



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2022 – 12:14 AM JST

PDB ID : 7DXQ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
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) : 2.27

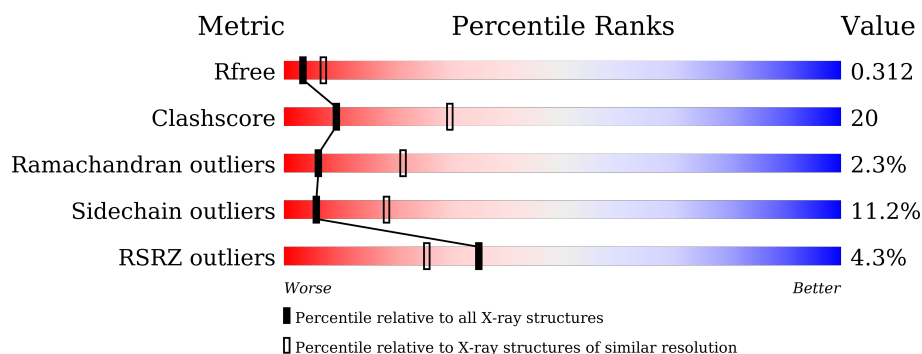
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>26%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	519	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>31%</div> <div>5%</div> <div>9%</div> </div> </div>
1	C	519	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>24%</div> <div>6%</div> <div>10%</div> </div> </div>
1	D	519	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>30%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	519	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>27%</div> <div>•</div> <div>10%</div> </div> </div>
1	F	519	<div> <div>6%</div> <div> <div></div> <div>56%</div> <div>31%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition [i](#)

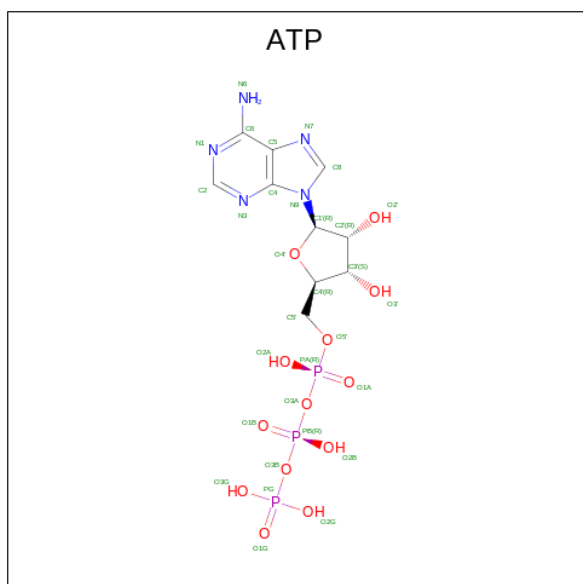
There are 4 unique types of molecules in this entry. The entry contains 21020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



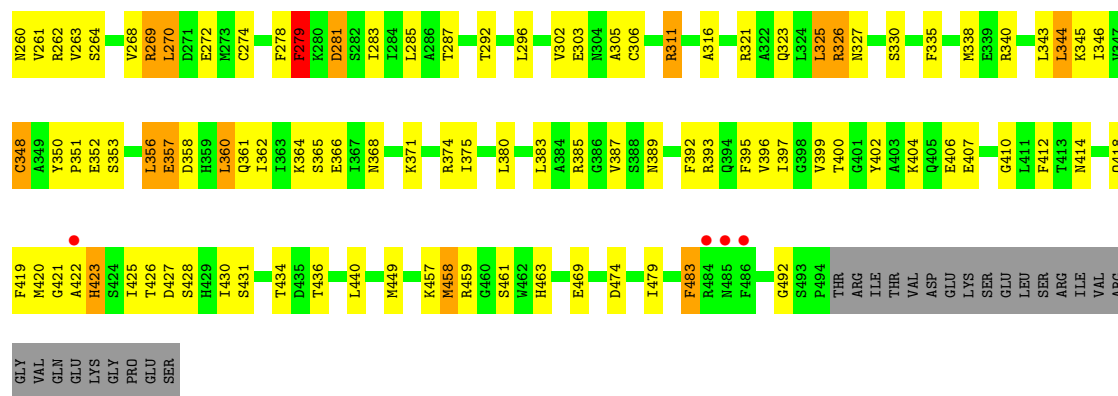
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F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

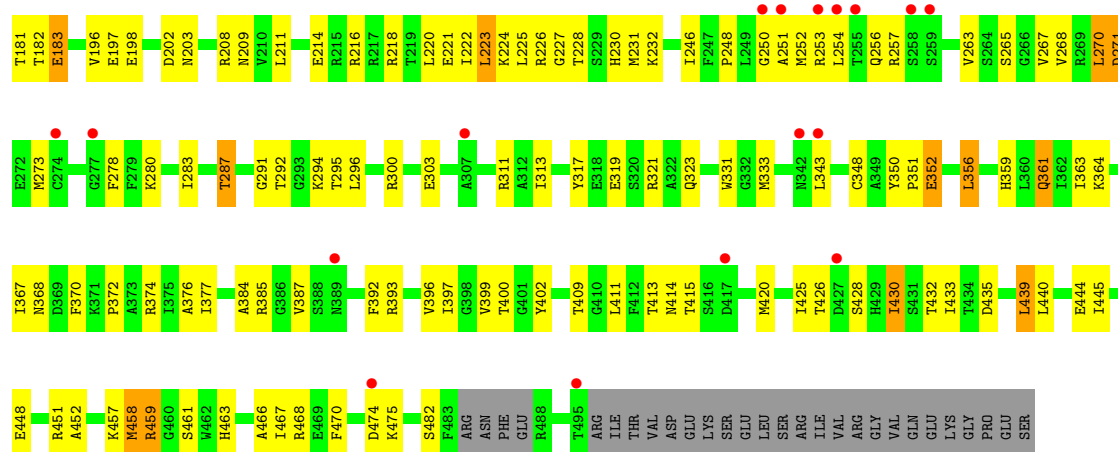
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		

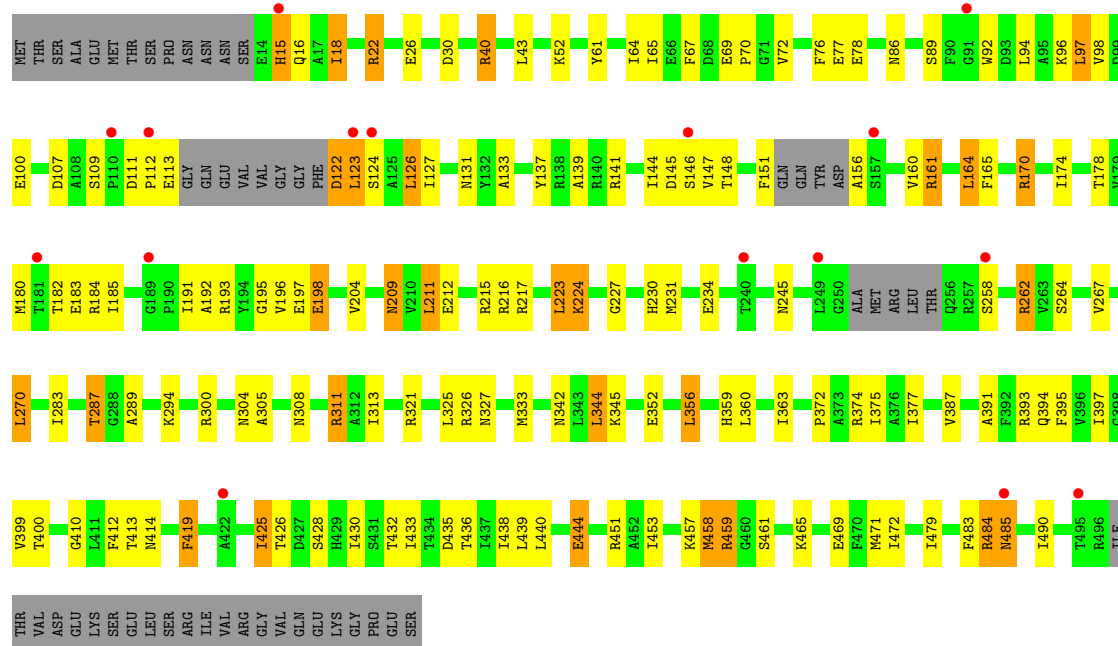
- Molecule 4 is water.

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

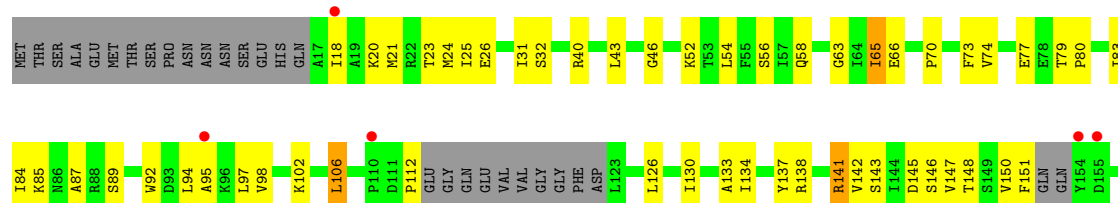


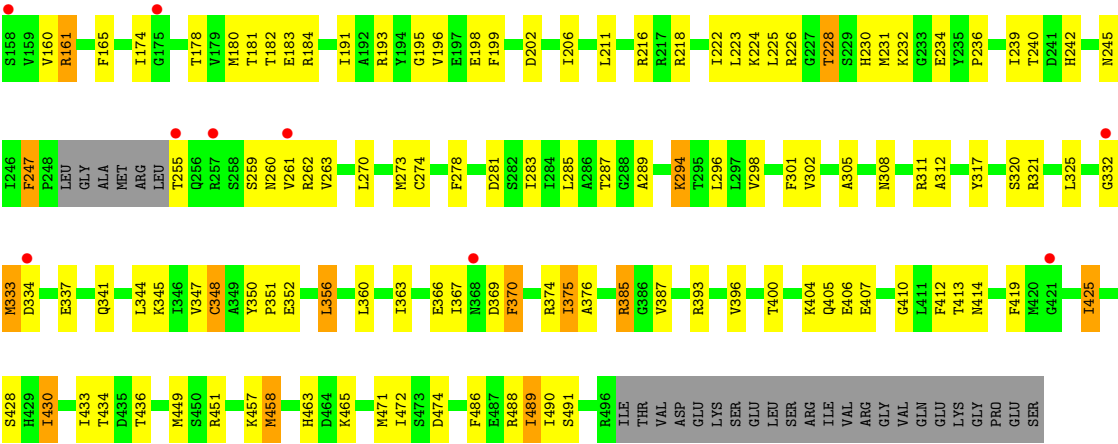


• Molecule 1: Circadian clock protein kinase KaiC



• 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 29.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.4 (29.96-2.80) 87.6 (29.94-2.80)	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 (4.93%)	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 , 49.8	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: ATP, MG, SEP, TPO

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	0.68	0/3315	0.74	0/4510
1	B	0.65	0/3600	0.72	0/4870
1	C	0.66	0/3508	0.73	0/4750
1	D	0.66	0/3467	0.73	0/4702
1	E	0.67	0/3426	0.73	0/4647
1	F	0.67	0/3439	0.73	0/4669
All	All	0.66	0/20755	0.73	0/28148

There are no bond length outliers.

There are no bond angle outliers.

