



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2020 – 08:31 PM BST

PDB ID : 6VZR
Title : Engineered TTL6 bound to the initiation analog
Authors : Mahalingan, K.K.; Keenen, E.K.; Strickland, M.; Li, Y.; Liu, Y.; Ball, H.L.;
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Deposited on : 2020-02-28
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

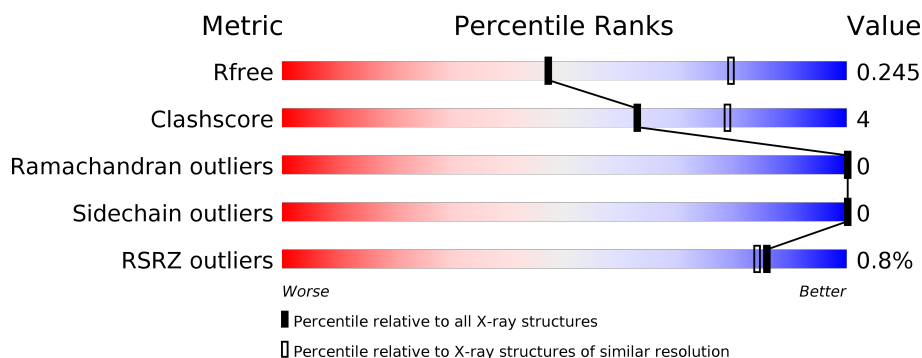
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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 ≥ 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 style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 79% 10% 12% </div> </div>
1	B	453	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 79% 10% 11% </div> </div>
1	C	453	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 80% 9% 11% </div> </div>
1	D	453	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 78% 11% 11% </div> </div>
2	F	12	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 100% </div> </div>
3	G	11	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 100% </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13457 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	400	Total	C	N	O	S	0	4	0
			3155	2022	542	570	21			
1	B	402	Total	C	N	O	S	0	3	0
			3142	2018	536	567	21			
1	C	404	Total	C	N	O	S	0	2	0
			3136	2009	536	571	20			
1	D	404	Total	C	N	O	S	0	0	0
			3139	2010	540	570	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	ALA	CYS	engineered mutation	UNP A4Q9E8
A	180	ARG	GLN	engineered mutation	UNP A4Q9E8
A	362	ILE	HIS	engineered mutation	UNP A4Q9E8
B	179	ALA	CYS	engineered mutation	UNP A4Q9E8
B	180	ARG	GLN	engineered mutation	UNP A4Q9E8
B	362	ILE	HIS	engineered mutation	UNP A4Q9E8
C	179	ALA	CYS	engineered mutation	UNP A4Q9E8
C	180	ARG	GLN	engineered mutation	UNP A4Q9E8
C	362	ILE	HIS	engineered mutation	UNP A4Q9E8
D	179	ALA	CYS	engineered mutation	UNP A4Q9E8
D	180	ARG	GLN	engineered mutation	UNP A4Q9E8
D	362	ILE	HIS	engineered mutation	UNP A4Q9E8

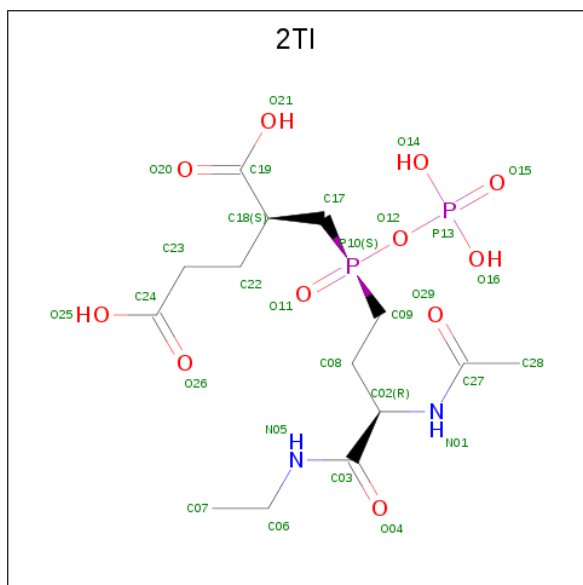
- Molecule 2 is a protein called TTLL6 unregistered chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	12	Total	C	N	O	0	0	0
			60	36	12	12			

- Molecule 3 is a protein called TTLL6 unregistered chain.

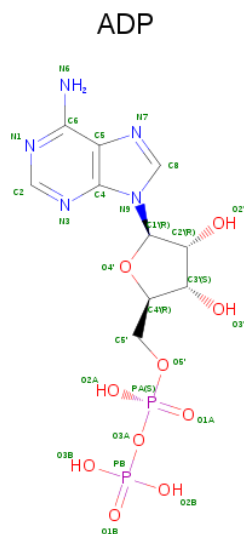
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	11	Total	C	N	O	0	0	0
			55	33	11	11			

- Molecule 4 is (2 {S})-2-[[[(3 {R})-3-acetamido-4-(ethylamino)-4-oxidanylidene-butyl]-phosphonoxy-phosphoryl]methyl]pentanedioic acid (three-letter code: 2TI) (formula: C₁₄H₂₆N₂O₁₁P₂).



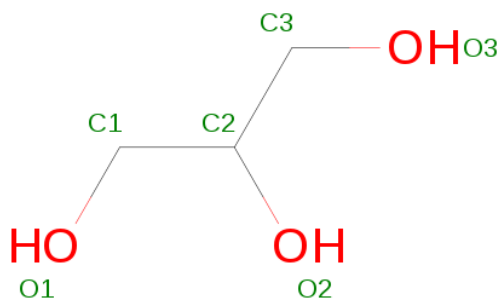
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	14	2	11	2		
4	B	1	Total	C	N	O	P	0	0
			29	14	2	11	2		
4	C	1	Total	C	N	O	P	0	0
			29	14	2	11	2		
4	D	1	Total	C	N	O	P	0	0
			29	14	2	11	2		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

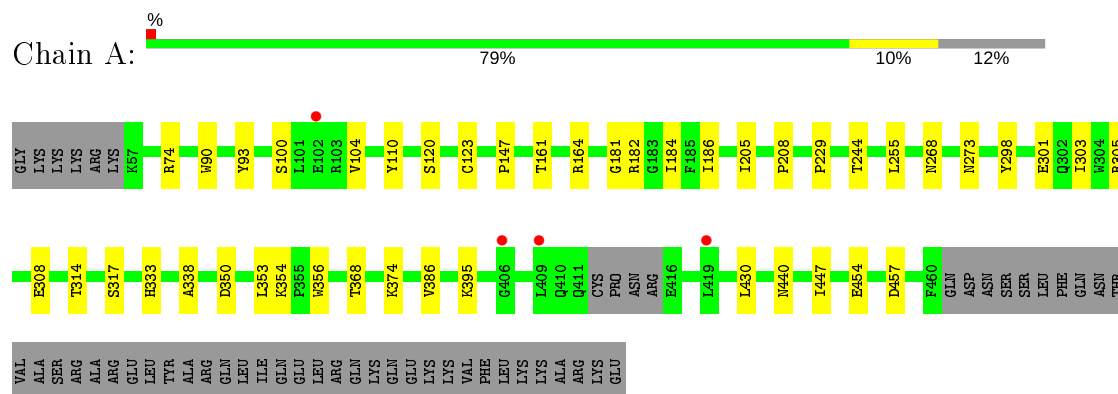
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	111	Total	O	0	0
			111	111		
8	B	81	Total	O	0	0
			81	81		
8	C	120	Total	O	0	0
			120	120		
8	D	70	Total	O	0	0
			70	70		

