



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:31 PM UTC

PDB ID : 8VR7 / pdb_00008vr7
Title : crystal structure of the Pcryo_0619 N-acetyltransferase from Psychrobacter cryohalolentis K5 in the presence of acetyl coenzyme A
Authors : Dunsirn, M.M.; Bockhaus, N.J.; Thoden, J.B.; Holden, H.M.
Deposited on : 2024-01-20
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

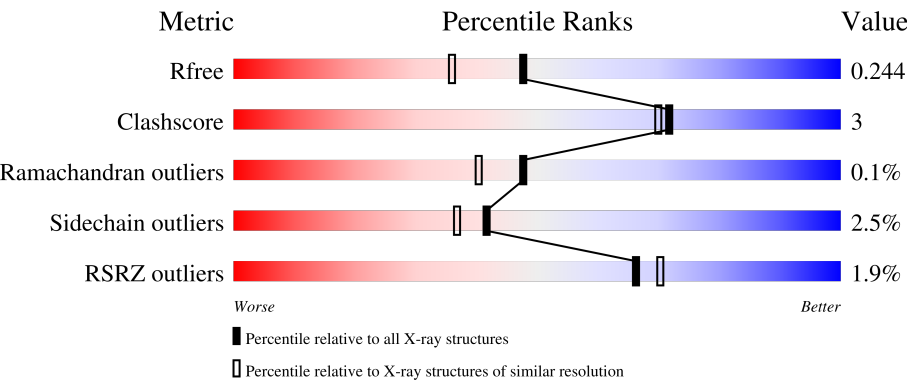
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	182	2% 92% 5% ...
1	B	182	% 87% 10% ...
1	C	182	2% 90% 5% ...
1	D	182	2% 88% 7% ...
1	E	182	2% 92% 6% ...

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Mol	Chain	Length	Quality of chain
1	F	182	% 91% 6% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9179 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 Acetyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	3	0
			1373	881	231	256	5			
1	B	177	Total	C	N	O	S	0	4	0
			1368	879	229	255	5			
1	C	176	Total	C	N	O	S	0	3	0
			1350	867	224	254	5			
1	D	175	Total	C	N	O	S	0	3	0
			1347	863	225	254	5			
1	E	180	Total	C	N	O	S	0	1	0
			1367	872	229	261	5			
1	F	178	Total	C	N	O	S	0	1	0
			1347	860	225	257	5			

There are 24 discrepancies between the modelled and reference sequences:

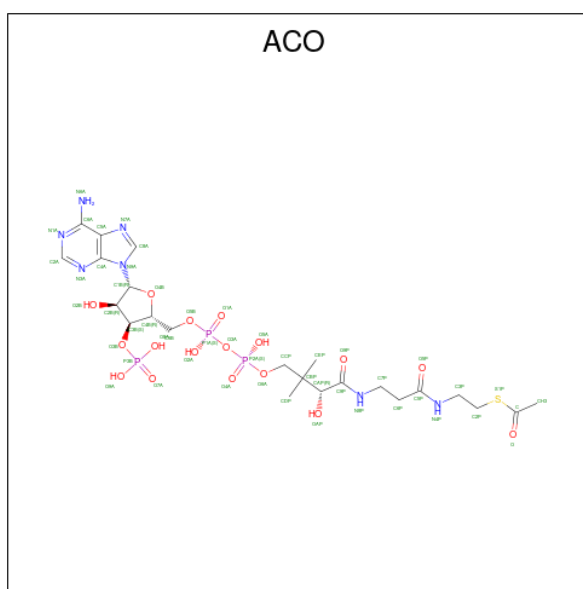
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q1QD51
A	-2	GLY	-	expression tag	UNP Q1QD51
A	-1	GLY	-	expression tag	UNP Q1QD51
A	0	HIS	-	expression tag	UNP Q1QD51
B	-3	GLY	-	expression tag	UNP Q1QD51
B	-2	GLY	-	expression tag	UNP Q1QD51
B	-1	GLY	-	expression tag	UNP Q1QD51
B	0	HIS	-	expression tag	UNP Q1QD51
C	-3	GLY	-	expression tag	UNP Q1QD51
C	-2	GLY	-	expression tag	UNP Q1QD51
C	-1	GLY	-	expression tag	UNP Q1QD51
C	0	HIS	-	expression tag	UNP Q1QD51
D	-3	GLY	-	expression tag	UNP Q1QD51
D	-2	GLY	-	expression tag	UNP Q1QD51
D	-1	GLY	-	expression tag	UNP Q1QD51
D	0	HIS	-	expression tag	UNP Q1QD51
E	-3	GLY	-	expression tag	UNP Q1QD51

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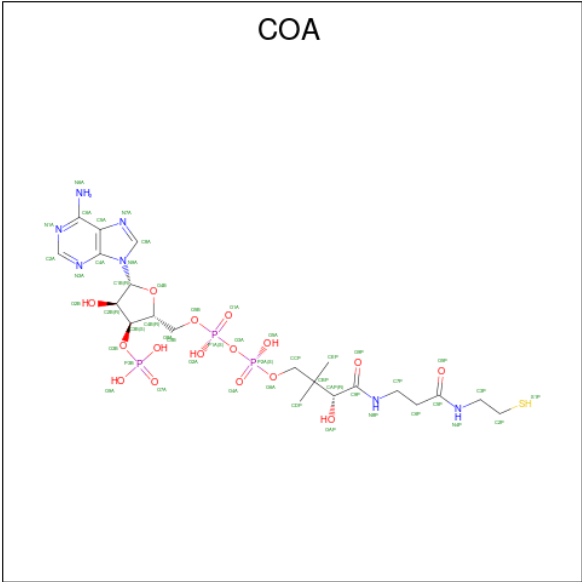
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q1QD51
E	-1	GLY	-	expression tag	UNP Q1QD51
E	0	HIS	-	expression tag	UNP Q1QD51
F	-3	GLY	-	expression tag	UNP Q1QD51
F	-2	GLY	-	expression tag	UNP Q1QD51
F	-1	GLY	-	expression tag	UNP Q1QD51
F	0	HIS	-	expression tag	UNP Q1QD51

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



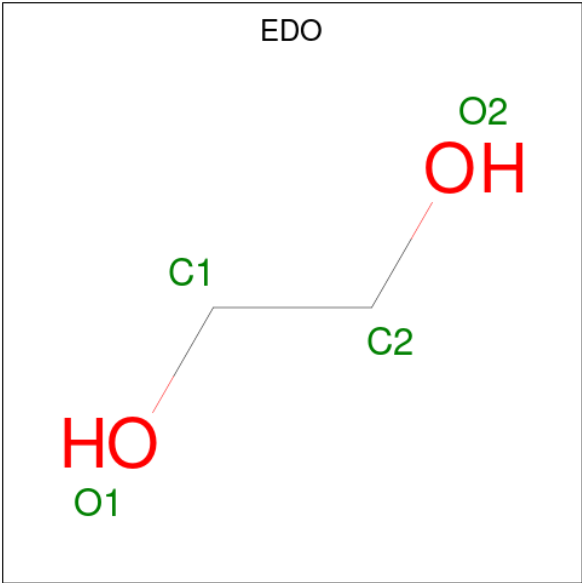
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



