WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 18, 2023 – 03:01 am GMT

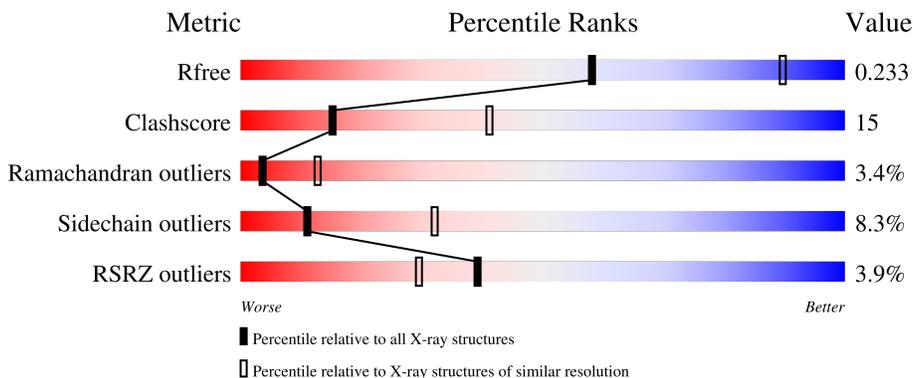|		
PDB ID	:	4TWB
Title	:	Sulfolobus solfataricus ribose-phosphate pyrophosphokinase
Authors	:	Kadziola, A.
Deposited on	:	2014-06-30
Resolution	:	2.80 Å(reported)

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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 2.80 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	Percentile Ranks	Value
Rfree		0.233
Clashscore		15
Ramachandran outliers		3.4%
Sidechain outliers		8.3%
RSRZ outliers		3.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of 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 <=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	291	3% / 68% 22% · · ·
1	B	291	5% / 64% 26% 5% · ·
1	C	291	3% / 63% 27% · · ·
1	D	291	3% / 63% 27% · · ·
1	E	291	4% / 66% 24% · · ·

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W O R L D W I D E
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Mol	Chain	Length	Quality of chain
1	F	291	4% ▇▇▇▇▇▇▇▇▇▇▇▇▇▇▇▇▇▇▇▇ 67% ▇▇▇▇▇ 23% ▇ · · ·

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:

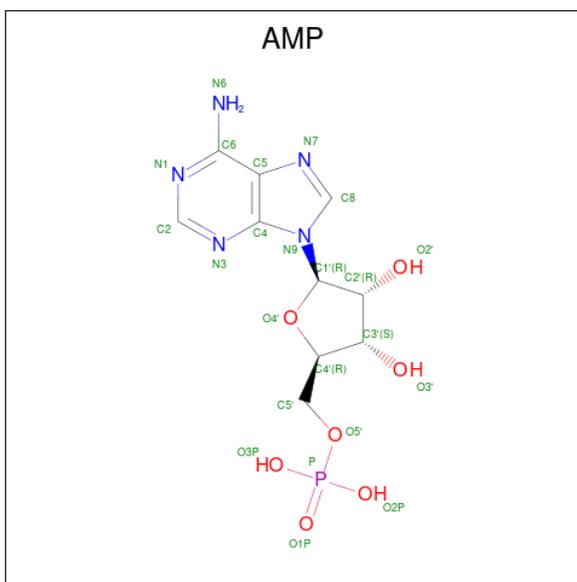| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	D	301	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13194 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.

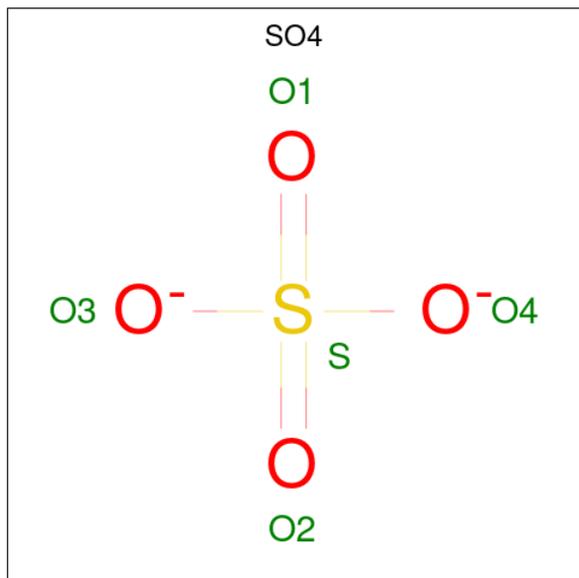- Molecule 1 is a protein called Ribose-phosphate pyrophosphokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2167	1386	368	412	1			
1	B	278	Total	C	N	O	S	0	0	0
			2167	1386	368	412	1			
1	C	278	Total	C	N	O	S	0	0	0
			2167	1386	368	412	1			
1	D	278	Total	C	N	O	S	0	0	0
			2167	1386	368	412	1			
1	E	278	Total	C	N	O	S	0	0	0
			2167	1386	368	412	1			
1	F	278	Total	C	N	O	S	0	0	0
			2167	1386	368	412	1			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	F	1	Total 23	C 10	N 5	O 7	P 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	E	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

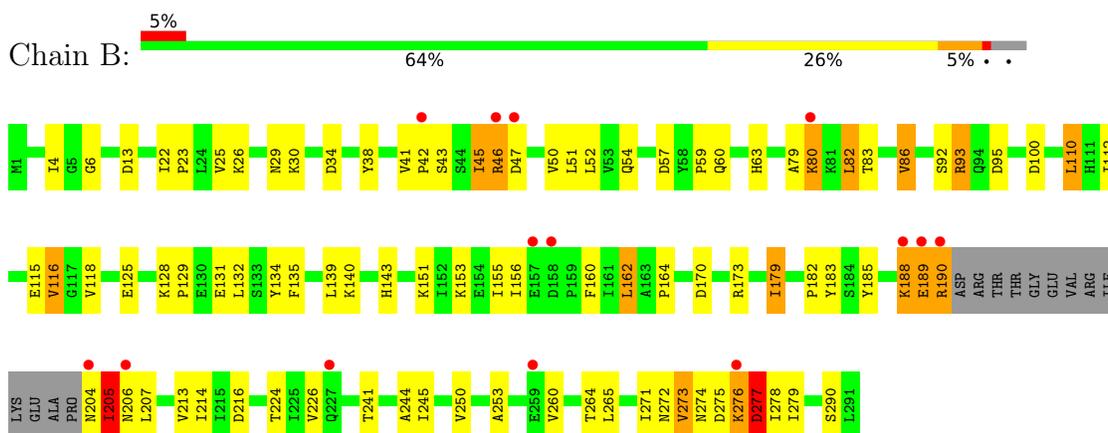| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	O 4	0	0
4	B	4	Total 4	O 4	0	0
4	C	4	Total 4	O 4	0	0
4	D	4	Total 4	O 4	0	0
4	E	4	Total 4	O 4	0	0
4	F	4	Total 4	O 4	0	0

