



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:09 PM BST

PDB ID : 6VZV
Title : TTLL6 bound to gamma-elongation 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 : 2.33 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

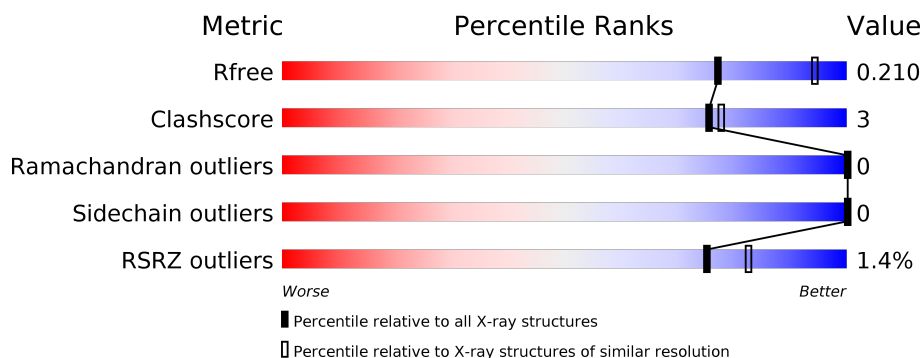
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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>2%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>11%</div> </div> </div>
1	B	453	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
1	C	453	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>11%</div> </div> </div>
1	D	453	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>11%</div> </div> </div>
2	I	15	<div> <div></div> <div>100%</div> </div>
3	J	16	<div> <div></div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	S37	D	612	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14100 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	404	Total	C	N	O	S	0	4	0
			3204	2047	548	588	21			
1	B	404	Total	C	N	O	S	0	4	0
			3239	2071	560	588	20			
1	C	405	Total	C	N	O	S	0	4	0
			3218	2054	555	586	23			
1	D	403	Total	C	N	O	S	0	5	0
			3226	2059	559	586	22			

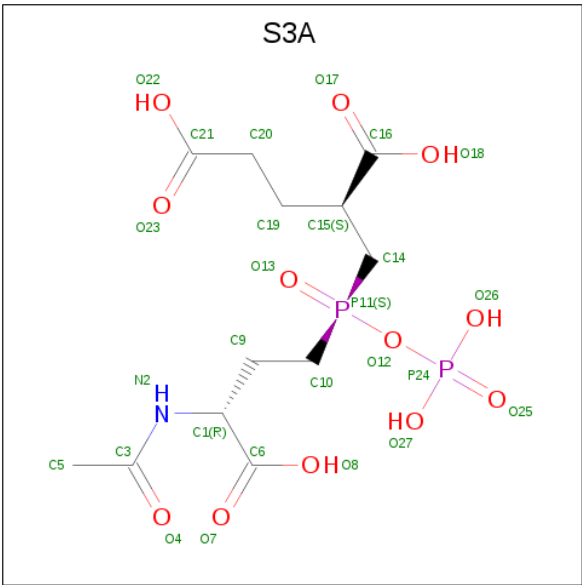
- Molecule 2 is a protein called TTLL6 unregistered chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	15	Total	C	N	O	0	0	0
			75	45	15	15			

- Molecule 3 is a protein called TTLL6 unregistered chain.

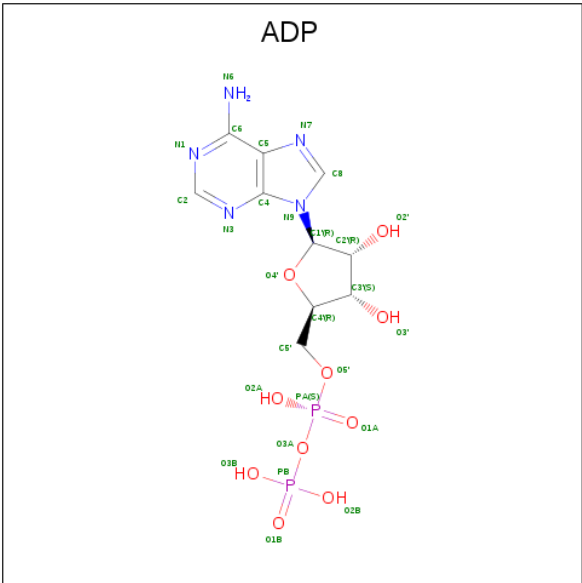
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	16	Total	C	N	O	0	0	0
			80	48	16	16			

- Molecule 4 is (2 {S})-2-[[[(3 {R})-3-acetamido-4-oxidanyl-4-oxidanylidene-butyl]-p
hosphonooxy-phosphoryl]methyl]pentanedioic acid (three-letter code: S3A) (formula:
C₁₂H₂₁NO₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	12	1	12	2		
4	B	1	Total	C	N	O	P	0	0
			27	12	1	12	2		
4	C	1	Total	C	N	O	P	0	0
			27	12	1	12	2		
4	D	1	Total	C	N	O	P	0	0
			27	12	1	12	2		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

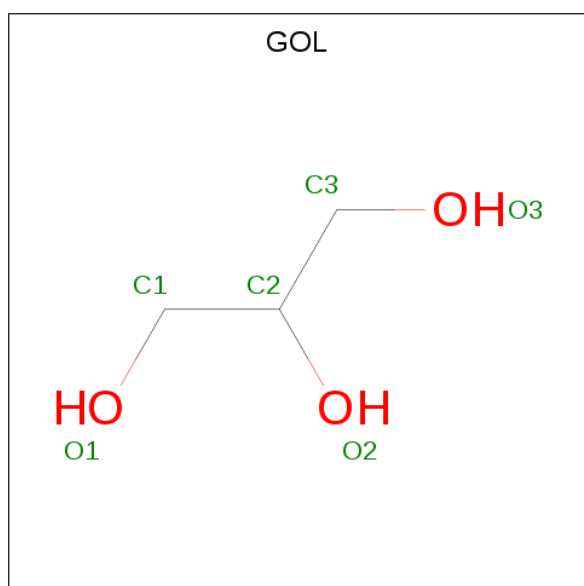


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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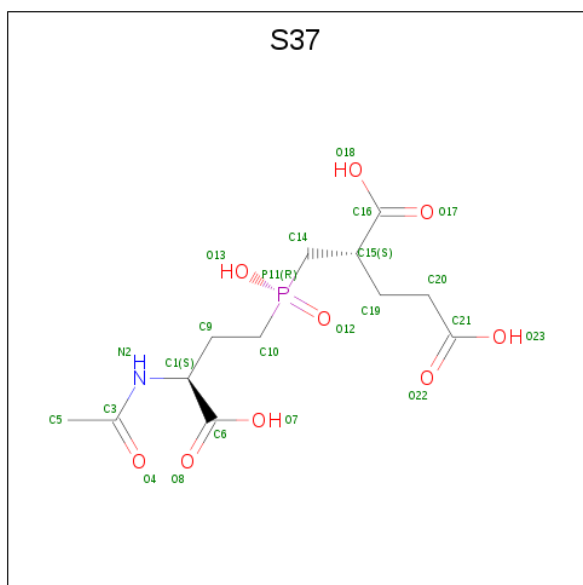
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total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

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

- Molecule 8 is (2 {S})-2-[[[(3 {S})-3-acetamido-4-oxidanyl-4-oxidanylidene-butyl]-oxidanyl-phosphoryl]methyl]pentanedioic acid (three-letter code: S37) (formula: C₁₂H₂₀NO₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			23	12	1	9	1		
8	D	1	Total	C	N	O	P	0	0
			23	12	1	9	1		

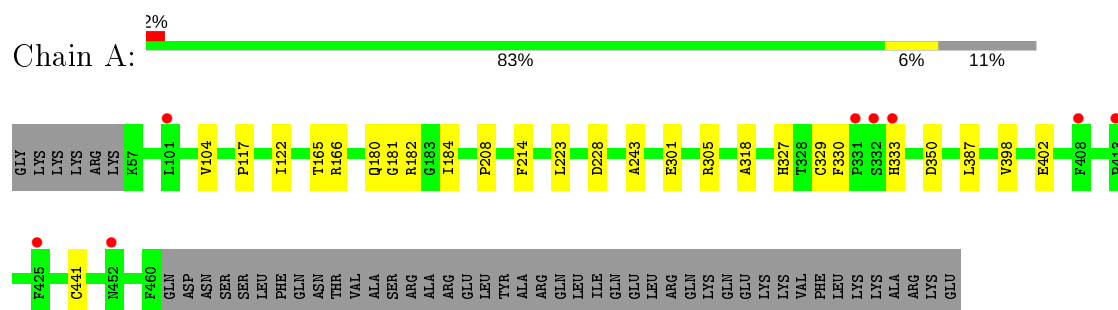
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	140	Total 140	O 140	0	0
9	B	155	Total 155	O 155	0	0
9	C	145	Total 145	O 145	0	0
9	D	156	Total 156	O 156	0	0

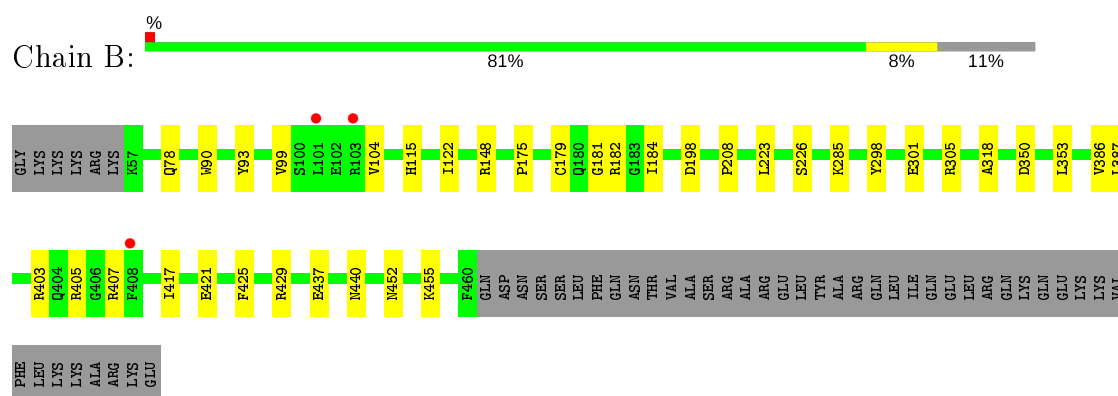
3 Residue-property plots

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.

