



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:10 pm BST

PDB ID : 1AQU
Title : ESTROGEN SULFOTRANSFERASE WITH BOUND INACTIVE COFACT-
TOR PAP AND 17-BETA ESTRADIOL
Authors : Kakuta, Y.; Negishi, M.; Pedersen, L.C.
Deposited on : 1997-08-01
Resolution : 1.60 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 : 2.11
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) : 2.11

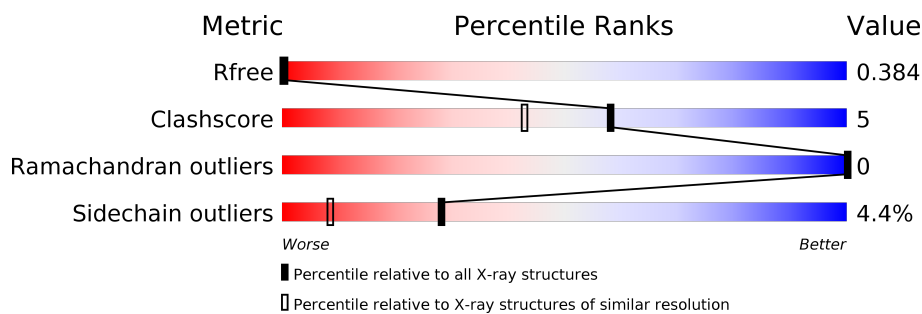
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	297	
1	B	297	

2 Entry composition [i](#)

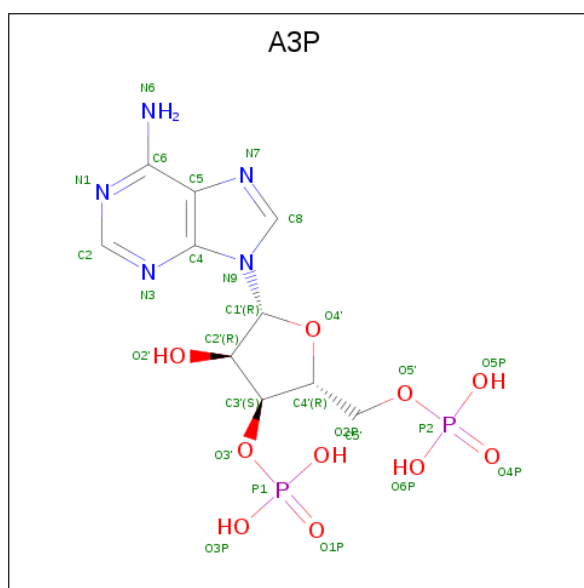
There are 4 unique types of molecules in this entry. The entry contains 5143 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ESTROGEN SULFOTRANSFERASE.

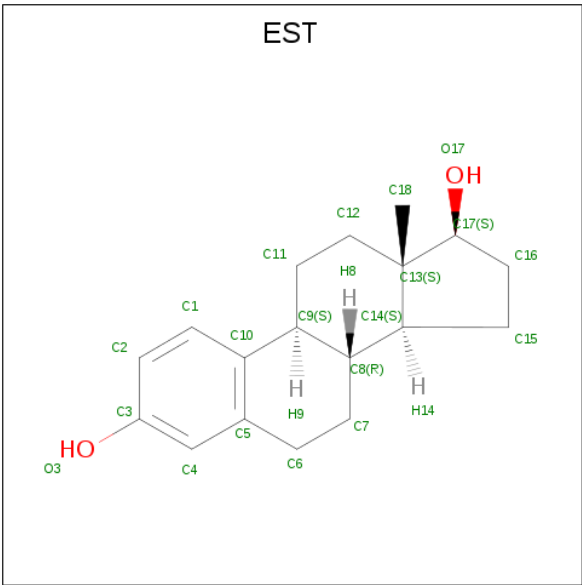
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2389	1549	393	427	20			
1	B	280	Total	C	N	O	S	0	0	0
			2381	1545	392	424	20			

- Molecule 2 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is ESTRADIOL (three-letter code: EST) (formula: $C_{18}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			20	18	2		

