



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:14 AM BST

PDB ID : 6KSH  
Title : Crystal structure of pyruvate kinase (PYK) from Plasmodium falciparum in complex with oxalate and ATP  
Authors : Zhong, W.; Cai, Q.; Li, K.; Lescar, J.; Dedon, P.C.  
Deposited on : 2019-08-23  
Resolution : 2.60 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](mailto: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.

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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 : 2.14.4.dev1  
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) : 2.14.4.dev1

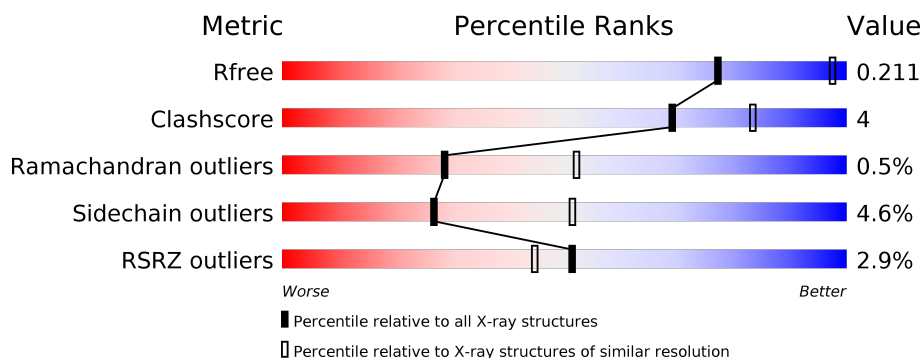
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	514	<div> <div>81%</div> <div>13% • 5%</div> </div>
1	B	514	<div>4%</div> <div>83%</div> <div>11% • 5%</div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16095 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	3	0
			3759	2364	650	715	30			
1	B	490	Total	C	N	O	S	0	2	0
			3751	2360	649	712	30			
1	C	490	Total	C	N	O	S	0	0	0
			3733	2350	645	708	30			
1	D	490	Total	C	N	O	S	0	1	0
			3742	2355	647	710	30			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP C6KTA4
A	-1	GLY	-	expression tag	UNP C6KTA4
A	0	HIS	-	expression tag	UNP C6KTA4
B	-2	GLY	-	expression tag	UNP C6KTA4
B	-1	GLY	-	expression tag	UNP C6KTA4
B	0	HIS	-	expression tag	UNP C6KTA4
C	-2	GLY	-	expression tag	UNP C6KTA4
C	-1	GLY	-	expression tag	UNP C6KTA4
C	0	HIS	-	expression tag	UNP C6KTA4
D	-2	GLY	-	expression tag	UNP C6KTA4
D	-1	GLY	-	expression tag	UNP C6KTA4
D	0	HIS	-	expression tag	UNP C6KTA4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

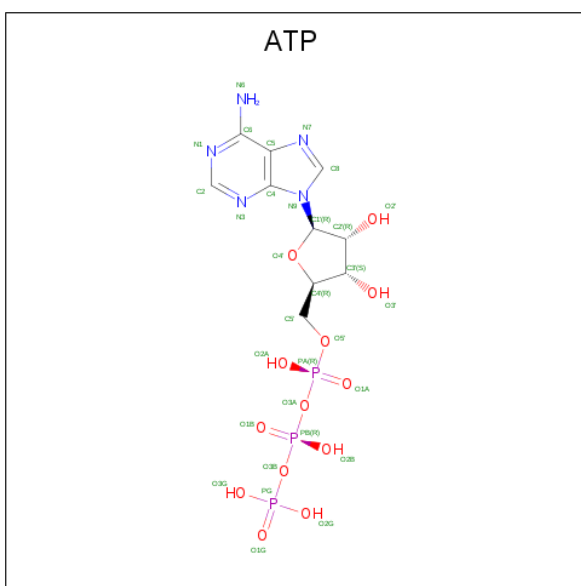
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ) (labeled as "Ligand of Interest" by author).



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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by author).

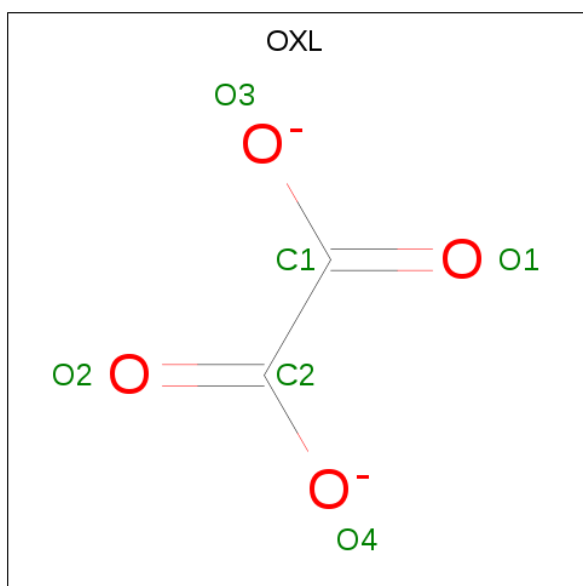
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is OXALATE ION (three-letter code: OXL) (formula:  $C_2O_4$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	2	4		
5	B	1	Total	C	O	0	0
			6	2	4		
5	C	1	Total	C	O	0	0
			6	2	4		
5	D	1	Total	C	O	0	0
			6	2	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	301	Total	O	0	0
			301	301		
6	B	186	Total	O	0	0
			186	186		

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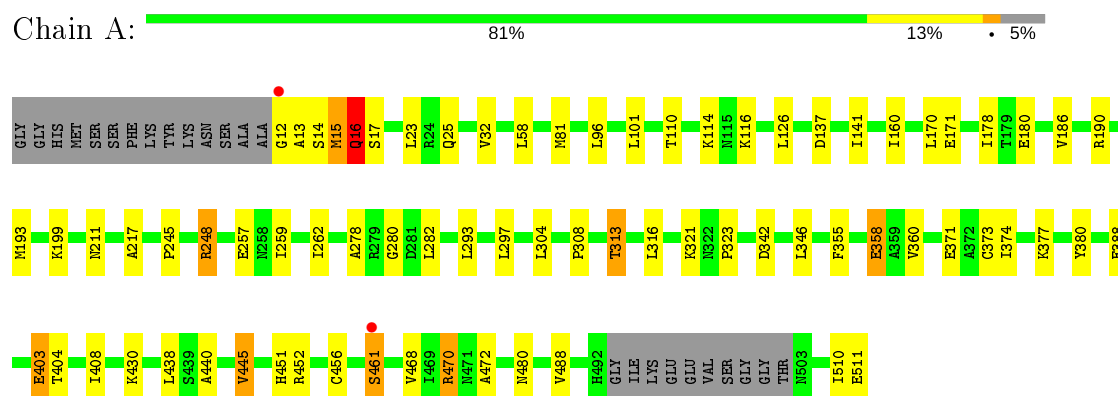
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	187	Total	O	0	0
			187	187		
6	D	276	Total	O	0	0
			276	276		

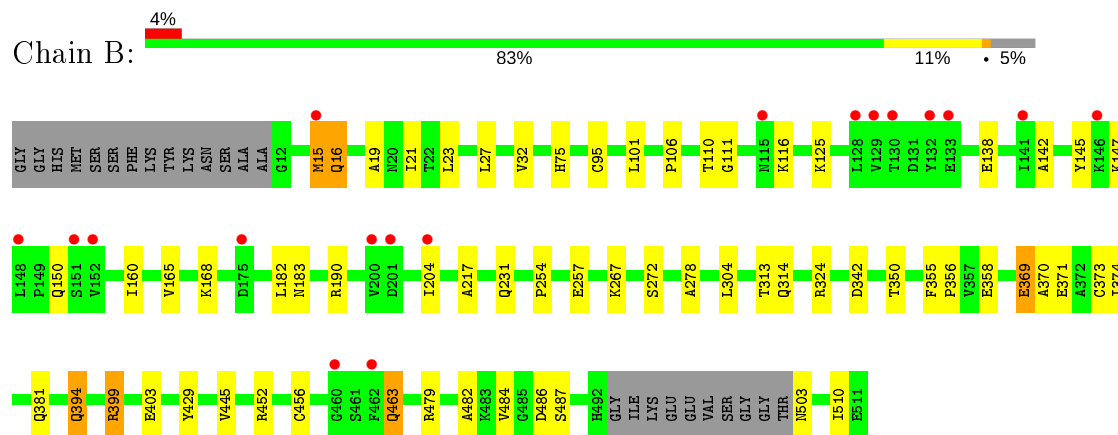
### 3 Residue-property plots [i](#)

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

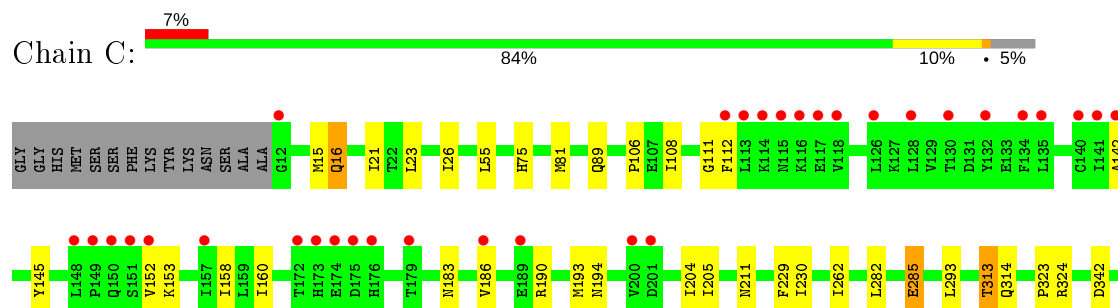
#### • Molecule 1: Pyruvate kinase



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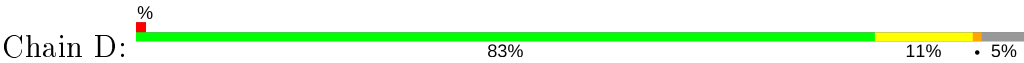