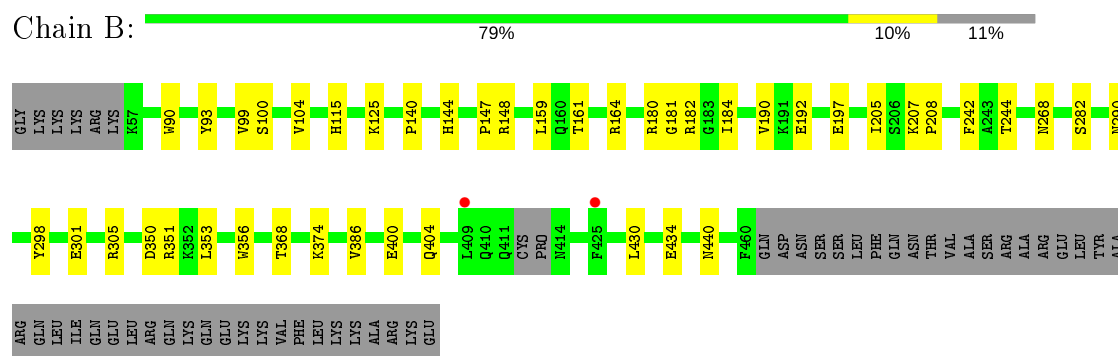
3 Residue-property plots

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

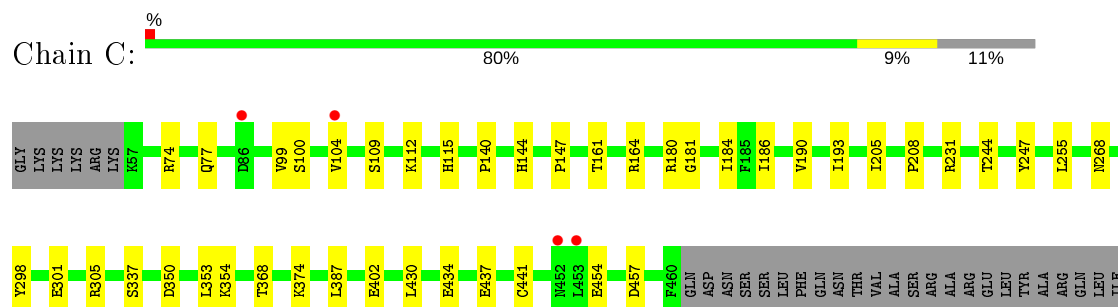
• Molecule 1: Tubulin polyglutamylase TTL6



• Molecule 1: Tubulin polyglutamylase TTL6




• Molecule 1: Tubulin polyglutamylase TTL6



GLN
GLU
LEU
ARG
GLN
LYS
GLN
GLU
LYS
VAL
PHE
LEU
LYS
ALA
ALA
LYS
ARG
GLU

• Molecule 1: Tubulin polyglutamylase TTLL6

Chain D:  78% 11% 11%

GLY
LYS
LYS
LYS
ARG
LYS
K57
V61
W90
Y93
V99
S109
I113
H114
H115
S120
E121
I122
C123
P140
H144
T161
R164
S177
G181
R182
G183
I184
F185
I186
E192
K207
P208
L223
P229
T244
L255
N268
Y298

E301
Q302
T303
R304
R305
T314
S317
A318
H333
T334
A338
D350
R351
K352
L353
K354
P355
W356
S367
T368
K374
V386
L387
E402
R405
I419
L430
N440
E460
GLN
ASP
ASN
SER
SER
LEU
PHE
GLN
ASN
THR
VAL
ALA
SER
ARG
ALA
ARG

GLU
LEU
TYR
ALA
ARG
GLN
LEU
ILE
GLN
GLU
LEU
ARG
GLN
LYS
GLN
GLU
LYS
VAL
PHE
LEU
LYS
LYS
ALA
ARG
LYS
GLU

• Molecule 2: TTLL6 unregistered chain

Chain F:  100%

There are no outlier residues recorded for this chain.

• Molecule 3: TTLL6 unregistered chain

Chain G:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.10Å 108.81Å 171.62Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	45.95 – 2.60 45.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.95-2.60) 99.8 (45.95-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.230 , 0.249 0.226 , 0.245	Depositor DCC
R_{free} test set	4223 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13457	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 52.75 % 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 4.6523e-05. 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	0/3242	0.40	0/4392
1	B	0.24	0/3227	0.39	0/4375
1	C	0.24	0/3219	0.39	0/4368
1	D	0.24	0/3215	0.39	0/4361
All	All	0.24	0/12903	0.39	0/17496

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	3155	0	2977	25	0
1	B	3142	0	2955	30	0
1	C	3136	0	2916	25	0
1	D	3139	0	2931	30	0
2	F	60	0	14	0	0
3	G	55	0	13	0	0
4	A	29	0	0	0	0
4	B	29	0	0	1	0
4	C	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	29	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
5	C	27	0	12	0	0
5	D	27	0	12	0	0
6	A	48	0	64	0	0
6	B	42	0	56	3	0
6	C	54	0	72	2	0
6	D	12	0	16	1	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
8	A	111	0	0	2	0
8	B	81	0	0	1	0
8	C	120	0	0	2	0
8	D	70	0	0	0	0
All	All	13457	0	12062	108	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.

The worst 5 of 108 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:D:334:THR:HG21	1:D:405:ARG:HD2	1.70	0.73
1:B:208:PRO:HA	1:B:350:ASP:HA	1.75	0.67
1:C:208:PRO:HA	1:C:350:ASP:HA	1.76	0.67
1:B:207:LYS:HB3	1:B:351:ARG:HD3	1.77	0.65
1:A:208:PRO:HA	1:A:350:ASP:HA	1.80	0.64

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	400/453 (88%)	389 (97%)	11 (3%)	0	100	100
1	B	401/453 (88%)	391 (98%)	10 (2%)	0	100	100
1	C	404/453 (89%)	393 (97%)	11 (3%)	0	100	100
1	D	402/453 (89%)	389 (97%)	13 (3%)	0	100	100
All	All	1607/1812 (89%)	1562 (97%)	45 (3%)	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	322/415 (78%)	322 (100%)	0	100	100
1	B	321/415 (77%)	321 (100%)	0	100	100
1	C	316/415 (76%)	316 (100%)	0	100	100
1	D	315/415 (76%)	315 (100%)	0	100	100
All	All	1274/1660 (77%)	1274 (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 ⓘ

There are no RNA molecules in this entry.

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

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 42 ligands modelled in this entry, 8 are monoatomic - leaving 34 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	GOL	A	604	-	5,5,5	0.91	0	5,5,5	0.99	0
6	GOL	C	604	-	5,5,5	1.03	0	5,5,5	1.12	0
6	GOL	B	611	-	5,5,5	0.91	0	5,5,5	1.00	0
6	GOL	A	606	-	5,5,5	0.88	0	5,5,5	1.22	0
6	GOL	A	608	-	5,5,5	0.91	0	5,5,5	1.00	0
6	GOL	A	603	-	5,5,5	0.98	0	5,5,5	1.07	0
6	GOL	C	613	-	5,5,5	0.89	0	5,5,5	1.00	0
5	ADP	D	602	7	24,29,29	0.97	1 (4%)	29,45,45	1.32	4 (13%)
5	ADP	A	602	7	24,29,29	0.97	1 (4%)	29,45,45	1.32	4 (13%)
5	ADP	C	602	7	24,29,29	0.98	1 (4%)	29,45,45	1.26	4 (13%)
6	GOL	C	610	-	5,5,5	0.93	0	5,5,5	1.07	1 (20%)
6	GOL	B	603	-	5,5,5	0.77	0	5,5,5	1.10	0
6	GOL	A	605	-	5,5,5	0.96	0	5,5,5	1.00	0
6	GOL	C	603	-	5,5,5	1.01	0	5,5,5	1.03	0
6	GOL	B	608	-	5,5,5	0.88	0	5,5,5	1.19	1 (20%)
6	GOL	D	603	-	5,5,5	0.95	0	5,5,5	1.04	0
6	GOL	A	609	-	5,5,5	0.92	0	5,5,5	1.00	0
6	GOL	A	612	-	5,5,5	0.91	0	5,5,5	1.00	0
6	GOL	C	612	-	5,5,5	0.91	0	5,5,5	1.02	0
5	ADP	B	602	7	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)
6	GOL	B	605	-	5,5,5	0.87	0	5,5,5	1.20	0
6	GOL	C	605	-	5,5,5	0.93	0	5,5,5	1.00	0
6	GOL	C	607	-	5,5,5	0.87	0	5,5,5	1.19	1 (20%)
4	2TI	A	601	7	17,28,28	2.00	5 (29%)	20,39,39	1.54	6 (30%)
4	2TI	B	601	7	17,28,28	2.03	5 (29%)	20,39,39	1.55	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	607	-	5,5,5	0.93	0	5,5,5	1.03	0
6	GOL	B	610	-	5,5,5	0.95	0	5,5,5	1.08	1 (20%)
6	GOL	D	606	-	5,5,5	0.88	0	5,5,5	1.18	1 (20%)
6	GOL	C	611	-	5,5,5	0.92	0	5,5,5	1.00	0
4	2TI	C	601	7	17,28,28	1.99	5 (29%)	20,39,39	1.53	4 (20%)
6	GOL	B	609	-	5,5,5	0.89	0	5,5,5	1.18	0
6	GOL	C	606	-	5,5,5	0.90	0	5,5,5	0.99	0
6	GOL	B	604	-	5,5,5	0.87	0	5,5,5	1.21	1 (20%)
4	2TI	D	601	7	17,28,28	1.97	5 (29%)	20,39,39	1.59	6 (30%)