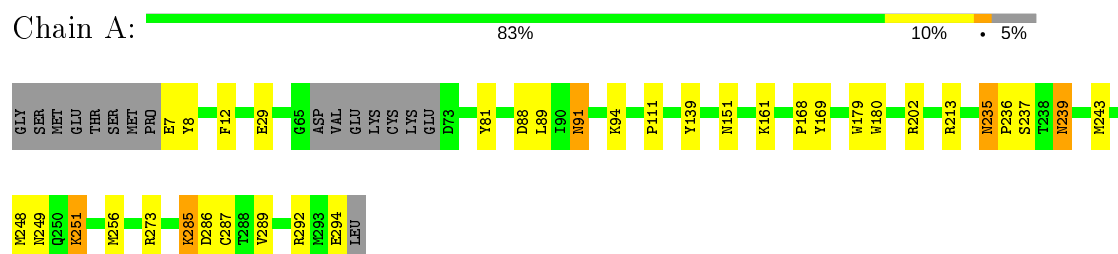
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	125	Total	O	0	0
			125	125		

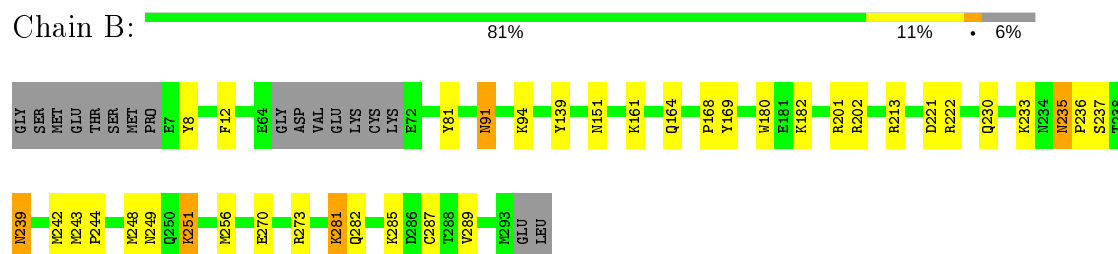
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: ESTROGEN SULFOTRANSFERASE



• Molecule 1: ESTROGEN SULFOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.38Å 80.39Å 80.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 19.13 – 1.58	Depositor EDS
% Data completeness (in resolution range)	81.7 (50.00-1.60) 78.6 (19.13-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 1.58Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.251 0.383 , 0.384	Depositor DCC
R_{free} test set	7229 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,l,k	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	5143	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A3P, EST

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	0.51	0/2456	0.60	0/3306
1	B	0.49	0/2448	0.59	0/3296
All	All	0.50	0/4904	0.60	0/6602

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2389	0	2348	22	1
1	B	2381	0	2341	26	2
2	A	27	0	11	1	0
2	B	27	0	11	0	0
3	A	20	0	24	0	0
3	B	20	0	24	0	0
4	A	154	0	0	1	1
4	B	125	0	0	2	1
All	All	5143	0	4759	46	3