#### • Molecule 1: Pyruvate kinase





● Molecule 1: Pyruvate kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.41Å 139.41Å 453.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.99 – 2.60 55.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.99-2.60) 100.0 (55.25-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.151 , 0.207 0.159 , 0.211	Depositor DCC
$R_{free}$ test set	4017 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OXL, MG, K, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.50	0/3804	0.71	1/5135 (0.0%)
1	B	0.51	0/3796	0.71	1/5124 (0.0%)
1	C	0.49	0/3778	0.72	1/5100 (0.0%)
1	D	0.49	0/3787	0.71	1/5112 (0.0%)
All	All	0.50	0/15165	0.71	4/20471 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	MET	C-N-CA	8.17	142.12	121.70
1	B	15	MET	C-N-CA	6.61	138.23	121.70
1	D	15	MET	C-N-CA	6.51	137.97	121.70
1	C	15	MET	C-N-CA	5.96	136.60	121.70

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	3759	0	3903	37	0
1	B	3751	0	3900	31	0
1	C	3733	0	3886	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3742	0	3893	30	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
6	A	301	0	0	0	0
6	B	186	0	0	1	0
6	C	187	0	0	0	0
6	D	276	0	0	1	0
All	All	16095	0	15630	114	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 4.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:PHE:HB3	1:A:358:GLU:HG2	1.50	0.93
1:D:355:PHE:HB3	1:D:358:GLU:HG2	1.62	0.82
1:D:262:ILE:HD11	1:D:282:LEU:HD11	1.63	0.81
1:B:394[B]:GLN:HG2	1:B:503:ASN:HD21	1.48	0.78
1:B:355:PHE:HB3	1:B:358:GLU:HG2	1.67	0.76
1:A:445:VAL:HG22	1:A:456:CYS:HB3	1.70	0.73
1:D:438:LEU:HD23	1:D:468:VAL:HG12	1.76	0.66
1:C:355:PHE:HB3	1:C:358:GLU:HG2	1.79	0.64
1:A:262:ILE:HD11	1:A:282:LEU:HD11	1.80	0.63
1:B:313:THR:HG22	1:B:314:GLN:HG3	1.82	0.62
1:B:486:ASP:HB2	1:B:510:ILE:HD12	1.80	0.62
1:A:438:LEU:HD21	1:A:472:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:HA	1:A:374:ILE:HD12	1.83	0.59
1:C:438:LEU:HD21	1:C:472:ALA:HB2	1.85	0.57
1:A:25[A]:GLN:HE22	1:A:373:CYS:HB3	1.70	0.56
1:C:293:LEU:HD11	1:D:369:GLU:HG3	1.88	0.56
1:A:355:PHE:HB3	1:A:358:GLU:CG	2.33	0.55
1:C:194:ASN:HD21	1:C:285:GLU:HG2	1.72	0.55
1:A:380:TYR:CE2	1:A:403:GLU:HG3	2.43	0.54
1:A:245:PRO:O	1:A:248:ARG:HD2	2.09	0.53
1:C:262:ILE:HD11	1:C:282:LEU:HD11	1.91	0.52
1:A:101:LEU:HD13	1:A:217:ALA:HB2	1.92	0.52
1:C:26:ILE:O	1:D:290:LYS:HG2	2.10	0.52
1:B:101:LEU:HD13	1:B:217:ALA:HB2	1.92	0.52
1:C:342:ASP:HA	1:C:452:ARG:HB2	1.91	0.51
1:D:416:LEU:HD11	1:D:469:ILE:HD11	1.92	0.51
1:C:399:ARG:HD2	1:C:429:TYR:CZ	2.45	0.50
1:C:369:GLU:HG3	1:D:293:LEU:HD11	1.93	0.50
1:C:55:LEU:HD11	1:C:81:MET:CE	2.42	0.50
1:D:371:GLU:HA	1:D:374:ILE:HD12	1.94	0.49
1:A:14:SER:HA	1:B:19:ALA:O	2.13	0.49
1:D:96:LEU:HD13	1:D:445:VAL:HG13	1.95	0.49
1:A:160:ILE:HG12	1:A:193:MET:HG2	1.93	0.49
1:C:313:THR:HG22	1:C:314:GLN:HG3	1.94	0.49
1:C:23:LEU:HD21	6:D:879:HOH:O	2.12	0.48
1:C:355:PHE:HB3	1:C:358:GLU:CG	2.44	0.48
1:C:152:VAL:HG21	1:C:158:ILE:HD11	1.94	0.48
1:C:111:GLY:HA3	1:C:142:ALA:HB3	1.94	0.48
1:D:257:GLU:HB3	1:D:278:ALA:HB3	1.96	0.48
1:D:459:VAL:HG11	1:D:468:VAL:HG13	1.94	0.48
1:A:12:GLY:HA2	1:B:21:ILE:O	2.13	0.47
1:B:257:GLU:HB3	1:B:278:ALA:HB3	1.97	0.47
1:B:399:ARG:HD2	1:B:429:TYR:CZ	2.49	0.47
1:B:342:ASP:HA	1:B:452:ARG:HB2	1.96	0.47
1:D:101:LEU:HD13	1:D:217:ALA:HB2	1.97	0.47
1:C:436:LEU:HD11	1:C:457:ILE:CD1	2.45	0.46
1:C:21:ILE:O	1:D:12:GLY:HA3	2.16	0.46
1:D:210:LYS:HG3	1:D:242:LEU:HD11	1.97	0.46
1:B:111:GLY:HA3	1:B:142:ALA:HB3	1.97	0.46
1:C:112:PHE:CZ	1:C:190:ARG:HD2	2.51	0.46
1:A:96:LEU:HD13	1:A:445:VAL:HG13	1.96	0.46
1:A:280:GLY:HA3	1:A:313:THR:HG21	1.98	0.46
1:D:254:PRO:HD2	1:D:274:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:GLN:HE22	1:D:385:ASN:HD21	1.64	0.46
1:A:470:ARG:HA	1:A:470:ARG:HD3	1.84	0.45
1:B:110:THR:O	1:B:190:ARG:HA	2.16	0.45
1:C:183:ASN:HB3	1:D:323:PRO:HD3	1.98	0.45
1:B:355:PHE:HB3	1:B:358:GLU:CG	2.43	0.45
1:A:404:THR:O	1:A:408:ILE:HG12	2.15	0.45
1:A:257:GLU:HB3	1:A:278:ALA:HB3	1.98	0.45
1:D:15:MET:HB2	1:D:16:GLN:H	1.59	0.45
1:A:440:ALA:HB1	1:A:461:SER:HA	1.97	0.45
1:B:106:PRO:HG3	1:B:204:ILE:HD13	1.98	0.45
1:B:204:ILE:HD11	1:B:231:GLN:HE21	1.82	0.45
1:A:470:ARG:HH21	1:A:511:GLU:HG2	1.82	0.45
1:A:316:LEU:HD12	1:A:346:LEU:HD21	1.99	0.44
1:D:40:HIS:O	1:D:343:CYS:HA	2.18	0.44
1:B:160:ILE:HB	1:B:165:VAL:HB	2.00	0.44
1:A:13:ALA:HB3	1:A:297:LEU:HD12	1.98	0.44
1:A:293:LEU:HD11	1:B:369:GLU:HG3	2.00	0.44
1:B:168:LYS:HB2	1:B:182:LEU:HD11	1.99	0.44
1:C:436:LEU:HD11	1:C:457:ILE:HD12	1.99	0.44
1:B:482:ALA:HB1	1:B:510:ILE:CD1	2.49	0.43
1:D:438:LEU:HD21	1:D:472:ALA:HB2	2.00	0.43
1:C:108:ILE:HG12	1:C:145:TYR:HB2	2.00	0.43
1:C:404:THR:O	1:C:408:ILE:HG12	2.18	0.43
1:C:399:ARG:HD2	1:C:429:TYR:CE2	2.52	0.43
1:D:342:ASP:HA	1:D:452:ARG:HB2	2.00	0.43
1:C:323:PRO:HD3	1:D:183:ASN:HB3	1.99	0.43
1:B:482:ALA:HB1	1:B:510:ILE:HD13	2.00	0.43
1:A:308:PRO:HD3	1:A:451:HIS:CE1	2.53	0.43
1:B:254:PRO:CD	1:B:272:SER:HB2	2.49	0.42
1:C:160:ILE:HG13	1:C:193:MET:HG2	2.01	0.42
1:D:160:ILE:HB	1:D:165:VAL:HB	2.00	0.42
1:B:394[A]:GLN:HG3	1:B:503:ASN:HD21	1.83	0.42
1:A:377:LYS:CE	1:C:389:THR:HG21	2.49	0.42
1:D:204:ILE:HG12	1:D:235:ASP:HB3	2.01	0.42
1:A:342:ASP:HA	1:A:452:ARG:HB2	2.01	0.42
1:A:259:ILE:HG23	1:B:27:LEU:HD22	2.01	0.42
1:C:106:PRO:HD2	1:C:229:PHE:HB2	2.01	0.42
1:A:114:LYS:HE3	1:A:137:ASP:HB3	2.00	0.42
1:A:171:GLU:HG2	1:A:178:ILE:HB	2.02	0.42
1:B:371:GLU:HA	1:B:374:ILE:HD12	2.00	0.42
1:D:233:ALA:HB1	1:D:271:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ALA:O	1:B:373:CYS:HB2	2.20	0.41
1:A:488:VAL:HG13	1:A:510:ILE:HD11	2.02	0.41
1:B:445:VAL:HG22	1:B:456:CYS:HB3	2.01	0.41
1:D:404:THR:O	1:D:408:ILE:HG12	2.20	0.41
1:A:15:MET:HB3	1:A:16:GLN:H	1.64	0.41
1:B:484:VAL:HA	1:B:510:ILE:HG22	2.01	0.41
1:D:316:LEU:HD12	1:D:346:LEU:HD21	2.03	0.41
1:B:145:TYR:CE2	1:B:147:LYS:HB2	2.56	0.41
1:A:170:LEU:HD11	1:A:180:GLU:HB2	2.03	0.41
1:A:323:PRO:HD3	1:B:183:ASN:HB3	2.03	0.41
1:C:204:ILE:HD11	1:C:230:ILE:HD13	2.02	0.41
1:D:279:ARG:NH2	1:D:315:MET:HG2	2.35	0.41
1:A:110:THR:O	1:A:190:ARG:HA	2.21	0.41
1:A:58:LEU:HD22	1:A:360:VAL:HG21	2.03	0.41
1:D:280:GLY:CA	1:D:313:THR:HG21	2.51	0.41
1:D:445:VAL:HG22	1:D:456:CYS:HB3	2.03	0.41
1:A:126:LEU:HD11	1:A:141:ILE:HD12	2.02	0.41
1:A:323:PRO:HD2	6:B:742:HOH:O	2.22	0.40
1:B:350:THR:HA	1:B:356:PRO:HB3	2.03	0.40
1:C:204:ILE:HD11	1:C:230:ILE:HA	2.03	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	489/514 (95%)	476 (97%)	11 (2%)	2 (0%)	34 57
1	B	488/514 (95%)	475 (97%)	10 (2%)	3 (1%)	25 47
1	C	486/514 (95%)	472 (97%)	12 (2%)	2 (0%)	34 57
1	D	487/514 (95%)	477 (98%)	8 (2%)	2 (0%)	34 57
All	All	1950/2056 (95%)	1900 (97%)	41 (2%)	9 (0%)	29 52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	D	16	GLN
1	B	16	GLN
1	B	463	GLN
1	A	313	THR
1	B	116	LYS
1	C	16	GLN
1	C	313	THR
1	D	313	THR

