.2
1	F	277	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	157	SER	3.2
1	F	423	HIS	3.2
1	D	95	ALA	3.2
1	C	420	MET	3.2
1	A	140	ARG	3.1
1	F	343	LEU	3.1
1	F	152	GLN	3.1
1	A	63	GLY	3.1
1	E	347	VAL	3.1
1	B	493	SER	3.1
1	A	495	THR	3.1
1	F	255	THR	3.1
1	E	99	ASP	3.0
1	F	155	ASP	3.0
1	E	417	ASP	3.0
1	F	122	ASP	3.0
1	B	251	ALA	3.0
1	D	421	GLY	2.9
1	C	14	GLU	2.9
1	E	111	ASP	2.9
1	A	248	PRO	2.9
1	C	111	ASP	2.9
1	F	335	PHE	2.9
1	E	496	ARG	2.9
1	A	111	ASP	2.8
1	E	17	ALA	2.8
1	A	68	ASP	2.8
1	A	494	PRO	2.8
1	E	253	ARG	2.8
1	A	103	LEU	2.8
1	C	485	ASN	2.8
1	A	419	PHE	2.7
1	C	112	PRO	2.7
1	A	148	THR	2.7
1	E	255	THR	2.7
1	A	329	TYR	2.7
1	F	477	PRO	2.7
1	D	484	ARG	2.7
1	D	336	GLU	2.7
1	A	307	ALA	2.6
1	F	342	ASN	2.6
1	F	157	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	488	ARG	2.6
1	C	92	TRP	2.6
1	A	430	ILE	2.6
1	F	159	VAL	2.6
1	E	112	PRO	2.5
1	E	348	CYS	2.5
1	C	156	ALA	2.5
1	C	488	ARG	2.5
1	E	371	LYS	2.5
1	A	112	PRO	2.5
1	E	490	ILE	2.5
1	B	122	ASP	2.5
1	B	155	ASP	2.5
1	A	164	LEU	2.5
1	C	110	PRO	2.5
1	B	422	ALA	2.5
1	F	47	THR	2.5
1	C	496	ARG	2.4
1	A	441	GLN	2.4
1	A	110	PRO	2.4
1	B	417	ASP	2.4
1	D	241	ASP	2.4
1	E	461	SER	2.4
1	D	169	ALA	2.4
1	A	152	GLN	2.4
1	A	490	ILE	2.4
1	B	250	GLY	2.3
1	F	253	ARG	2.3
1	A	192	ALA	2.3
1	B	256	GLN	2.3
1	D	124	SER	2.3
1	D	149	SER	2.3
1	A	254	LEU	2.3
1	A	242	HIS	2.3
1	E	125	ALA	2.3
1	D	94	LEU	2.3
1	A	493	SER	2.3
1	A	56	SER	2.3
1	F	260	ASN	2.2
1	D	84	ILE	2.2
1	E	495	THR	2.2
1	D	146	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	100	GLU	2.2
1	F	489	ILE	2.2
1	C	423	HIS	2.2
1	A	147	VAL	2.2
1	A	317	TYR	2.2
1	E	124	SER	2.2
1	C	146	SER	2.2
1	E	492	GLY	2.2
1	D	332	GLY	2.2
1	B	385[A]	ARG	2.2
1	E	153	GLN	2.2
1	E	110	PRO	2.2
1	D	261	VAL	2.2
1	E	189	GLY	2.2
1	A	99	ASP	2.2
1	B	252	MET	2.2
1	E	175	GLY	2.2
1	A	344	LEU	2.2
1	F	158	SER	2.2
1	C	77	GLU	2.2
1	F	417	ASP	2.1
1	B	92	TRP	2.1
1	E	344	LEU	2.1
1	F	149	SER	2.1
1	F	274	CYS	2.1
1	E	407	GLU	2.1
1	B	419	PHE	2.1
1	E	176	ALA	2.1
1	C	108	ALA	2.1
1	D	329	TYR	2.1
1	E	493	SER	2.1
1	A	81	GLN	2.1
1	B	441	GLN	2.1
1	A	196	VAL	2.1
1	B	485	ASN	2.1
1	C	147	VAL	2.1
1	A	227	GLY	2.1
1	F	407	GLU	2.1
1	E	491	SER	2.1
1	C	158	SER	2.1
1	C	258	SER	2.1
1	A	420	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	80	PRO	2.1
1	F	308	ASN	2.1
1	A	460	GLY	2.1
1	E	332	GLY	2.1
1	F	492	GLY	2.1
1	E	445	ILE	2.1
1	D	489	ILE	2.1
1	A	146	SER	2.0
1	E	485	ASN	2.0
1	D	106	LEU	2.0
1	C	250	GLY	2.0
1	A	427	ASP	2.0
1	A	497	ILE	2.0
1	B	134	ILE	2.0
1	C	369	ASP	2.0
1	D	490	ILE	2.0
1	A	310	GLU	2.0
1	B	420	MET	2.0
1	E	416	SER	2.0
1	D	308	ASN	2.0
1	D	403	ALA	2.0
1	A	357	GLU	2.0
1	B	481	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	E	431	10/11	0.81	0.16	40,42,44,44	0
1	TPO	F	432	11/12	0.81	0.17	42,43,47,47	0
1	SEP	B	431	10/11	0.82	0.15	38,39,41,42	0
1	TPO	D	432	11/12	0.83	0.14	34,34,35,35	4
1	TPO	E	432	11/12	0.84	0.14	38,38,39,39	4
1	SEP	D	431	10/11	0.85	0.13	36,38,39,40	0
1	SEP	F	431	10/11	0.86	0.15	43,45,48,48	0
1	SEP	A	431	10/11	0.86	0.15	44,46,49,50	0
1	TPO	C	432	11/12	0.87	0.12	32,33,34,34	4
1	TPO	B	432	11/12	0.87	0.12	38,39,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SEP	C	431	10/11	0.87	0.15	34,36,38,38	0
1	TPO	A	432	11/12	0.91	0.11	43,43,45,45	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