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	131	0
1	B	3560	0	3445	161	0
1	C	3474	0	3343	138	0
1	D	3425	0	3262	140	0
1	E	3393	0	3166	143	0
1	F	3403	0	3162	153	0
2	A	62	0	24	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	795	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 (795) 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:C:147:VAL:HG11	1:C:180:MET:HE3	1.50	0.92
1:A:463:HIS:HE2	2:F:602:ATP:HO2'	1.10	0.92
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.49	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:273:MET:HE1	1:E:479:ILE:HD13	1.60	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: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: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
2:B:602:ATP:O3G	1:C:457:LYS:NZ	2.15	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
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:F:267:VAL:HG11	1:F:270:LEU:HB3	1.67	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: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:D:147:VAL:HG11	1:D:180:MET:HE1	1.68	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:D:301:PHE:C	1:D:374:ARG:HH21	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:490:ILE:HD11	1:D:449:MET:HE2	1.69	0.74
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:147:VAL:HG11	1:C:180:MET:HE2	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:273:MET:HE2	1:E:479:ILE:HG21	1.79	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:147:VAL:CG1	1:D:180:MET:HE1	2.27	0.64
1:D:225:LEU:HB2	1:D:230:HIS:CD2	2.33	0.63
1:A:463:HIS:CD2	2:F:602:ATP:HO2'	2.15	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:A:147:VAL:HG11	1:A:180:MET:HE3	1.81	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
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
1:A:457:LYS:NZ	2:F:602:ATP:O3G	2.33	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:300:ARG:HD3	1:C:333:MET:HE3	1.82	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:F:52:LYS:NZ	2:F:601:ATP:O3G	2.40	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:D:147:VAL:CG1	1:D:180:MET:CE	2.84	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:NH2	1:B:461:SER:HB2	2.23	0.54
1:F:458:MET:HE2	1:F:461:SER:HB3	1.90	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: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:D:191:ILE:HD12	1:D:206:ILE:HD11	1.89	0.53
1:D:332:GLY:C	1:D:333:MET:HG2	2.27	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:184:ARG:C	1:C:185:ILE:HD13	2.30	0.52
1:C:191:ILE:HB	1:C:198:GLU:HG2	1.91	0.52
1:D:56:SER:HG	1:D:73:PHE:HE1	1.57	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
1:E:321:ARG:O	1:E:325:LEU:HG	2.10	0.51
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: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:A:52:LYS:HD2	1:A:182:THR:O	2.10	0.51
1:A:234:GLU:OE2	1:F:211:LEU:HD21	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:602:ATP:O2G	1:D:457:LYS:NZ	2.42	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: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: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: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
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:E:273:MET:HE3	1:E:479:ILE:HD13	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385[A]:ARG:HD2	1:C:393:ARG:CD	2.43	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:F:267:VAL:C	1:F:268:VAL:HG23	2.33	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
2:E:602:ATP:HO2'	1:F:463:HIS:CD2	2.24	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:E:273:MET:HE1	1:E:479:ILE:HG21	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:C:483:PHE:C	1:C:485:ASN:CB	2.83	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: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:A:419:PHE:HD1	1:A:420:MET:HE2	1.79	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:A:269:ARG:O	1:A:272:GLU:N	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:HA	1:A:173:GLN:NE2	2.29	0.47
1:A:404:LYS:C	1:A:406:GLU:H	2.17	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:C:300:ARG:HG2	1:C:333:MET:HE1	1.96	0.47
1:B:292:THR:HB	1:B:440:LEU:HB3	1.97	0.46
1:F:300:ARG:HA	1:F:333:MET:HE3	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
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:C:64:ILE:HG21	1:C:97:LEU:HD12	1.97	0.46
1:A:147:VAL:C	1:A:150:VAL:HG12	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:387:VAL:HG12	1:C:391:ALA:HB3	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:110:PRO:HB2	1:E:111:ASP:C	2.37	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
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: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:B:147:VAL:HG21	1:B:180:MET:CE	2.48	0.44
1:E:463:HIS:NE2	2:D:602:ATP:O2'	2.46	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: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: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:240:THR:C	1:D:242:HIS:H	2.22	0.43
1:D:296:LEU:HD22	1:D:472:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:300:ARG:CD	1:C:333:MET:HE1	2.48	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:B:45:SER:CB	1:B:182:THR:HB	2.49	0.43
1:B:303:GLU:HA	1:B:338:MET:HE3	2.00	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
1:C:161:ARG:CB	1:C:196:VAL:HG11	2.49	0.43
1:B:134:ILE:HD13	1:B:134:ILE:C	2.38	0.43
1:E:296:LEU:HD12	1:E:296:LEU:O	2.19	0.43
1:C:483:PHE:O	1:C:484:ARG:C	2.57	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
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:392:PHE:O	1:A:395:PHE:HB3	2.18	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:A:57:ILE:HD11	1:A:73:PHE:CE1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:ILE:HD13	1:E:73:PHE:CE1	2.54	0.42
1:F:303:GLU:CB	1:F:333:MET:HE2	2.49	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:A:281:ASP:CG	1:A:407:GLU:HG3	2.40	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
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: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:A:458:MET:HB3	1:A:458:MET:HE2	1.83	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
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:B:70:PRO:HB2	1:B:139:ALA:HA	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASN:C	1:B:134:ILE:HG22	2.40	0.41
1:E:184:ARG:C	1:E:185:ILE:HD13	2.41	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
1:D:305:ALA:HB2	1:D:374:ARG:HD3	2.02	0.41
1:A:64:ILE:C	1:A:66:GLU:H	2.23	0.41
1:A:307:ALA:C	1:A:309:LYS:H	2.23	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: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
2:B:601:ATP:HO2'	1:C:230:HIS:CD2	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:F:231:MET:HE1	1:F:251:ALA:O	2.21	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:F:361:GLN:NE2	1:F:361:GLN:CA	2.79	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:B:303:GLU:HA	1:B:338:MET:CE	2.50	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:C:156:ALA:C	1:C:160:VAL:HG23	2.41	0.40
1:C:165:PHE:CD2	1:C:165:PHE:C	2.93	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%)	4	15
1	B	463/519 (89%)	418 (90%)	35 (8%)	10 (2%)	6	22
1	C	456/519 (88%)	411 (90%)	38 (8%)	7 (2%)	10	33
1	D	454/519 (88%)	416 (92%)	30 (7%)	8 (2%)	8	28
1	E	455/519 (88%)	398 (88%)	46 (10%)	11 (2%)	6	20
1	F	458/519 (88%)	397 (87%)	48 (10%)	13 (3%)	5	17
All	All	2739/3114 (88%)	2419 (88%)	258 (9%)	62 (2%)	6	21

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	257 (87%)	38 (13%)	4	13
1	B	359/442 (81%)	317 (88%)	42 (12%)	5	16
1	C	347/442 (78%)	309 (89%)	38 (11%)	6	19
1	D	337/442 (76%)	299 (89%)	38 (11%)	6	18
1	E	320/442 (72%)	283 (88%)	37 (12%)	5	17
1	F	324/442 (73%)	294 (91%)	30 (9%)	9	26
All	All	1982/2652 (75%)	1759 (89%)	223 (11%)	6	18

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
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	260	ASN

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Mol	Chain	Res	Type
1	A	269	ARG
1	A	270	LEU
1	A	281	ASP
1	A	294	LYS
1	A	300	ARG
1	A	329	TYR
1	A	333	MET
1	A	342	ASN
1	A	352	GLU
1	A	356	LEU
1	A	360	LEU
1	A	368	ASN
1	A	374	ARG
1	A	375	ILE
1	A	385	ARG
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	474	ASP
1	B	20	LYS
1	B	24	MET
1	B	75	THR
1	B	81	GLN
1	B	92	TRP
1	B	124	SER
1	B	134	ILE
1	B	135	GLN
1	B	140	ARG
1	B	161	ARG
1	B	164	LEU
1	B	191	ILE
1	B	193	ARG
1	B	198	GLU
1	B	209	ASN
1	B	223	LEU
1	B	228	THR
1	B	245	ASN
1	B	257	ARG

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Mol	Chain	Res	Type
1	B	269	ARG
1	B	270	LEU
1	B	279	PHE
1	B	296	LEU
1	B	311	ARG
1	B	323	GLN
1	B	325	LEU
1	B	326	ARG
1	B	340	ARG
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	361	GLN
1	B	365	SER
1	B	366	GLU
1	B	406	GLU
1	B	427	ASP
1	B	457	LYS
1	B	458	MET
1	B	483	PHE
1	E	18	ILE
1	E	20	LYS
1	E	30	ASP
1	E	40	ARG
1	E	68	ASP
1	E	69	GLU
1	E	96	LYS
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	221	GLU
1	E	223	LEU
1	E	228	THR
1	E	232	LYS
1	E	245	ASN
1	E	254	LEU

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Mol	Chain	Res	Type
1	E	270	LEU
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	385	ARG
1	E	390	ASN
1	E	428	SER
1	E	441	GLN
1	E	458	MET
1	E	469	GLU
1	E	474	ASP
1	F	22	ARG
1	F	24	MET
1	F	26	GLU
1	F	40	ARG
1	F	45	SER
1	F	99	ASP
1	F	131	ASN
1	F	140	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
1	F	232	LYS
1	F	252	MET
1	F	270	LEU
1	F	271	ASP
1	F	287	THR
1	F	350	TYR
1	F	352	GLU
1	F	356	LEU
1	F	361	GLN

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Mol	Chain	Res	Type
1	F	370	PHE
1	F	430	ILE
1	F	439	LEU
1	F	458	MET
1	F	459	ARG
1	F	470	PHE
1	C	18	ILE
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	131	ASN
1	C	161	ARG
1	C	164	LEU
1	C	170	ARG
1	C	178	THR
1	C	198	GLU
1	C	209	ASN
1	C	211	LEU
1	C	223	LEU
1	C	224	LYS
1	C	231	MET
1	C	234	GLU
1	C	258	SER
1	C	262	ARG
1	C	270	LEU
1	C	287	THR
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

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Mol	Chain	Res	Type
1	C	459	ARG
1	C	471	MET
1	D	24	MET
1	D	79	THR
1	D	106	LEU
1	D	141	ARG
1	D	161	ARG
1	D	193	ARG
1	D	223	LEU
1	D	228	THR
1	D	232	LYS
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	294	LYS
1	D	344	LEU
1	D	345	LYS
1	D	348	CYS
1	D	352	GLU
1	D	356	LEU
1	D	360	LEU
1	D	369	ASP
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	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 (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	173	GLN
1	A	209	ASN
1	A	260	ASN
1	A	368	ASN
1	A	414	ASN
1	B	209	ASN
1	B	245	ASN
1	B	260	ASN
1	B	368	ASN
1	B	414	ASN
1	B	418	GLN
1	E	173	GLN
1	E	209	ASN
1	E	256	GLN
1	E	414	ASN
1	F	131	ASN
1	F	209	ASN
1	F	245	ASN
1	F	361	GLN
1	F	389	ASN
1	F	414	ASN
1	C	62	ASN
1	C	209	ASN
1	C	304	ASN
1	C	414	ASN
1	C	418	GLN
1	C	441	GLN
1	D	209	ASN
1	D	256	GLN
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	SEP	D	431	1	8,9,10	0.59	0	8,12,14	0.66	0
1	SEP	B	431	1	8,9,10	0.62	0	8,12,14	0.61	0
1	TPO	F	432	1	8,10,11	0.83	0	10,14,16	0.81	0
1	TPO	E	432	1	8,10,11	0.81	0	10,14,16	0.84	0
1	SEP	A	431	1	8,9,10	0.59	0	8,12,14	0.65	0
1	TPO	A	432	1	8,10,11	0.70	0	10,14,16	0.86	0
1	TPO	C	432	1	8,10,11	0.76	0	10,14,16	0.86	0
1	SEP	E	431	1	8,9,10	0.59	0	8,12,14	0.66	0
1	SEP	C	431	1	8,9,10	0.62	0	8,12,14	0.60	0
1	TPO	B	432	1	8,10,11	0.84	0	10,14,16	0.87	0
1	TPO	D	432	1	8,10,11	0.84	0	10,14,16	0.88	0
1	SEP	F	431	1	8,9,10	0.62	0	8,12,14	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	D	431	1	-	1/5/8/10	-
1	SEP	B	431	1	-	2/5/8/10	-
1	TPO	F	432	1	-	0/9/11/13	-
1	TPO	E	432	1	-	0/9/11/13	-
1	SEP	A	431	1	-	1/5/8/10	-
1	TPO	A	432	1	-	1/9/11/13	-
1	TPO	C	432	1	-	0/9/11/13	-
1	SEP	E	431	1	-	1/5/8/10	-
1	SEP	C	431	1	-	1/5/8/10	-
1	TPO	B	432	1	-	0/9/11/13	-
1	TPO	D	432	1	-	1/9/11/13	-
1	SEP	F	431	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) 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	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

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	F	432	TPO	1	0
1	A	432	TPO	2	0
1	C	432	TPO	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	26,33,33	0.65	0	31,52,52	0.96	2 (6%)
2	ATP	B	601	3	26,33,33	0.66	0	31,52,52	1.00	2 (6%)
2	ATP	E	601	3	26,33,33	0.67	0	31,52,52	0.99	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	D	601	3	26,33,33	0.66	0	31,52,52	0.90	2 (6%)
2	ATP	A	601	3	26,33,33	0.67	0	31,52,52	0.95	2 (6%)
2	ATP	A	602	3	26,33,33	0.67	0	31,52,52	1.04	2 (6%)
2	ATP	C	601	3	26,33,33	0.66	0	31,52,52	0.99	2 (6%)
2	ATP	D	602	3	26,33,33	0.66	0	31,52,52	0.81	1 (3%)
2	ATP	F	602	3	26,33,33	0.67	0	31,52,52	0.77	1 (3%)
2	ATP	B	602	3	26,33,33	0.66	0	31,52,52	0.88	2 (6%)
2	ATP	E	602	3	26,33,33	0.67	0	31,52,52	0.94	2 (6%)
2	ATP	C	602	3	26,33,33	0.66	0	31,52,52	0.92	2 (6%)

