Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 02:50 AM EDT

PDB ID	:	7K09
Title	:	Puromycin N-acetyltransferase in complex with acetyl-CoA
Authors	:	Caputo, A.T.; Newman, J.; Adams, T.E.; Peat, T.S.
Deposited on	:	2020-09-03
Resolution	:	2.31 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

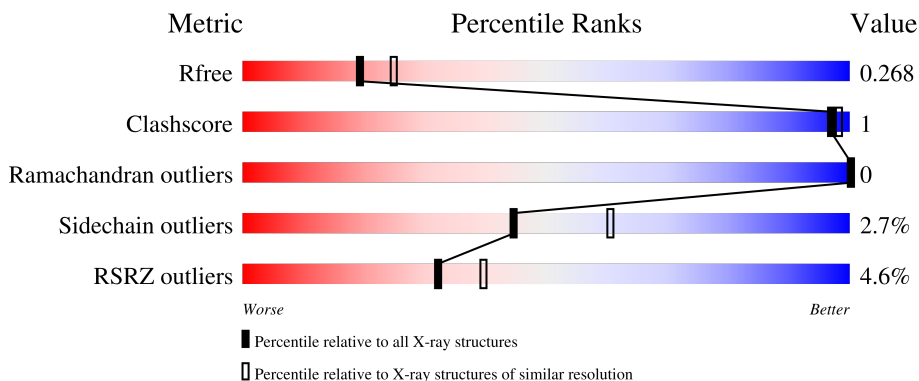|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.31 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		0.268
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		2.7%
RSRZ outliers		4.6%

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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	208	7% 91% • 7%
1	B	208	3% 89% • 8%
1	C	208	3% 91% • 7%
1	D	208	3% 91% • 6%
1	E	208	9% 86% 7% 7%

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Mol	Chain	Length	Quality of chain
1	F	208	% 88% 5% 6%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 18145 atoms, of which 8986 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 Puromycin N-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	194	Total	C	H	N	O	S	1456	0	0
			2927	929	1457	264	273	4			
1	B	192	Total	C	H	N	O	S	1448	0	0
			2910	924	1449	262	271	4			
1	C	194	Total	C	H	N	O	S	1457	0	0
			2927	929	1457	264	273	4			
1	D	195	Total	C	H	N	O	S	1469	0	0
			2948	935	1469	266	274	4			
1	E	194	Total	C	H	N	O	S	1457	0	0
			2927	929	1457	264	273	4			
1	F	195	Total	C	H	N	O	S	1468	0	0
			2948	935	1469	266	274	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P13249
A	0	GLY	-	expression tag	UNP P13249
A	1	SER	-	expression tag	UNP P13249
A	200	SER	-	expression tag	UNP P13249
A	201	HIS	-	expression tag	UNP P13249
A	202	HIS	-	expression tag	UNP P13249
A	203	HIS	-	expression tag	UNP P13249
A	204	HIS	-	expression tag	UNP P13249
A	205	HIS	-	expression tag	UNP P13249
A	206	HIS	-	expression tag	UNP P13249
B	-1	MET	-	initiating methionine	UNP P13249
B	0	GLY	-	expression tag	UNP P13249
B	1	SER	-	expression tag	UNP P13249
B	200	SER	-	expression tag	UNP P13249
B	201	HIS	-	expression tag	UNP P13249
B	202	HIS	-	expression tag	UNP P13249
B	203	HIS	-	expression tag	UNP P13249

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Chain	Residue	Modelled	Actual	Comment	Reference
B	204	HIS	-	expression tag	UNP P13249
B	205	HIS	-	expression tag	UNP P13249
B	206	HIS	-	expression tag	UNP P13249
C	-1	MET	-	initiating methionine	UNP P13249
C	0	GLY	-	expression tag	UNP P13249
C	1	SER	-	expression tag	UNP P13249
C	200	SER	-	expression tag	UNP P13249
C	201	HIS	-	expression tag	UNP P13249
C	202	HIS	-	expression tag	UNP P13249
C	203	HIS	-	expression tag	UNP P13249
C	204	HIS	-	expression tag	UNP P13249
C	205	HIS	-	expression tag	UNP P13249
C	206	HIS	-	expression tag	UNP P13249
D	-1	MET	-	initiating methionine	UNP P13249
D	0	GLY	-	expression tag	UNP P13249
D	1	SER	-	expression tag	UNP P13249
D	200	SER	-	expression tag	UNP P13249
D	201	HIS	-	expression tag	UNP P13249
D	202	HIS	-	expression tag	UNP P13249
D	203	HIS	-	expression tag	UNP P13249
D	204	HIS	-	expression tag	UNP P13249
D	205	HIS	-	expression tag	UNP P13249
D	206	HIS	-	expression tag	UNP P13249
E	-1	MET	-	initiating methionine	UNP P13249
E	0	GLY	-	expression tag	UNP P13249
E	1	SER	-	expression tag	UNP P13249
E	200	SER	-	expression tag	UNP P13249
E	201	HIS	-	expression tag	UNP P13249
E	202	HIS	-	expression tag	UNP P13249
E	203	HIS	-	expression tag	UNP P13249
E	204	HIS	-	expression tag	UNP P13249
E	205	HIS	-	expression tag	UNP P13249
E	206	HIS	-	expression tag	UNP P13249
F	-1	MET	-	initiating methionine	UNP P13249
F	0	GLY	-	expression tag	UNP P13249
F	1	SER	-	expression tag	UNP P13249
F	200	SER	-	expression tag	UNP P13249
F	201	HIS	-	expression tag	UNP P13249
F	202	HIS	-	expression tag	UNP P13249
F	203	HIS	-	expression tag	UNP P13249
F	204	HIS	-	expression tag	UNP P13249
F	205	HIS	-	expression tag	UNP P13249

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Chain	Residue	Modelled	Actual	Comment	Reference
F	206	HIS	-	expression tag	UNP P13249

