



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:46 PM BST

PDB ID : 6VZW
Title : TTLL6 bound to the initiation analog
Authors : Mahalingan, K.K.; Keenen, E.K.; Strickland, M.; Li, Y.; Liu, Y.; Ball, H.L.;
Tanner, T.E.; Tjandra, N.; Roll-Mecak, A.
Deposited on : 2020-02-28
Resolution : 2.50 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 : 2.13.1
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) : 2.13.1

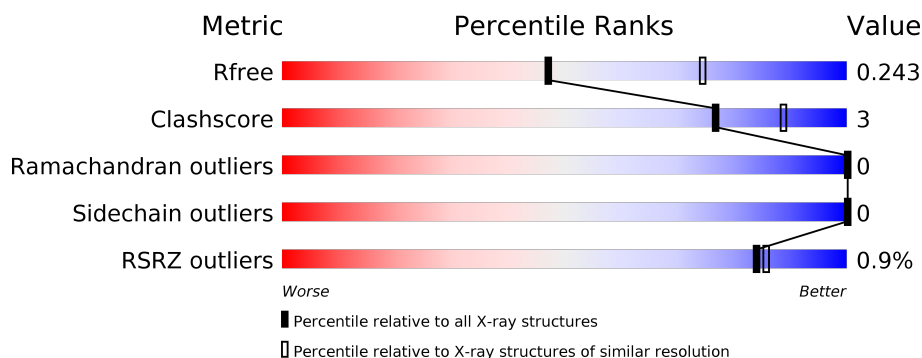
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	453	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>11%</div> </div> </div>
1	B	453	<div> <div></div> <div>81%</div> <div>7%</div> <div>12%</div> </div>
1	C	453	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>11%</div> </div> </div>
1	D	453	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>11%</div> </div> </div>

2 Entry composition [i](#)

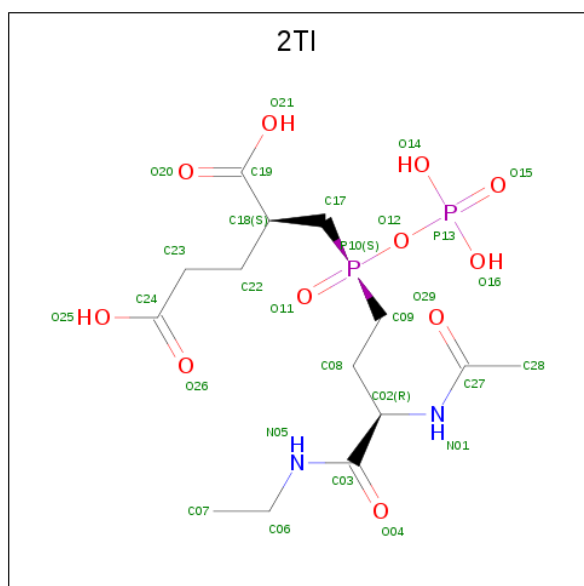
There are 6 unique types of molecules in this entry. The entry contains 13131 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tubulin polyglutamylase TTLL6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3100	1989	527	563	21			
1	B	398	Total	C	N	O	S	0	3	0
			3147	2010	547	570	20			
1	C	401	Total	C	N	O	S	0	0	0
			3098	1983	529	565	21			
1	D	402	Total	C	N	O	S	0	1	0
			3140	2013	542	565	20			

- Molecule 2 is (2 {S})-2-[[[(3 {R})-3-acetamido-4-(ethylamino)-4-oxidanylidene-butyl]-phosphonoxy-phosphoryl]methyl]pentanedioic acid (three-letter code: 2TI) (formula: C₁₄H₂₆N₂O₁₁P₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	14	2	11	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			29	14	2	11	2		
2	C	1	Total	C	N	O	P	0	0
			29	14	2	11	2		
2	D	1	Total	C	N	O	P	0	0
			29	14	2	11	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



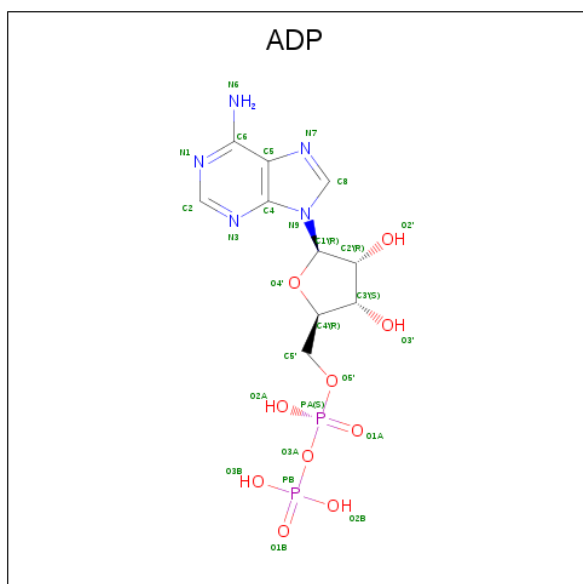
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

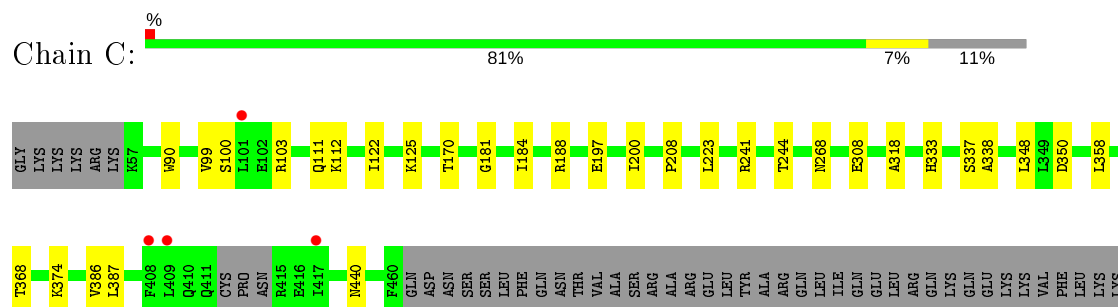
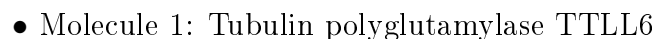
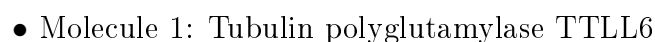
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

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

- Molecule 6 is water.

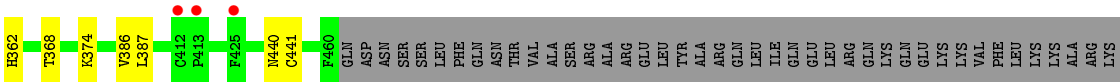
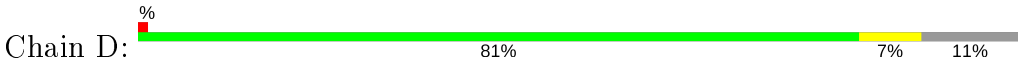
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		
6	B	115	Total	O	0	0
			115	115		
6	C	31	Total	O	0	0
			31	31		
6	D	117	Total	O	0	0
			117	117		

- Molecule 1: Tubulin polyglutamylase TTL6



ALA
ARG
LYS
GLU

● Molecule 1: Tubulin polyglutamylase TTL6



GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.25Å 110.58Å 173.58Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	19.92 – 2.50 19.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.92-2.50) 99.1 (19.92-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.50Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.217 , 0.243 0.216 , 0.243	Depositor DCC
R_{free} test set	4815 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13131	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4055e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: GOL, MG, 2TI, ADP

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	0.24	0/3176	0.39	0/4312
1	B	0.24	0/3232	0.40	0/4375
1	C	0.24	0/3174	0.39	0/4309
1	D	0.24	0/3220	0.39	0/4364
All	All	0.24	0/12802	0.39	0/17360

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	3100	0	2866	19	0
1	B	3147	0	2963	19	0
1	C	3098	0	2847	19	0
1	D	3140	0	2944	20	0
2	A	29	0	0	1	0
2	B	29	0	0	0	0
2	C	29	0	0	1	0
2	D	29	0	0	0	0
3	A	12	0	16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	64	0	0
3	C	18	0	24	1	0
3	D	42	0	56	2	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	31	0	0	0	0
6	B	115	0	0	0	0
6	C	31	0	0	0	0
6	D	117	0	0	0	0
All	All	13131	0	11828	75	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 3.