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	-	5/18/38/38	0/3/3/3
2	ATP	B	601	3	-	7/18/38/38	0/3/3/3
2	ATP	E	601	3	-	0/18/38/38	0/3/3/3
2	ATP	D	601	3	-	6/18/38/38	0/3/3/3
2	ATP	A	601	3	-	5/18/38/38	0/3/3/3
2	ATP	A	602	3	-	5/18/38/38	0/3/3/3
2	ATP	C	601	3	-	5/18/38/38	0/3/3/3
2	ATP	D	602	3	-	1/18/38/38	0/3/3/3
2	ATP	F	602	3	-	5/18/38/38	0/3/3/3
2	ATP	B	602	3	-	0/18/38/38	0/3/3/3
2	ATP	E	602	3	-	1/18/38/38	0/3/3/3
2	ATP	C	602	3	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	ATP	C3'-C2'-C1'	3.41	106.12	100.98
2	B	601	ATP	C3'-C2'-C1'	3.03	105.54	100.98
2	E	601	ATP	C3'-C2'-C1'	2.89	105.33	100.98
2	C	601	ATP	C3'-C2'-C1'	2.82	105.22	100.98
2	A	601	ATP	C3'-C2'-C1'	2.63	104.94	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	ATP	C3'-C2'-C1'	2.63	104.93	100.98
2	E	602	ATP	C3'-C2'-C1'	2.61	104.91	100.98
2	C	602	ATP	C3'-C2'-C1'	2.52	104.78	100.98
2	A	601	ATP	C5-C6-N6	2.41	124.01	120.35
2	F	601	ATP	C5-C6-N6	2.39	123.98	120.35
2	C	601	ATP	C5-C6-N6	2.36	123.94	120.35
2	D	601	ATP	C3'-C2'-C1'	2.32	104.46	100.98
2	E	601	ATP	C5-C6-N6	2.30	123.85	120.35
2	B	601	ATP	C5-C6-N6	2.29	123.84	120.35
2	D	602	ATP	C5-C6-N6	2.29	123.83	120.35
2	B	602	ATP	C5-C6-N6	2.28	123.81	120.35
2	D	601	ATP	C5-C6-N6	2.27	123.81	120.35
2	C	602	ATP	C5-C6-N6	2.24	123.76	120.35
2	E	602	ATP	C5-C6-N6	2.22	123.73	120.35
2	A	602	ATP	C5-C6-N6	2.22	123.73	120.35
2	B	602	ATP	C3'-C2'-C1'	2.22	104.31	100.98
2	F	602	ATP	C5-C6-N6	2.20	123.69	120.35

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A
2	A	601	ATP	C5'-O5'-PA-O2A
2	A	602	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	C5'-O5'-PA-O2A
2	F	601	ATP	C5'-O5'-PA-O1A
2	F	601	ATP	C5'-O5'-PA-O2A
2	F	601	ATP	O4'-C4'-C5'-O5'
2	F	601	ATP	C3'-C4'-C5'-O5'
2	F	602	ATP	C5'-O5'-PA-O1A
2	F	602	ATP	C3'-C4'-C5'-O5'
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	A	602	ATP	C3'-C4'-C5'-O5'
2	B	601	ATP	C3'-C4'-C5'-O5'
2	A	601	ATP	O4'-C4'-C5'-O5'
2	C	601	ATP	C3'-C4'-C5'-O5'
2	F	602	ATP	O4'-C4'-C5'-O5'

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

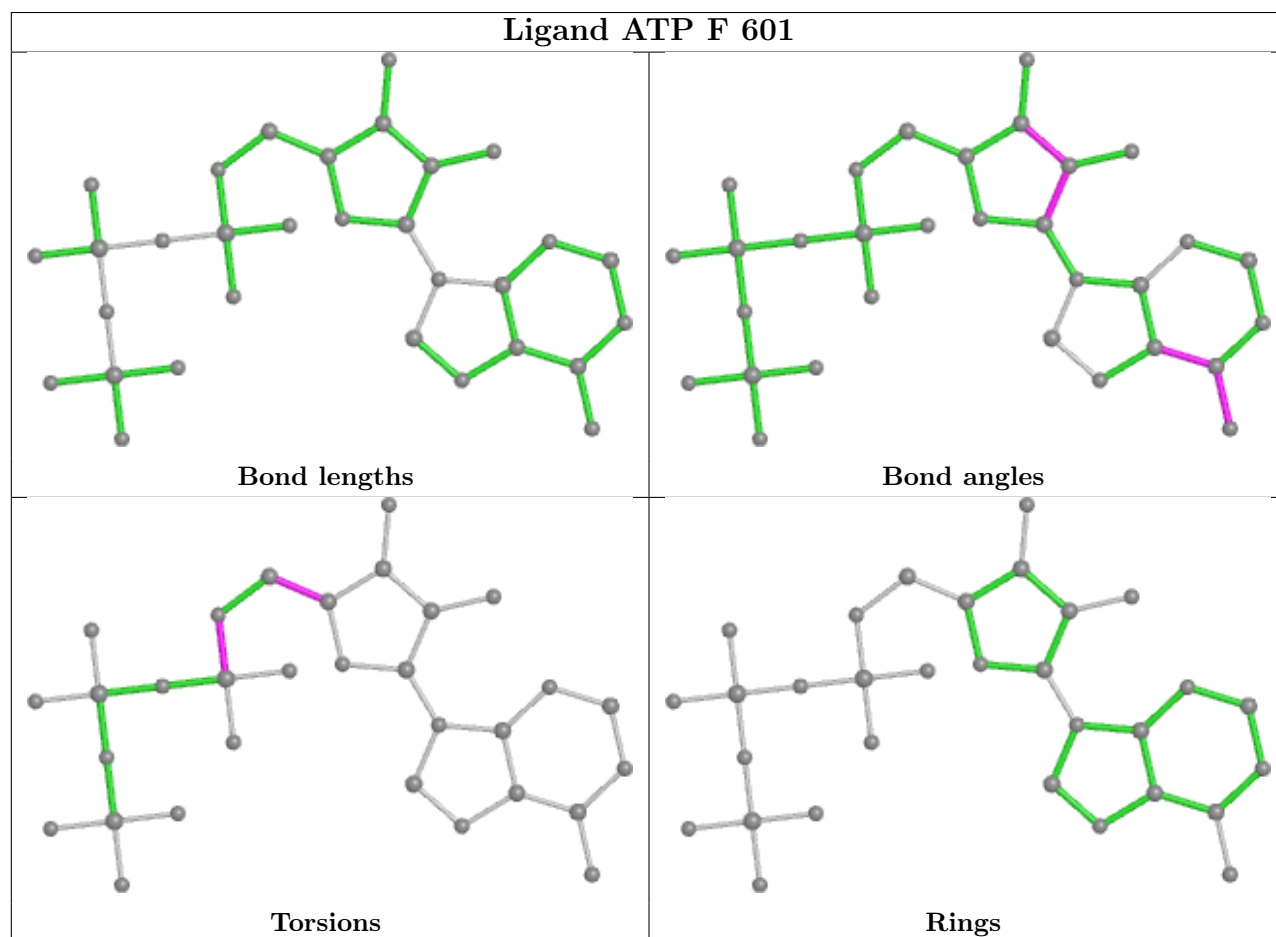
There are no ring outliers.

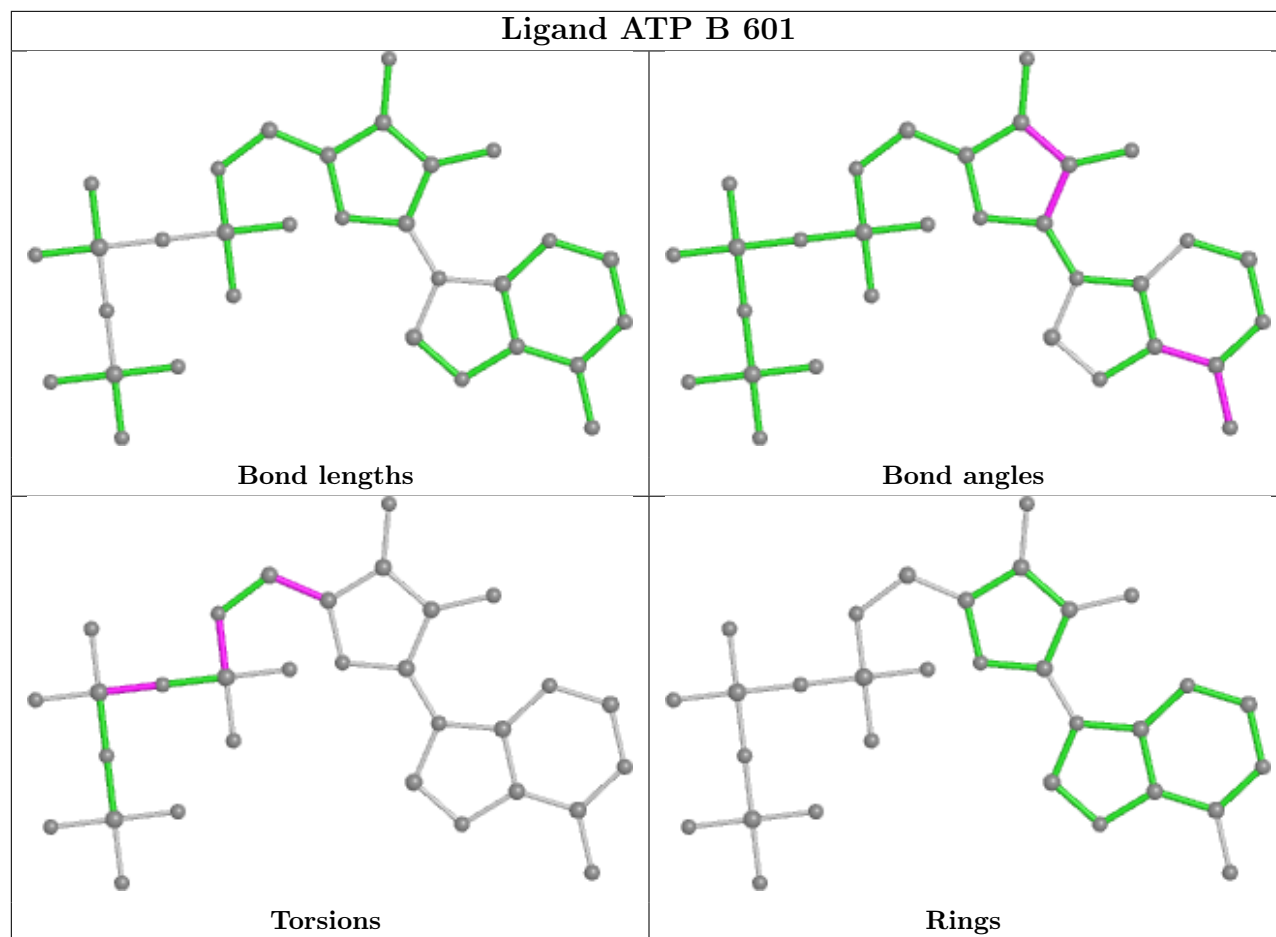
11 monomers are involved in 36 short contacts:

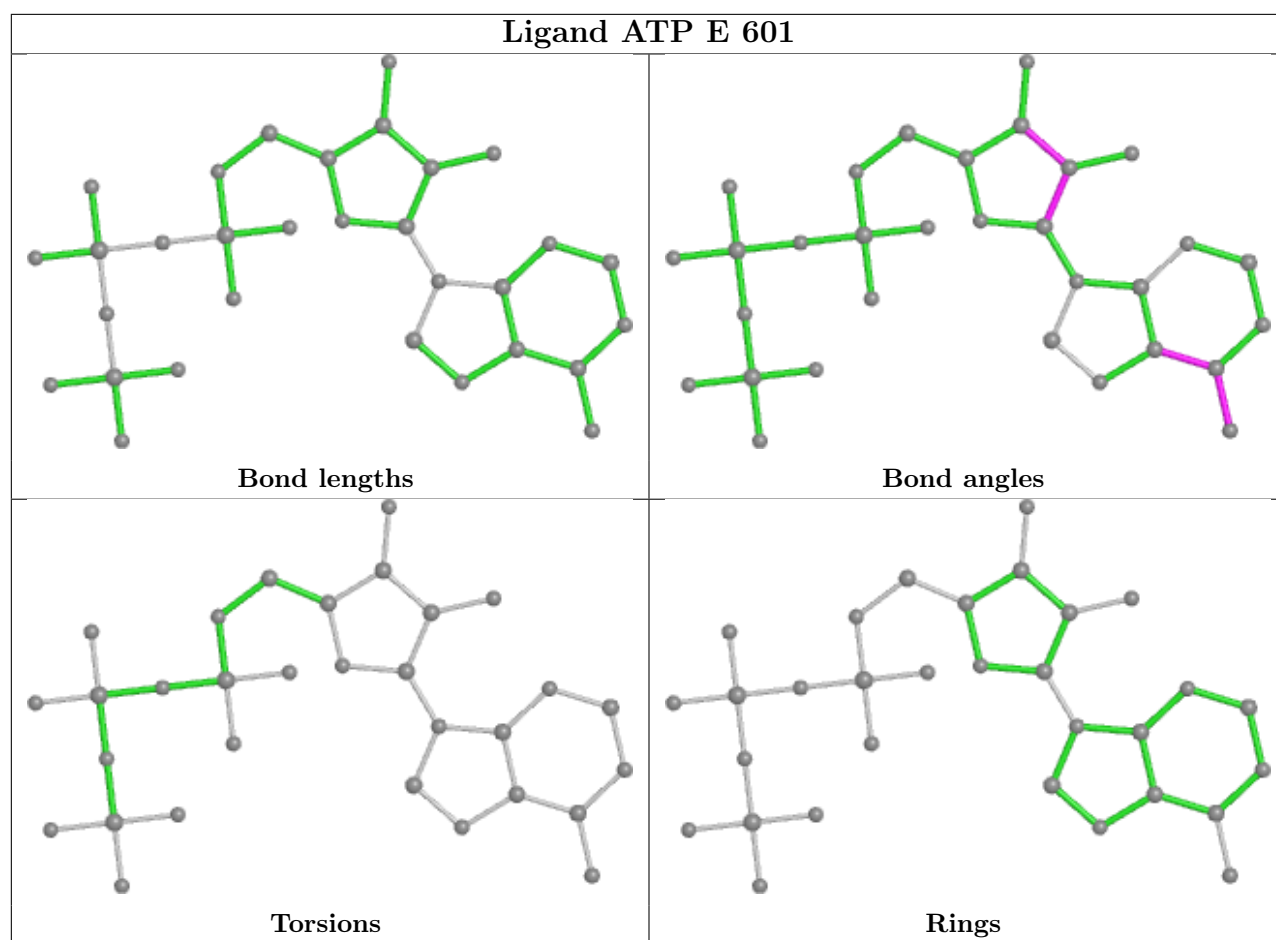
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	ATP	3	0
2	B	601	ATP	2	0
2	E	601	ATP	4	0
2	A	601	ATP	3	0
2	A	602	ATP	4	0
2	C	601	ATP	4	0
2	D	602	ATP	1	0
2	F	602	ATP	6	0
2	B	602	ATP	3	0
2	E	602	ATP	4	0
2	C	602	ATP	2	0