### 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	425/439 (97%)	404 (95%)	21 (5%)	25	48
1	B	424/439 (97%)	404 (95%)	20 (5%)	26	50
1	C	422/439 (96%)	403 (96%)	19 (4%)	27	52
1	D	423/439 (96%)	404 (96%)	19 (4%)	27	52
All	All	1694/1756 (96%)	1615 (95%)	79 (5%)	27	50

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	17	SER
1	A	23	LEU
1	A	32	VAL
1	A	81	MET
1	A	116	LYS
1	A	186	VAL
1	A	199	LYS
1	A	211	ASN
1	A	248	ARG
1	A	304	LEU

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Mol	Chain	Res	Type
1	A	321	LYS
1	A	358	GLU
1	A	388	GLU
1	A	403	GLU
1	A	430	LYS
1	A	445	VAL
1	A	461	SER
1	A	468	VAL
1	A	470	ARG
1	A	480	ASN
1	B	15	MET
1	B	16	GLN
1	B	23	LEU
1	B	32	VAL
1	B	75	HIS
1	B	95	CYS
1	B	125	LYS
1	B	138	GLU
1	B	150	GLN
1	B	267	LYS
1	B	304	LEU
1	B	324	ARG
1	B	369	GLU
1	B	394[A]	GLN
1	B	394[B]	GLN
1	B	399	ARG
1	B	403	GLU
1	B	463	GLN
1	B	479	ARG
1	B	487	SER
1	C	16	GLN
1	C	75	HIS
1	C	89	GLN
1	C	153	LYS
1	C	186	VAL
1	C	205	ILE
1	C	211	ASN
1	C	285	GLU
1	C	324	ARG
1	C	358	GLU
1	C	388	GLU
1	C	389	THR

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Mol	Chain	Res	Type
1	C	399	ARG
1	C	416	LEU
1	C	442	ASP
1	C	461	SER
1	C	467	ILE
1	C	470	ARG
1	C	474	GLU
1	D	15	MET
1	D	16	GLN
1	D	32	VAL
1	D	81	MET
1	D	172	THR
1	D	197	ASN
1	D	260	GLU
1	D	290	LYS
1	D	304	LEU
1	D	382	SER
1	D	388	GLU
1	D	389	THR
1	D	400	SER
1	D	438	LEU
1	D	442	ASP
1	D	445	VAL
1	D	458	LYS
1	D	479	ARG
1	D	506	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	409	GLN
1	B	211	ASN
1	B	215	ASN
1	B	231	GLN
1	B	409	GLN
1	B	471	ASN
1	B	503	ASN
1	C	20	ASN
1	C	156	ASN
1	C	194	ASN
1	D	83	ASN

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Mol	Chain	Res	Type
1	D	150	GLN
1	D	385	ASN
1	D	471	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ATP	A	603	2,4	26,33,33	0.70	0	31,52,52	0.83	1 (3%)
3	ATP	C	603	2,4	26,33,33	0.58	0	31,52,52	0.68	1 (3%)
3	ATP	D	603	2,4	26,33,33	0.66	0	31,52,52	0.79	2 (6%)
5	OXL	A	605	2	0,5,5	0.00	-	0,6,6	0.00	-
5	OXL	C	605	2	0,5,5	0.00	-	0,6,6	0.00	-
3	ATP	B	603	2,4	26,33,33	0.61	0	31,52,52	0.72	1 (3%)
5	OXL	D	605	2	0,5,5	0.00	-	0,6,6	0.00	-
5	OXL	B	605	2	0,5,5	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	603	2,4	-	3/18/38/38	0/3/3/3
3	ATP	C	603	2,4	-	3/18/38/38	0/3/3/3
3	ATP	D	603	2,4	-	2/18/38/38	0/3/3/3
5	OXL	A	605	2	-	0/0/4/4	-
5	OXL	C	605	2	-	0/0/4/4	-
3	ATP	B	603	2,4	-	4/18/38/38	0/3/3/3
5	OXL	D	605	2	-	0/0/4/4	-
5	OXL	B	605	2	-	0/0/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	ATP	C5-C6-N6	2.30	123.84	120.35
3	D	603	ATP	C5-C6-N6	2.29	123.83	120.35
3	C	603	ATP	C5-C6-N6	2.29	123.83	120.35
3	B	603	ATP	C5-C6-N6	2.20	123.69	120.35
3	D	603	ATP	O3'-C3'-C4'	2.05	116.99	111.05

There are no chirality outliers.

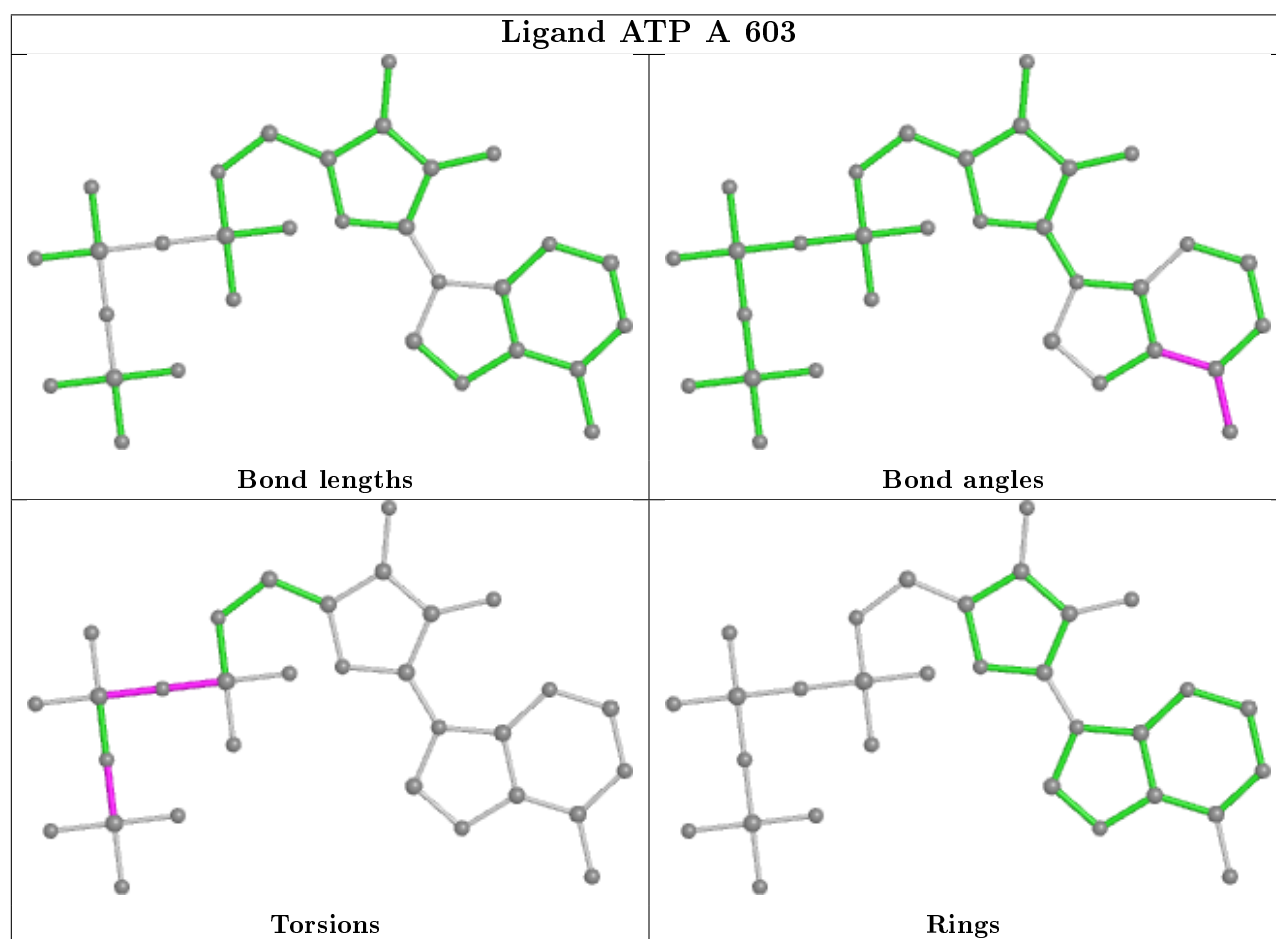
All (12) torsion outliers are listed below:

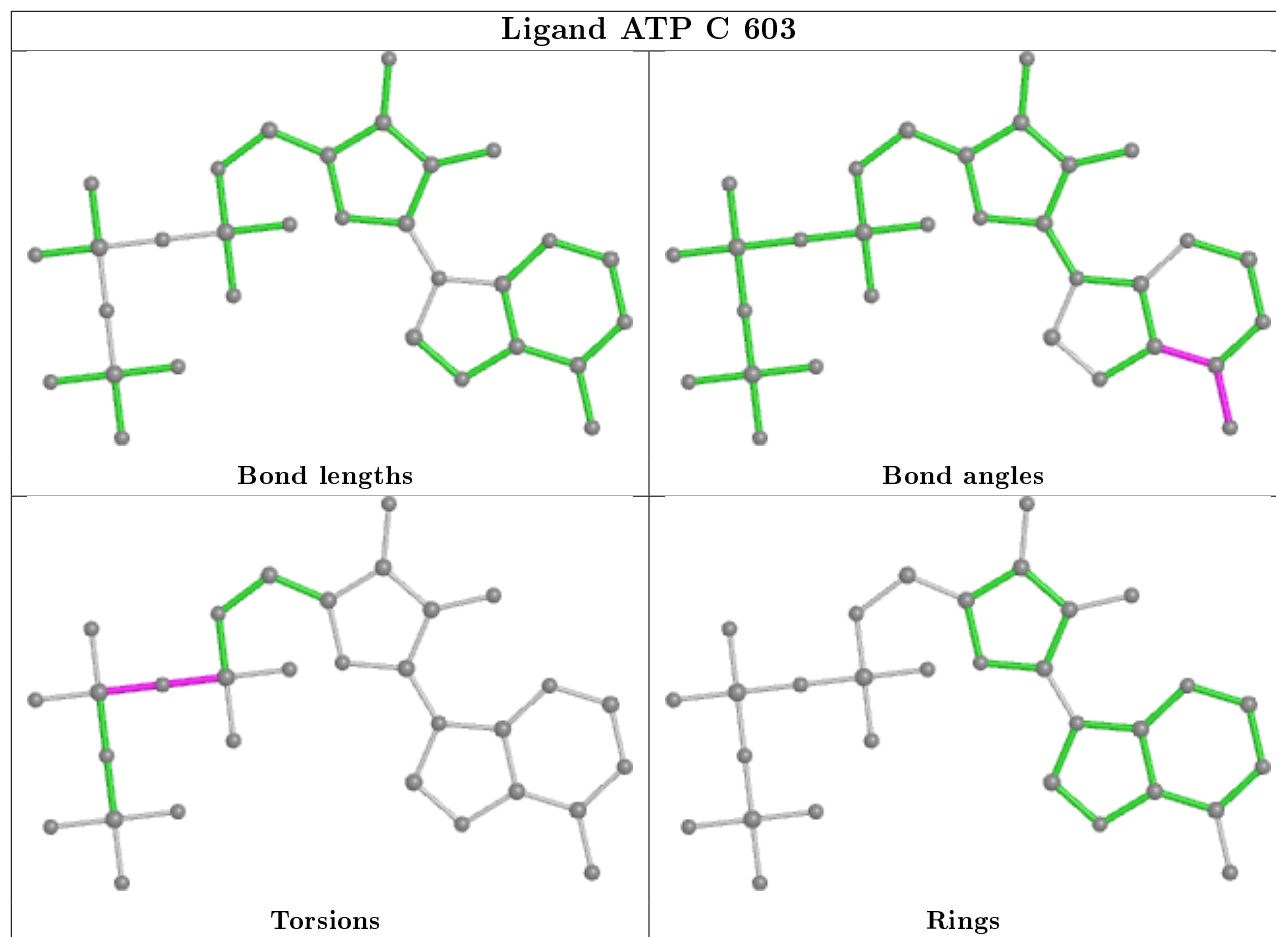
Mol	Chain	Res	Type	Atoms
3	D	603	ATP	PB-O3B-PG-O2G
3	D	603	ATP	PB-O3B-PG-O3G
3	A	603	ATP	PB-O3B-PG-O3G
3	C	603	ATP	PA-O3A-PB-O1B
3	B	603	ATP	PA-O3A-PB-O1B
3	C	603	ATP	PB-O3A-PA-O2A
3	B	603	ATP	PB-O3A-PA-O2A
3	A	603	ATP	PA-O3A-PB-O2B
3	A	603	ATP	PB-O3A-PA-O2A
3	C	603	ATP	PB-O3A-PA-O1A
3	B	603	ATP	PA-O3A-PB-O2B
3	B	603	ATP	PB-O3A-PA-O1A

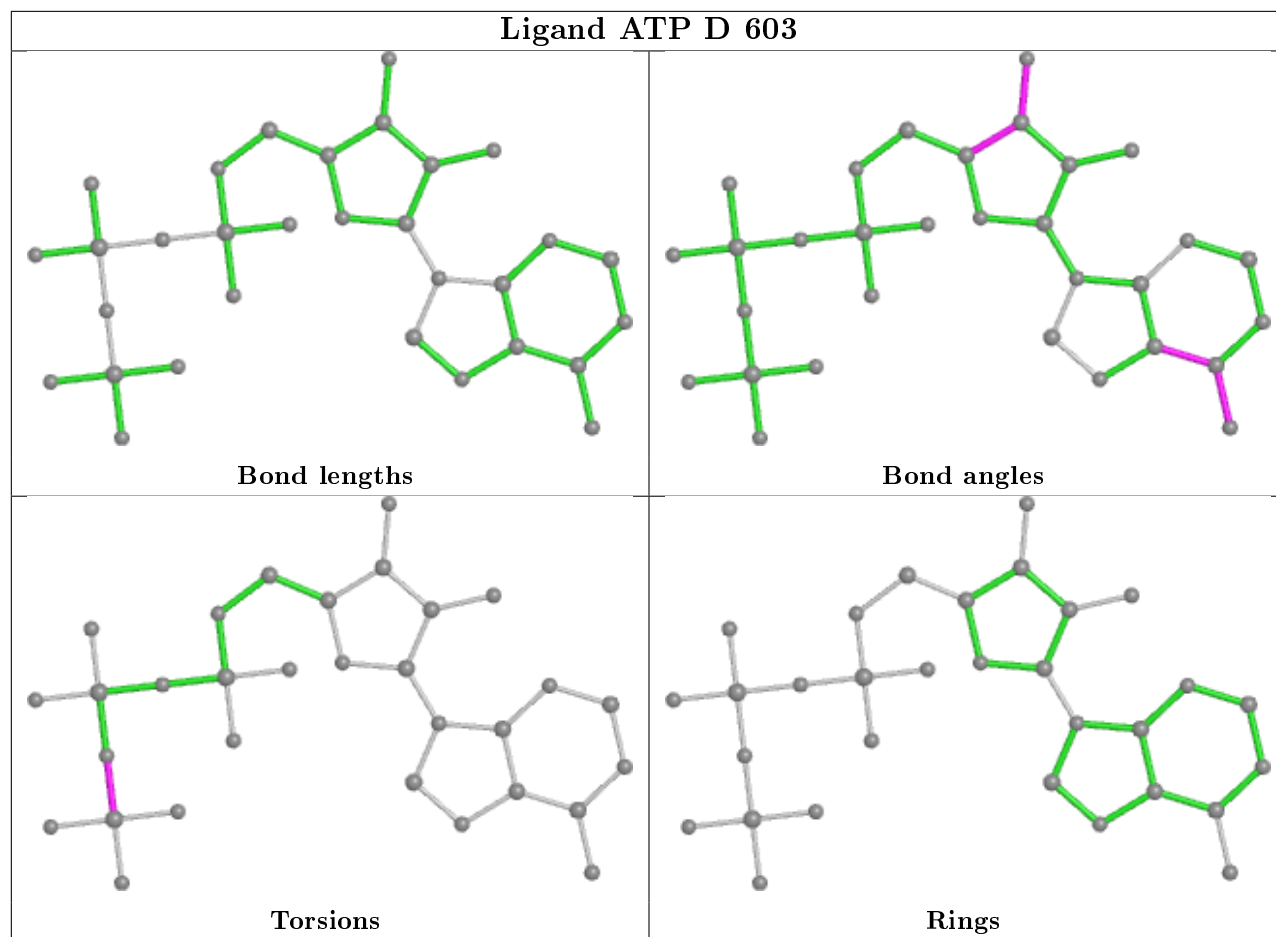
There are no ring outliers.