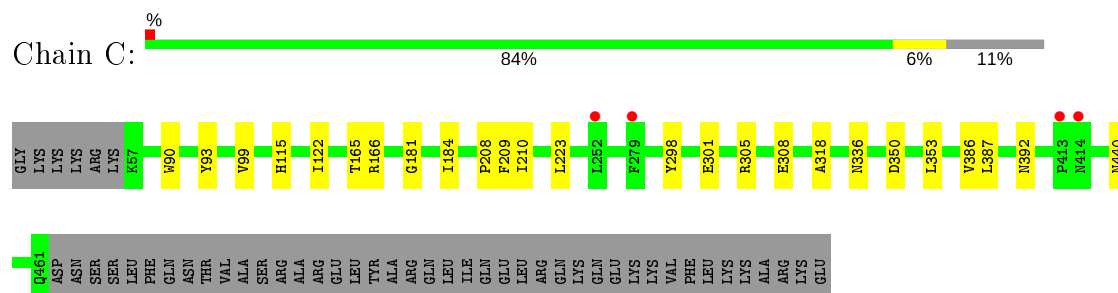
- Molecule 1: Tubulin polyglutamylase TTL6



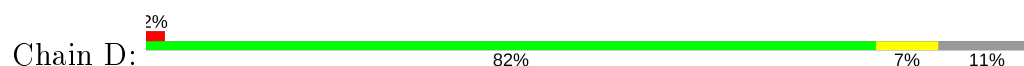
- Molecule 1: Tubulin polyglutamylase TTLL6

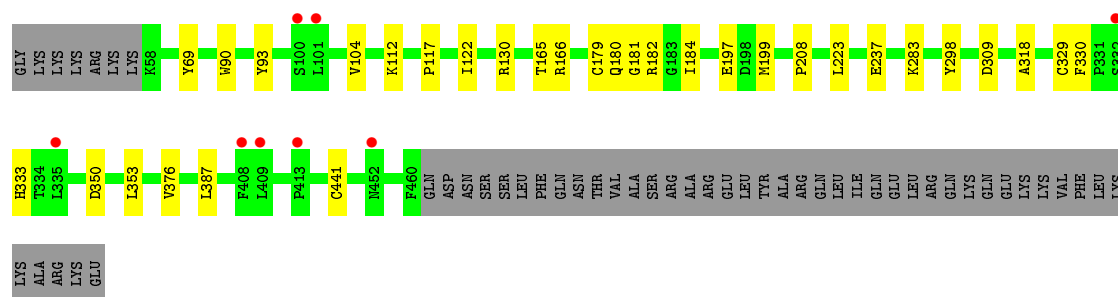


- Molecule 1: Tubulin polyglutamylase TTL6



- Molecule 1: Tubulin polyglutamylase TTLL6





- Molecule 2: TTLL6 unregistered chain

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: TTLL6 unregistered chain

Chain J:  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	75.07Å 109.72Å 173.03Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	45.84 – 2.33 45.84 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.84-2.33) 97.8 (45.84-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.182 , 0.211 0.181 , 0.210	Depositor DCC
R_{free} test set	5968 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.380 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14100	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 39.75 % 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 3.0320e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, S3A, S37, 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	0.25	0/3288	0.42	0/4457
1	B	0.25	0/3324	0.42	0/4498
1	C	0.25	0/3299	0.42	0/4470
1	D	0.25	0/3310	0.42	0/4480
All	All	0.25	0/13221	0.42	0/17905

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	3204	0	3013	17	0
1	B	3239	0	3094	23	0
1	C	3218	0	3042	17	0
1	D	3226	0	3063	24	0
2	I	75	0	17	0	0
3	J	80	0	18	0	0
4	A	27	0	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	27	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	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	A	66	0	88	3	0
7	B	48	0	64	2	0
7	C	36	0	48	5	0
7	D	42	0	56	4	0
8	A	23	0	0	0	0
8	D	23	0	0	0	0
9	A	140	0	0	0	0
9	B	155	0	0	2	0
9	C	145	0	0	0	0
9	D	156	0	0	3	0
All	All	14100	0	12551	81	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 (81) 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:C:210:ILE:H	7:C:610:GOL:H12	1.54	0.72
1:D:208:PRO:HA	1:D:350:ASP:HA	1.80	0.63
1:B:208:PRO:HA	1:B:350:ASP:HA	1.84	0.60
1:C:208:PRO:HA	1:C:350:ASP:HA	1.84	0.59
1:D:69:TYR:HA	7:D:606:GOL:H12	1.86	0.58
1:D:180:GLN:OE1	1:D:182[B]:ARG:NH2	2.37	0.58
1:A:104:VAL:HG21	1:A:117:PRO:HG3	1.86	0.58
1:D:104:VAL:HG21	1:D:117:PRO:HG3	1.87	0.57
1:B:175:PRO:HB3	7:D:609:GOL:H2	1.86	0.57
1:D:130[A]:ARG:NH2	9:D:703:HOH:O	2.38	0.57
1:A:208:PRO:HA	1:A:350:ASP:HA	1.87	0.55
1:B:285:LYS:HD2	7:B:611:GOL:H2	1.88	0.54
1:D:104:VAL:HG12	1:D:329:CYS:HB3	1.90	0.54
1:A:223:LEU:HD23	1:A:387:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASP:OD2	1:A:327:HIS:NE2	2.26	0.54
1:A:330:PHE:HB3	1:A:333:HIS:HB2	1.90	0.54
1:D:181:GLY:HA2	1:D:184:ILE:HD12	1.89	0.53
1:A:180:GLN:OE1	1:A:182:ARG:NH2	2.42	0.53
1:C:336:ASN:OD1	1:C:392:ASN:ND2	2.34	0.53
1:A:301:GLU:OE2	7:A:607:GOL:H31	2.08	0.53
1:B:99:VAL:HG13	1:B:115:HIS:HB2	1.89	0.53
1:D:330:PHE:HB3	1:D:333:HIS:HB2	1.90	0.53
1:D:298:TYR:CD1	1:D:353:LEU:HD11	2.44	0.53
1:D:197:GLU:OE2	1:D:199:MET:HE3	2.08	0.52
1:A:104:VAL:HG13	1:A:330:PHE:CZ	2.45	0.52
1:C:165:THR:OG1	1:C:166:ARG:NH2	2.41	0.52
1:B:223:LEU:HD23	1:B:387:LEU:HD23	1.92	0.52
1:D:104:VAL:HG13	1:D:330:PHE:CZ	2.44	0.52
1:A:181:GLY:HA2	1:A:184:ILE:HD12	1.92	0.52
1:C:210:ILE:HB	7:C:610:GOL:H31	1.92	0.52
1:B:298:TYR:CD1	1:B:353:LEU:HD11	2.45	0.51
1:B:179:CYS:SG	1:B:182:ARG:NH1	2.84	0.51
1:A:104:VAL:HG12	1:A:329:CYS:HB3	1.92	0.51
1:C:99:VAL:HG13	1:C:115:HIS:HB2	1.92	0.50
1:A:214:PHE:CD2	7:A:611:GOL:H11	2.46	0.50
1:B:122:ILE:HG23	1:B:318:ALA:HB2	1.94	0.50
1:C:223:LEU:HD23	1:C:387:LEU:HD23	1.92	0.50
1:A:165:THR:OG1	1:A:166:ARG:NH2	2.45	0.50
1:C:298:TYR:CD1	1:C:353:LEU:HD11	2.48	0.49
1:D:223:LEU:HD23	1:D:387:LEU:HD23	1.94	0.49
1:D:309:ASP:OD2	7:D:607:GOL:H31	2.14	0.48
1:D:122:ILE:HG23	1:D:318:ALA:HB2	1.95	0.48
1:D:283:LYS:NZ	9:D:702:HOH:O	2.46	0.48
1:D:165:THR:OG1	1:D:166:ARG:NH2	2.46	0.48
1:B:148:ARG:NH2	9:B:708:HOH:O	2.39	0.48
1:D:387:LEU:HD13	1:D:441:CYS:HA	1.95	0.48
1:C:122:ILE:HG23	1:C:318:ALA:HB2	1.97	0.47
1:A:398:VAL:O	1:A:402:GLU:HG2	2.15	0.46
1:C:209:PHE:CE1	7:C:610:GOL:H11	2.50	0.46
1:D:197:GLU:HB3	1:D:199:MET:HE3	1.97	0.46
1:B:181:GLY:HA2	1:B:184:ILE:HD12	1.97	0.46
1:B:452:ASN:O	1:B:455:LYS:HG2	2.16	0.46
1:B:301:GLU:O	1:B:305:ARG:HG2	2.16	0.45
1:A:122:ILE:HG23	1:A:318:ALA:HB2	1.98	0.45
1:C:181:GLY:HA2	1:C:184:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLU:O	1:A:305:ARG:HG2	2.16	0.45
1:D:112:LYS:NZ	9:D:701:HOH:O	2.30	0.44
1:A:243:ALA:O	7:A:611:GOL:O2	2.34	0.44
1:D:298:TYR:HD1	1:D:353:LEU:HD11	1.83	0.44
1:B:417:ILE:O	1:B:421:GLU:HG2	2.18	0.44
1:B:437:GLU:OE1	9:B:701:HOH:O	2.21	0.44
1:A:387:LEU:HD13	1:A:441:CYS:HA	1.99	0.44
1:C:308:GLU:OE2	7:C:609:GOL:O2	2.36	0.43
1:B:198:ASP:O	7:D:609:GOL:O1	2.35	0.43
1:C:301:GLU:O	1:C:305:ARG:HG2	2.18	0.43
1:C:298:TYR:HD1	1:C:353:LEU:HD11	1.83	0.43
1:D:179:CYS:SG	1:D:182[A]:ARG:NH2	2.92	0.42
1:B:386:VAL:HG12	1:B:440:ASN:HB3	2.01	0.42
1:B:90:TRP:CZ3	1:B:93:TYR:HB2	2.54	0.42
1:B:405:ARG:HD2	1:B:425:PHE:CZ	2.54	0.42
1:D:237:GLU:HG3	1:D:376:VAL:HG22	2.02	0.42
1:C:90:TRP:CZ3	1:C:93:TYR:HB2	2.54	0.42
1:D:179:CYS:O	1:D:182[A]:ARG:HG2	2.20	0.42
1:C:301:GLU:OE2	7:C:608:GOL:H11	2.21	0.41
1:B:298:TYR:HD1	1:B:353:LEU:HD11	1.83	0.41
1:D:90:TRP:CZ3	1:D:93:TYR:HB2	2.55	0.41
1:C:386:VAL:HG12	1:C:440:ASN:HB3	2.02	0.40
1:B:226:SER:OG	1:B:429:ARG:NH1	2.55	0.40
1:B:99:VAL:HB	1:B:104:VAL:HG21	2.03	0.40
1:B:78:GLN:OE1	7:B:609:GOL:O1	2.31	0.40
1:B:403:ARG:O	1:B:407:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/453 (90%)	398 (98%)	8 (2%)	0	100	100
1	B	406/453 (90%)	398 (98%)	8 (2%)	0	100	100
1	C	407/453 (90%)	398 (98%)	9 (2%)	0	100	100
1	D	406/453 (90%)	398 (98%)	8 (2%)	0	100	100
All	All	1625/1812 (90%)	1592 (98%)	33 (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	335/416 (80%)	335 (100%)	0	100	100
1	B	341/416 (82%)	341 (100%)	0	100	100
1	C	338/416 (81%)	338 (100%)	0	100	100
1	D	339/416 (82%)	339 (100%)	0	100	100
All	All	1353/1664 (81%)	1353 (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 50 ligands modelled in this entry, 8 are monoatomic - leaving 42 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	$\# Z > 2$
4	S3A	B	601	6	12,26,26	0.48	0	14,37,37	1.06	2 (14%)
7	GOL	A	615	-	5,5,5	0.93	0	5,5,5	0.98	0
7	GOL	B	611	-	5,5,5	0.88	0	5,5,5	1.02	0
7	GOL	C	610	-	5,5,5	0.86	0	5,5,5	0.93	0
7	GOL	B	609	-	5,5,5	0.88	0	5,5,5	1.02	0
7	GOL	B	607	-	5,5,5	0.93	0	5,5,5	1.00	0
7	GOL	C	607	-	5,5,5	0.87	0	5,5,5	1.08	0
7	GOL	A	608	-	5,5,5	0.99	0	5,5,5	1.01	0
7	GOL	A	612	-	5,5,5	0.90	0	5,5,5	1.01	0
7	GOL	C	609	-	5,5,5	0.94	0	5,5,5	0.99	0
7	GOL	B	605	-	5,5,5	0.90	0	5,5,5	0.99	0
7	GOL	A	605	-	5,5,5	0.84	0	5,5,5	1.02	0
7	GOL	C	605	-	5,5,5	0.96	0	5,5,5	1.05	0
8	S37	A	616	-	9,22,22	0.83	1 (11%)	9,30,30	1.39	2 (22%)
7	GOL	A	610	-	5,5,5	1.06	0	5,5,5	0.91	0
5	ADP	D	602	6	24,29,29	1.00	1 (4%)	29,45,45	1.19	3 (10%)
7	GOL	A	613	-	5,5,5	0.92	0	5,5,5	0.94	0
7	GOL	A	614	-	5,5,5	0.90	0	5,5,5	0.98	0
7	GOL	D	608	-	5,5,5	0.88	0	5,5,5	0.95	0
7	GOL	A	607	-	5,5,5	0.91	0	5,5,5	1.06	0
7	GOL	C	608	-	5,5,5	0.87	0	5,5,5	1.01	0
7	GOL	B	610	-	5,5,5	0.91	0	5,5,5	0.99	0
4	S3A	C	601	6	12,26,26	0.48	0	14,37,37	0.98	2 (14%)
5	ADP	B	602	6	24,29,29	0.98	1 (4%)	29,45,45	1.19	3 (10%)
7	GOL	D	606	-	5,5,5	0.91	0	5,5,5	1.06	1 (20%)
4	S3A	A	601	6	12,26,26	0.47	0	14,37,37	1.09	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	S37	D	612	-	9,22,22	0.78	1 (11%)	9,30,30	1.33	2 (22%)
7	GOL	C	606	-	5,5,5	0.94	0	5,5,5	0.98	0
5	ADP	C	602	6	24,29,29	0.99	1 (4%)	29,45,45	1.17	3 (10%)
7	GOL	B	612	-	5,5,5	0.94	0	5,5,5	0.99	0
7	GOL	A	611	-	5,5,5	0.97	0	5,5,5	1.00	0
7	GOL	D	607	-	5,5,5	0.92	0	5,5,5	0.99	0
7	GOL	B	608	-	5,5,5	1.06	0	5,5,5	0.90	0
7	GOL	D	611	-	5,5,5	0.93	0	5,5,5	0.94	0
7	GOL	A	609	-	5,5,5	0.92	0	5,5,5	0.97	0
7	GOL	D	605	-	5,5,5	0.90	0	5,5,5	1.00	0
4	S3A	D	601	6	12,26,26	0.49	0	14,37,37	0.98	1 (7%)
7	GOL	D	609	-	5,5,5	0.85	0	5,5,5	0.98	0
7	GOL	A	606	-	5,5,5	0.93	0	5,5,5	0.94	0
7	GOL	B	606	-	5,5,5	0.92	0	5,5,5	1.05	0
7	GOL	D	610	-	5,5,5	1.00	0	5,5,5	1.02	0
5	ADP	A	602	6	24,29,29	0.99	1 (4%)	29,45,45	1.18	3 (10%)

