



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:17 PM UTC

PDB ID : 6YBU / pdb_00006ybu
Title : Crystal structure of a native BcsE (349-523) RQ complex with c-di-GMP and ATP bound
Authors : Abidi, W.; Zouhir, S.; Roche, S.; Krasteva, P.V.
Deposited on : 2020-03-17
Resolution : 2.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

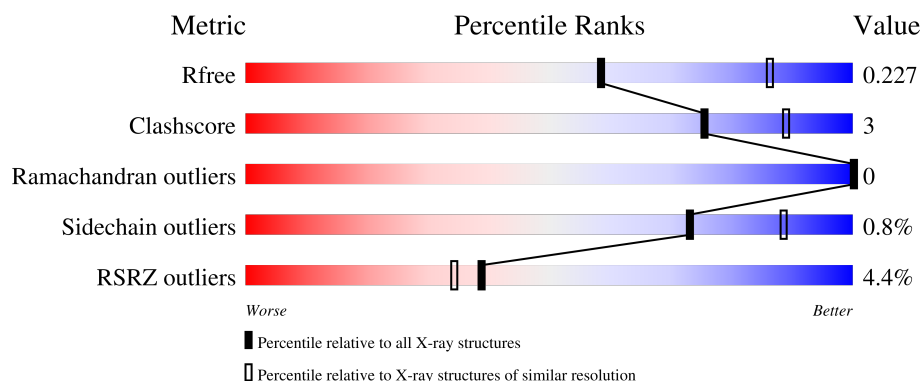
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

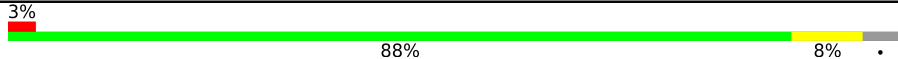
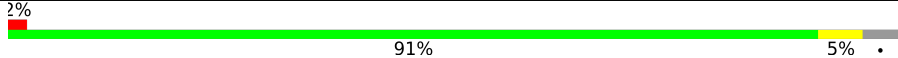
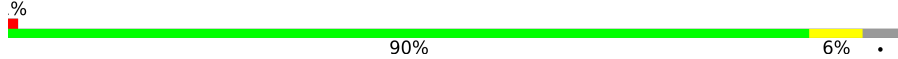
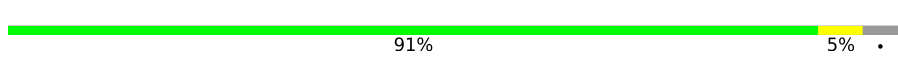
The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	250	
1	B	250	
1	G	250	
1	H	250	
2	C	67	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	67	
2	I	67	
2	J	67	
3	E	179	
3	F	179	
3	K	179	
3	L	179	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14546 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 Bacterial cellulose secretion regulator BcsQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1891	1187	342	352	10			
1	B	240	Total	C	N	O	S	0	0	0
			1891	1187	342	352	10			
1	G	240	Total	C	N	O	S	0	1	0
			1899	1191	343	355	10			
1	H	239	Total	C	N	O	S	0	0	0
			1887	1185	341	351	10			

- Molecule 2 is a protein called Bacterial cellulose secretion regulator BcsR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	29	Total	C	N	O	0	0	0
			235	151	40	44			
2	D	29	Total	C	N	O	0	0	0
			237	151	41	45			
2	I	30	Total	C	N	O	0	0	0
			243	157	41	45			
2	J	33	Total	C	N	O	0	0	0
			265	172	44	49			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP J7QAC9
C	-3	PRO	-	expression tag	UNP J7QAC9
C	-2	MET	-	expression tag	UNP J7QAC9
C	-1	GLY	-	expression tag	UNP J7QAC9
C	0	SER	-	expression tag	UNP J7QAC9
D	-4	GLY	-	expression tag	UNP J7QAC9
D	-3	PRO	-	expression tag	UNP J7QAC9
D	-2	MET	-	expression tag	UNP J7QAC9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP J7QAC9
D	0	SER	-	expression tag	UNP J7QAC9
I	-4	GLY	-	expression tag	UNP J7QAC9
I	-3	PRO	-	expression tag	UNP J7QAC9
I	-2	MET	-	expression tag	UNP J7QAC9
I	-1	GLY	-	expression tag	UNP J7QAC9
I	0	SER	-	expression tag	UNP J7QAC9
J	-4	GLY	-	expression tag	UNP J7QAC9
J	-3	PRO	-	expression tag	UNP J7QAC9
J	-2	MET	-	expression tag	UNP J7QAC9
J	-1	GLY	-	expression tag	UNP J7QAC9
J	0	SER	-	expression tag	UNP J7QAC9

- Molecule 3 is a protein called Bacterial cellulose secretion regulator BcsE, residues 349-523.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	168	Total	C	N	O	S	0	0	0
			1339	853	241	233	12			
3	F	166	Total	C	N	O	S	0	0	0
			1322	841	239	231	11			
3	K	166	Total	C	N	O	S	0	0	0
			1322	841	239	231	11			
3	L	162	Total	C	N	O	S	0	0	0
			1292	825	235	221	11			

There are 16 discrepancies between the modelled and reference sequences:

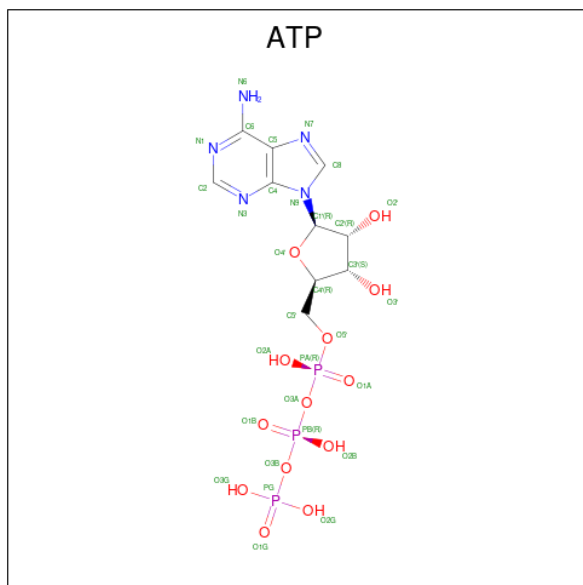
Chain	Residue	Modelled	Actual	Comment	Reference
E	345	MET	-	initiating methionine	UNP P37657
E	346	GLY	-	expression tag	UNP P37657
E	347	SER	-	expression tag	UNP P37657
E	348	MET	-	expression tag	UNP P37657
F	345	MET	-	initiating methionine	UNP P37657
F	346	GLY	-	expression tag	UNP P37657
F	347	SER	-	expression tag	UNP P37657
F	348	MET	-	expression tag	UNP P37657
K	345	MET	-	initiating methionine	UNP P37657
K	346	GLY	-	expression tag	UNP P37657
K	347	SER	-	expression tag	UNP P37657
K	348	MET	-	expression tag	UNP P37657
L	345	MET	-	initiating methionine	UNP P37657
L	346	GLY	-	expression tag	UNP P37657

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	347	SER	-	expression tag	UNP P37657
L	348	MET	-	expression tag	UNP P37657

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

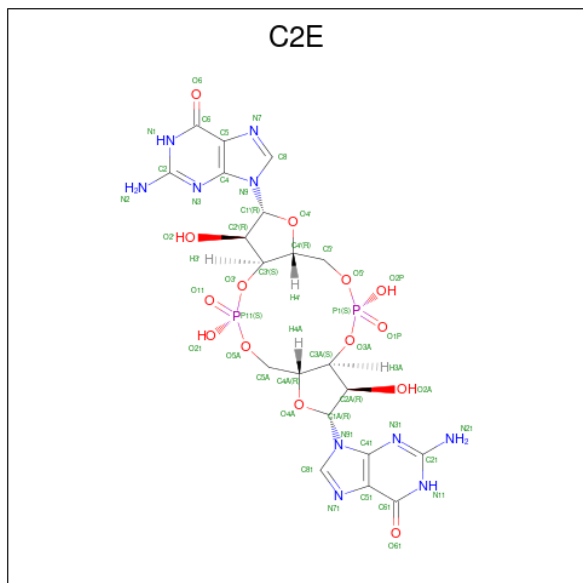
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
6	E	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
6	F	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
6	F	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
6	K	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
6	K	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
6	L	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
6	L	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

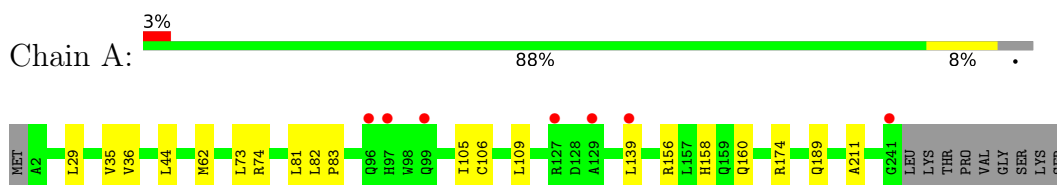
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	36	Total 36	O 36	0	0
7	B	35	Total 35	O 35	0	0
7	D	3	Total 3	O 3	0	0
7	E	18	Total 18	O 18	0	0
7	F	18	Total 18	O 18	0	0
7	G	35	Total 35	O 35	0	0
7	H	36	Total 36	O 36	0	0
7	I	3	Total 3	O 3	0	0
7	J	1	Total 1	O 1	0	0
7	K	20	Total 20	O 20	0	0
7	L	22	Total 22	O 22	0	0

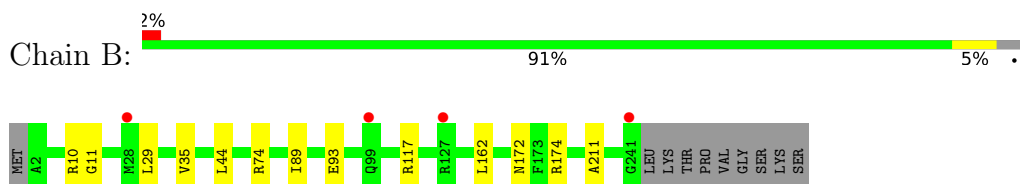
3 Residue-property plots [i](#)

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

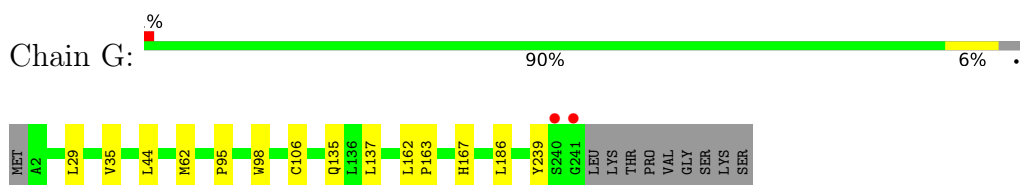
- Molecule 1: Bacterial cellulose secretion regulator BcsQ



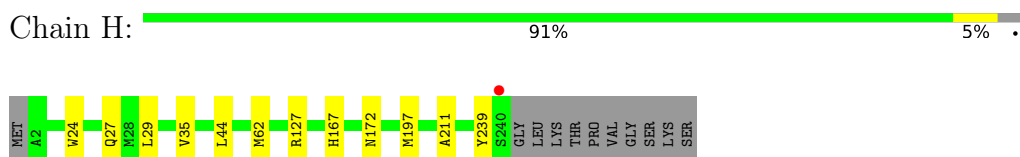
- Molecule 1: Bacterial cellulose secretion regulator BcsQ



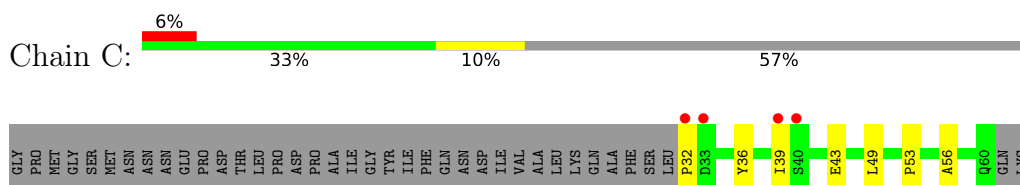
- Molecule 1: Bacterial cellulose secretion regulator BcsQ



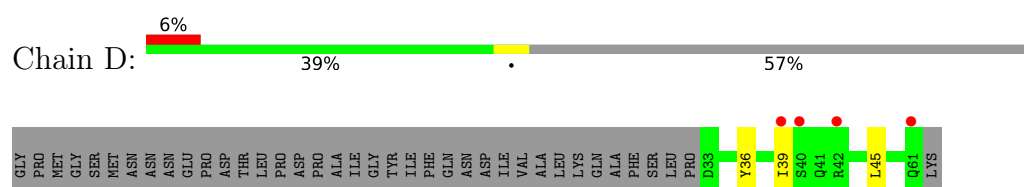
- Molecule 1: Bacterial cellulose secretion regulator BcsQ



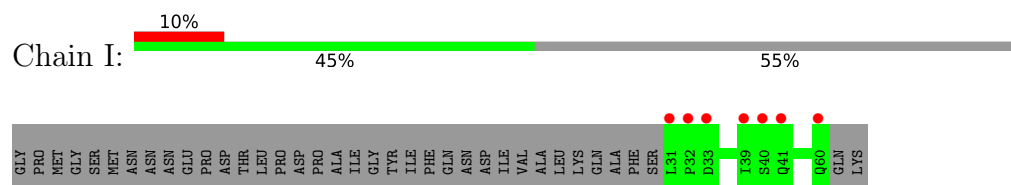
- Molecule 2: Bacterial cellulose secretion regulator BcsR



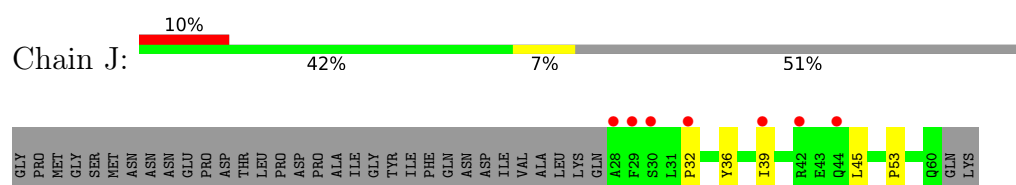
- Molecule 2: Bacterial cellulose secretion regulator BcsR