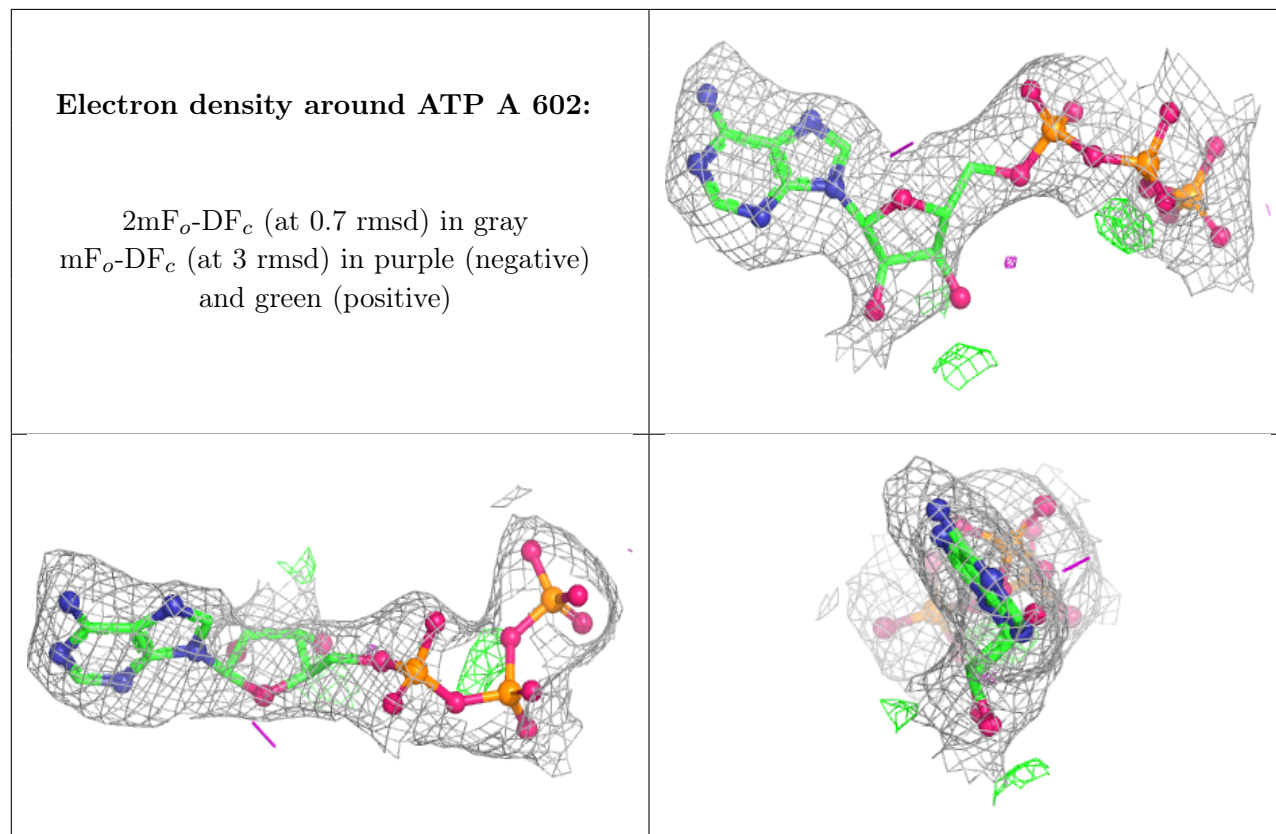
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	ATP	A	602	31/31	0.89	0.12	41,46,47,48	0
3	MG	F	603	1/1	0.90	0.06	25,25,25,25	0
3	MG	D	603	1/1	0.90	0.07	39,39,39,39	0
3	MG	F	604	1/1	0.91	0.06	50,50,50,50	0
2	ATP	F	601	31/31	0.92	0.10	30,32,34,34	0
2	ATP	E	602	31/31	0.92	0.10	40,45,49,49	0
2	ATP	D	601	31/31	0.93	0.11	38,39,41,41	0
2	ATP	A	601	31/31	0.93	0.09	35,36,37,37	0
2	ATP	F	602	31/31	0.93	0.09	51,55,58,59	0
2	ATP	C	601	31/31	0.93	0.09	32,34,36,36	0
3	MG	B	604	1/1	0.94	0.06	29,29,29,29	0
2	ATP	C	602	31/31	0.94	0.08	30,35,38,38	0
2	ATP	B	602	31/31	0.94	0.08	26,27,27,27	0
2	ATP	D	602	31/31	0.94	0.09	35,38,40,40	0
2	ATP	E	601	31/31	0.95	0.08	37,39,41,41	0
3	MG	A	604	1/1	0.96	0.10	43,43,43,43	0
3	MG	D	604	1/1	0.96	0.08	28,28,28,28	0
3	MG	A	603	1/1	0.97	0.06	63,63,63,63	0
3	MG	E	603	1/1	0.97	0.05	56,56,56,56	0
2	ATP	B	601	31/31	0.97	0.07	20,22,23,23	0
3	MG	E	604	1/1	0.98	0.03	39,39,39,39	0
3	MG	B	603	1/1	0.99	0.03	27,27,27,27	0
3	MG	C	603	1/1	0.99	0.02	28,28,28,28	0
3	MG	C	604	1/1	1.00	0.04	21,21,21,21	0

