



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 08:26 PM BST

PDB ID : 6VZU
Title : TTLL6 bound to alpha-elongation analog
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Deposited on : 2020-02-28
Resolution : 1.98 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

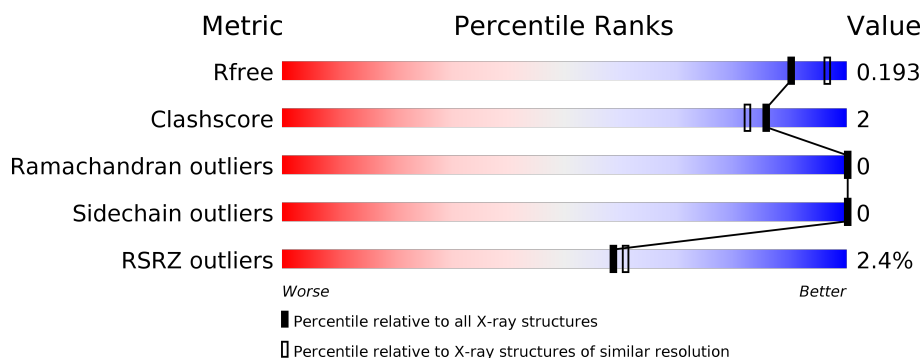
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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>3%</div> <div>84%</div> <div>6%</div> <div>11%</div> </div>
1	B	453	<div> <div>84%</div> <div>5%</div> <div>11%</div> </div>
1	C	453	<div> <div>2%</div> <div>82%</div> <div>5%</div> <div>13%</div> </div>
1	D	453	<div> <div>3%</div> <div>85%</div> <div>5%</div> <div>11%</div> </div>
2	M	13	<div> <div>100%</div> </div>
3	N	15	<div> <div>100%</div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14501 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	405	Total	C	N	O	S	0	14	0
			3279	2094	567	595	23			
1	B	404	Total	C	N	O	S	0	7	0
			3270	2086	567	594	23			
1	C	396	Total	C	N	O	S	0	8	0
			3180	2028	550	580	22			
1	D	405	Total	C	N	O	S	0	14	0
			3259	2084	563	589	23			

- Molecule 2 is a protein called TTLL6 unregistered chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	13	Total	C	N	O	0	0	0
			65	39	13	13			

- Molecule 3 is a protein called TTLL6 unregistered chain.

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



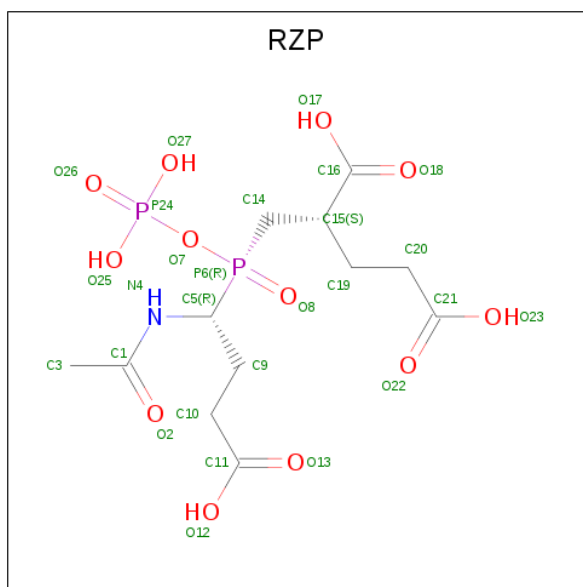
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total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

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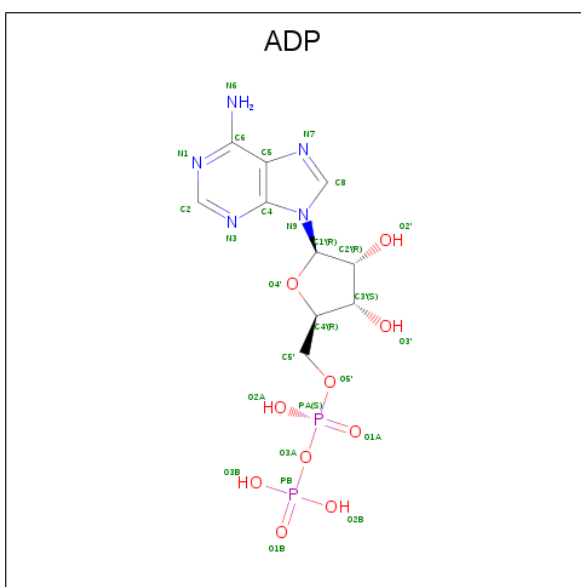
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is (2 {S})-2-[[[(1 {R})-1-acetamido-4-oxidanyl-4-oxidanylidene-butyl]-p hosphonoxy-phosphoryl]methyl]pentanedioic acid (three-letter code: RZP) (formula: C₁₂H₂₁NO₁₂P₂).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

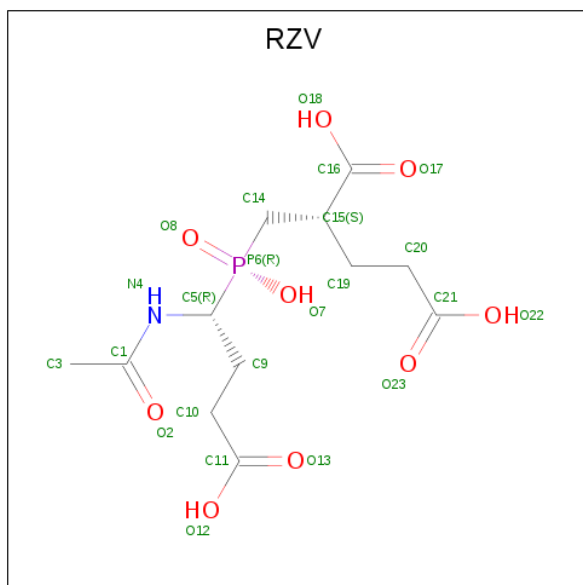
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Cl 1 1	0	0

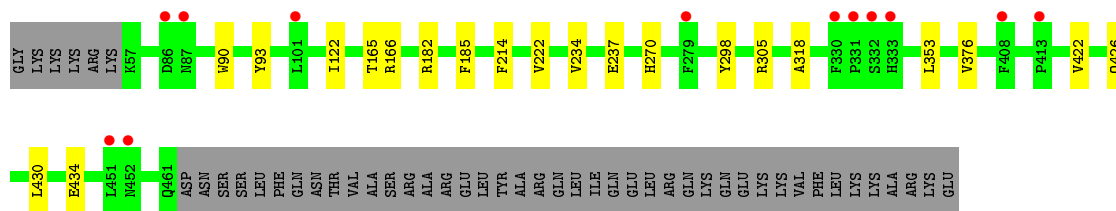
- Molecule 9 is (2 {S})-2-[[[(1 {R})-1-acetamido-4-oxidanyl-4-oxidanylidene-butyl]-oxidanyl-phosphoryl]methyl]pentanedioic acid (three-letter code: RZV) (formula: C₁₂H₂₀NO₉P).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	245	Total O 245 245	0	0
10	B	259	Total O 259 259	0	0
10	C	257	Total O 257 257	0	0
10	D	267	Total O 267 267	0	0



- Molecule 2: TTL6 unregistered chain

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: TTL6 unregistered chain

Chain N:  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	75.26Å 110.63Å 173.37Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	46.63 – 1.98 46.63 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.63-1.98) 96.6 (46.63-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.174 , 0.193 0.174 , 0.193	Depositor DCC
R_{free} test set	9697 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.400 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14501	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 40.11 % 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 2.8701e-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, ADP, CL, RZV, RZP

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	0.39	0/3385	0.53	0/4575
1	B	0.42	0/3356	0.55	0/4533
1	C	0.41	0/3270	0.55	0/4422
1	D	0.41	0/3363	0.54	0/4552
All	All	0.41	0/13374	0.54	0/18082

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	3279	0	3148	16	0
1	B	3270	0	3142	16	0
1	C	3180	0	3031	15	0
1	D	3259	0	3113	14	0
2	M	65	0	15	0	0
3	N	75	0	17	0	0
4	A	24	0	32	2	0
4	B	24	0	32	1	0
4	C	6	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	42	0	56	3	0
5	A	27	0	0	0	0
5	B	27	0	0	0	0
5	C	27	0	0	0	0
5	D	27	0	0	0	0
6	A	27	0	12	0	0
6	B	27	0	12	0	0
6	C	27	0	12	0	0
6	D	27	0	12	0	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	1	0	0	0	0
8	D	1	0	0	0	0
9	C	23	0	0	0	0
10	A	245	0	0	1	0
10	B	259	0	0	0	0
10	C	257	0	0	2	0
10	D	267	0	0	1	0
All	All	14501	0	12641	57	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 2.