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
4	S3A	B	601	6	-	2/20/34/34	-
7	GOL	A	615	-	-	0/4/4/4	-
7	GOL	B	611	-	-	0/4/4/4	-
7	GOL	C	610	-	-	1/4/4/4	-
7	GOL	B	609	-	-	0/4/4/4	-
7	GOL	B	607	-	-	0/4/4/4	-
7	GOL	C	607	-	-	1/4/4/4	-
7	GOL	A	608	-	-	1/4/4/4	-
7	GOL	A	612	-	-	0/4/4/4	-
7	GOL	C	609	-	-	0/4/4/4	-
7	GOL	B	605	-	-	0/4/4/4	-
7	GOL	A	605	-	-	0/4/4/4	-
7	GOL	C	605	-	-	1/4/4/4	-
8	S37	A	616	-	-	9/18/28/28	-
7	GOL	A	610	-	-	0/4/4/4	-
5	ADP	D	602	6	-	3/12/32/32	0/3/3/3
7	GOL	A	613	-	-	0/4/4/4	-
7	GOL	A	614	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	D	608	-	-	0/4/4/4	-
7	GOL	A	607	-	-	0/4/4/4	-
7	GOL	C	608	-	-	0/4/4/4	-
7	GOL	B	610	-	-	0/4/4/4	-
4	S3A	C	601	6	-	2/20/34/34	-
5	ADP	B	602	6	-	5/12/32/32	0/3/3/3
7	GOL	D	606	-	-	0/4/4/4	-
4	S3A	A	601	6	-	2/20/34/34	-
8	S37	D	612	-	-	3/18/28/28	-
7	GOL	C	606	-	-	0/4/4/4	-
5	ADP	C	602	6	-	1/12/32/32	0/3/3/3
7	GOL	B	612	-	-	0/4/4/4	-
7	GOL	A	611	-	-	2/4/4/4	-
7	GOL	D	607	-	-	0/4/4/4	-
7	GOL	B	608	-	-	2/4/4/4	-
7	GOL	D	611	-	-	0/4/4/4	-
7	GOL	A	609	-	-	0/4/4/4	-
7	GOL	D	605	-	-	0/4/4/4	-
4	S3A	D	601	6	-	2/20/34/34	-
7	GOL	D	609	-	-	0/4/4/4	-
7	GOL	A	606	-	-	0/4/4/4	-
7	GOL	B	606	-	-	0/4/4/4	-
7	GOL	D	610	-	-	0/4/4/4	-
5	ADP	A	602	6	-	1/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	602	ADP	C5-C4	2.56	1.47	1.40
5	A	602	ADP	C5-C4	2.54	1.47	1.40
5	C	602	ADP	C5-C4	2.48	1.47	1.40
5	B	602	ADP	C5-C4	2.46	1.47	1.40
8	A	616	S37	P11-C14	2.19	1.81	1.79
8	D	612	S37	P11-C14	2.14	1.81	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	602	ADP	N3-C2-N1	-3.09	123.85	128.68
5	C	602	ADP	N3-C2-N1	-3.06	123.89	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	ADP	N3-C2-N1	-2.92	124.12	128.68
5	D	602	ADP	N3-C2-N1	-2.91	124.14	128.68
8	A	616	S37	P11-C10-C9	-2.91	109.14	114.56
4	A	601	S3A	C19-C20-C21	-2.78	107.60	113.59
4	D	601	S3A	C19-C20-C21	-2.64	107.91	113.59
5	A	602	ADP	C4-C5-N7	-2.53	106.76	109.40
5	D	602	ADP	C4-C5-N7	-2.52	106.77	109.40
4	B	601	S3A	C19-C20-C21	-2.50	108.21	113.59
8	D	612	S37	P11-C10-C9	-2.49	109.91	114.56
5	B	602	ADP	C4-C5-N7	-2.48	106.81	109.40
8	A	616	S37	C19-C15-C16	-2.46	108.86	112.53
5	C	602	ADP	C4-C5-N7	-2.36	106.94	109.40
4	A	601	S3A	C19-C15-C16	-2.31	109.09	112.53
4	B	601	S3A	C19-C15-C16	-2.31	109.10	112.53
4	C	601	S3A	C19-C20-C21	-2.27	108.72	113.59
5	A	602	ADP	C3'-C2'-C1'	2.25	104.37	100.98
5	B	602	ADP	C3'-C2'-C1'	2.24	104.35	100.98
5	C	602	ADP	C3'-C2'-C1'	2.22	104.31	100.98
5	D	602	ADP	C3'-C2'-C1'	2.21	104.31	100.98
8	D	612	S37	C19-C15-C16	-2.20	109.26	112.53
4	C	601	S3A	C19-C15-C16	-2.18	109.28	112.53
7	D	606	GOL	C3-C2-C1	-2.03	103.81	111.70

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	602	ADP	PA-O3A-PB-O2B
8	A	616	S37	C6-C1-C9-C10
8	A	616	S37	C9-C10-P11-O13
8	A	616	S37	C15-C14-P11-O12
5	B	602	ADP	PA-O3A-PB-O2B
5	B	602	ADP	PA-O3A-PB-O3B
8	D	612	S37	C6-C1-C9-C10
8	D	612	S37	N2-C1-C9-C10
8	D	612	S37	C15-C19-C20-C21
8	A	616	S37	C16-C15-C19-C20
8	A	616	S37	C15-C19-C20-C21
8	A	616	S37	C9-C10-P11-C14
8	A	616	S37	N2-C1-C9-C10
7	A	611	GOL	C1-C2-C3-O3
7	B	608	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	A	616	S37	C14-C15-C19-C20
5	D	602	ADP	PB-O3A-PA-O1A
7	C	610	GOL	O1-C1-C2-C3
7	A	608	GOL	O1-C1-C2-C3
7	B	608	GOL	O2-C2-C3-O3
7	A	611	GOL	O2-C2-C3-O3
7	C	607	GOL	O1-C1-C2-O2
4	B	601	S3A	P11-C14-C15-C16
4	C	601	S3A	P11-C14-C15-C16
4	A	601	S3A	P11-C14-C15-C16
4	D	601	S3A	P11-C14-C15-C16
4	B	601	S3A	P11-C14-C15-C19
4	C	601	S3A	P11-C14-C15-C19
4	A	601	S3A	P11-C14-C15-C19
4	D	601	S3A	P11-C14-C15-C19
5	D	602	ADP	PB-O3A-PA-O2A
7	C	605	GOL	O1-C1-C2-O2
5	B	602	ADP	PB-O3A-PA-O1A
5	A	602	ADP	PB-O3A-PA-O1A
5	B	602	ADP	PA-O3A-PB-O1B
5	D	602	ADP	PA-O3A-PB-O2B
5	B	602	ADP	PB-O3A-PA-O2A
8	A	616	S37	C9-C10-P11-O12

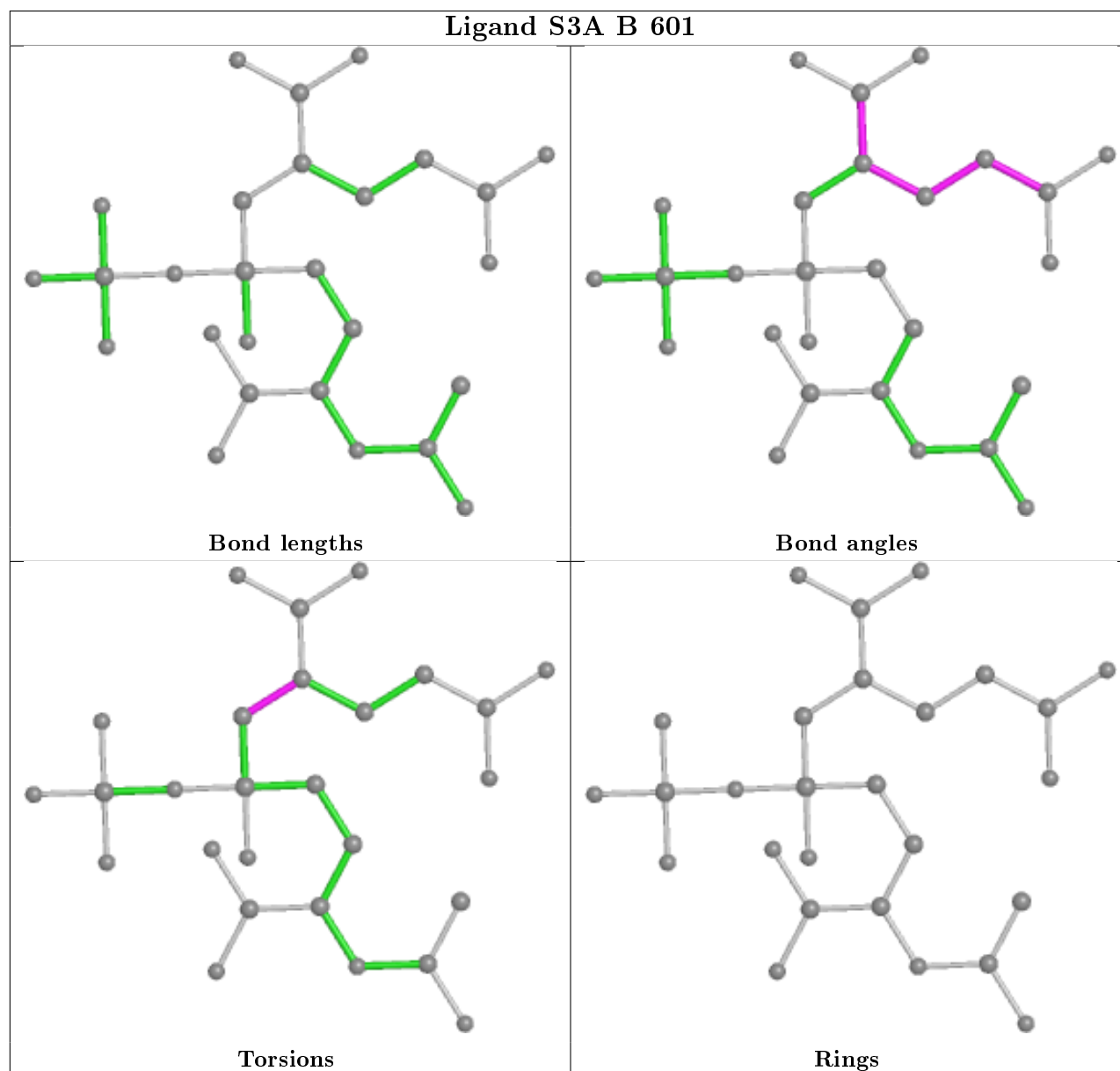
There are no ring outliers.