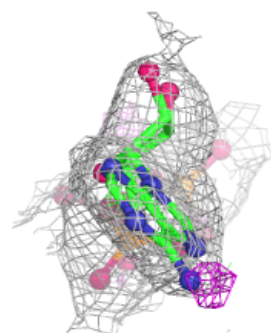
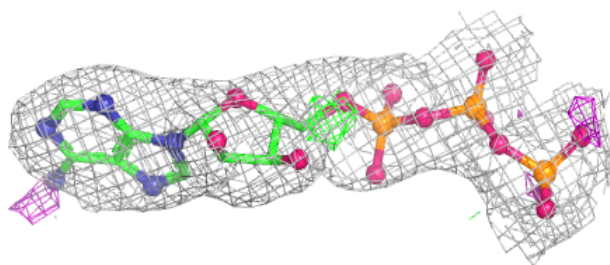
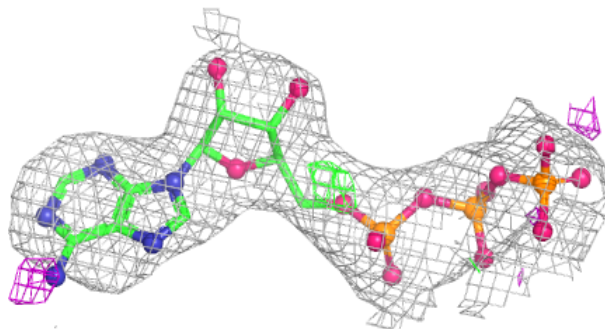
The following is a graphical depiction of the model fit to experimental electron density of all