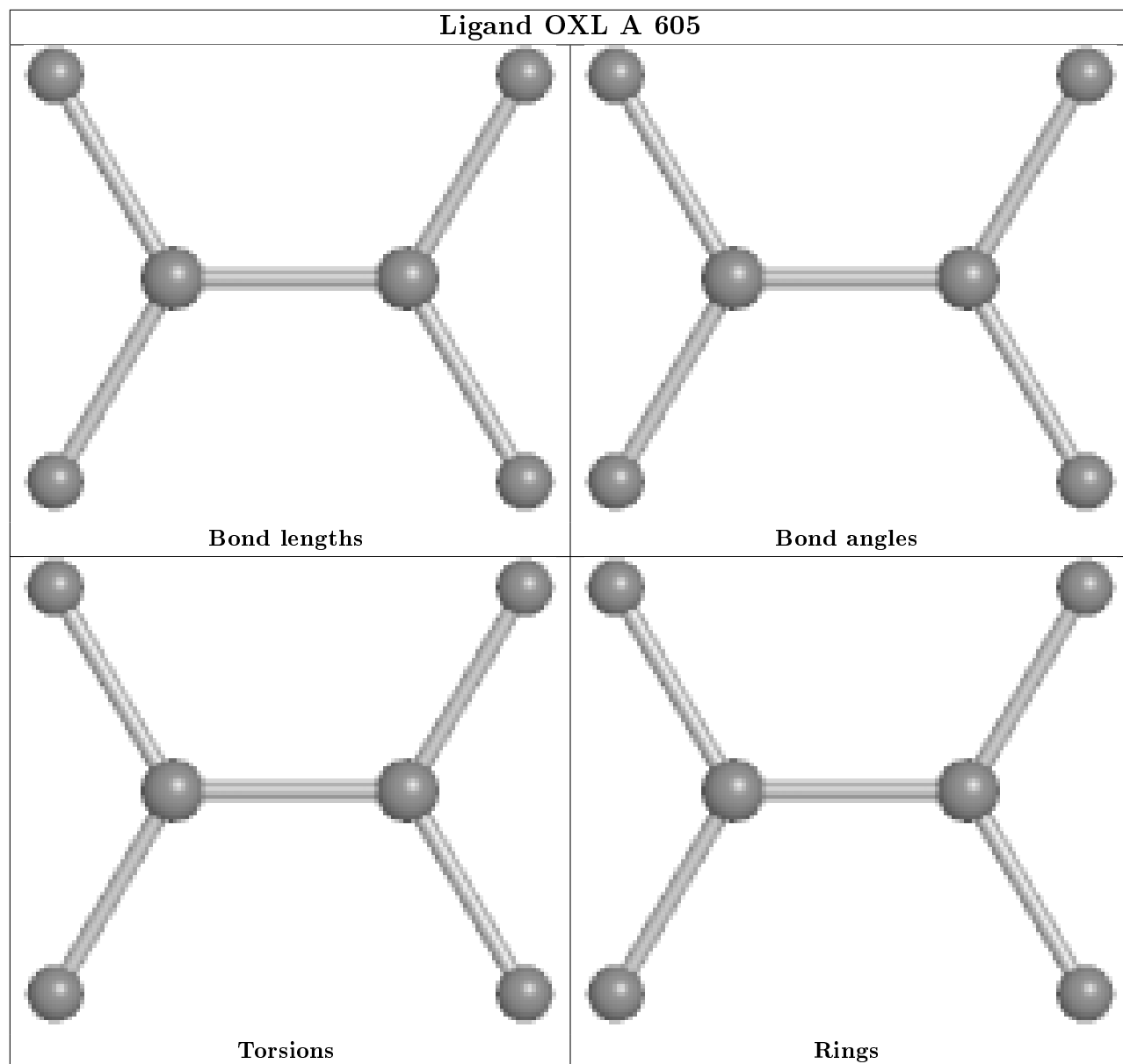
No monomer is involved in short contacts.

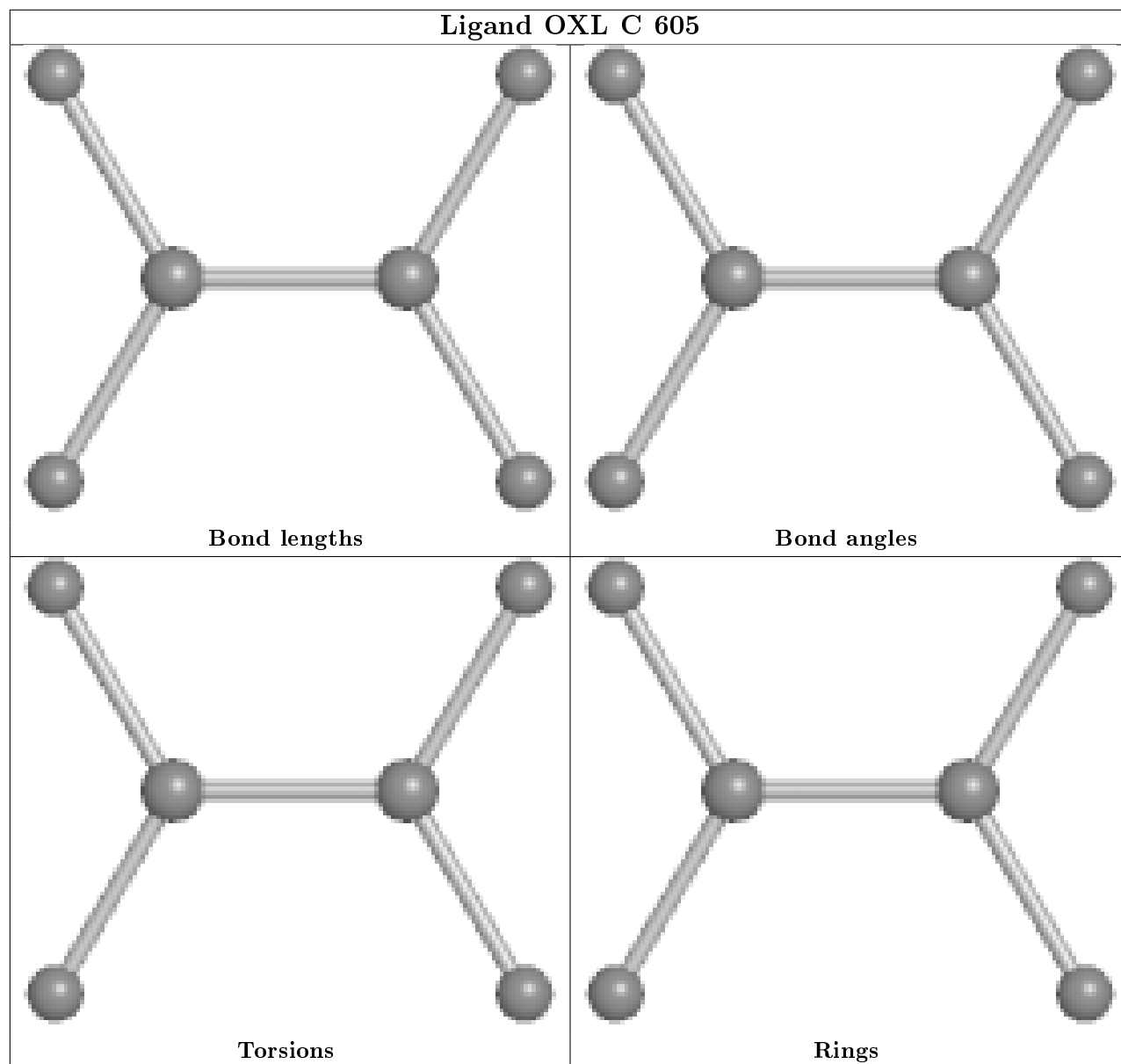
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