All (57) 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:165:THR:OG1	1:C:166[A]:ARG:NH2	2.18	0.77
1:A:104:VAL:HB	1:A:330:PHE:CZ	2.25	0.71
1:B:100:SER:H	1:B:103:ARG:HE	1.45	0.65
1:D:222:VAL:HG22	1:D:234[B]:VAL:HG12	1.79	0.64
1:A:301:GLU:OE2	4:A:603:GOL:H31	1.97	0.64
1:C:209:PHE:CE1	4:C:704:GOL:H32	2.36	0.61
1:B:99:VAL:HA	1:B:103:ARG:HE	1.66	0.60
1:B:334:THR:OG1	1:B:402:GLU:OE2	2.22	0.57
1:D:305:ARG:HG3	4:D:603:GOL:H11	1.87	0.56
1:D:165:THR:OG1	1:D:166:ARG:HD2	2.06	0.56
1:B:207:LYS:HB3	1:B:351[A]:ARG:HD3	1.89	0.55
1:C:441[B]:CYS:SG	10:C:801:HOH:O	2.59	0.53
1:D:237:GLU:HG3	1:D:376:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ARG:O	1:B:411:GLN:HG2	2.08	0.53
1:A:214:PHE:CE2	4:A:601:GOL:H2	2.44	0.52
1:B:100:SER:H	1:B:103:ARG:NE	2.06	0.52
1:C:101:LEU:O	1:C:105:MET:HG3	2.09	0.52
1:A:165:THR:HB	1:A:166:ARG:HD2	1.92	0.51
1:D:298:TYR:CD1	1:D:353:LEU:HD11	2.44	0.51
1:C:374[A]:LYS:NZ	10:C:805:HOH:O	2.44	0.50
1:D:214:PHE:CE2	4:D:605:GOL:H2	2.47	0.49
1:A:182:ARG:HD2	1:C:185:PHE:CE2	2.47	0.49
1:B:298:TYR:CD1	1:B:353:LEU:HD11	2.48	0.49
1:A:222:VAL:HG22	1:A:234[B]:VAL:HG22	1.95	0.48
1:B:100:SER:OG	1:B:103:ARG:HG3	2.13	0.48
1:D:270:HIS:HE1	10:D:913:HOH:O	1.97	0.48
1:D:305:ARG:HG3	4:D:603:GOL:C1	2.44	0.47
1:B:182:ARG:HD2	1:D:185:PHE:CE2	2.49	0.47
1:A:298:TYR:CD1	1:A:353:LEU:HD11	2.49	0.47
1:B:101:LEU:O	1:B:105:MET:HG3	2.15	0.47
1:C:298:TYR:CD1	1:C:353:LEU:HD11	2.51	0.46
1:B:185:PHE:CE2	1:D:182:ARG:HD2	2.51	0.46
1:C:401:GLU:O	1:C:405:ARG:HG3	2.16	0.46
1:D:430:LEU:HD21	1:D:434:GLU:OE2	2.15	0.46
1:B:90:TRP:CZ3	1:B:93:TYR:HB2	2.51	0.45
1:D:122:ILE:HG23	1:D:318:ALA:HB2	1.98	0.45
1:C:140:PRO:O	1:C:144:HIS:NE2	2.50	0.44
1:B:308:GLU:OE1	4:B:603:GOL:O2	2.35	0.44
1:B:223:LEU:HD23	1:B:387:LEU:HD23	1.99	0.44
1:A:101:LEU:HG	1:A:329:CYS:SG	2.58	0.44
1:A:122:ILE:HG23	1:A:318:ALA:HB2	2.00	0.44
1:A:452:ASN:HB2	1:A:455:LYS:NZ	2.33	0.44
1:A:270:HIS:HE1	10:A:892:HOH:O	2.02	0.43
1:C:223:LEU:HD23	1:C:387:LEU:HD23	2.01	0.43
1:C:122:ILE:HG23	1:C:318:ALA:HB2	2.00	0.43
1:A:423:LYS:HA	1:A:423:LYS:HD3	1.79	0.43
1:D:90:TRP:CZ3	1:D:93:TYR:HB2	2.54	0.43
1:B:417:ILE:O	1:B:421:GLU:HG2	2.19	0.42
1:A:412:CYS:SG	1:A:421:GLU:HG3	2.59	0.42
1:C:90:TRP:CZ3	1:C:93:TYR:HB2	2.53	0.42
1:D:422:VAL:O	1:D:426:GLN:HG3	2.19	0.42
1:A:237:GLU:HG3	1:A:376:VAL:HG22	2.02	0.42
1:B:109:SER:HA	1:B:333:HIS:CE1	2.55	0.42
1:A:185:PHE:CE2	1:C:182:ARG:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:THR:HG1	1:C:166[A]:ARG:NH2	2.16	0.41
1:A:422:VAL:O	1:A:426:GLN:HG3	2.20	0.41
1:C:147:PRO:HB3	1:C:205:ILE:HD11	2.03	0.41

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	416/453 (92%)	406 (98%)	10 (2%)	0	100	100
1	B	409/453 (90%)	397 (97%)	12 (3%)	0	100	100
1	C	400/453 (88%)	390 (98%)	10 (2%)	0	100	100
1	D	417/453 (92%)	407 (98%)	10 (2%)	0	100	100
All	All	1642/1812 (91%)	1600 (97%)	42 (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	348/416 (84%)	348 (100%)	0	100	100
1	B	346/416 (83%)	346 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	337/416 (81%)	337 (100%)	0	100	100
1	D	342/416 (82%)	342 (100%)	0	100	100
All	All	1373/1664 (82%)	1373 (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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 35 ligands modelled in this entry, 10 are monoatomic - leaving 25 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	ADP	A	606	7	24,29,29	1.08	2 (8%)	29,45,45	1.28	1 (3%)
4	GOL	A	604	-	5,5,5	0.98	0	5,5,5	0.99	0
6	ADP	B	606	7	24,29,29	1.07	3 (12%)	29,45,45	1.37	4 (13%)
4	GOL	B	603	-	5,5,5	1.09	0	5,5,5	0.94	0
4	GOL	D	603	-	5,5,5	1.14	0	5,5,5	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	RZP	D	608	7	12,26,26	1.37	1 (8%)	18,37,37	1.57	4 (22%)
4	GOL	D	606	-	5,5,5	1.06	0	5,5,5	0.86	0
4	GOL	D	601	-	5,5,5	0.98	0	5,5,5	0.99	0
4	GOL	B	602	-	5,5,5	0.94	0	5,5,5	1.14	0
4	GOL	C	704	-	5,5,5	1.57	0	5,5,5	1.10	1 (20%)
4	GOL	D	604	-	5,5,5	0.99	0	5,5,5	0.85	0
4	GOL	A	602	-	5,5,5	0.98	0	5,5,5	1.15	0
4	GOL	B	604	-	5,5,5	1.01	0	5,5,5	0.96	0
5	RZP	A	605	7	12,26,26	1.32	1 (8%)	18,37,37	1.48	5 (27%)
9	RZV	C	701	-	10,22,22	1.12	1 (10%)	11,30,30	1.15	1 (9%)
5	RZP	C	705	7	12,26,26	1.36	1 (8%)	18,37,37	1.51	4 (22%)
4	GOL	D	602	-	5,5,5	0.82	0	5,5,5	1.34	1 (20%)
4	GOL	D	607	-	5,5,5	0.93	0	5,5,5	0.98	0
6	ADP	C	706	7	24,29,29	1.18	3 (12%)	29,45,45	1.29	2 (6%)
6	ADP	D	609	7	24,29,29	1.13	3 (12%)	29,45,45	1.29	3 (10%)
4	GOL	D	605	-	5,5,5	1.01	0	5,5,5	1.16	0
4	GOL	A	603	-	5,5,5	0.76	0	5,5,5	1.21	0
5	RZP	B	605	7	12,26,26	1.27	1 (8%)	18,37,37	1.65	4 (22%)
4	GOL	A	601	-	5,5,5	1.02	0	5,5,5	1.18	0
4	GOL	B	601	-	5,5,5	0.95	0	5,5,5	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	A	606	7	-	1/12/32/32	0/3/3/3
4	GOL	A	604	-	-	0/4/4/4	-
6	ADP	B	606	7	-	5/12/32/32	0/3/3/3
4	GOL	B	603	-	-	0/4/4/4	-
4	GOL	D	603	-	-	2/4/4/4	-
5	RZP	D	608	7	-	0/21/35/35	-
4	GOL	D	606	-	-	0/4/4/4	-
4	GOL	D	601	-	-	0/4/4/4	-
4	GOL	B	602	-	-	0/4/4/4	-
4	GOL	C	704	-	-	2/4/4/4	-
4	GOL	D	604	-	-	2/4/4/4	-
4	GOL	A	602	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	604	-	-	0/4/4/4	-
5	RZP	A	605	7	-	0/21/35/35	-
9	RZV	C	701	-	-	6/16/29/29	-
5	RZP	C	705	7	-	1/21/35/35	-
4	GOL	D	602	-	-	1/4/4/4	-
4	GOL	D	607	-	-	0/4/4/4	-
6	ADP	C	706	7	-	1/12/32/32	0/3/3/3
6	ADP	D	609	7	-	5/12/32/32	0/3/3/3
4	GOL	D	605	-	-	0/4/4/4	-
4	GOL	A	603	-	-	2/4/4/4	-
5	RZP	B	605	7	-	0/21/35/35	-
4	GOL	A	601	-	-	0/4/4/4	-
4	GOL	B	601	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	705	RZP	P6-C14	4.03	1.83	1.79
5	D	608	RZP	P6-C14	3.98	1.83	1.79
5	A	605	RZP	P6-C14	3.85	1.83	1.79
5	B	605	RZP	P6-C14	3.78	1.83	1.79
9	C	701	RZV	P6-C14	3.06	1.82	1.79
6	C	706	ADP	C2-N3	2.76	1.36	1.32
6	B	606	ADP	C2-N3	2.75	1.36	1.32
6	A	606	ADP	C2-N3	2.61	1.36	1.32
6	D	609	ADP	C2-N3	2.54	1.36	1.32
6	A	606	ADP	C5-C4	2.37	1.47	1.40
6	D	609	ADP	C2'-C1'	-2.26	1.50	1.53
6	C	706	ADP	C5-C4	2.24	1.46	1.40
6	C	706	ADP	O4'-C1'	2.23	1.44	1.41
6	B	606	ADP	C5-C4	2.23	1.46	1.40
6	B	606	ADP	O4'-C1'	2.20	1.44	1.41
6	D	609	ADP	C5-C4	2.18	1.46	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	606	ADP	N3-C2-N1	-3.87	122.63	128.68
5	B	605	RZP	O7-P6-C5	3.77	112.98	103.40
6	A	606	ADP	N3-C2-N1	-3.77	122.79	128.68
5	D	608	RZP	C19-C15-C16	-3.39	107.49	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	706	ADP	N3-C2-N1	-3.39	123.39	128.68
6	D	609	ADP	N3-C2-N1	-3.30	123.52	128.68
5	C	705	RZP	O7-P6-C5	3.27	111.71	103.40
6	C	706	ADP	N6-C6-N1	2.79	124.36	118.57
5	A	605	RZP	C19-C20-C21	-2.77	107.63	113.59
9	C	701	RZV	C19-C15-C16	2.73	116.60	112.53
5	D	608	RZP	O7-P6-C5	2.69	110.22	103.40
5	C	705	RZP	C19-C20-C21	-2.68	107.82	113.59
5	D	608	RZP	C19-C20-C21	-2.68	107.83	113.59
5	B	605	RZP	P6-C14-C15	-2.67	106.65	114.10
5	A	605	RZP	O7-P6-C5	2.64	110.11	103.40
5	B	605	RZP	C19-C20-C21	-2.62	107.97	113.59
5	A	605	RZP	C19-C15-C16	-2.52	108.78	112.53
6	B	606	ADP	O3B-PB-O2B	2.51	117.24	107.64
5	C	705	RZP	P6-C14-C15	-2.50	107.10	114.10
6	D	609	ADP	N6-C6-N1	2.39	123.53	118.57
5	C	705	RZP	C19-C15-C16	-2.38	108.99	112.53
4	C	704	GOL	C3-C2-C1	-2.35	102.56	111.70
6	B	606	ADP	N6-C6-N1	2.35	123.45	118.57
5	D	608	RZP	P6-C14-C15	-2.31	107.65	114.10
5	A	605	RZP	P6-C14-C15	-2.30	107.69	114.10
5	B	605	RZP	C19-C15-C16	-2.27	109.15	112.53
5	A	605	RZP	O27-P24-O7	2.24	112.14	104.64
4	D	602	GOL	C3-C2-C1	-2.23	103.03	111.70
6	D	609	ADP	O3B-PB-O2B	2.19	116.00	107.64
6	B	606	ADP	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	606	ADP	PA-O3A-PB-O3B
4	D	604	GOL	C1-C2-C3-O3
6	B	606	ADP	PA-O3A-PB-O2B
6	B	606	ADP	PA-O3A-PB-O3B
9	C	701	RZV	C3-C1-N4-C5
9	C	701	RZV	O2-C1-N4-C5
6	D	609	ADP	PA-O3A-PB-O2B
6	D	609	ADP	PA-O3A-PB-O3B
6	C	706	ADP	PA-O3A-PB-O3B
9	C	701	RZV	N4-C5-C9-C10
4	D	604	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	603	GOL	C1-C2-C3-O3
4	A	602	GOL	O1-C1-C2-C3
4	A	603	GOL	C1-C2-C3-O3
4	A	602	GOL	O1-C1-C2-O2
9	C	701	RZV	C11-C10-C9-C5
4	D	603	GOL	O2-C2-C3-O3
4	C	704	GOL	O1-C1-C2-O2
4	D	602	GOL	O2-C2-C3-O3
4	A	603	GOL	O2-C2-C3-O3
4	C	704	GOL	O1-C1-C2-C3
9	C	701	RZV	C9-C5-P6-O8
6	B	606	ADP	PB-O3A-PA-O1A
6	D	609	ADP	PB-O3A-PA-O1A
6	B	606	ADP	PB-O3A-PA-O2A
6	D	609	ADP	PB-O3A-PA-O2A
6	B	606	ADP	PA-O3A-PB-O1B
6	D	609	ADP	PA-O3A-PB-O1B
5	C	705	RZP	P6-C14-C15-C16
9	C	701	RZV	C16-C15-C19-C20