All (75) 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:B:194:LYS:HB3	3:D:602:GOL:H31	1.72	0.71
1:D:208:PRO:HA	1:D:350:ASP:HA	1.78	0.66
1:A:208:PRO:HA	1:A:350:ASP:HA	1.79	0.65
1:D:104:VAL:HG21	1:D:117:PRO:HG3	1.81	0.62
1:B:208:PRO:HA	1:B:350:ASP:HA	1.80	0.62
1:C:368:THR:HB	1:C:374:LYS:HG3	1.81	0.61
4:C:605:ADP:H8	4:C:605:ADP:H5'1	1.65	0.61
1:C:208:PRO:HA	1:C:350:ASP:HA	1.81	0.61
1:B:161:THR:HG22	1:B:164:ARG:HH22	1.67	0.60
1:B:368:THR:HB	1:B:374:LYS:HG3	1.83	0.59
1:A:368:THR:HB	1:A:374:LYS:HG3	1.84	0.59
1:C:241:ARG:NH1	2:C:601:2TI:O20	2.36	0.58
1:C:223:LEU:HD23	1:C:387:LEU:HD23	1.86	0.57
1:C:112:LYS:NZ	1:C:337:SER:O	2.35	0.57
1:D:105:MET:HG2	1:D:329:CYS:HA	1.88	0.56
1:B:223:LEU:HD23	1:B:387:LEU:HD23	1.89	0.55
1:B:333:HIS:CG	1:B:338:ALA:HB2	2.43	0.54
1:D:223:LEU:HD23	1:D:387:LEU:HD23	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:NH1	2:A:601:2TI:O21	2.42	0.53
1:D:368:THR:HB	1:D:374:LYS:HG3	1.91	0.52
1:D:112:LYS:NZ	1:D:337:SER:O	2.38	0.51
1:C:333:HIS:CG	1:C:338:ALA:HB2	2.46	0.50
1:D:97:TYR:HA	3:D:602:GOL:H12	1.93	0.50
1:C:99:VAL:HG12	1:C:103:ARG:HE	1.76	0.50
1:D:165:THR:HB	1:D:166:ARG:HD2	1.94	0.50
1:D:123:CYS:SG	1:D:362:HIS:HB3	2.51	0.50
1:B:112:LYS:NZ	1:B:337:SER:O	2.41	0.49
1:C:125:LYS:HB3	1:C:200:ILE:HD13	1.94	0.49
1:A:122:ILE:HG23	1:A:318:ALA:HB2	1.95	0.49
1:D:387:LEU:HD13	1:D:441:CYS:HA	1.94	0.49
1:A:223:LEU:HD23	1:A:387:LEU:HD23	1.95	0.49
1:B:298:TYR:CD1	1:B:353:LEU:HD11	2.49	0.48
1:A:181:GLY:HA2	1:A:184:ILE:HD12	1.95	0.47
1:B:207:LYS:HB3	1:B:351:ARG:HD3	1.96	0.47
1:D:330:PHE:HB3	1:D:333:HIS:HB3	1.96	0.47
1:A:188:ARG:HG3	1:A:255:LEU:HD11	1.97	0.47
1:A:244:THR:HG23	1:A:268:ASN:HB3	1.96	0.47
1:C:100:SER:H	1:C:103:ARG:HD3	1.80	0.47
1:C:181:GLY:HA2	1:C:184:ILE:HD12	1.97	0.47
1:D:122:ILE:HG23	1:D:318:ALA:HB2	1.97	0.47
1:B:386:VAL:HG12	1:B:440:ASN:HB3	1.97	0.46
1:B:181:GLY:HA2	1:B:184:ILE:HD12	1.96	0.46
1:A:367:SER:O	1:A:377:LYS:NZ	2.44	0.46
1:D:101:LEU:O	1:D:105:MET:HG3	2.16	0.46
1:C:386:VAL:HG12	1:C:440:ASN:HB3	1.98	0.46
1:A:348:LEU:HB2	1:A:358:LEU:HD11	1.98	0.45
1:A:105:MET:HB2	1:A:105:MET:HE3	1.88	0.44
1:C:308:GLU:OE1	3:C:603:GOL:O2	2.34	0.44
1:C:122:ILE:HG23	1:C:318:ALA:HB2	1.98	0.43
1:A:242:PHE:HB2	1:A:282:SER:HA	2.00	0.43
1:B:122:ILE:HG23	1:B:318:ALA:HB2	1.99	0.43
1:D:298:TYR:CD1	1:D:353:LEU:HD11	2.53	0.43
1:C:348:LEU:HB2	1:C:358:LEU:HD11	2.00	0.43
1:B:165:THR:HB	1:B:166:ARG:HD2	2.00	0.43
1:A:140:PRO:O	1:A:144:HIS:NE2	2.52	0.43
1:D:301:GLU:O	1:D:305:ARG:HG2	2.19	0.43
1:B:185:PHE:CE2	1:D:182[B]:ARG:HD3	2.54	0.42
1:A:125:LYS:HB3	1:A:200:ILE:HD13	2.01	0.42
1:C:333:HIS:CD2	1:C:338:ALA:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LEU:HD23	1:B:453:LEU:H	1.85	0.42
1:B:162:TYR:OH	1:B:169:LYS:NZ	2.53	0.42
1:B:197:GLU:OE2	1:D:182[A]:ARG:NH2	2.52	0.42
1:D:386:VAL:HG12	1:D:440:ASN:HB3	2.00	0.42
1:C:170:THR:OG1	1:C:188:ARG:NH1	2.52	0.42
1:C:244:THR:HG23	1:C:268:ASN:HB3	2.02	0.42
1:B:245:THR:HB	1:B:260:MET:HB2	2.02	0.41
1:A:177:SER:O	1:C:197:GLU:HG2	2.20	0.41
1:A:387:LEU:HD13	1:A:441:CYS:HA	2.03	0.41
1:B:168:ASN:OD1	1:B:168:ASN:N	2.53	0.41
1:D:245:THR:HB	1:D:260:MET:HB2	2.02	0.41
1:A:239:LEU:HD13	1:A:283:LYS:HZ2	1.86	0.41
1:A:301:GLU:O	1:A:305:ARG:HG2	2.20	0.41
1:C:90:TRP:CZ3	1:C:111:GLN:HB3	2.56	0.41
1:D:341:GLU:OE1	1:D:362:HIS:HB2	2.21	0.41
1:A:453:LEU:HD23	1:A:453:LEU:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/453 (88%)	386 (97%)	12 (3%)	0	100	100
1	B	397/453 (88%)	385 (97%)	12 (3%)	0	100	100
1	C	397/453 (88%)	384 (97%)	13 (3%)	0	100	100
1	D	399/453 (88%)	389 (98%)	10 (2%)	0	100	100
All	All	1591/1812 (88%)	1544 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/416 (74%)	310 (100%)	0	100	100
1	B	324/416 (78%)	324 (100%)	0	100	100
1	C	309/416 (74%)	309 (100%)	0	100	100
1	D	318/416 (76%)	318 (100%)	0	100	100
All	All	1261/1664 (76%)	1261 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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	GOL	B	603	-	5,5,5	0.88	0	5,5,5	1.05	0
3	GOL	D	603	-	5,5,5	0.89	0	5,5,5	1.00	0
3	GOL	B	605	-	5,5,5	0.87	0	5,5,5	1.11	0
2	2TI	C	601	5	17,28,28	2.04	5 (29%)	20,39,39	1.62	5 (25%)
3	GOL	B	609	-	5,5,5	0.90	0	5,5,5	1.01	0
4	ADP	C	605	5	24,29,29	0.95	1 (4%)	29,45,45	1.41	4 (13%)
3	GOL	C	602	-	5,5,5	0.91	0	5,5,5	1.00	0
4	ADP	D	609	5	24,29,29	0.97	1 (4%)	29,45,45	1.27	3 (10%)
3	GOL	D	605	-	5,5,5	0.90	0	5,5,5	1.08	0
3	GOL	B	602	-	5,5,5	0.96	0	5,5,5	1.25	1 (20%)
3	GOL	B	606	-	5,5,5	0.91	0	5,5,5	0.99	0
3	GOL	D	602	-	5,5,5	1.01	0	5,5,5	0.96	0
4	ADP	B	610	5	24,29,29	0.97	1 (4%)	29,45,45	1.28	4 (13%)
2	2TI	D	601	5	17,28,28	1.96	5 (29%)	20,39,39	1.63	6 (30%)
3	GOL	A	603	-	5,5,5	0.86	0	5,5,5	1.23	1 (20%)
3	GOL	D	607	-	5,5,5	0.89	0	5,5,5	1.11	0
3	GOL	A	602	-	5,5,5	0.92	0	5,5,5	1.01	0
3	GOL	B	604	-	5,5,5	0.91	0	5,5,5	1.01	0
3	GOL	B	607	-	5,5,5	0.88	0	5,5,5	1.16	0
3	GOL	B	608	-	5,5,5	0.92	0	5,5,5	0.99	0
3	GOL	D	608	-	5,5,5	0.91	0	5,5,5	0.99	0
2	2TI	A	601	5	17,28,28	1.98	5 (29%)	20,39,39	1.60	4 (20%)
4	ADP	A	604	5	24,29,29	0.95	1 (4%)	29,45,45	1.33	4 (13%)
3	GOL	D	604	-	5,5,5	0.90	0	5,5,5	1.09	0
2	2TI	B	601	5	17,28,28	1.96	5 (29%)	20,39,39	1.61	6 (30%)
3	GOL	D	606	-	5,5,5	0.90	0	5,5,5	1.11	0
3	GOL	C	603	-	5,5,5	0.88	0	5,5,5	1.10	1 (20%)
3	GOL	C	604	-	5,5,5	0.89	0	5,5,5	1.06	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
3	GOL	B	603	-	-	0/4/4/4	-
3	GOL	D	603	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	605	-	-	0/4/4/4	-
2	2TI	C	601	5	-	5/27/37/37	-
3	GOL	B	609	-	-	0/4/4/4	-
4	ADP	C	605	5	-	7/12/32/32	0/3/3/3
3	GOL	C	602	-	-	0/4/4/4	-
4	ADP	D	609	5	-	0/12/32/32	0/3/3/3
3	GOL	D	605	-	-	0/4/4/4	-
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	B	606	-	-	0/4/4/4	-
3	GOL	D	602	-	-	0/4/4/4	-
4	ADP	B	610	5	-	0/12/32/32	0/3/3/3
2	2TI	D	601	5	-	1/27/37/37	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	D	607	-	-	0/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-
3	GOL	B	604	-	-	0/4/4/4	-
3	GOL	B	607	-	-	0/4/4/4	-
3	GOL	B	608	-	-	0/4/4/4	-
3	GOL	D	608	-	-	0/4/4/4	-
2	2TI	A	601	5	-	7/27/37/37	-
4	ADP	A	604	5	-	1/12/32/32	0/3/3/3
3	GOL	D	604	-	-	0/4/4/4	-
2	2TI	B	601	5	-	2/27/37/37	-
3	GOL	D	606	-	-	0/4/4/4	-
3	GOL	C	603	-	-	0/4/4/4	-
3	GOL	C	604	-	-	0/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	2TI	C03-N05	5.90	1.46	1.33
2	A	601	2TI	C03-N05	5.51	1.45	1.33
2	B	601	2TI	C03-N05	5.41	1.45	1.33
2	D	601	2TI	C03-N05	5.34	1.45	1.33
2	C	601	2TI	C27-N01	3.34	1.45	1.34
2	A	601	2TI	C27-N01	3.26	1.45	1.34
2	B	601	2TI	C27-N01	3.26	1.45	1.34
2	D	601	2TI	C27-N01	3.25	1.45	1.34
4	C	605	ADP	C5-C4	2.52	1.47	1.40
4	B	610	ADP	C5-C4	2.52	1.47	1.40
4	D	609	ADP	C5-C4	2.50	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	ADP	C5-C4	2.49	1.47	1.40
2	D	601	2TI	O04-C03	-2.31	1.18	1.23
2	B	601	2TI	O04-C03	-2.31	1.18	1.23
2	A	601	2TI	O04-C03	-2.25	1.18	1.23
2	D	601	2TI	P13-O14	-2.24	1.46	1.54
2	B	601	2TI	P13-O14	-2.22	1.46	1.54
2	A	601	2TI	P13-O14	-2.21	1.46	1.54
2	C	601	2TI	P13-O14	-2.19	1.46	1.54
2	A	601	2TI	P13-O16	-2.18	1.46	1.54
2	D	601	2TI	P13-O16	-2.17	1.46	1.54
2	C	601	2TI	P13-O16	-2.17	1.46	1.54
2	C	601	2TI	O04-C03	-2.16	1.19	1.23
2	B	601	2TI	P13-O16	-2.16	1.46	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	2TI	O16-P13-O12	3.31	115.74	104.64
2	A	601	2TI	O16-P13-O12	3.20	115.37	104.64
4	C	605	ADP	PA-O3A-PB	-3.18	121.92	132.83
2	B	601	2TI	O16-P13-O12	3.14	115.17	104.64
2	D	601	2TI	O16-P13-O12	3.14	115.17	104.64
4	B	610	ADP	N3-C2-N1	-3.09	123.84	128.68
4	C	605	ADP	C3'-C2'-C1'	3.09	105.62	100.98
4	A	604	ADP	N3-C2-N1	-3.08	123.86	128.68
4	C	605	ADP	N3-C2-N1	-3.08	123.87	128.68
4	D	609	ADP	N3-C2-N1	-3.07	123.88	128.68
4	A	604	ADP	C3'-C2'-C1'	3.01	105.50	100.98
2	C	601	2TI	C08-C02-C03	-2.93	103.35	110.20
4	D	609	ADP	C3'-C2'-C1'	2.81	105.21	100.98
2	A	601	2TI	C22-C23-C24	-2.79	107.60	113.59
4	B	610	ADP	C3'-C2'-C1'	2.71	105.05	100.98
2	C	601	2TI	O14-P13-O12	2.68	113.64	104.64
4	D	609	ADP	C4-C5-N7	-2.62	106.67	109.40
2	A	601	2TI	O14-P13-O12	2.59	113.32	104.64
4	A	604	ADP	PA-O3A-PB	-2.58	123.97	132.83
4	B	610	ADP	C4-C5-N7	-2.55	106.75	109.40
2	D	601	2TI	O14-P13-O12	2.54	113.15	104.64
4	A	604	ADP	C4-C5-N7	-2.54	106.75	109.40
3	B	602	GOL	C3-C2-C1	-2.52	101.89	111.70
2	D	601	2TI	C22-C23-C24	-2.52	108.17	113.59
2	B	601	2TI	C22-C23-C24	-2.50	108.21	113.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	2TI	C28-C27-N01	2.46	120.26	116.10
2	B	601	2TI	O14-P13-O12	2.40	112.67	104.64
2	D	601	2TI	C02-C03-N05	2.38	121.34	116.54
4	C	605	ADP	C4-C5-N7	-2.37	106.93	109.40
2	B	601	2TI	C02-C03-N05	2.34	121.26	116.54
2	C	601	2TI	C22-C23-C24	-2.29	108.67	113.59
4	B	610	ADP	PA-O3A-PB	-2.29	124.98	132.83
2	B	601	2TI	C22-C18-C19	-2.28	109.14	112.53
2	B	601	2TI	C28-C27-N01	2.15	119.73	116.10
3	A	603	GOL	C3-C2-C1	-2.12	103.46	111.70
2	D	601	2TI	C22-C18-C19	-2.07	109.46	112.53
2	A	601	2TI	C28-C27-N01	2.06	119.59	116.10
2	D	601	2TI	C28-C27-N01	2.05	119.58	116.10
3	C	603	GOL	C3-C2-C1	-2.04	103.76	111.70