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).
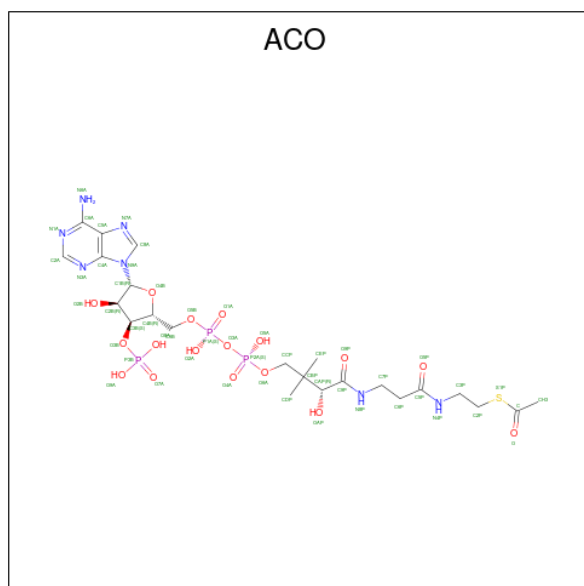
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	38	0
			89	23	38	7	17	3	1		
2	B	1	Total	C	H	N	O	P	S	38	0
			89	23	38	7	17	3	1		
2	C	1	Total	C	H	N	O	P	S	38	0
			89	23	38	7	17	3	1		
2	D	1	Total	C	H	N	O	P	S	38	0
			89	23	38	7	17	3	1		
2	E	1	Total	C	H	N	O	P	S	38	0
			89	23	38	7	17	3	1		
2	F	1	Total	C	H	N	O	P	S	38	0
			89	23	38	7	17	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		

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

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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.
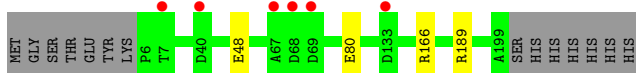
- Molecule 1: Puromycin N-acetyltransferase
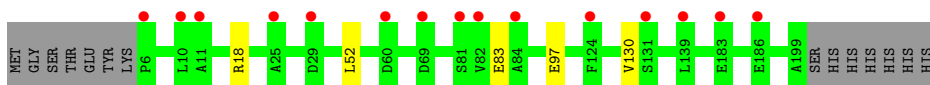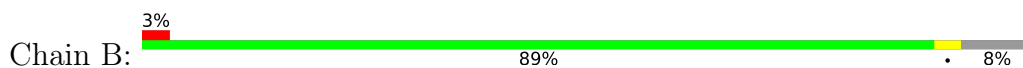
- Molecule 1: Puromycin N-acetyltransferase

- Molecule 1: Puromycin N-acetyltransferase
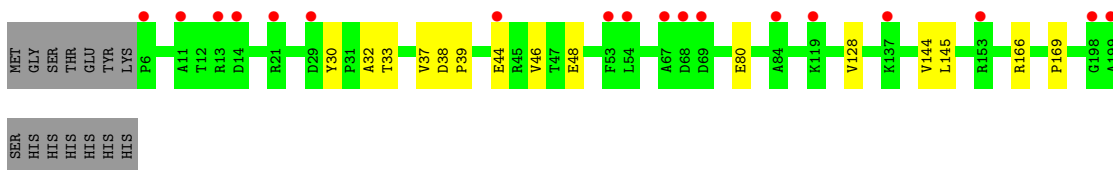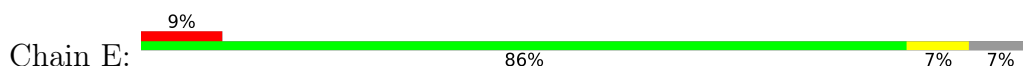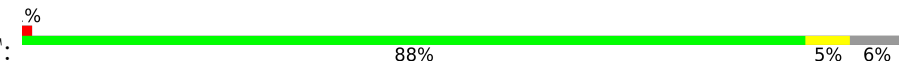

- Molecule 1: Puromycin N-acetyltransferase

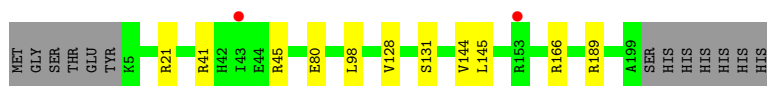- Molecule 1: Puromycin N-acetyltransferase

• Molecule 1: Puromycin N-acetyltransferase

Chain F:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	149.07Å 73.63Å 106.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.24 – 2.31 106.24 – 2.31	Depositor EDS
% Data completeness (in resolution range)	53.7 (106.24-2.31) 53.7 (106.24-2.31)	Depositor EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.32Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.236 , 0.252 0.251 , 0.268	Depositor DCC
R_{free} test set	1346 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.0	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18145	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 29.06 % 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 1.6547e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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: ACO

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	0/1507	0.62	0/2060
1	B	0.48	0/1498	0.61	0/2048
1	C	0.53	0/1507	0.62	0/2060
1	D	0.52	0/1516	0.62	0/2072
1	E	0.53	0/1507	0.64	0/2060
1	F	0.51	0/1516	0.61	0/2072
All	All	0.52	0/9051	0.62	0/12372

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	1470	1457	1457	3	0
1	B	1461	1449	1449	1	0
1	C	1470	1457	1457	1	0
1	D	1479	1469	1469	1	0
1	E	1470	1457	1457	5	0
1	F	1479	1469	1469	3	0
2	A	51	38	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	51	38	34	0	0
2	C	51	38	34	2	0
2	D	51	38	34	1	0
2	E	51	38	34	0	0
2	F	51	38	34	1	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
3	E	6	0	0	0	0
3	F	4	0	0	0	0
All	All	9159	8986	8962	17	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 1.