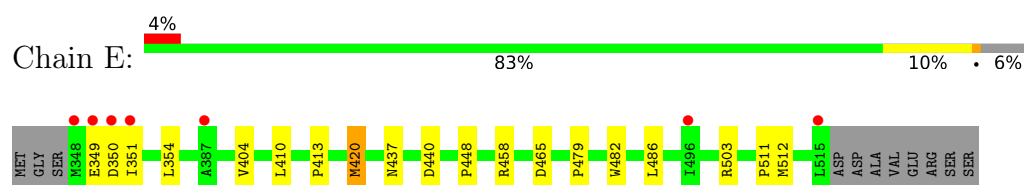
- Molecule 2: Bacterial cellulose secretion regulator BcsR



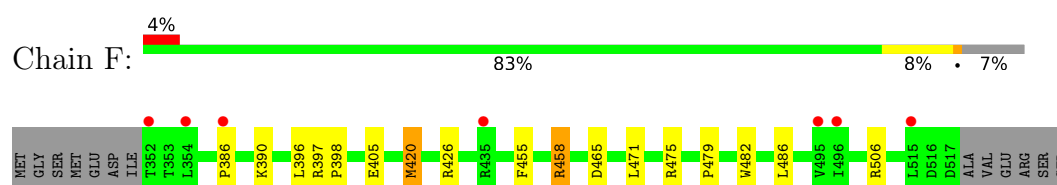
- Molecule 2: Bacterial cellulose secretion regulator BcsR



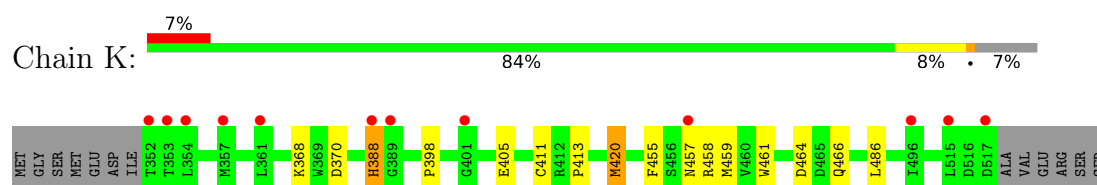
- Molecule 3: Bacterial cellulose secretion regulator BcsE, residues 349-523



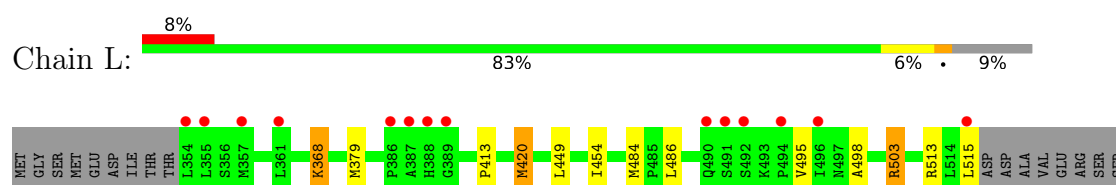
- Molecule 3: Bacterial cellulose secretion regulator BcsE, residues 349-523



- Molecule 3: Bacterial cellulose secretion regulator BcsE, residues 349-523



- Molecule 3: Bacterial cellulose secretion regulator BcsE, residues 349-523



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.99Å 72.57Å 161.25Å 90.00° 98.37° 90.00°	Depositor
Resolution (Å)	47.71 – 2.49 47.71 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.71-2.49) 99.0 (47.71-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.17rc2_3619	Depositor
R, R_{free}	0.181 , 0.225 0.184 , 0.227	Depositor DCC
R_{free} test set	4331 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14546	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, C2E

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	0.10	0/1928	0.29	0/2623
1	B	0.09	0/1928	0.28	0/2623
1	G	0.10	0/1936	0.29	0/2634
1	H	0.10	0/1924	0.29	0/2618
2	C	0.11	0/240	0.28	0/325
2	D	0.10	0/241	0.27	0/326
2	I	0.11	0/248	0.27	0/337
2	J	0.13	0/271	0.30	0/368
3	E	0.11	0/1371	0.31	0/1864
3	F	0.11	0/1354	0.31	0/1842
3	K	0.12	0/1354	0.31	0/1842
3	L	0.12	0/1324	0.33	0/1800
All	All	0.10	0/14119	0.30	0/19202

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

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	1891	0	1861	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1891	0	1861	11	0
1	G	1899	0	1864	10	0
1	H	1887	0	1858	8	0
2	C	235	0	230	4	0
2	D	237	0	230	4	0
2	I	243	0	240	0	0
2	J	265	0	259	4	0
3	E	1339	0	1361	14	1
3	F	1322	0	1339	12	0
3	K	1322	0	1339	10	0
3	L	1292	0	1317	9	1
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	G	31	0	12	0	0
4	H	31	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	E	92	0	44	0	0
6	F	92	0	44	0	1
6	K	92	0	44	1	1
6	L	92	0	44	0	0
7	A	36	0	0	0	0
7	B	35	0	0	2	0
7	D	3	0	0	0	0
7	E	18	0	0	0	0
7	F	18	0	0	0	0
7	G	35	0	0	0	0
7	H	36	0	0	1	0
7	I	3	0	0	0	0
7	J	1	0	0	0	0
7	K	20	0	0	0	0
7	L	22	0	0	0	0
All	All	14546	0	13983	86	2

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 3.

All (86) 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)
3:K:413:PRO:HG3	3:K:420:MET:HE1	1.63	0.81
3:L:413:PRO:HG3	3:L:420:MET:HE1	1.69	0.74
3:E:413:PRO:HG3	3:E:420:MET:HE1	1.72	0.71
2:J:39:ILE:HG23	2:J:45:LEU:HD23	1.77	0.66
1:B:172:ASN:ND2	7:B:401:HOH:O	2.31	0.64
1:A:174:ARG:HH22	1:B:174:ARG:HE	1.48	0.61
1:A:189:GLN:HG3	2:D:45:LEU:HD11	1.82	0.60
3:E:349:GLU:HG3	3:E:354:LEU:HD21	1.83	0.60
1:A:74:ARG:HB2	3:E:512:MET:HG2	1.84	0.60
1:A:35:VAL:HG22	1:A:44:LEU:HD21	1.84	0.59
1:H:127:ARG:NH1	7:H:401:HOH:O	2.24	0.58
3:K:457:ASN:OD1	3:K:458:ARG:N	2.37	0.58
1:G:167:HIS:HD1	1:G:239:TYR:HH	1.51	0.58
1:B:35:VAL:HG22	1:B:44:LEU:HD21	1.87	0.57
3:F:398:PRO:HA	3:F:455:PHE:HA	1.87	0.57
1:B:162:LEU:HG	2:C:32:PRO:HG3	1.87	0.57
1:H:35:VAL:HG22	1:H:44:LEU:HD21	1.86	0.57
1:B:74:ARG:HH12	1:B:117:ARG:HH22	1.51	0.57
1:G:35:VAL:HG22	1:G:44:LEU:HD21	1.88	0.56
1:G:29:LEU:HA	3:K:486:LEU:HD13	1.89	0.54
1:B:174:ARG:NH1	7:B:402:HOH:O	2.41	0.54
3:E:465:ASP:N	3:E:465:ASP:OD1	2.41	0.53
1:H:211:ALA:HA	2:J:53:PRO:HD2	1.91	0.53
3:F:397:ARG:HH11	3:F:426:ARG:HH22	1.58	0.52
1:H:29:LEU:HA	3:L:486:LEU:HD13	1.91	0.52
1:B:29:LEU:HA	3:F:486:LEU:HD13	1.91	0.52
2:C:36:TYR:HD1	2:C:39:ILE:HG13	1.75	0.52
1:A:36:VAL:HG12	1:A:82:LEU:HB3	1.92	0.51
1:G:167:HIS:ND1	1:G:239:TYR:OH	2.38	0.51
1:A:29:LEU:HA	3:E:486:LEU:HD13	1.92	0.50
1:H:167:HIS:ND1	1:H:239:TYR:OH	2.41	0.49
3:L:368:LYS:HG2	3:L:484:MET:HE1	1.94	0.49
1:B:211:ALA:O	3:F:506:ARG:NH2	2.36	0.49
3:K:405:GLU:HB3	3:K:486:LEU:HG	1.94	0.49
3:L:495:VAL:HG23	3:L:498:ALA:HB2	1.96	0.48
1:A:105:ILE:HG13	1:A:109:LEU:HD13	1.94	0.47
3:K:466:GLN:N	3:K:466:GLN:OE1	2.47	0.47
3:E:349:GLU:N	3:E:349:GLU:OE2	2.47	0.47
3:E:440:ASP:OD1	3:E:458:ARG:NH2	2.46	0.47
1:A:106:CYS:HA	1:A:139:LEU:HD11	1.97	0.46
3:F:396:LEU:HD23	3:F:458:ARG:HB2	1.97	0.46
3:F:420:MET:HE2	3:F:420:MET:HB3	1.70	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:420:MET:HB3	3:L:420:MET:HE2	1.60	0.46
3:F:386:PRO:O	3:F:390:LYS:NZ	2.38	0.45
3:E:479:PRO:HA	3:E:482:TRP:CE2	2.52	0.45
1:B:10:ARG:HD2	1:B:11:GLY:O	2.17	0.45
3:K:388:HIS:CD2	3:K:464:ASP:H	2.36	0.44
3:K:398:PRO:HA	3:K:455:PHE:HA	1.98	0.44
1:A:158:HIS:NE2	2:D:36:TYR:OH	2.39	0.44
3:F:465:ASP:OD1	3:F:465:ASP:N	2.50	0.44
1:H:24:TRP:O	1:H:27:GLN:HG3	2.17	0.44
1:A:81:LEU:HD12	1:A:83:PRO:HD3	2.00	0.44
1:G:106:CYS:SG	1:G:135:GLN:HB3	2.57	0.44
1:H:62:MET:HE2	1:H:62:MET:HB3	1.87	0.44
3:L:379:MET:HE3	3:L:379:MET:HB2	1.80	0.44
3:L:513:ARG:HG2	3:L:515:LEU:HD12	1.99	0.44
1:B:74:ARG:HH12	1:B:117:ARG:NH2	2.15	0.43
2:D:36:TYR:HD1	2:D:39:ILE:HD11	1.83	0.43
3:E:350:ASP:OD1	3:E:351:ILE:N	2.52	0.43
3:F:479:PRO:HA	3:F:482:TRP:CE2	2.54	0.43
2:C:49:LEU:O	2:C:56:ALA:HB2	2.19	0.43
3:E:410:LEU:O	3:E:448:PRO:HD3	2.18	0.43
1:G:137:LEU:HD21	1:G:163:PRO:HG3	2.00	0.43
1:G:162:LEU:HD22	2:J:32:PRO:HG3	2.01	0.42
1:H:197:MET:HE2	1:H:197:MET:HB3	1.92	0.42
1:A:62:MET:HE1	1:A:105:ILE:N	2.33	0.42
2:D:36:TYR:CD1	2:D:39:ILE:HD11	2.54	0.42
3:E:479:PRO:HA	3:E:482:TRP:CD2	2.54	0.42
1:A:211:ALA:HA	2:C:53:PRO:HD2	2.00	0.42
3:L:413:PRO:CG	3:L:420:MET:HE1	2.45	0.42
3:L:449:LEU:HB2	3:L:454:ILE:HD11	2.01	0.42
3:E:420:MET:HE2	3:E:420:MET:HB3	1.67	0.42
1:G:62:MET:HE2	1:G:62:MET:HB3	1.84	0.42
3:E:437:ASN:OD1	3:E:437:ASN:N	2.47	0.42
6:K:601:C2E:H81	6:K:601:C2E:O5A	2.19	0.42
1:G:186:LEU:HD21	2:J:36:TYR:HE1	1.85	0.42
3:F:405:GLU:HB2	3:F:486:LEU:HG	2.02	0.41
3:F:471:LEU:O	3:F:475:ARG:HG3	2.20	0.41
1:G:95:PRO:HA	1:G:98:TRP:NE1	2.35	0.41
3:K:459:MET:HG2	3:K:461:TRP:CZ2	2.56	0.41
1:B:89:ILE:O	1:B:93:GLU:HG2	2.21	0.41
3:K:411:CYS:SG	3:K:420:MET:HE2	2.60	0.41
1:A:73:LEU:HD23	3:E:511:PRO:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:O	1:A:160:GLN:HG2	2.20	0.40
3:F:479:PRO:HA	3:F:482:TRP:CD2	2.56	0.40
3:K:370:ASP:OD1	3:K:370:ASP:N	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:503:ARG:NH2	6:K:601:C2E:O2P[1_455]	1.30	0.90
3:L:503:ARG:NH1	6:F:602:C2E:O2P[1_655]	1.30	0.90

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	238/250 (95%)	237 (100%)	1 (0%)	0	100	100
1	B	238/250 (95%)	237 (100%)	1 (0%)	0	100	100
1	G	239/250 (96%)	234 (98%)	5 (2%)	0	100	100
1	H	237/250 (95%)	233 (98%)	4 (2%)	0	100	100
2	C	27/67 (40%)	24 (89%)	3 (11%)	0	100	100
2	D	27/67 (40%)	27 (100%)	0	0	100	100
2	I	28/67 (42%)	27 (96%)	1 (4%)	0	100	100
2	J	31/67 (46%)	28 (90%)	3 (10%)	0	100	100
3	E	166/179 (93%)	165 (99%)	1 (1%)	0	100	100
3	F	164/179 (92%)	162 (99%)	2 (1%)	0	100	100
3	K	164/179 (92%)	160 (98%)	4 (2%)	0	100	100
3	L	160/179 (89%)	158 (99%)	2 (1%)	0	100	100
All	All	1719/1984 (87%)	1692 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	202/211 (96%)	202 (100%)	0	100	100
1	B	202/211 (96%)	202 (100%)	0	100	100
1	G	203/211 (96%)	203 (100%)	0	100	100
1	H	202/211 (96%)	201 (100%)	1 (0%)	81	92
2	C	23/55 (42%)	22 (96%)	1 (4%)	26	51
2	D	23/55 (42%)	23 (100%)	0	100	100
2	I	24/55 (44%)	24 (100%)	0	100	100
2	J	26/55 (47%)	26 (100%)	0	100	100
3	E	150/159 (94%)	148 (99%)	2 (1%)	61	82
3	F	148/159 (93%)	146 (99%)	2 (1%)	59	81
3	K	148/159 (93%)	145 (98%)	3 (2%)	48	75
3	L	144/159 (91%)	141 (98%)	3 (2%)	47	74
All	All	1495/1700 (88%)	1483 (99%)	12 (1%)	73	88