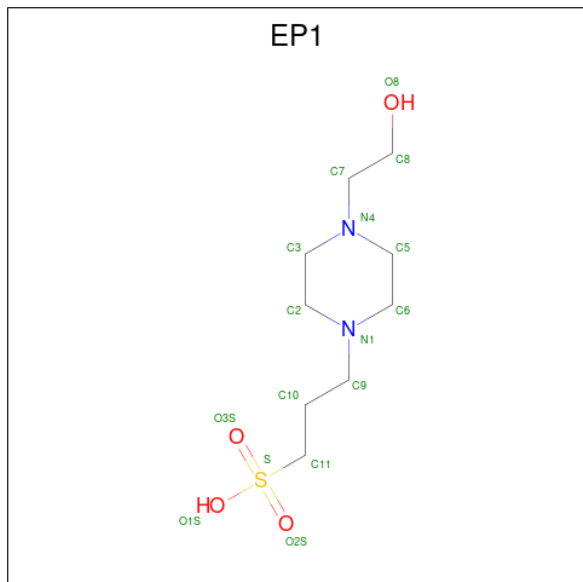
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



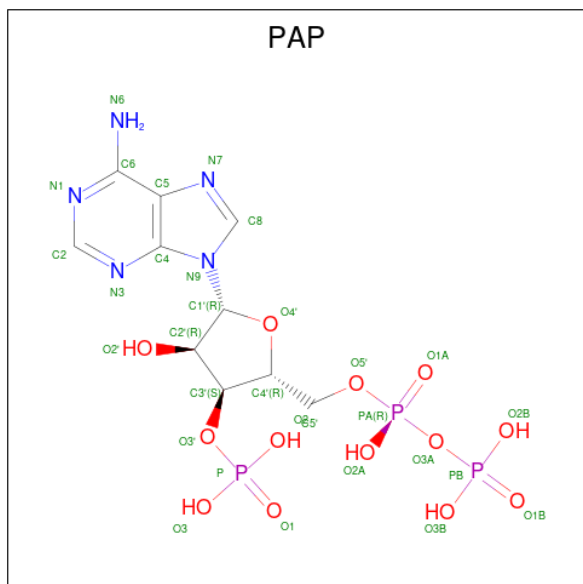
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	C O	0	0
			4	2 2		
4	F	1	Total	C O	0	0
			4	2 2		

- Molecule 5 is 3-[4-(2-HYDROXYETHYL)PIPERAZIN-1-YL]PROPANE-1-SULFONIC ACID (CCD ID: EP1) (formula: $C_9H_{20}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			16	9	2	4	1		

- Molecule 6 is 3'-PHOSPHATE-ADENOSINE-5'-DIPHOSPHATE (CCD ID: PAP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	112	Total 112	O 112	0	0
7	B	95	Total 95	O 95	0	0
7	C	114	Total 114	O 114	0	0
7	D	108	Total 108	O 108	0	0
7	E	113	Total 113	O 113	0	0
7	F	130	Total 130	O 130	0	0

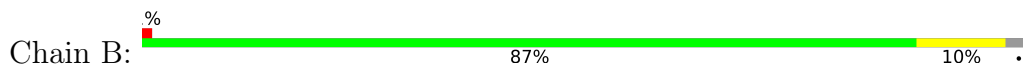
3 Residue-property plots [i](#)

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: Acetyltransferase, putative



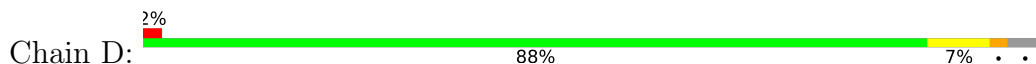
- Molecule 1: Acetyltransferase, putative



- Molecule 1: Acetyltransferase, putative



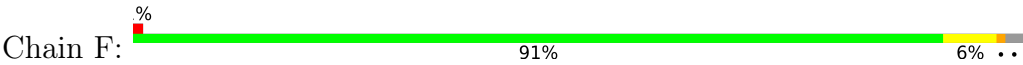
- Molecule 1: Acetyltransferase, putative



- Molecule 1: Acetyltransferase, putative



- Molecule 1: Acetyltransferase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.89Å 157.82Å 66.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 1.90 29.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.69-1.90) 99.7 (29.69-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.197 , 0.240 0.203 , 0.244	Depositor DCC
R_{free} test set	4466 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9179	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: PAP, ACO, COA, EP1, EDO

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	0.55	0/1405	0.93	1/1893 (0.1%)
1	B	0.53	0/1403	0.92	0/1892
1	C	0.53	0/1382	0.90	2/1864 (0.1%)
1	D	0.55	0/1377	0.91	0/1856
1	E	0.57	0/1392	0.95	2/1880 (0.1%)
1	F	0.54	0/1372	0.95	1/1852 (0.1%)
All	All	0.54	0/8331	0.93	6/11237 (0.1%)

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	C	0	1
1	D	0	2
1	F	0	2
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	ASP	CB-CA-C	6.38	121.84	110.16
1	A	0	HIS	CB-CA-C	5.77	119.93	110.88
1	F	32	ILE	N-CA-C	-5.65	106.30	111.67
1	E	46	GLU	CB-CA-C	5.15	119.02	109.54
1	C	99	ASP	CA-CB-CG	5.15	117.75	112.60
1	E	66	THR	CA-CB-OG1	-5.02	102.08	109.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	24	ARG	Sidechain
1	D	102	ARG	Sidechain
1	D	14	ARG	Sidechain
1	F	102	ARG	Sidechain
1	F	35	ARG	Sidechain