All (17) 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:A:97:GLU:OE1	1:D:134:HIS:NE2	2.36	0.57
2:A:301:ACO:H8A	2:A:301:ACO:H143	1.89	0.54
1:C:48:GLU:OE1	1:F:21:ARG:HD3	2.08	0.53
1:A:83:GLU:HA	1:A:83:GLU:OE2	2.11	0.50
1:A:130:VAL:HG23	2:A:301:ACO:H132	1.96	0.47
2:C:301:ACO:H32	2:C:301:ACO:HH33	1.96	0.46
1:E:128:VAL:HG21	1:E:144:VAL:CG1	2.45	0.46
1:E:30:TYR:CE2	1:E:32:ALA:HB3	2.51	0.45
1:F:128:VAL:HG21	1:F:144:VAL:CG1	2.47	0.44
1:E:166:ARG:O	1:E:169:PRO:HD2	2.16	0.44
1:E:38:ASP:OD1	1:E:39:PRO:HD2	2.18	0.44
1:B:87:VAL:O	1:B:91:ILE:HG12	2.20	0.41
2:C:301:ACO:HH33	2:C:301:ACO:C3P	2.50	0.41
2:D:301:ACO:O9P	2:D:301:ACO:H62	2.21	0.41
1:E:37:VAL:HG11	1:E:46:VAL:HG23	2.03	0.41
1:F:45:ARG:HD3	1:F:98:LEU:O	2.21	0.41
2:F:301:ACO:H32	2:F:301:ACO:HH33	2.02	0.41

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	192/208 (92%)	188 (98%)	4 (2%)	0	100	100
1	B	190/208 (91%)	188 (99%)	2 (1%)	0	100	100
1	C	192/208 (92%)	187 (97%)	5 (3%)	0	100	100
1	D	193/208 (93%)	187 (97%)	6 (3%)	0	100	100
1	E	192/208 (92%)	187 (97%)	5 (3%)	0	100	100
1	F	193/208 (93%)	189 (98%)	4 (2%)	0	100	100
All	All	1152/1248 (92%)	1126 (98%)	26 (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	150/163 (92%)	148 (99%)	2 (1%)	69	81
1	B	150/163 (92%)	146 (97%)	4 (3%)	44	60
1	C	150/163 (92%)	147 (98%)	3 (2%)	55	71
1	D	151/163 (93%)	147 (97%)	4 (3%)	46	62
1	E	150/163 (92%)	145 (97%)	5 (3%)	38	52
1	F	151/163 (93%)	145 (96%)	6 (4%)	31	44
All	All	902/978 (92%)	878 (97%)	24 (3%)	44	60

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	52	LEU
1	B	15	ASP
1	B	21	ARG
1	B	80	GLU
1	B	109	MET
1	C	80	GLU
1	C	166	ARG
1	C	189	ARG
1	D	21	ARG
1	D	80	GLU
1	D	99	SER
1	D	145	LEU
1	E	33	THR
1	E	44	GLU
1	E	48	GLU
1	E	80	GLU
1	E	145	LEU
1	F	41	ARG
1	F	80	GLU
1	F	131	SER
1	F	145	LEU
1	F	166	ARG
1	F	189	ARG

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

Mol	Chain	Res	Type
1	C	108	GLN

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)

6 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	ACO	A	301	-	45,53,53	0.94	3 (6%)	56,79,79	0.99	4 (7%)
2	ACO	B	301	-	45,53,53	0.82	2 (4%)	56,79,79	1.07	3 (5%)
2	ACO	C	301	-	45,53,53	0.85	1 (2%)	56,79,79	1.07	6 (10%)
2	ACO	E	301	-	45,53,53	0.81	1 (2%)	56,79,79	0.80	1 (1%)
2	ACO	F	301	-	45,53,53	0.72	1 (2%)	56,79,79	0.86	2 (3%)
2	ACO	D	301	-	45,53,53	0.86	2 (4%)	56,79,79	0.81	2 (3%)

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	ACO	A	301	-	-	9/47/67/67	0/3/3/3
2	ACO	B	301	-	-	8/47/67/67	0/3/3/3
2	ACO	C	301	-	-	10/47/67/67	0/3/3/3
2	ACO	E	301	-	-	6/47/67/67	0/3/3/3
2	ACO	F	301	-	-	8/47/67/67	0/3/3/3
2	ACO	D	301	-	-	9/47/67/67	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ACO	C8A-N7A	-3.81	1.27	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ACO	P3B-O3B	3.55	1.66	1.59
2	E	301	ACO	P3B-O3B	3.42	1.65	1.59
2	D	301	ACO	P3B-O3B	3.37	1.65	1.59
2	B	301	ACO	C4A-N3A	-2.54	1.32	1.35
2	F	301	ACO	C8A-N7A	-2.54	1.30	1.34
2	B	301	ACO	P3B-O3B	2.51	1.64	1.59
2	D	301	ACO	P3B-O7A	2.47	1.58	1.50
2	A	301	ACO	P1A-O2A	-2.04	1.45	1.55
2	A	301	ACO	P1A-O5B	2.01	1.67	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ACO	C4A-C5A-N7A	5.08	114.69	109.40
2	A	301	ACO	C1B-N9A-C4A	3.92	133.53	126.64
2	C	301	ACO	C2P-S1P-C	3.66	120.93	101.68
2	D	301	ACO	C2P-S1P-C	3.39	119.50	101.68
2	F	301	ACO	C1B-N9A-C4A	3.38	132.59	126.64
2	B	301	ACO	C2P-S1P-C	2.91	117.00	101.68
2	F	301	ACO	C2P-S1P-C	2.89	116.88	101.68
2	A	301	ACO	C4A-C5A-N7A	-2.71	106.58	109.40
2	E	301	ACO	C5A-C6A-N6A	2.61	124.32	120.35
2	C	301	ACO	C2P-C3P-N4P	2.47	117.60	112.42
2	A	301	ACO	C2P-S1P-C	2.44	114.54	101.68
2	D	301	ACO	C5A-C6A-N6A	2.35	123.92	120.35
2	B	301	ACO	C2P-C3P-N4P	2.31	117.27	112.42
2	C	301	ACO	C5A-C6A-N6A	2.26	123.79	120.35
2	C	301	ACO	CDP-CBP-CAP	-2.22	104.96	108.82
2	A	301	ACO	C5A-C6A-N6A	2.22	123.72	120.35
2	C	301	ACO	C6P-C5P-N4P	-2.07	112.94	116.42
2	C	301	ACO	C4A-C5A-N7A	2.02	111.50	109.40