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

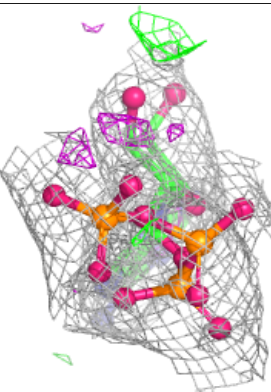
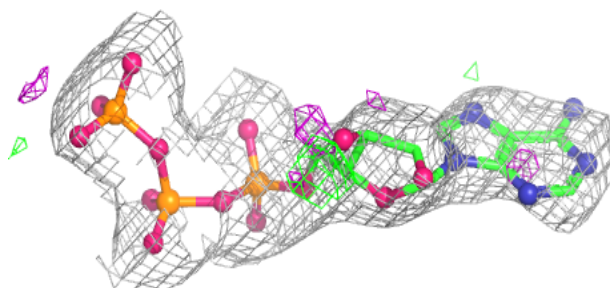
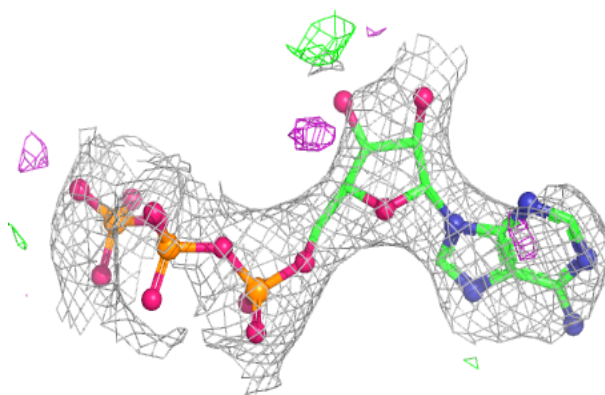


Electron density around ATP F 601:

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

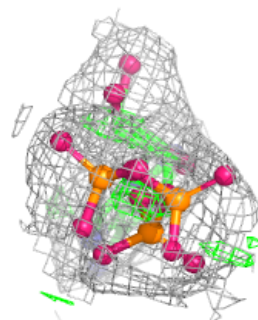
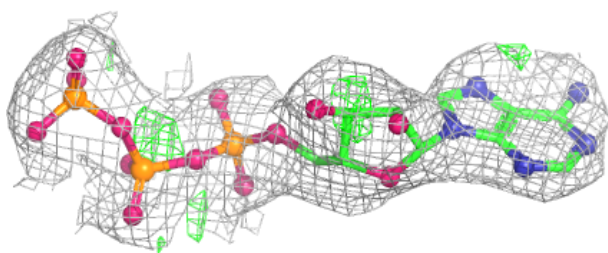
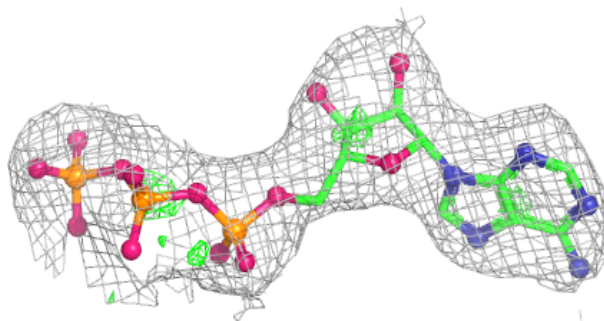
**Electron density around ATP E 602:**