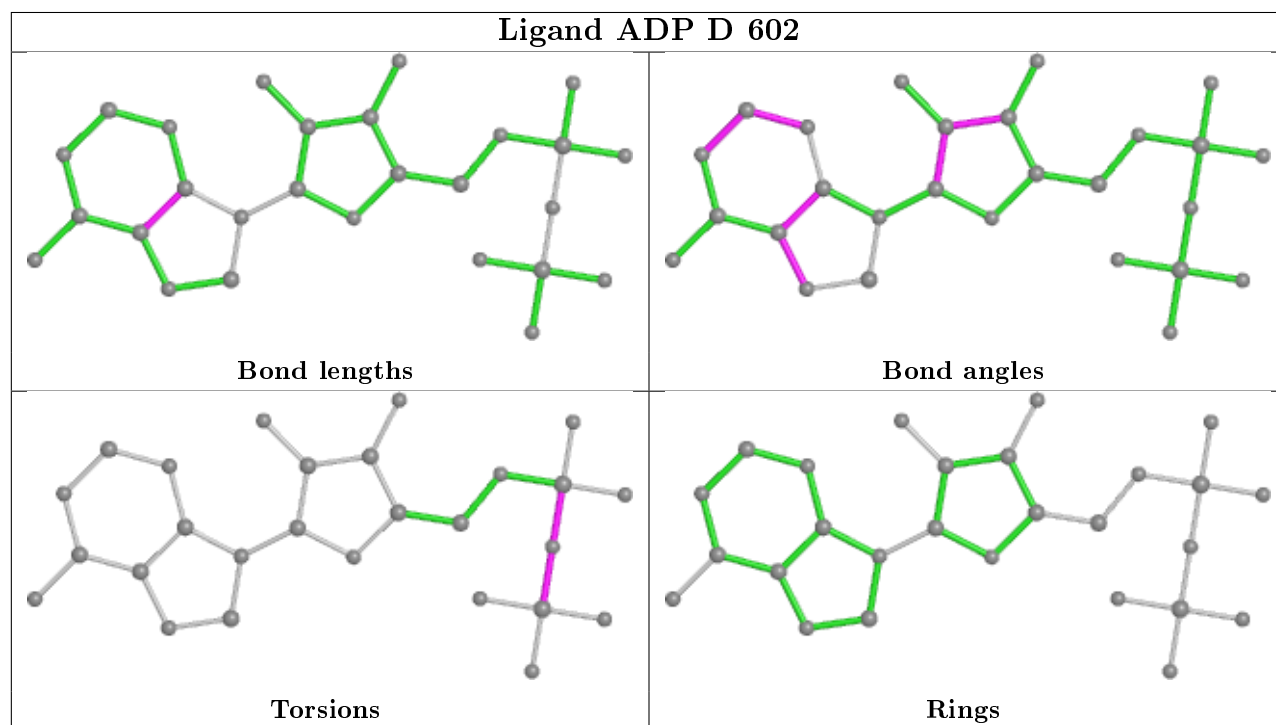
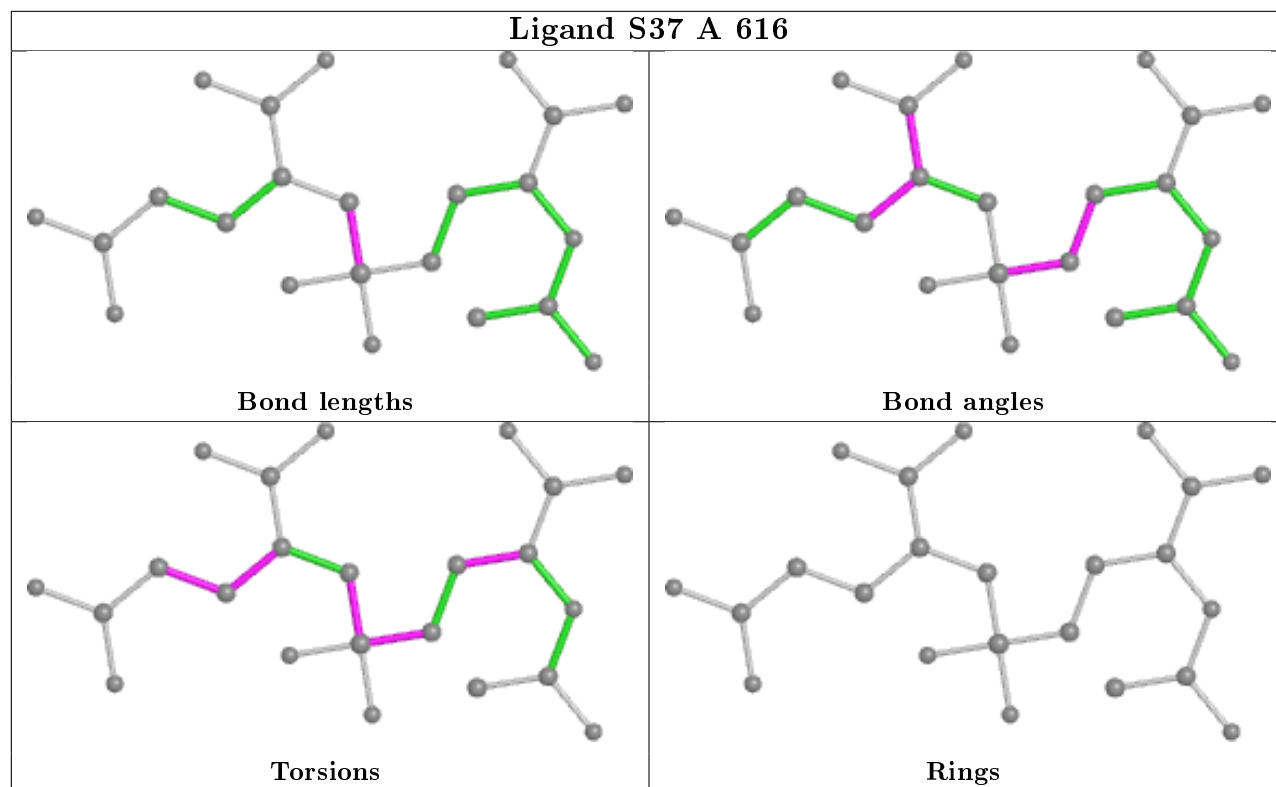
10 monomers are involved in 14 short contacts:

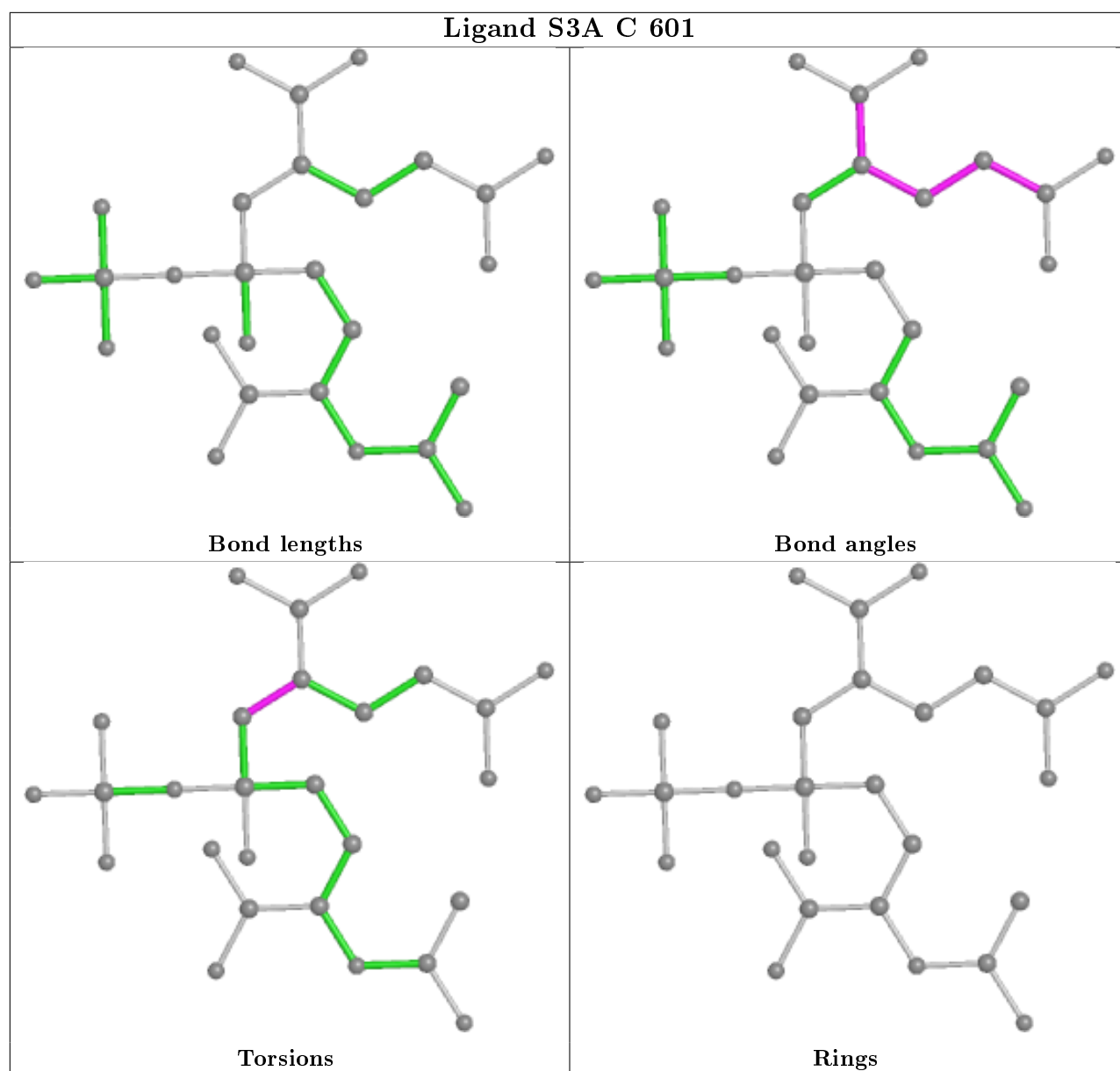
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	611	GOL	1	0
7	C	610	GOL	3	0
7	B	609	GOL	1	0
7	C	609	GOL	1	0
7	A	607	GOL	1	0
7	C	608	GOL	1	0
7	D	606	GOL	1	0
7	A	611	GOL	2	0
7	D	607	GOL	1	0
7	D	609	GOL	2	0