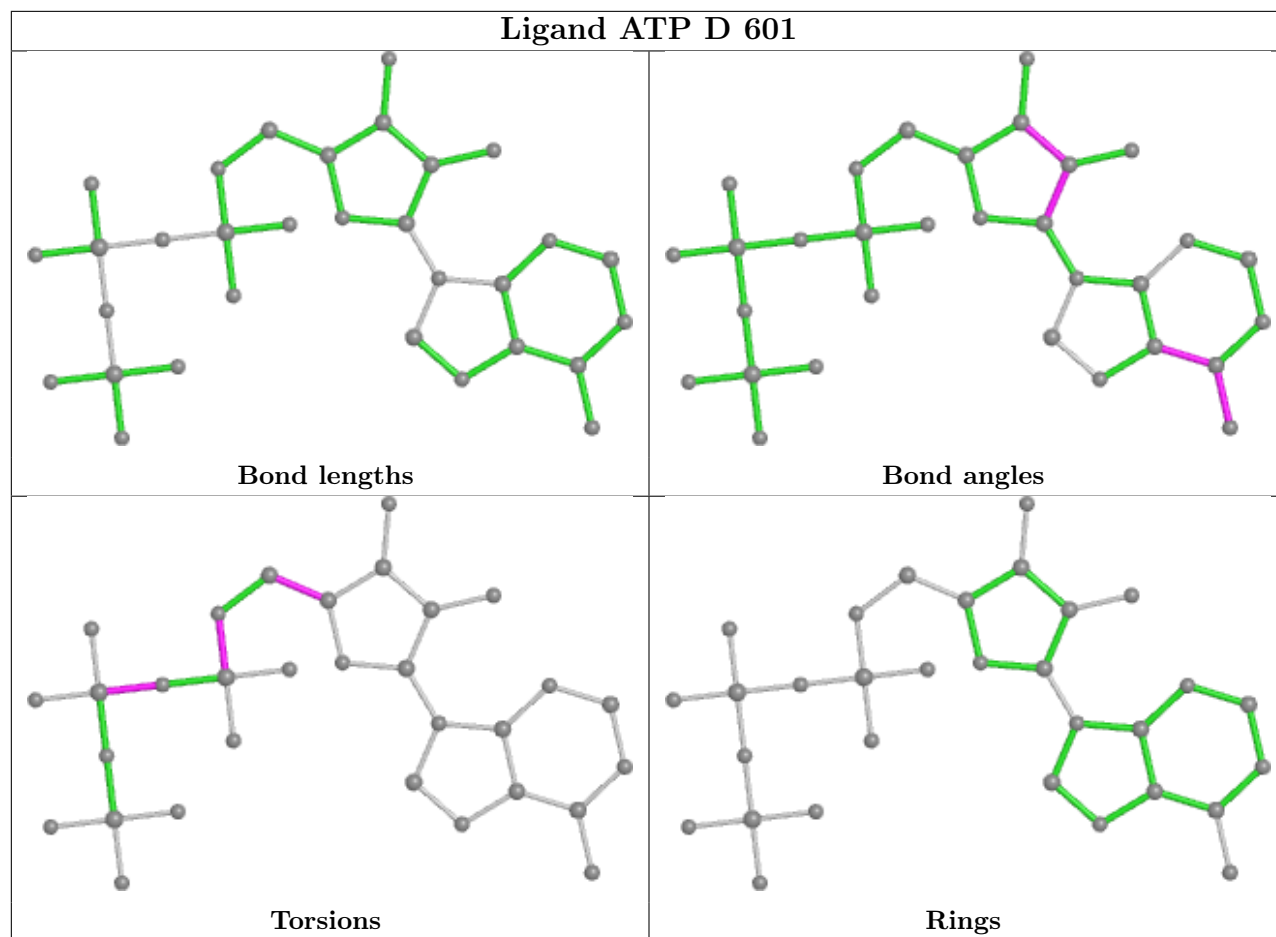
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

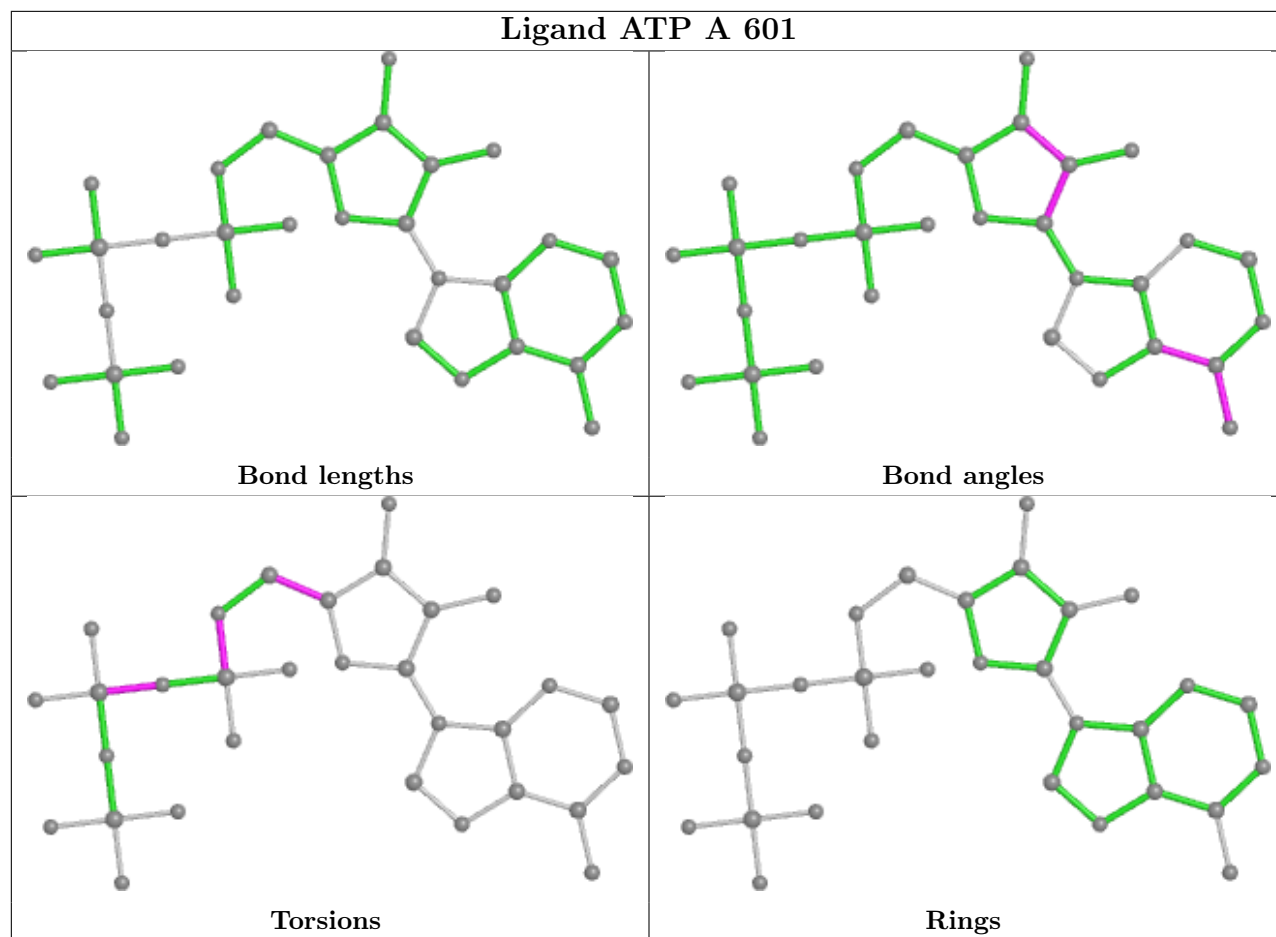
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