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	1373	0	1427	11	0
1	B	1368	0	1426	10	0
1	C	1350	0	1401	9	0
1	D	1347	0	1407	9	0
1	E	1367	0	1403	6	0
1	F	1347	0	1383	6	0
2	A	51	0	34	1	0
2	C	51	0	34	2	0
2	D	51	0	34	0	0
2	E	51	0	34	2	0
3	B	48	0	32	1	0
3	F	48	0	32	2	0
4	B	4	0	6	0	0
4	F	4	0	6	0	0
5	B	16	0	20	0	0
6	E	31	0	11	3	0
7	A	112	0	0	2	1
7	B	95	0	0	2	0
7	C	114	0	0	3	0
7	D	108	0	0	1	0
7	E	113	0	0	1	0
7	F	130	0	0	1	0
All	All	9179	0	8690	56	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (56) 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:99:ASP:CG	7:C:301:HOH:O	2.06	0.96
1:F:173:TYR:OH	3:F:201:COA:O5A	2.01	0.77
1:B:28:PHE:CE1	1:B:32[B]:ILE:HD11	2.21	0.75
6:E:202:PAP:C5'	6:E:202:PAP:H8	2.17	0.73
1:D:11:PHE:CD2	1:D:31:MET:HE1	2.24	0.72
1:C:99:ASP:OD1	7:C:301:HOH:O	2.07	0.67
1:A:100:THR:OG1	2:C:201:ACO:HH33	1.96	0.65
6:E:202:PAP:H8	6:E:202:PAP:H5'1	1.80	0.64
7:A:378:HOH:O	2:C:201:ACO:HH32	1.97	0.61
1:C:99:ASP:CB	7:C:301:HOH:O	2.43	0.60
1:D:175:ARG:HH21	1:D:175:ARG:HB3	1.65	0.60
3:B:201:COA:O4A	3:B:201:COA:O5B	2.21	0.59
1:B:168:THR:OG1	1:B:169:ASP:N	2.39	0.55
1:E:124:TYR:OH	2:E:201:ACO:H62	2.07	0.55
1:A:118:ARG:HH21	1:A:118:ARG:CB	2.19	0.55
6:E:202:PAP:H8	6:E:202:PAP:H5'2	1.88	0.53
1:E:133:LYS:NZ	7:E:303:HOH:O	2.35	0.52
1:B:64:LYS:HG3	1:E:46:GLU:OE2	2.10	0.52
1:C:169:ASP:OD1	1:C:171:LEU:HB2	2.10	0.51
1:C:94:GLN:NE2	1:C:96:TYR:OH	2.43	0.51
1:E:173:TYR:OH	2:E:201:ACO:O5A	2.27	0.50
1:F:94:GLN:NE2	1:F:96:TYR:OH	2.44	0.50
1:B:133:LYS:NZ	7:B:303:HOH:O	2.43	0.50
1:D:99[A]:ASP:OD2	7:D:301:HOH:O	2.19	0.50
1:A:172:ASN:HD22	1:A:172:ASN:H	1.58	0.50
1:D:11:PHE:CE2	1:D:31:MET:HE1	2.47	0.49
3:F:201:COA:H52A	7:F:362:HOH:O	2.12	0.49
1:D:119:ILE:HD13	1:D:125:LEU:HD11	1.95	0.48
1:C:131:ILE:HD12	1:C:137:ILE:HD11	1.95	0.48
1:A:60:VAL:O	1:A:61:LYS:HD2	2.14	0.48
1:B:159:VAL:HG12	1:B:166:ILE:HA	1.94	0.48
1:C:135:VAL:C	1:C:136:LYS:HD3	2.40	0.47
1:B:122:ASP:O	1:B:140:ARG:HA	2.14	0.47
1:A:118:ARG:HH21	1:A:118:ARG:HB2	1.79	0.47
1:A:172:ASN:HD22	1:A:172:ASN:N	2.13	0.46
1:F:159:VAL:HG12	1:F:166:ILE:HA	1.98	0.46
1:E:167:ILE:O	1:E:168:THR:HG23	2.14	0.46
1:D:75:ASP:HB3	1:D:96:TYR:HA	1.97	0.45
1:F:172:ASN:H	1:F:172:ASN:HD22	1.65	0.44
1:F:118:ARG:HB3	1:F:136:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TYR:HH	2:A:201:ACO:HN4	1.65	0.42
1:B:119:ILE:HG12	1:B:137:ILE:HD12	2.00	0.42
1:D:175:ARG:HB3	1:D:175:ARG:NH2	2.33	0.42
1:D:94:GLN:NE2	1:D:96:TYR:OH	2.52	0.42
1:A:0:HIS:CD2	7:B:327:HOH:O	2.72	0.42
1:C:131:ILE:HD13	1:C:149:VAL:CG2	2.50	0.42
1:F:38:LYS:O	1:F:42:LEU:HG	2.20	0.42
1:B:94:GLN:NE2	1:B:96:TYR:OH	2.53	0.41
1:C:48:THR:HG23	1:C:66:THR:O	2.20	0.41
1:A:102:ARG:HD3	7:A:401:HOH:O	2.20	0.41
1:B:21[B]:LYS:HB3	1:B:21[B]:LYS:HE2	1.72	0.41
1:B:65:ASP:O	1:B:86:ASN:HA	2.20	0.41
1:A:159:VAL:HG12	1:A:166:ILE:HA	2.02	0.41

All (1) 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)
7:A:361:HOH:O	7:A:361:HOH:O[2_555]	1.95	0.25

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	180/182 (99%)	176 (98%)	4 (2%)	0	100	100
1	B	179/182 (98%)	177 (99%)	2 (1%)	0	100	100
1	C	177/182 (97%)	171 (97%)	6 (3%)	0	100	100
1	D	176/182 (97%)	169 (96%)	7 (4%)	0	100	100
1	E	179/182 (98%)	175 (98%)	3 (2%)	1 (1%)	21	13
1	F	177/182 (97%)	171 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1068/1092 (98%)	1039 (97%)	28 (3%)	1 (0%)	48 40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	172	ASN

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	152/152 (100%)	149 (98%)	3 (2%)	48 46
1	B	153/152 (101%)	152 (99%)	1 (1%)	76 78
1	C	151/152 (99%)	148 (98%)	3 (2%)	48 46
1	D	151/152 (99%)	143 (95%)	8 (5%)	20 12
1	E	152/152 (100%)	146 (96%)	6 (4%)	28 21
1	F	149/152 (98%)	147 (99%)	2 (1%)	61 61
All	All	908/912 (100%)	885 (98%)	23 (2%)	42 37

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

Mol	Chain	Res	Type
1	A	118	ARG
1	A	172	ASN
1	A	175	ARG
1	B	109	LYS
1	C	99	ASP
1	C	136	LYS
1	C	171	LEU
1	D	14	ARG
1	D	23	ASN
1	D	66	THR
1	D	99[A]	ASP

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Mol	Chain	Res	Type
1	D	99[B]	ASP
1	D	159	VAL
1	D	168	THR
1	D	175	ARG
1	E	46	GLU
1	E	59	GLU
1	E	66	THR
1	E	127	PRO
1	E	136	LYS
1	E	159	VAL
1	F	136	LYS
1	F	172	ASN

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

Mol	Chain	Res	Type
1	A	86	ASN
1	A	94	GLN
1	A	128	ASN
1	A	172	ASN
1	B	86	ASN
1	B	94	GLN
1	B	128	ASN
1	C	94	GLN
1	C	128	ASN
1	D	94	GLN
1	E	86	ASN
1	E	128	ASN
1	F	86	ASN
1	F	94	GLN
1	F	128	ASN
1	F	172	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	C	201	-	51,53,53	0.42	0	73,79,79	0.83	3 (4%)
2	ACO	A	201	-	51,53,53	0.57	1 (1%)	73,79,79	0.85	1 (1%)
4	EDO	F	202	-	3,3,3	0.14	0	2,2,2	0.07	0
2	ACO	D	201	-	51,53,53	0.54	1 (1%)	73,79,79	0.83	3 (4%)
4	EDO	B	202	-	3,3,3	0.22	0	2,2,2	0.49	0
3	COA	B	201	-	47,50,50	0.61	1 (2%)	69,75,75	0.87	3 (4%)
5	EP1	B	203	-	16,16,16	0.66	1 (6%)	21,21,21	0.81	1 (4%)
2	ACO	E	201	-	51,53,53	0.60	1 (1%)	73,79,79	0.86	5 (6%)
3	COA	F	201	-	47,50,50	0.53	1 (2%)	69,75,75	0.85	3 (4%)
6	PAP	E	202	-	32,33,33	0.70	1 (3%)	50,52,52	0.93	3 (6%)