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	GOL	A	604	-	-	0/4/4/4	-
6	GOL	C	604	-	-	0/4/4/4	-
6	GOL	B	611	-	-	2/4/4/4	-
6	GOL	A	606	-	-	0/4/4/4	-
6	GOL	A	608	-	-	0/4/4/4	-
6	GOL	A	603	-	-	0/4/4/4	-
6	GOL	C	613	-	-	0/4/4/4	-
5	ADP	D	602	7	-	1/12/32/32	0/3/3/3
5	ADP	A	602	7	-	2/12/32/32	0/3/3/3
5	ADP	C	602	7	-	1/12/32/32	0/3/3/3
6	GOL	C	610	-	-	0/4/4/4	-
6	GOL	B	603	-	-	0/4/4/4	-
6	GOL	A	605	-	-	0/4/4/4	-
6	GOL	C	603	-	-	0/4/4/4	-
6	GOL	B	608	-	-	0/4/4/4	-
6	GOL	D	603	-	-	0/4/4/4	-
6	GOL	A	609	-	-	0/4/4/4	-
6	GOL	A	612	-	-	0/4/4/4	-
6	GOL	C	612	-	-	0/4/4/4	-
5	ADP	B	602	7	-	1/12/32/32	0/3/3/3
6	GOL	B	605	-	-	0/4/4/4	-
6	GOL	C	605	-	-	1/4/4/4	-
6	GOL	C	607	-	-	0/4/4/4	-
4	2TI	A	601	7	-	4/27/37/37	-
4	2TI	B	601	7	-	6/27/37/37	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	607	-	-	0/4/4/4	-
6	GOL	B	610	-	-	0/4/4/4	-
6	GOL	D	606	-	-	0/4/4/4	-
6	GOL	C	611	-	-	1/4/4/4	-
4	2TI	C	601	7	-	3/27/37/37	-
6	GOL	B	609	-	-	0/4/4/4	-
6	GOL	C	606	-	-	0/4/4/4	-
6	GOL	B	604	-	-	0/4/4/4	-
4	2TI	D	601	7	-	6/27/37/37	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	2TI	C03-N05	5.88	1.46	1.33
4	C	601	2TI	C03-N05	5.68	1.46	1.33
4	A	601	2TI	C03-N05	5.66	1.46	1.33
4	D	601	2TI	C03-N05	5.51	1.45	1.33
4	D	601	2TI	C27-N01	3.26	1.45	1.34

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	2TI	O16-P13-O12	3.42	116.09	104.64
4	A	601	2TI	O16-P13-O12	3.38	115.97	104.64
4	D	601	2TI	O16-P13-O12	3.22	115.44	104.64
5	A	602	ADP	N3-C2-N1	-3.21	123.66	128.68
4	B	601	2TI	O16-P13-O12	3.19	115.33	104.64

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

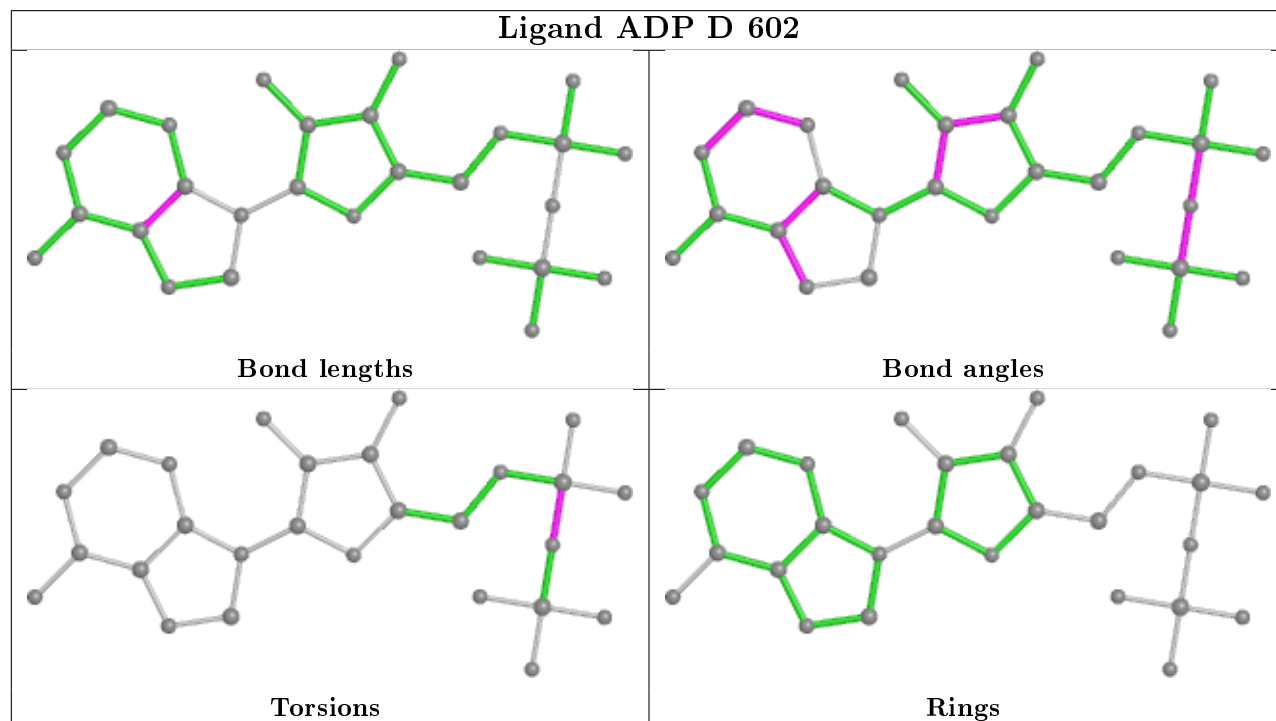
Mol	Chain	Res	Type	Atoms
6	B	611	GOL	O1-C1-C2-C3
4	A	601	2TI	C08-C09-P10-O12
4	B	601	2TI	C07-C06-N05-C03
4	B	601	2TI	C08-C09-P10-O12
4	C	601	2TI	C08-C09-P10-O11