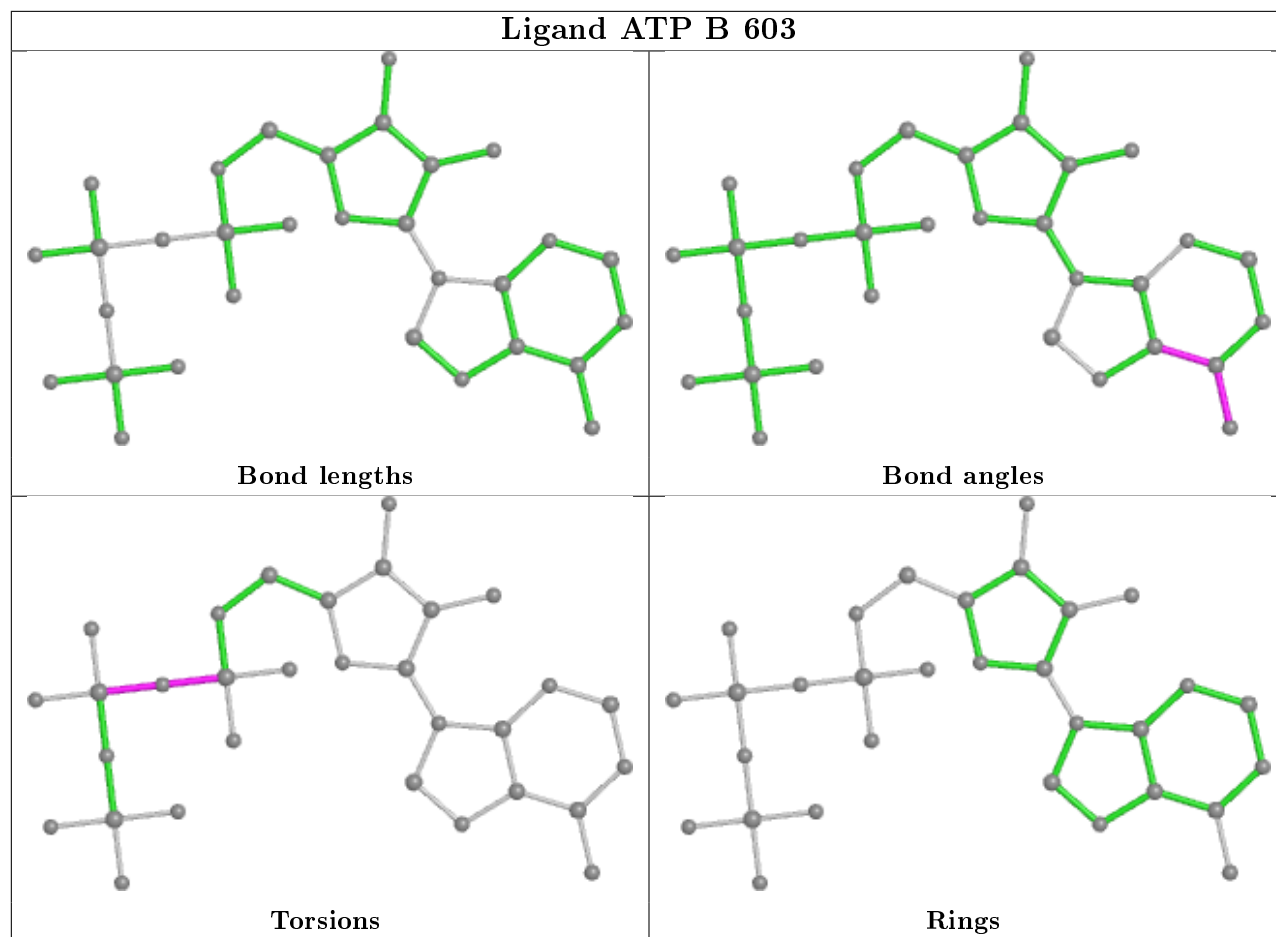


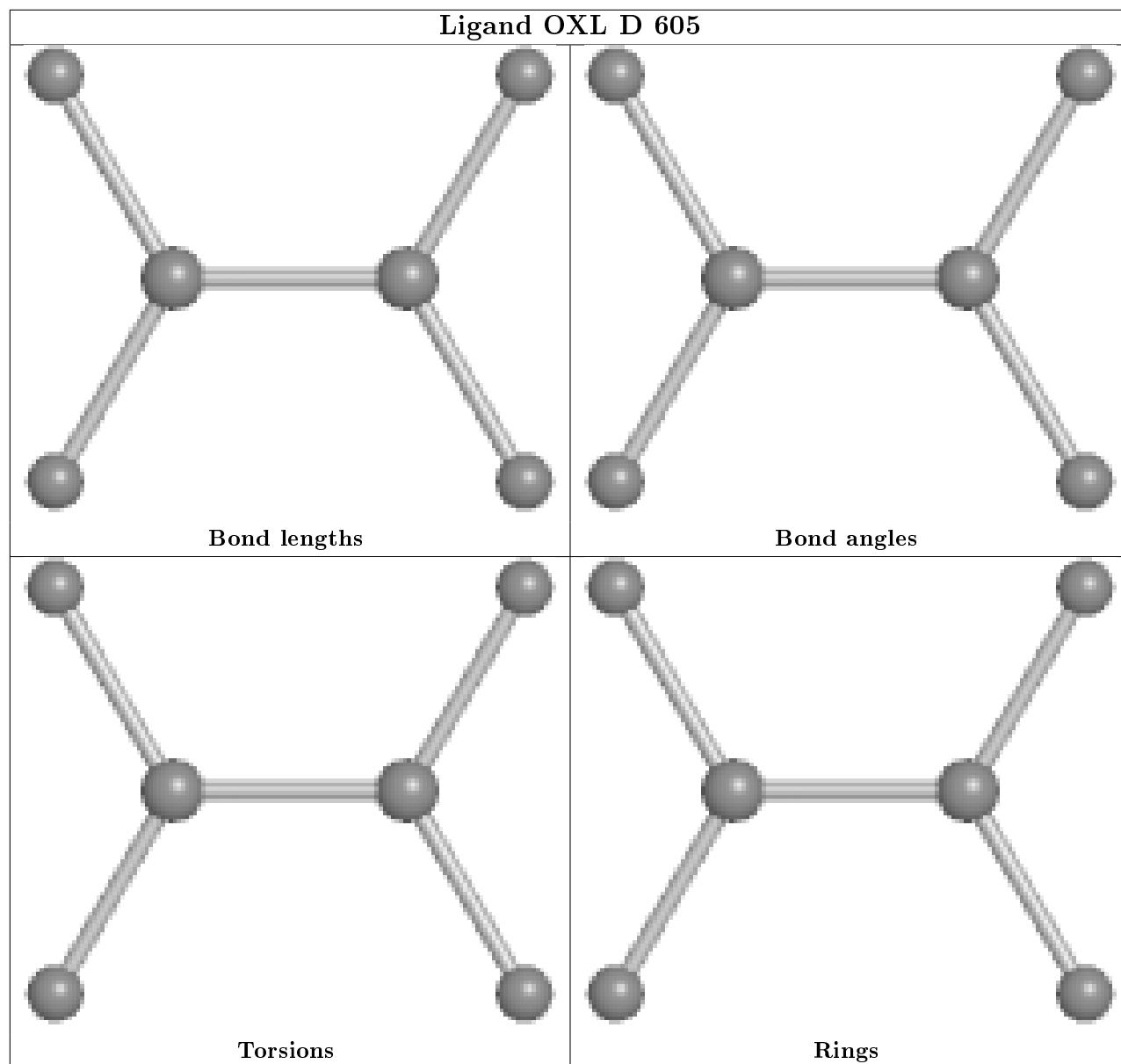


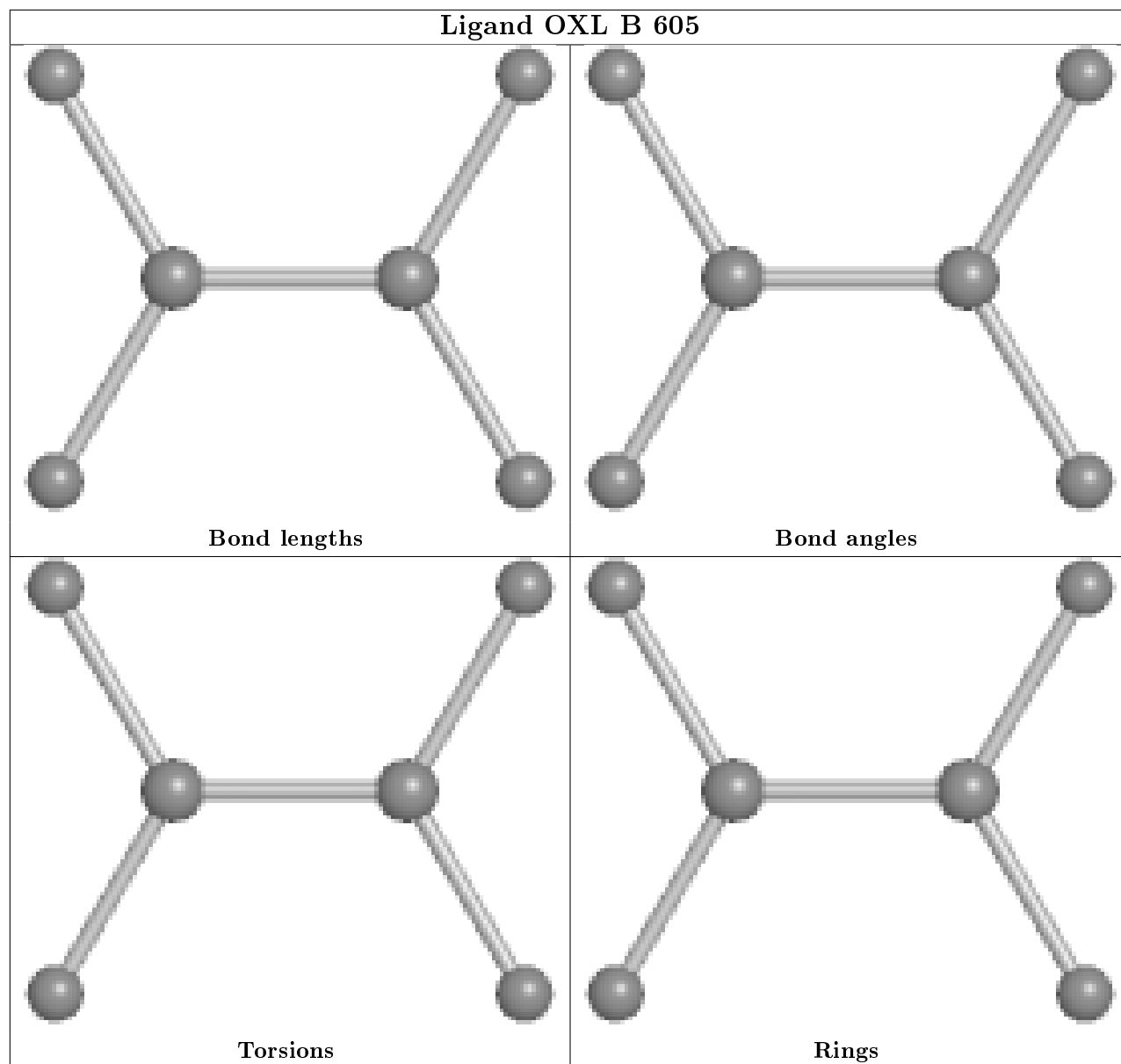












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	490/514 (95%)	-0.45	2 (0%) 92 91	30, 46, 79, 115	0
1	B	490/514 (95%)	-0.15	18 (3%) 41 34	28, 55, 88, 117	0
1	C	490/514 (95%)	-0.02	34 (6%) 16 12	33, 56, 105, 131	0
1	D	490/514 (95%)	-0.50	3 (0%) 89 88	31, 45, 77, 108	0
All	All	1960/2056 (95%)	-0.28	57 (2%) 51 45	28, 50, 90, 131	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	462	PHE	6.8
1	C	152	VAL	6.5
1	C	149	PRO	5.7
1	C	148	LEU	5.7
1	C	141	ILE	4.7
1	C	12	GLY	4.3
1	C	179	THR	4.1
1	C	115	ASN	3.9
1	C	140	CYS	3.9
1	C	117	GLU	3.9
1	C	174	GLU	3.8
1	C	112	PHE	3.5
1	B	129	VAL	3.5
1	C	173	HIS	3.5
1	C	132	TYR	3.5
1	C	126	LEU	3.4
1	C	175	ASP	3.3
1	C	134	PHE	3.1
1	C	176	HIS	3.1
1	A	461	SER	3.1
1	B	175	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	152	VAL	2.9
1	D	511	GLU	2.8
1	C	157	ILE	2.8
1	B	132	TYR	2.8
1	B	148	LEU	2.8
1	C	200	VAL	2.7
1	C	128	LEU	2.7
1	C	150	GLN	2.7
1	C	186	VAL	2.7
1	C	201	ASP	2.7
1	B	130	THR	2.6
1	C	135	LEU	2.4
1	C	151	SER	2.4
1	C	462	PHE	2.4
1	C	130	THR	2.4
1	D	484	VAL	2.4
1	C	114	LYS	2.4
1	B	201	ASP	2.4
1	B	204	ILE	2.4
1	A	12	GLY	2.3
1	B	115	ASN	2.3
1	B	133	GLU	2.2
1	C	142	ALA	2.2
1	B	146	LYS	2.2
1	B	151	SER	2.2
1	B	128	LEU	2.2
1	B	200	VAL	2.1
1	C	172	THR	2.1
1	B	460	GLY	2.1
1	C	113	LEU	2.1
1	B	15	MET	2.1
1	C	118	VAL	2.1
1	B	141	ILE	2.1
1	D	510	ILE	2.1
1	C	116	LYS	2.0
1	C	189	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