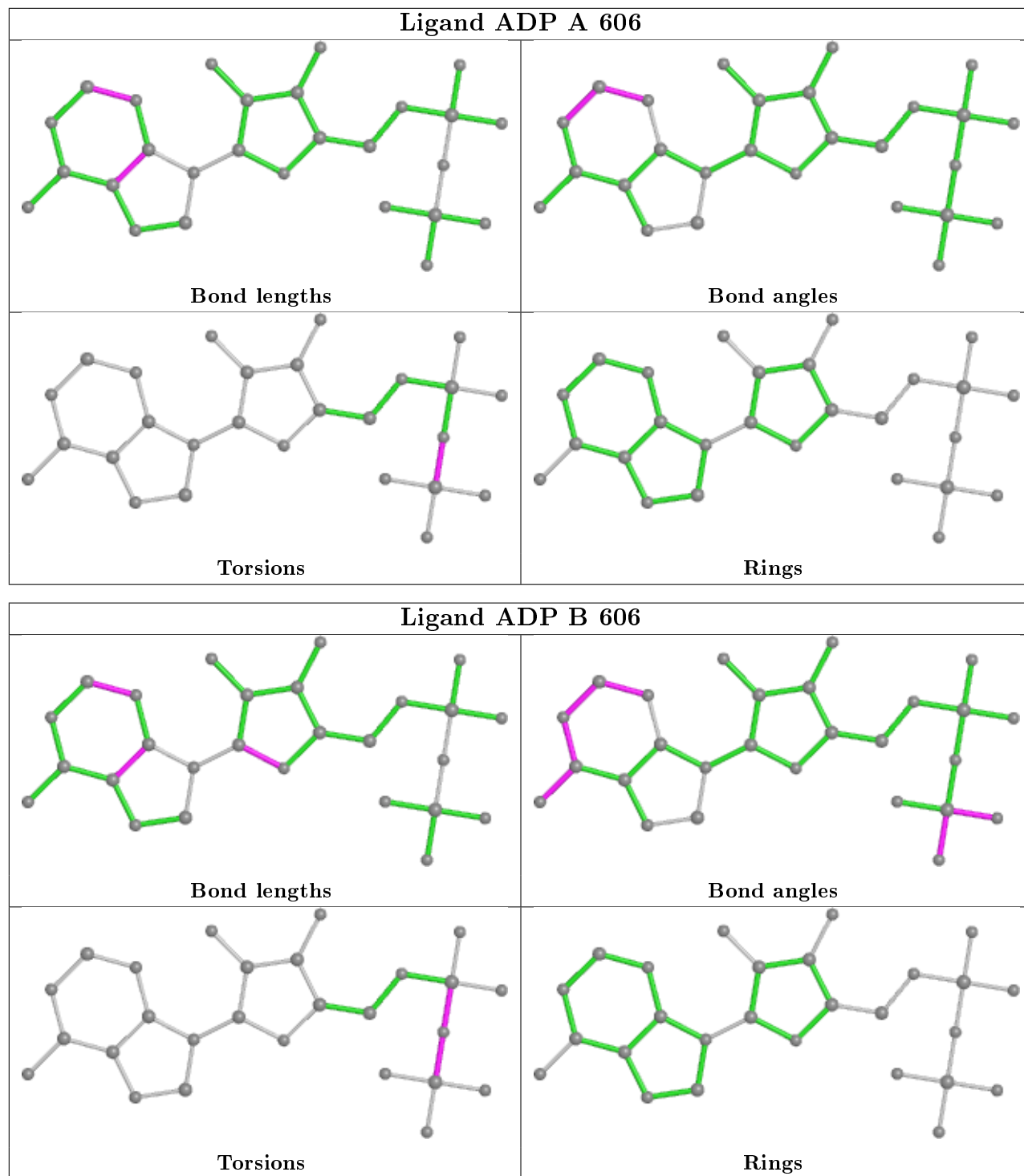
There are no ring outliers.