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

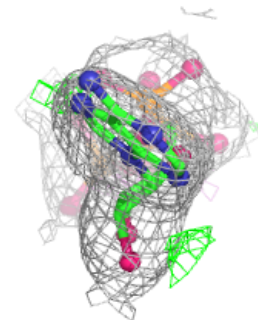
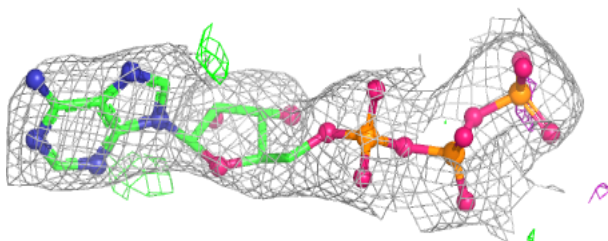
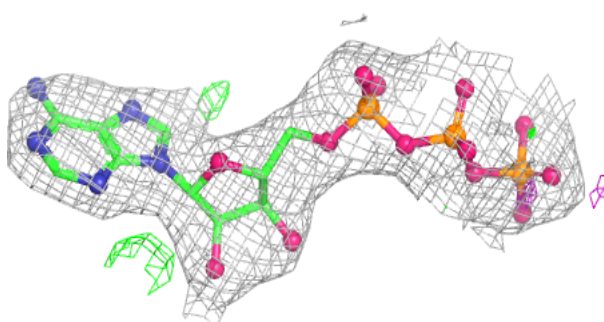


Electron density around ATP D 601:

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

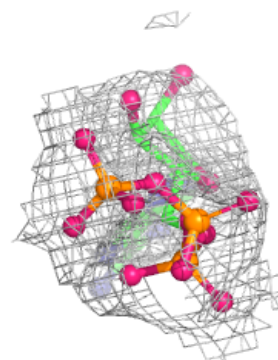
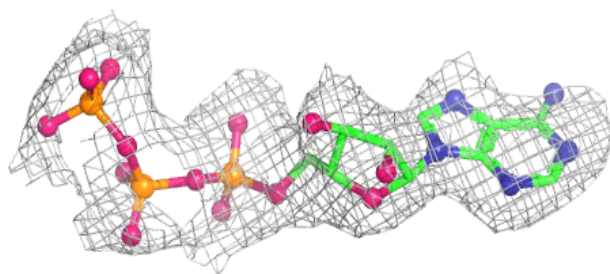
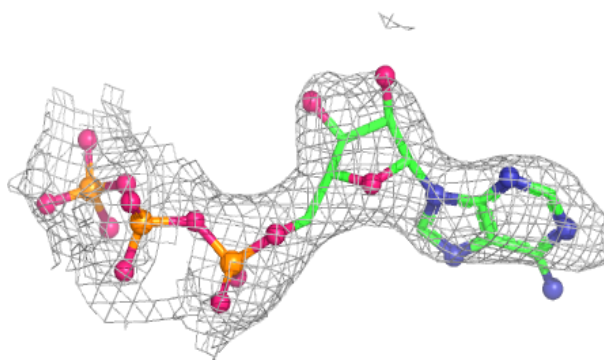
**Electron density around ATP A 601:**

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and green (positive)