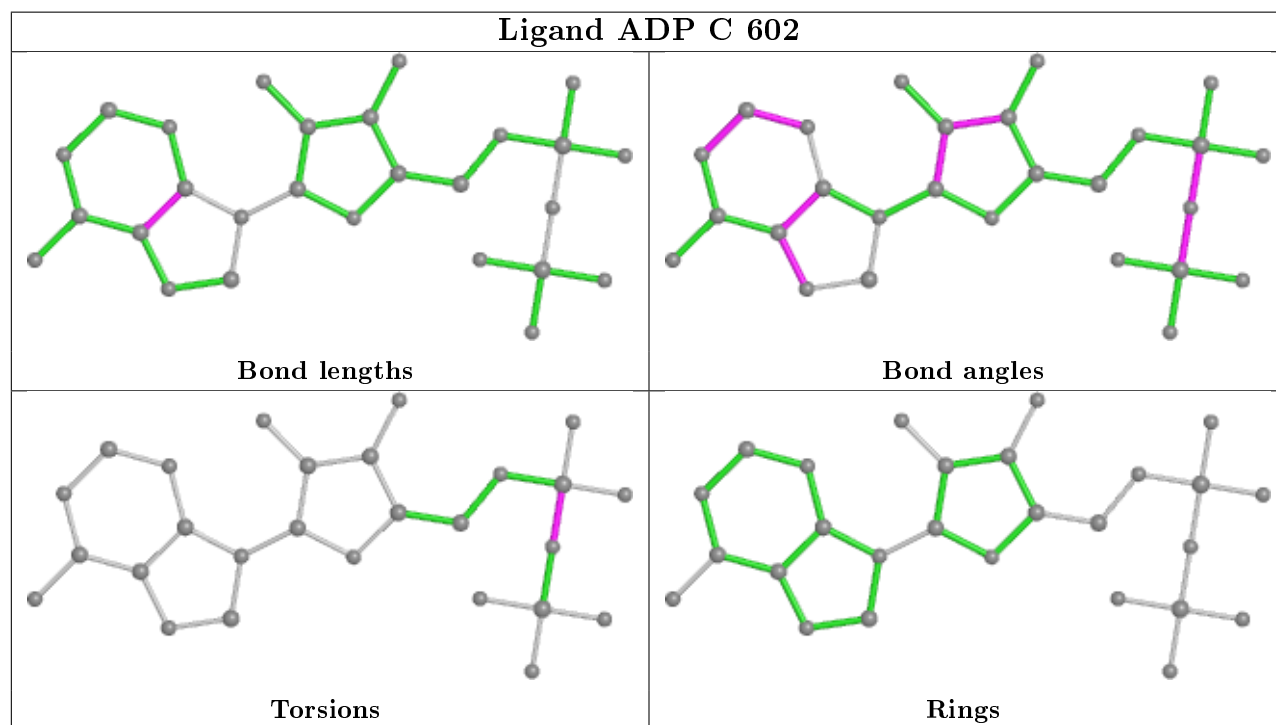
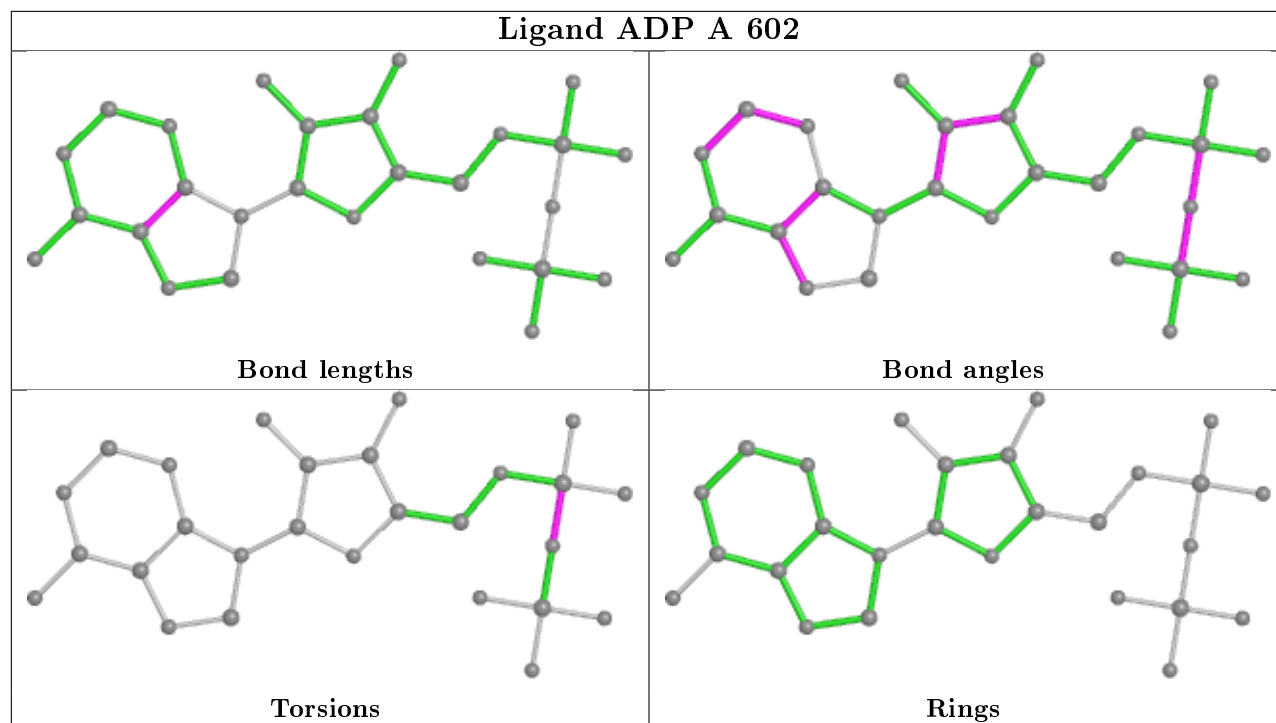
There are no ring outliers.

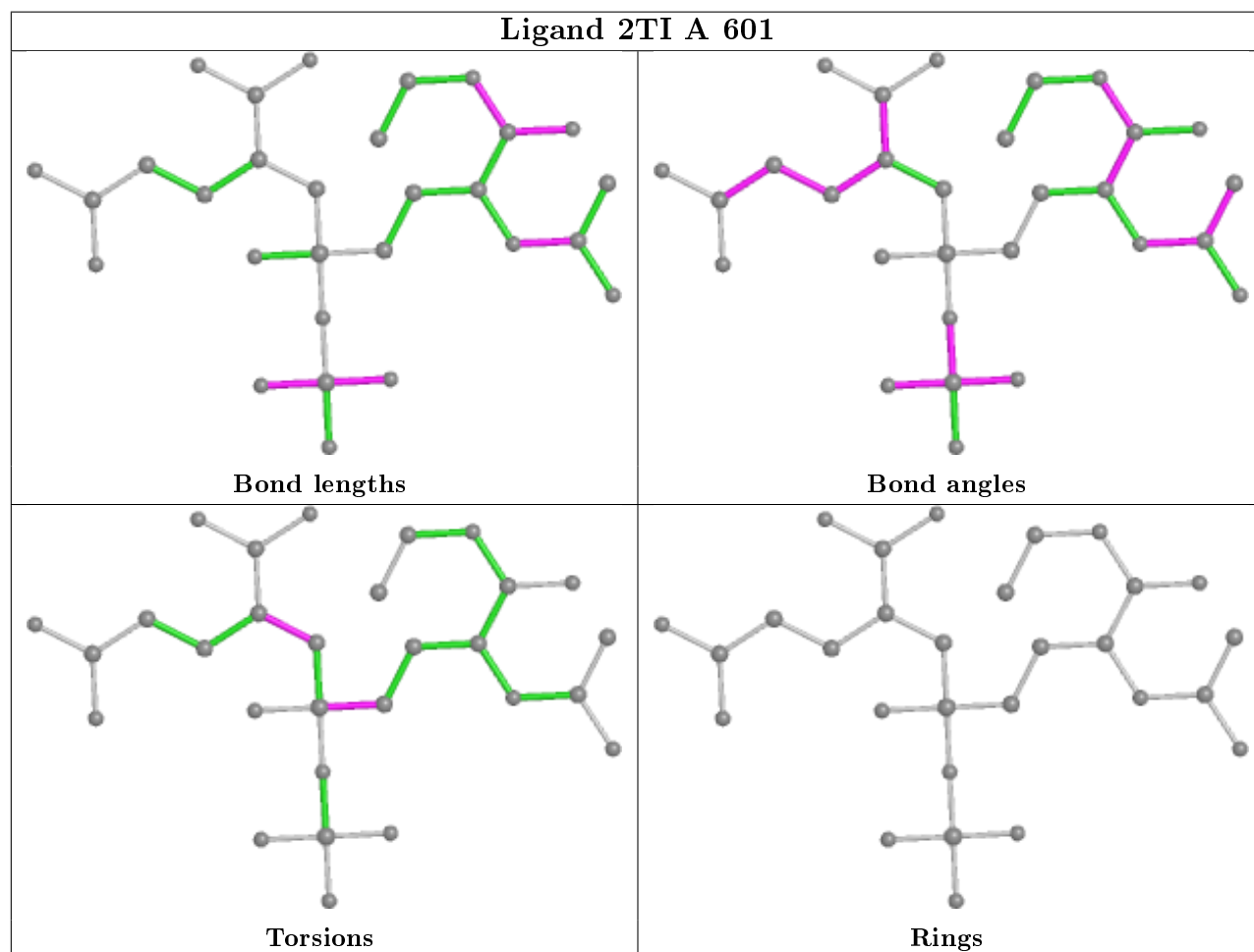
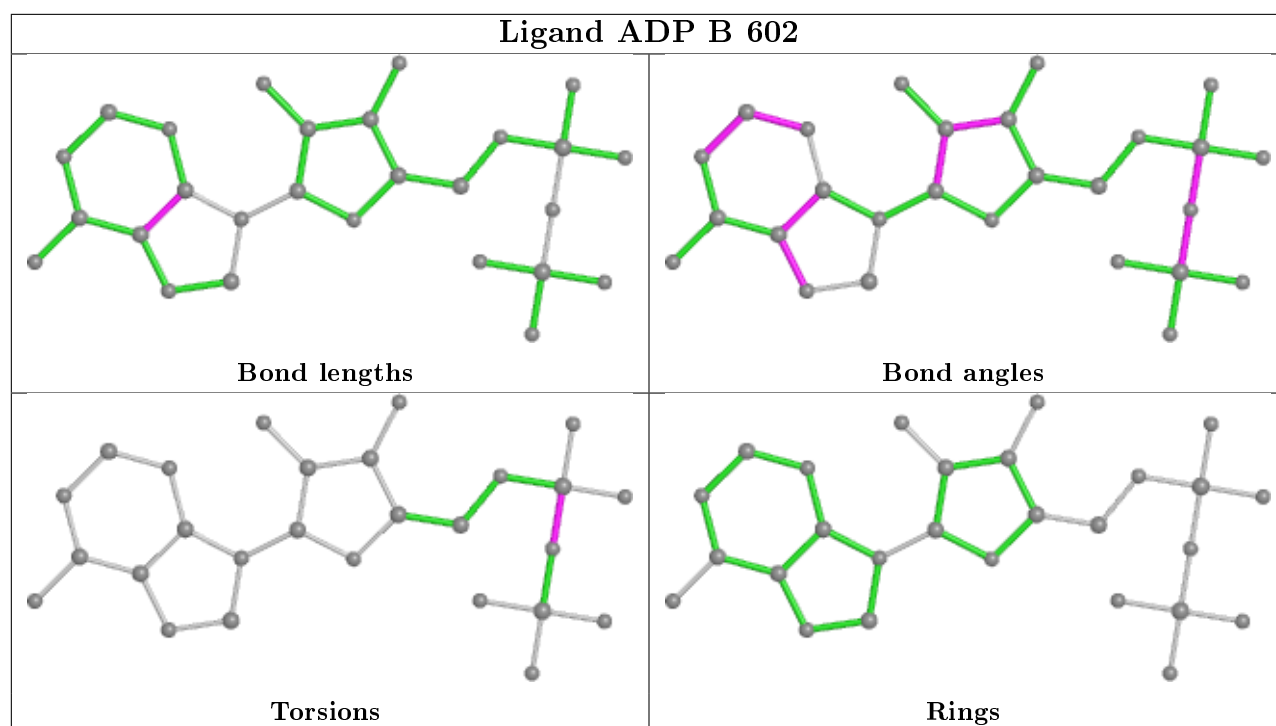
7 monomers are involved in 7 short contacts:

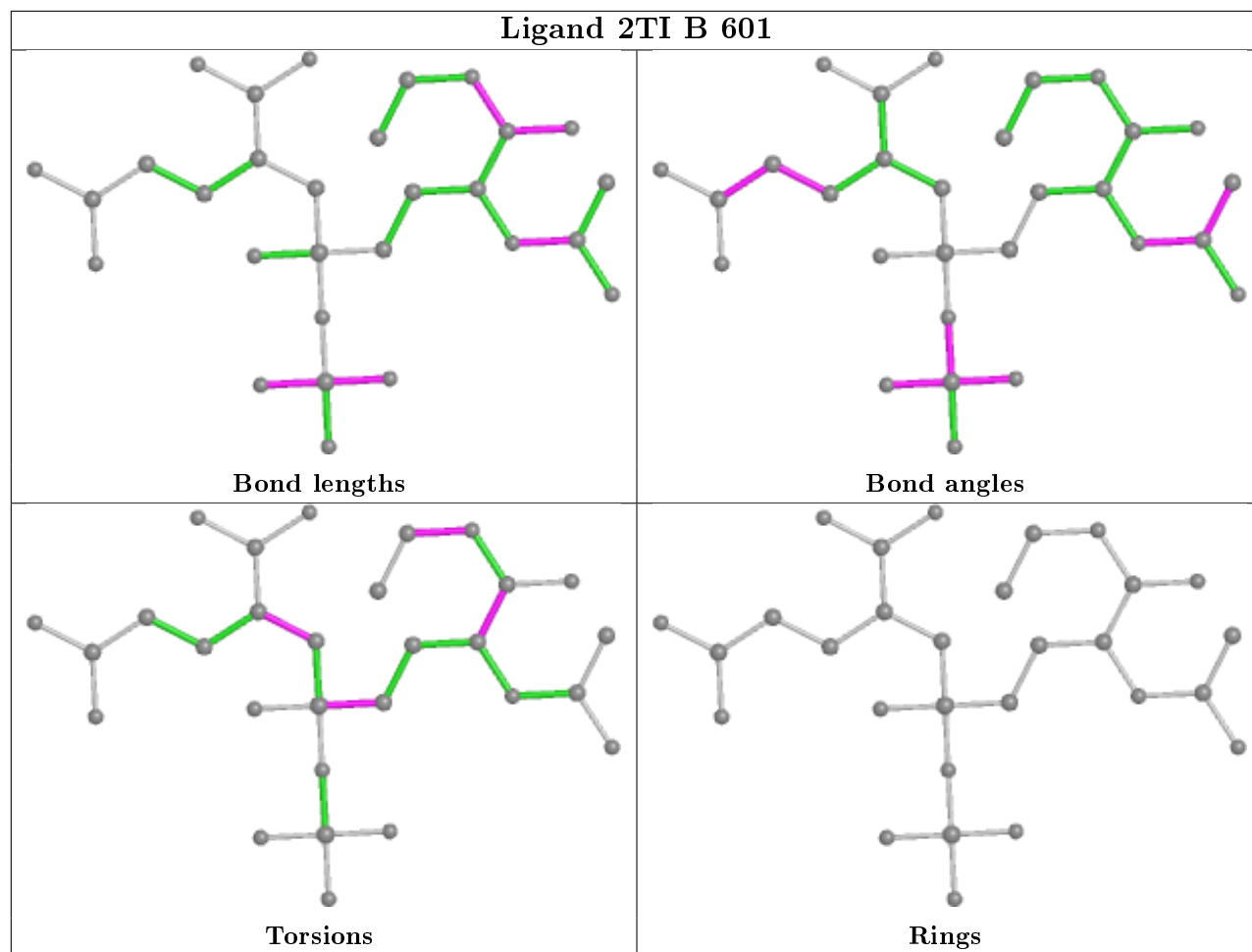
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	603	GOL	1	0
6	B	608	GOL	1	0
6	D	603	GOL	1	0
6	B	605	GOL	1	0
6	C	607	GOL	1	0
4	B	601	2TI	1	0
6	B	609	GOL	2	0

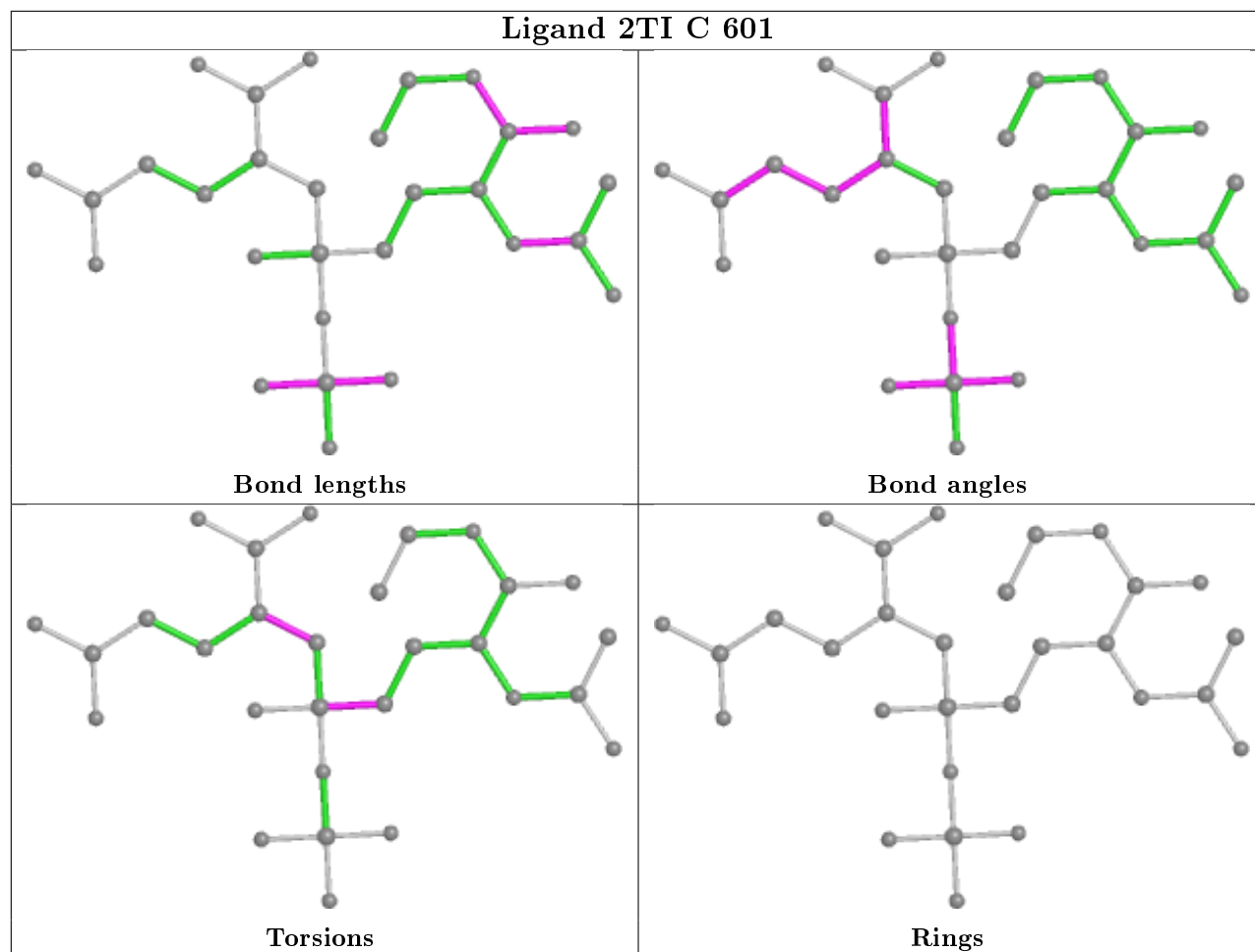
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