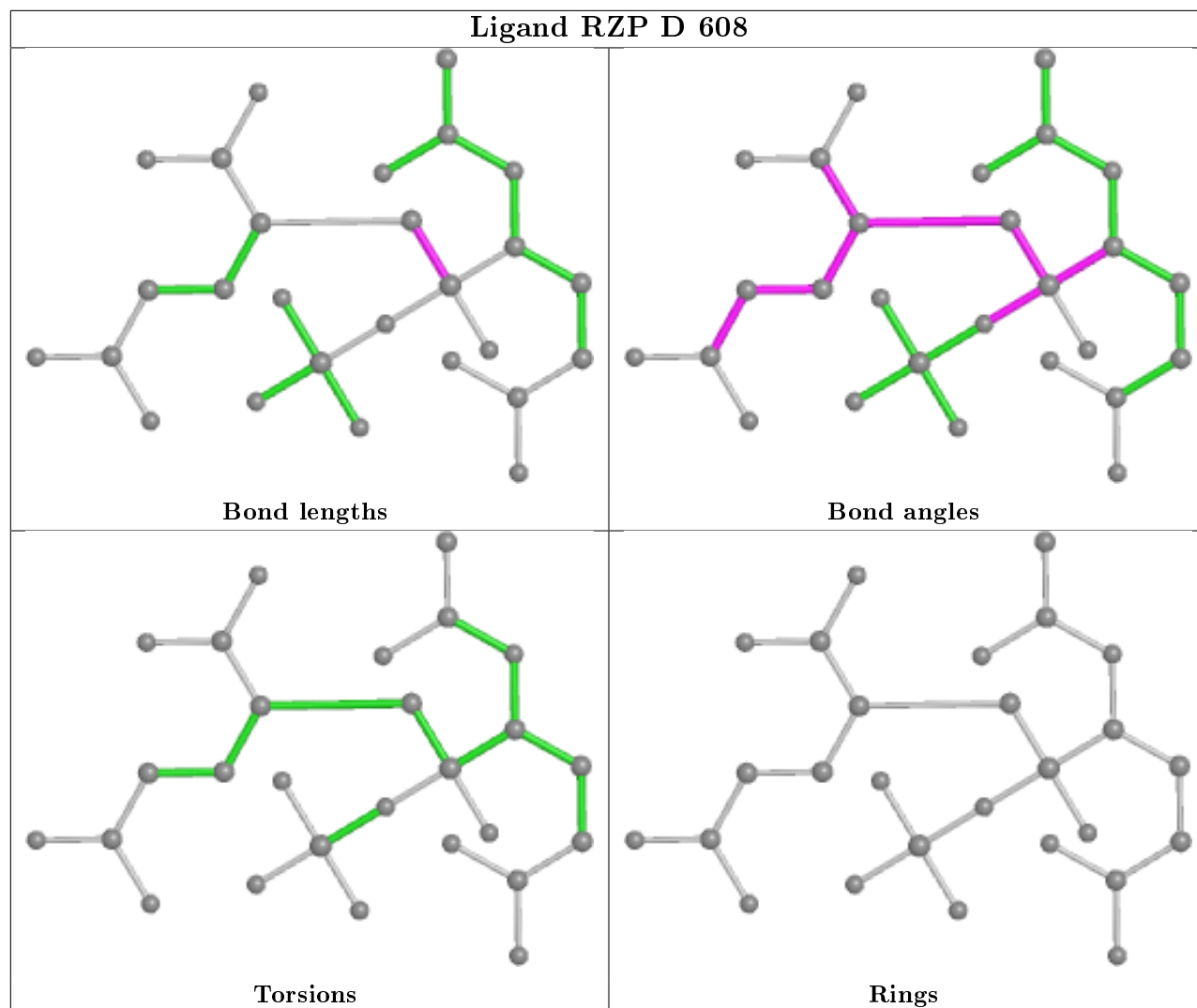
6 monomers are involved in 7 short contacts:

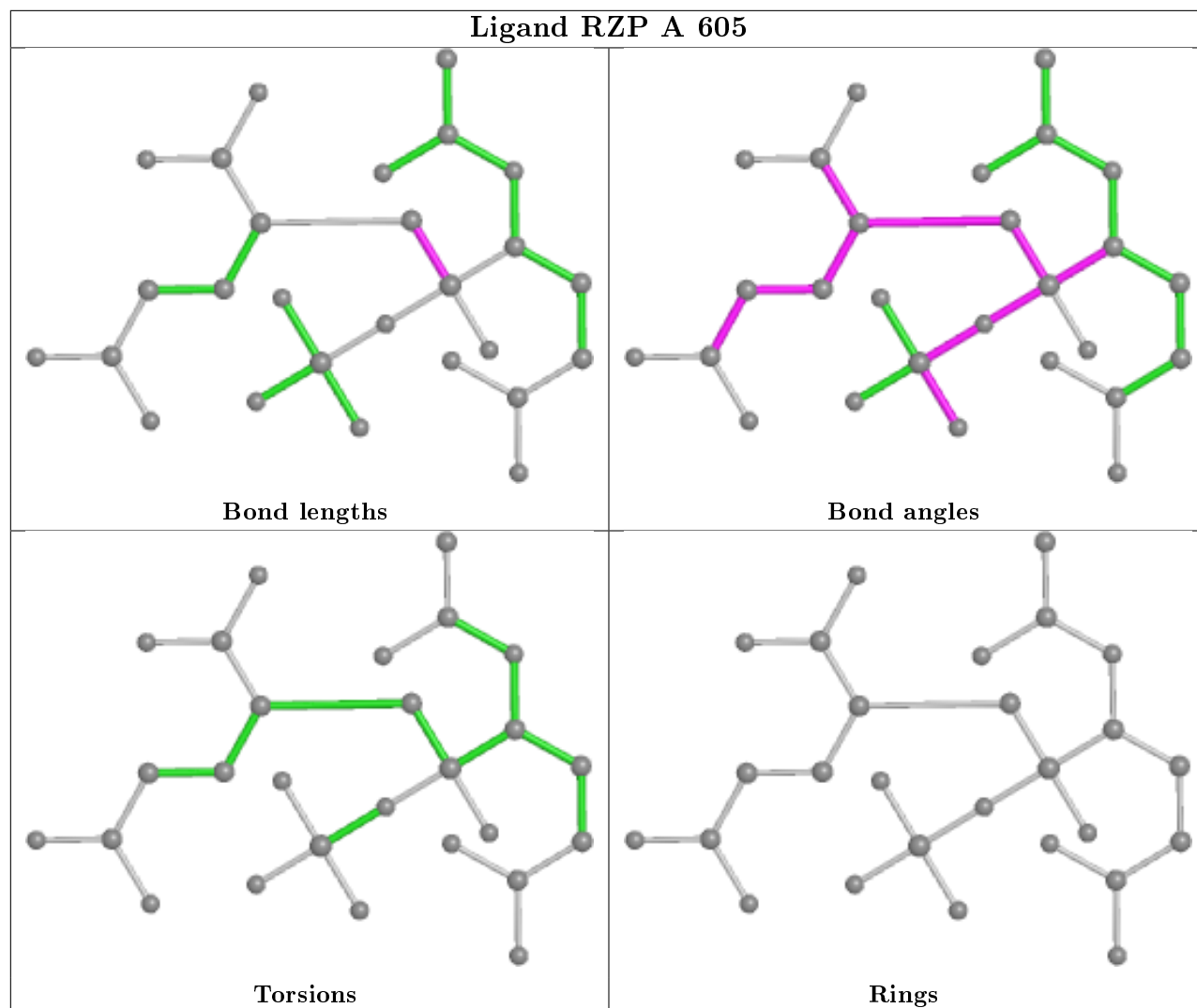
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	GOL	1	0
4	D	603	GOL	2	0
4	C	704	GOL	1	0
4	D	605	GOL	1	0
4	A	603	GOL	1	0
4	A	601	GOL	1	0

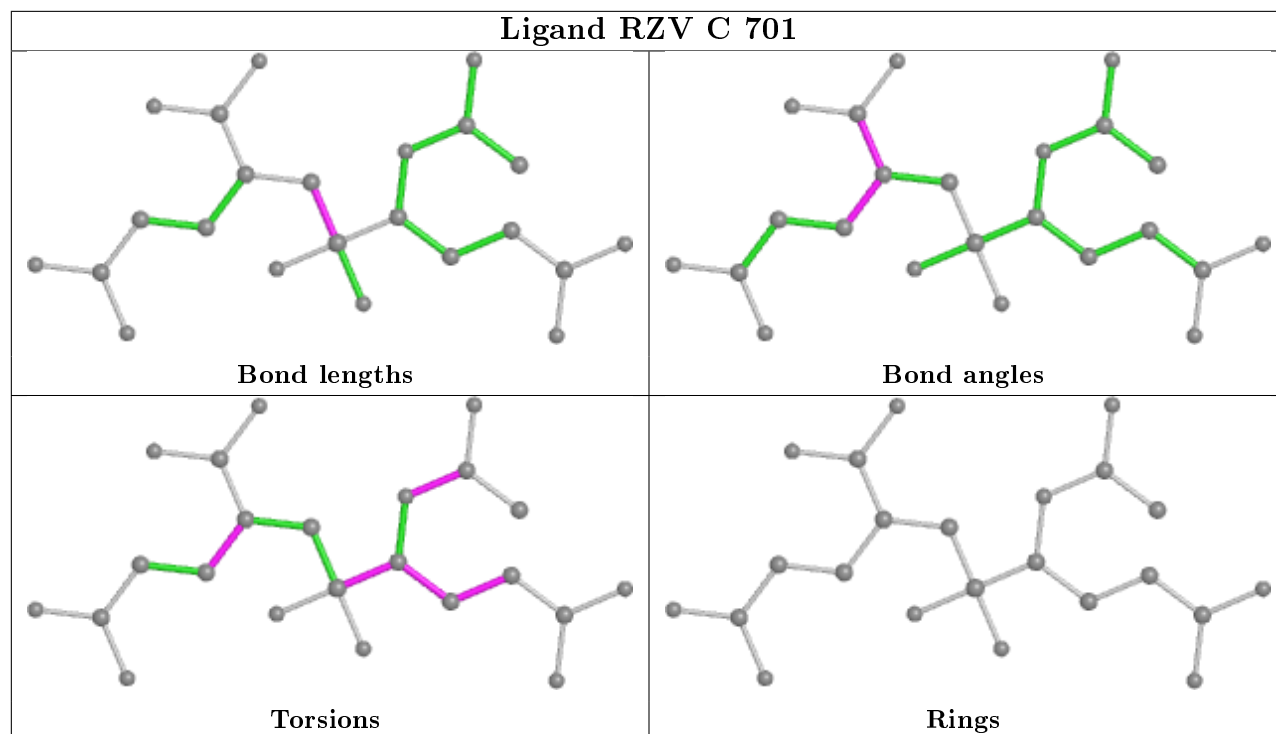
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