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 5.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:CYS:SG	1:B:289:VAL:HG23	2.19	0.82
1:B:202:ARG:HH11	1:B:202:ARG:HG3	1.47	0.80
1:A:202:ARG:HH11	1:A:202:ARG:HG3	1.47	0.79
1:A:287:CYS:SG	1:A:289:VAL:HG23	2.22	0.79
1:B:233:LYS:HA	1:B:256:MET:HG3	1.76	0.67
1:B:151:ASN:ND2	4:B:371:HOH:O	2.30	0.65
1:A:151:ASN:ND2	4:A:328:HOH:O	2.32	0.62
1:B:202:ARG:NH1	1:B:202:ARG:HG3	2.14	0.59
1:A:202:ARG:NH1	1:A:202:ARG:HG3	2.14	0.57
1:A:235:ASN:ND2	1:A:237:SER:H	2.05	0.55
1:A:29:GLU:H	1:A:29:GLU:CD	2.11	0.54
1:B:239:ASN:C	1:B:239:ASN:HD22	2.11	0.53
1:A:243:MET:HG2	1:A:248:MET:SD	2.49	0.53
1:A:89:LEU:HD23	1:B:244:PRO:HG2	1.89	0.53
1:A:235:ASN:HD22	1:A:235:ASN:C	2.12	0.53
1:A:91:ASN:C	1:A:91:ASN:HD22	2.12	0.53
1:B:235:ASN:ND2	1:B:237:SER:H	2.06	0.53
1:A:239:ASN:C	1:A:239:ASN:HD22	2.13	0.52
1:B:235:ASN:HD22	1:B:235:ASN:C	2.13	0.51
1:B:282:GLN:HE22	1:B:285:LYS:NZ	2.09	0.51
1:B:180:TRP:CG	1:B:289:VAL:HG22	2.46	0.50
1:B:91:ASN:HD22	1:B:91:ASN:C	2.14	0.50
1:B:243:MET:HG2	1:B:248:MET:SD	2.51	0.50
1:A:12:PHE:CE1	1:A:168:PRO:HG3	2.46	0.50
1:A:256:MET:CE	2:A:301:A3P:H8	2.42	0.50
1:B:12:PHE:CE1	1:B:168:PRO:HG3	2.47	0.50
1:B:180:TRP:CD2	1:B:289:VAL:HG22	2.46	0.49
1:A:249:ASN:OD1	1:A:251:LYS:HB2	2.13	0.48
1:B:249:ASN:OD1	1:B:251:LYS:HB2	2.13	0.48
1:B:282:GLN:OE1	1:B:285:LYS:HE3	2.14	0.48
1:B:281:LYS:O	1:B:285:LYS:HG3	2.14	0.47
1:A:180:TRP:CD2	1:A:289:VAL:HG22	2.50	0.47
1:B:201:ARG:NH2	1:B:221:ASP:OD1	2.45	0.46
1:A:168:PRO:O	1:A:169:TYR:HB2	2.17	0.45
1:A:111:PRO:HD3	1:A:179:TRP:CD1	2.52	0.45
1:A:8:TYR:CZ	1:A:161:LYS:HE2	2.51	0.45
1:B:235:ASN:HD22	1:B:236:PRO:N	2.16	0.44
1:A:88:ASP:HB2	1:B:242:MET:HB3	1.99	0.44
1:B:287:CYS:SG	1:B:289:VAL:CG2	3.01	0.44
1:B:281:LYS:HE3	1:B:285:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:HD22	1:A:236:PRO:N	2.16	0.43
1:B:168:PRO:O	1:B:169:TYR:HB2	2.18	0.42
1:A:292:ARG:O	1:A:294:GLU:HG2	2.19	0.42
1:B:8:TYR:CZ	1:B:161:LYS:HE2	2.55	0.41
1:B:182:LYS:HE2	4:B:407:HOH:O	2.21	0.41
1:A:285:LYS:H	1:A:285:LYS:HG3	1.50	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLU:OE1	4:B:367:HOH:O[4_456]	1.51	0.69
1:B:270:GLU:CG	1:B:270:GLU:CG[2_565]	1.86	0.34
1:B:164:GLN:O	4:A:308:HOH:O[3_556]	1.90	0.30

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	277/297 (93%)	267 (96%)	10 (4%)	0	100	100
1	B	276/297 (93%)	262 (95%)	14 (5%)	0	100	100
All	All	553/594 (93%)	529 (96%)	24 (4%)	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	263/278 (95%)	252 (96%)	11 (4%)	30	9
1	B	262/278 (94%)	250 (95%)	12 (5%)	27	8
All	All	525/556 (94%)	502 (96%)	23 (4%)	28	8

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	TYR
1	A	91	ASN
1	A	94	LYS
1	A	139	TYR
1	A	213	ARG
1	A	235	ASN
1	A	239	ASN
1	A	251	LYS
1	A	273	ARG
1	A	285	LYS
1	A	286	ASP
1	B	81	TYR
1	B	91	ASN
1	B	94	LYS
1	B	139	TYR
1	B	213	ARG
1	B	222	ARG
1	B	230	GLN
1	B	235	ASN
1	B	239	ASN
1	B	251	LYS
1	B	273	ARG
1	B	281	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	122	ASN
1	A	151	ASN
1	A	166	GLN