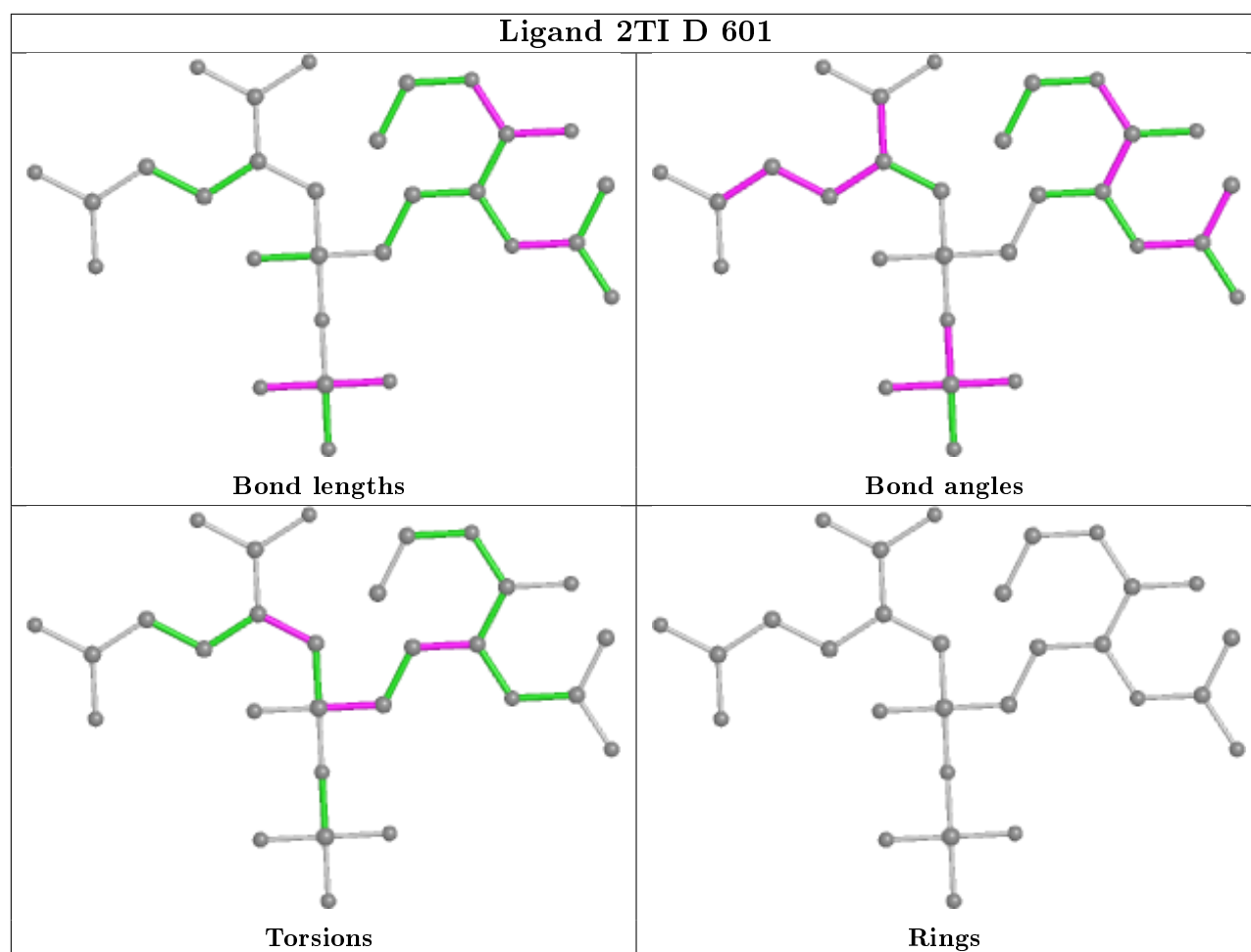












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	400/453 (88%)	-0.04	4 (1%) 82 80	22, 45, 97, 128	0
1	B	402/453 (88%)	0.06	2 (0%) 91 89	33, 58, 95, 130	0
1	C	404/453 (89%)	-0.06	4 (0%) 82 80	24, 46, 93, 120	0
1	D	404/453 (89%)	0.04	3 (0%) 87 86	35, 58, 103, 136	0
2	F	0/12	-	-	-	-
3	G	0/11	-	-	-	-
All	All	1610/1835 (87%)	-0.00	13 (0%) 86 84	22, 52, 98, 136	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	LEU	4.5
1	A	409	LEU	3.6
1	C	86	ASP	3.2
1	C	453	LEU	2.8
1	B	409	LEU	2.7

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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	B	611	6/6	0.69	0.26	84,88,90,91	0
6	GOL	C	603	6/6	0.70	0.30	69,74,79,80	0
6	GOL	A	609	6/6	0.70	0.25	80,89,89,90	0
6	GOL	B	609	6/6	0.70	0.24	77,82,83,86	0
6	GOL	D	603	6/6	0.73	0.34	56,68,76,79	0
6	GOL	A	603	6/6	0.73	0.34	93,99,100,102	0
6	GOL	B	608	6/6	0.73	0.19	83,90,98,99	0
6	GOL	B	605	6/6	0.74	0.26	60,67,76,78	0
6	GOL	C	607	6/6	0.76	0.39	63,64,65,69	0
6	GOL	B	603	6/6	0.78	0.19	82,84,89,89	0
6	GOL	B	610	6/6	0.79	0.23	80,84,90,93	0
6	GOL	C	613	6/6	0.81	0.30	68,75,82,85	0
6	GOL	A	606	6/6	0.81	0.30	79,83,85,88	0
6	GOL	A	604	6/6	0.82	0.22	45,54,62,63	0
6	GOL	C	606	6/6	0.82	0.32	75,88,90,91	0
6	GOL	C	604	6/6	0.85	0.20	43,61,64,66	0
6	GOL	C	610	6/6	0.85	0.23	39,63,68,69	0
6	GOL	A	612	6/6	0.86	0.15	85,87,90,93	0
6	GOL	C	611	6/6	0.87	0.24	54,58,62,64	0
6	GOL	A	608	6/6	0.88	0.18	45,49,51,60	0
6	GOL	A	607	6/6	0.88	0.33	48,55,59,59	0
6	GOL	B	604	6/6	0.88	0.17	58,69,73,73	0
7	MG	C	609	1/1	0.89	0.12	35,35,35,35	0
6	GOL	A	605	6/6	0.89	0.36	32,59,62,64	0
6	GOL	C	605	6/6	0.89	0.33	64,73,76,80	0
6	GOL	D	606	6/6	0.89	0.20	54,59,65,74	0
6	GOL	C	612	6/6	0.90	0.19	67,71,74,75	0
4	2TI	B	601	29/29	0.96	0.18	32,43,59,65	0
7	MG	A	610	1/1	0.96	0.14	26,26,26,26	0
5	ADP	C	602	27/27	0.97	0.17	10,22,33,48	0
5	ADP	B	602	27/27	0.97	0.18	29,40,48,53	0
4	2TI	C	601	29/29	0.97	0.19	13,29,50,61	0
4	2TI	D	601	29/29	0.97	0.19	34,42,59,62	0
7	MG	A	611	1/1	0.98	0.11	35,35,35,35	0
7	MG	B	607	1/1	0.98	0.18	48,48,48,48	0
5	ADP	D	602	27/27	0.98	0.14	30,39,46,55	0
4	2TI	A	601	29/29	0.98	0.18	16,29,50,60	0
7	MG	B	606	1/1	0.98	0.06	42,42,42,42	0
5	ADP	A	602	27/27	0.98	0.16	10,25,35,42	0
7	MG	C	608	1/1	0.98	0.11	24,24,24,24	0
7	MG	D	604	1/1	0.99	0.10	38,38,38,38	0