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	43	GLU
3	E	404	VAL
3	E	420	MET
3	F	420	MET
3	F	458	ARG
1	H	172	ASN
3	K	368	LYS
3	K	388	HIS
3	K	420	MET
3	L	368	LYS
3	L	420	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	503	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	148	ASN
1	A	189	GLN
1	B	159	GLN
1	B	172	ASN
3	E	378	ASN
3	F	374	ASN
3	F	466	GLN
1	G	134	HIS
1	G	148	ASN
1	G	172	ASN
1	G	213	GLN
1	H	32	ASN
1	H	134	HIS
1	H	148	ASN
3	K	504	HIS
3	L	378	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 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	$\# Z > 2$
6	C2E	L	602	-	52,52,52	0.25	0	78,82,82	0.33	0
6	C2E	K	602	-	52,52,52	0.26	0	78,82,82	0.33	0
6	C2E	K	601	-	52,52,52	0.23	0	78,82,82	0.33	0
6	C2E	E	601	-	52,52,52	0.26	0	78,82,82	0.33	0
4	ATP	H	301	5	32,33,33	0.29	0	48,52,52	0.29	0
6	C2E	L	601	-	52,52,52	0.25	0	78,82,82	0.33	0
4	ATP	A	301	5	32,33,33	0.28	0	48,52,52	0.29	0
6	C2E	F	602	-	52,52,52	0.25	0	78,82,82	0.33	0
4	ATP	B	301	5	32,33,33	0.25	0	48,52,52	0.31	0
6	C2E	E	602	-	52,52,52	0.25	0	78,82,82	0.33	0
6	C2E	F	601	-	52,52,52	0.26	0	78,82,82	0.32	0
4	ATP	G	301	5	32,33,33	0.28	0	48,52,52	0.32	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
6	C2E	L	602	-	-	0/30/62/62	0/6/7/7
6	C2E	K	602	-	-	0/30/62/62	0/6/7/7
6	C2E	K	601	-	-	0/30/62/62	0/6/7/7
6	C2E	E	601	-	-	0/30/62/62	0/6/7/7
4	ATP	H	301	5	-	3/22/38/38	0/3/3/3
6	C2E	L	601	-	-	0/30/62/62	0/6/7/7
4	ATP	A	301	5	-	0/22/38/38	0/3/3/3
6	C2E	F	602	-	-	0/30/62/62	0/6/7/7
4	ATP	B	301	5	-	3/22/38/38	0/3/3/3
6	C2E	E	602	-	-	0/30/62/62	0/6/7/7
6	C2E	F	601	-	-	0/30/62/62	0/6/7/7
4	ATP	G	301	5	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	ATP	PB-O3B-PG-O3G
4	H	301	ATP	PB-O3B-PG-O3G
4	B	301	ATP	PB-O3B-PG-O1G
4	H	301	ATP	PB-O3B-PG-O1G
4	B	301	ATP	PB-O3B-PG-O2G
4	H	301	ATP	PB-O3B-PG-O2G

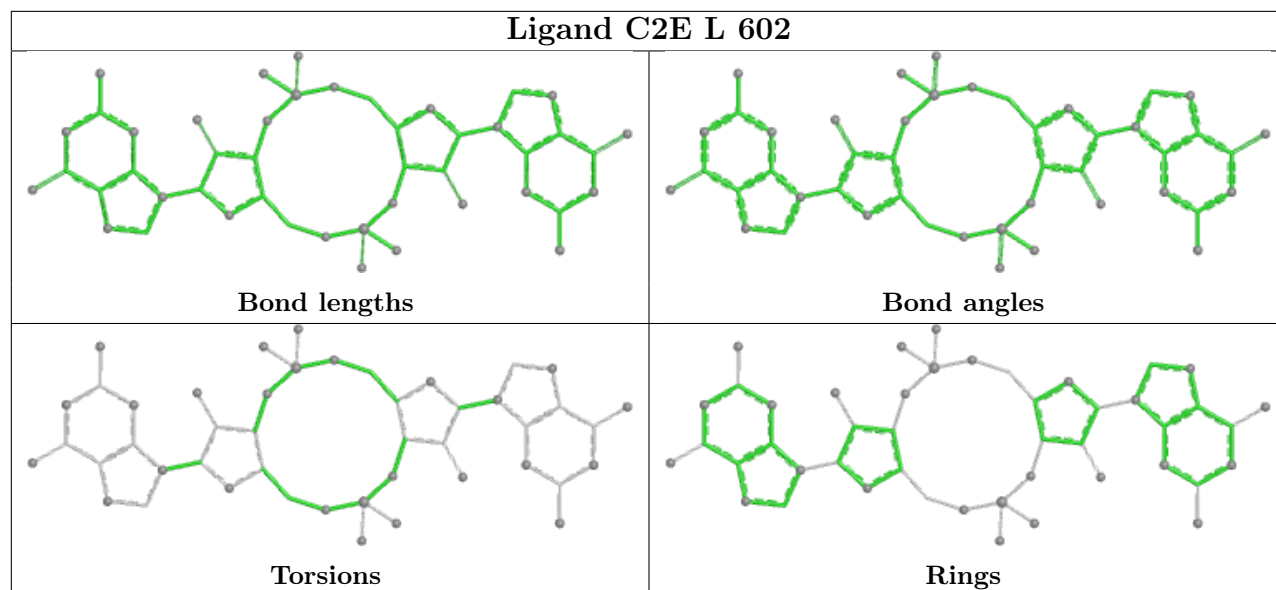
There are no ring outliers.

2 monomers are involved in 3 short contacts:

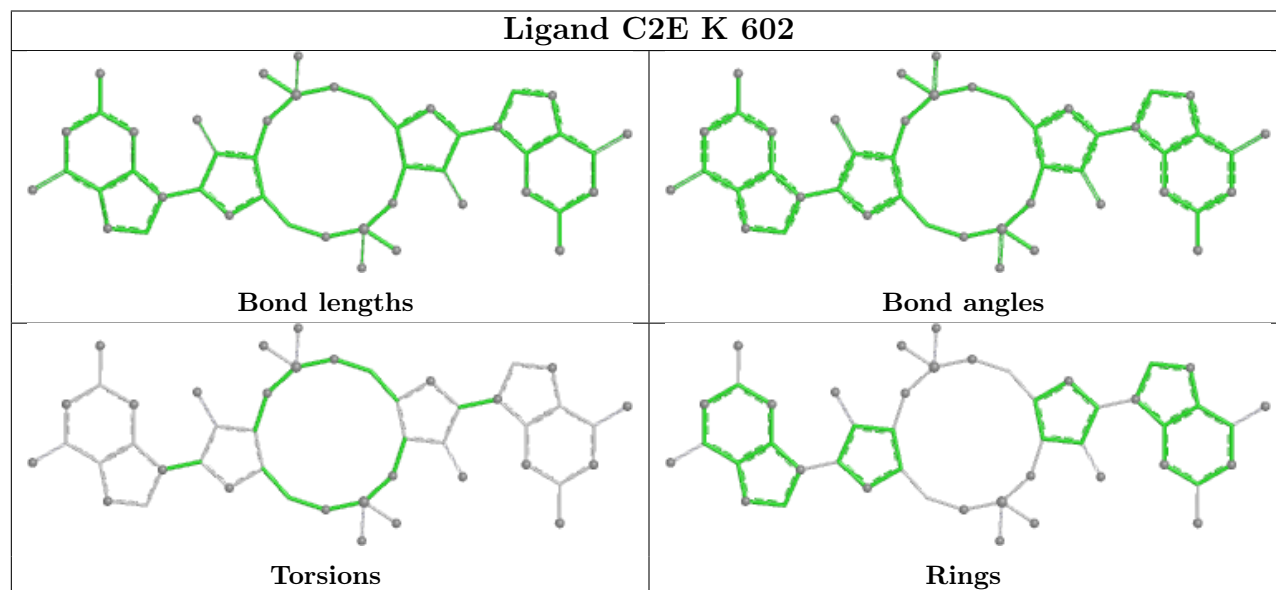
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	601	C2E	1	1
6	F	602	C2E	0	1

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.