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Mol	Chain	Res	Type
1	A	234	ASN
1	A	235	ASN
1	A	239	ASN
1	B	91	ASN
1	B	95	GLN
1	B	122	ASN
1	B	151	ASN
1	B	166	GLN
1	B	226	HIS
1	B	235	ASN
1	B	239	ASN
1	B	282	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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
2	A3P	B	302	-	26,29,29	1.11	1 (3%)	31,45,45	0.97	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EST	B	303	-	23,23,23	2.07	9 (39%)	36,36,36	1.04	4 (11%)
2	A3P	A	301	-	26,29,29	1.15	3 (11%)	31,45,45	0.94	2 (6%)
3	EST	A	304	-	23,23,23	1.96	8 (34%)	36,36,36	1.05	3 (8%)

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
2	A3P	B	302	-	-	0/11/31/31	0/3/3/3
3	EST	B	303	-	-	-	0/4/4/4
2	A3P	A	301	-	-	0/11/31/31	0/3/3/3
3	EST	A	304	-	-	-	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	EST	C5-C10	3.89	1.46	1.40
3	A	304	EST	C5-C10	3.61	1.45	1.40
3	B	303	EST	C9-C8	3.39	1.58	1.54
3	B	303	EST	C1-C10	3.38	1.44	1.39
3	A	304	EST	C1-C10	3.25	1.44	1.39
3	A	304	EST	C9-C8	3.02	1.57	1.54
3	B	303	EST	C8-C14	3.00	1.59	1.53
2	B	302	A3P	C2-N3	2.84	1.36	1.32
3	A	304	EST	C8-C14	2.83	1.59	1.53
3	A	304	EST	C4-C3	2.70	1.43	1.39
3	B	303	EST	C4-C5	2.61	1.44	1.39
2	A	301	A3P	C2-N3	2.55	1.36	1.32
3	A	304	EST	C4-C5	2.42	1.43	1.39
3	A	304	EST	C18-C13	2.37	1.58	1.54
3	B	303	EST	C13-C14	2.34	1.59	1.55
3	B	303	EST	C4-C3	2.26	1.42	1.39
3	B	303	EST	C18-C13	2.16	1.58	1.54
3	A	304	EST	C10-C9	2.07	1.55	1.52
2	A	301	A3P	P1-O2P	-2.06	1.46	1.54
2	A	301	A3P	P2-O5P	-2.04	1.47	1.54
3	B	303	EST	C10-C9	2.04	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	EST	C15-C14-C8	2.54	123.26	119.08
2	A	301	A3P	P2-O5'-C5'	2.41	124.94	118.30
3	A	304	EST	C16-C17-C13	2.40	106.44	104.53
3	B	303	EST	C15-C14-C8	2.37	122.99	119.08
3	B	303	EST	C16-C17-C13	2.22	106.29	104.53
2	A	301	A3P	C5-C6-N6	2.21	123.71	120.35
2	B	302	A3P	P2-O5'-C5'	2.17	124.27	118.30
2	B	302	A3P	O2'-C2'-C3'	2.12	117.19	111.17
2	B	302	A3P	C5-C6-N6	2.06	123.49	120.35
3	B	303	EST	C13-C14-C8	-2.04	111.36	114.38
3	B	303	EST	C11-C9-C8	-2.04	108.65	111.39
3	A	304	EST	C13-C14-C8	-2.03	111.37	114.38

There are no chirality outliers.

There are no torsion outliers.