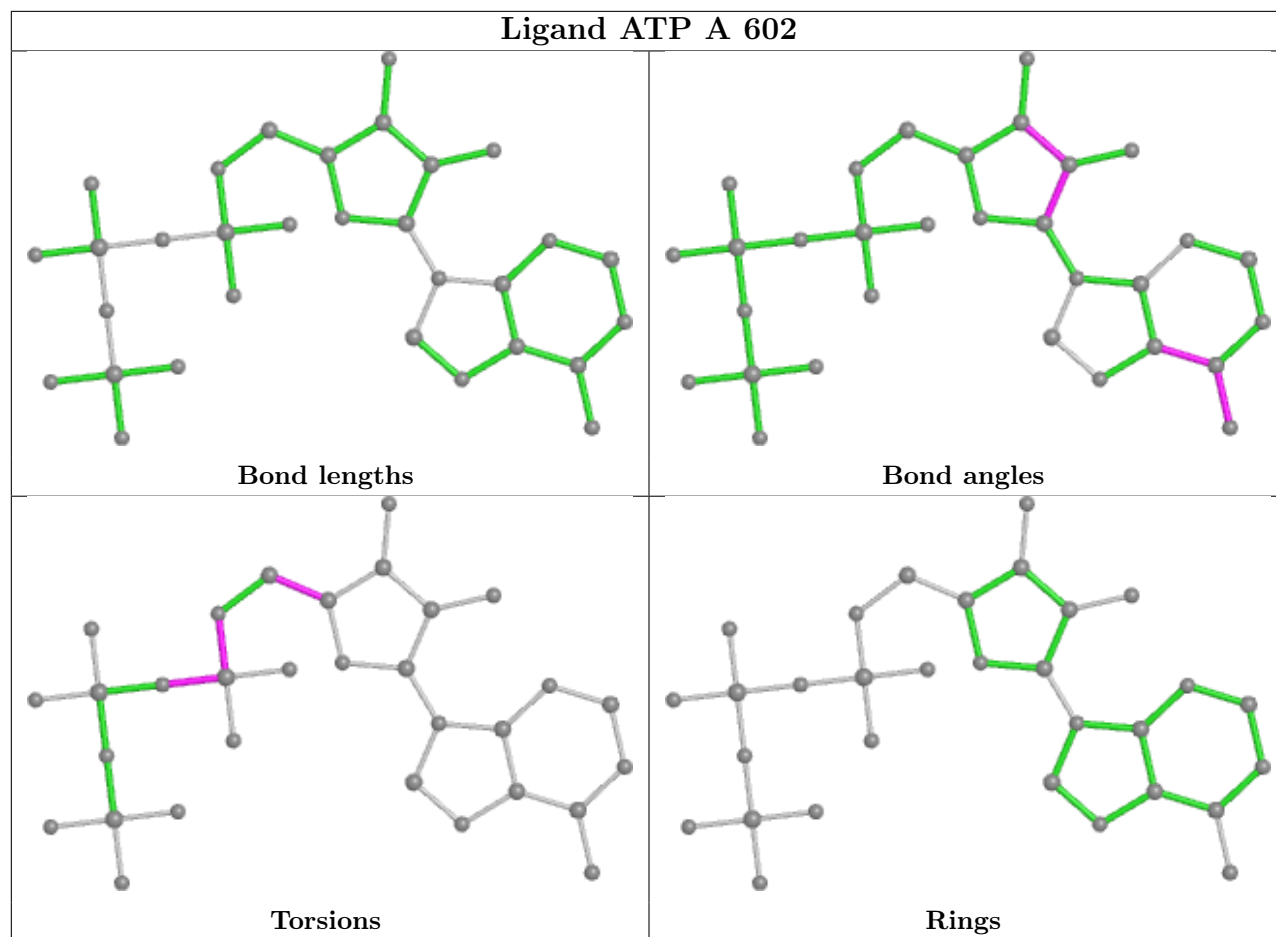


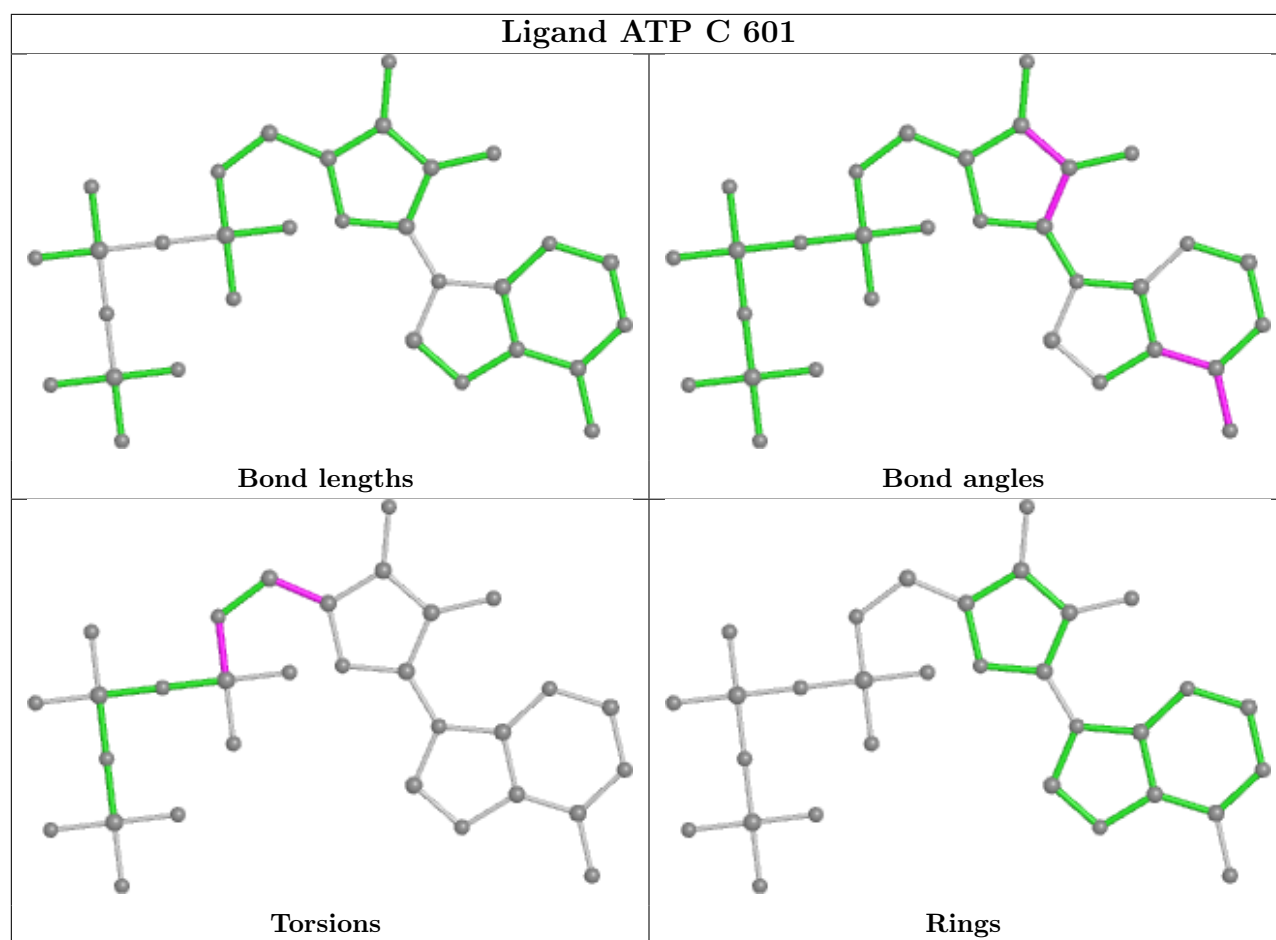


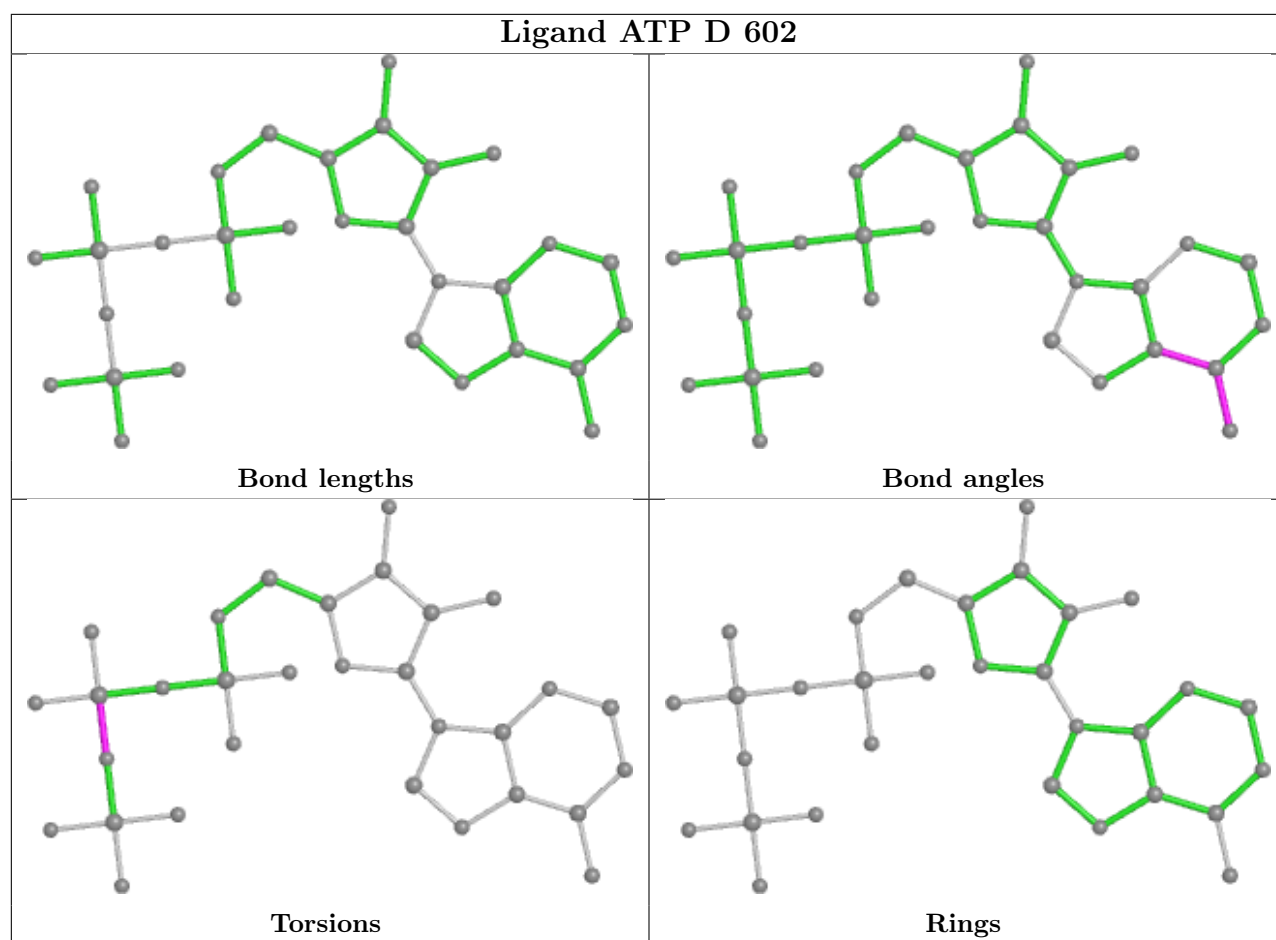




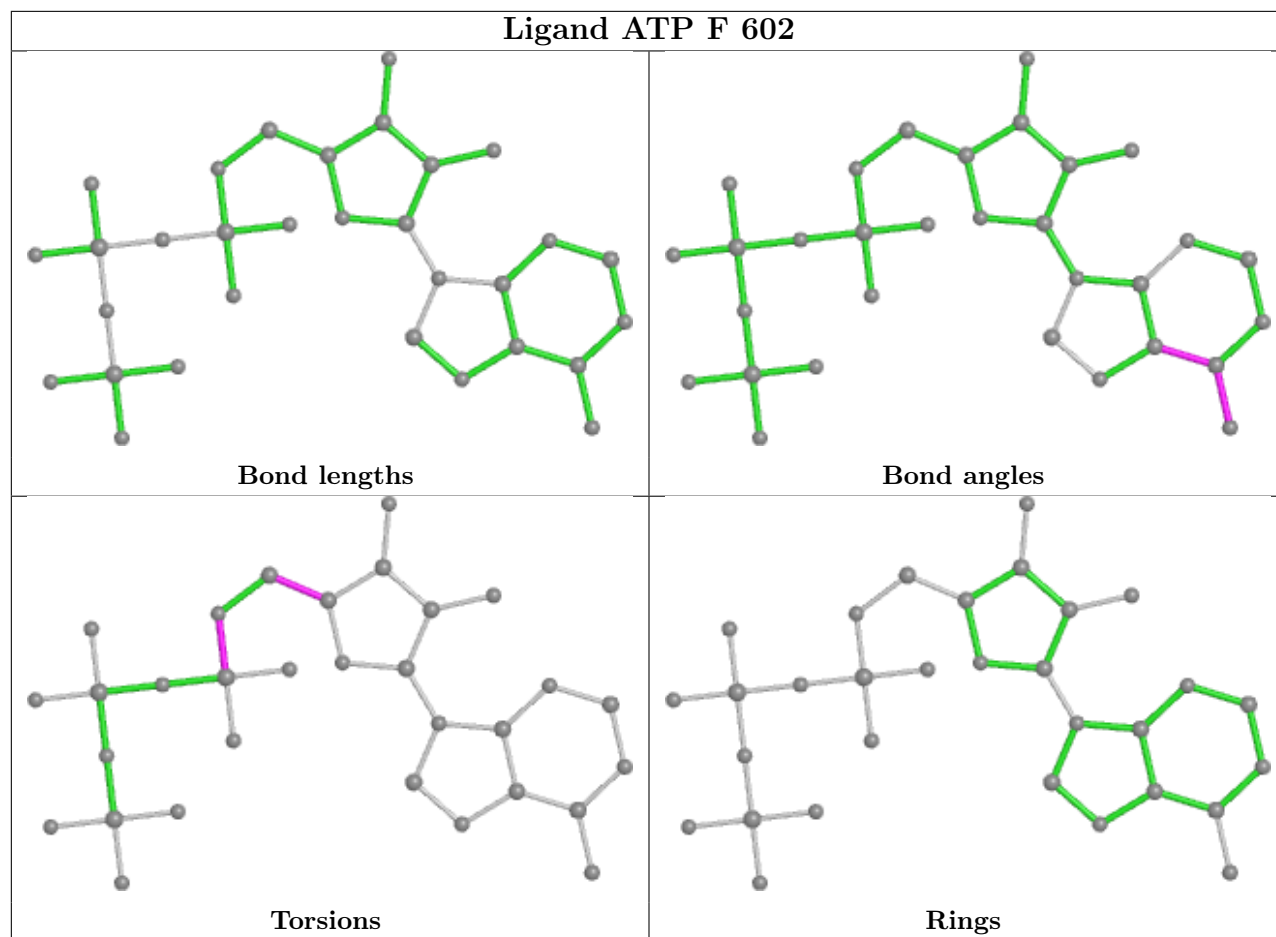




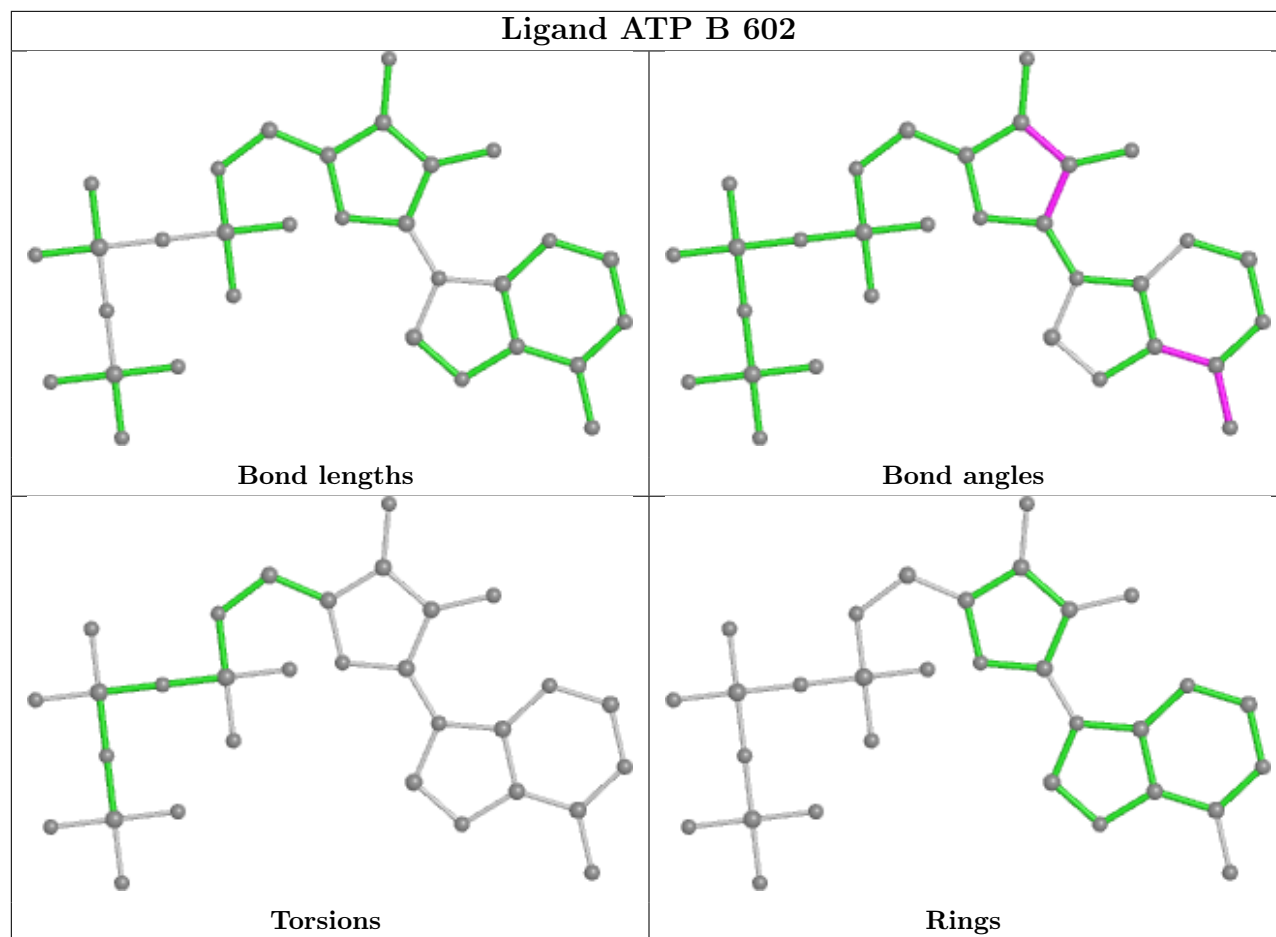




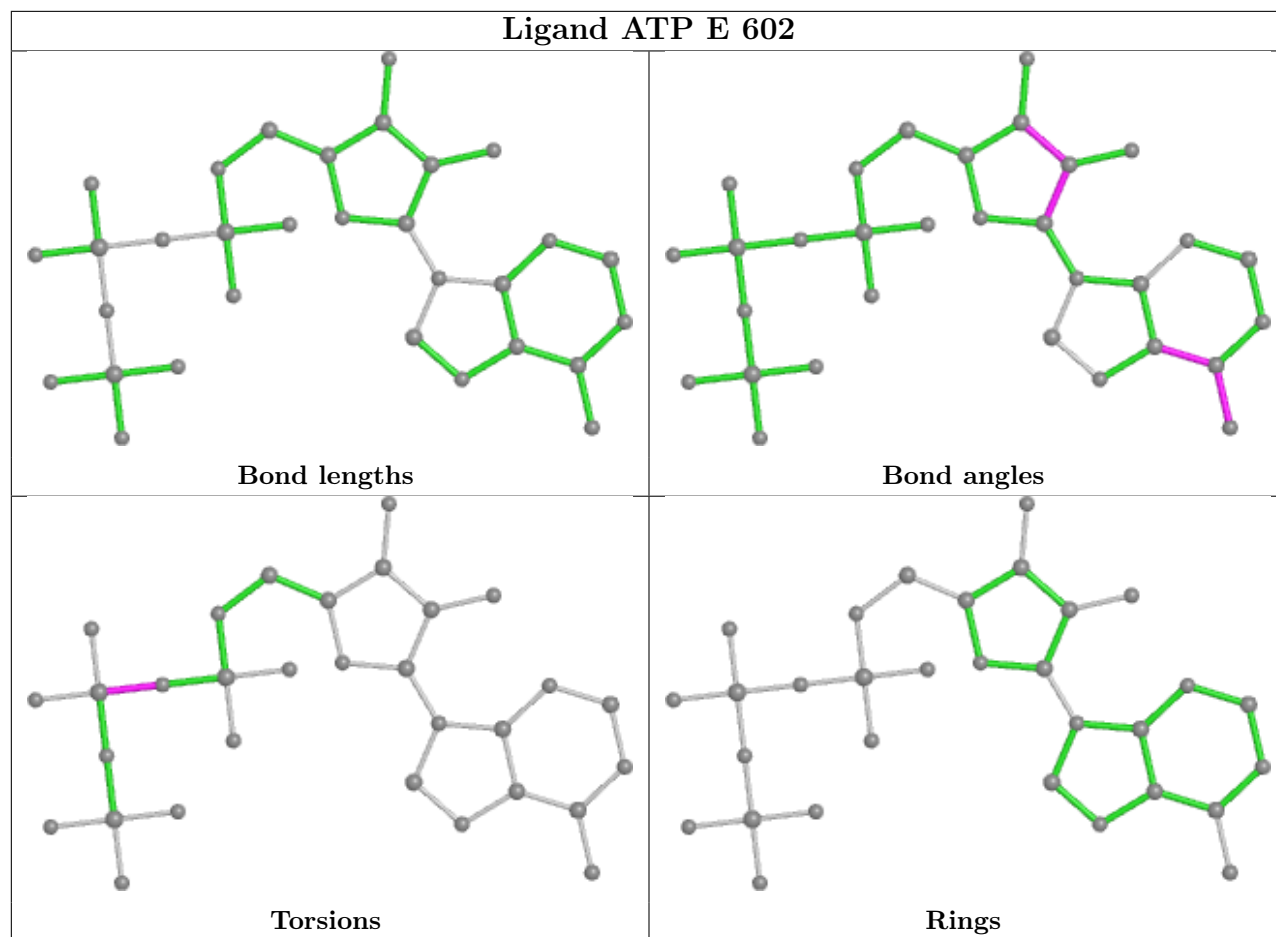
Ligand ATP F 602

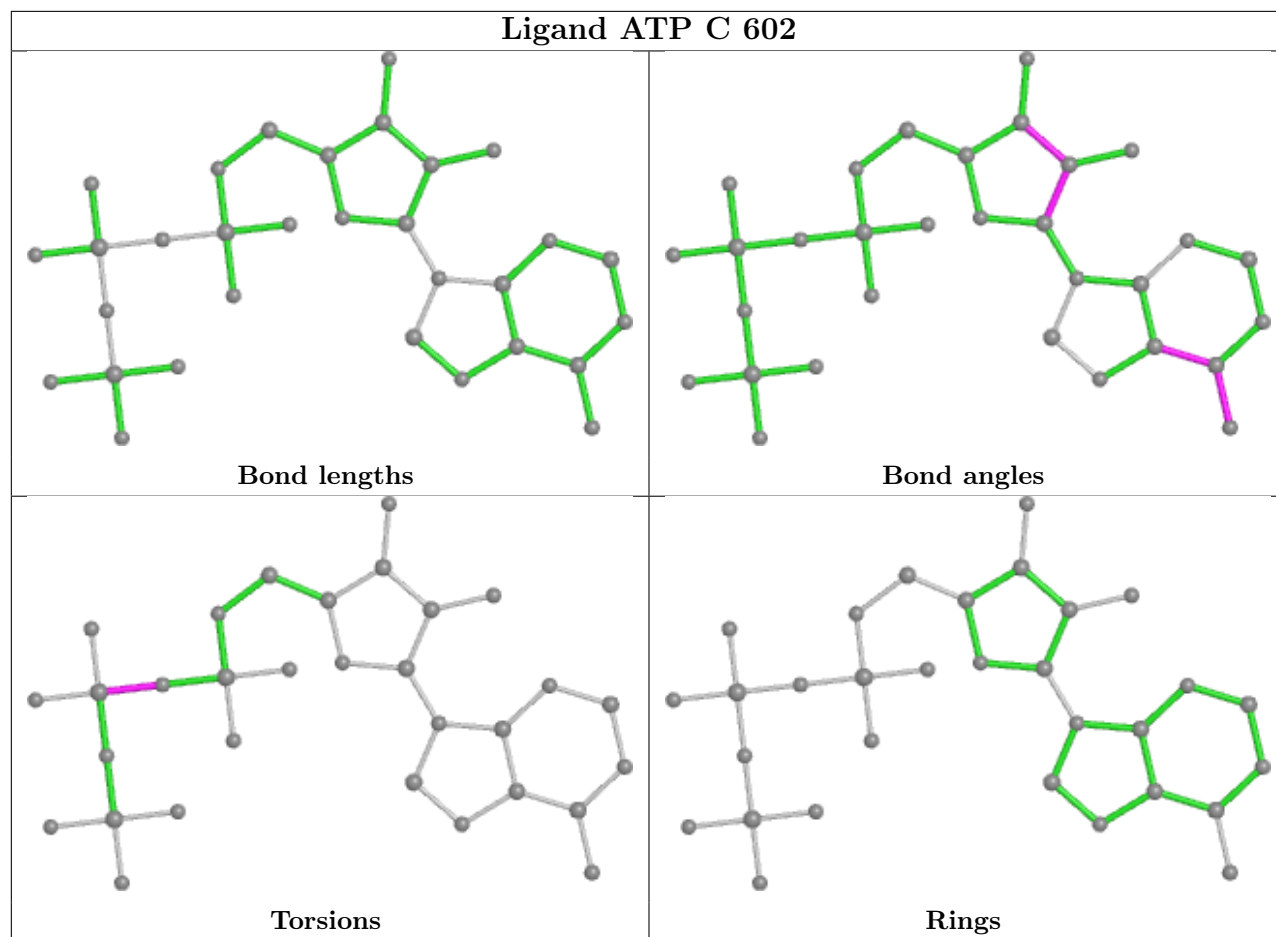


Ligand ATP B 602



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%)	0.34	23 (4%)	28	19	25, 55, 78, 95	0
1	B	468/519 (90%)	0.11	16 (3%)	45	35	17, 38, 71, 88	0
1	C	464/519 (89%)	0.12	16 (3%)	45	35	17, 38, 65, 105	0
1	D	460/519 (88%)	0.22	14 (3%)	50	40	22, 47, 67, 89	0
1	E	463/519 (89%)	0.31	21 (4%)	33	23	22, 47, 76, 97	0
1	F	465/519 (89%)	0.36	29 (6%)	20	13	21, 50, 75, 92	0
All	All	2781/3114 (89%)	0.24	119 (4%)	35	25	17, 45, 73, 105	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	254	LEU	5.3
1	B	112	PRO	5.3
1	A	421	GLY	5.2
1	E	112	PRO	4.8
1	A	495	THR	4.5
1	D	154	TYR	4.5
1	F	251	ALA	4.4
1	F	343	LEU	4.3
1	E	484	ARG	4.3
1	E	111	ASP	4.3
1	B	485	ASN	4.2
1	D	421	GLY	4.0
1	C	485	ASN	4.0
1	F	16	GLN	3.9
1	D	95	ALA	3.9
1	A	152	GLN	3.8
1	B	15	HIS	3.8
1	F	417	ASP	3.8
1	F	255	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	111	ASP	3.7
1	C	112	PRO	3.7
1	C	189	GLY	3.7
1	F	307	ALA	3.6
1	E	255	THR	3.5
1	B	158	SER	3.5
1	F	15	HIS	3.5
1	F	277	GLY	3.5
1	B	16	GLN	3.5
1	E	124	SER	3.4
1	A	63	GLY	3.4
1	F	99	ASP	3.4
1	E	253	ARG	3.3
1	E	421	GLY	3.3
1	F	254	LEU	3.3
1	F	14	GLU	3.3