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.
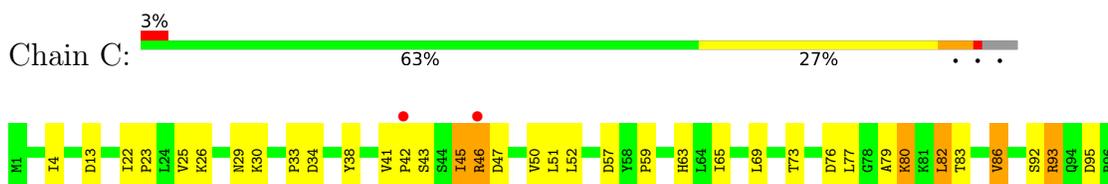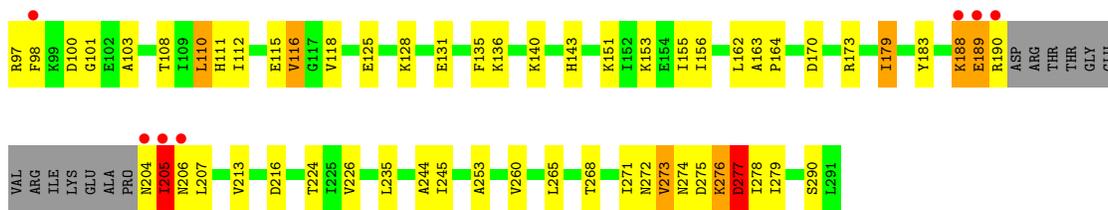
- Molecule 1: Ribose-phosphate pyrophosphokinase

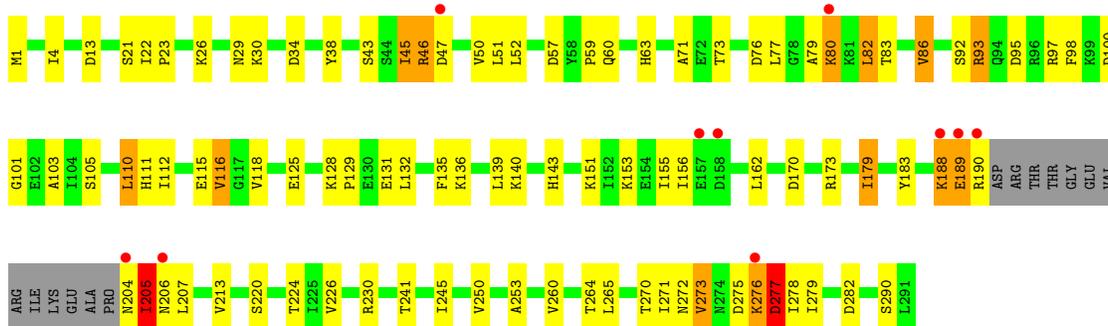- Molecule 1: Ribose-phosphate pyrophosphokinase
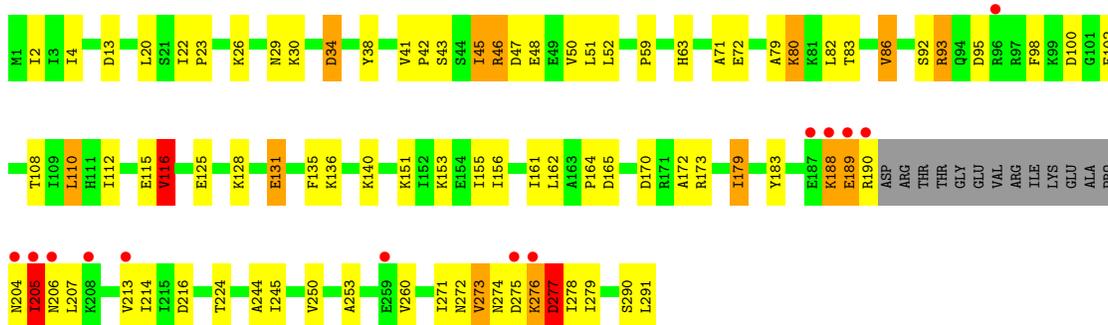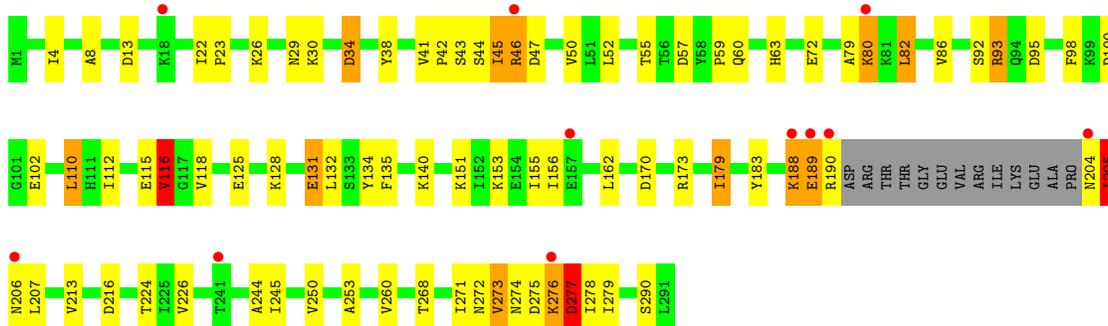

- Molecule 1: Ribose-phosphate pyrophosphokinase

R97 F98 K99 D100 G101 E102 A103 T108 I109 L110 H111 I112 E115 V116 G117 V118 E125 K128 E131 F135 K136 K140 H143 K151 I152 K153 I155 I156 L162 A163 P164 D170 R173 I179 Y183 K188 E189 R190 ASP ARG THR GLY GLU

VAL ARG ILE LYS GLU ALA PRO N204 I205 N206 L207 V213 D216 T224 I225 V226 L235 A244 I245 A253 V260 L265 T268 I271 N272 V273 N274 D275 K276 D277 I278 I279 S290 L291

• Molecule 1: Ribose-phosphate pyrophosphokinase

Chain D:

3% | 63% | 27% | • • •

M1 I4 D13 S21 I22 P23 K26 N29 K30 D34 Y38 S43 S44 I45 R46 D47 V50 L51 L52 D57 Y58 P59 Q60 H63 A71 E72 T73 D76 L77 G78 A79 K80 K81 L82 T83 V86 S92 R93 Q94 D95 R96 F98 K99 D100