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ACO	N8P-C9P-CAP-OAP
2	A	301	ACO	C5P-C6P-C7P-N8P
2	A	301	ACO	C2P-C3P-N4P-C5P
2	A	301	ACO	O-C-S1P-C2P
2	A	301	ACO	CH3-C-S1P-C2P
2	B	301	ACO	N8P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
2	B	301	ACO	C6P-C5P-N4P-C3P
2	B	301	ACO	S1P-C2P-C3P-N4P
2	B	301	ACO	O-C-S1P-C2P
2	B	301	ACO	CH3-C-S1P-C2P
2	C	301	ACO	N8P-C9P-CAP-OAP
2	C	301	ACO	S1P-C2P-C3P-N4P
2	C	301	ACO	C3P-C2P-S1P-C
2	C	301	ACO	O-C-S1P-C2P
2	C	301	ACO	CH3-C-S1P-C2P
2	D	301	ACO	N8P-C9P-CAP-OAP
2	D	301	ACO	C6P-C5P-N4P-C3P
2	D	301	ACO	S1P-C2P-C3P-N4P
2	D	301	ACO	O-C-S1P-C2P
2	D	301	ACO	CH3-C-S1P-C2P
2	E	301	ACO	S1P-C2P-C3P-N4P
2	E	301	ACO	O-C-S1P-C2P
2	E	301	ACO	CH3-C-S1P-C2P
2	F	301	ACO	N8P-C9P-CAP-OAP
2	F	301	ACO	C6P-C5P-N4P-C3P
2	F	301	ACO	S1P-C2P-C3P-N4P
2	F	301	ACO	O-C-S1P-C2P
2	F	301	ACO	CH3-C-S1P-C2P
2	B	301	ACO	O5P-C5P-N4P-C3P
2	D	301	ACO	O5P-C5P-N4P-C3P
2	F	301	ACO	O5P-C5P-N4P-C3P
2	D	301	ACO	C6P-C7P-N8P-C9P
2	C	301	ACO	C6P-C7P-N8P-C9P
2	C	301	ACO	C6P-C5P-N4P-C3P
2	B	301	ACO	C6P-C7P-N8P-C9P
2	F	301	ACO	C6P-C7P-N8P-C9P
2	C	301	ACO	O5P-C5P-N4P-C3P
2	A	301	ACO	C2B-C3B-O3B-P3B
2	A	301	ACO	C4B-C3B-O3B-P3B
2	E	301	ACO	C2B-C3B-O3B-P3B
2	E	301	ACO	C4B-C3B-O3B-P3B
2	A	301	ACO	O9P-C9P-CAP-OAP
2	B	301	ACO	O9P-C9P-CAP-OAP
2	C	301	ACO	O9P-C9P-CAP-OAP
2	D	301	ACO	O9P-C9P-CAP-OAP
2	F	301	ACO	O9P-C9P-CAP-OAP
2	A	301	ACO	C3B-O3B-P3B-O9A
2	C	301	ACO	C3B-O3B-P3B-O9A

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Mol	Chain	Res	Type	Atoms
2	D	301	ACO	C3P-C2P-S1P-C
2	E	301	ACO	P2A-O3A-P1A-O2A

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ACO	2	0
2	C	301	ACO	2	0
2	F	301	ACO	1	0
2	D	301	ACO	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 ACO A 301