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	C	201	-	-	8/51/67/67	0/3/3/3
2	ACO	A	201	-	-	9/51/67/67	0/3/3/3
4	EDO	F	202	-	-	1/1/1/1	-
2	ACO	D	201	-	-	8/51/67/67	0/3/3/3
4	EDO	B	202	-	-	1/1/1/1	-
3	COA	B	201	-	-	6/48/64/64	0/3/3/3
5	EP1	B	203	-	-	5/10/20/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	E	201	-	-	11/51/67/67	0/3/3/3
3	COA	F	201	-	-	8/48/64/64	0/3/3/3
6	PAP	E	202	-	-	4/21/37/37	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	ACO	P3B-O3B	2.99	1.64	1.59
2	A	201	ACO	P3B-O3B	2.86	1.64	1.59
6	E	202	PAP	P-O3'	2.69	1.64	1.59
2	D	201	ACO	P3B-O3B	2.36	1.63	1.59
3	B	201	COA	P3B-O3B	2.34	1.63	1.59
5	B	203	EP1	O1S-S	2.28	1.55	1.47
3	F	201	COA	P3B-O3B	2.19	1.63	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	202	PAP	P-O3'-C3'	-3.81	113.26	123.43
2	A	201	ACO	P3B-O3B-C3B	-3.59	113.84	123.43
2	D	201	ACO	P3B-O3B-C3B	-3.26	114.73	123.43
5	B	203	EP1	O1S-S-C11	-2.78	100.56	106.00
2	C	201	ACO	C2P-S1P-C	2.74	114.58	101.42
2	E	201	ACO	C3P-N4P-C5P	2.66	127.77	122.82
2	E	201	ACO	P3B-O3B-C3B	-2.58	116.53	123.43
2	C	201	ACO	P3B-O3B-C3B	-2.52	116.70	123.43
3	F	201	COA	C7P-C6P-C5P	2.51	116.57	112.39
3	B	201	COA	C7P-C6P-C5P	2.37	116.34	112.39
2	E	201	ACO	C2P-C3P-N4P	2.28	117.18	112.41
3	F	201	COA	P3B-O3B-C3B	-2.24	117.45	123.43
6	E	202	PAP	O4'-C1'-N9	2.17	112.26	108.09
2	E	201	ACO	C2B-C1B-N9A	2.12	118.58	113.30
2	D	201	ACO	O9A-P3B-O3B	-2.10	97.68	105.85
2	D	201	ACO	C2P-S1P-C	2.09	111.47	101.42
6	E	202	PAP	PA-O5'-C5'	-2.06	109.55	121.35
2	C	201	ACO	O2A-P1A-O1A	2.05	121.96	112.44
3	B	201	COA	O5P-C5P-C6P	-2.02	118.36	122.02
3	B	201	COA	C3P-N4P-C5P	2.01	126.57	122.82
2	E	201	ACO	O5A-P2A-O4A	2.01	121.80	112.44
3	F	201	COA	O3A-P1A-O1A	-2.01	104.66	110.70

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	ACO	C5B-O5B-P1A-O1A
2	A	201	ACO	C5B-O5B-P1A-O2A
2	A	201	ACO	C5B-O5B-P1A-O3A
2	A	201	ACO	P2A-O3A-P1A-O5B
2	C	201	ACO	C5B-O5B-P1A-O1A
2	C	201	ACO	C5B-O5B-P1A-O2A
2	C	201	ACO	C5B-O5B-P1A-O3A
2	C	201	ACO	P2A-O3A-P1A-O5B
2	D	201	ACO	C5B-O5B-P1A-O1A
2	D	201	ACO	C5B-O5B-P1A-O2A
2	D	201	ACO	C5B-O5B-P1A-O3A
2	D	201	ACO	P2A-O3A-P1A-O5B
2	D	201	ACO	O-C-S1P-C2P
2	D	201	ACO	CH3-C-S1P-C2P
2	E	201	ACO	C5B-O5B-P1A-O1A
2	E	201	ACO	C5B-O5B-P1A-O2A
2	E	201	ACO	C5B-O5B-P1A-O3A
2	E	201	ACO	P2A-O3A-P1A-O5B
3	F	201	COA	C5B-O5B-P1A-O2A
3	F	201	COA	C5B-O5B-P1A-O3A
5	B	203	EP1	C9-C10-C11-S
5	B	203	EP1	C11-C10-C9-N1
5	B	203	EP1	C8-C7-N4-C5
6	E	202	PAP	PA-O3A-PB-O3B
6	E	202	PAP	O4'-C4'-C5'-O5'
6	E	202	PAP	C3'-C4'-C5'-O5'
5	B	203	EP1	C10-C9-N1-C6
5	B	203	EP1	C10-C9-N1-C2
2	C	201	ACO	O-C-S1P-C2P
2	C	201	ACO	CH3-C-S1P-C2P
2	E	201	ACO	O-C-S1P-C2P
2	E	201	ACO	CH3-C-S1P-C2P
3	B	201	COA	O4B-C4B-C5B-O5B
4	F	202	EDO	O1-C1-C2-O2
3	B	201	COA	P2A-O3A-P1A-O5B
3	F	201	COA	P2A-O3A-P1A-O5B
2	E	201	ACO	O5P-C5P-N4P-C3P
2	E	201	ACO	C3P-C2P-S1P-C
2	A	201	ACO	CCP-O6A-P2A-O4A
2	C	201	ACO	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
2	D	201	ACO	CCP-O6A-P2A-O4A
2	E	201	ACO	CCP-O6A-P2A-O4A
3	B	201	COA	C5B-O5B-P1A-O1A
3	F	201	COA	C5B-O5B-P1A-O1A
3	F	201	COA	CCP-O6A-P2A-O4A
3	B	201	COA	C3B-C4B-C5B-O5B
2	A	201	ACO	C3B-O3B-P3B-O8A
3	F	201	COA	C3B-O3B-P3B-O8A
2	E	201	ACO	S1P-C2P-C3P-N4P
4	B	202	EDO	O1-C1-C2-O2
6	E	202	PAP	PA-O3A-PB-O1B
2	A	201	ACO	C2B-C3B-O3B-P3B
2	A	201	ACO	C4B-C3B-O3B-P3B
2	A	201	ACO	N8P-C9P-CAP-OAP
2	C	201	ACO	N8P-C9P-CAP-OAP
2	D	201	ACO	N8P-C9P-CAP-OAP
2	E	201	ACO	N8P-C9P-CAP-OAP
3	B	201	COA	N8P-C9P-CAP-OAP
3	F	201	COA	N8P-C9P-CAP-OAP
3	B	201	COA	P1A-O3A-P2A-O5A
3	F	201	COA	P1A-O3A-P2A-O5A