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	2TI	C03-C02-C08-C09
2	C	601	2TI	C07-C06-N05-C03
4	C	605	ADP	PA-O3A-PB-O3B
4	C	605	ADP	C5'-O5'-PA-O1A
4	C	605	ADP	C5'-O5'-PA-O2A
3	B	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
2	A	601	2TI	P10-C17-C18-C22
2	C	601	2TI	N01-C02-C08-C09
3	A	603	GOL	C1-C2-C3-O3
3	A	603	GOL	O2-C2-C3-O3
2	A	601	2TI	N01-C02-C03-O04
4	C	605	ADP	PB-O3A-PA-O5'
2	A	601	2TI	N01-C02-C03-N05
2	C	601	2TI	P10-C17-C18-C19
2	A	601	2TI	P10-C17-C18-C19
2	B	601	2TI	P10-C17-C18-C19
2	C	601	2TI	P10-C17-C18-C22
2	A	601	2TI	C08-C09-P10-O12
2	B	601	2TI	P10-C17-C18-C22
2	A	601	2TI	C08-C02-C03-O04
4	C	605	ADP	PA-O3A-PB-O1B
2	A	601	2TI	C08-C02-C03-N05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	604	ADP	PB-O3A-PA-O2A
4	C	605	ADP	C5'-O5'-PA-O3A
4	C	605	ADP	O4'-C4'-C5'-O5'
2	D	601	2TI	P10-C17-C18-C19

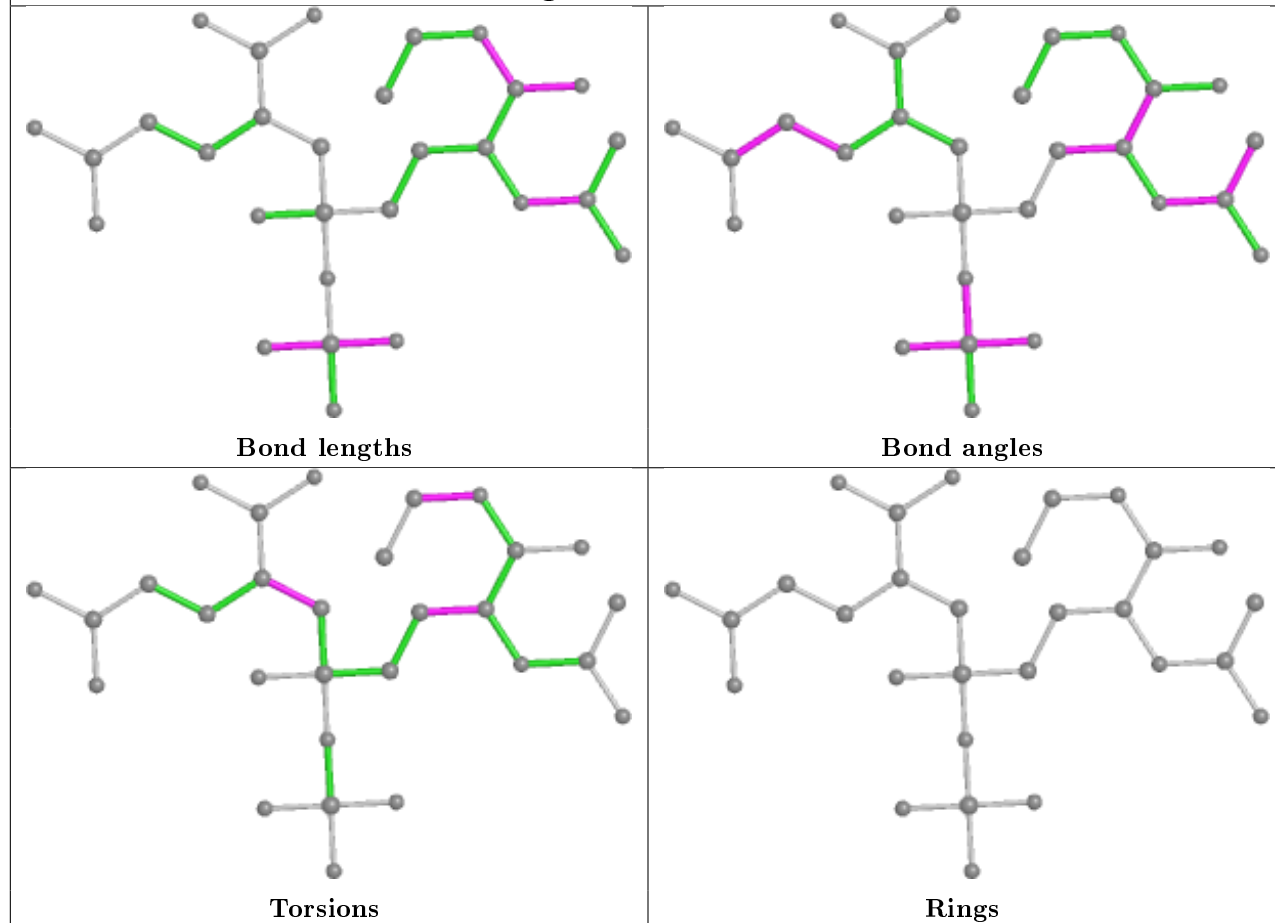
There are no ring outliers.

5 monomers are involved in 6 short contacts:

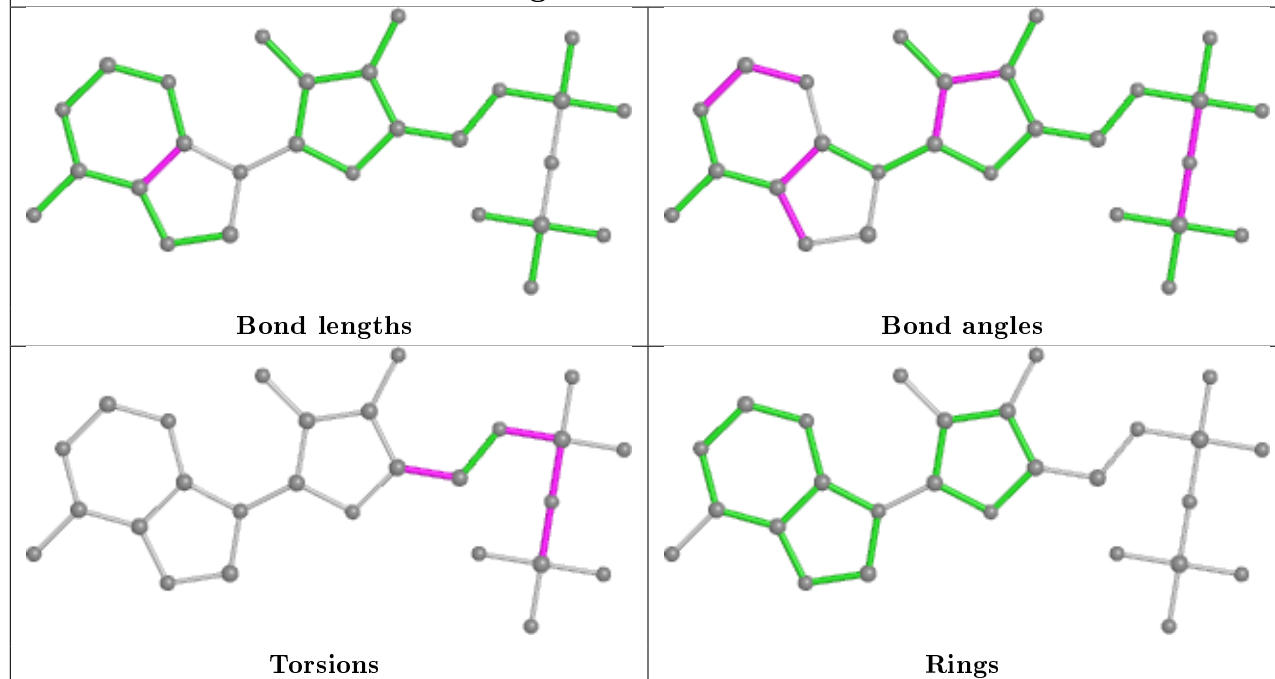
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	2TI	1	0
4	C	605	ADP	1	0
3	D	602	GOL	2	0
2	A	601	2TI	1	0
3	C	603	GOL	1	0