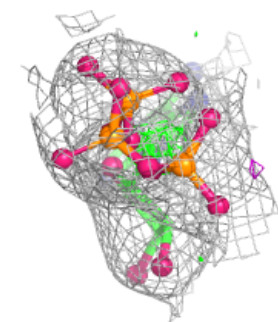
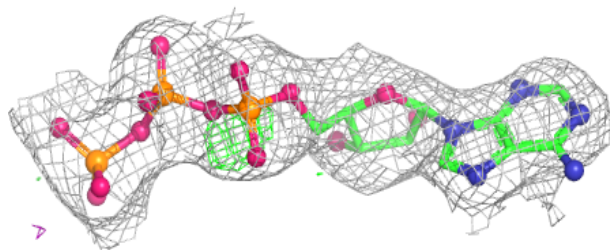
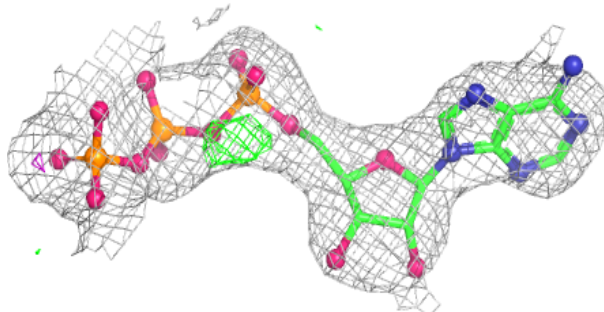


Electron density around ATP F 602:

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

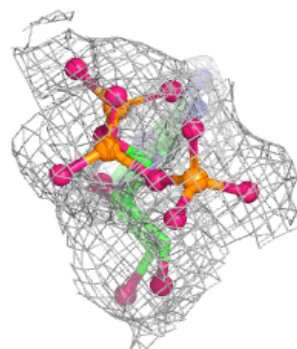
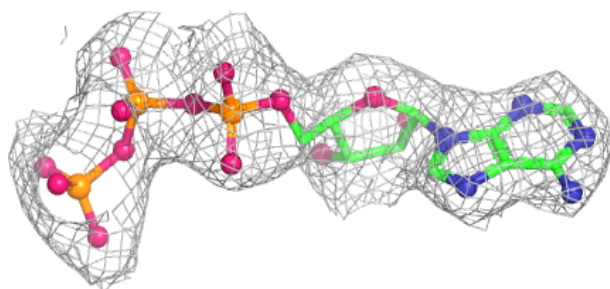
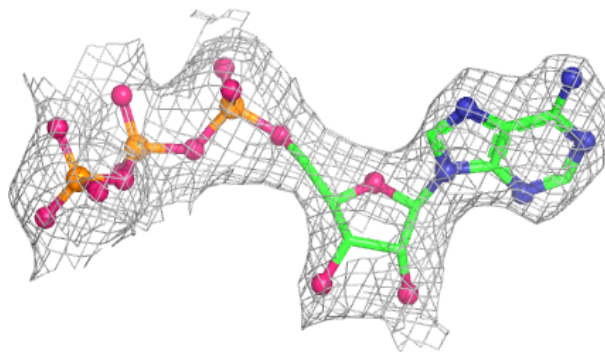
**Electron density around ATP C 601:**