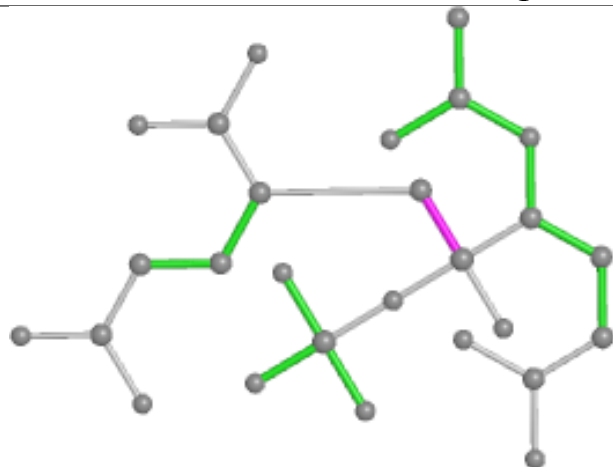




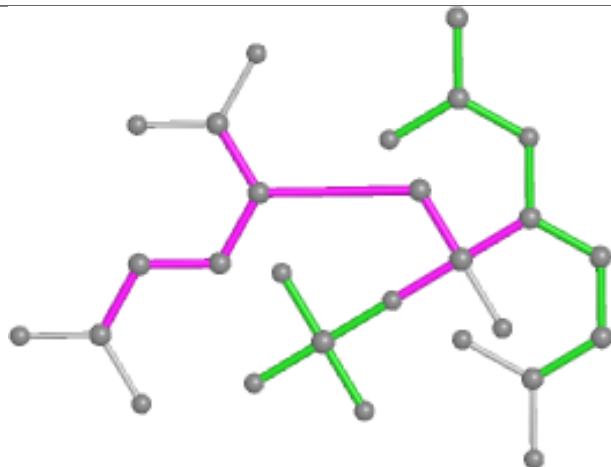




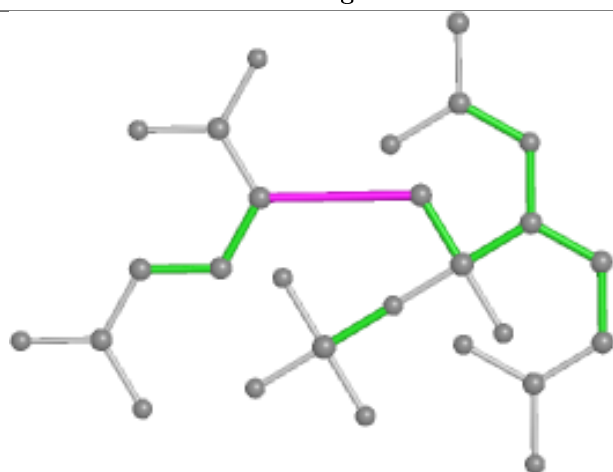
Ligand RZP C 705



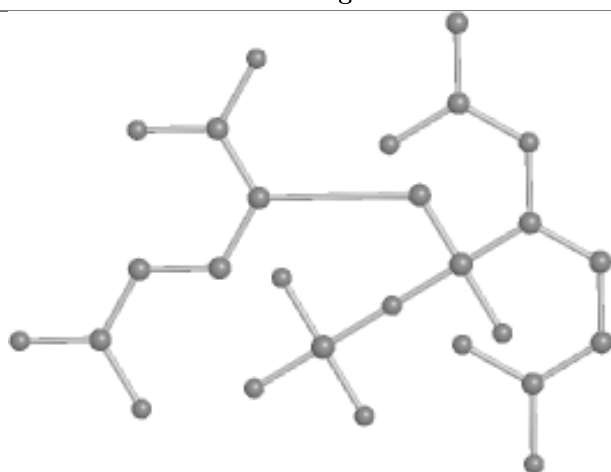
Bond lengths



Bond angles

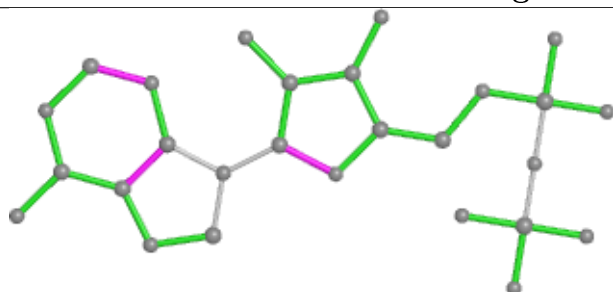


Torsions

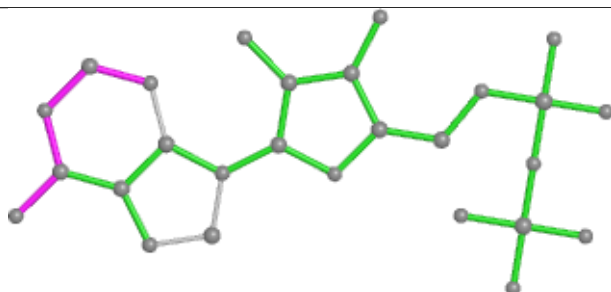


Rings

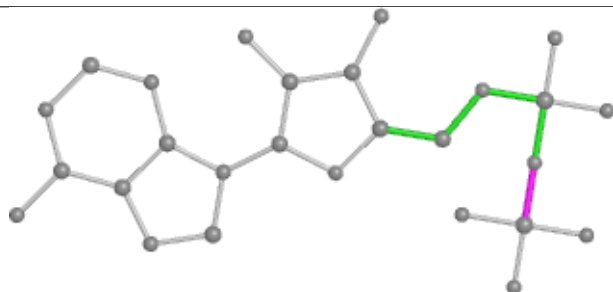
Ligand ADP C 706



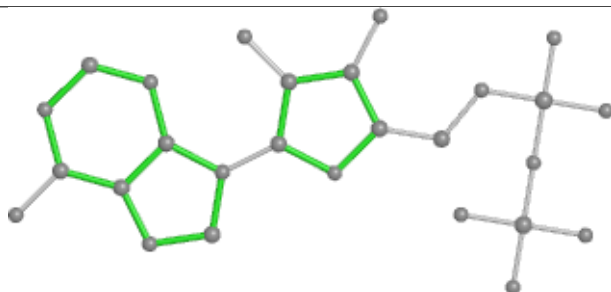
Bond lengths



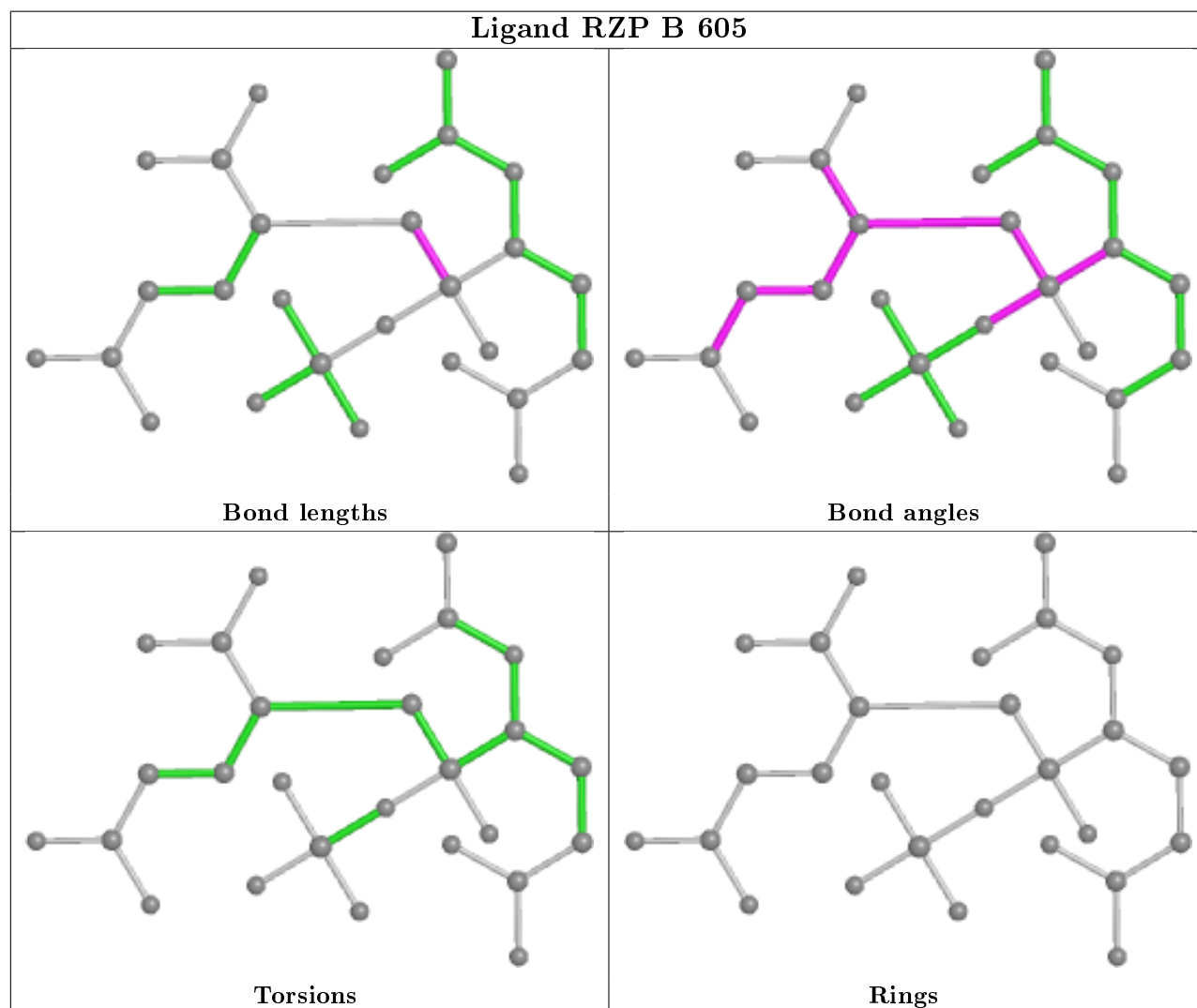
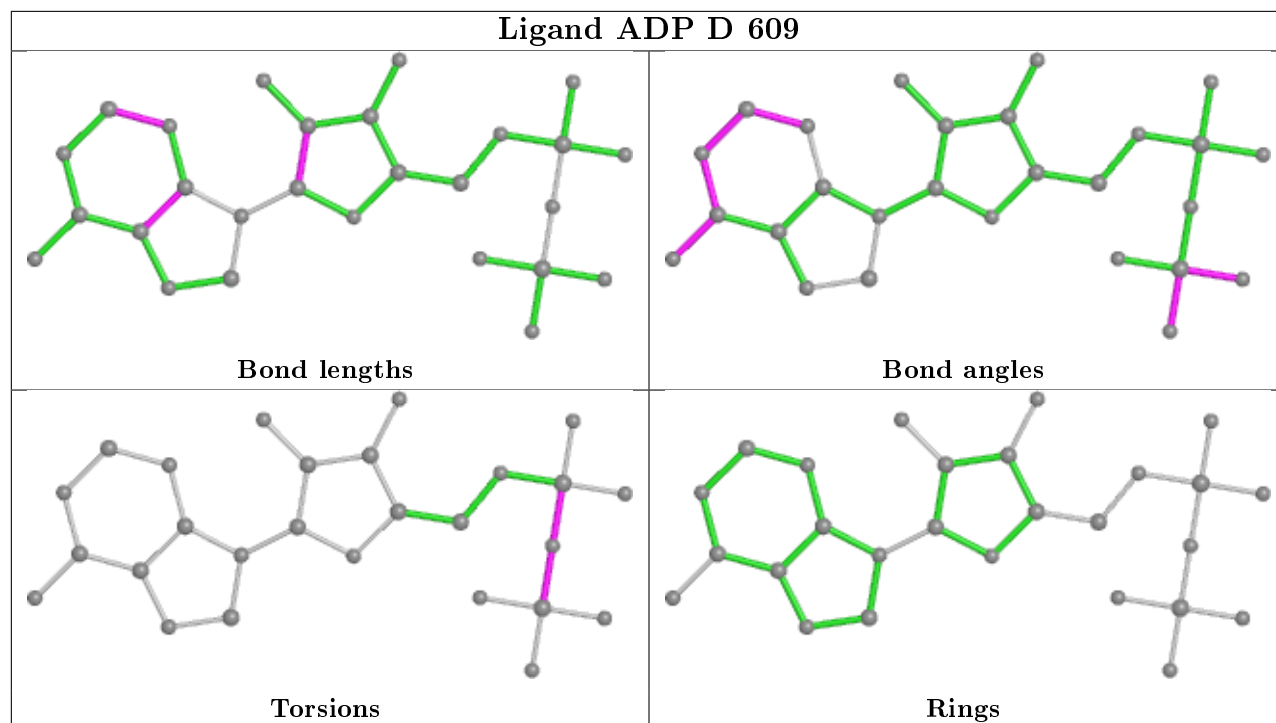
Bond angles



Torsions



Rings



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	405/453 (89%)	0.06	13 (3%) 47 50	27, 41, 85, 99	0
1	B	404/453 (89%)	0.10	2 (0%) 91 91	24, 41, 81, 119	0
1	C	396/453 (87%)	0.16	11 (2%) 53 55	24, 42, 86, 110	0
1	D	405/453 (89%)	0.03	12 (2%) 50 52	26, 40, 84, 111	0
2	M	0/13	-	-	-	-
3	N	0/15	-	-	-	-
All	All	1610/1840 (87%)	0.09	38 (2%) 59 61	24, 41, 85, 119	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	101	LEU	8.2
1	A	101	LEU	5.7
1	B	101	LEU	5.4
1	D	101	LEU	4.9
1	D	451	LEU	4.9
1	A	451	LEU	4.3
1	D	279	PHE	4.0
1	A	332	SER	3.9
1	D	413	PRO	3.3
1	D	86	ASP	3.2
1	C	424	GLY	3.1
1	A	279	PHE	3.0
1	A	413	PRO	2.9
1	A	452	ASN	2.9
1	C	405	ARG	2.8
1	C	422	VAL	2.7
1	C	425	PHE	2.7
1	D	330	PHE	2.7
1	A	412	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	332	SER	2.6
1	D	333	HIS	2.5
1	D	87	ASN	2.4
1	C	406	GLY	2.3
1	A	408	PHE	2.3
1	A	331	PRO	2.3
1	A	100	SER	2.3
1	D	331	PRO	2.2
1	C	417	ILE	2.2
1	A	330	PHE	2.2
1	C	86	ASP	2.2
1	A	57	LYS	2.2
1	C	398	VAL	2.2
1	D	452	ASN	2.1
1	B	452	ASN	2.1
1	A	422	VAL	2.1
1	D	408	PHE	2.1
1	C	452	ASN	2.0
1	C	402	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