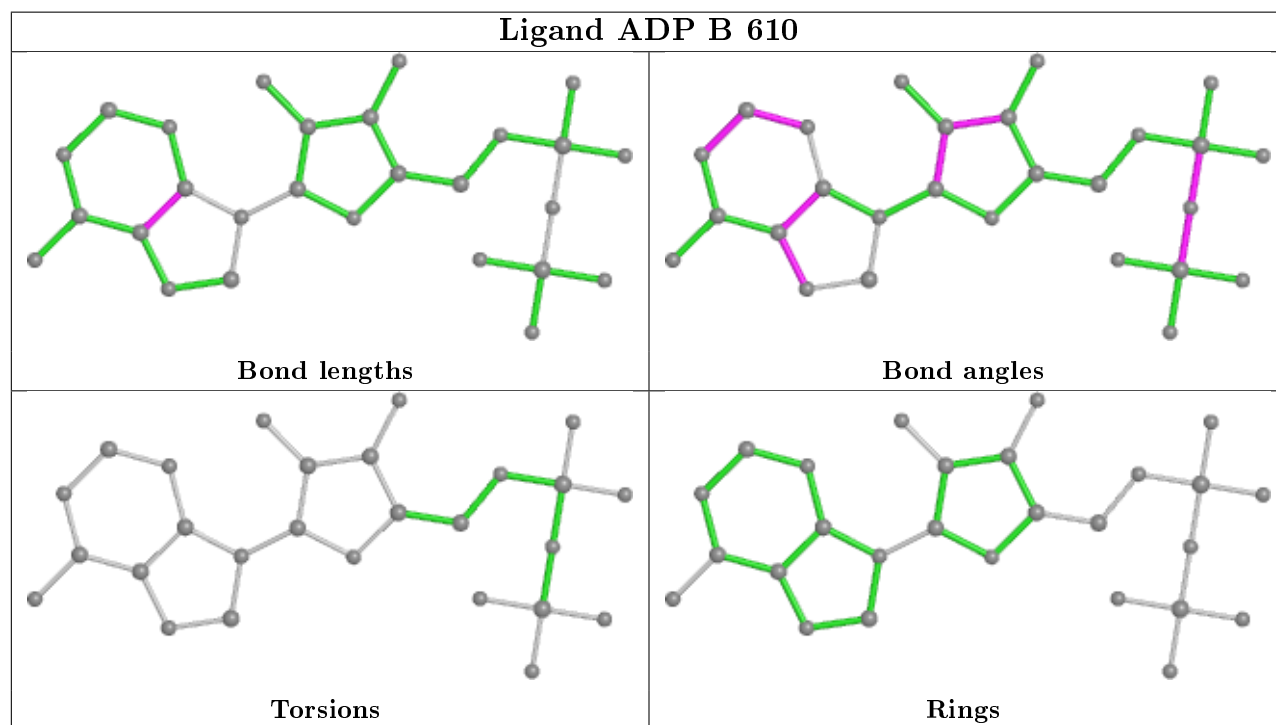
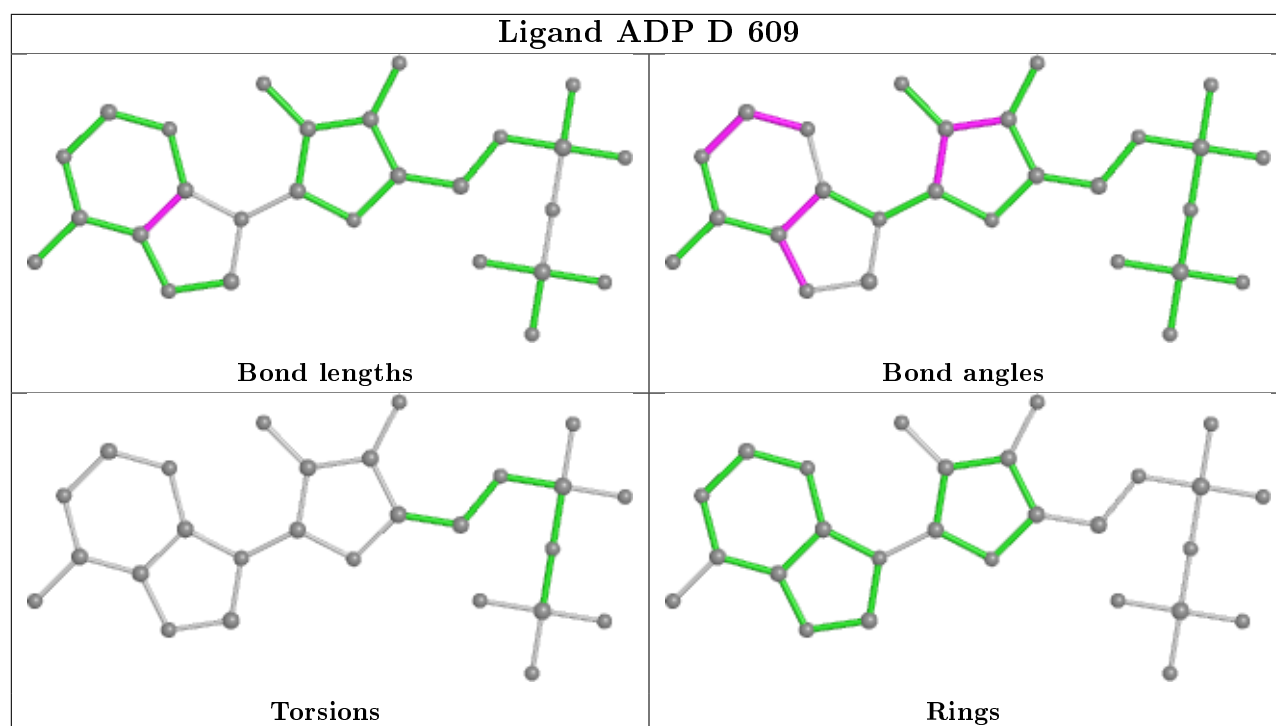
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