G101 E102 A103 I104 S105 L110 H111 I112 E115 V116 G117 V118 E125 K128 P129 E130 E131 L132 F135 K136 L139 K140 H143 K151 I152 K153 E154 I155 I156 E157 D158 L162 D170 R173 I179 Y183 K188 E189 R190 ASP ARG THR GLY GLU VAL

ARG ILE LYS GLU ALA PRO N204 I205 N206 L207 V213 S220 T224 I225 V226 R230 T241 I245 V250 A253 V260 T264 L265 T270 I271 N272 V273 N274 D275 K276 D277 I278 I279 D282 S290 L291

• Molecule 1: Ribose-phosphate pyrophosphokinase

Chain E:

4% | 66% | 24% | • • •

M1 I2 I3 I4 D13 L20 S21 I22 P23 K26 N29 K30 D34 Y38 V41 P42 S43 S44 I45 R46 D47 E48 E49 V50 L51 L52 P59 H63 A71 E72 A79 K80 K81 L82 T83 V86 S92 R93 Q94 D95 R96 R97 F98 K99 D100 G101 E102

T108 I109 L110 H111 I112 E115 V116 E125 K128 E131 F135 K136 K140 K151 I152 K153 E154 I155 I156 I161 L162 A163 P164 D165 D170 R171 A172 R173 I179 Y183 E187 K188 E189 R190 ASP ARG THR GLY GLU VAL ARG ILE LYS GLU ALA PRO

N204 I205 N206 L207 K208 V213 I214 I215 D216 T224 A244 I245 V250 A253 E259 V260 I271 N272 V273 N274 D275 K276 D277 I278 I279 S290 L291

• Molecule 1: Ribose-phosphate pyrophosphokinase

Chain F:

4% | 67% | 23% | • • •

M1 I4 A8 D13 K18 I22 P23 K26 N29 K30 D34 Y38 V41 P42 S43 S44 I45 R46 D47 V50 L51 L52 T55 T56 D57 Y58 P59 Q60 H63 E72 A79 K80 K81 L82 V86 S92 R93 Q94 D95 F98 K99 D100

G101 E102 L110 H111 I112 E115 V118 G117 V118 E125 K128 E131 L132 S133 Y134 F135 K140 K151 I152 K153 E154 I155 I156 E157 L162 D170 R173 I179 Y183 K188 E189 R190 ASP ARG THR GLY GLU VAL ARG ILE LYS GLU ALA PRO N204 I205

N206 L207 V213 V226 D216 T224 I225 T241 A244 I245 V250 A253 V260 T268 I271 N272 V273 N274 D275 K276 D277 I278 I279 S290 L291

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4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.22Å 92.85Å 138.34Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.98-2.80) 96.8 (19.98-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.235 , 0.265 0.231 , 0.233	Depositor DCC
R_{free} test set	2447 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.0	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13194	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: AMP, SO4

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	0.38	0/2196	0.59	1/2971 (0.0%)
1	B	0.45	0/2196	0.63	1/2971 (0.0%)
1	C	0.46	0/2196	0.63	1/2971 (0.0%)
1	D	0.46	0/2196	0.65	1/2971 (0.0%)
1	E	0.44	0/2196	0.63	1/2971 (0.0%)
1	F	0.44	0/2196	0.64	1/2971 (0.0%)
All	All	0.44	0/13176	0.63	6/17826 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	277	ASP	N-CA-C	-5.89	95.09	111.00
1	F	277	ASP	N-CA-C	-5.82	95.28	111.00
1	A	277	ASP	N-CA-C	-5.64	95.77	111.00
1	D	277	ASP	N-CA-C	-5.61	95.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	277	ASP	N-CA-C	-5.47	96.23	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	LYS	Peptide
1	A	277	ASP	Peptide
1	B	276	LYS	Peptide
1	B	277	ASP	Peptide
1	C	276	LYS	Peptide

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	2167	0	2278	60	0
1	B	2167	0	2278	65	2
1	C	2167	0	2278	76	0
1	D	2167	0	2278	86	1
1	E	2167	0	2278	71	0
1	F	2167	0	2278	64	0
2	A	46	0	24	1	0
2	C	46	0	24	2	0
2	E	23	0	12	4	0
2	F	23	0	12	4	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	1
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	4	0	0	0	0
All	All	13194	0	13740	404	2

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 15.

The worst 5 of 404 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:F:277:ASP:HB3	1:F:278:ILE:HA	1.31	1.13
1:E:277:ASP:HB3	1:E:278:ILE:HA	1.31	1.10
1:D:277:ASP:HB3	1:D:278:ILE:HA	1.31	1.10
1:C:277:ASP:HB3	1:C:278:ILE:HA	1.30	1.09
1:A:277:ASP:HB3	1:A:278:ILE:HA	1.32	1.06

All (2) 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:B:190:ARG:NH2	3:D:301:SO4:O3[2_646]	1.80	0.40
1:B:185:TYR:OH	1:D:230:ARG:NH2[2_646]	2.09	0.11

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	274/291 (94%)	245 (89%)	20 (7%)	9 (3%)	4	13
1	B	274/291 (94%)	246 (90%)	19 (7%)	9 (3%)	4	13
1	C	274/291 (94%)	248 (90%)	17 (6%)	9 (3%)	4	13
1	D	274/291 (94%)	245 (89%)	20 (7%)	9 (3%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	274/291 (94%)	245 (89%)	19 (7%)	10 (4%)	3	11
1	F	274/291 (94%)	245 (89%)	19 (7%)	10 (4%)	3	11
All	All	1644/1746 (94%)	1474 (90%)	114 (7%)	56 (3%)	3	13

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	116	VAL
1	A	205	ILE
1	A	253	ALA
1	B	46	ARG

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	241/252 (96%)	221 (92%)	20 (8%)	11	32
1	B	241/252 (96%)	222 (92%)	19 (8%)	12	34
1	C	241/252 (96%)	221 (92%)	20 (8%)	11	32
1	D	241/252 (96%)	222 (92%)	19 (8%)	12	34
1	E	241/252 (96%)	220 (91%)	21 (9%)	10	30
1	F	241/252 (96%)	220 (91%)	21 (9%)	10	30
All	All	1446/1512 (96%)	1326 (92%)	120 (8%)	11	32

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	273	VAL
1	F	162	LEU
1	D	179	ILE
1	F	116	VAL
1	F	273	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	10	ASN