4	GOL	B	604	6/6	0.75	0.26	60,70,74,76	0
9	RZV	C	701	23/23	0.77	0.29	30,55,82,88	23
4	GOL	D	603	6/6	0.85	0.33	36,54,65,68	0
4	GOL	A	604	6/6	0.85	0.20	74,81,84,85	0

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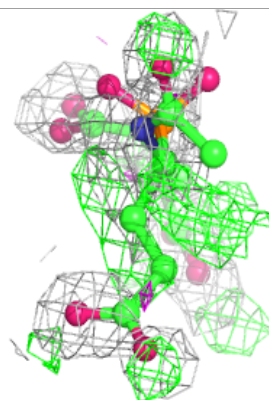
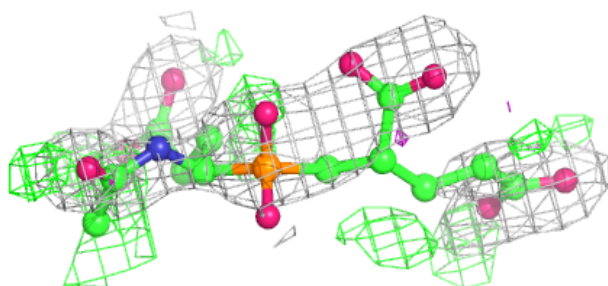
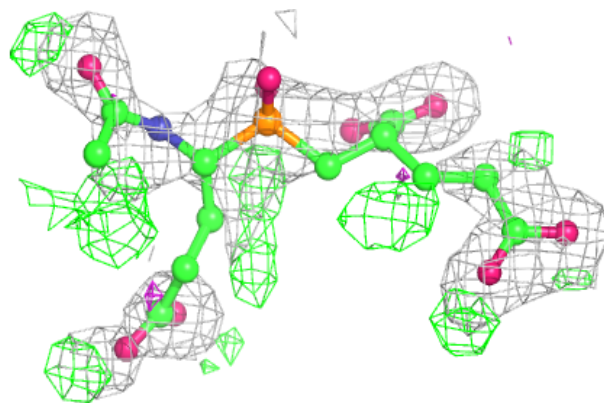
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	603	6/6	0.85	0.27	47,66,74,75	0
4	GOL	D	607	6/6	0.87	0.26	57,82,87,88	0
4	GOL	D	606	6/6	0.90	0.30	47,59,69,73	0
4	GOL	A	601	6/6	0.91	0.30	34,49,55,55	0
4	GOL	A	603	6/6	0.92	0.11	51,64,67,72	0
4	GOL	B	602	6/6	0.93	0.11	55,55,61,63	0
4	GOL	D	605	6/6	0.93	0.34	31,46,52,54	0
4	GOL	C	704	6/6	0.94	0.21	33,38,54,55	0
4	GOL	D	601	6/6	0.94	0.15	49,54,63,70	0
4	GOL	A	602	6/6	0.94	0.13	36,48,54,57	0
4	GOL	B	601	6/6	0.94	0.18	33,47,58,69	0
4	GOL	D	602	6/6	0.96	0.11	32,49,55,65	0
4	GOL	D	604	6/6	0.96	0.15	41,47,56,61	0
7	MG	C	703	1/1	0.97	0.08	24,24,24,24	0
7	MG	B	608	1/1	0.97	0.13	26,26,26,26	0
6	ADP	C	706	27/27	0.98	0.11	22,25,28,30	0
5	RZP	B	605	27/27	0.98	0.10	22,26,34,37	0
8	CL	A	609	1/1	0.98	0.06	46,46,46,46	0
7	MG	A	608	1/1	0.98	0.12	25,25,25,25	0
7	MG	D	610	1/1	0.99	0.07	23,23,23,23	0
8	CL	D	612	1/1	0.99	0.06	45,45,45,45	0
5	RZP	C	705	27/27	0.99	0.11	22,28,35,37	0
6	ADP	D	609	27/27	0.99	0.11	23,27,29,32	0
5	RZP	D	608	27/27	0.99	0.10	23,28,35,37	0
7	MG	B	607	1/1	0.99	0.09	25,25,25,25	0
7	MG	C	702	1/1	0.99	0.13	26,26,26,26	0
5	RZP	A	605	27/27	0.99	0.10	23,29,36,37	0
6	ADP	B	606	27/27	0.99	0.11	21,24,28,29	0
6	ADP	A	606	27/27	0.99	0.10	23,26,29,31	0
7	MG	D	611	1/1	0.99	0.10	26,26,26,26	0
7	MG	A	607	1/1	0.99	0.07	22,22,22,22	0