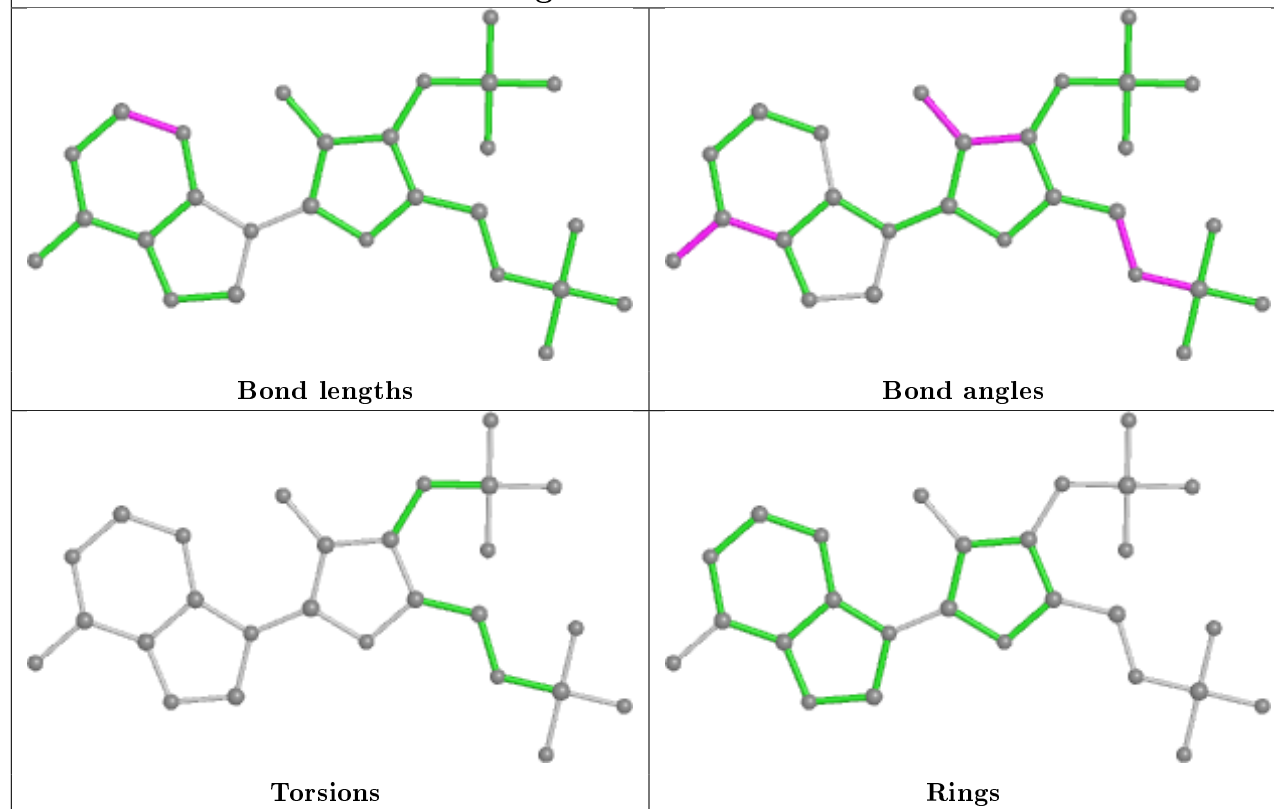
There are no ring outliers.

1 monomer is involved in 1 short contact:

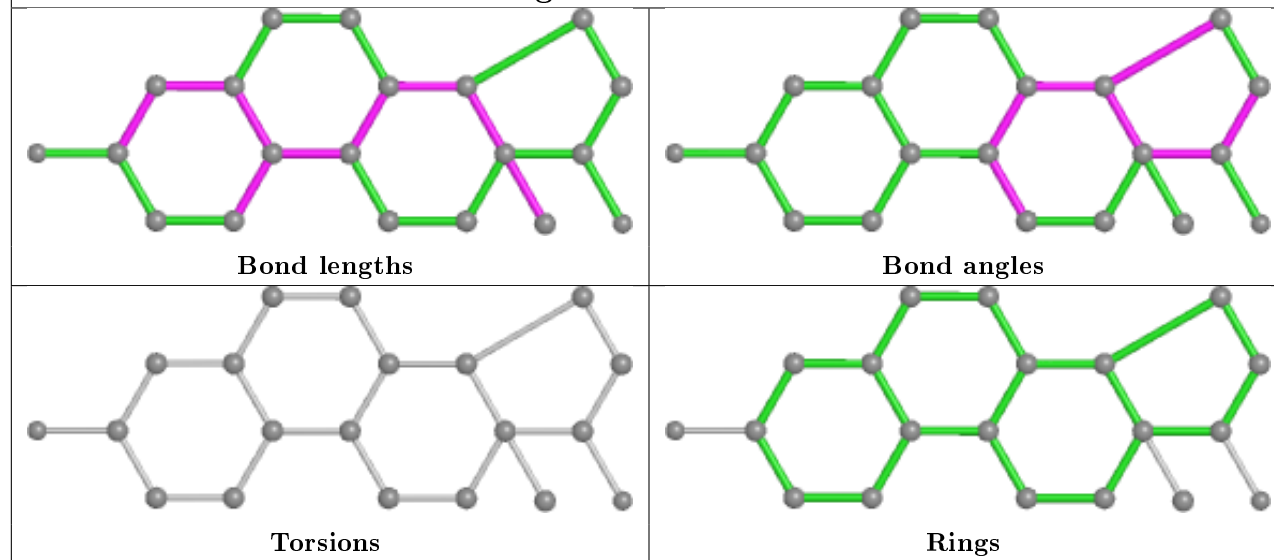
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	A3P	1	0