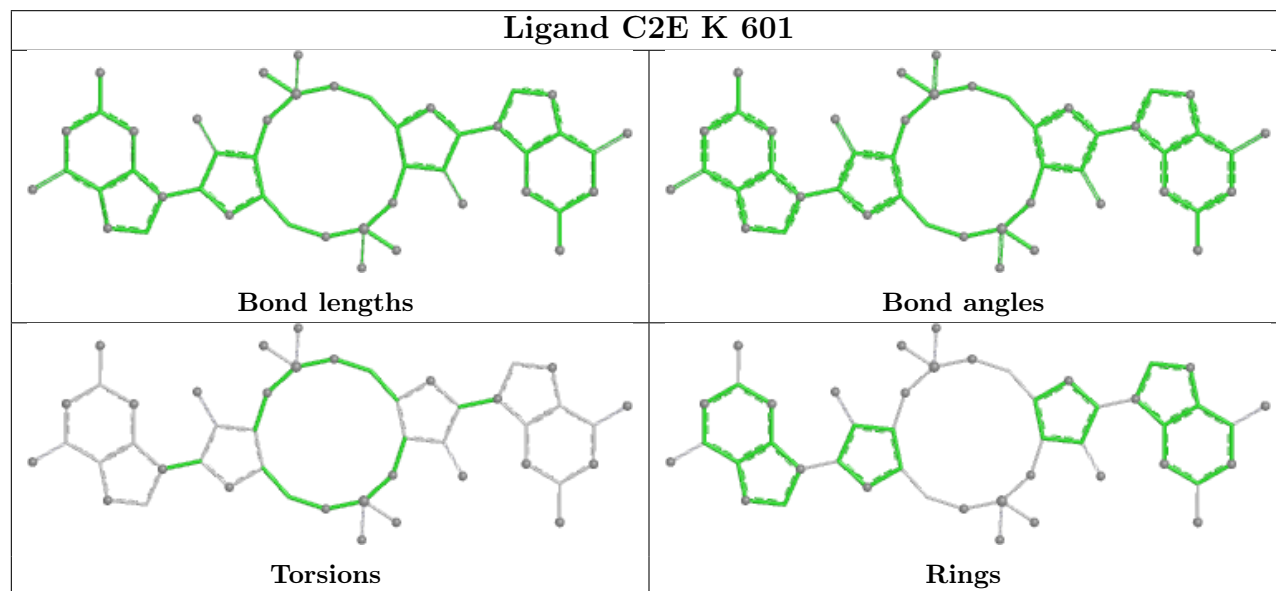
Ligand C2E L 602



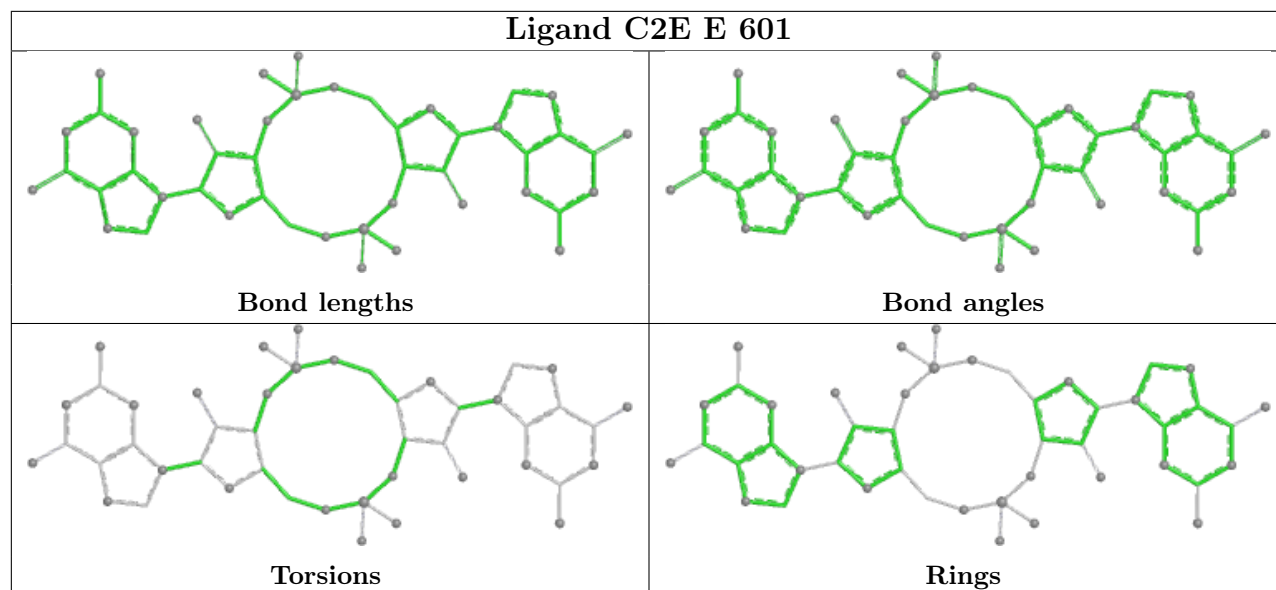
Ligand C2E K 602



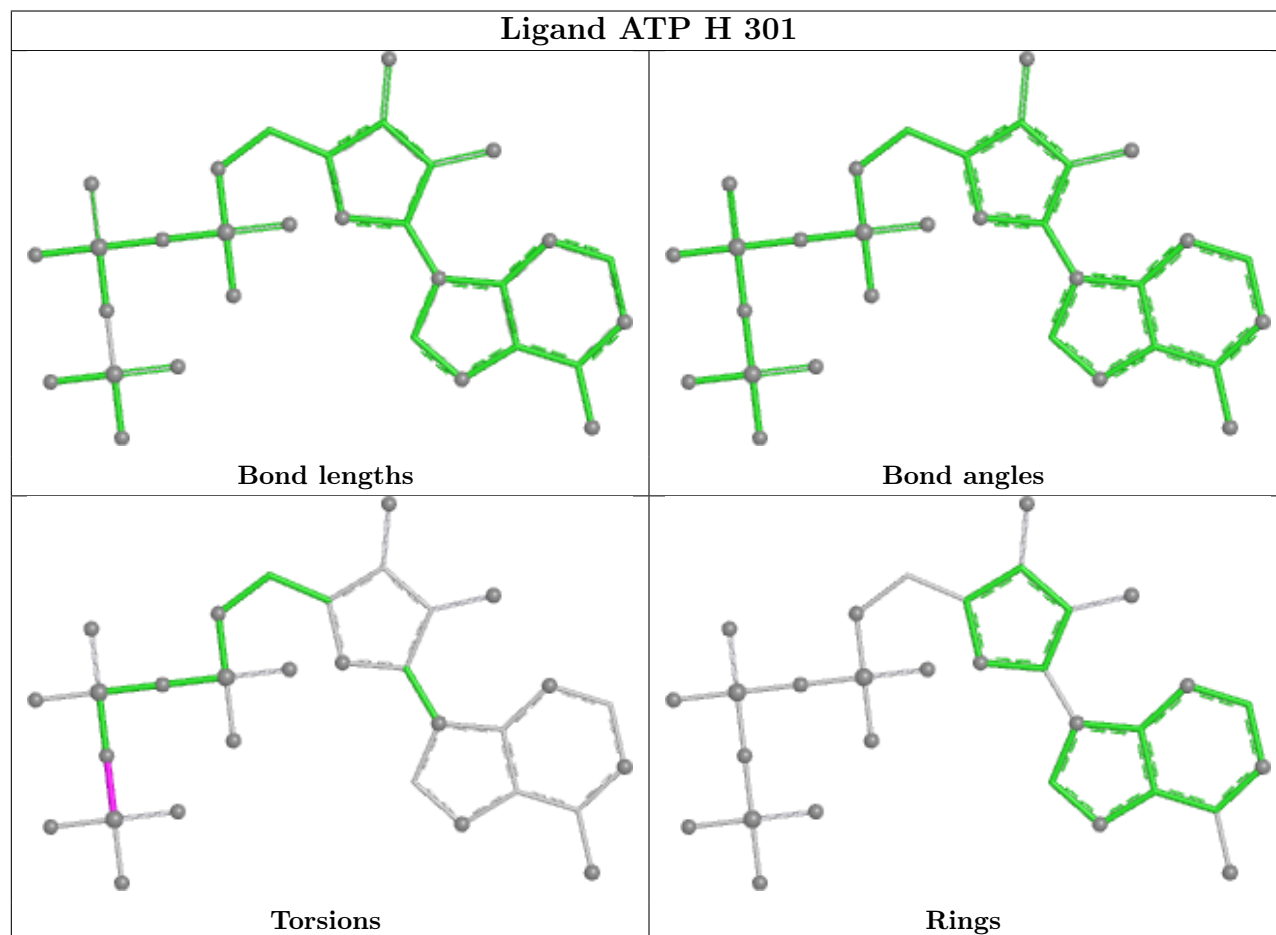
Ligand C2E K 601



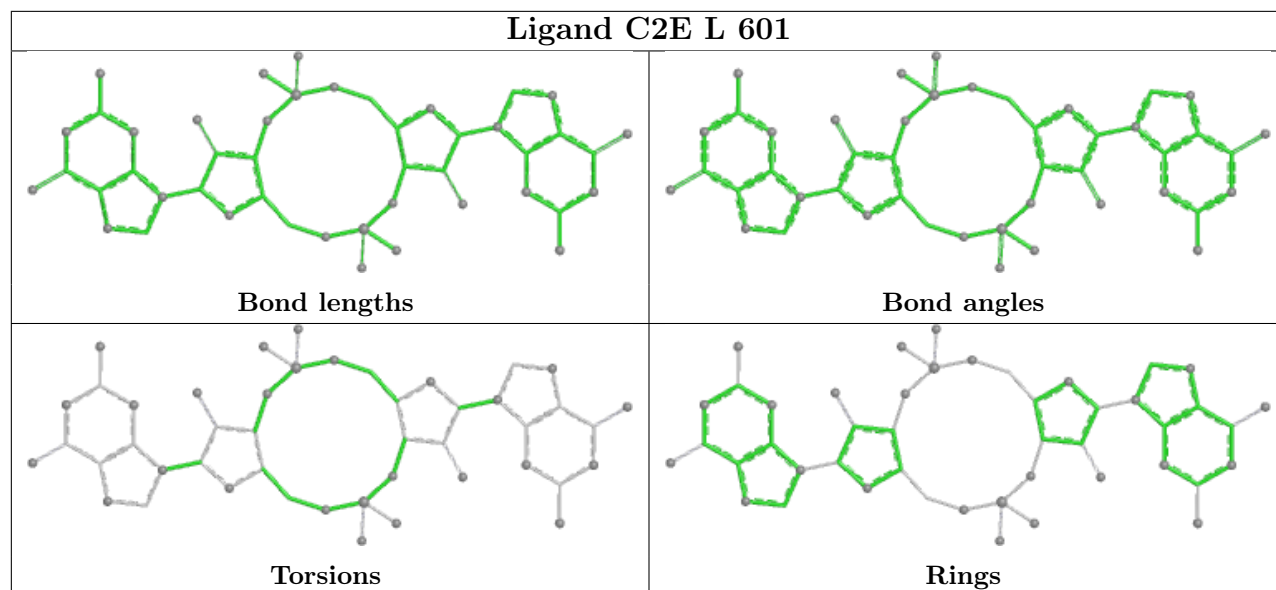
Ligand C2E E 601



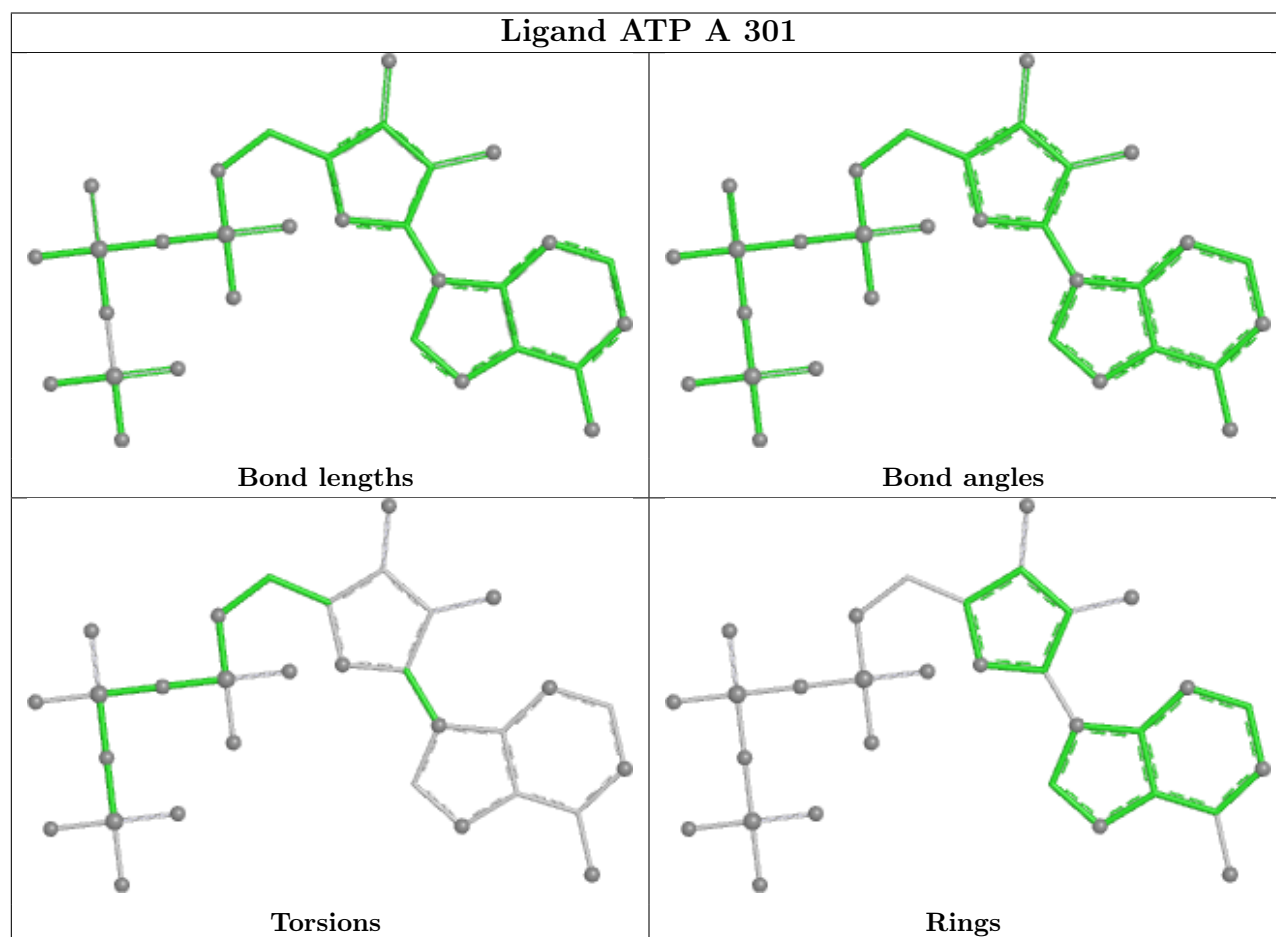
Ligand ATP H 301



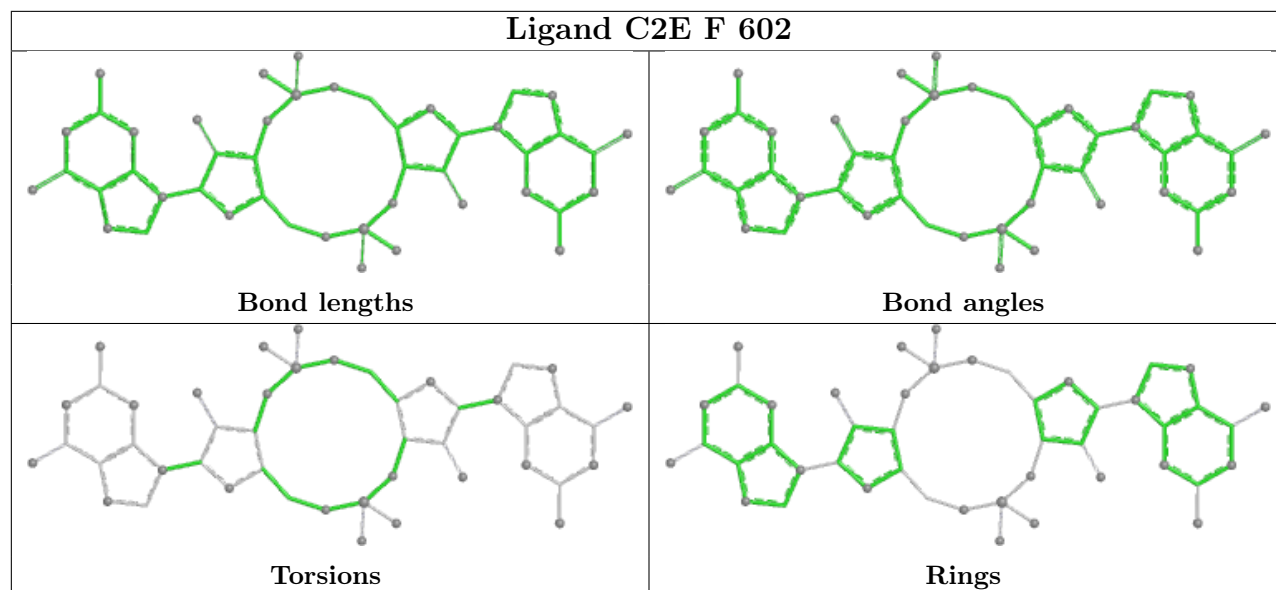
Ligand C2E L 601



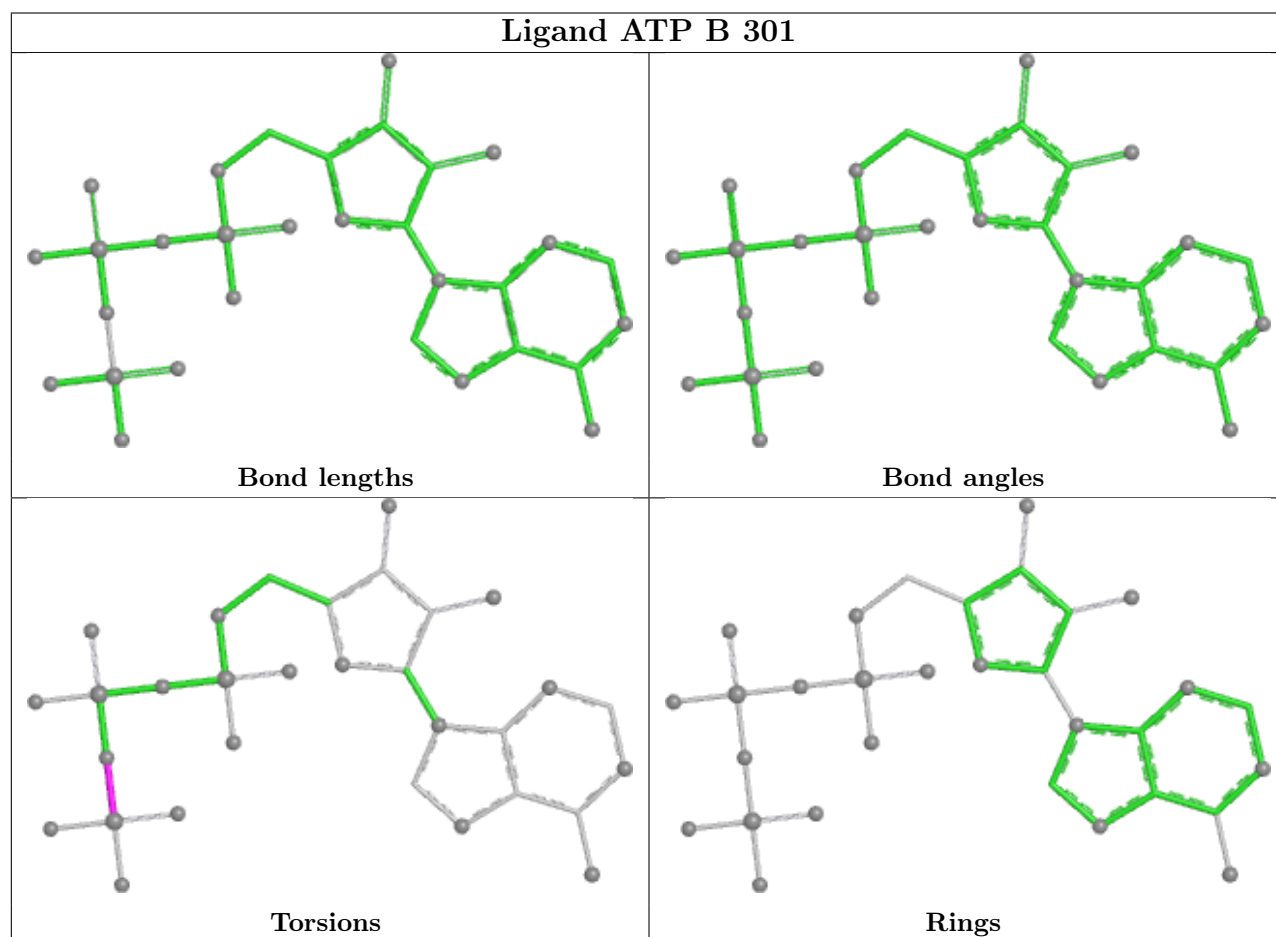
Ligand ATP A 301



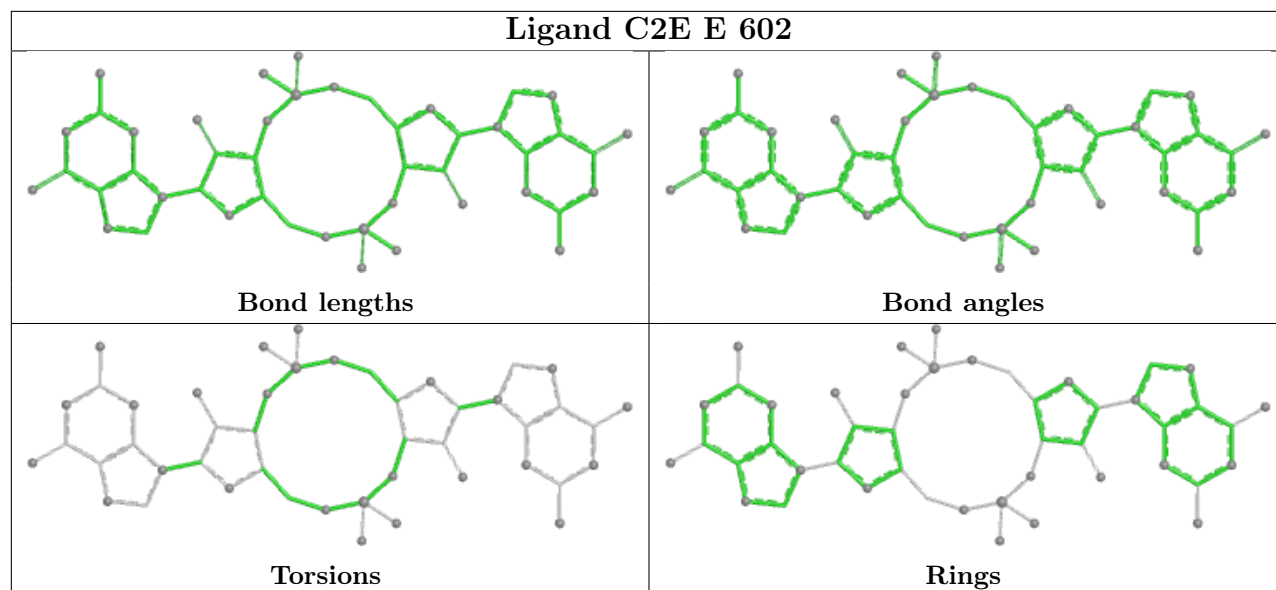
Ligand C2E F 602



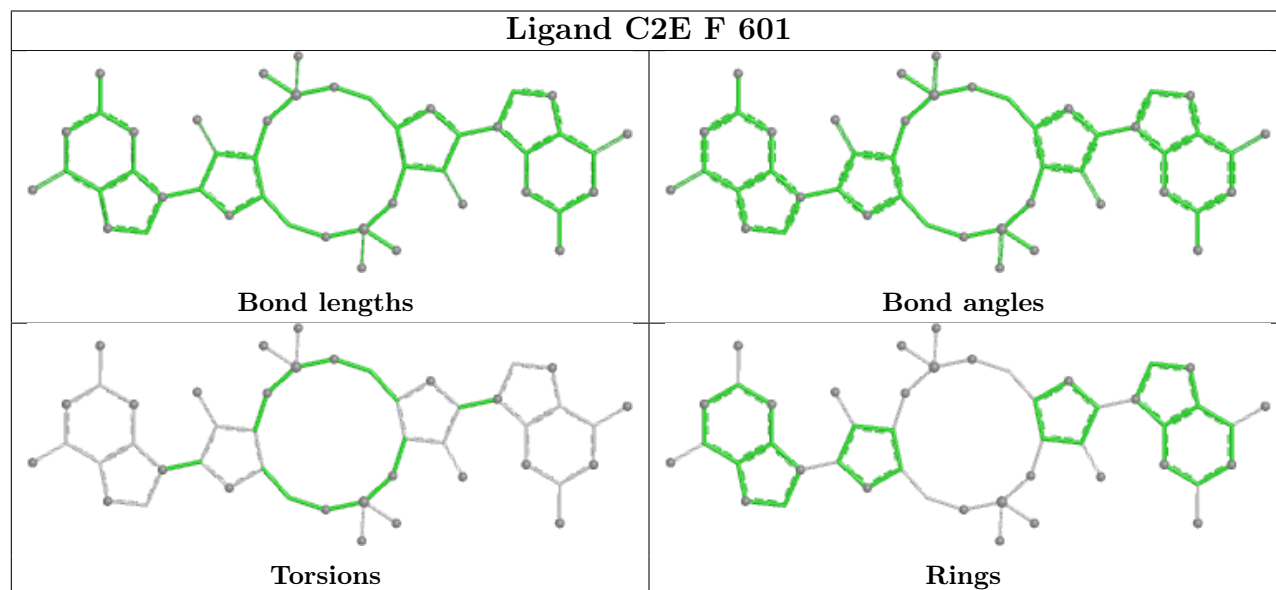
Ligand ATP B 301

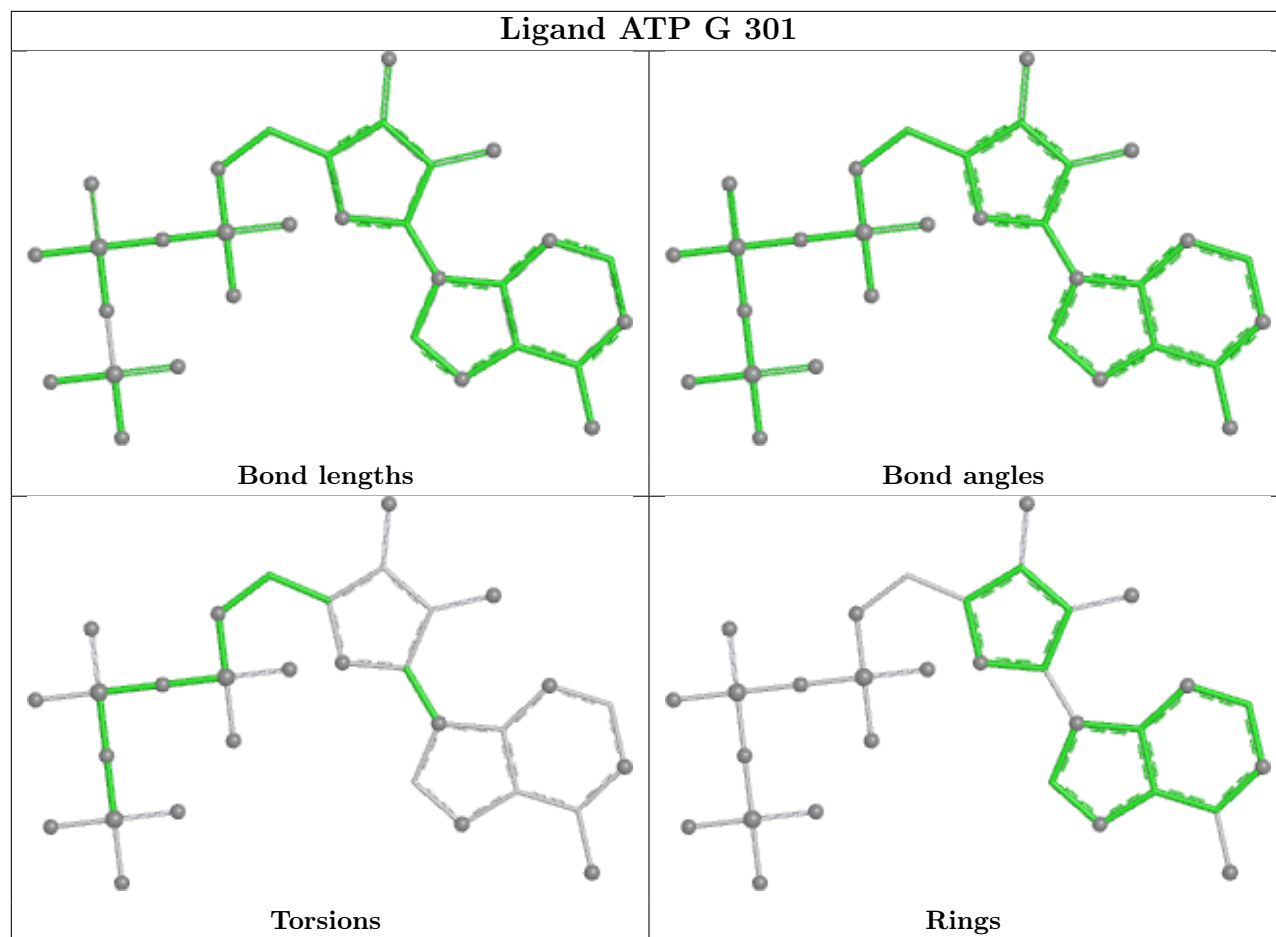


Ligand C2E E 602



Ligand C2E F 601





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	240/250 (96%)	0.04	7 (2%) 53 49	41, 56, 101, 135	0
1	B	240/250 (96%)	-0.07	4 (1%) 69 65	40, 56, 89, 102	0
1	G	240/250 (96%)	-0.09	2 (0%) 82 80	27, 52, 83, 93	1 (0%)
1	H	239/250 (95%)	-0.12	1 (0%) 88 86	37, 52, 87, 110	0
2	C	29/67 (43%)	1.12	4 (13%) 6 5	52, 86, 137, 153	0
2	D	29/67 (43%)	0.70	4 (13%) 6 5	48, 79, 140, 153	0
2	I	30/67 (44%)	0.86	7 (23%) 2 1	44, 73, 142, 153	0
2	J	33/67 (49%)	1.04	7 (21%) 2 2	49, 74, 127, 139	0
3	E	168/179 (93%)	0.18	7 (4%) 40 36	40, 59, 99, 141	0
3	F	166/179 (92%)	0.18	7 (4%) 40 36	41, 60, 90, 126	0
3	K	166/179 (92%)	0.23	12 (7%) 21 19	35, 54, 103, 131	0
3	L	162/179 (90%)	0.25	14 (8%) 16 14	37, 56, 103, 120	0