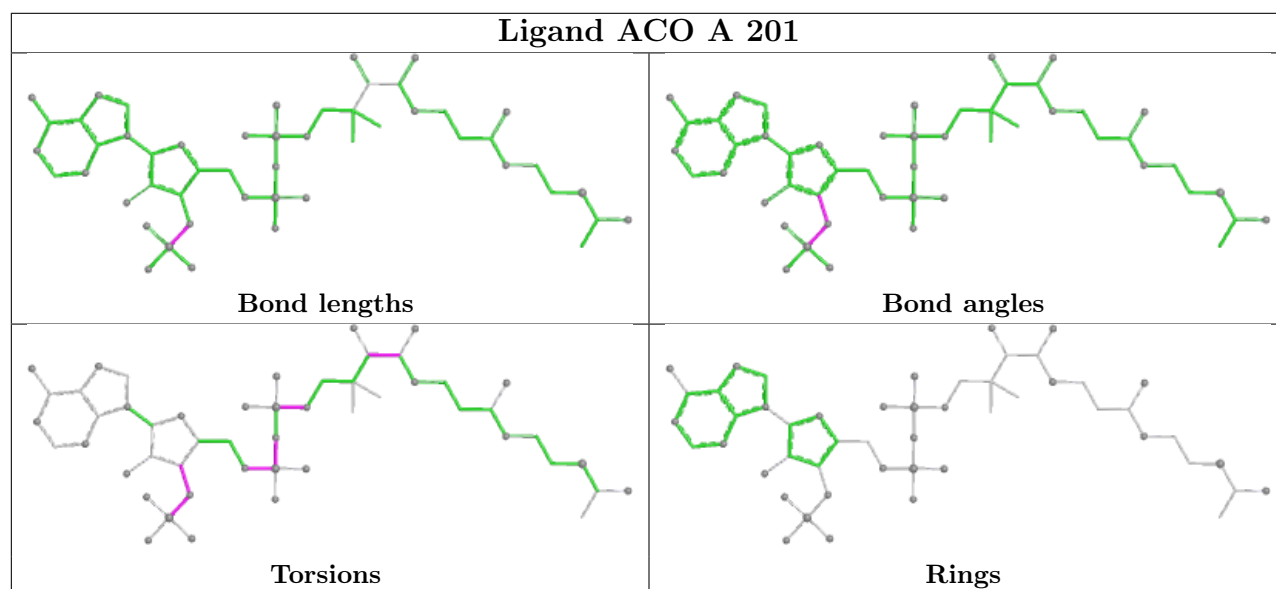
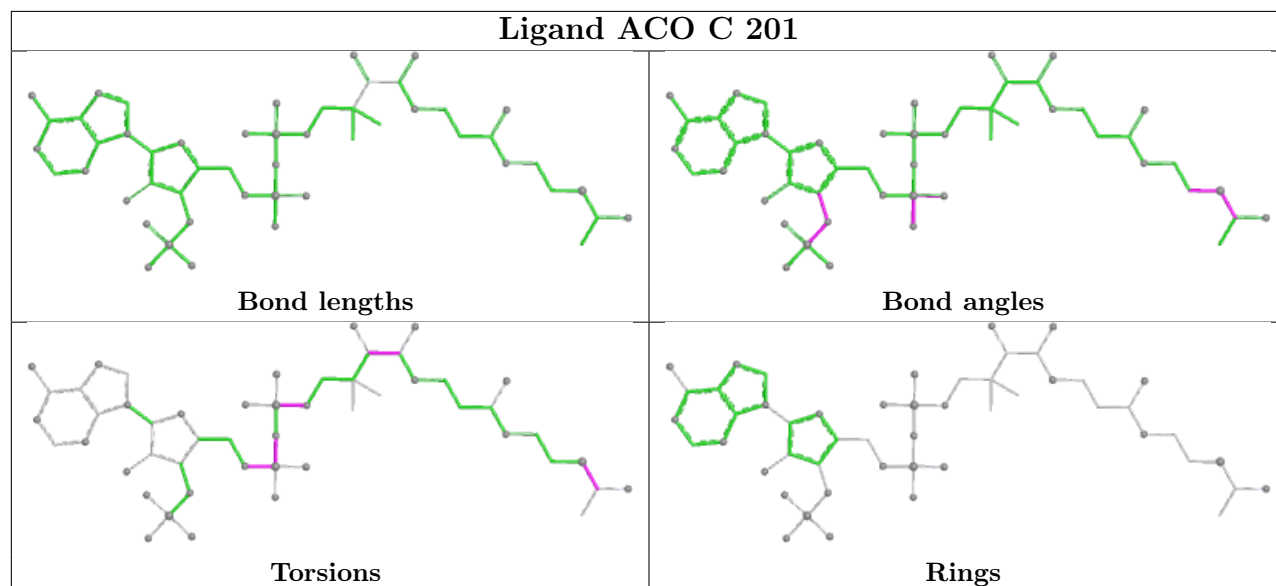
There are no ring outliers.