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

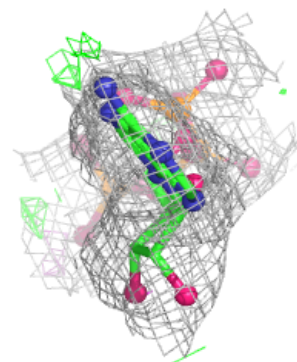
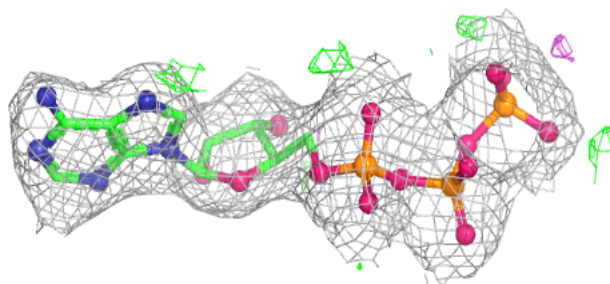
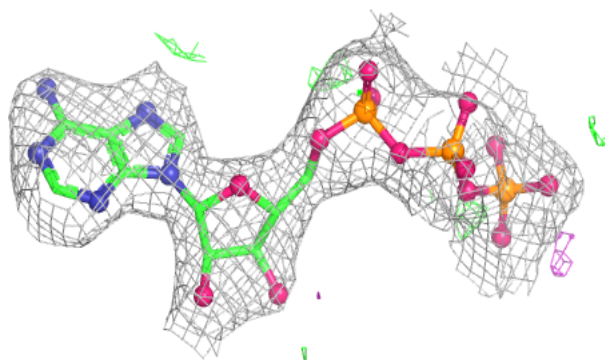


Electron density around ATP C 602:

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

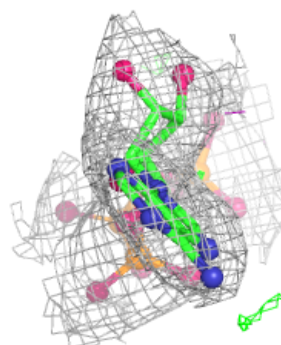
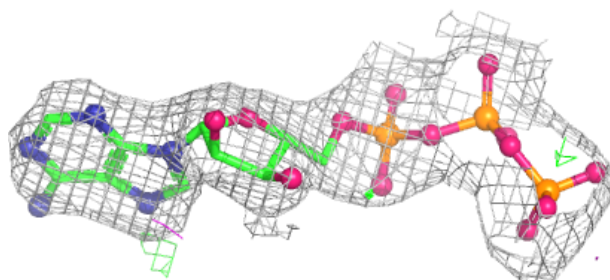
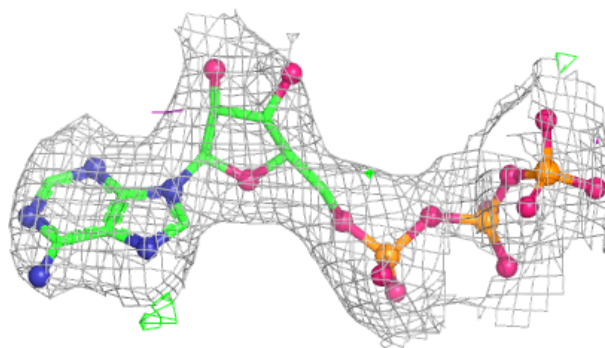
**Electron density around ATP B 602:**

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

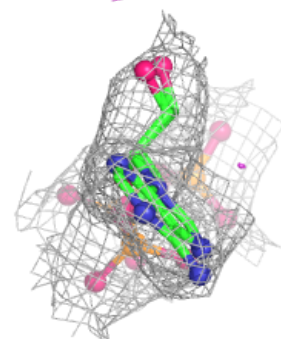
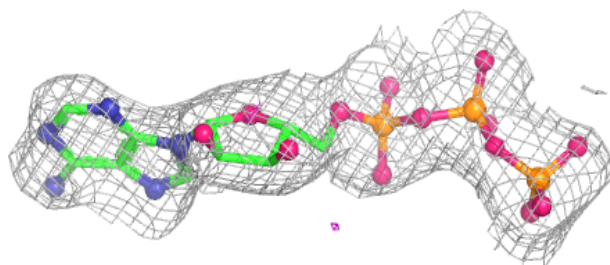
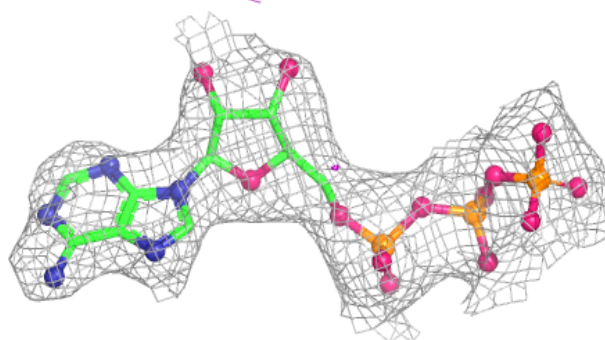