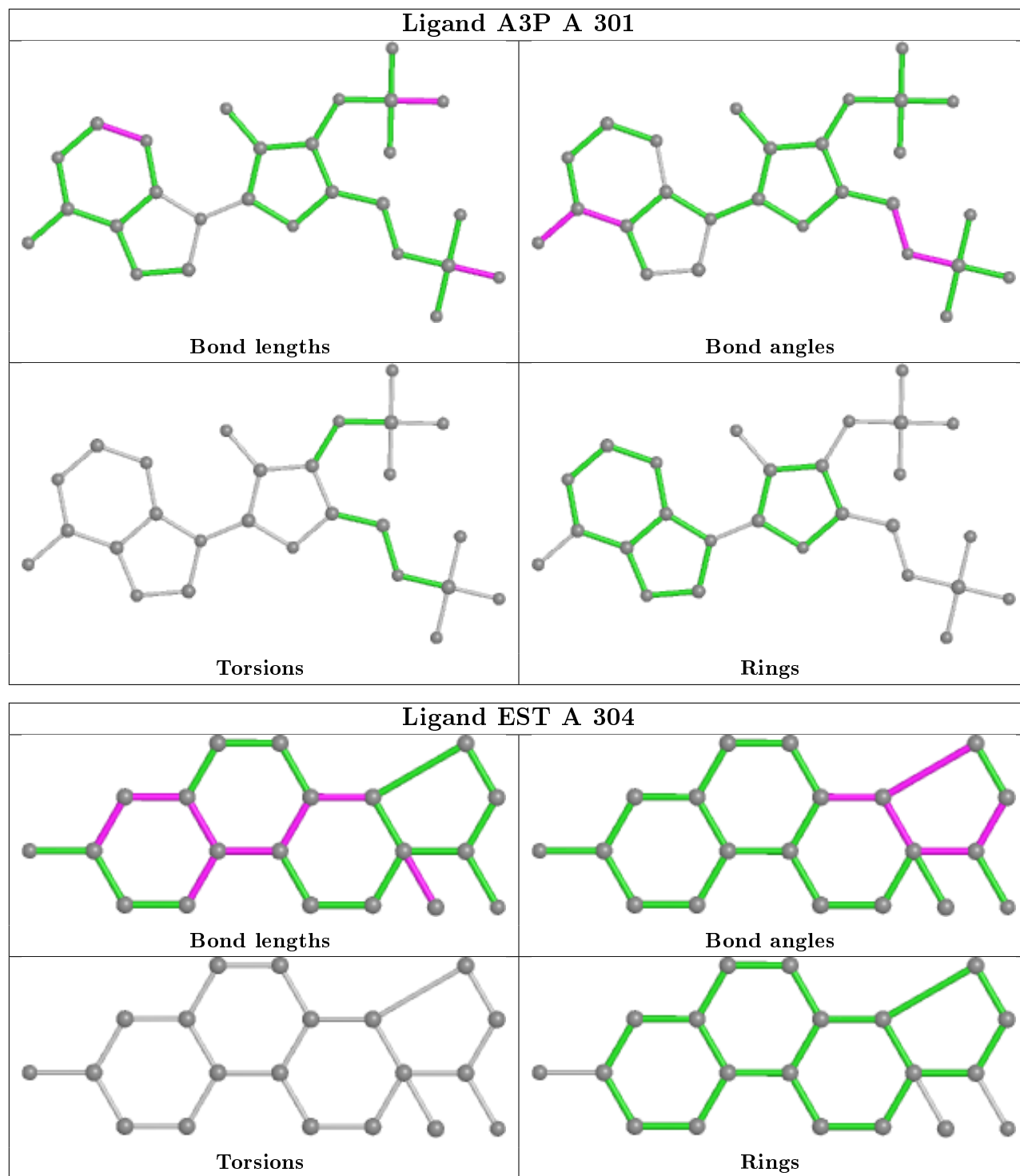
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A3P B 302