1	A	248	PRO	3.2
1	E	494	PRO	3.2
1	B	257	ARG	3.1
1	E	485	ASN	3.1
1	C	157	SER	3.1
1	D	255	THR	3.1
1	D	175	GLY	3.1
1	F	342	ASN	3.1
1	A	488	ARG	3.1
1	C	91	GLY	3.1
1	A	417	ASP	3.1
1	A	329	TYR	3.1
1	B	486	PHE	3.0
1	F	253	ARG	3.0
1	A	157	SER	3.0
1	E	110	PRO	3.0
1	B	111	ASP	2.9
1	E	150	VAL	2.9
1	F	110	PRO	2.9
1	A	306	CYS	2.9
1	E	125	ALA	2.9
1	C	110	PRO	2.9
1	A	140	ARG	2.8
1	A	101	GLY	2.7
1	F	157	SER	2.7
1	B	252	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	123	LEU	2.7
1	F	156	ALA	2.7
1	E	329	TYR	2.7
1	F	155	ASP	2.6
1	D	334	ASP	2.6
1	C	258	SER	2.6
1	E	493	SER	2.6
1	B	422	ALA	2.6
1	F	152	GLN	2.5
1	F	250	GLY	2.5
1	E	158	SER	2.5
1	C	146	SER	2.5
1	C	249	LEU	2.5
1	E	486	PHE	2.5
1	B	110	PRO	2.5
1	D	18	ILE	2.5
1	F	259	SER	2.5
1	A	99	ASP	2.5
1	A	497	ILE	2.5
1	F	389	ASN	2.5
1	A	276	GLY	2.5
1	A	494	PRO	2.4
1	A	422	ALA	2.4
1	B	251	ALA	2.4
1	D	257	ARG	2.4
1	A	103	LEU	2.4
1	F	427	ASP	2.4
1	A	340	ARG	2.4
1	D	261	VAL	2.3
1	A	112	PRO	2.3
1	A	56	SER	2.3
1	D	158	SER	2.3
1	C	495	THR	2.3
1	B	256	GLN	2.3
1	F	258	SER	2.3
1	D	368	ASN	2.2
1	E	492	GLY	2.2
1	D	110	PRO	2.2
1	B	135	GLN	2.2
1	F	153	GLN	2.2
1	E	487	GLU	2.2
1	C	15	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	474	ASP	2.1
1	C	124	SER	2.1
1	C	181	THR	2.1
1	F	111	ASP	2.1
1	E	332	GLY	2.1
1	F	274	CYS	2.1
1	D	332	GLY	2.1
1	E	181	THR	2.0
1	F	495	THR	2.0
1	B	484	ARG	2.0
1	D	155	ASP	2.0
1	A	373	ALA	2.0
1	B	17	ALA	2.0
1	F	17	ALA	2.0
1	C	422	ALA	2.0
1	C	240	THR	2.0