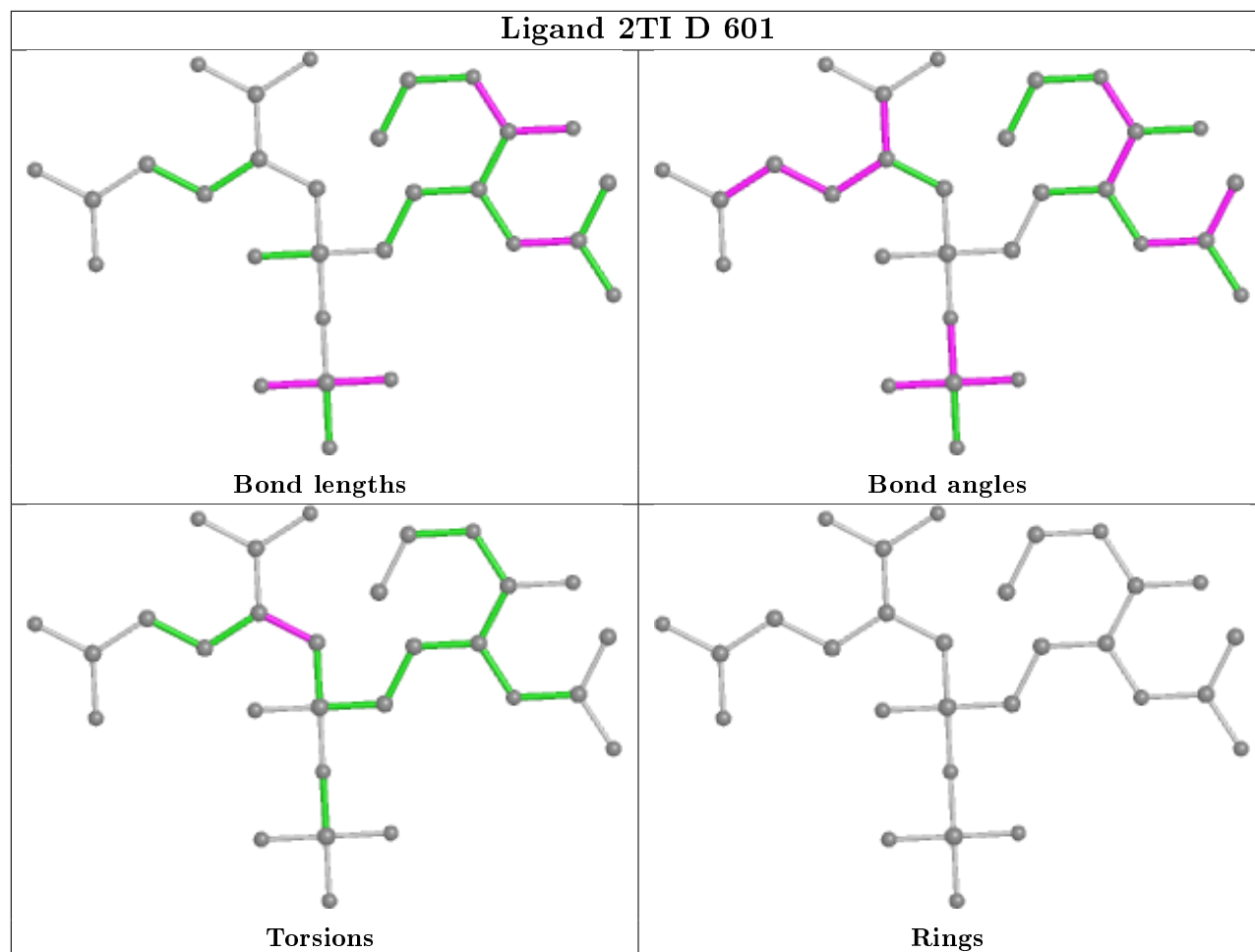
Ligand 2TI C 601



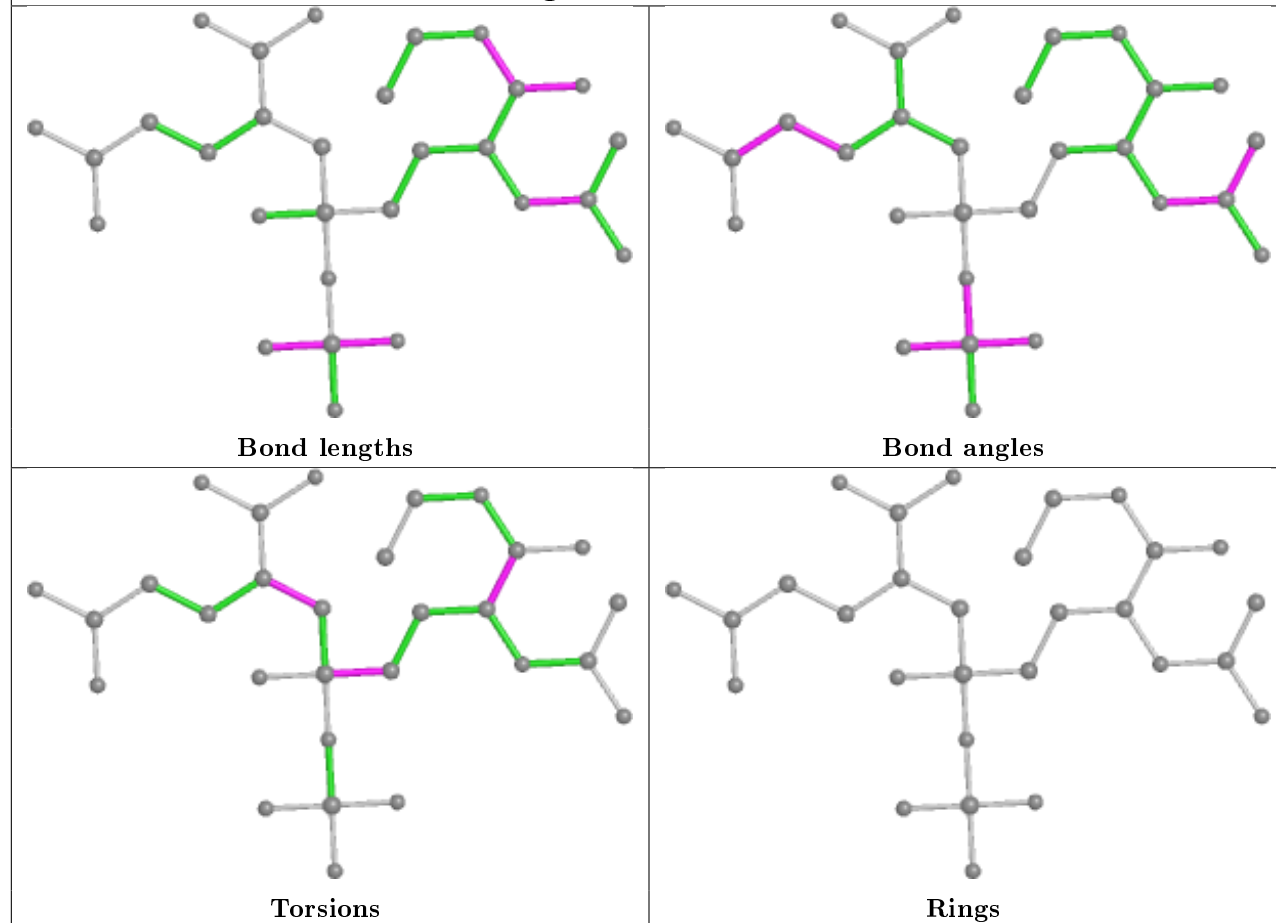
Ligand ADP C 605



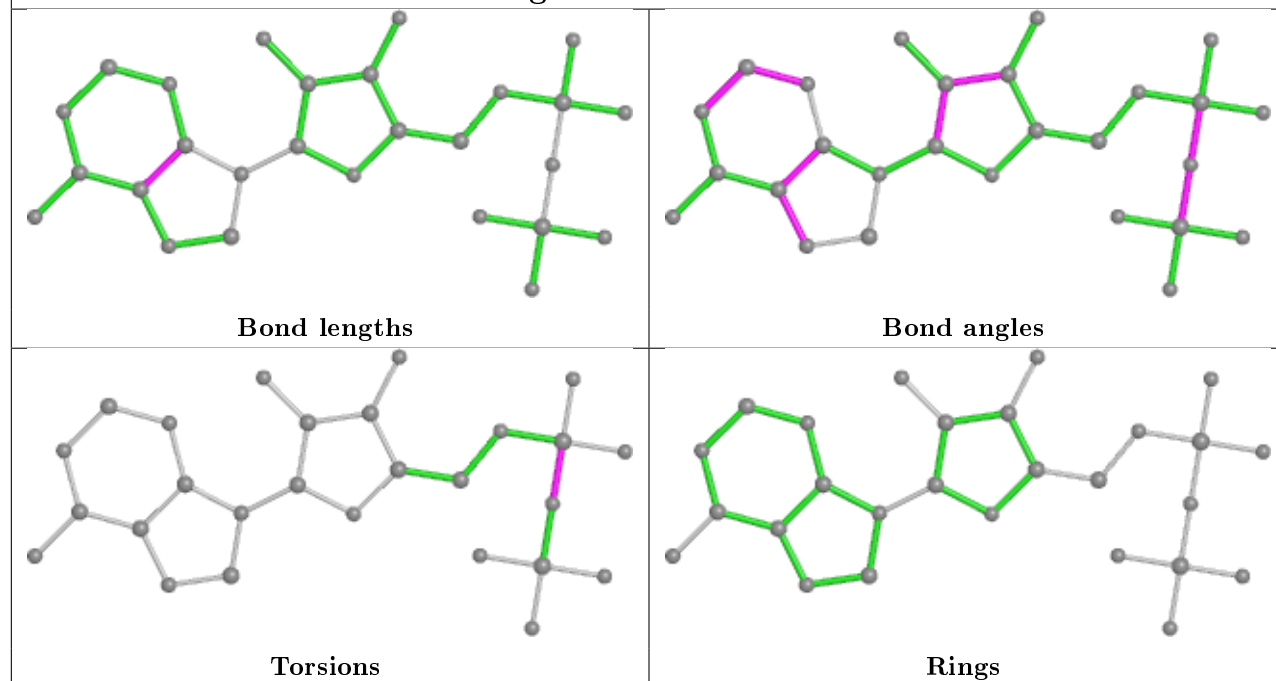


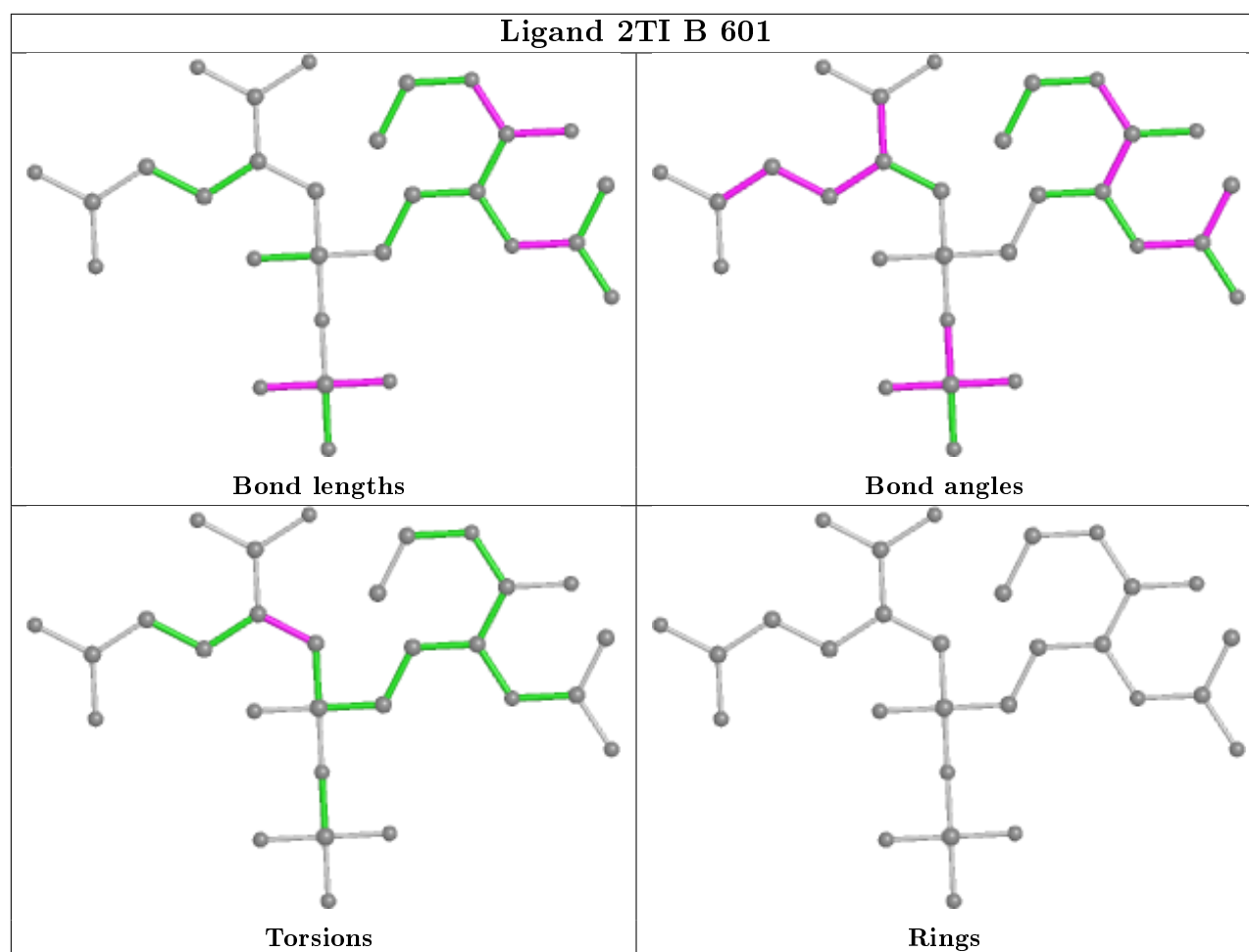


Ligand 2TI A 601



Ligand ADP A 604





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	402/453 (88%)	-0.09	4 (0%) 82 84	50, 67, 106, 155	0
1	B	398/453 (87%)	-0.15	2 (0%) 91 91	32, 50, 103, 151	0
1	C	401/453 (88%)	-0.02	4 (0%) 82 84	51, 68, 113, 144	0
1	D	402/453 (88%)	-0.11	4 (0%) 82 84	34, 52, 103, 143	0
All	All	1603/1812 (88%)	-0.09	14 (0%) 84 86	32, 61, 108, 155	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	LEU	4.8
1	D	413	PRO	3.9
1	C	101	LEU	3.9
1	B	409	LEU	3.3
1	A	86	ASP	3.3
1	A	327	HIS	2.8
1	C	409	LEU	2.7
1	D	86	ASP	2.6
1	C	417	ILE	2.4
1	D	425	PHE	2.4
1	D	412	CYS	2.4
1	A	279	PHE	2.2
1	A	101	LEU	2.1
1	C	408	PHE	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, 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	GOL	B	603	6/6	0.81	0.17	83,89,94,94	0
3	GOL	C	603	6/6	0.83	0.26	72,84,86,87	0
3	GOL	B	609	6/6	0.86	0.21	79,84,87,87	0
3	GOL	B	602	6/6	0.87	0.20	51,69,74,76	0
3	GOL	D	608	6/6	0.88	0.20	64,74,81,85	0
3	GOL	D	607	6/6	0.88	0.25	88,97,99,101	0
3	GOL	B	608	6/6	0.89	0.18	69,80,85,85	0
3	GOL	D	605	6/6	0.89	0.28	60,80,85,89	0
3	GOL	C	604	6/6	0.89	0.29	71,83,92,96	0
3	GOL	A	602	6/6	0.90	0.26	71,80,82,84	0
3	GOL	D	606	6/6	0.90	0.21	50,64,67,70	0
3	GOL	B	606	6/6	0.92	0.20	47,53,61,66	0
3	GOL	B	607	6/6	0.92	0.14	55,67,69,76	0
3	GOL	D	602	6/6	0.93	0.23	54,60,63,78	0
3	GOL	A	603	6/6	0.93	0.18	67,79,83,83	0
3	GOL	D	603	6/6	0.95	0.20	56,65,74,78	0
3	GOL	D	604	6/6	0.96	0.14	62,65,69,69	0
3	GOL	B	605	6/6	0.96	0.17	62,65,72,77	0
3	GOL	C	602	6/6	0.96	0.15	72,75,77,84	0
2	2TI	A	601	29/29	0.96	0.19	43,69,103,108	0
2	2TI	C	601	29/29	0.97	0.22	46,68,86,89	0
3	GOL	B	604	6/6	0.97	0.15	37,64,70,71	0
4	ADP	D	609	27/27	0.98	0.16	9,23,39,41	0
4	ADP	B	610	27/27	0.98	0.15	12,23,38,42	0
2	2TI	D	601	29/29	0.98	0.16	12,40,61,68	0
4	ADP	C	605	27/27	0.98	0.14	43,55,62,63	0
4	ADP	A	604	27/27	0.98	0.14	45,55,63,66	0
5	MG	C	606	1/1	0.98	0.14	48,48,48,48	0
5	MG	B	611	1/1	0.98	0.14	27,27,27,27	0
2	2TI	B	601	29/29	0.98	0.17	20,42,62,68	0
5	MG	A	606	1/1	0.98	0.10	43,43,43,43	0
5	MG	A	605	1/1	0.98	0.12	52,52,52,52	0

Continued on next page...

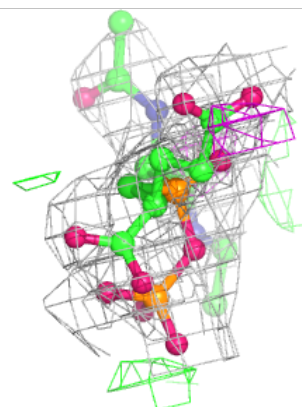
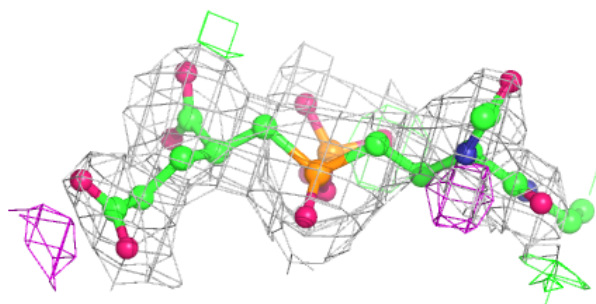
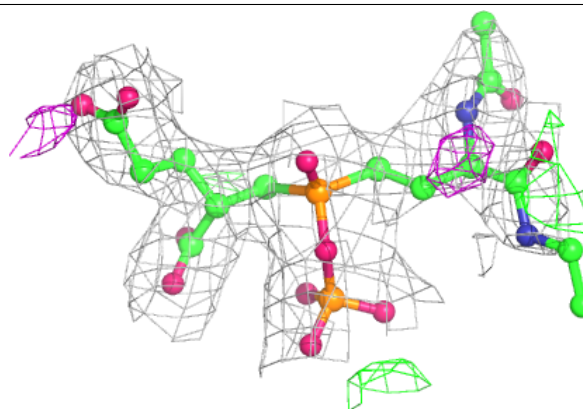
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	D	610	1/1	0.98	0.17	30,30,30,30	0
5	MG	D	611	1/1	0.99	0.15	24,24,24,24	0
5	MG	C	607	1/1	0.99	0.14	49,49,49,49	0
5	MG	B	612	1/1	0.99	0.14	33,33,33,33	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.