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 ⓘ

12 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	$\#|Z| > 2$
3	SO4	B	301	-	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	E	301	-	4,4,4	0.24	0	6,6,6	0.12	0
2	AMP	A	301	-	22,25,25	1.08	2 (9%)	25,38,38	1.30	2 (8%)
3	SO4	C	302	-	4,4,4	0.17	0	6,6,6	0.08	0
2	AMP	E	302	-	22,25,25	1.02	2 (9%)	25,38,38	1.33	3 (12%)
2	AMP	A	303	-	22,25,25	1.04	1 (4%)	25,38,38	1.39	3 (12%)
3	SO4	A	302	-	4,4,4	0.09	0	6,6,6	0.12	0
2	AMP	F	301	-	22,25,25	1.14	2 (9%)	25,38,38	1.29	3 (12%)
3	SO4	D	301	-	4,4,4	0.22	0	6,6,6	0.47	0
2	AMP	C	303	-	22,25,25	1.09	2 (9%)	25,38,38	1.37	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	SO4	F	302	-	4,4,4	0.19	0	6,6,6	0.20	0
2	AMP	C	301	-	22,25,25	1.02	1 (4%)	25,38,38	1.34	2 (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	AMP	A	301	-	-	3/6/26/26	0/3/3/3
2	AMP	E	302	-	-	3/6/26/26	0/3/3/3
2	AMP	A	303	-	-	3/6/26/26	0/3/3/3
2	AMP	F	301	-	-	3/6/26/26	0/3/3/3
2	AMP	C	303	-	-	3/6/26/26	0/3/3/3
2	AMP	C	301	-	-	3/6/26/26	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	AMP	C5-C4	2.96	1.48	1.40
2	A	301	AMP	C5-C4	2.86	1.48	1.40
2	C	303	AMP	C5-C4	2.84	1.48	1.40
2	C	301	AMP	C5-C4	2.77	1.48	1.40
2	E	302	AMP	C5-C4	2.67	1.48	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	303	AMP	N3-C2-N1	-3.89	122.59	128.68
2	C	303	AMP	N3-C2-N1	-3.49	123.22	128.68
2	C	301	AMP	N3-C2-N1	-3.43	123.32	128.68
2	A	301	AMP	N3-C2-N1	-3.26	123.59	128.68
2	E	302	AMP	N3-C2-N1	-3.15	123.76	128.68

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	AMP	C5'-O5'-P-O1P
2	A	301	AMP	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
2	A	301	AMP	C5'-O5'-P-O3P
2	A	303	AMP	C5'-O5'-P-O1P
2	A	303	AMP	C5'-O5'-P-O2P

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	AMP	1	0
2	E	302	AMP	4	0
2	F	301	AMP	4	0
3	D	301	SO4	1	1
2	C	303	AMP	1	0
2	C	301	AMP	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 then 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 AMP A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP E 302