Bond lengths   Bond angles

Torsions   Rings

Ligand ACO B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO D 301

Bond lengths

Bond angles

Torsions

Rings
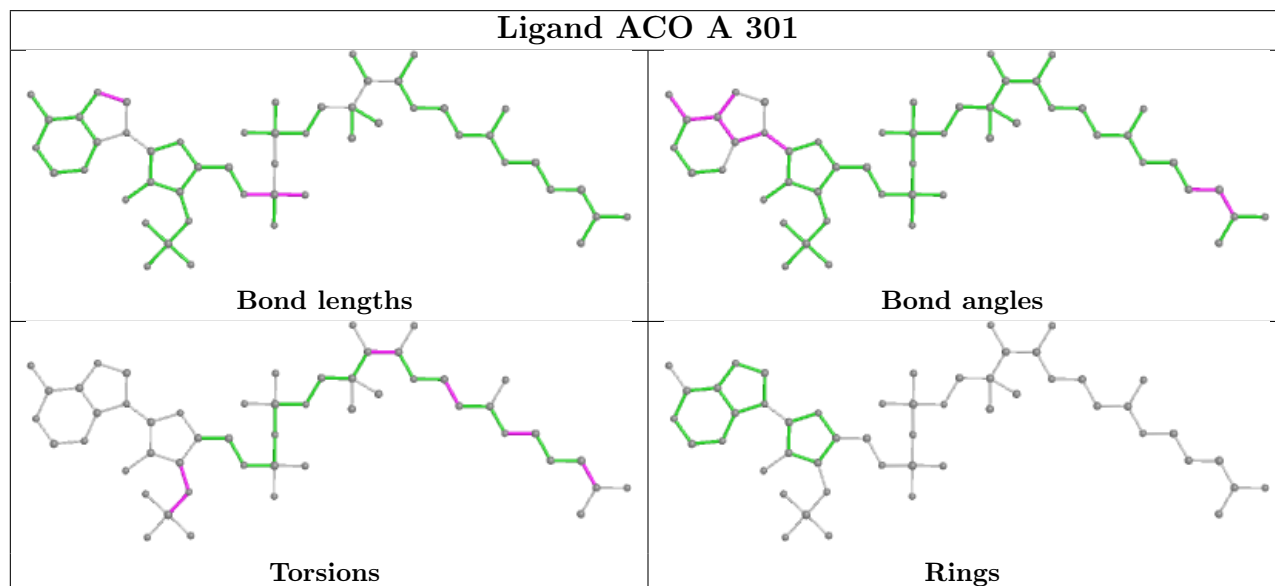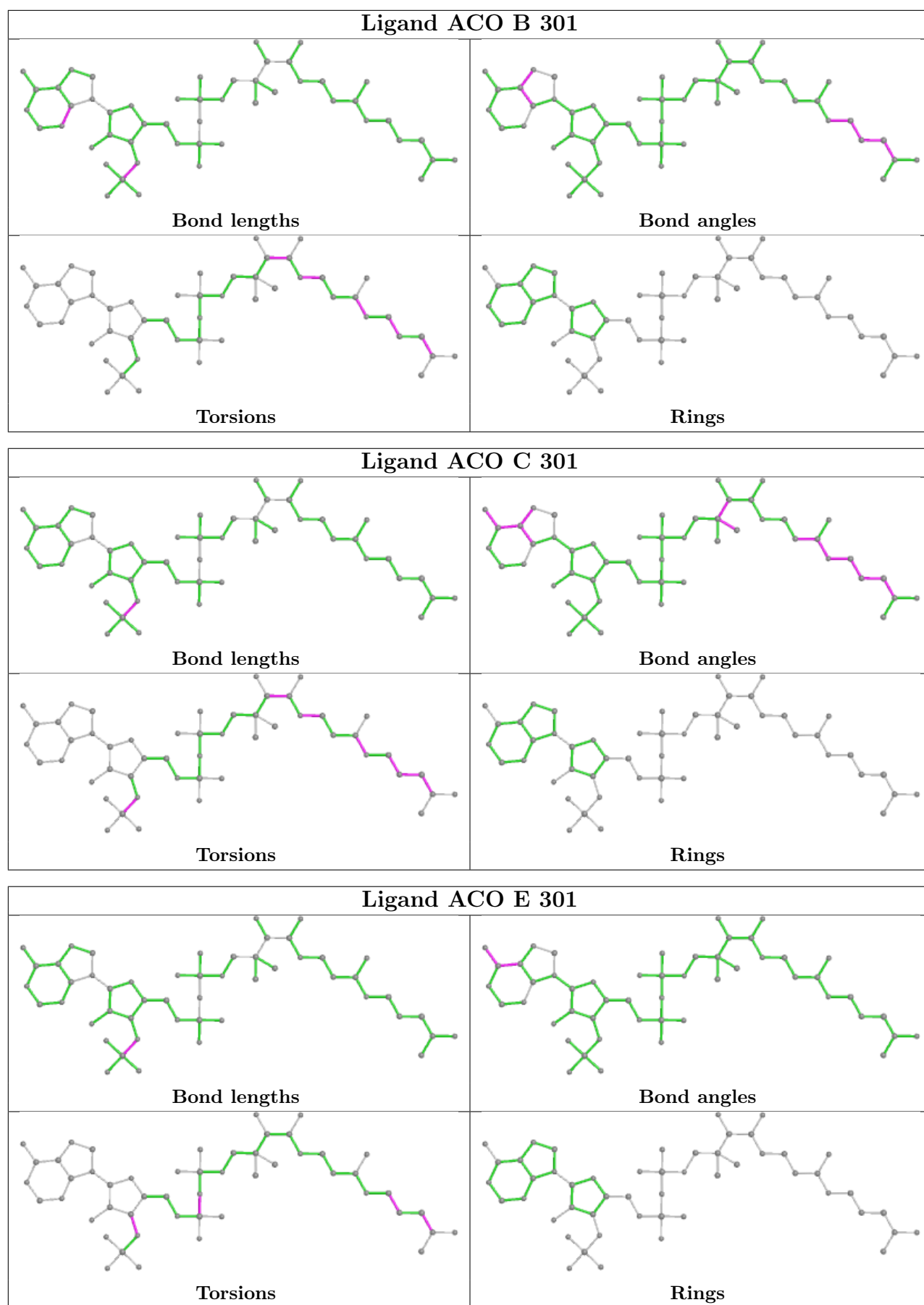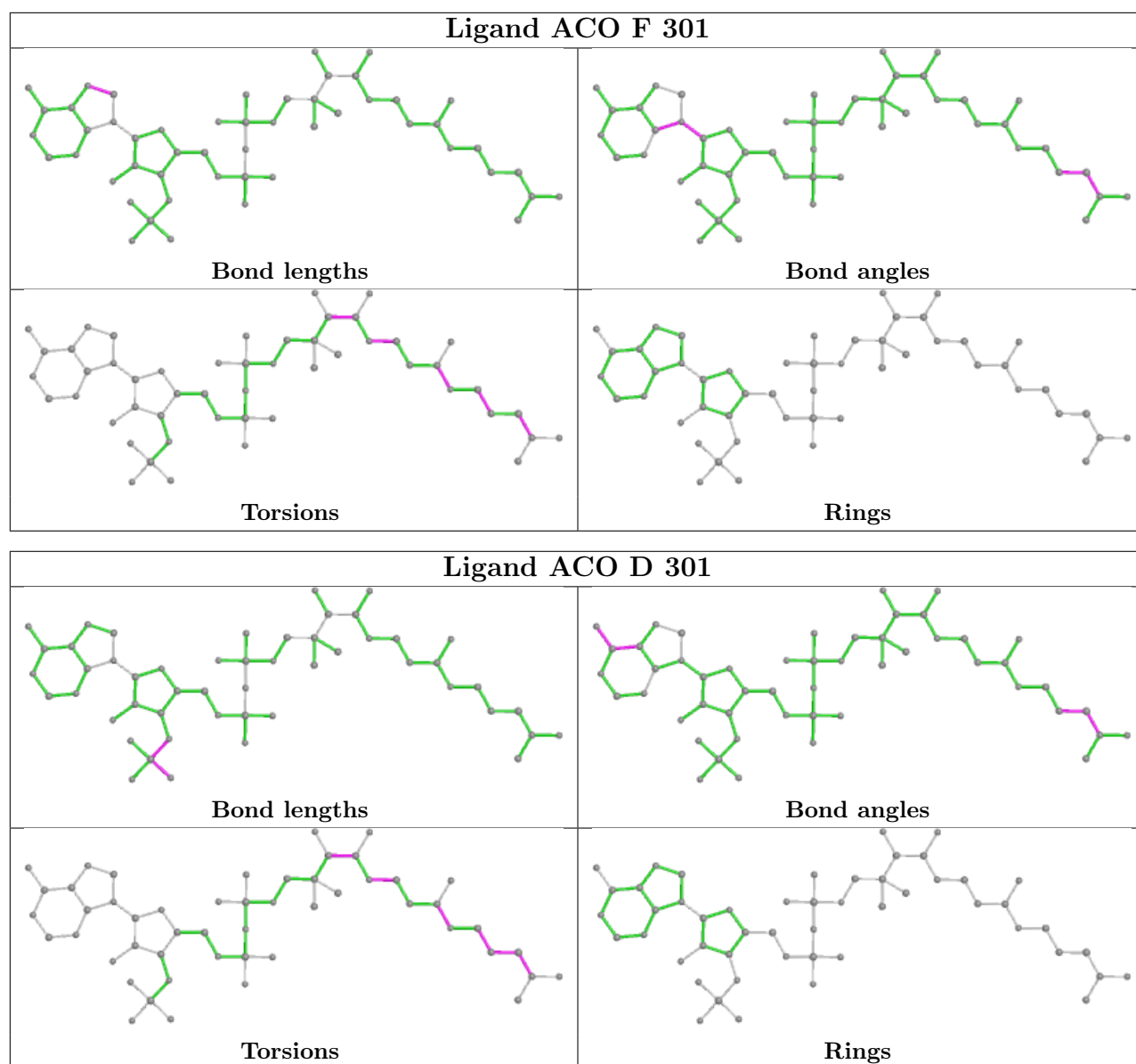
5.7 Other polymers ⓘ