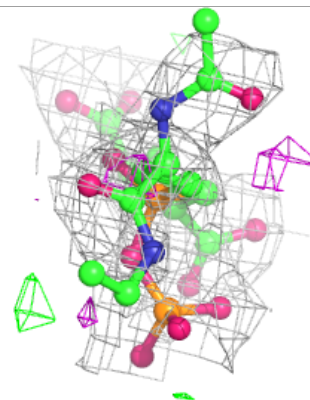
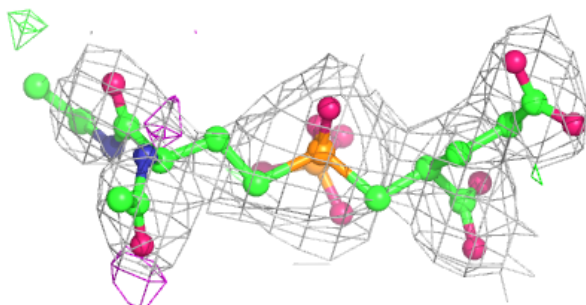
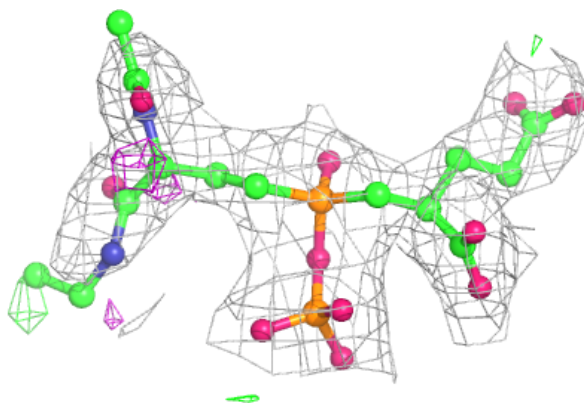
Electron density around 2TI A 601:

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



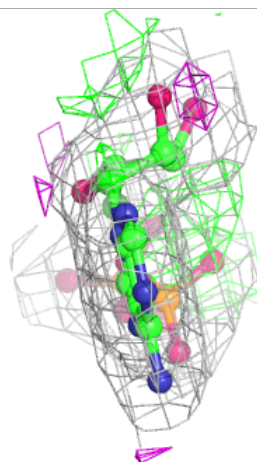
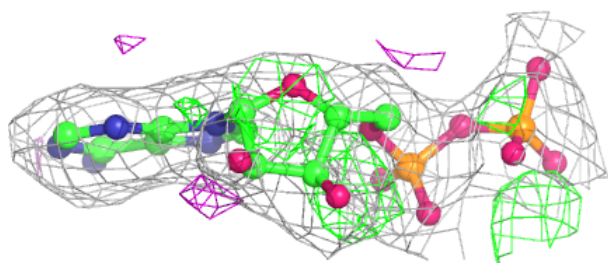
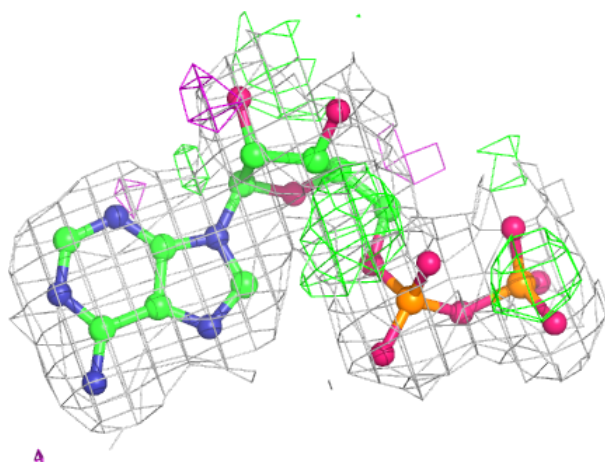
Electron density around 2TI C 601:

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



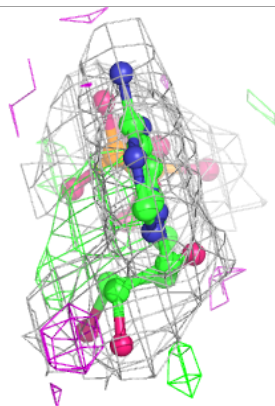
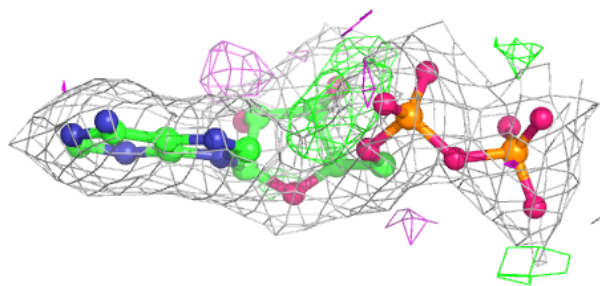
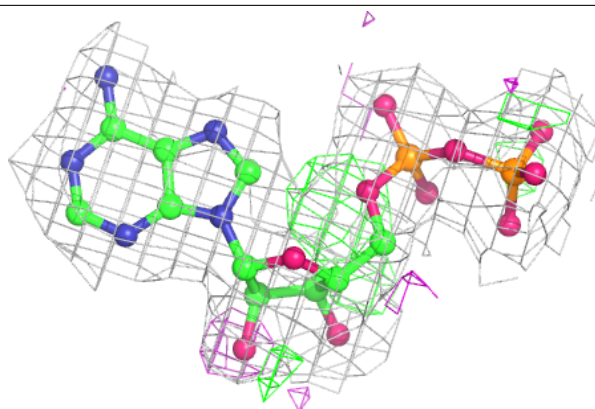
Electron density around ADP D 609:

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

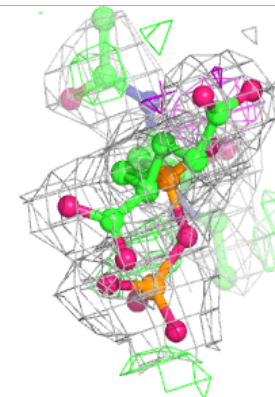
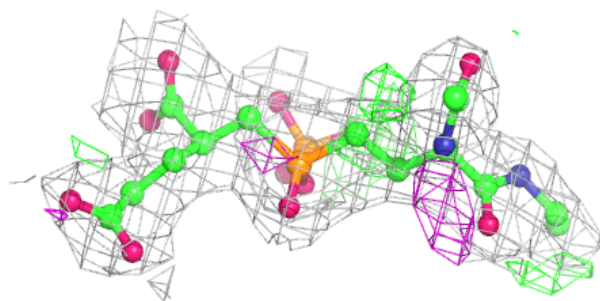
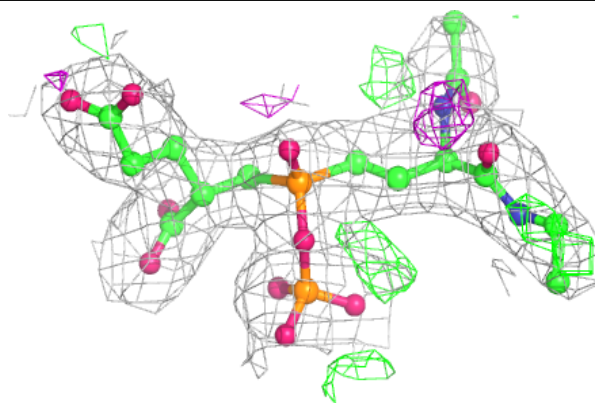


Electron density around ADP B 610:

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

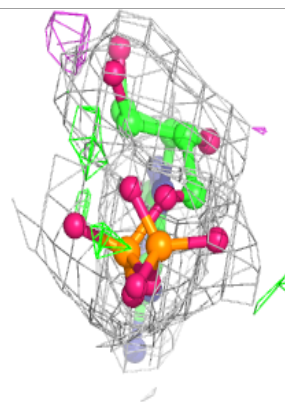
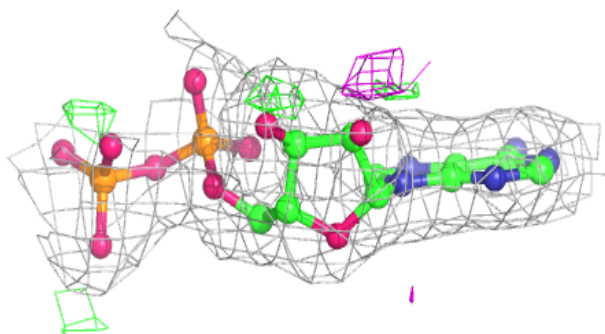
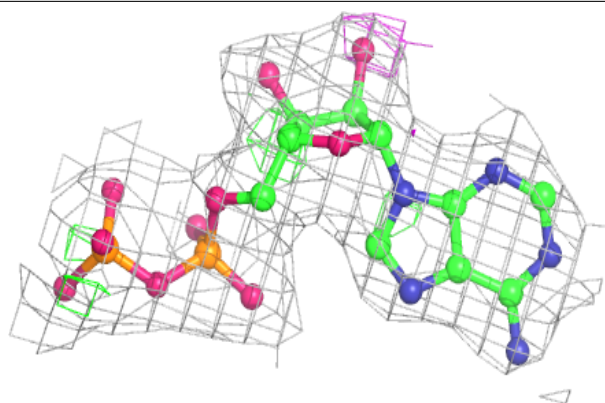
**Electron density around 2TI D 601:**

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

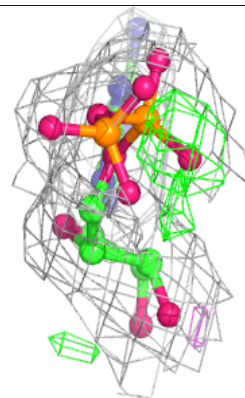
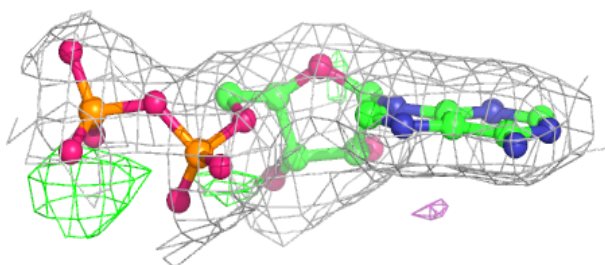
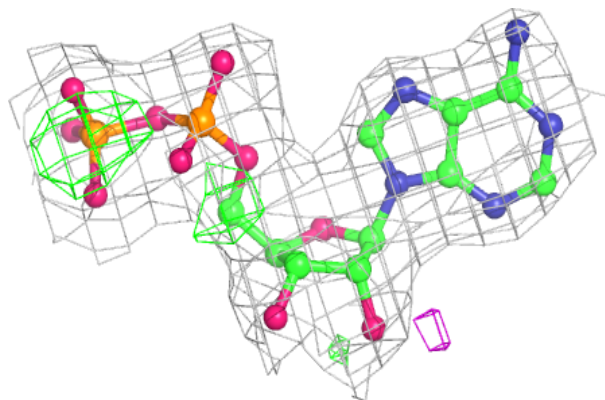


Electron density around ADP C 605:

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

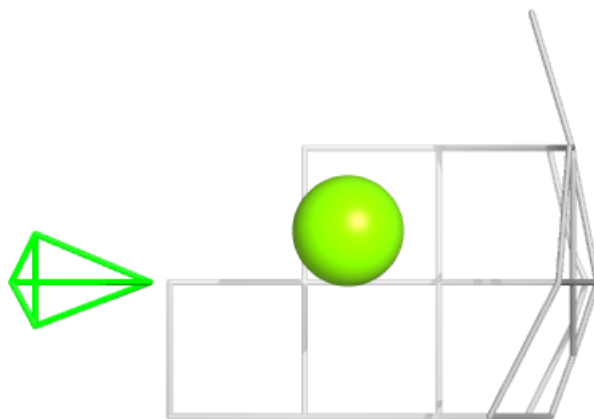
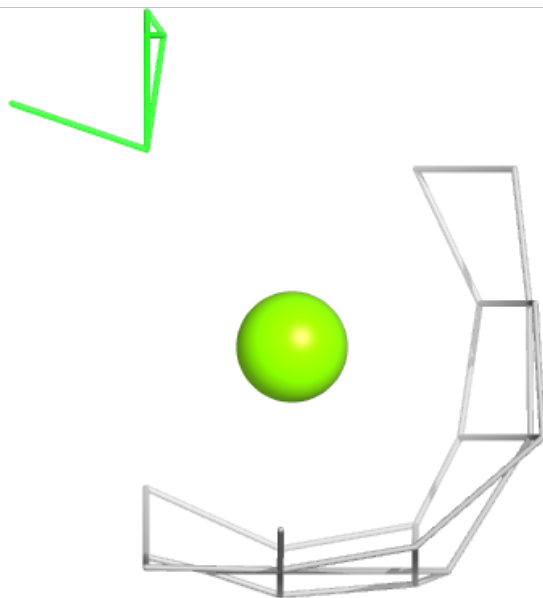
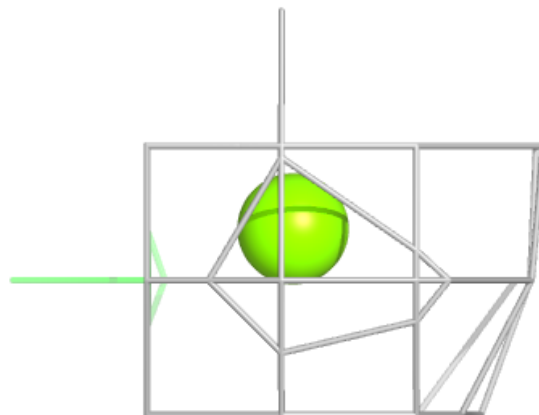
**Electron density around ADP A 604:**

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



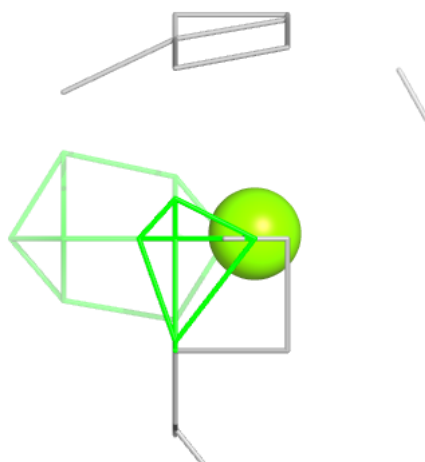
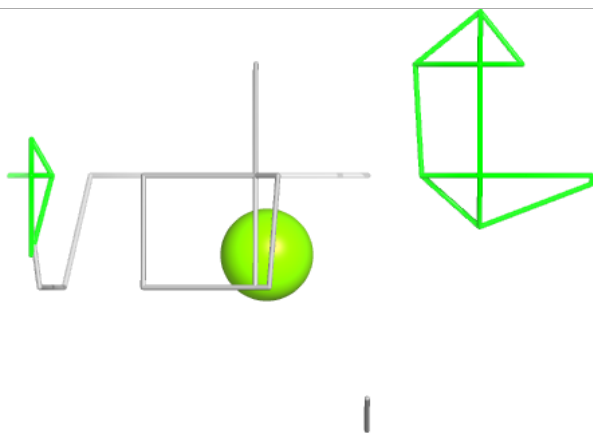
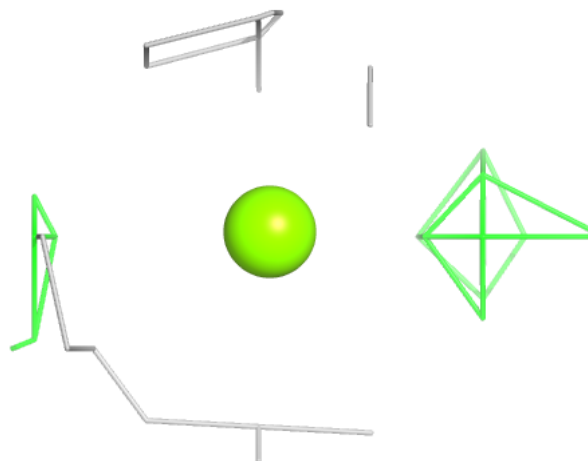
Electron density around MG C 606:

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



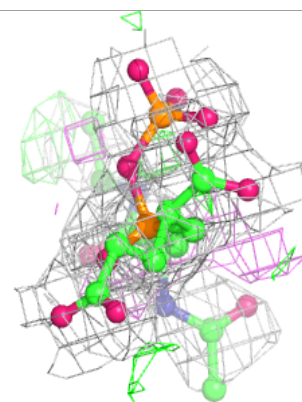
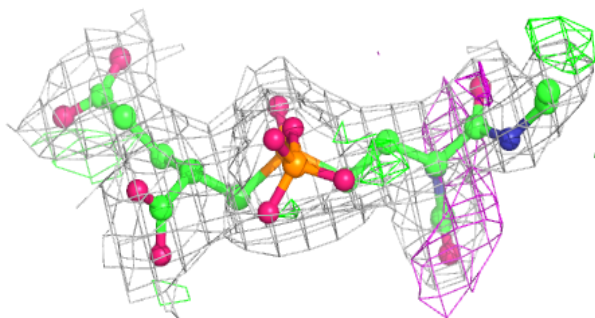
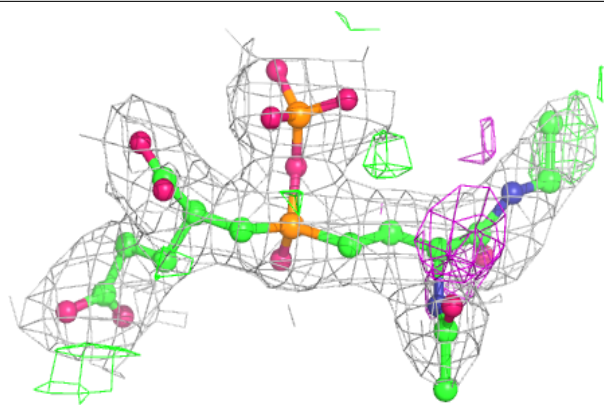
Electron density around MG B 611:

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



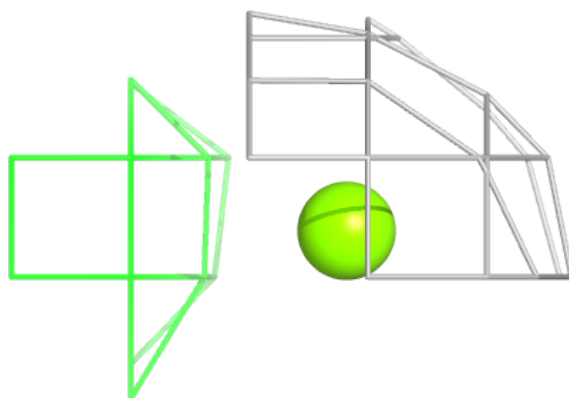
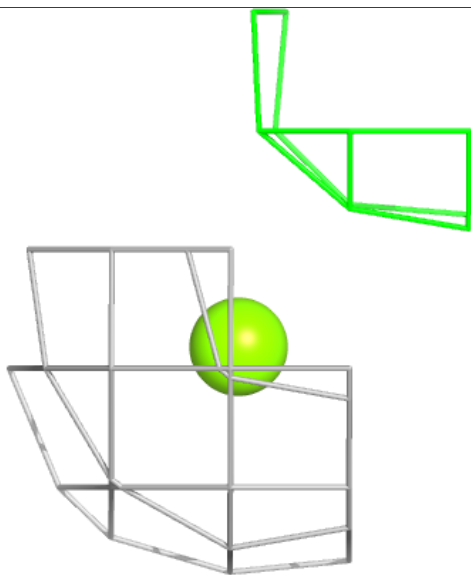
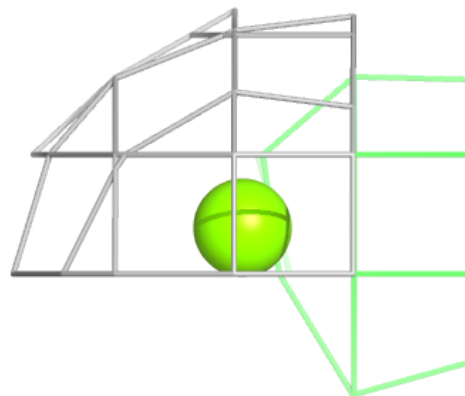
Electron density around 2TI B 601:

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



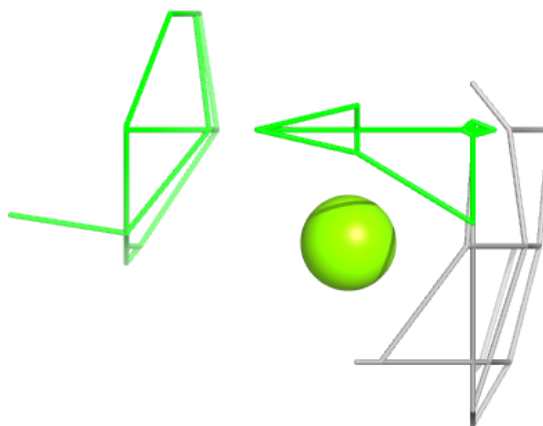
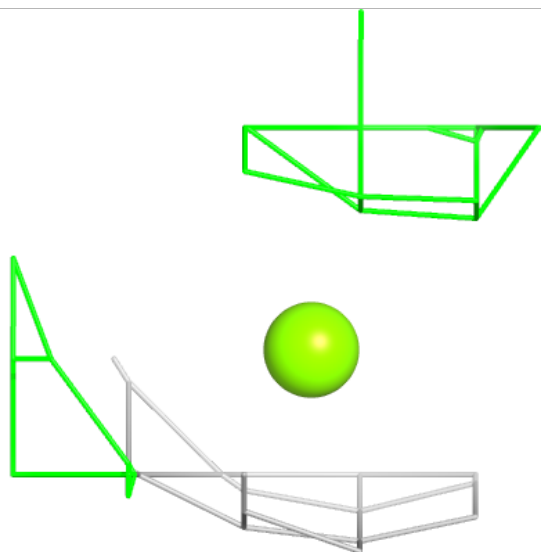
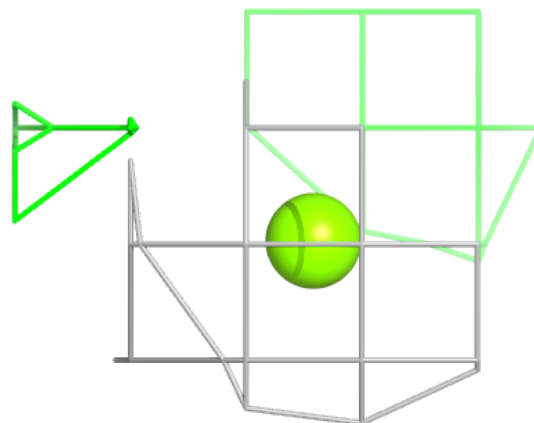
Electron density around MG A 606:

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



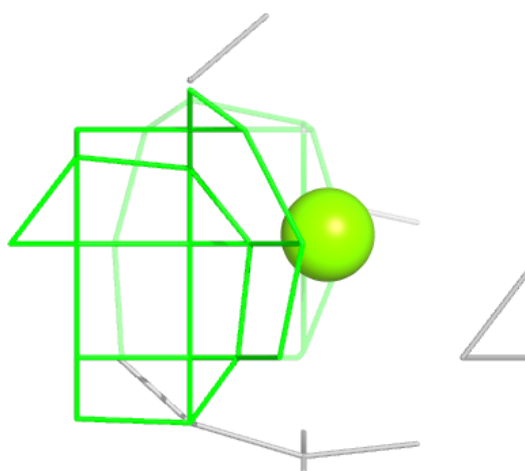
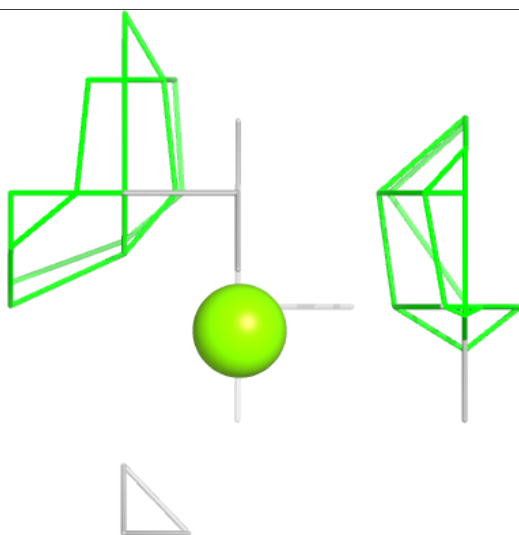
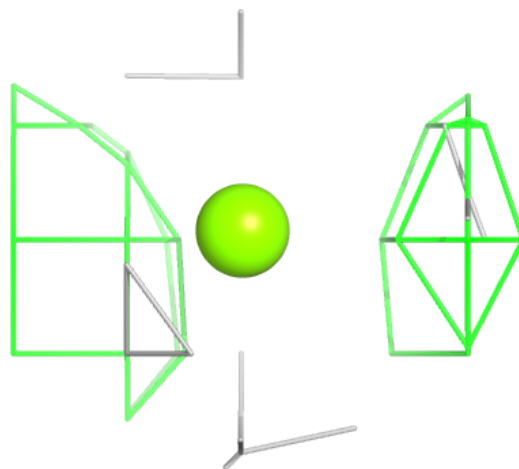
Electron density around MG A 605:

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



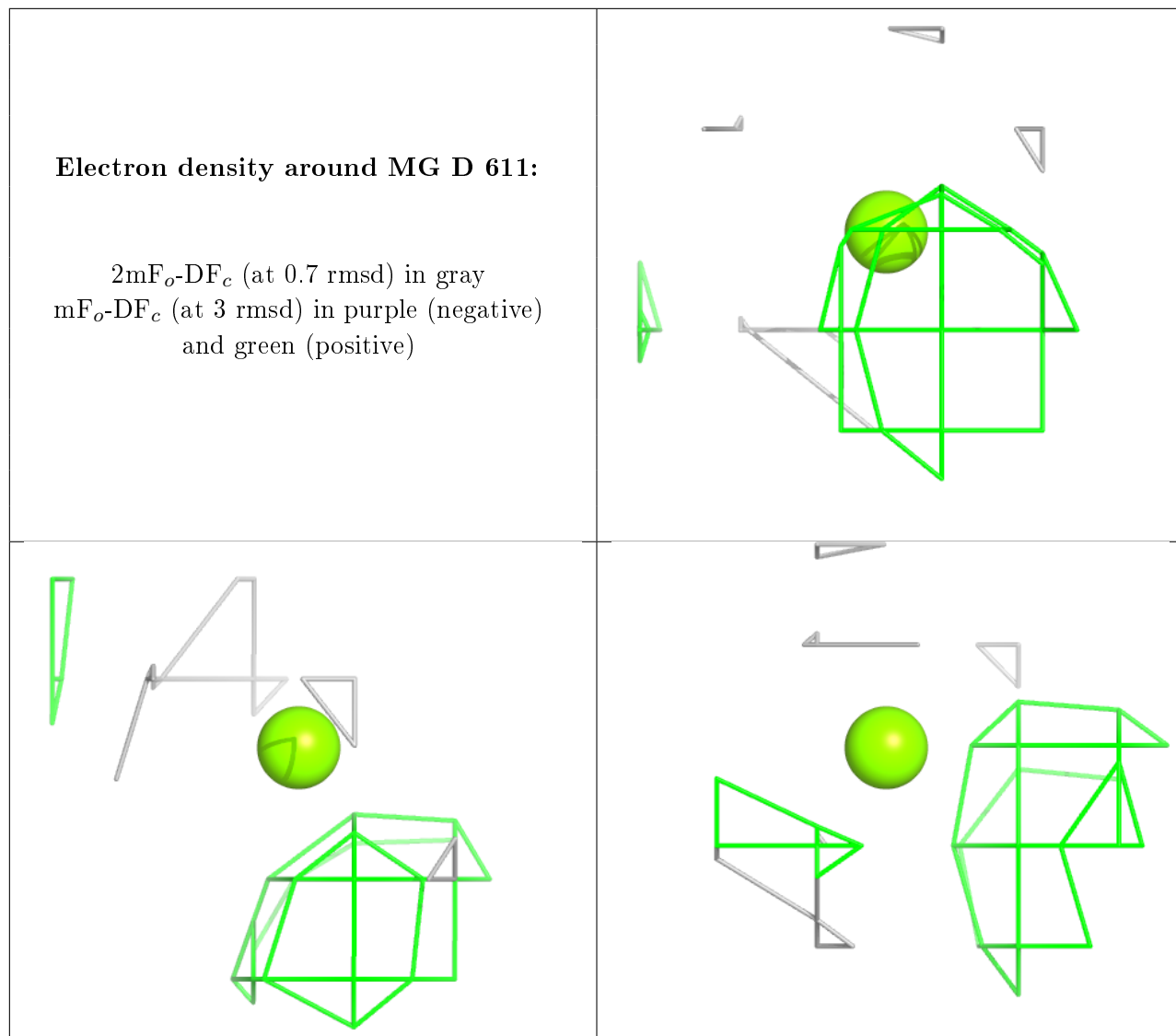
Electron density around MG D 610:

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



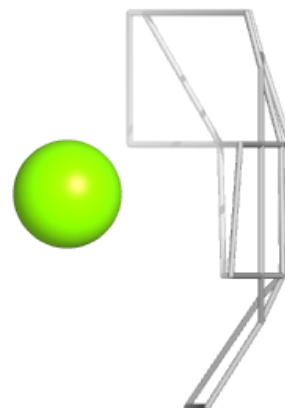
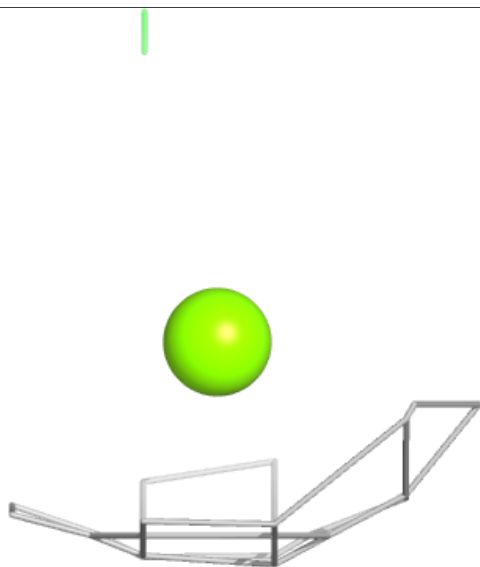
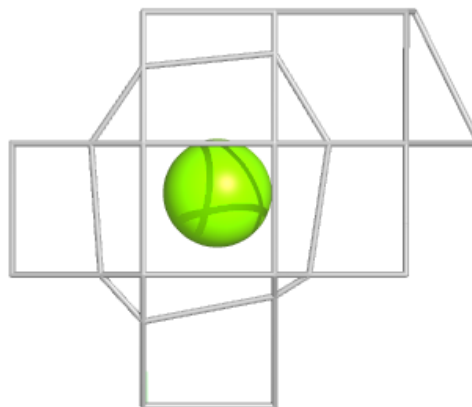
Electron density around MG D 611:

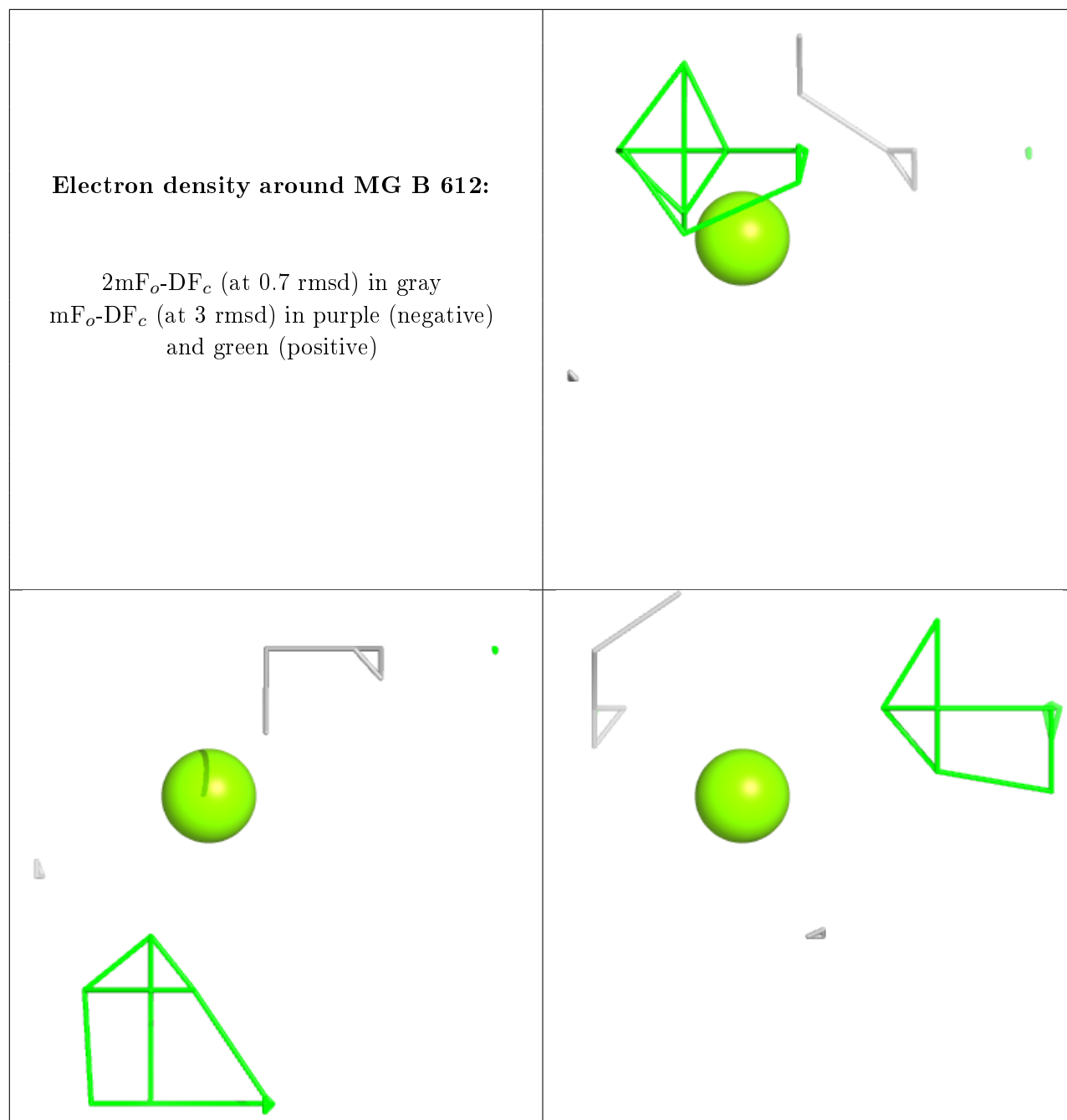
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG C 607:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.