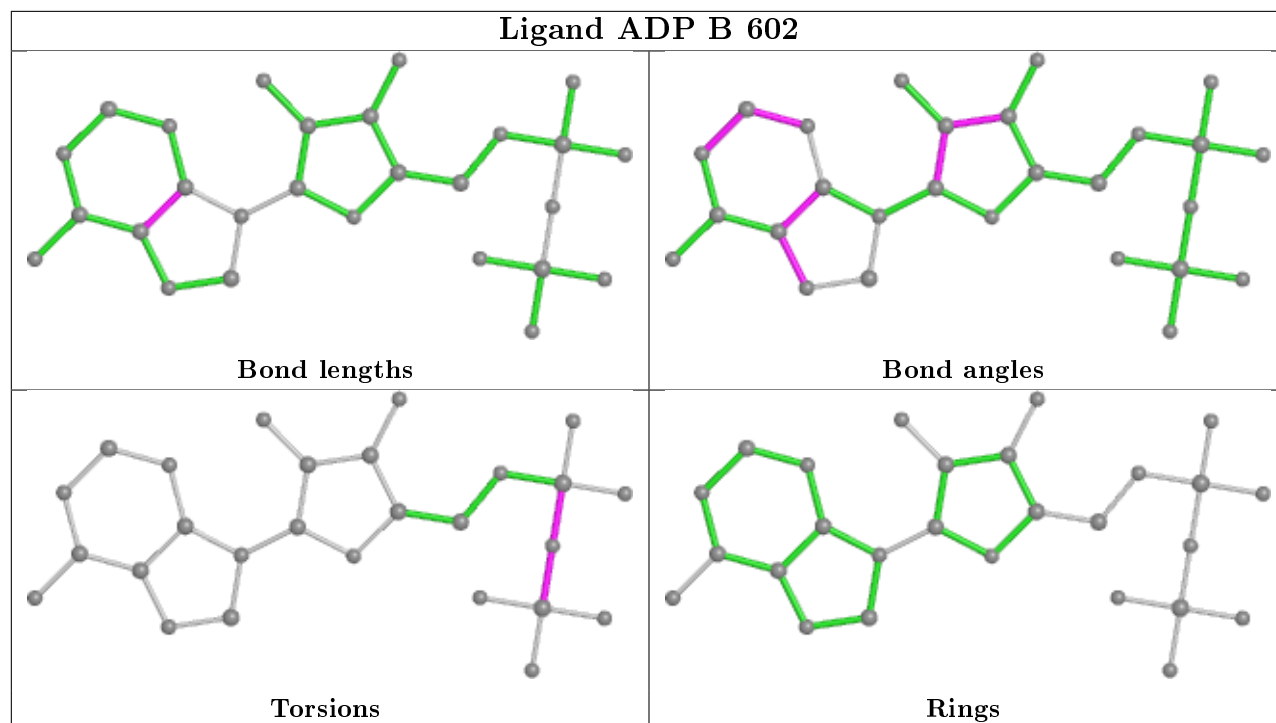
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

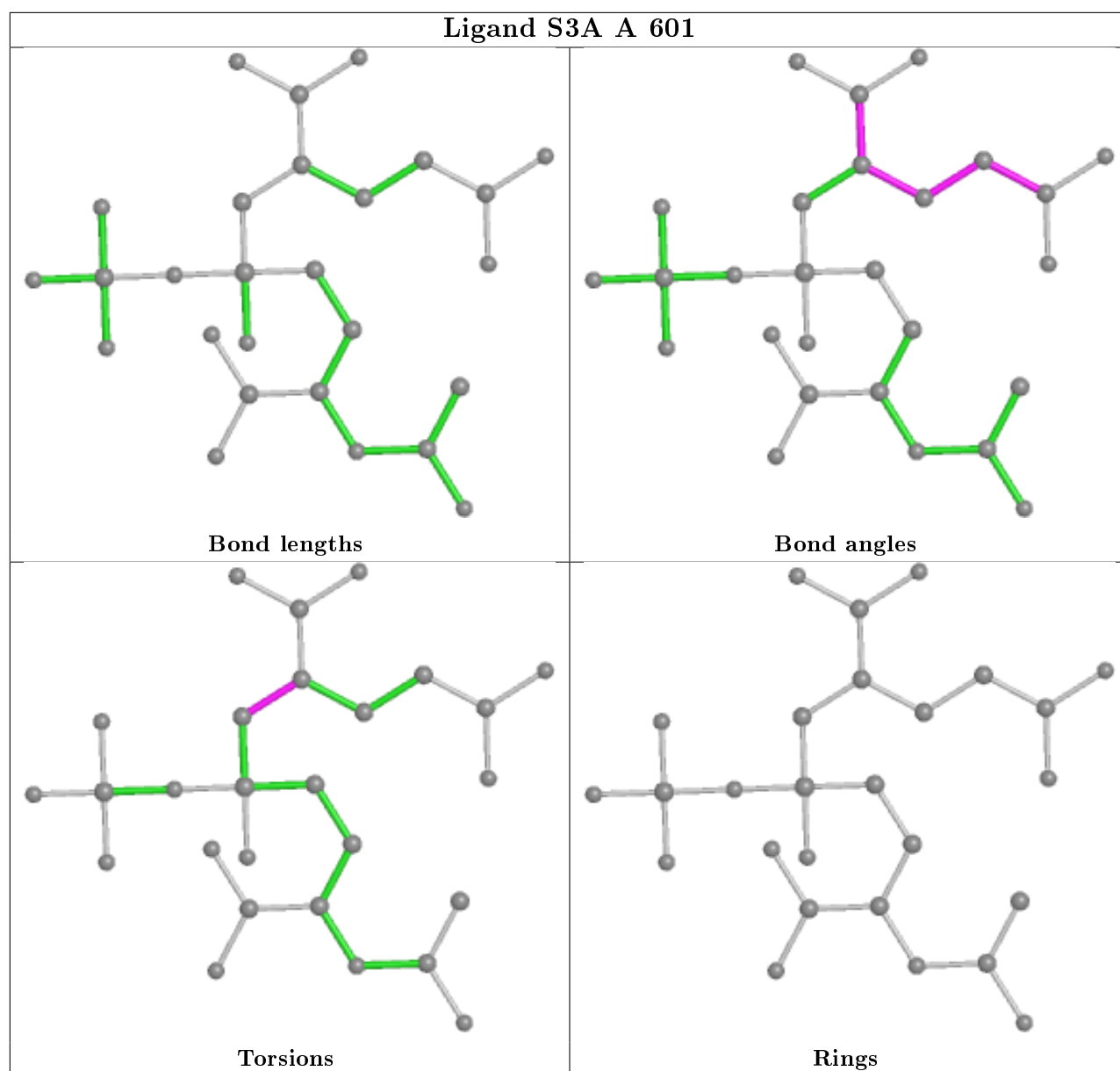
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

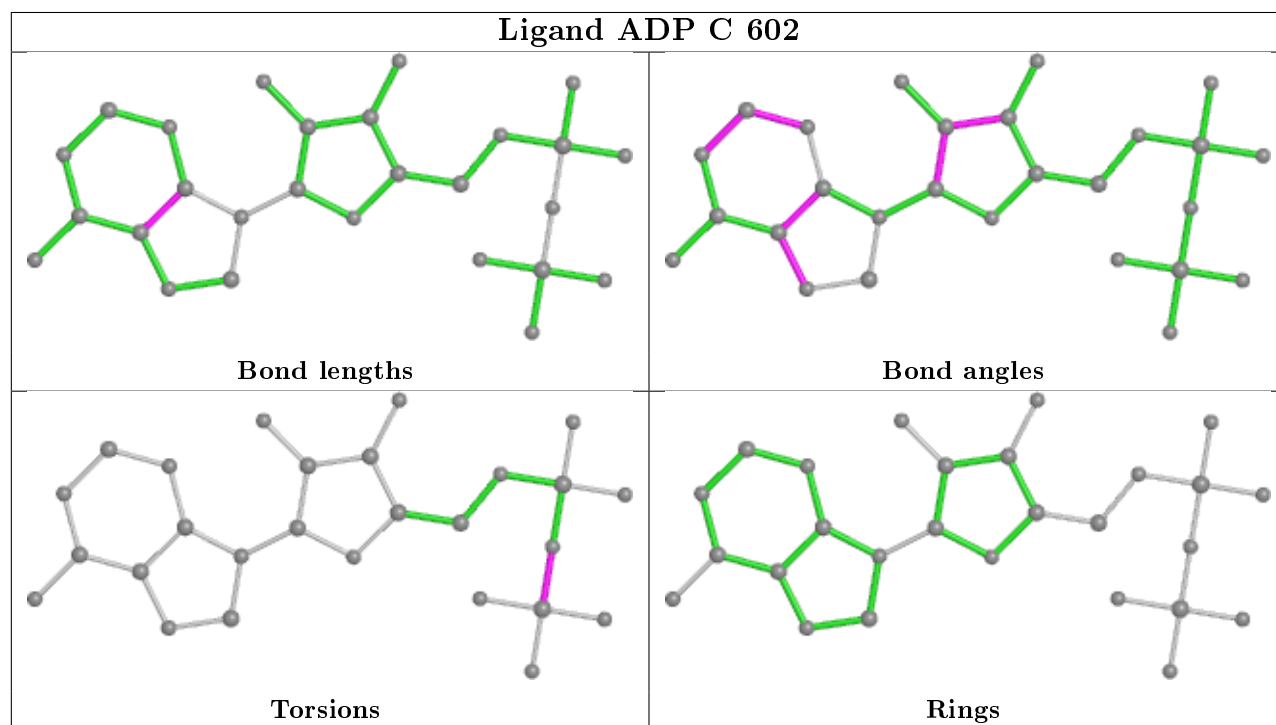
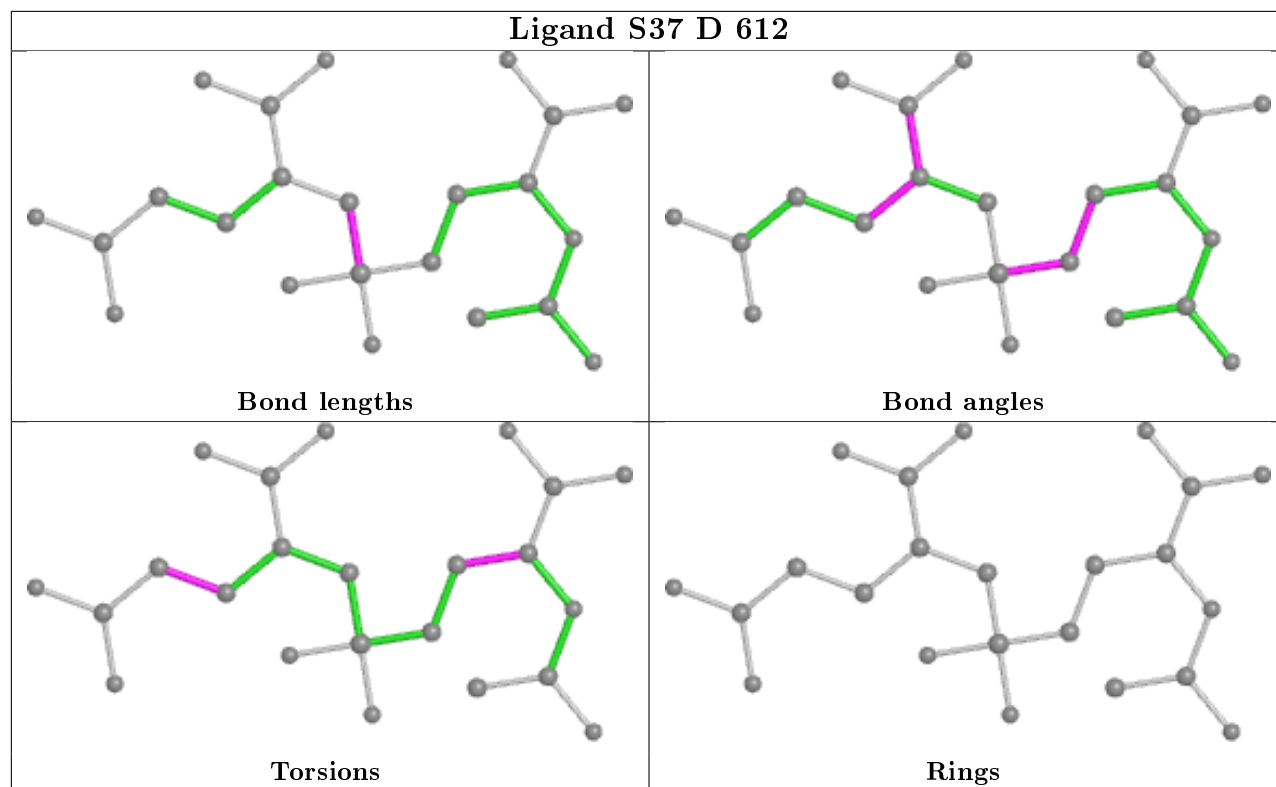