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP A 303

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP C 303

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP C 301

Bond lengths

Bond angles

Torsions

Rings
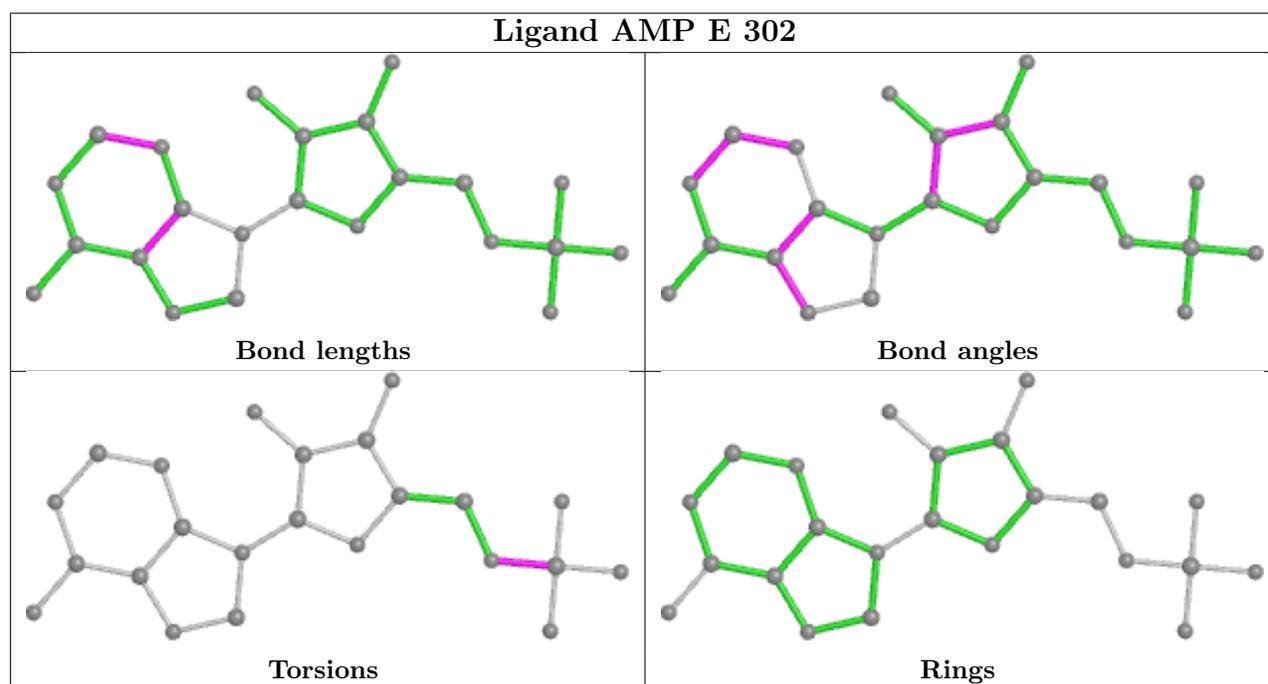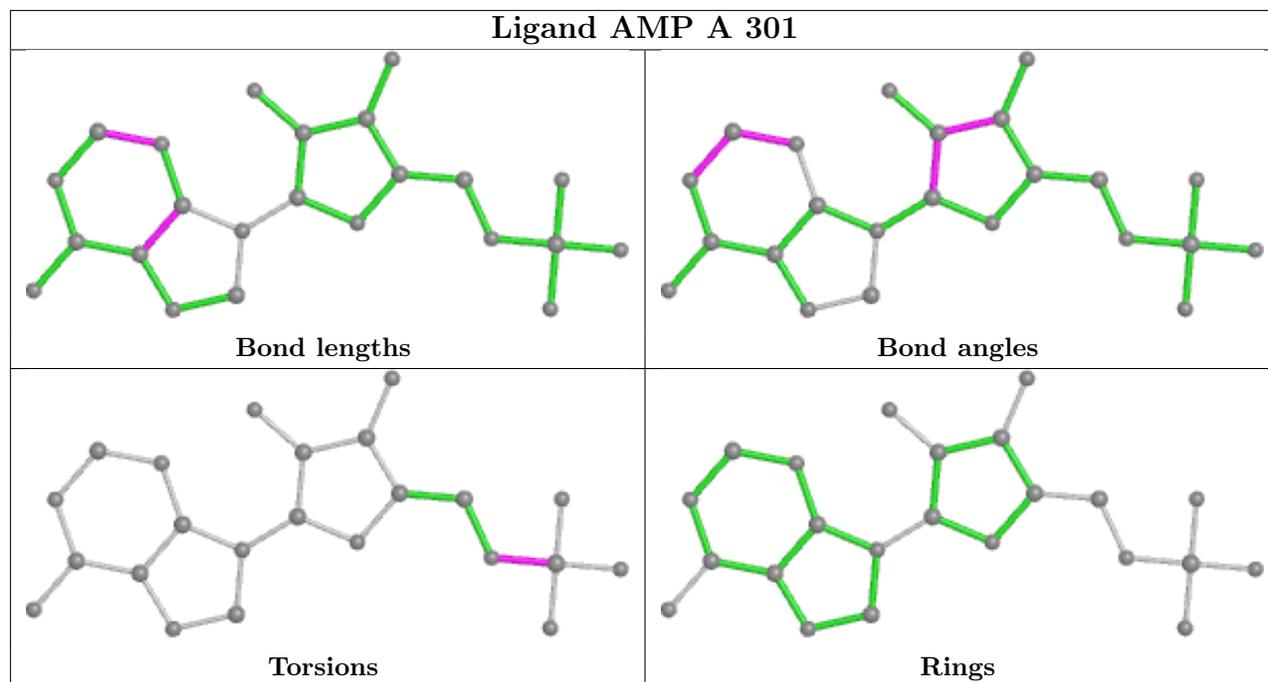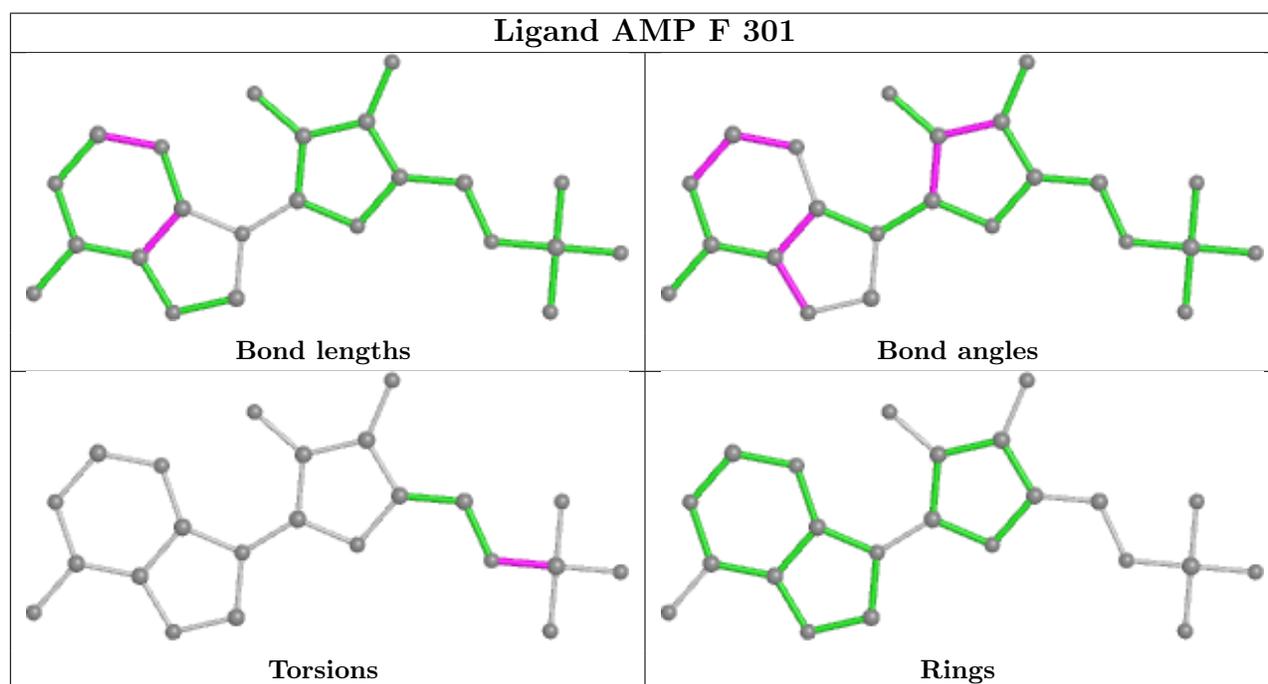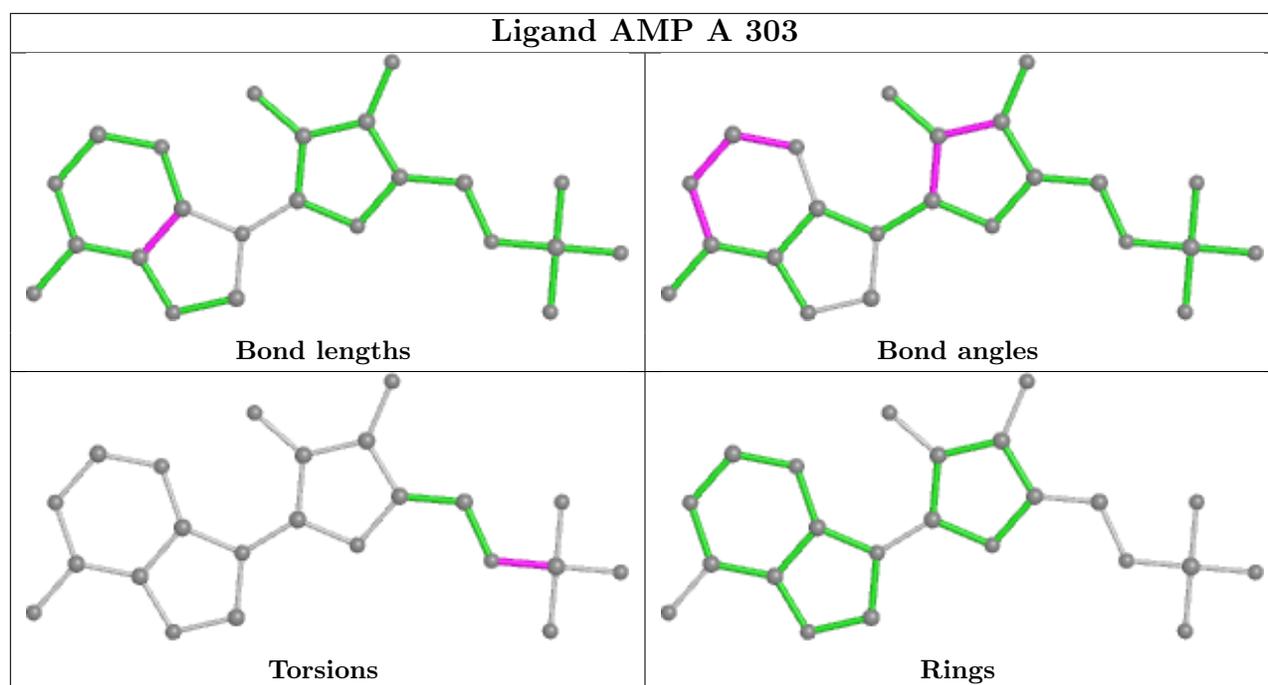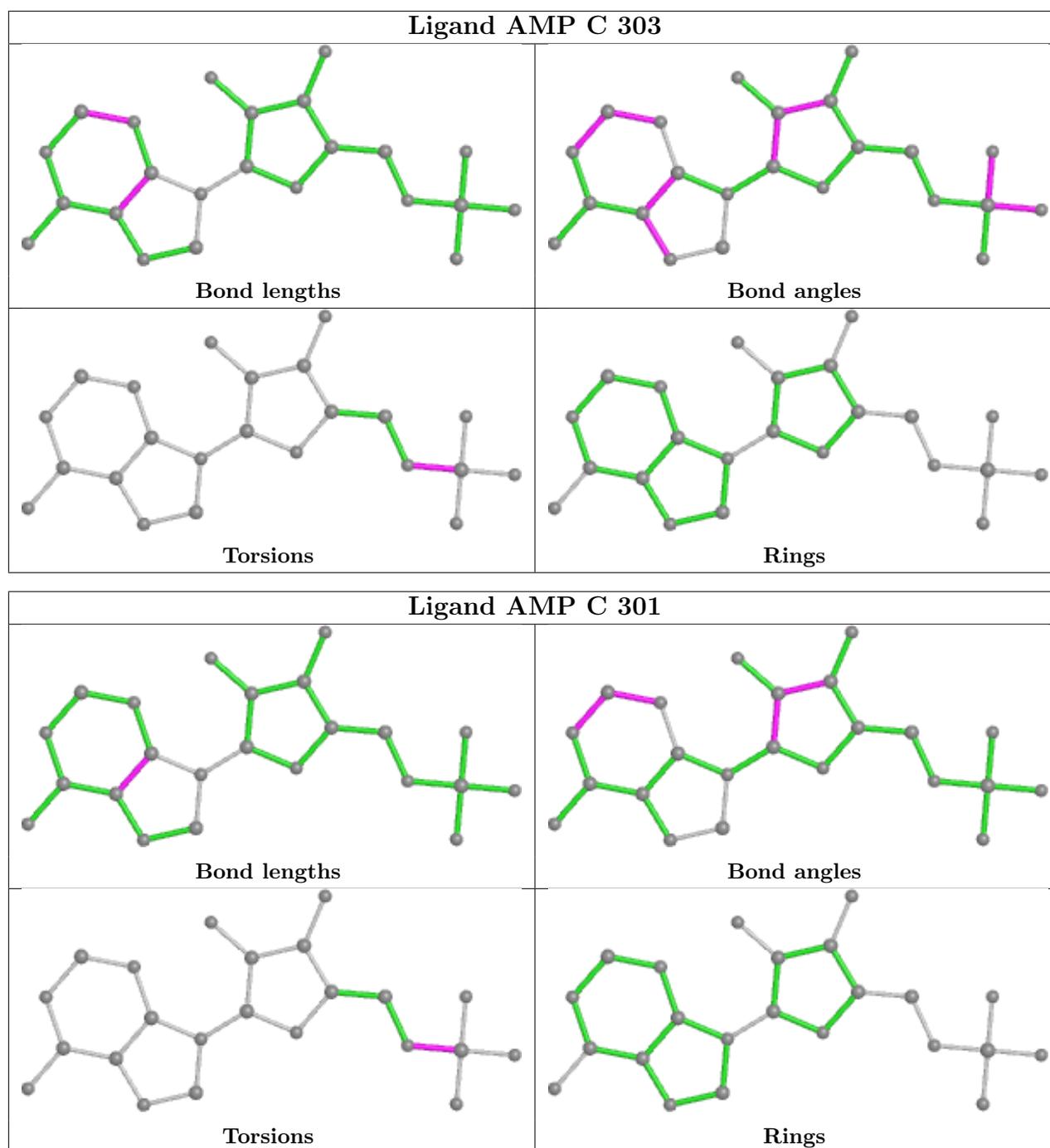
5.7 Other polymers ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	278/291 (95%)	-0.03	8 (2%)	51	41	28, 50, 88, 151	0
1	B	278/291 (95%)	-0.07	14 (5%)	28	19	30, 51, 92, 144	0
1	C	278/291 (95%)	-0.11	9 (3%)	47	37	25, 48, 88, 150	0
1	D	278/291 (95%)	-0.08	10 (3%)	42	32	26, 51, 90, 154	0
1	E	278/291 (95%)	-0.01	13 (4%)	31	22	26, 51, 93, 153	0
1	F	278/291 (95%)	-0.09	11 (3%)	38	28	27, 50, 88, 153	0
All	All	1668/1746 (95%)	-0.06	65 (3%)	39	29	25, 50, 91, 154	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	ASN	12.0
1	E	189	GLU	8.8
1	E	204	ASN	7.8
1	D	204	ASN	7.1
1	F	190	ARG	6.7