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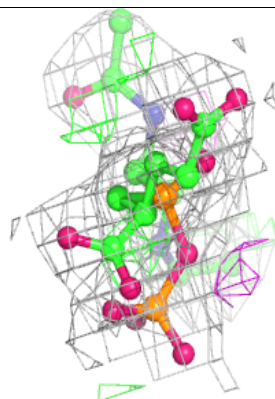
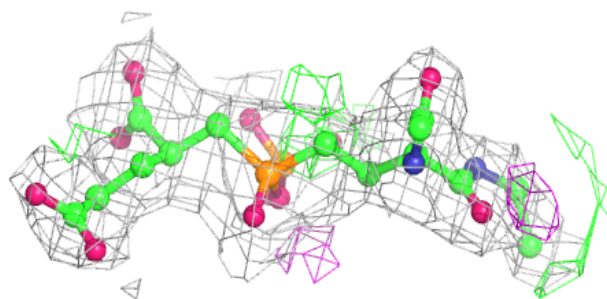
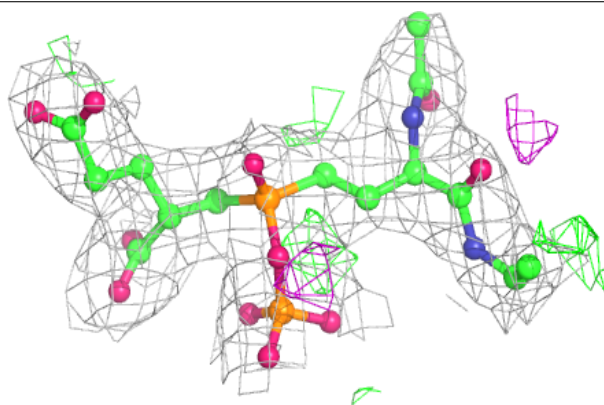
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	D	605	1/1	0.99	0.18	37,37,37,37	0

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.

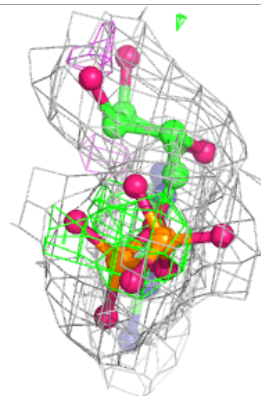
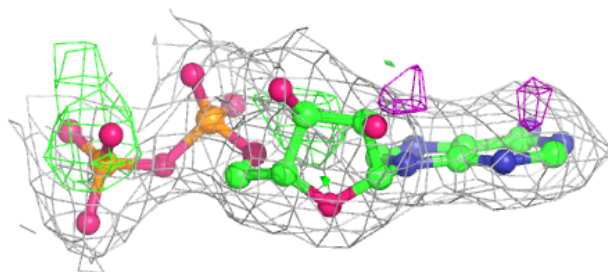
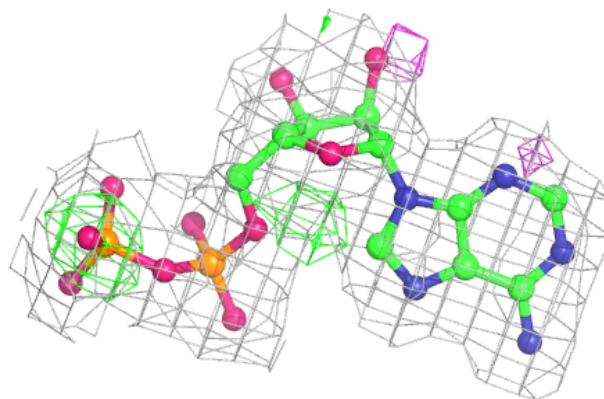
Electron density around 2TI B 601:

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

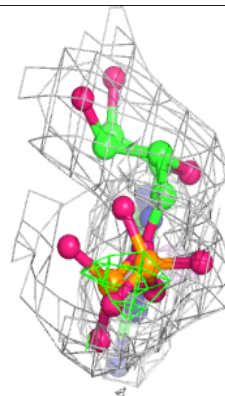
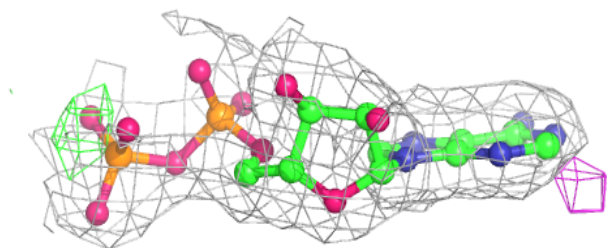
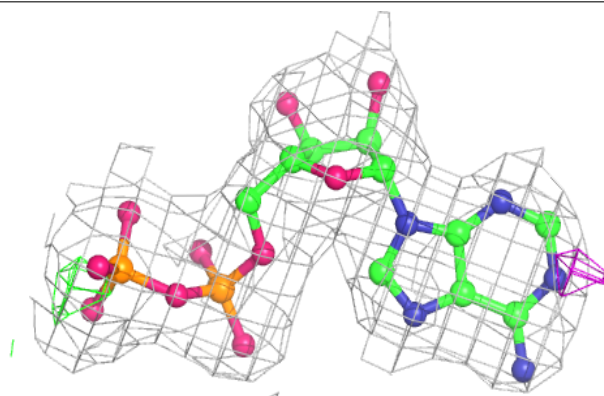


Electron density around ADP C 602:

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

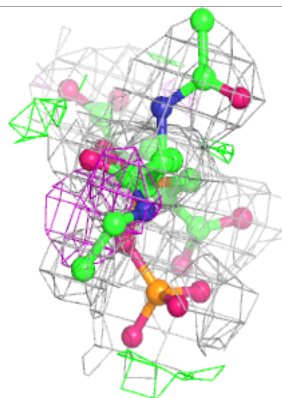
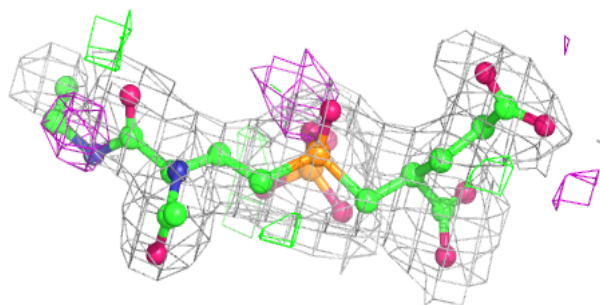
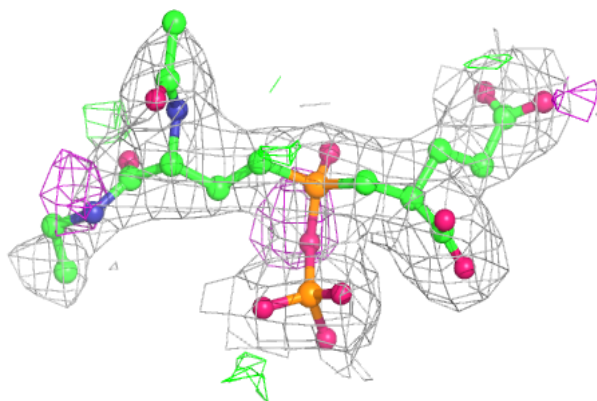
**Electron density around ADP B 602:**