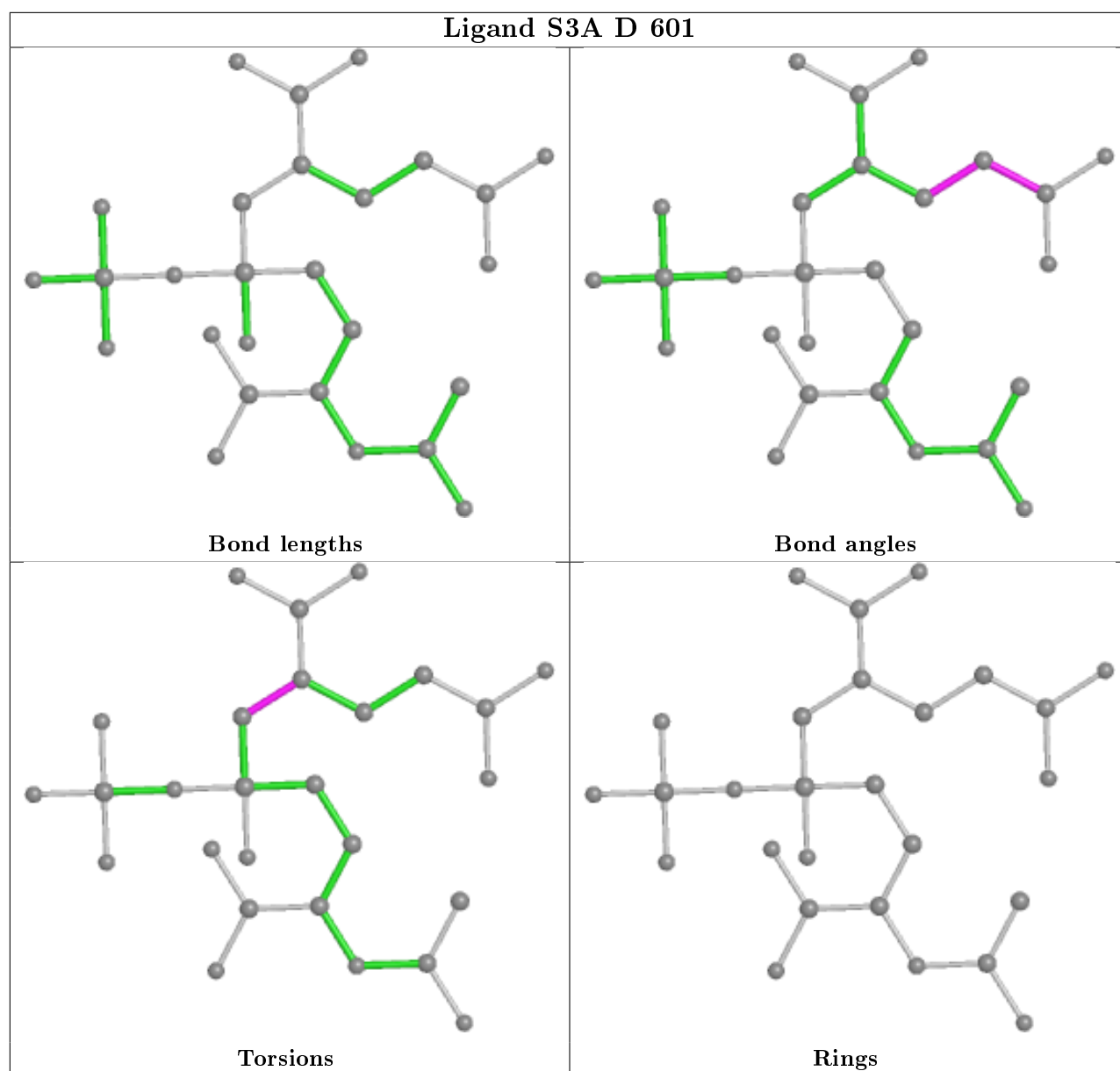


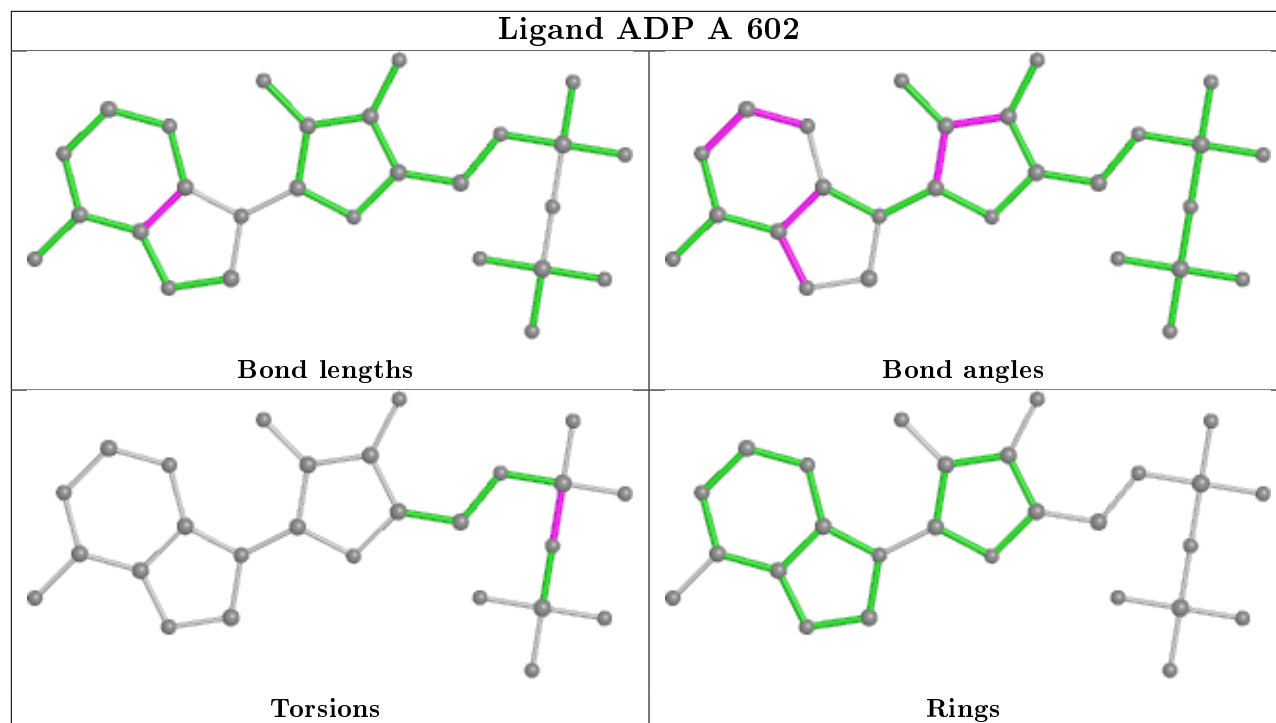












5.7 Other polymers [i](#)

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 ⓘ

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	404/453 (89%)	-0.03	8 (1%) 65 74	29, 44, 97, 126	0
1	B	404/453 (89%)	0.04	3 (0%) 87 92	29, 45, 95, 122	0
1	C	405/453 (89%)	-0.02	4 (0%) 82 88	27, 45, 97, 141	0
1	D	403/453 (88%)	-0.01	8 (1%) 65 74	29, 44, 96, 130	0
2	I	0/15	-	-	-	-
3	J	0/16	-	-	-	-
All	All	1616/1843 (87%)	-0.01	23 (1%) 75 82	27, 44, 97, 141	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	PRO	5.3
1	C	413	PRO	4.8
1	B	103	ARG	3.6
1	B	408	PHE	3.6
1	D	332	SER	3.5
1	C	414	ASN	3.4
1	A	332	SER	3.3
1	D	335	LEU	3.2
1	D	452	ASN	3.0
1	D	413	PRO	2.8
1	D	101	LEU	2.8
1	B	101	LEU	2.6
1	D	100	SER	2.6
1	A	408	PHE	2.5
1	C	252	LEU	2.5
1	D	409	LEU	2.5
1	A	333	HIS	2.4
1	A	425	PHE	2.4
1	A	452	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	279	PHE	2.2
1	A	331	PRO	2.1
1	D	408	PHE	2.1
1	A	101	LEU	2.1

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(\AA^2)	Q<0.9
7	GOL	A	613	6/6	0.62	0.36	61,66,70,71	0
8	S37	D	612	23/23	0.67	0.42	40,58,64,72	23
7	GOL	D	611	6/6	0.71	0.35	62,70,71,73	0
8	S37	A	616	23/23	0.73	0.40	72,102,115,118	0
7	GOL	A	605	6/6	0.76	0.36	52,63,69,71	0
7	GOL	B	612	6/6	0.76	0.27	55,65,67,70	0
7	GOL	C	610	6/6	0.78	0.33	56,60,64,64	0
7	GOL	C	609	6/6	0.79	0.31	59,65,67,68	0
7	GOL	D	609	6/6	0.80	0.36	40,51,52,53	6
7	GOL	D	610	6/6	0.80	0.31	53,66,68,74	0
7	GOL	A	612	6/6	0.82	0.22	99,104,105,105	0
7	GOL	A	606	6/6	0.82	0.18	70,78,82,85	0
7	GOL	D	607	6/6	0.82	0.17	84,87,90,91	0
7	GOL	C	606	6/6	0.83	0.34	54,65,66,70	0
7	GOL	B	611	6/6	0.83	0.40	72,82,86,89	0
7	GOL	D	608	6/6	0.83	0.33	72,77,79,79	0
7	GOL	C	607	6/6	0.86	0.33	66,71,73,74	0
7	GOL	A	609	6/6	0.87	0.29	70,79,80,81	0
7	GOL	A	608	6/6	0.88	0.20	49,56,60,61	0