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AMP	C	301	23/23	0.79	0.38	39,95,135,159	0
3	SO4	F	302	5/5	0.80	0.19	69,90,98,127	0
2	AMP	F	301	23/23	0.81	0.30	43,89,140,170	0
2	AMP	A	303	23/23	0.82	0.34	43,97,140,172	0
2	AMP	C	303	23/23	0.82	0.36	28,90,145,171	0
3	SO4	E	301	5/5	0.84	0.17	70,89,95,129	0
2	AMP	A	301	23/23	0.84	0.28	40,93,141,171	0
2	AMP	E	302	23/23	0.85	0.32	37,84,141,177	0
3	SO4	D	301	5/5	0.87	0.16	66,84,89,110	0
3	SO4	C	302	5/5	0.89	0.15	64,74,97,109	0
3	SO4	A	302	5/5	0.90	0.16	66,86,95,114	0
3	SO4	B	301	5/5	0.90	0.13	81,85,100,125	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.
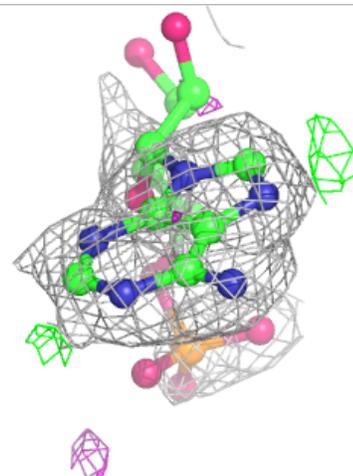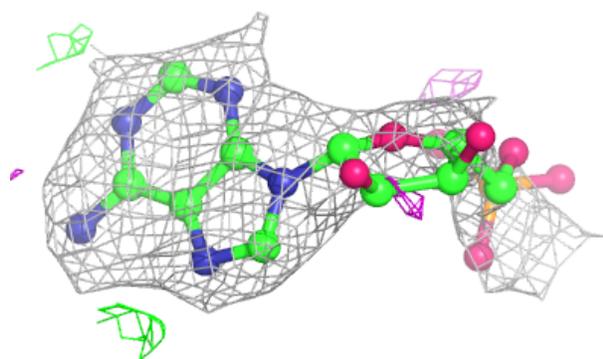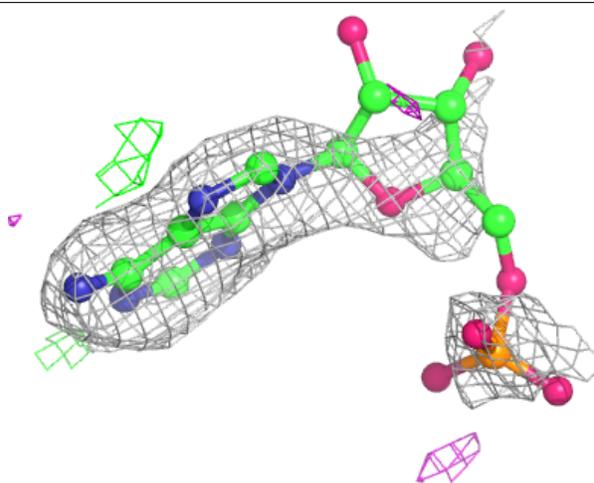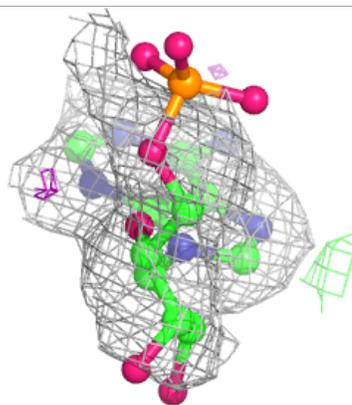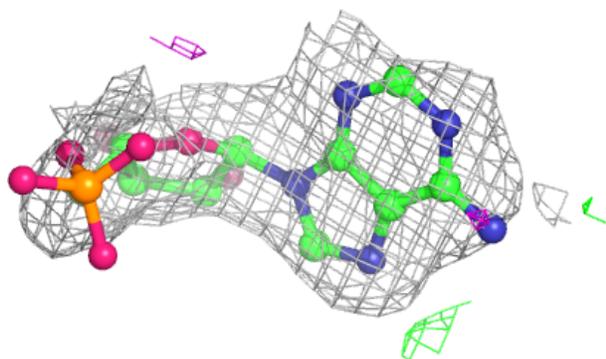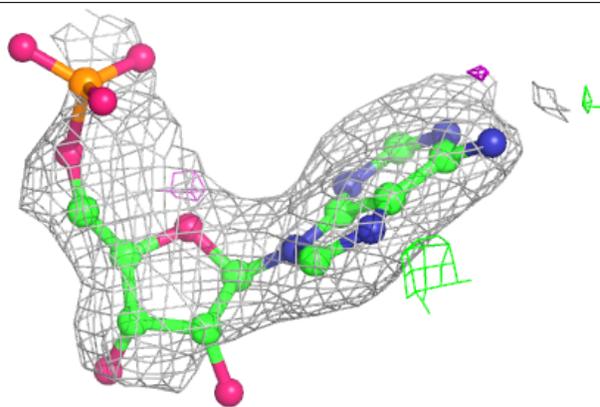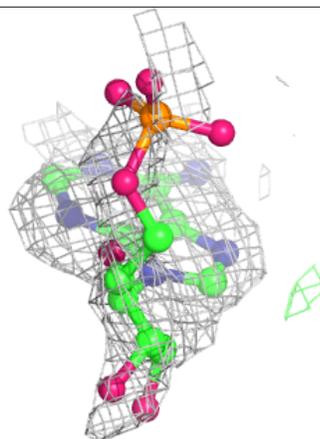