All	All	1742/1984 (87%)	0.11	76 (4%) 39 34	27, 56, 102, 153	1 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	32	PRO	5.3
3	K	352	THR	5.2
1	A	241	GLY	4.7
3	L	515	LEU	4.5
3	E	496	ILE	4.4
3	E	348	MET	4.3
2	I	32	PRO	4.1
1	G	241	GLY	4.0
3	E	515	LEU	4.0
3	E	387	ALA	3.8
3	F	496	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	40	SER	3.7
2	J	32	PRO	3.5
2	J	29	PHE	3.5
3	L	354	LEU	3.5
3	L	494	PRO	3.3
1	B	241	GLY	3.3
2	I	33	ASP	3.3
2	C	39	ILE	3.3
3	L	361	LEU	3.3
3	E	349	GLU	3.3
3	L	387	ALA	3.3
3	L	491	SER	3.2
1	A	127	ARG	3.2
3	F	515	LEU	3.2
3	L	496	ILE	3.2
3	K	496	ILE	3.1
3	K	515	LEU	3.1
2	D	39	ILE	3.1
2	I	31	LEU	3.0
1	A	96	GLN	3.0
3	L	355	LEU	2.8
3	E	351	ILE	2.8
1	A	99	GLN	2.8
3	K	389	GLY	2.7
2	J	39	ILE	2.7
2	I	40	SER	2.7
3	K	361	LEU	2.7
2	J	28	ALA	2.7
1	H	240	SER	2.6
2	D	61	GLN	2.6
1	G	240	SER	2.6
2	I	39	ILE	2.5
2	J	42	ARG	2.5
3	F	495	VAL	2.5
3	K	353	THR	2.5
1	B	127	ARG	2.5
3	F	354	LEU	2.4
3	L	357	MET	2.4
3	L	386	PRO	2.4
3	K	457	ASN	2.4
3	L	492	SER	2.4
1	A	97	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	2.4
2	I	60	GLN	2.3
3	L	388	HIS	2.3
3	K	357	MET	2.3
1	A	129	ALA	2.3
1	B	28	MET	2.3
2	C	33	ASP	2.3
2	D	42	ARG	2.3
2	J	44	GLN	2.3
3	K	354	LEU	2.2
3	K	388	HIS	2.2
2	D	40	SER	2.2
3	F	435	ARG	2.1
3	E	350	ASP	2.1
1	B	99	GLN	2.1
2	I	41	GLN	2.1
3	F	352	THR	2.1
3	L	389	GLY	2.1
3	L	490	GLN	2.1
3	K	401	GLY	2.1
2	J	30	SER	2.0
3	F	386	PRO	2.0
3	K	517	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Continued on next page...