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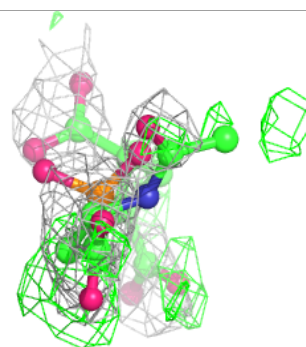
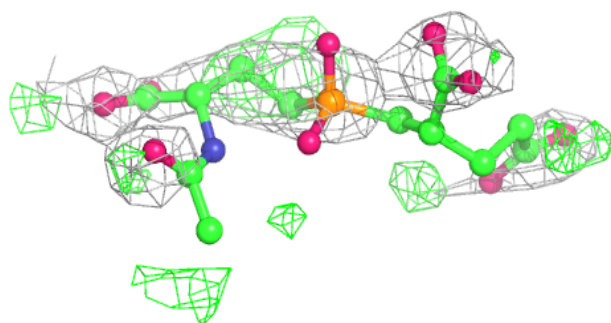
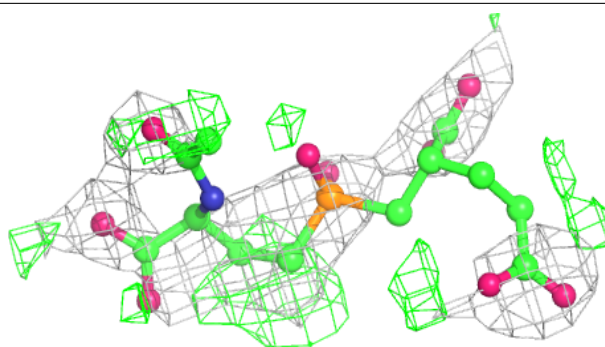
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	C	608	6/6	0.88	0.22	69,71,73,74	0
7	GOL	B	608	6/6	0.89	0.30	50,53,60,67	0
7	GOL	A	615	6/6	0.89	0.47	53,59,62,67	0
7	GOL	A	610	6/6	0.89	0.28	49,55,63,64	0
7	GOL	D	606	6/6	0.90	0.22	56,71,74,81	0
7	GOL	B	609	6/6	0.91	0.30	80,85,87,89	0
7	GOL	B	610	6/6	0.92	0.38	73,76,77,79	0
7	GOL	C	605	6/6	0.93	0.17	46,52,60,65	0
7	GOL	A	607	6/6	0.93	0.21	59,65,69,71	0
7	GOL	B	607	6/6	0.93	0.33	76,78,80,82	0
7	GOL	A	614	6/6	0.93	0.36	52,68,70,76	0
7	GOL	A	611	6/6	0.94	0.22	46,62,69,71	0
6	MG	C	604	1/1	0.94	0.12	30,30,30,30	0
7	GOL	B	605	6/6	0.95	0.16	60,63,65,66	0
7	GOL	B	606	6/6	0.96	0.17	45,53,62,69	0
7	GOL	D	605	6/6	0.96	0.18	58,63,64,69	0
6	MG	D	603	1/1	0.97	0.10	30,30,30,30	0
6	MG	B	603	1/1	0.97	0.11	31,31,31,31	0
4	S3A	C	601	27/27	0.98	0.14	25,32,37,42	0
6	MG	A	604	1/1	0.98	0.12	31,31,31,31	0
4	S3A	D	601	27/27	0.98	0.13	22,33,39,44	0
4	S3A	B	601	27/27	0.99	0.13	25,33,41,48	0
5	ADP	C	602	27/27	0.99	0.13	25,30,34,36	0
5	ADP	B	602	27/27	0.99	0.15	24,30,35,36	0
5	ADP	D	602	27/27	0.99	0.14	25,32,36,36	0
4	S3A	A	601	27/27	0.99	0.13	25,33,41,41	0
6	MG	B	604	1/1	0.99	0.15	31,31,31,31	0
6	MG	D	604	1/1	0.99	0.11	31,31,31,31	0
6	MG	C	603	1/1	0.99	0.13	29,29,29,29	0
6	MG	A	603	1/1	0.99	0.13	33,33,33,33	0
5	ADP	A	602	27/27	0.99	0.14	23,31,34,36	0

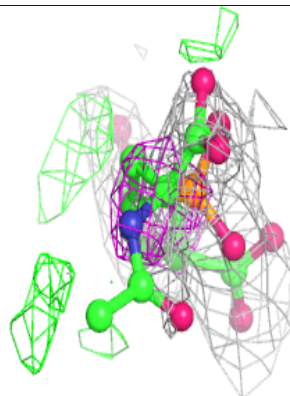
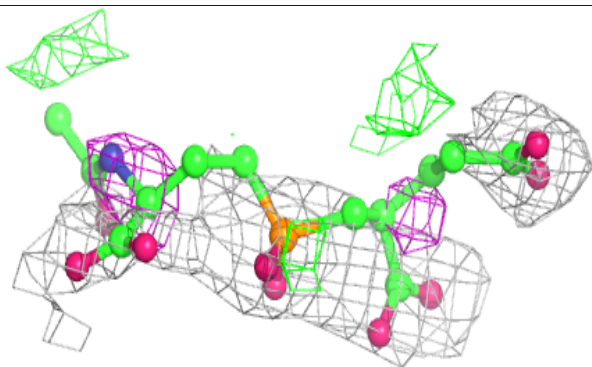
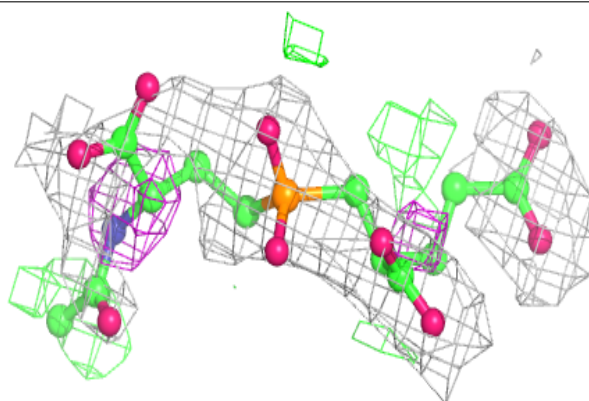
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around S37 D 612:

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

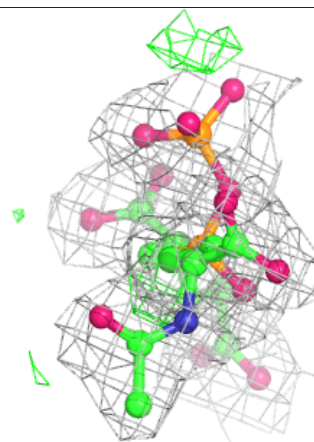
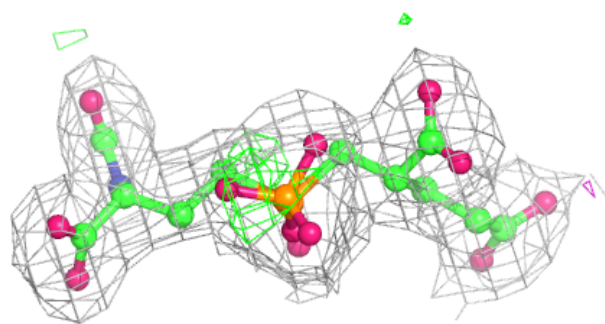
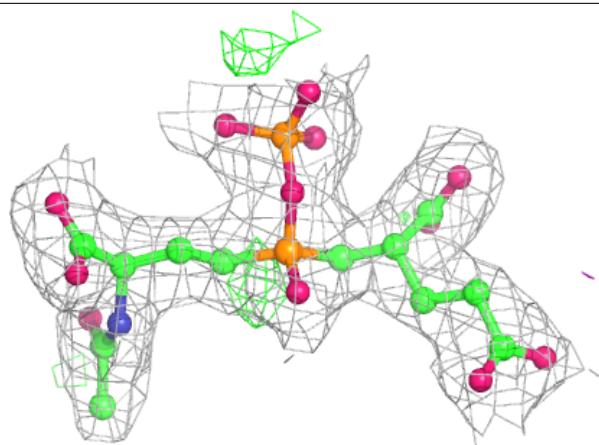
**Electron density around S37 A 616:**

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



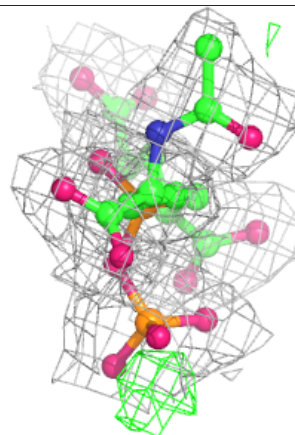
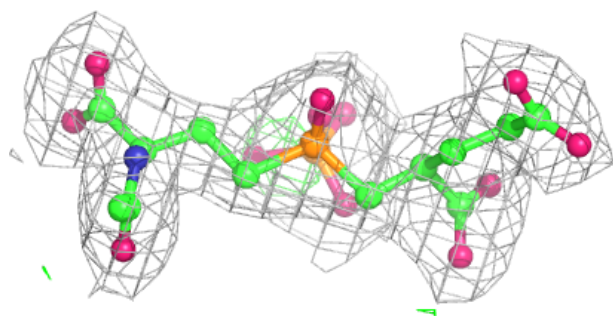
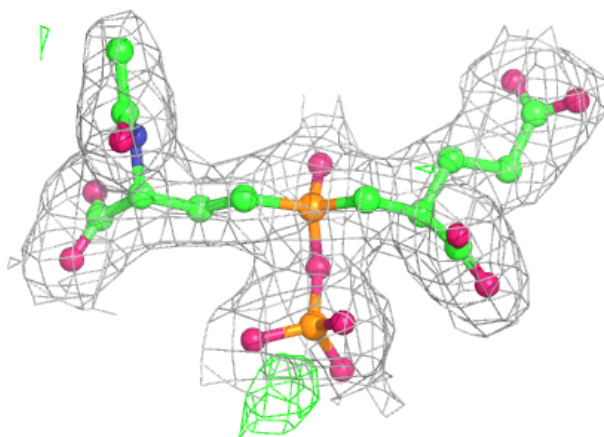
Electron density around S3A C 601:

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



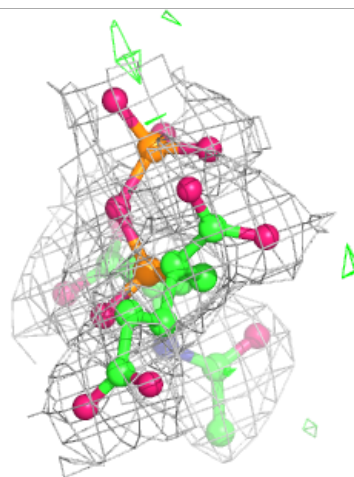
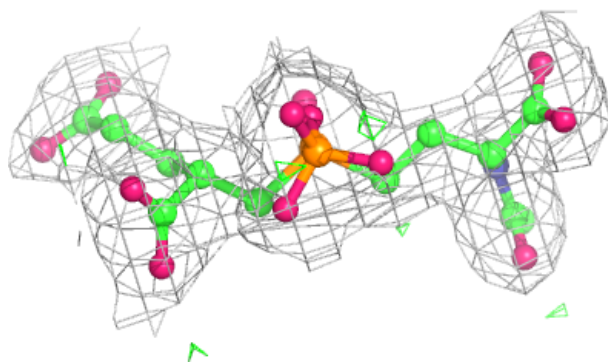
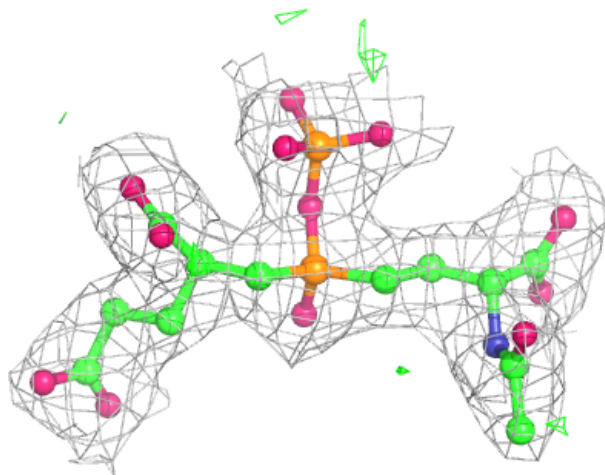
Electron density around S3A D 601:

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



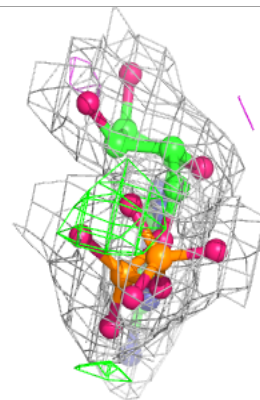
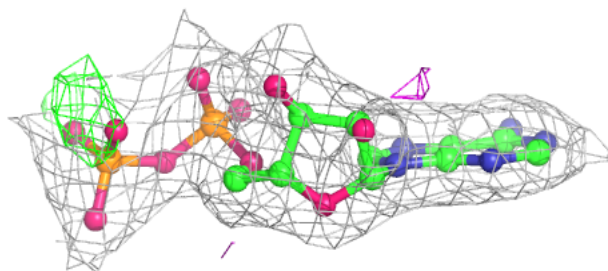
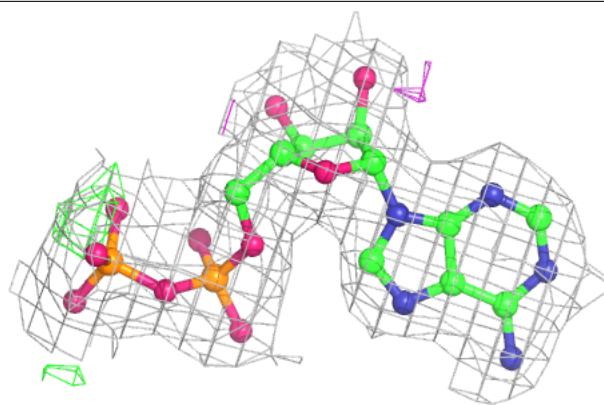
Electron density around S3A B 601:

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

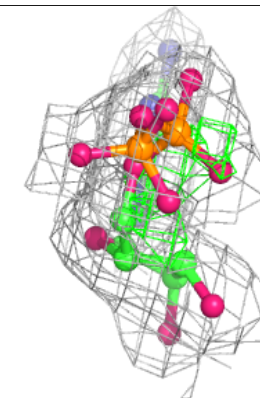
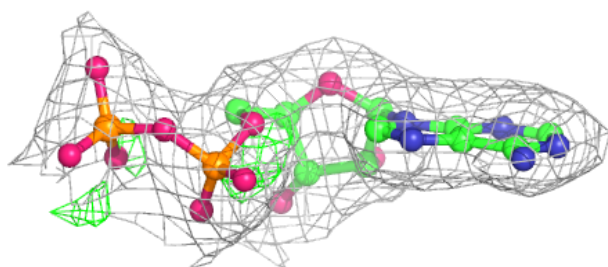
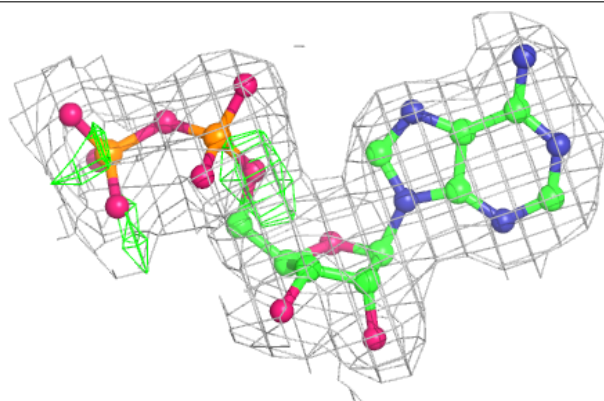


Electron density around ADP C 602:

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

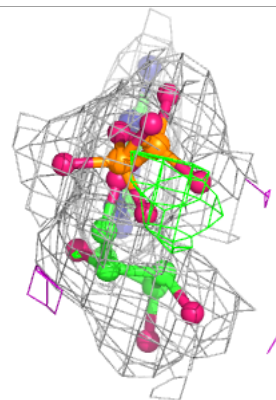
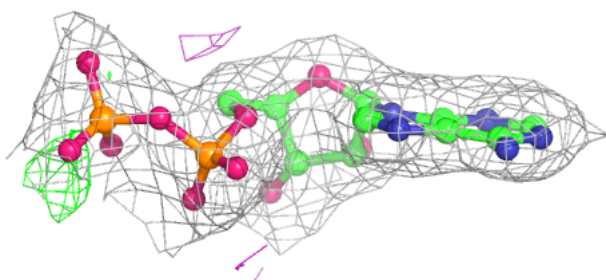
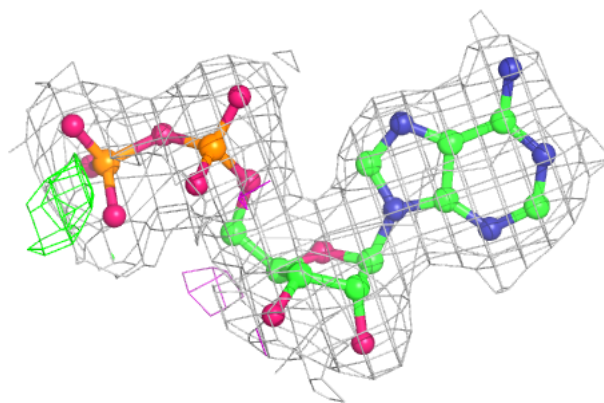
**Electron density around ADP B 602:**

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

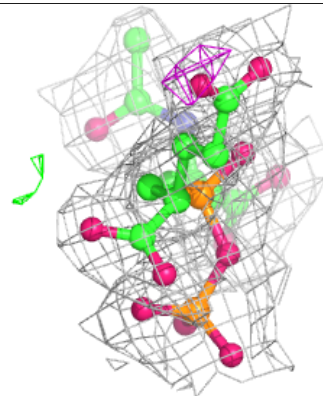
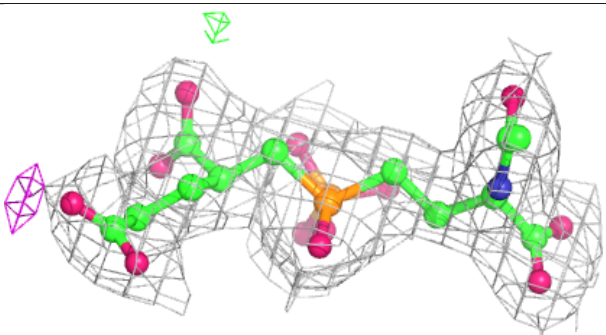
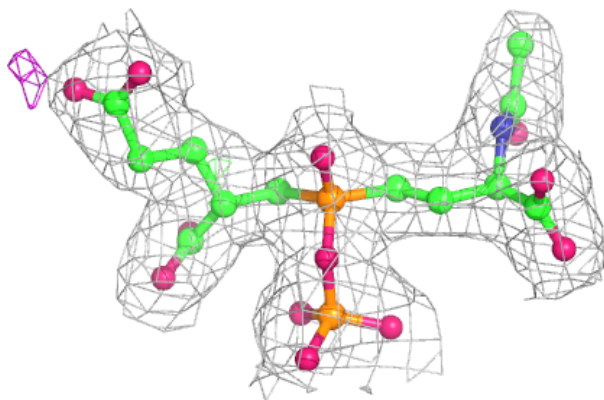


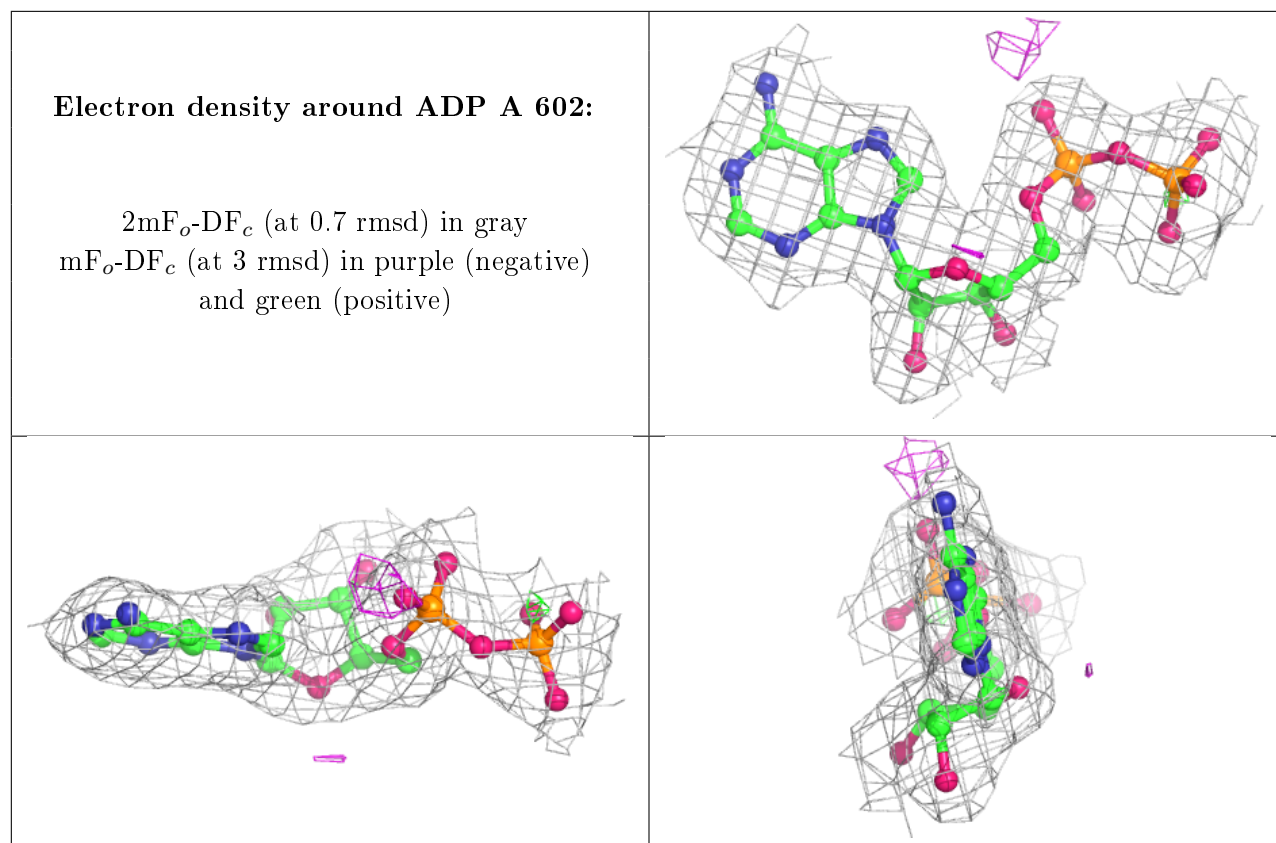
Electron density around ADP D 602:

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

**Electron density around S3A 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.