Ligand EST B 303





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

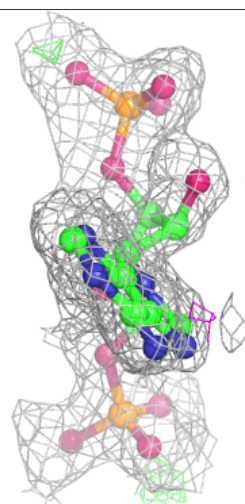
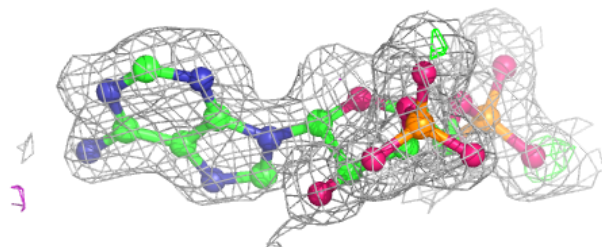
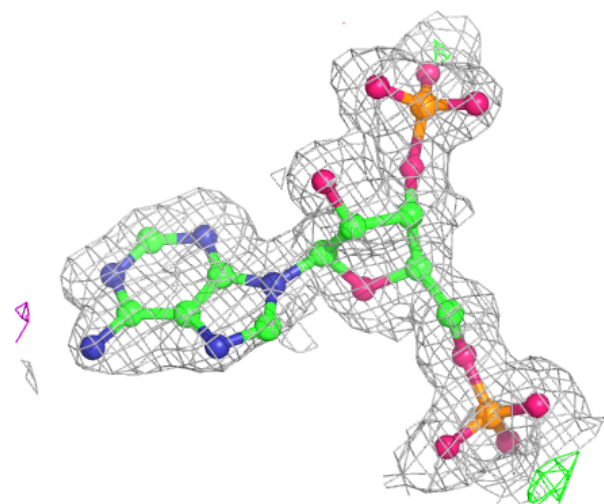
6.4 Ligands

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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.

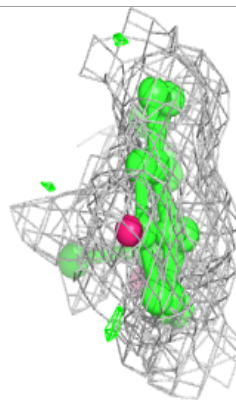
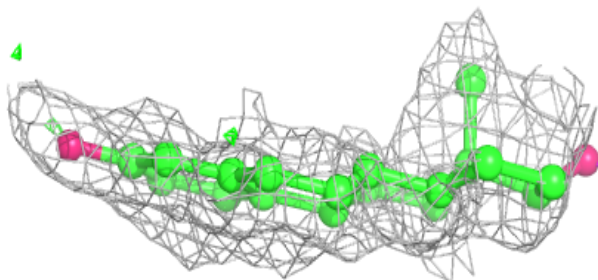
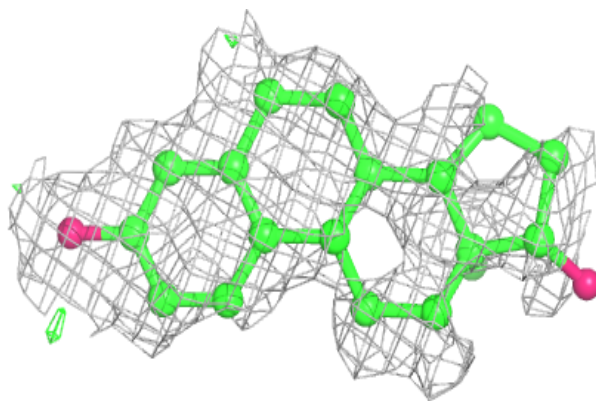
Electron density around A3P B 302:

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



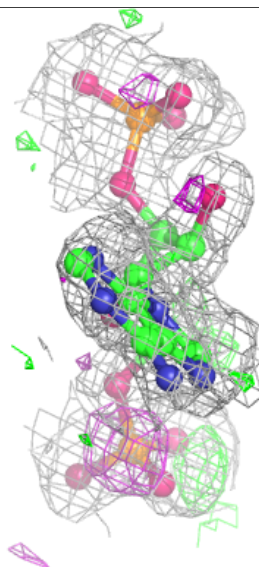
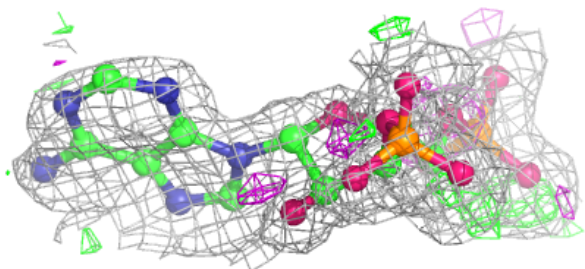
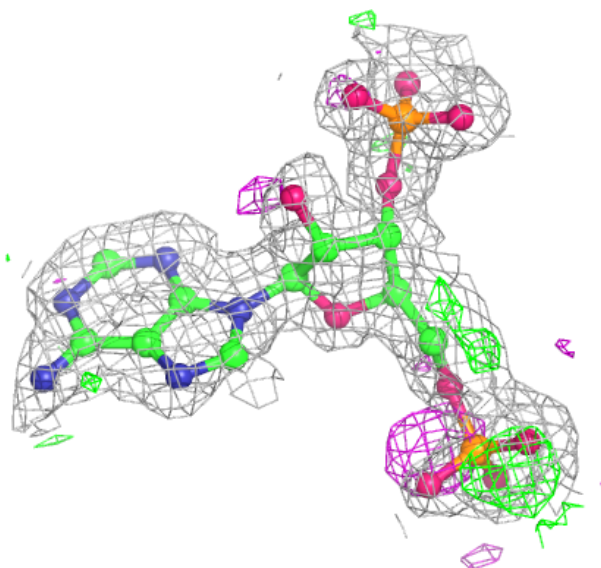
Electron density around EST B 303:

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



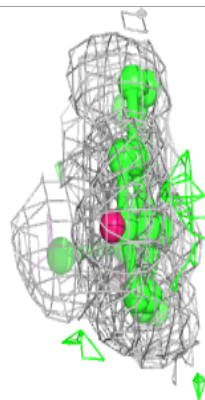
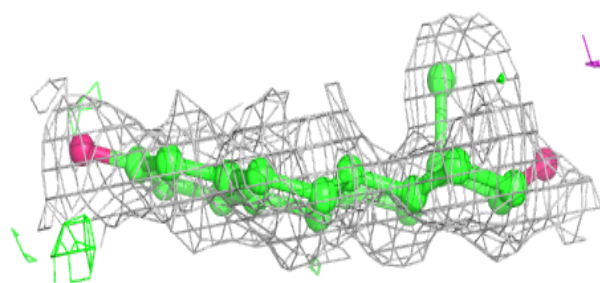
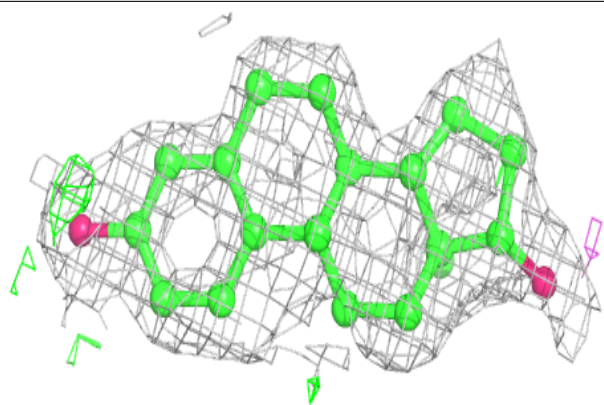
Electron density around A3P A 301:

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



Electron density around EST A 304:

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



6.5 Other polymers [i](#)

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