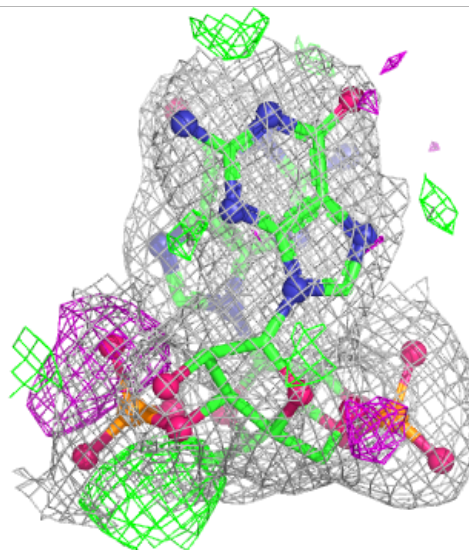
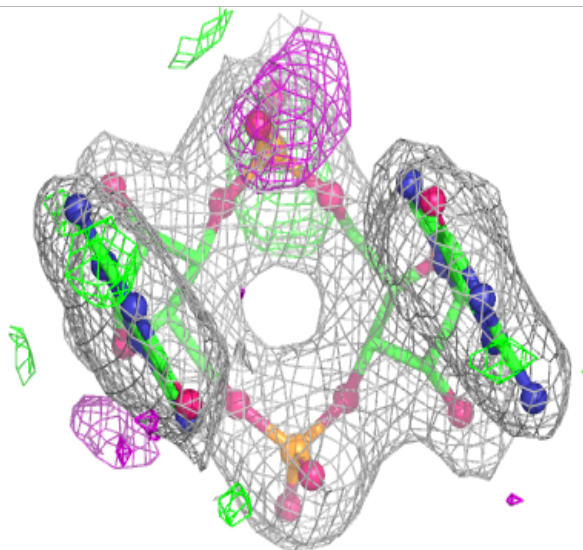
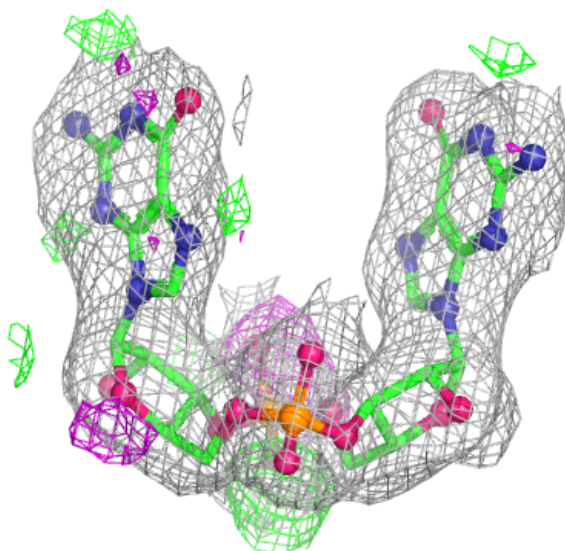
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	C2E	F	602	46/46	0.92	0.09	47,56,64,74	0
6	C2E	K	601	46/46	0.93	0.09	45,58,68,72	0
6	C2E	L	601	46/46	0.94	0.08	43,53,61,69	0
6	C2E	F	601	46/46	0.95	0.08	50,60,64,67	0
6	C2E	K	602	46/46	0.95	0.08	44,53,63,68	0
6	C2E	E	601	46/46	0.95	0.08	46,54,67,71	0
6	C2E	L	602	46/46	0.95	0.08	36,51,58,71	0
6	C2E	E	602	46/46	0.96	0.07	44,52,61,67	0
4	ATP	A	301	31/31	0.98	0.05	37,47,55,63	0
4	ATP	B	301	31/31	0.98	0.06	37,46,55,56	0
4	ATP	G	301	31/31	0.98	0.05	31,43,51,61	0
4	ATP	H	301	31/31	0.98	0.05	35,46,51,53	0
5	MG	H	302	1/1	0.99	0.02	46,46,46,46	0
5	MG	B	302	1/1	0.99	0.02	45,45,45,45	0
5	MG	G	302	1/1	0.99	0.04	43,43,43,43	0
5	MG	A	302	1/1	1.00	0.02	41,41,41,41	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.

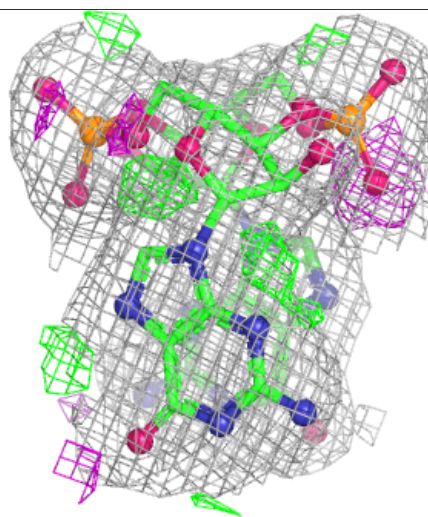
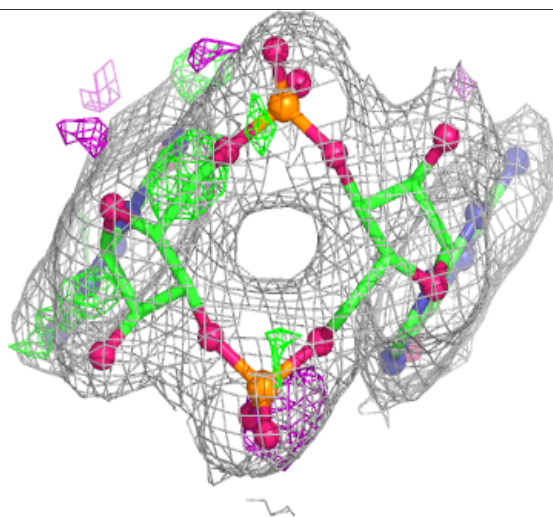
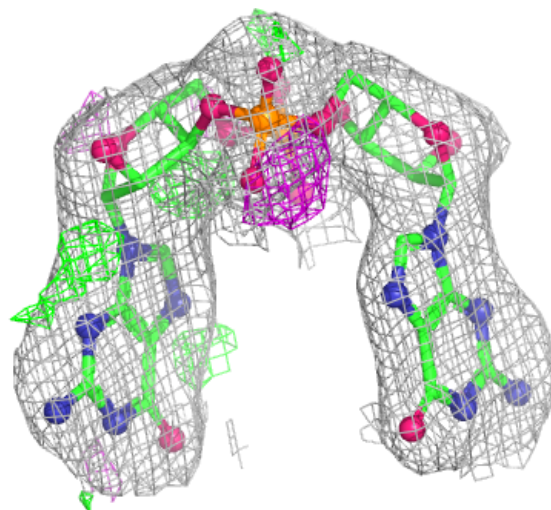
Electron density around C2E F 602:

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



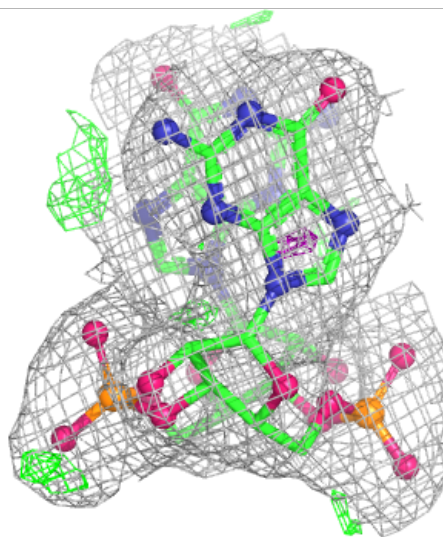
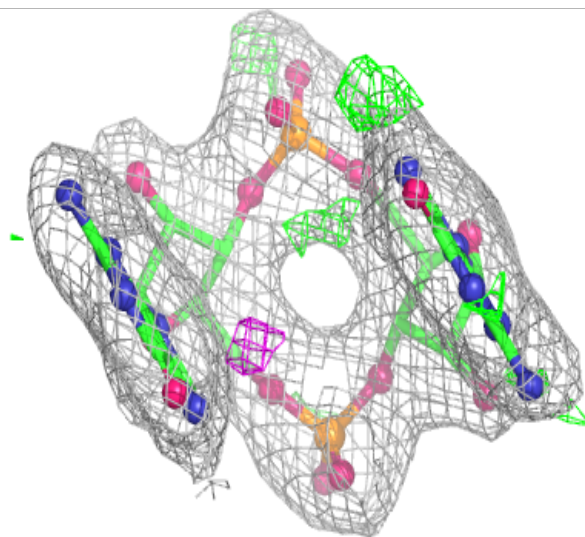
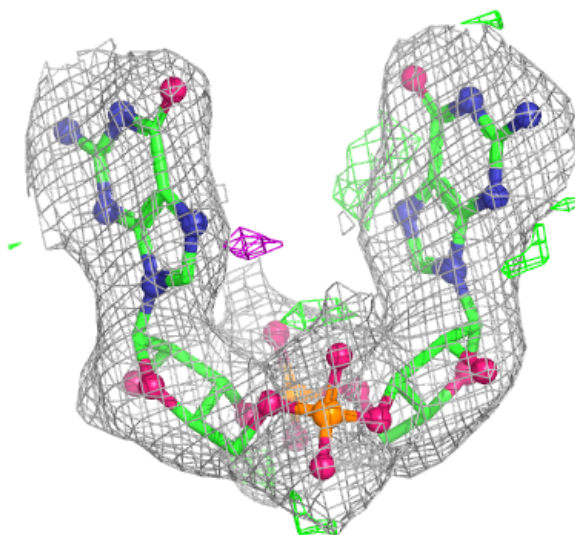
Electron density around C2E K 601:

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



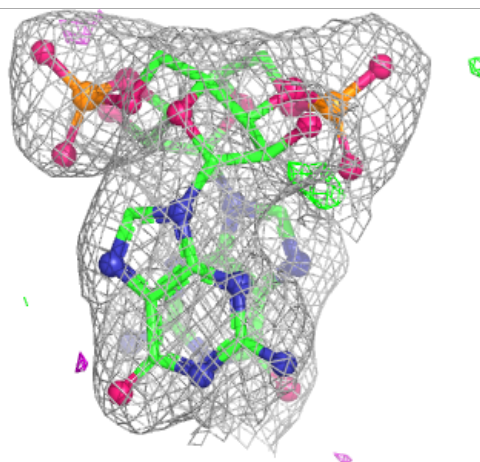
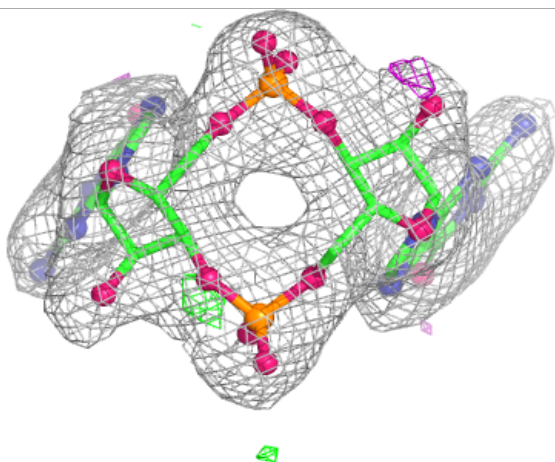
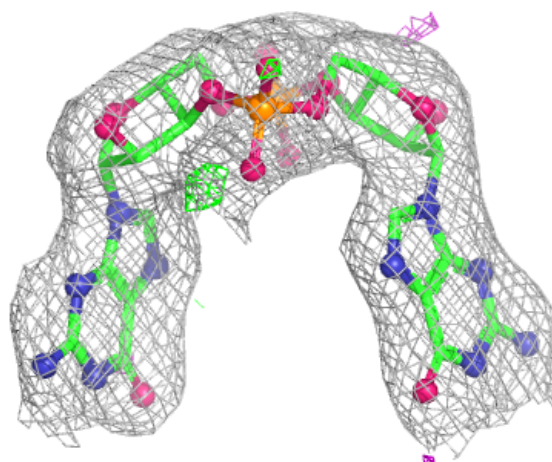
Electron density around C2E L 601:

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



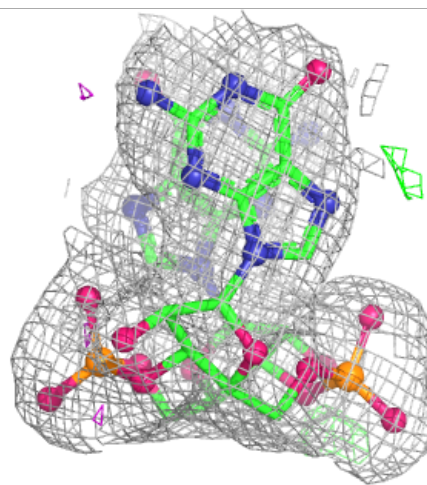
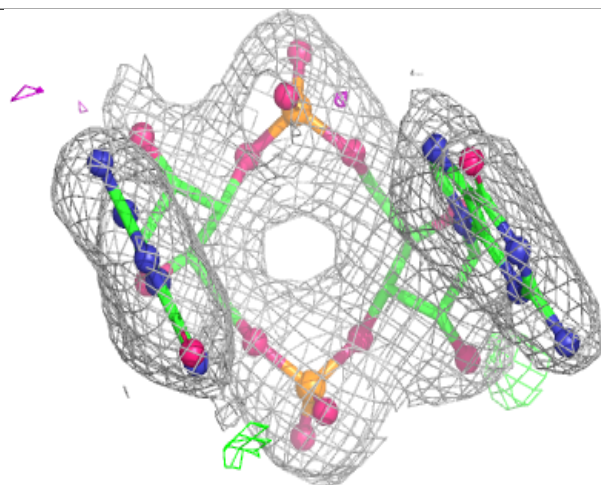
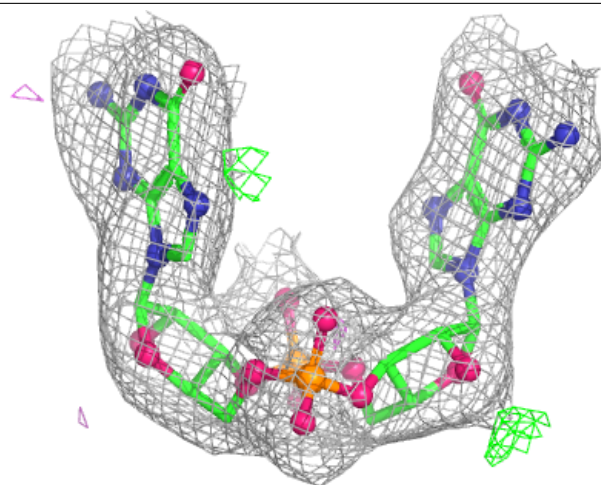
Electron density around C2E F 601:

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



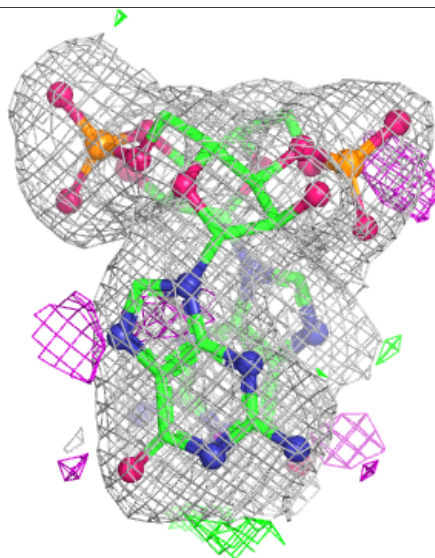
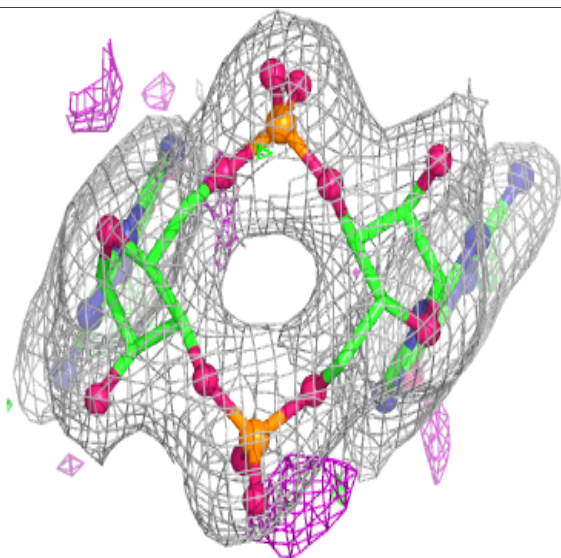
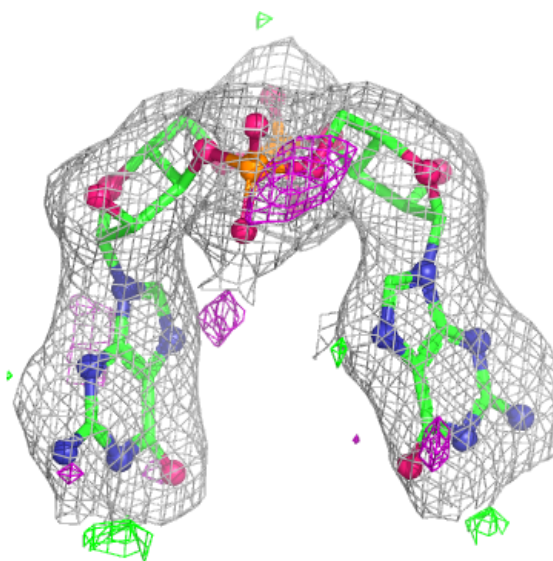
Electron density around C2E K 602:

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



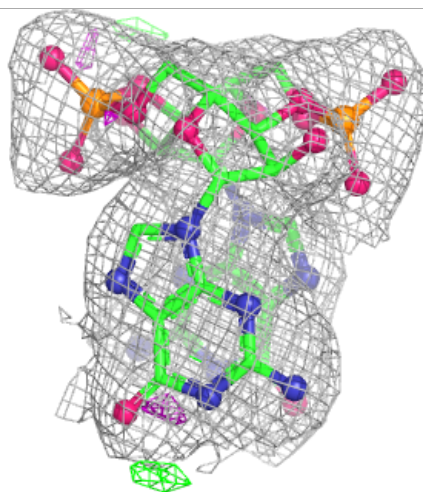
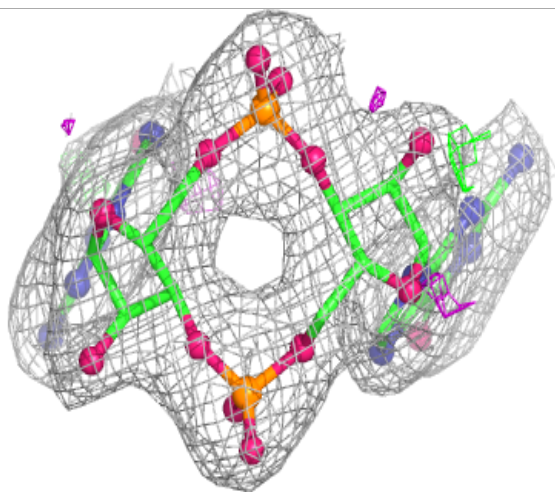
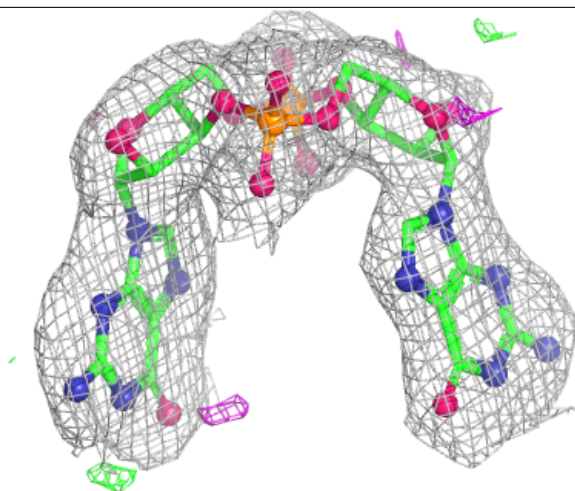
Electron density around C2E E 601:

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



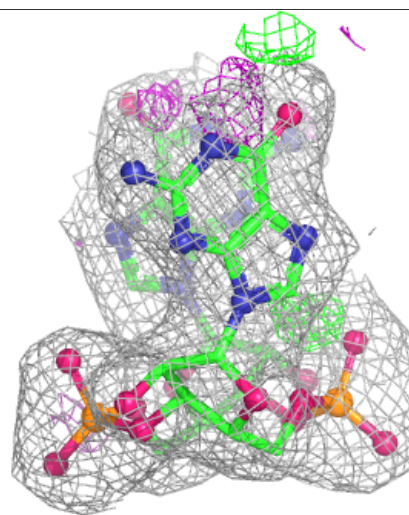
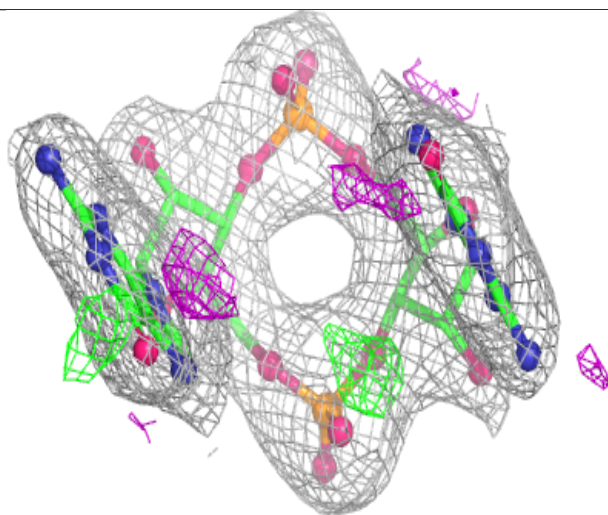
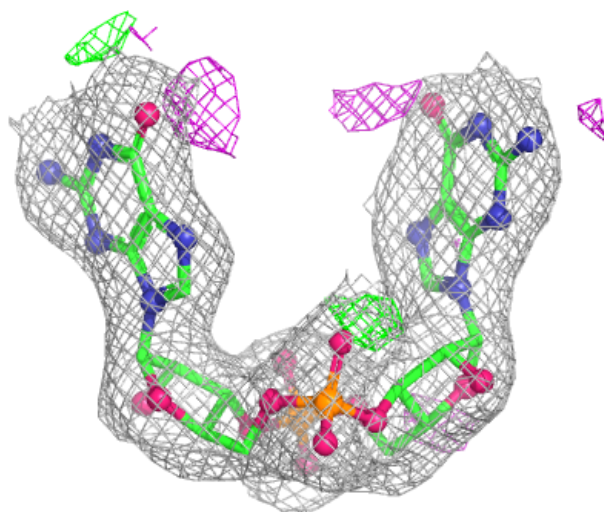
Electron density around C2E L 602:

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



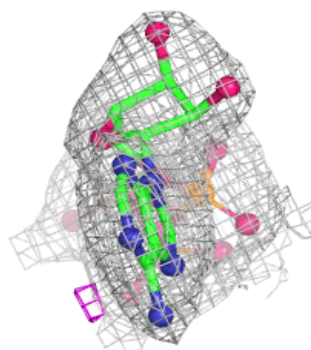
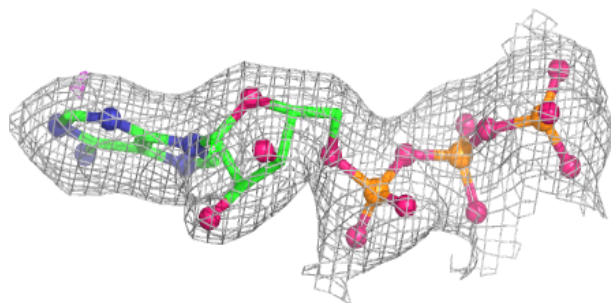
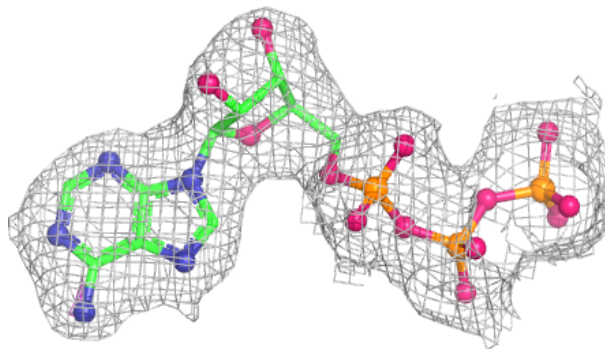
Electron density around C2E E 602:

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

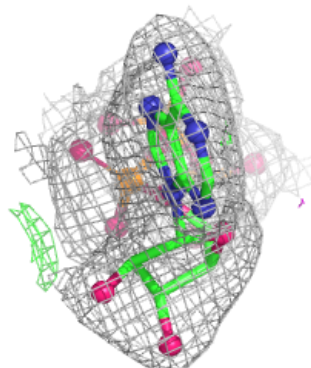
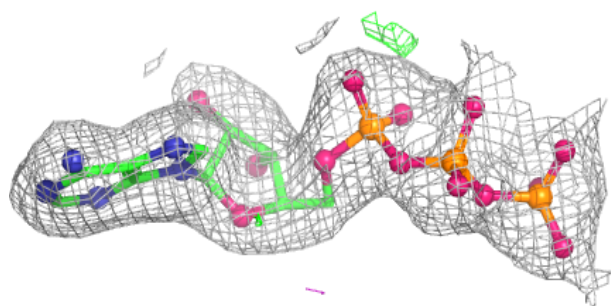
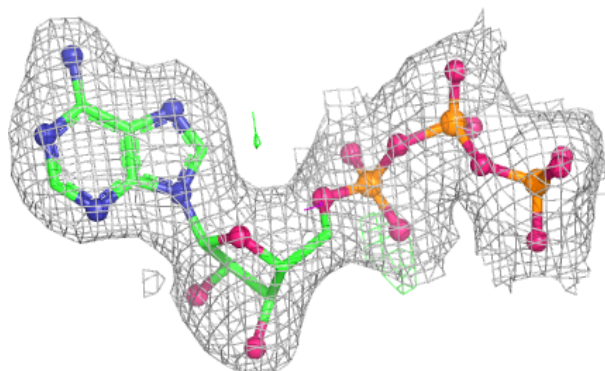


Electron density around ATP A 301:

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

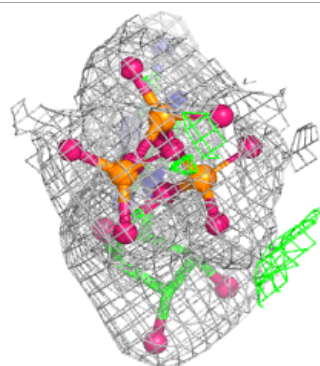
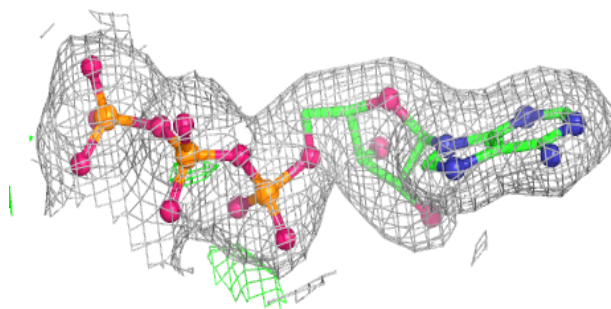
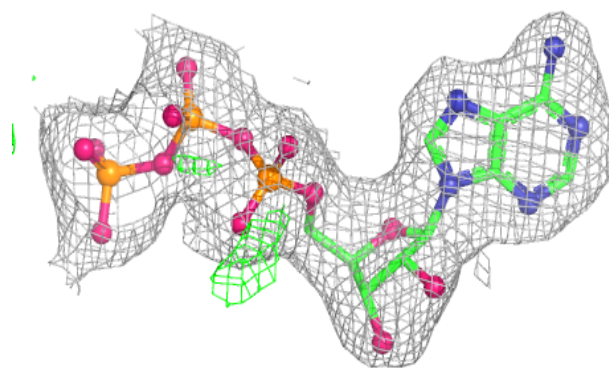
**Electron density around ATP B 301:**

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

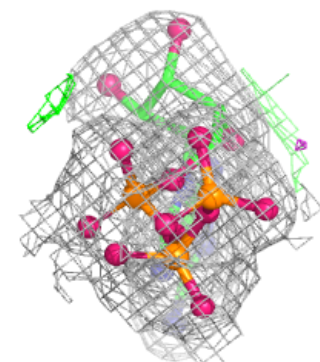
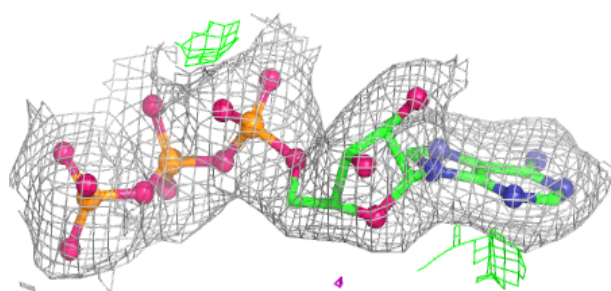
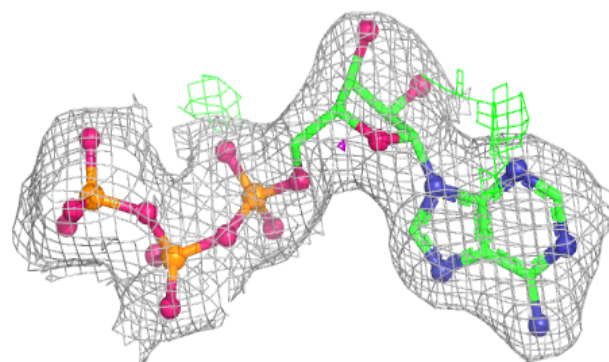


Electron density around ATP G 301:

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

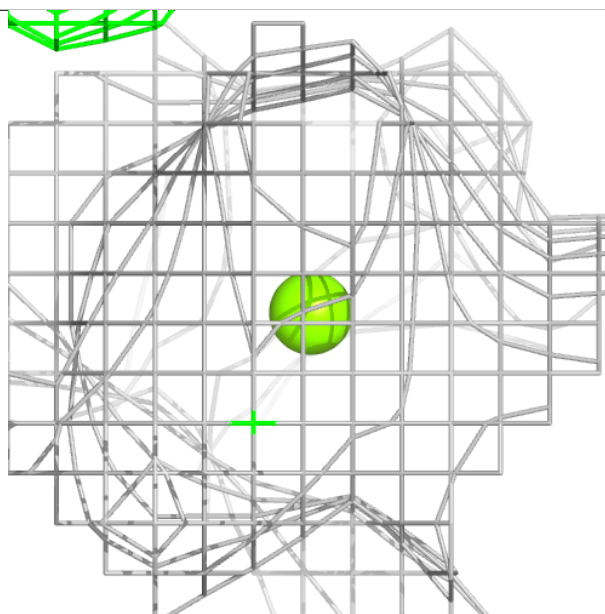
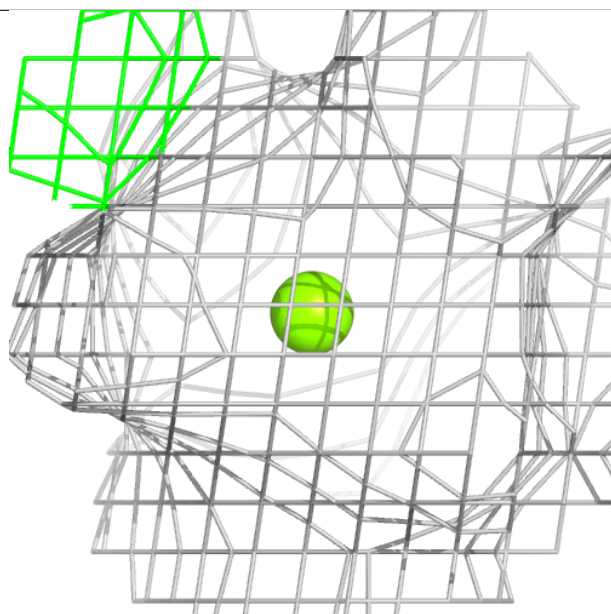
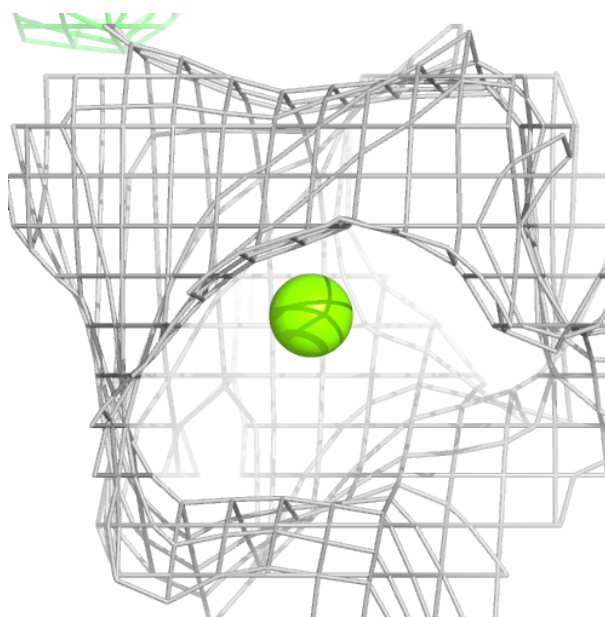
**Electron density around ATP H 301:**

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



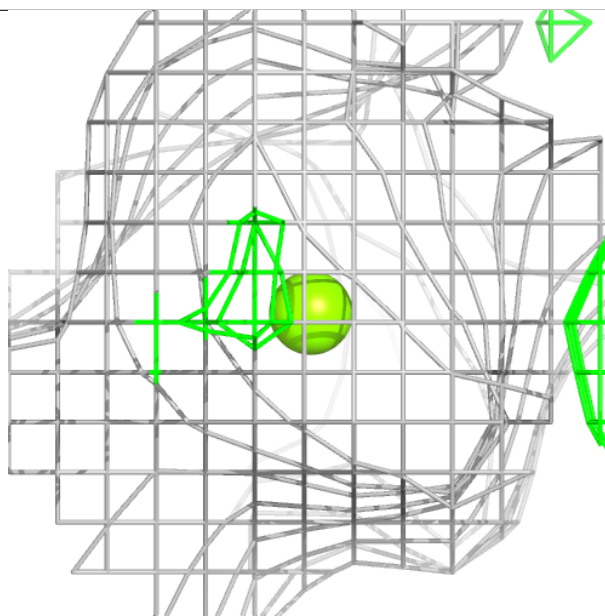
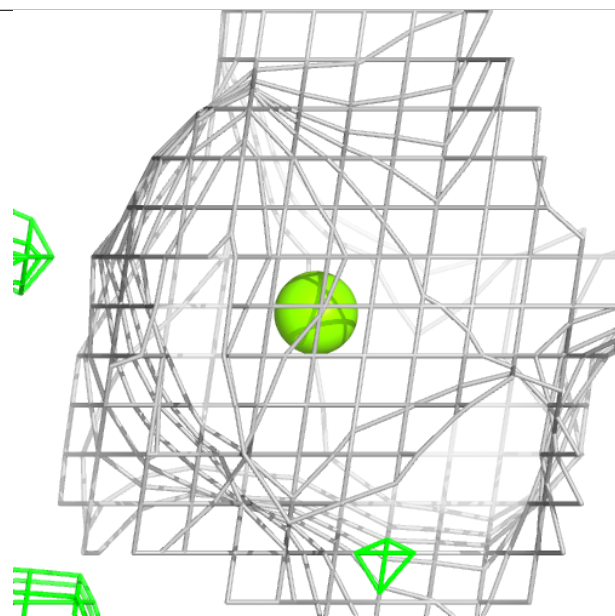
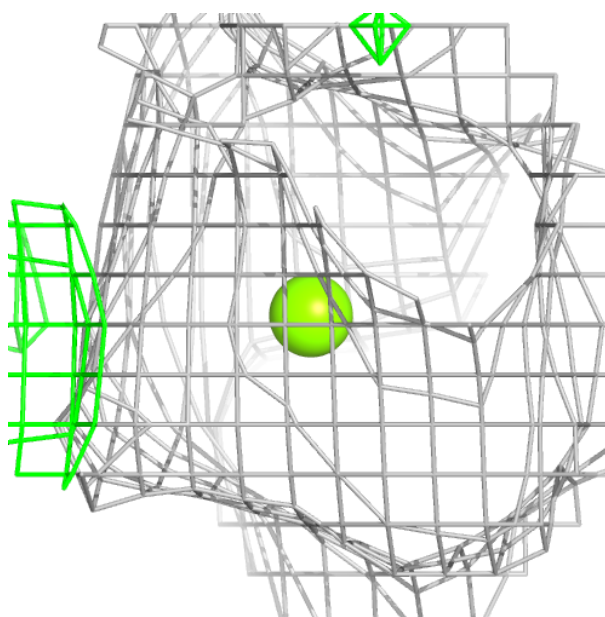
Electron density around MG H 302:

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



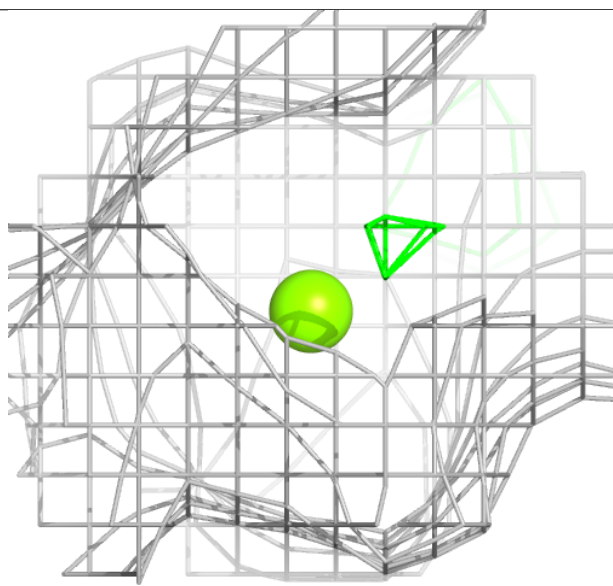
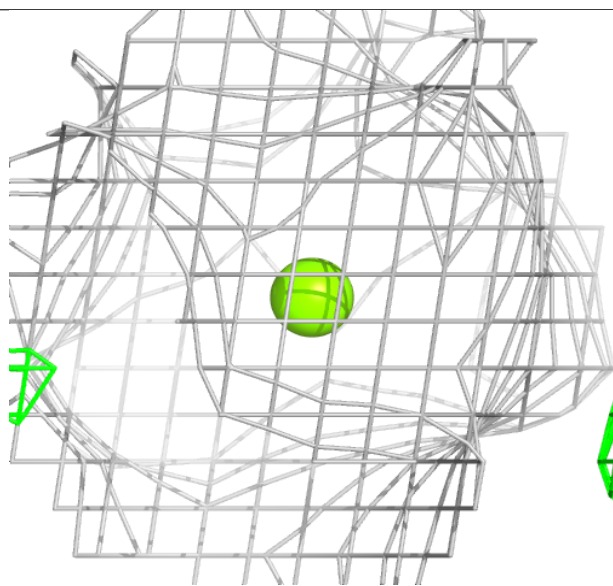
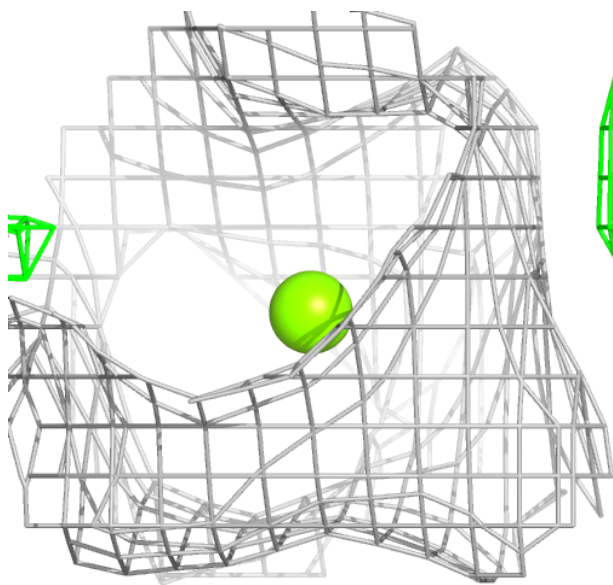
Electron density around MG B 302:

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



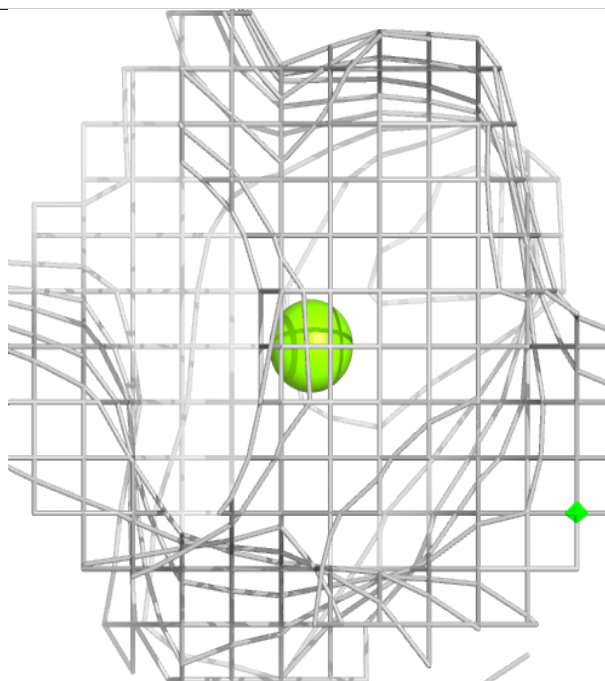
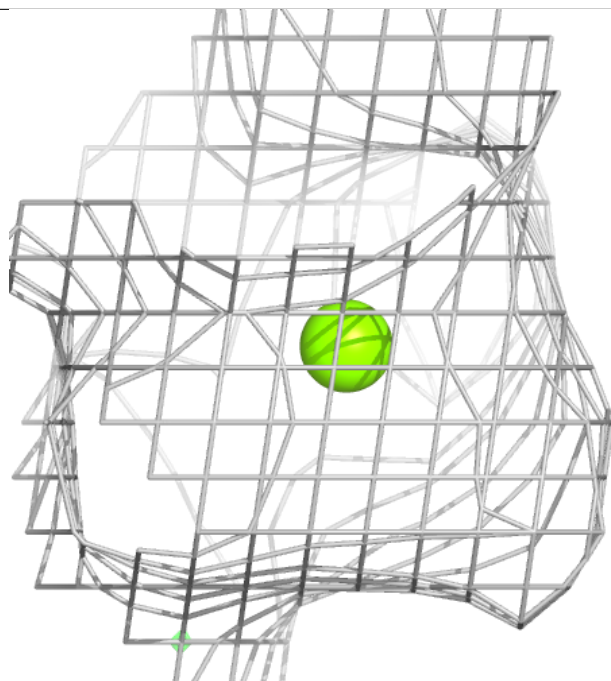
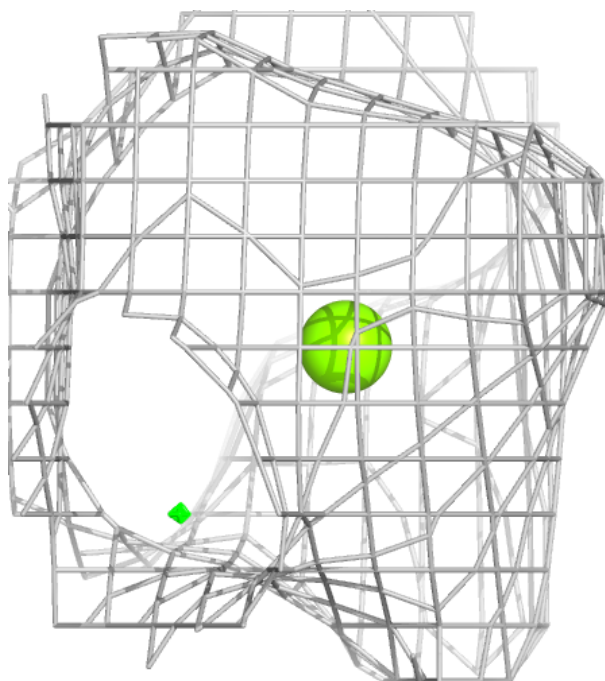
Electron density around MG G 302:

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



Electron density around MG A 302:

$2mF_o-DF_c$ (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.