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	194/208 (93%)	0.59	15 (7%)	13	18	27, 45, 67, 85	0
1	B	192/208 (92%)	0.39	6 (3%)	49	56	24, 43, 65, 85	0
1	C	194/208 (93%)	0.23	6 (3%)	49	56	14, 31, 59, 84	0
1	D	195/208 (93%)	0.40	7 (3%)	42	49	24, 39, 63, 88	0
1	E	194/208 (93%)	0.65	18 (9%)	8	12	26, 46, 72, 92	0
1	F	195/208 (93%)	0.03	2 (1%)	82	86	9, 27, 51, 87	0
All	All	1164/1248 (93%)	0.38	54 (4%)	32	40	9, 39, 65, 92	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	ASP	5.5
1	A	69	ASP	5.2
1	E	198	GLY	5.0
1	E	14	ASP	4.8
1	D	153	ARG	4.6
1	A	82	VAL	4.5
1	E	69	ASP	4.4
1	B	53	PHE	3.7
1	E	199	ALA	3.7
1	D	166	ARG	3.5
1	E	6	PRO	3.5
1	E	153	ARG	3.5
1	E	29	ASP	3.4
1	A	81	SER	3.4
1	D	199	ALA	3.3
1	A	84	ALA	3.0
1	D	13	ARG	2.8
1	A	186	GLU	2.8
1	E	54	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	198	GLY	2.8
1	B	41	ARG	2.8
1	E	84	ALA	2.8
1	E	21	ARG	2.7
1	B	133	ASP	2.7
1	A	60	ASP	2.6
1	E	68	ASP	2.6
1	E	11	ALA	2.6
1	A	183	GLU	2.5
1	D	119	LYS	2.5
1	C	68	ASP	2.5
1	A	6	PRO	2.4
1	E	137	LYS	2.4
1	A	124	PHE	2.4
1	E	67	ALA	2.3
1	C	69	ASP	2.3
1	B	29	ASP	2.3
1	E	44	GLU	2.3
1	E	13	ARG	2.3
1	E	53	PHE	2.3
1	A	11	ALA	2.3
1	F	153	ARG	2.2
1	A	29	ASP	2.2
1	C	7	THR	2.2
1	B	7	THR	2.2
1	F	43	ILE	2.2
1	A	10	LEU	2.1
1	B	186	GLU	2.1
1	A	25	ALA	2.1
1	A	139	LEU	2.1
1	E	119	LYS	2.1
1	C	40	ASP	2.0
1	C	67	ALA	2.0
1	A	131	SER	2.0
1	D	154	ALA	2.0