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

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	0.80	0.23	40,42,44,44	0
1	TPO	F	432	11/12	0.82	0.25	42,43,47,47	0
1	SEP	A	431	10/11	0.86	0.23	44,46,49,50	0
1	SEP	B	431	10/11	0.87	0.21	38,39,41,42	0
1	SEP	D	431	10/11	0.87	0.20	36,38,39,40	0
1	TPO	E	432	11/12	0.89	0.25	38,38,39,39	4
1	SEP	C	431	10/11	0.89	0.21	34,36,38,38	0
1	SEP	F	431	10/11	0.89	0.21	43,45,48,48	0
1	TPO	D	432	11/12	0.91	0.21	34,34,35,35	4
1	TPO	C	432	11/12	0.92	0.20	32,33,34,34	4
1	TPO	B	432	11/12	0.92	0.17	38,39,41,41	0
1	TPO	A	432	11/12	0.92	0.16	43,43,45,45	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

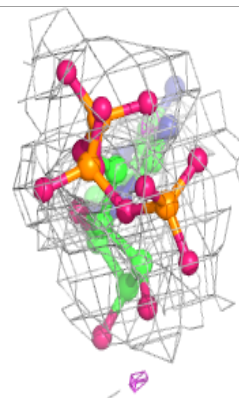
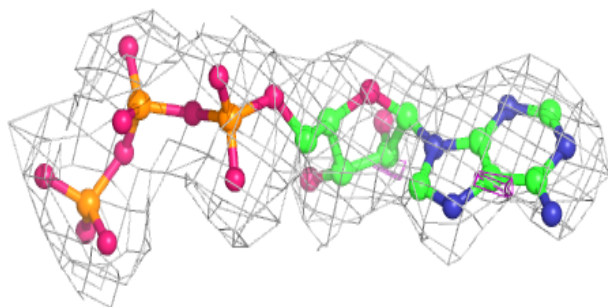
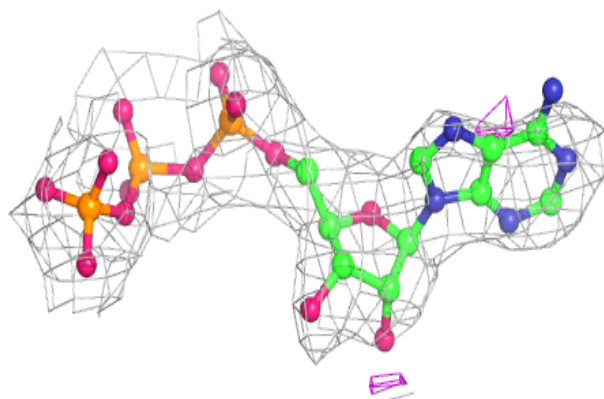
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	F	604	1/1	0.72	0.16	50,50,50,50	0
3	MG	F	603	1/1	0.80	0.17	25,25,25,25	0
2	ATP	F	602	31/31	0.89	0.20	51,55,58,59	0
2	ATP	E	602	31/31	0.91	0.21	40,45,49,49	0
2	ATP	C	601	31/31	0.92	0.18	32,34,36,36	0
2	ATP	D	601	31/31	0.92	0.21	38,39,41,41	0
2	ATP	C	602	31/31	0.93	0.17	30,35,38,38	0
2	ATP	F	601	31/31	0.93	0.17	30,32,34,34	0
2	ATP	D	602	31/31	0.93	0.18	35,38,40,40	0
3	MG	B	603	1/1	0.93	0.10	27,27,27,27	0
3	MG	B	604	1/1	0.93	0.13	29,29,29,29	0
2	ATP	A	602	31/31	0.93	0.17	41,46,47,48	0
2	ATP	A	601	31/31	0.93	0.18	35,36,37,37	0
3	MG	D	603	1/1	0.93	0.16	39,39,39,39	0
2	ATP	B	602	31/31	0.94	0.17	26,27,27,27	0
2	ATP	E	601	31/31	0.94	0.16	37,39,41,41	0
3	MG	E	604	1/1	0.95	0.18	39,39,39,39	0
3	MG	E	603	1/1	0.95	0.18	56,56,56,56	0
3	MG	A	603	1/1	0.97	0.29	63,63,63,63	0
2	ATP	B	601	31/31	0.97	0.14	20,22,23,23	0
3	MG	D	604	1/1	0.97	0.23	28,28,28,28	0
3	MG	A	604	1/1	0.98	0.25	43,43,43,43	0
3	MG	C	604	1/1	0.98	0.06	21,21,21,21	0
3	MG	C	603	1/1	0.99	0.16	28,28,28,28	0

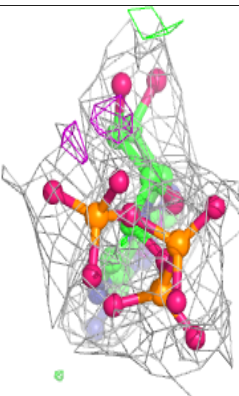
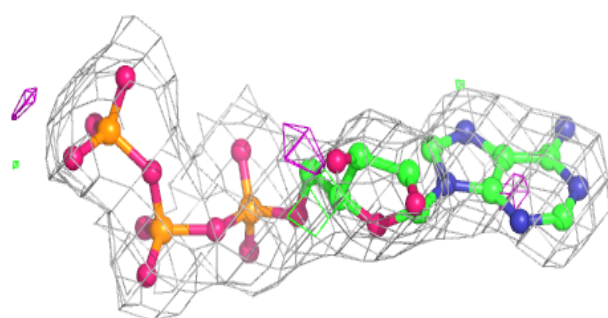
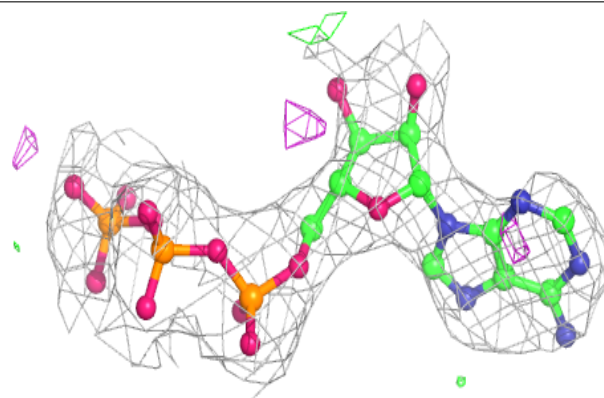
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP F 602:

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

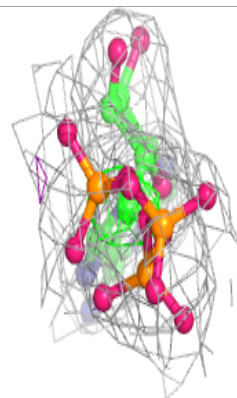
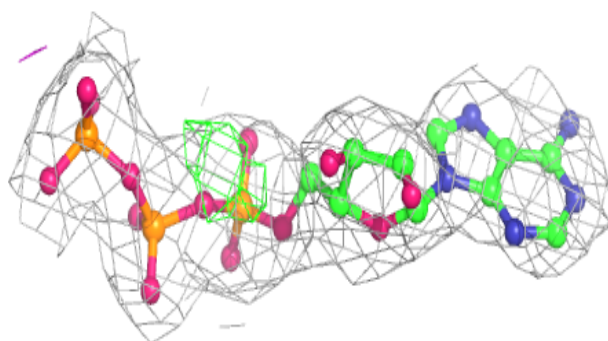
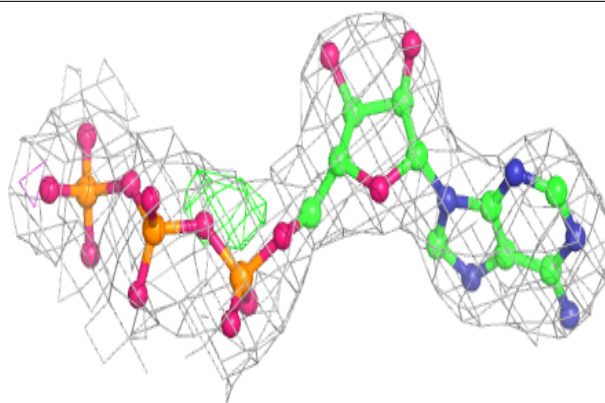
**Electron density around ATP E 602:**

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

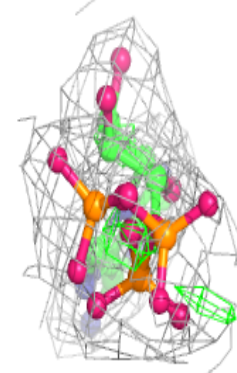
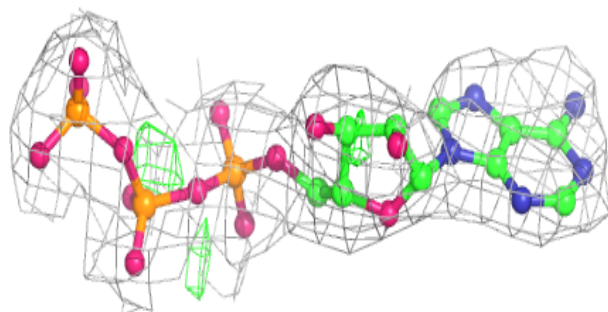
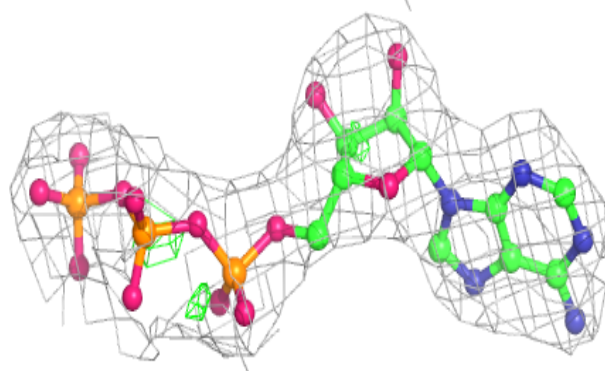


Electron density around ATP C 601:

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

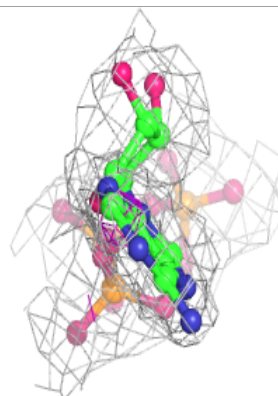
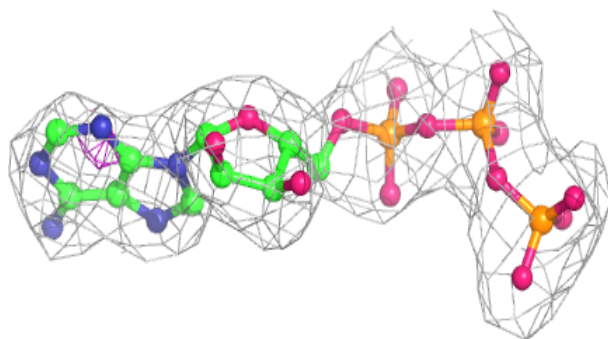
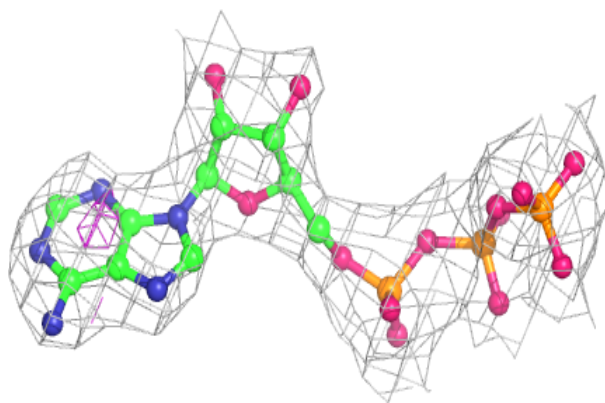
**Electron density around ATP D 601:**