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

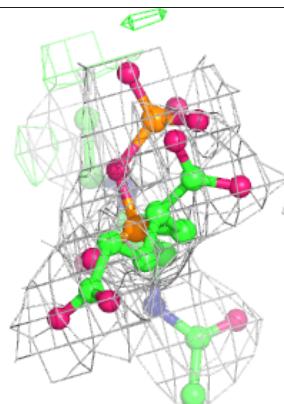
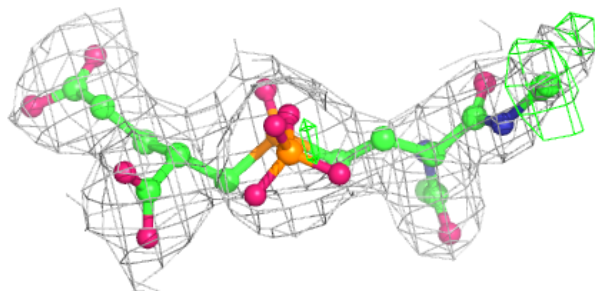
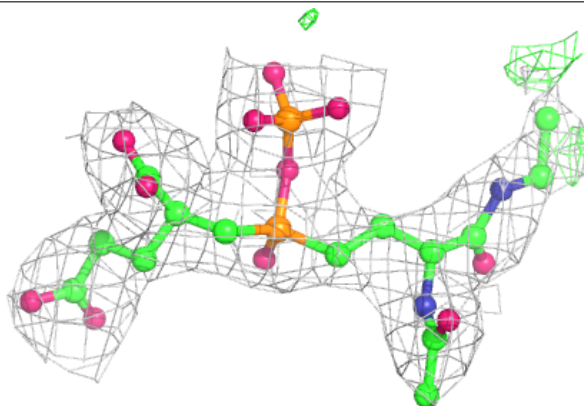


Electron density around 2TI C 601:

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

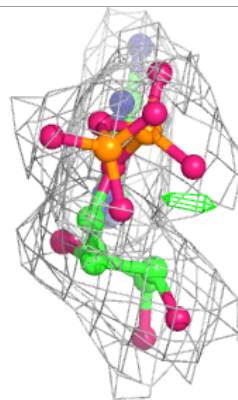
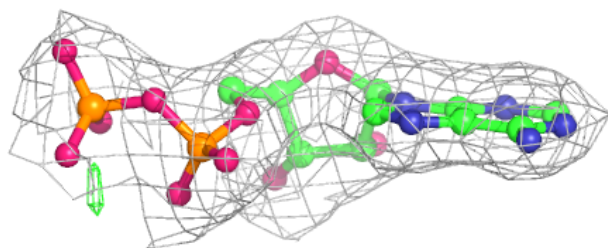
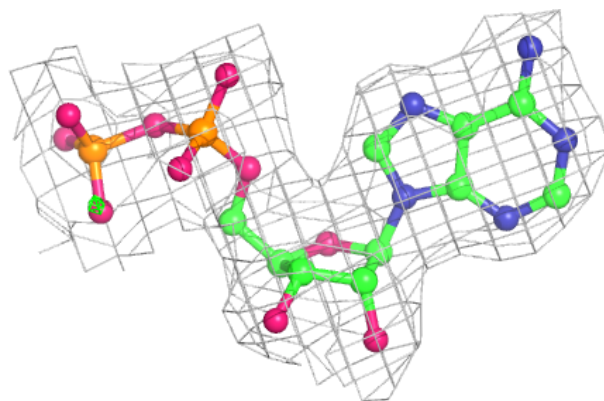
**Electron density around 2TI D 601:**

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

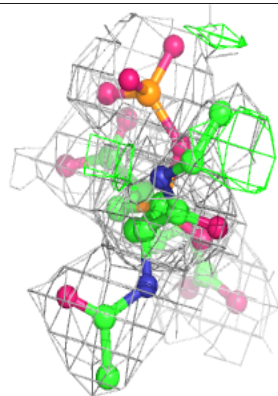
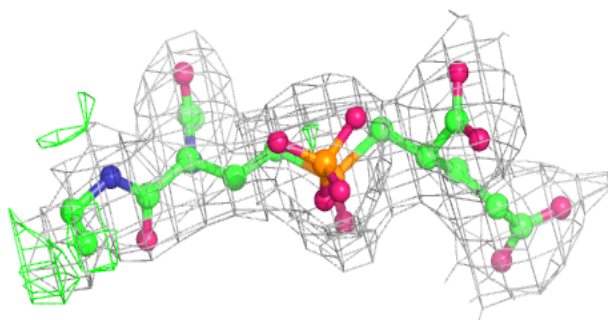
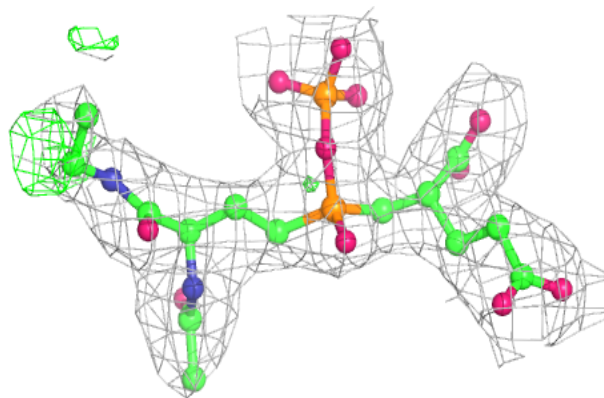


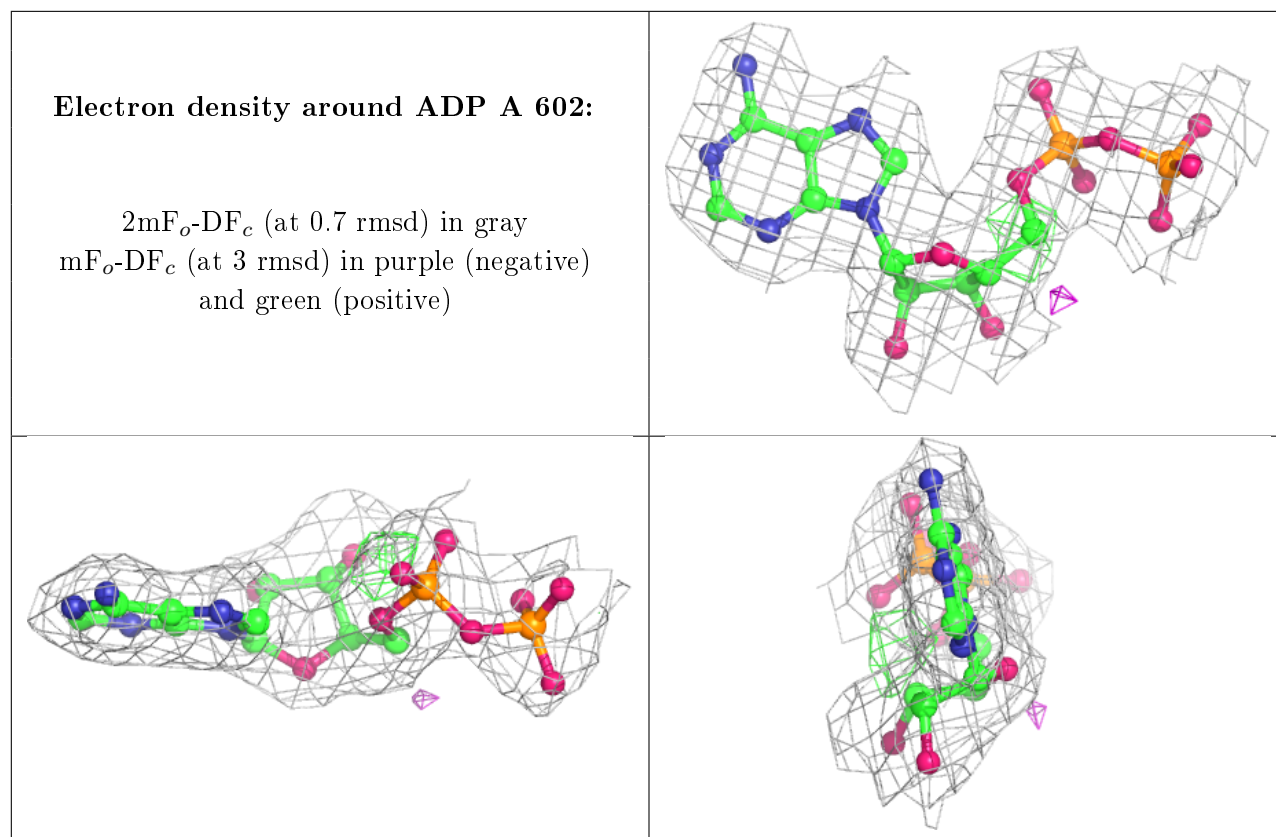
Electron density around ADP D 602:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.