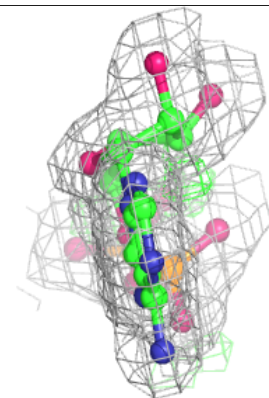
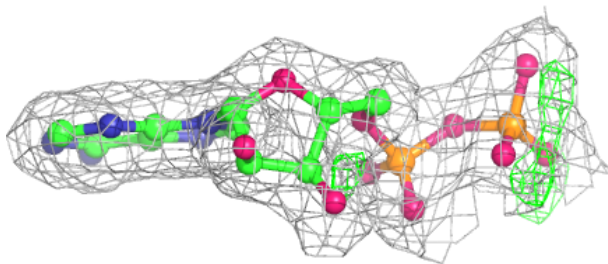
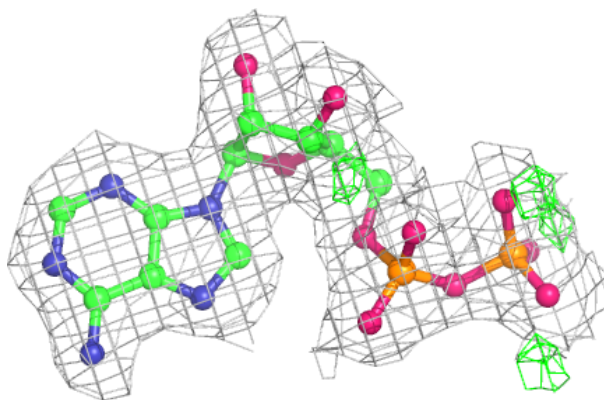
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RZV C 701:

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

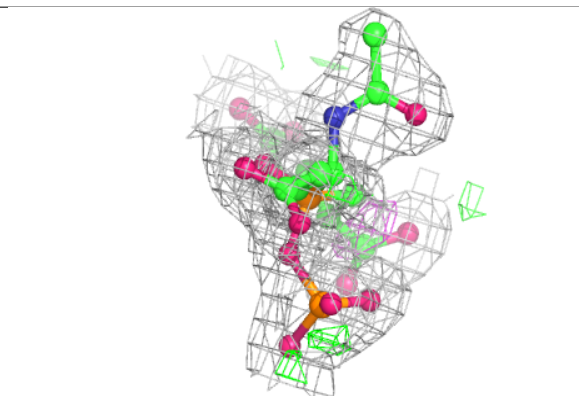
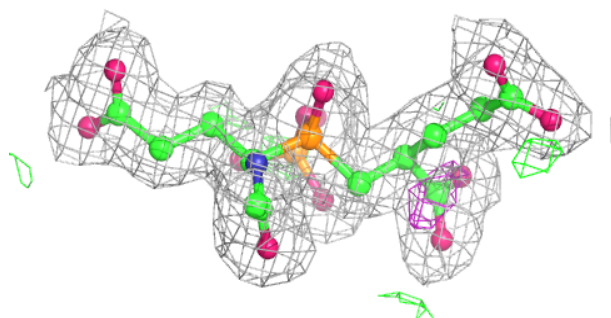
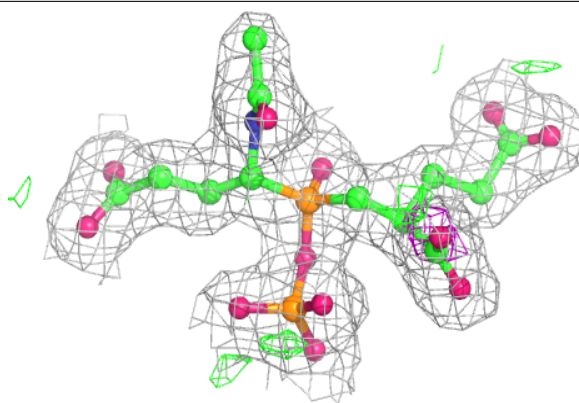
**Electron density around ADP C 706:**

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

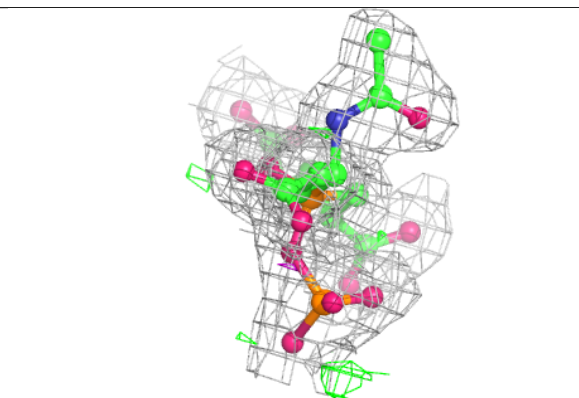
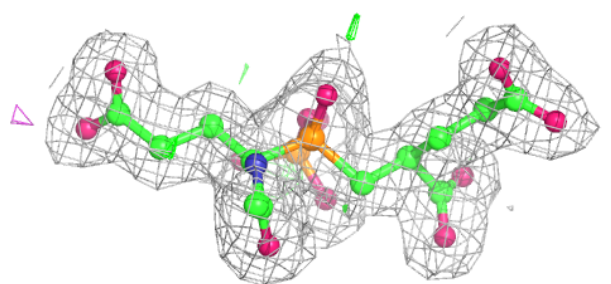
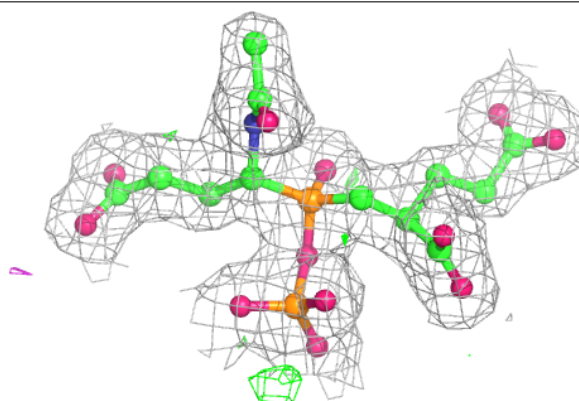


Electron density around RZP B 605:

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

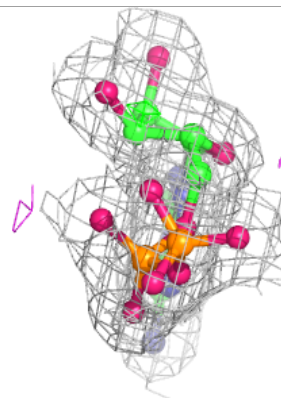
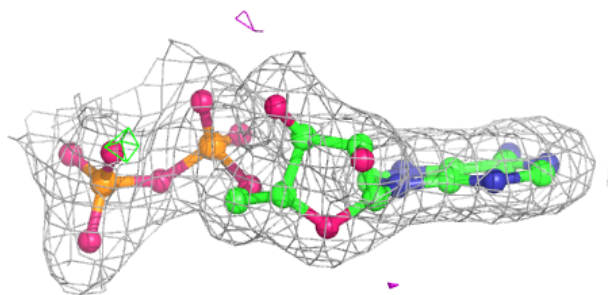
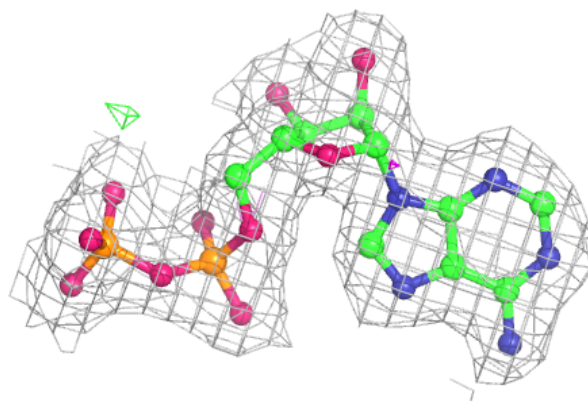
**Electron density around RZP C 705:**