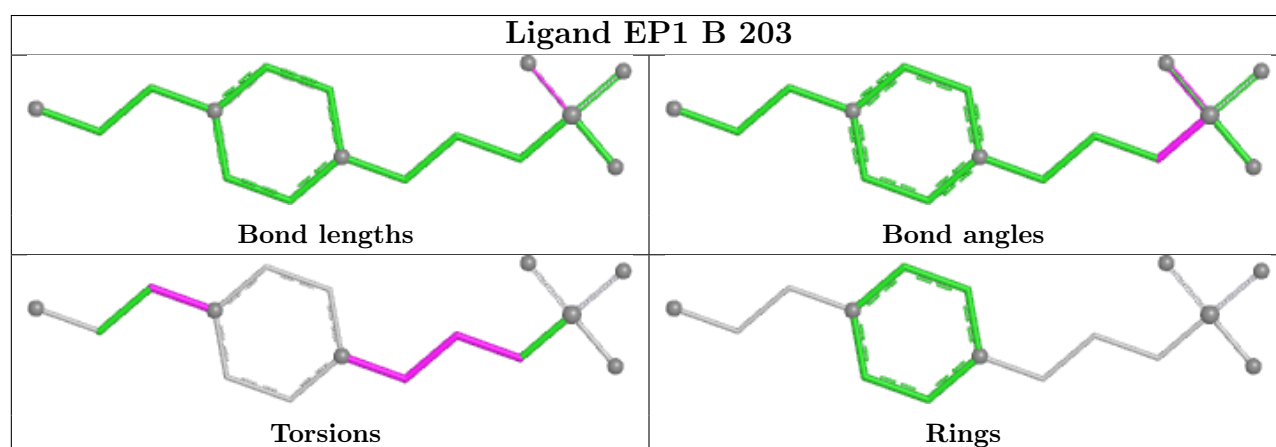
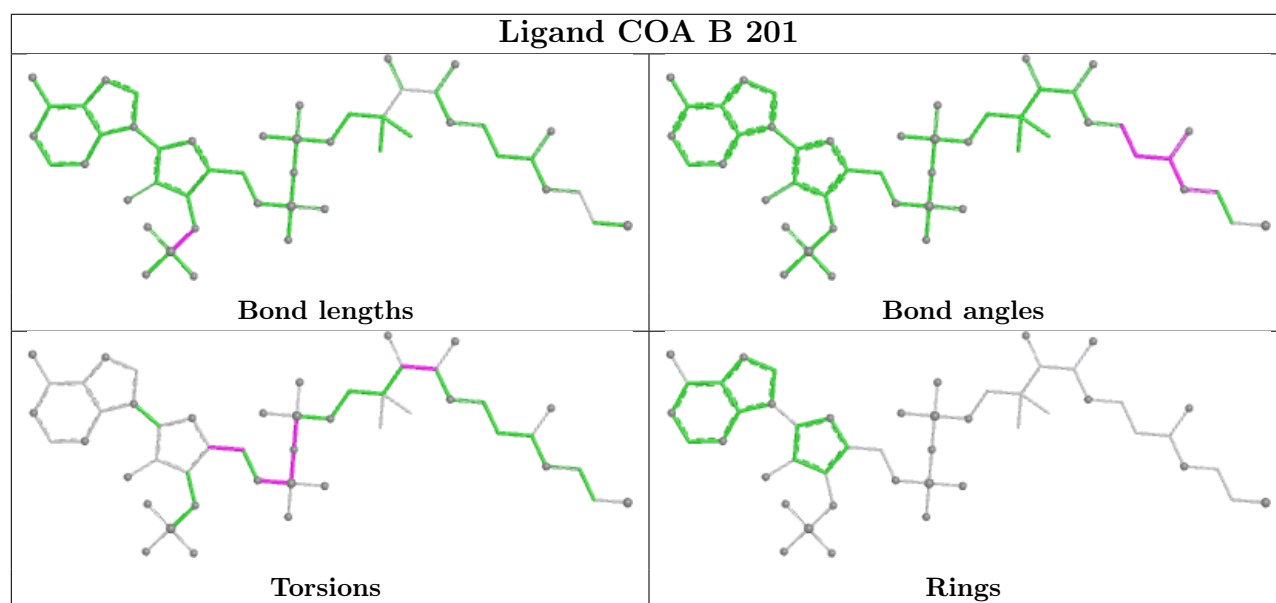
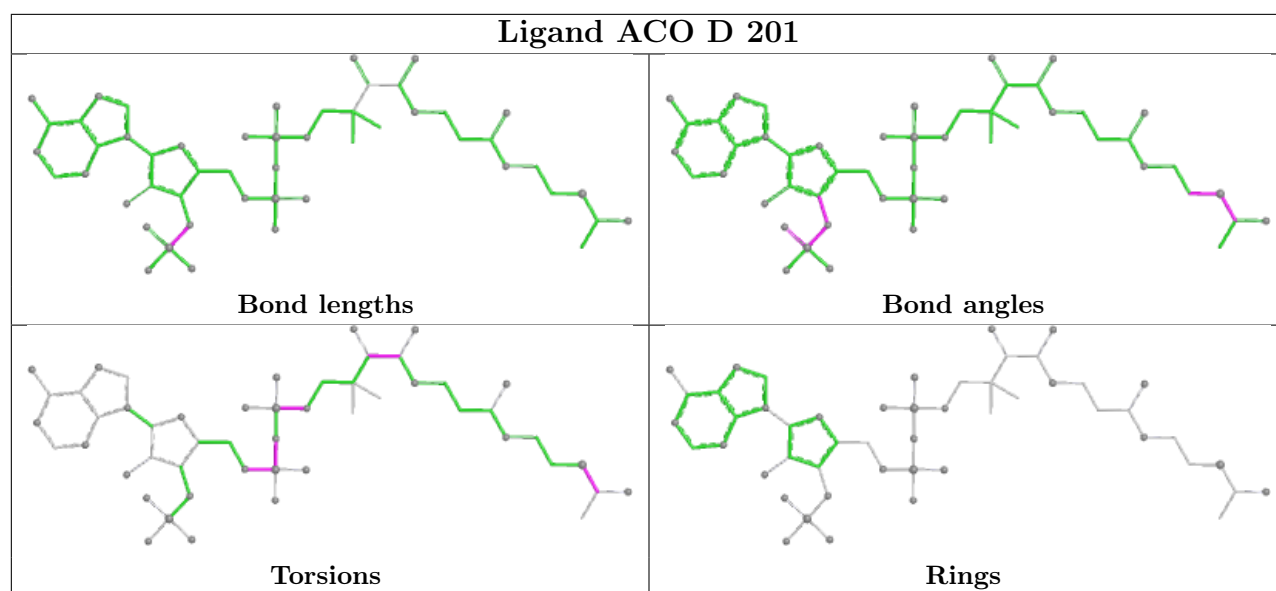
6 monomers are involved in 11 short contacts:

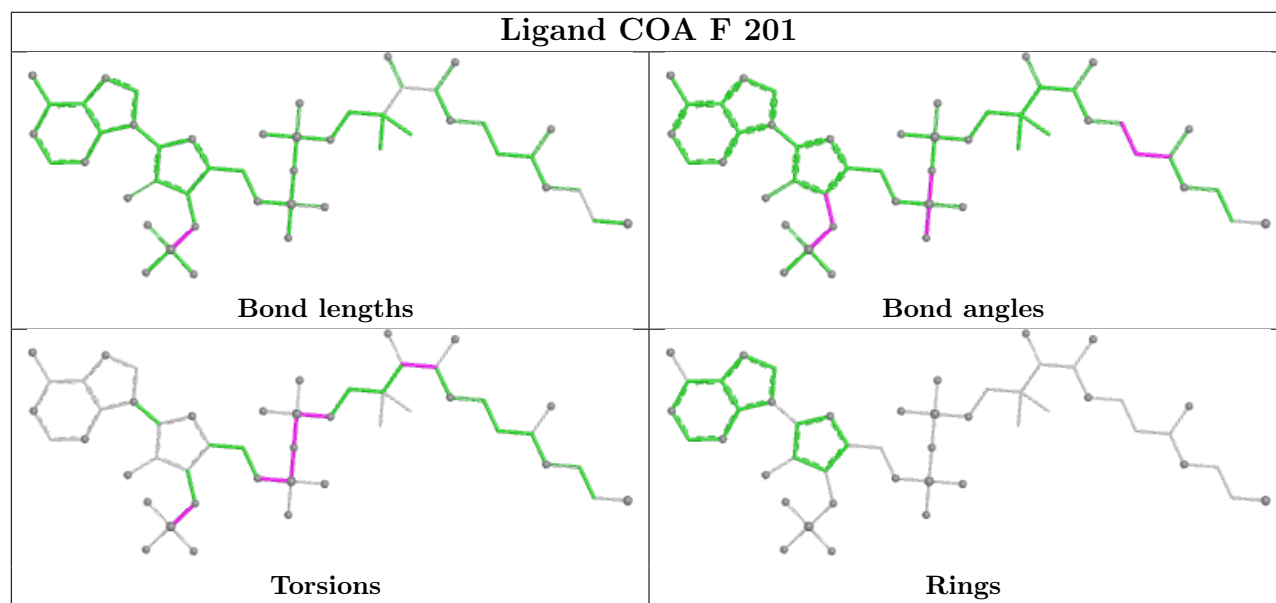
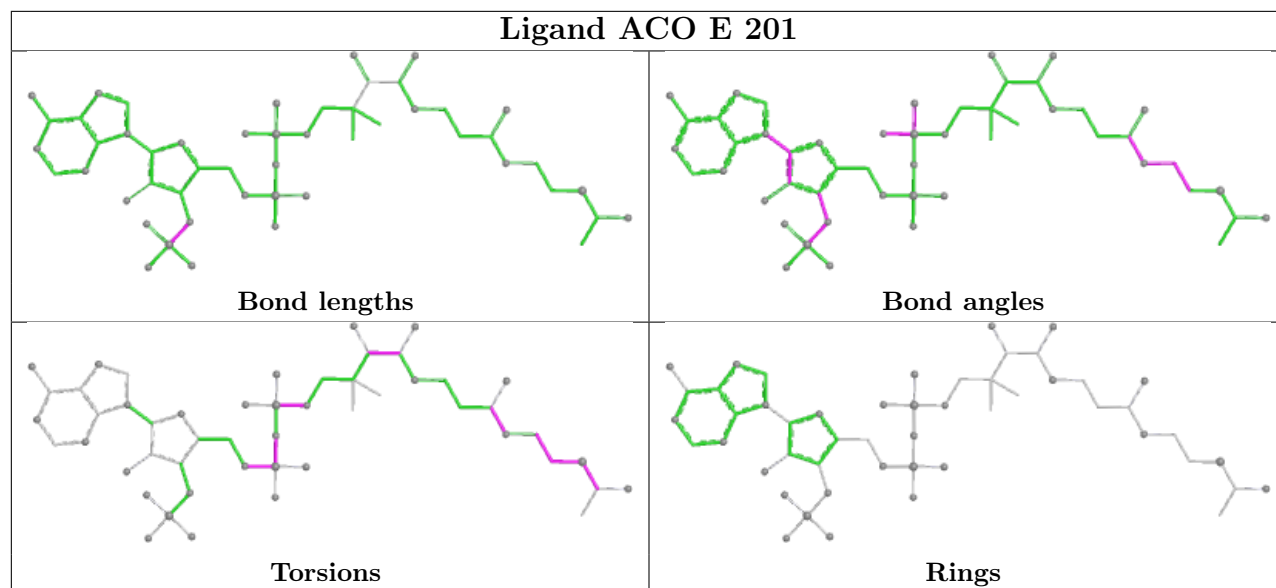
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	ACO	2	0
2	A	201	ACO	1	0
3	B	201	COA	1	0
2	E	201	ACO	2	0
3	F	201	COA	2	0
6	E	202	PAP	3	0