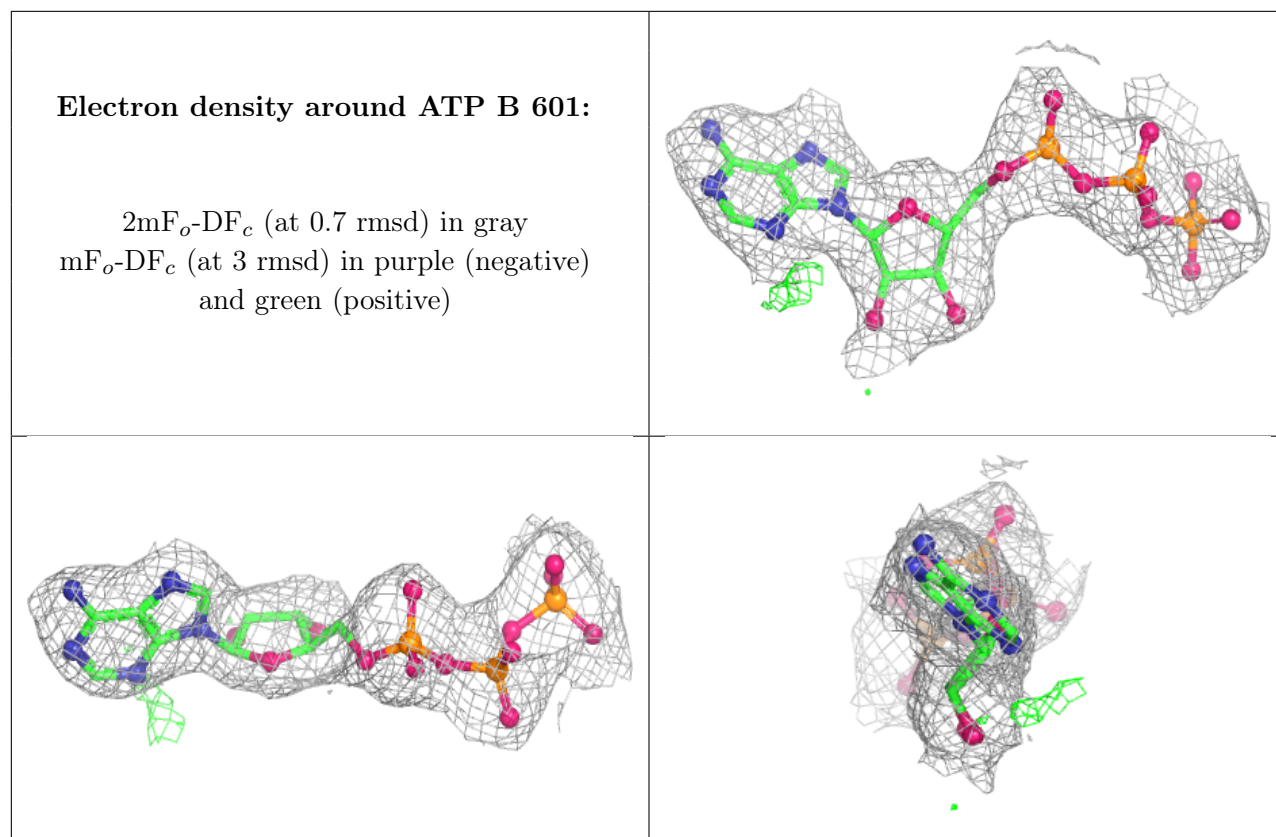
Electron density around ATP D 602:

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

**Electron density around ATP E 601:**

$2mF_o-DF_c$ (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.