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

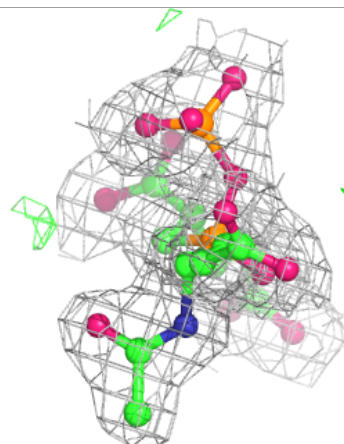
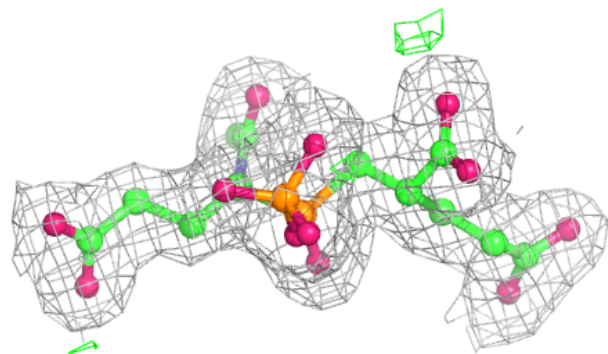
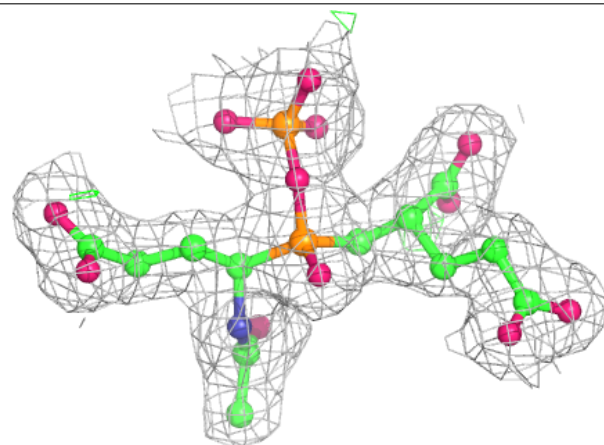


Electron density around ADP D 609:

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

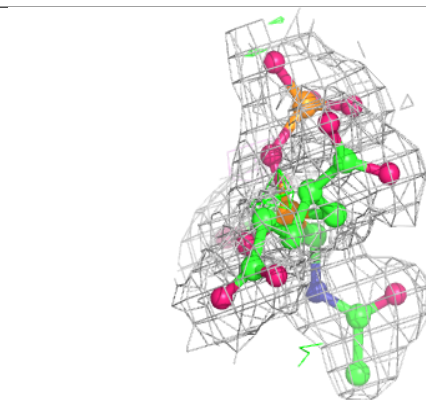
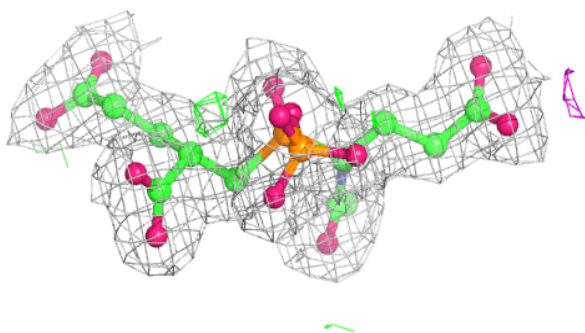
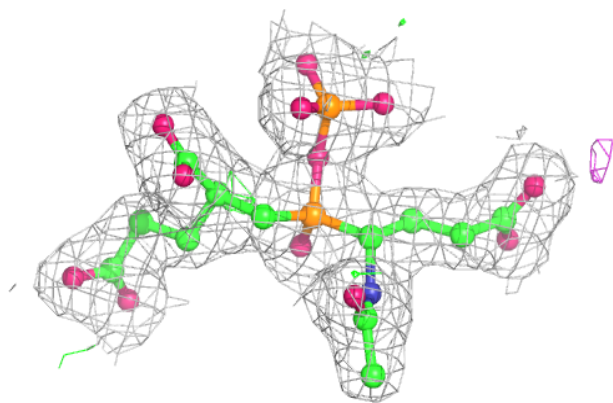
**Electron density around RZP D 608:**

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

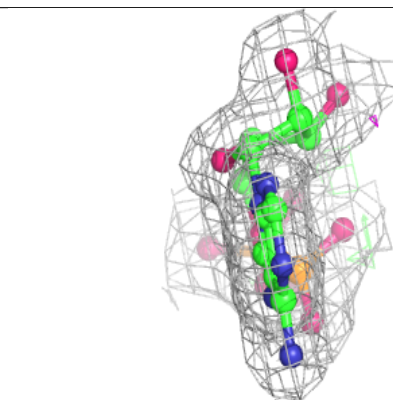
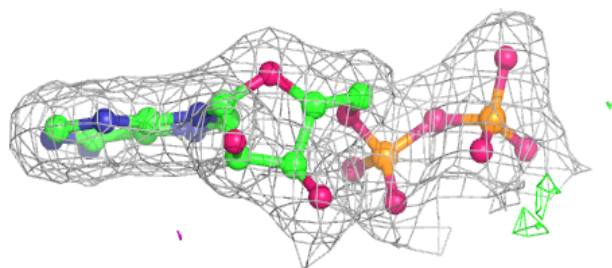
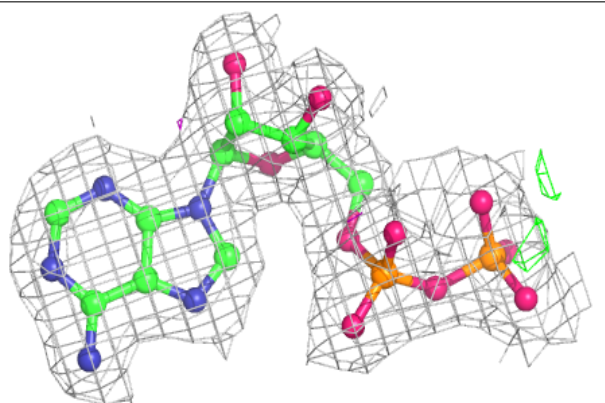


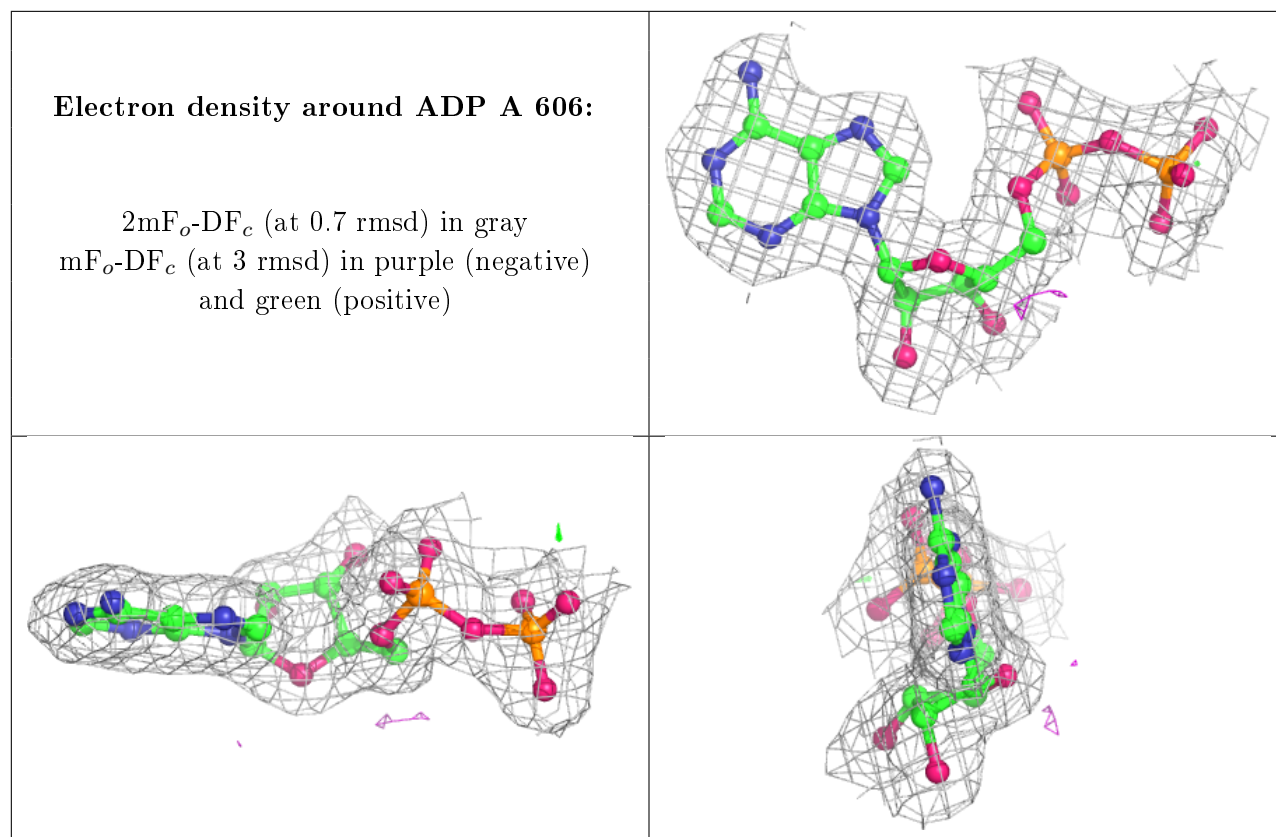
Electron density around RZP A 605:

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

**Electron density around ADP B 606:**

$2mF_o-DF_c$ (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.