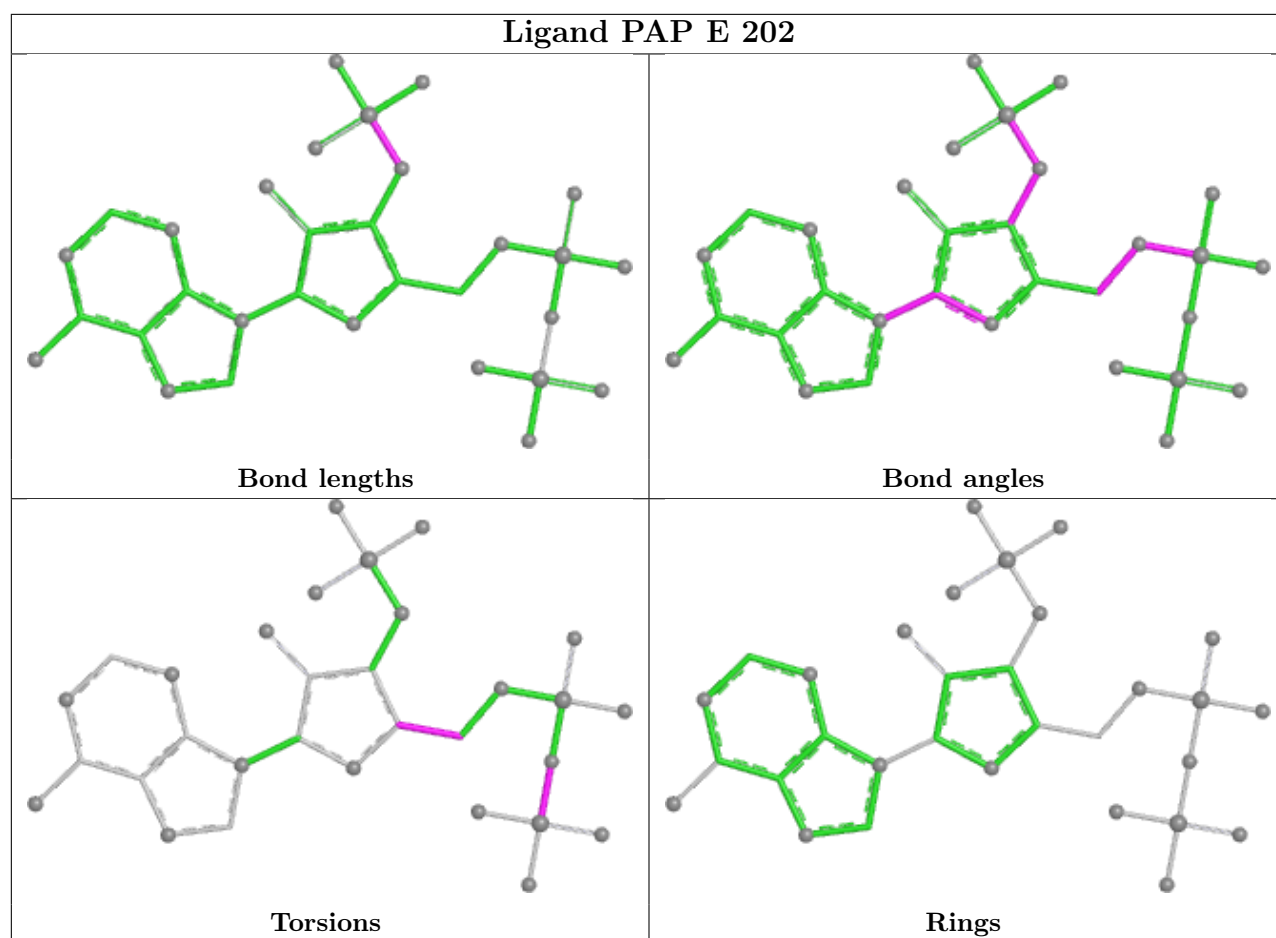
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	179/182 (98%)	-0.34	4 (2%)	62 66	7, 13, 34, 57	3 (1%)
1	B	177/182 (97%)	-0.16	2 (1%)	78 80	9, 18, 32, 50	4 (2%)
1	C	176/182 (96%)	-0.22	4 (2%)	61 65	7, 16, 31, 69	3 (1%)
1	D	175/182 (96%)	-0.15	4 (2%)	61 65	8, 18, 32, 70	3 (1%)
1	E	180/182 (98%)	-0.18	4 (2%)	62 66	7, 16, 37, 82	1 (0%)
1	F	178/182 (97%)	-0.22	2 (1%)	78 80	8, 16, 33, 48	1 (0%)
All	All	1065/1092 (97%)	-0.21	20 (1%)	66 70	7, 16, 33, 82	15 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-1	GLY	6.1
1	E	178	ILE	5.2
1	C	-1	GLY	4.3
1	E	0	HIS	3.9
1	E	1	MET	3.6
1	D	1	MET	3.5
1	A	176	ASN	3.5
1	F	-1	GLY	3.3
1	C	1	MET	2.9
1	A	17	TYR	2.7
1	D	175	ARG	2.7
1	D	172	ASN	2.6
1	B	1	MET	2.5
1	F	1	MET	2.5
1	A	20	LYS	2.3
1	A	12[A]	PHE	2.2
1	C	0	HIS	2.1
1	D	20	LYS	2.0
1	C	172	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	175	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