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

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

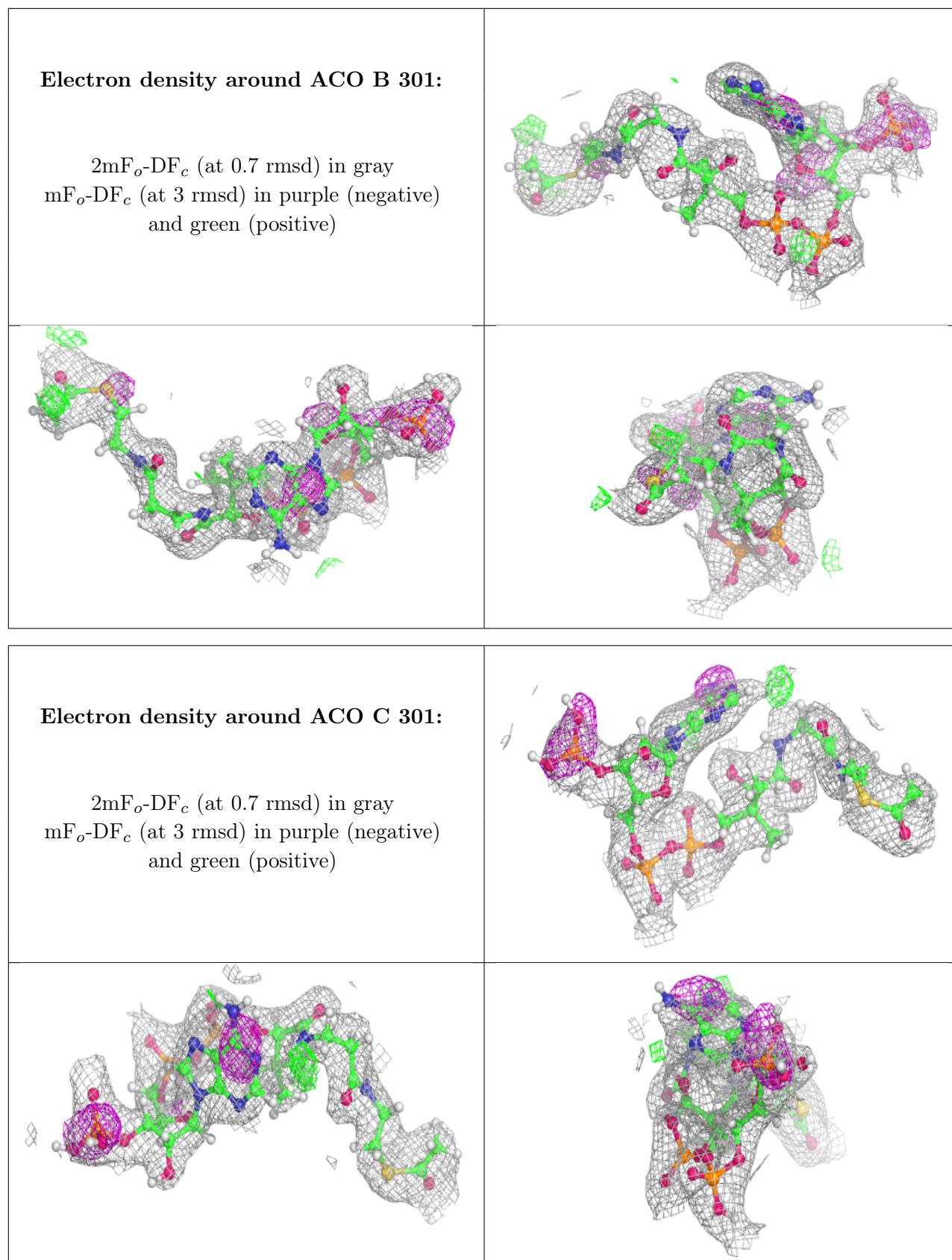## 6.3 Carbohydrates ⓘ

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	ACO	A	301	51/51	0.90	0.18	29,37,45,53	38
2	ACO	B	301	51/51	0.91	0.17	29,36,42,48	38
2	ACO	C	301	51/51	0.91	0.16	29,34,41,47	38
2	ACO	E	301	51/51	0.91	0.17	30,37,44,50	38
2	ACO	F	301	51/51	0.92	0.15	28,33,40,44	38
2	ACO	D	301	51/51	0.93	0.13	29,35,41,48	38

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.
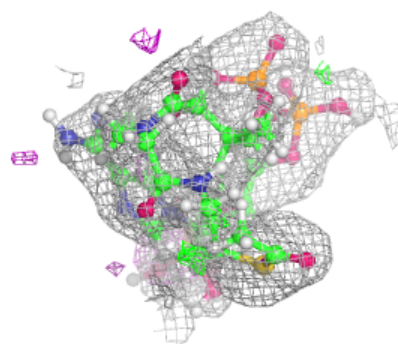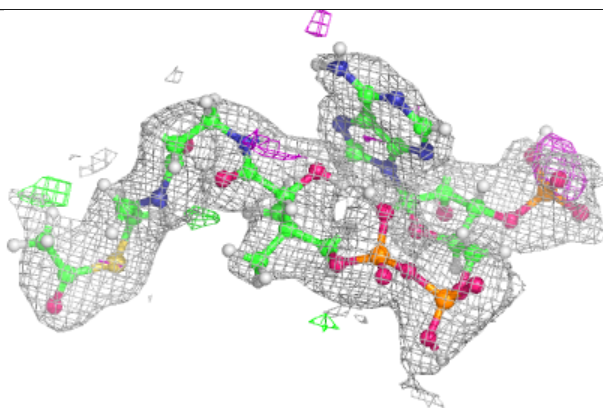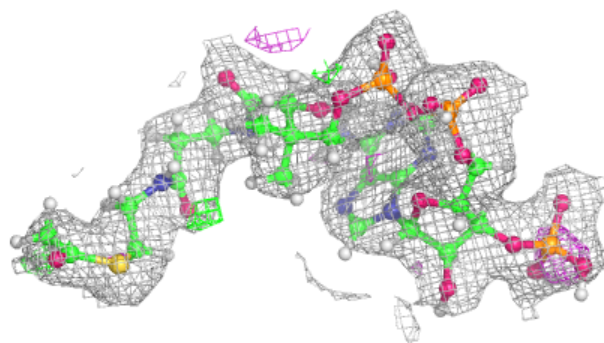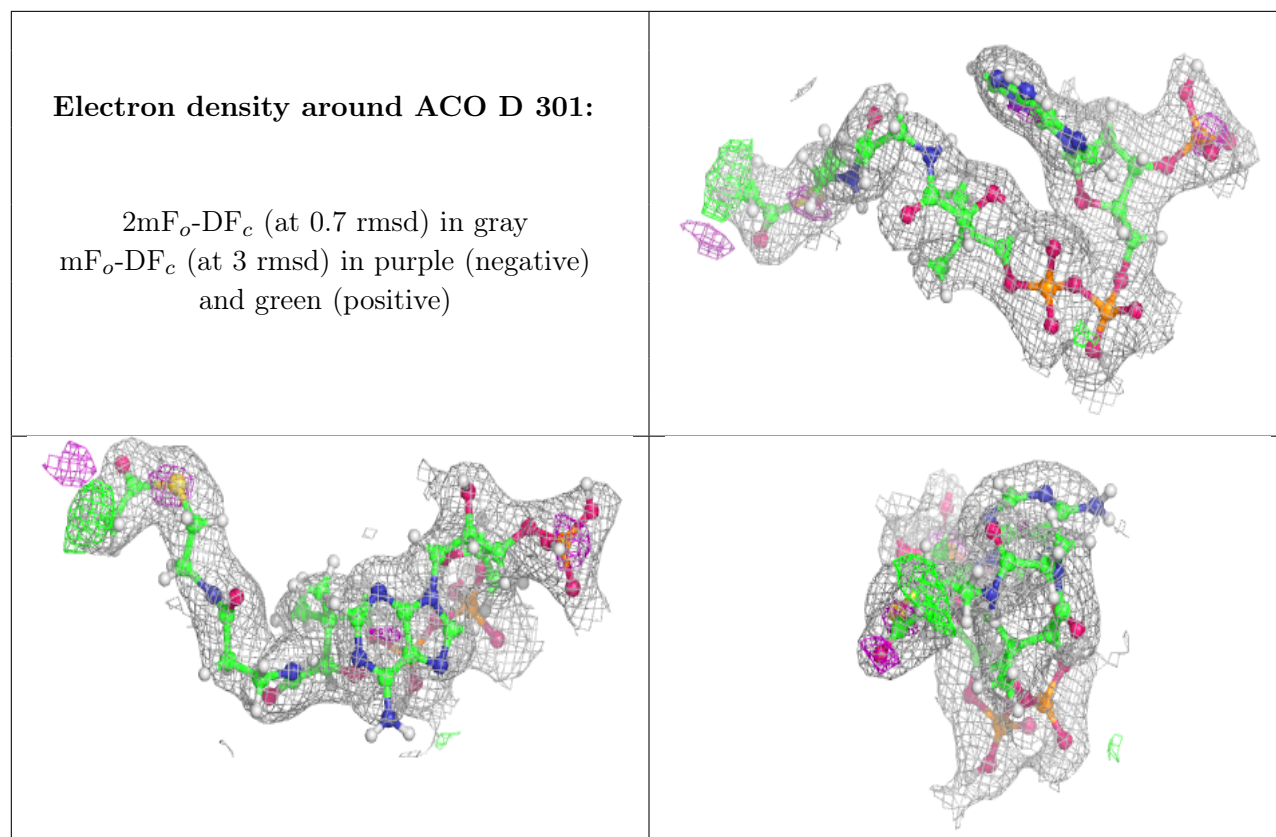
Electron density around ACO A 301:

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

Electron density around ACO B 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 ACO 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)
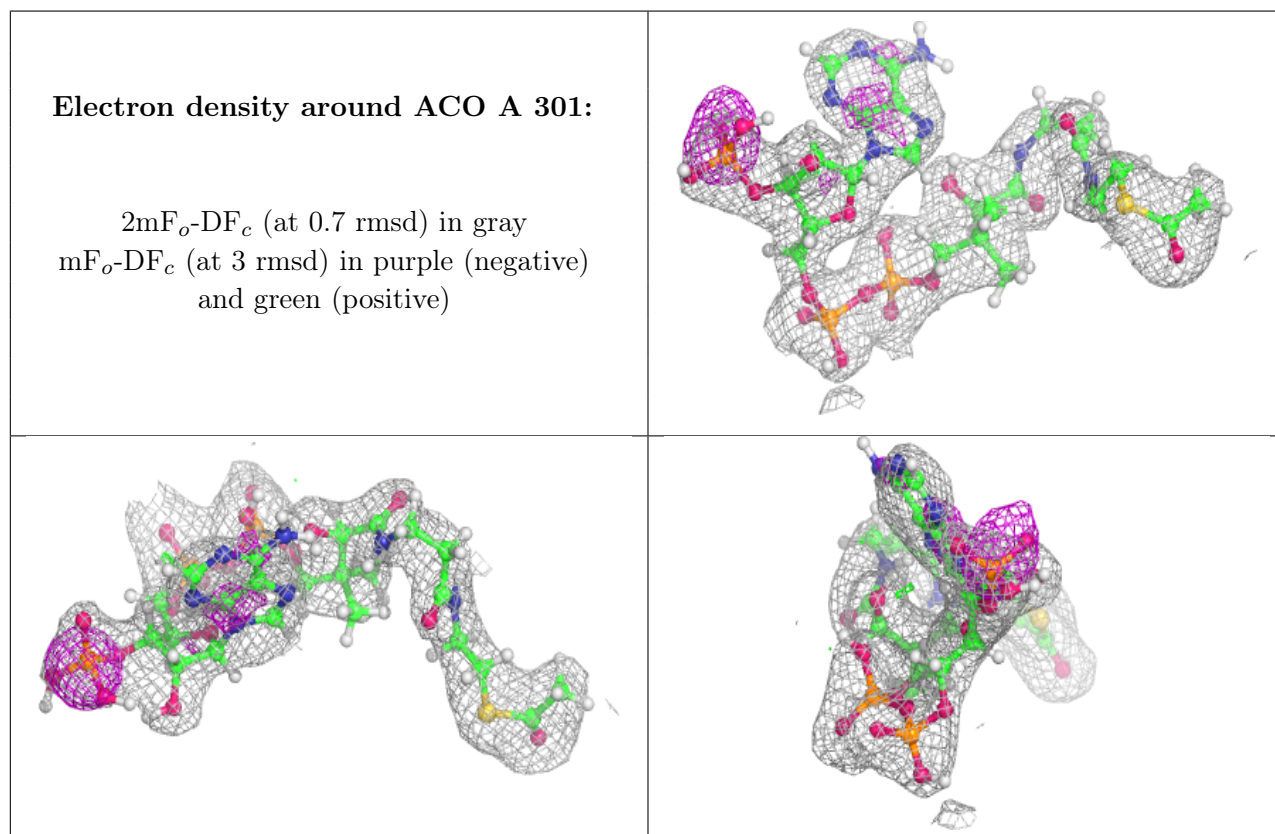
Electron density around ACO E 301:

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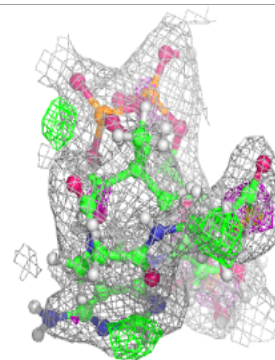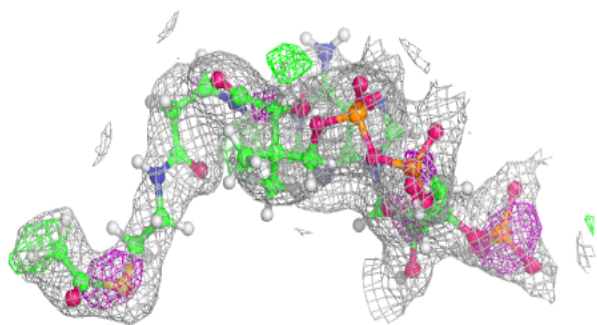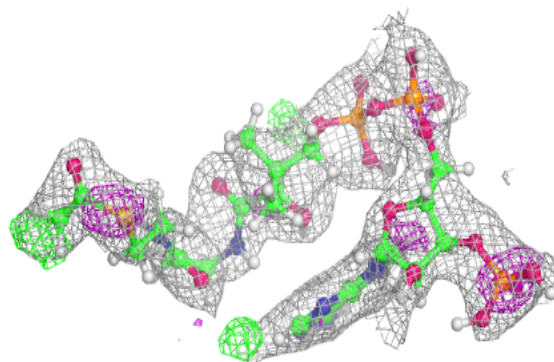
Electron density around ACO F 301:

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

Electron density around ACO D 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.