Electron density around AMP C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
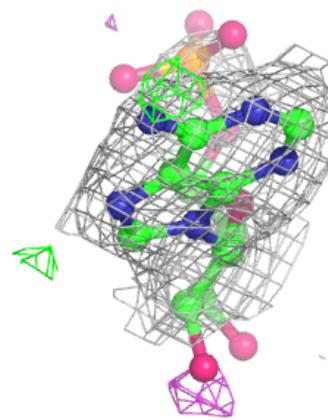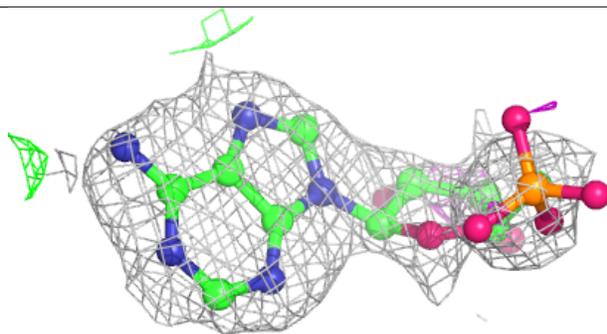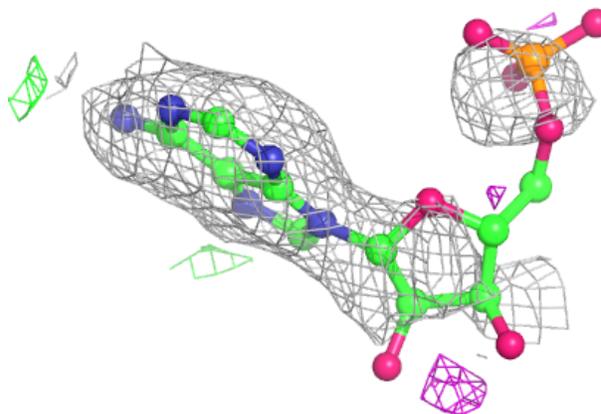
Electron density around AMP F 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
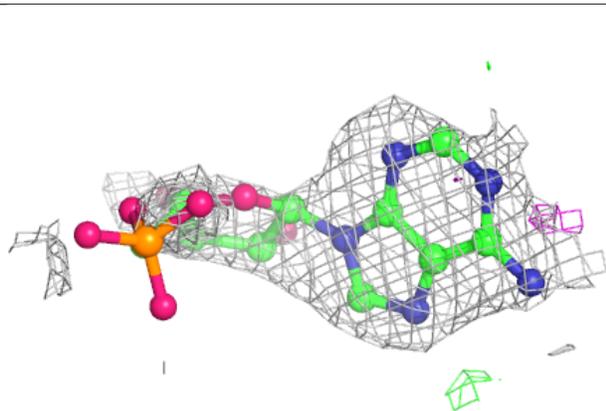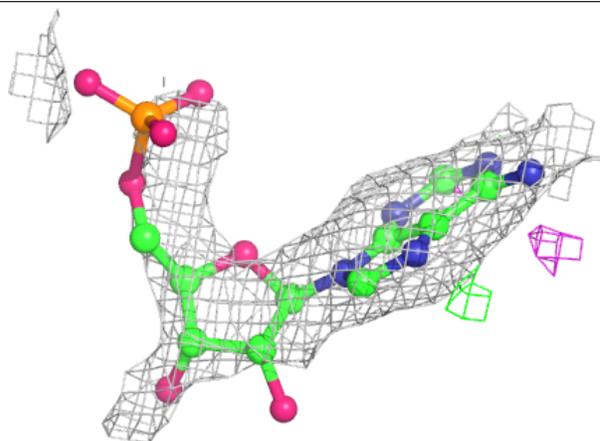and green (positive)
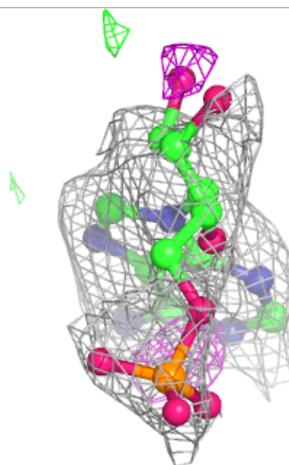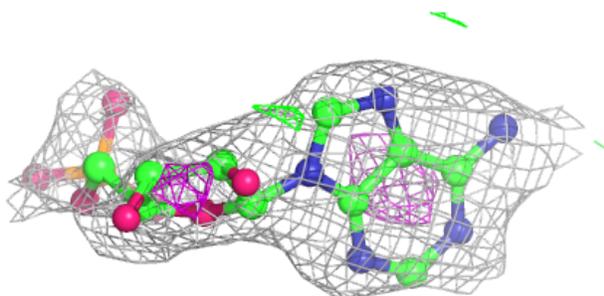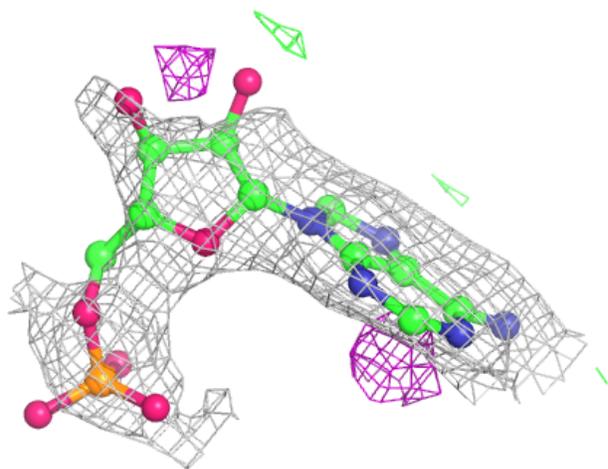
Electron density around AMP A 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
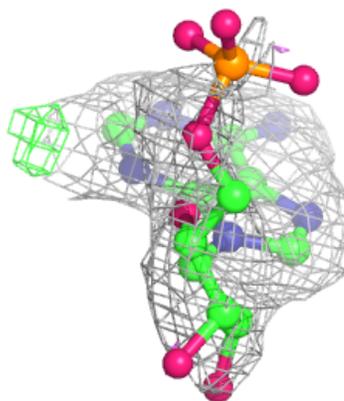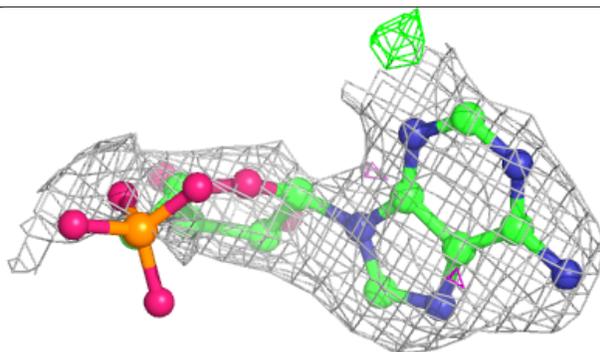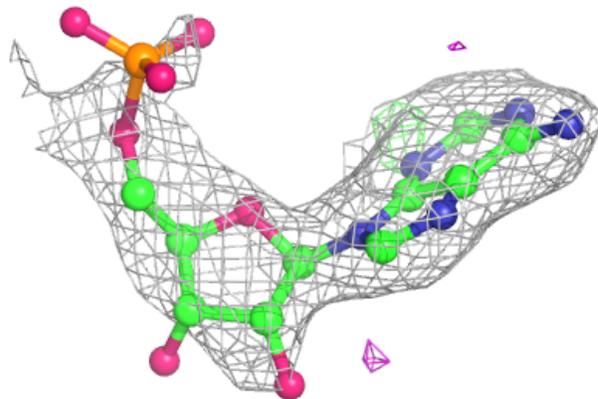
Electron density around AMP C 303:

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

Electron density around AMP 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 AMP E 302:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.