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

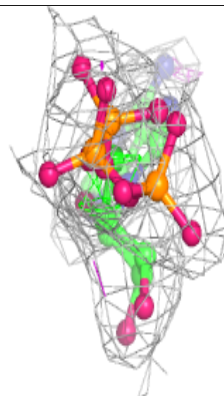
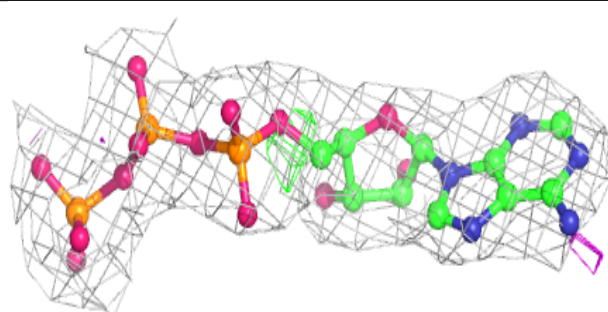
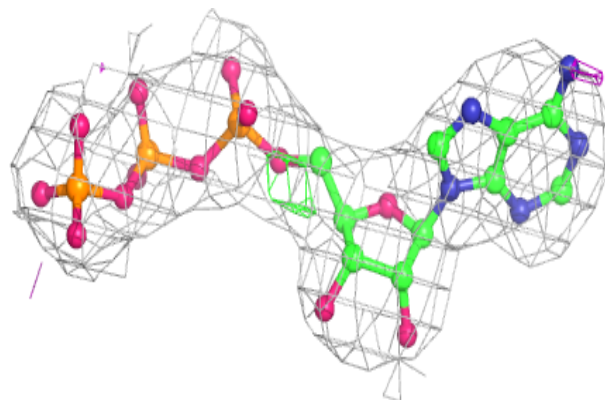


Electron density around ATP C 602:

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

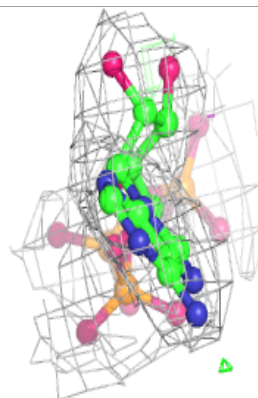
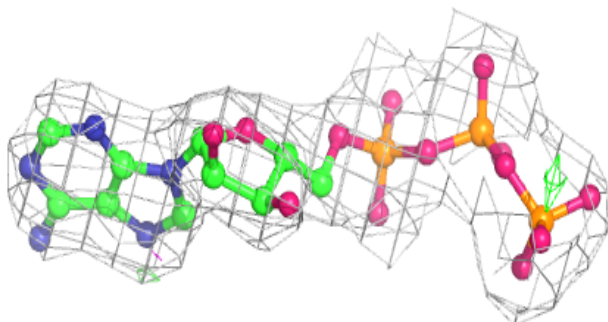
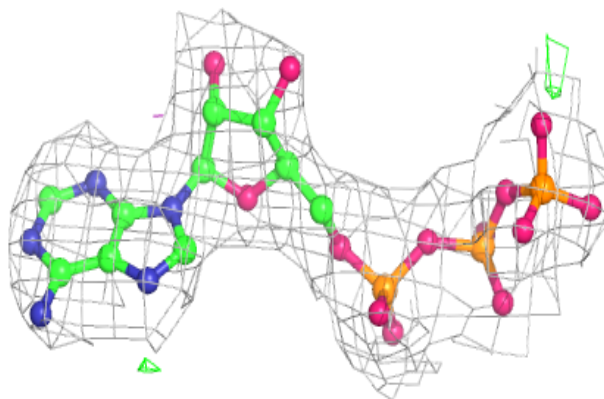
**Electron density around ATP F 601:**

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

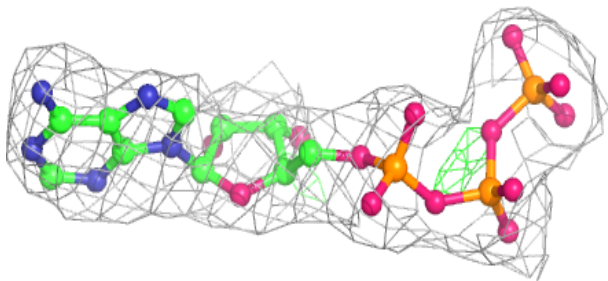
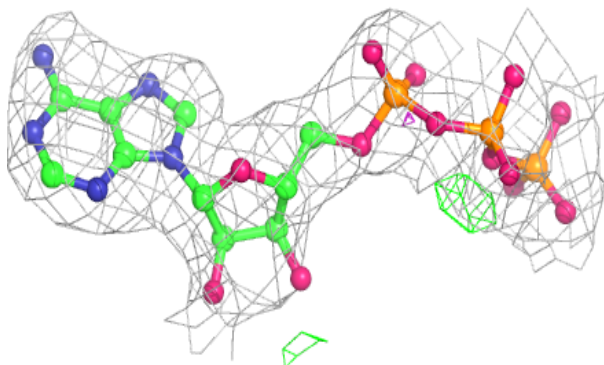


Electron density around ATP D 602:

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

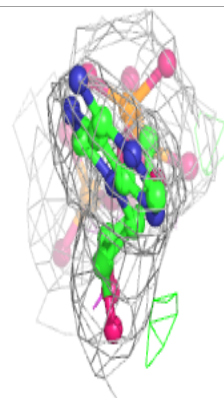
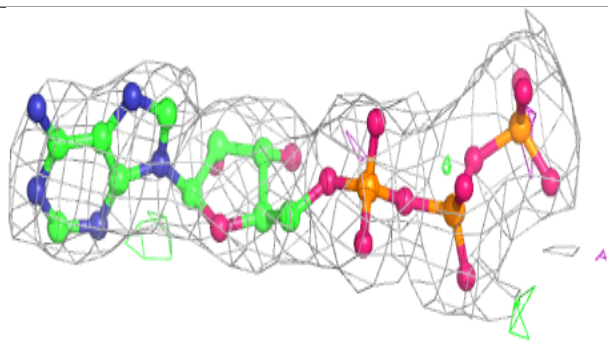
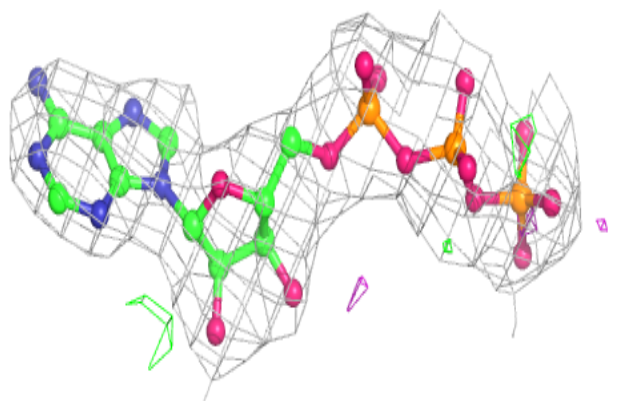
**Electron density around ATP A 602:**

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

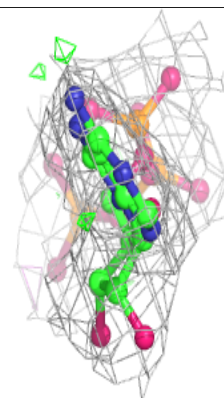
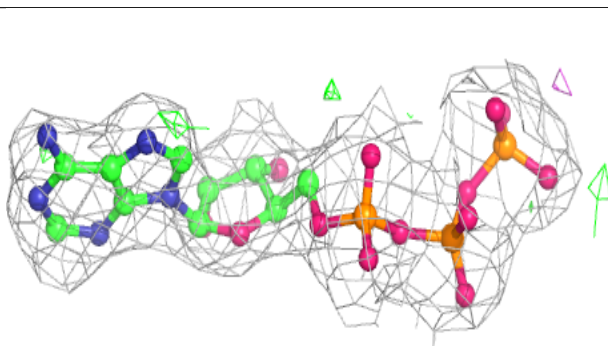
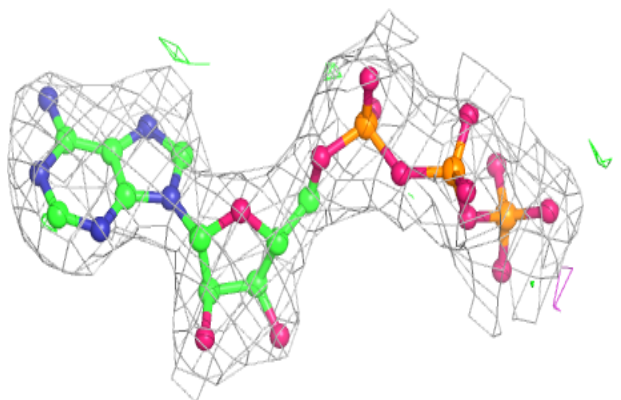


Electron density around ATP A 601:

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

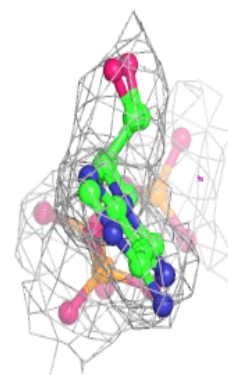
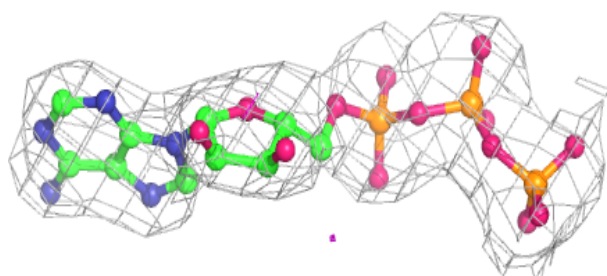
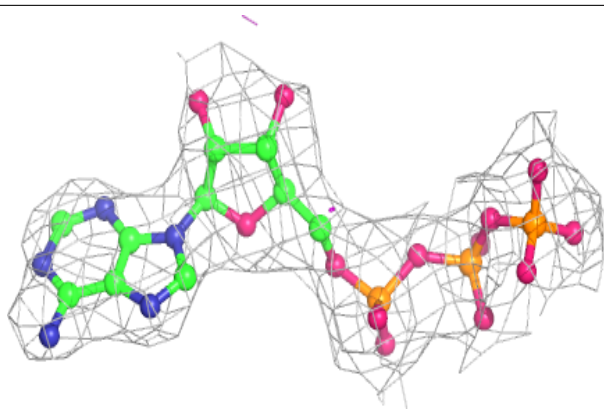
**Electron density around ATP B 602:**

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

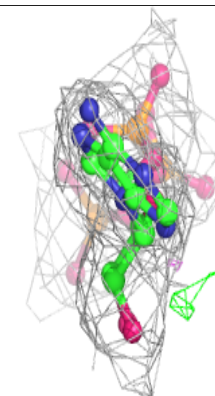
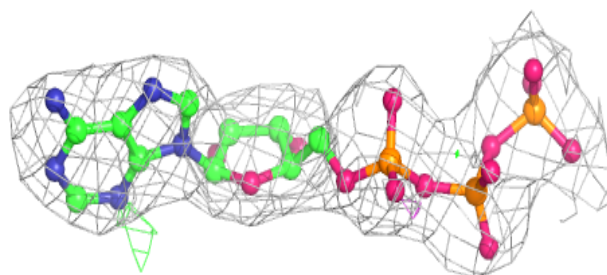
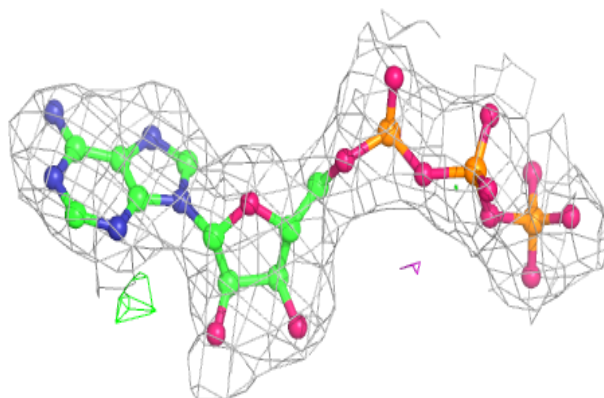


Electron density around ATP E 601:

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

**Electron density around ATP B 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.