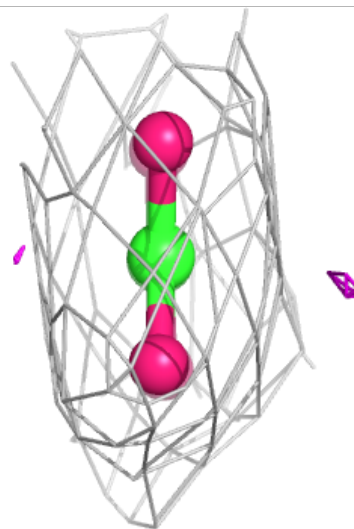
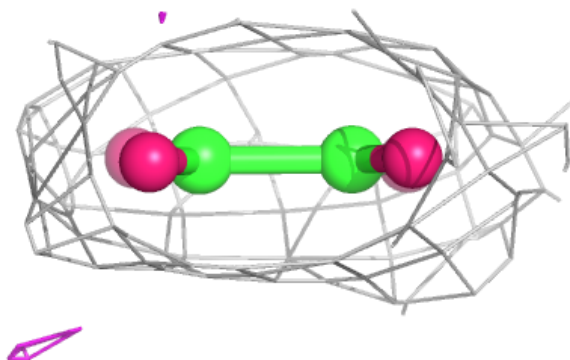
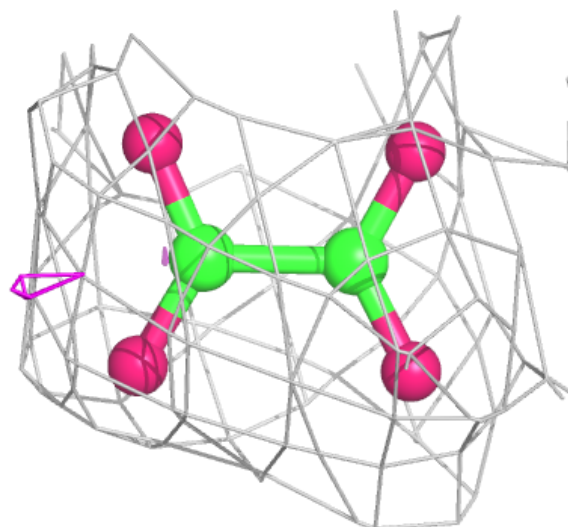
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	C	601	1/1	0.95	0.04	60,60,60,60	0
2	MG	C	602	1/1	0.96	0.06	56,56,56,56	0
5	OXL	C	605	6/6	0.96	0.12	57,59,59,61	0
5	OXL	B	605	6/6	0.96	0.13	53,58,61,61	0
3	ATP	C	603	31/31	0.97	0.17	59,71,75,76	0
5	OXL	D	605	6/6	0.97	0.11	45,48,49,49	0
4	K	C	604	1/1	0.98	0.08	60,60,60,60	0
3	ATP	B	603	31/31	0.98	0.11	53,61,65,65	0
4	K	B	604	1/1	0.98	0.07	51,51,51,51	0
5	OXL	A	605	6/6	0.98	0.11	42,43,47,48	0
2	MG	B	601	1/1	0.98	0.09	42,42,42,42	0
2	MG	A	602	1/1	0.98	0.09	33,33,33,33	0
2	MG	A	601	1/1	0.99	0.06	26,26,26,26	0
3	ATP	A	603	31/31	0.99	0.11	25,37,42,43	0
4	K	A	604	1/1	0.99	0.08	39,39,39,39	0
4	K	D	604	1/1	0.99	0.09	36,36,36,36	0
2	MG	D	602	1/1	0.99	0.07	29,29,29,29	0
2	MG	B	602	1/1	0.99	0.05	42,42,42,42	0
3	ATP	D	603	31/31	0.99	0.12	31,35,42,43	0
2	MG	D	601	1/1	1.00	0.14	30,30,30,30	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.

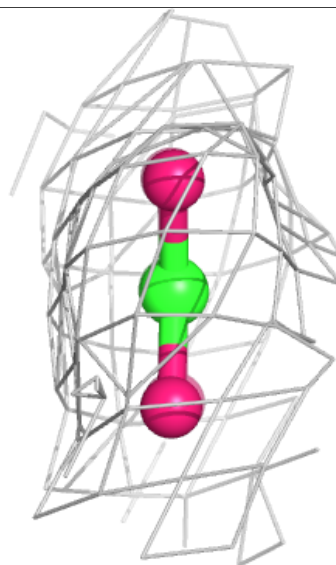
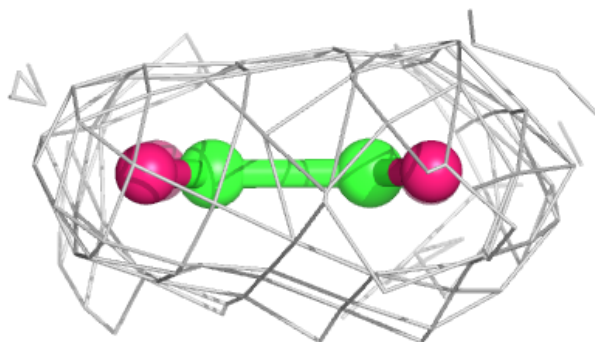
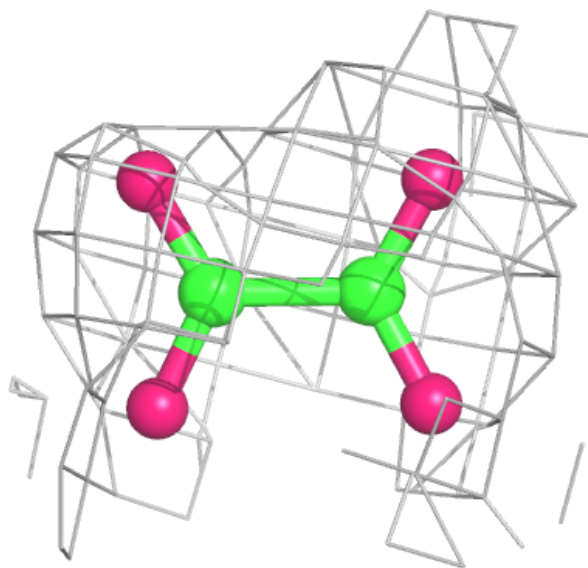
**Electron density around OXL C 605:**

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



**Electron density around OXL B 605:**

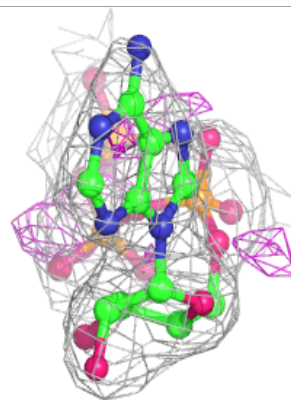
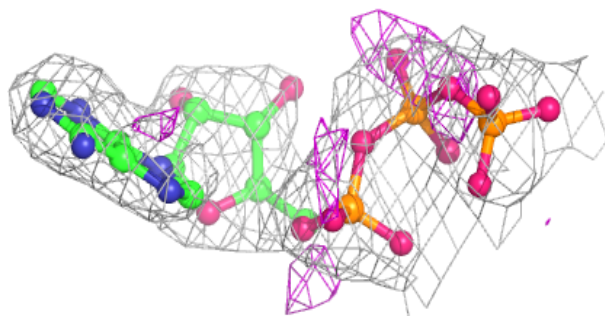
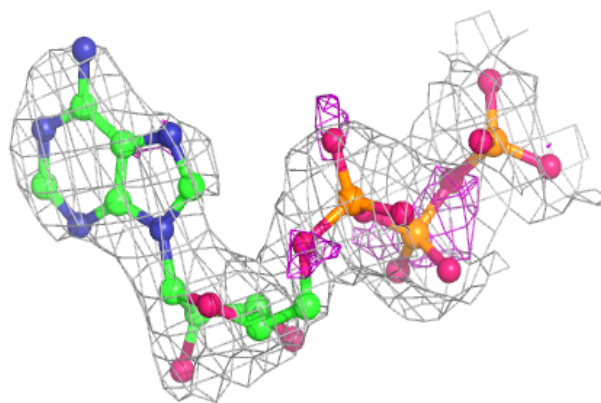
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





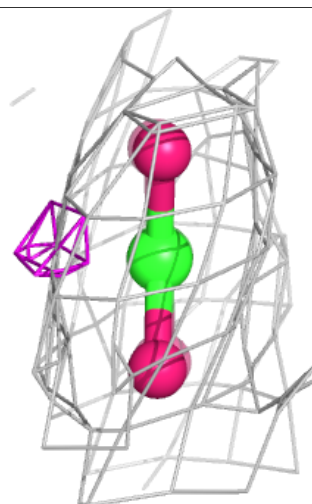
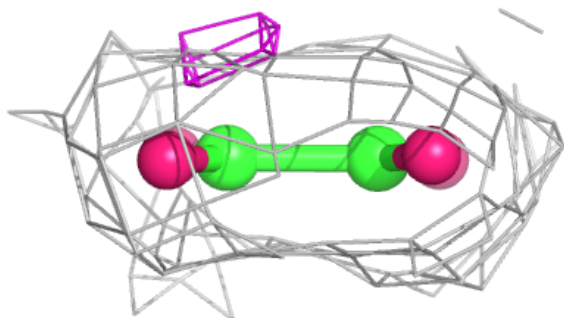
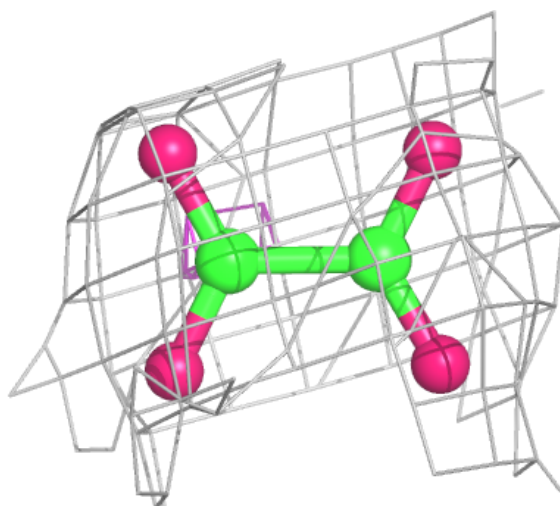
**Electron density around ATP C 603:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



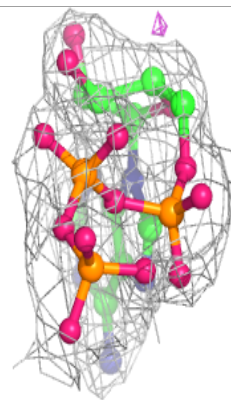
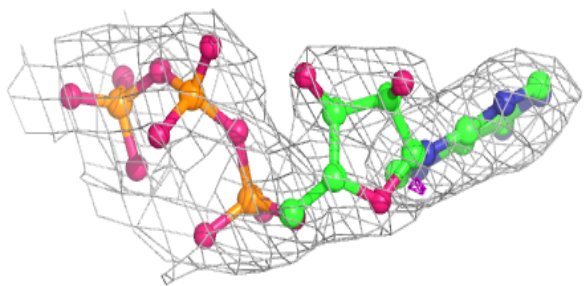
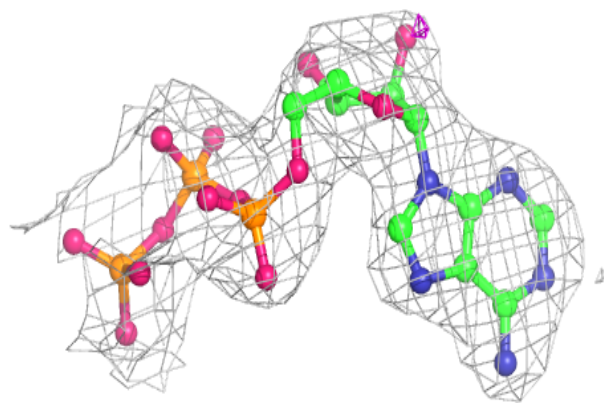
**Electron density around OXL D 605:**

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



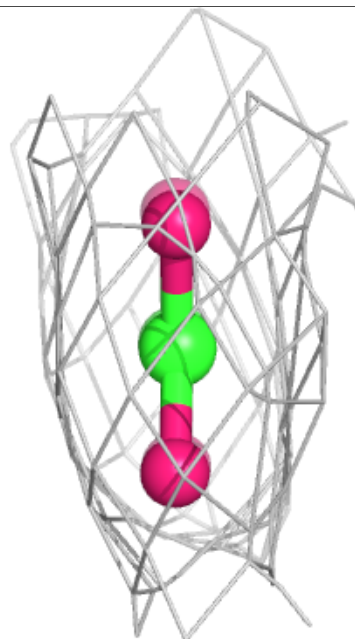
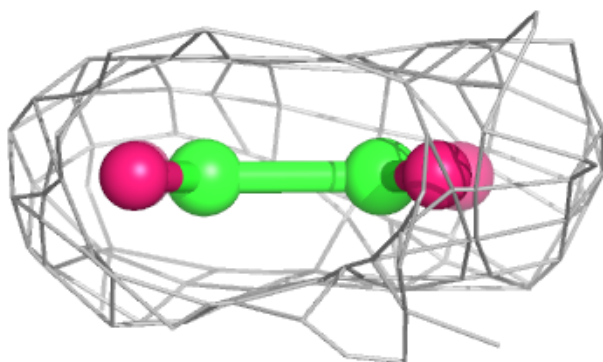
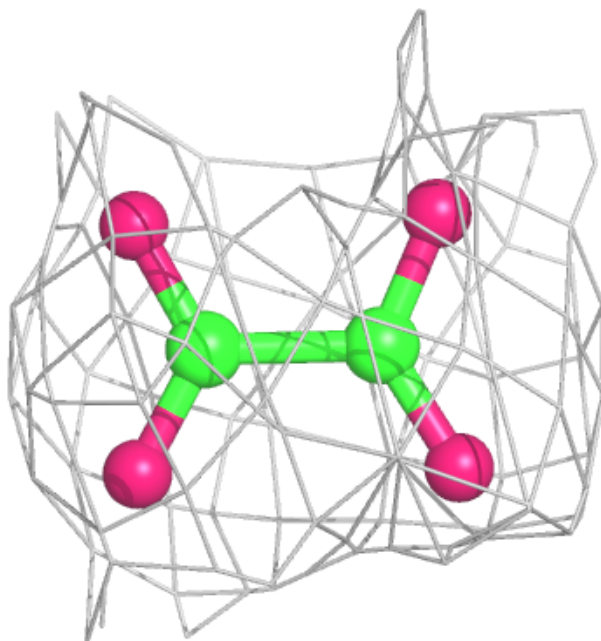
**Electron density around ATP B 603:**

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



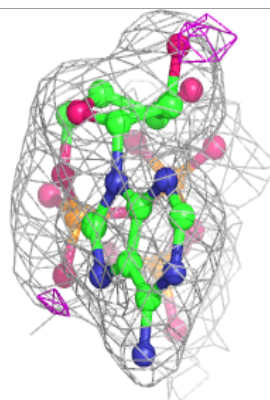
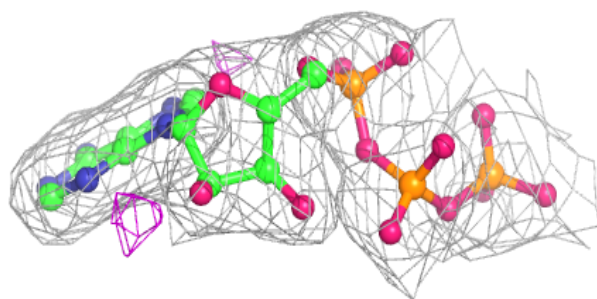
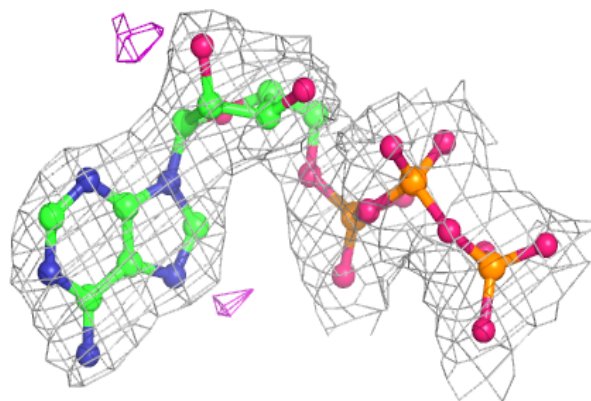
**Electron density around OXL A 605:**

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

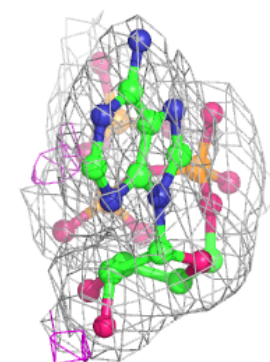
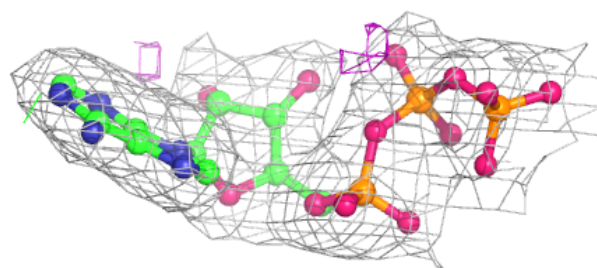
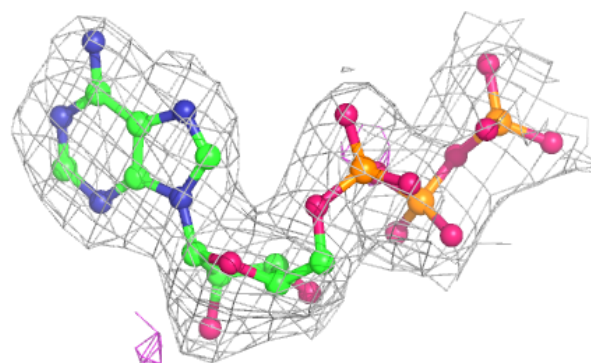


**Electron density around ATP A 603:**

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

**Electron density around ATP D 603:**

$2mF_o-DF_c$  (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.