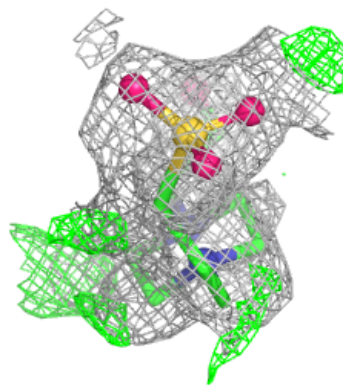
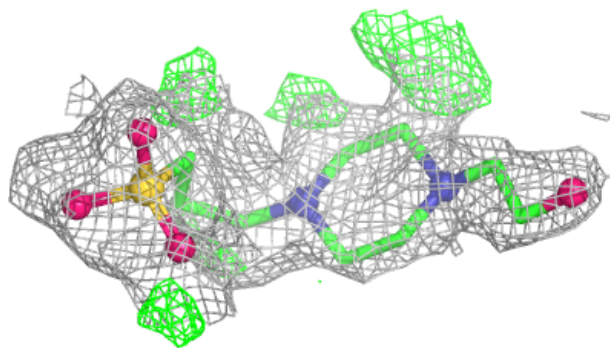
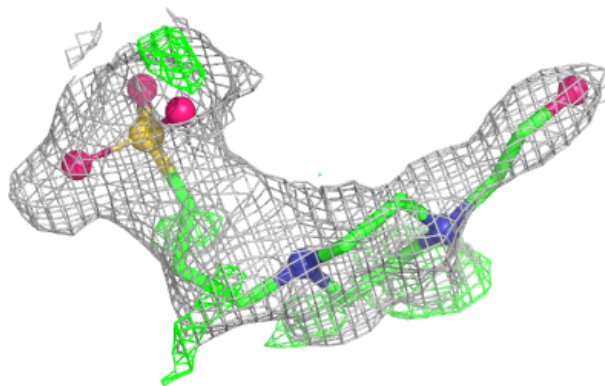
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EP1	B	203	16/16	0.72	0.20	60,66,71,71	0
4	EDO	F	202	4/4	0.88	0.16	30,31,31,32	0
6	PAP	E	202	31/31	0.90	0.09	24,32,62,64	0
3	COA	F	201	48/48	0.91	0.09	21,29,42,47	0
2	ACO	E	201	51/51	0.91	0.08	14,24,40,49	0
3	COA	B	201	48/48	0.92	0.08	14,18,36,51	0
4	EDO	B	202	4/4	0.93	0.12	25,26,27,27	0
2	ACO	C	201	51/51	0.93	0.07	18,23,37,45	0
2	ACO	D	201	51/51	0.95	0.07	12,21,31,34	0
2	ACO	A	201	51/51	0.96	0.06	13,17,26,32	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.

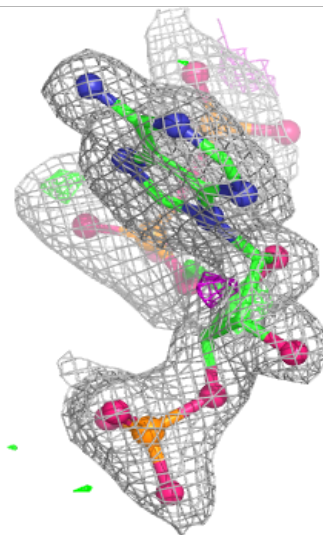
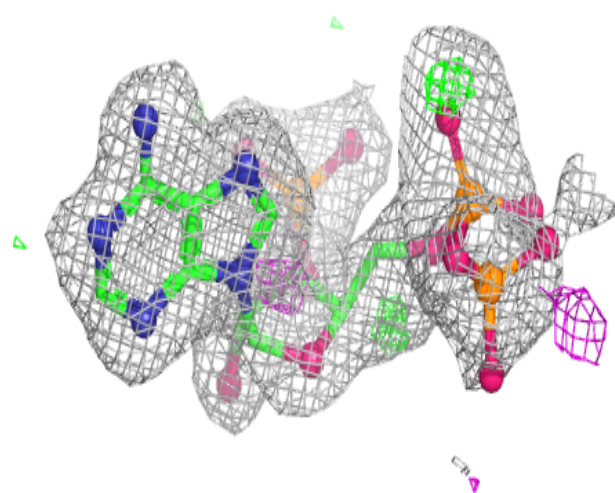
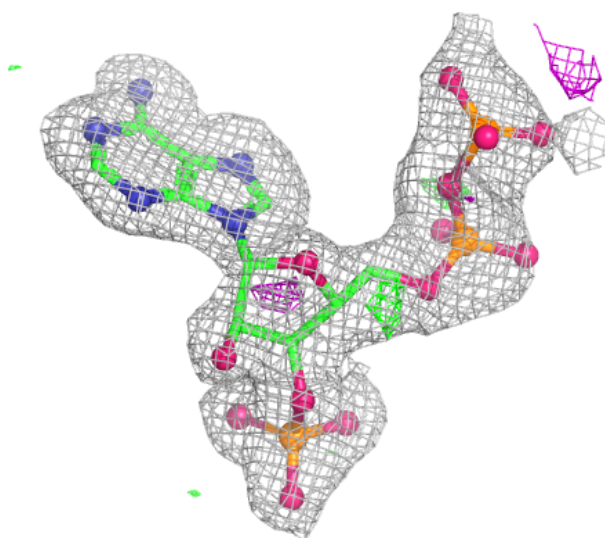
Electron density around EP1 B 203:

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



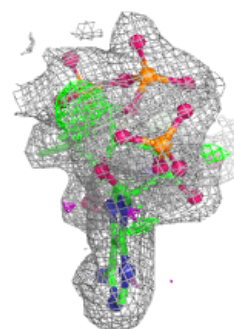
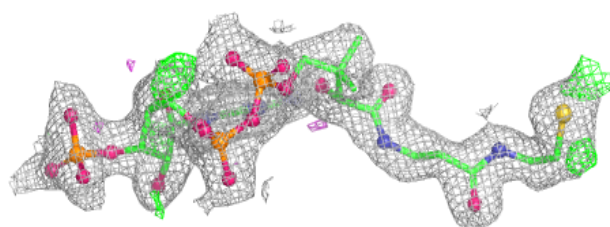
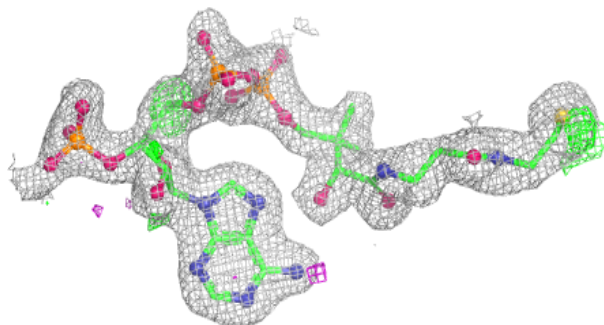
Electron density around PAP E 202:

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

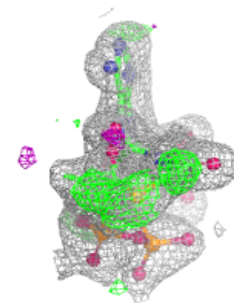
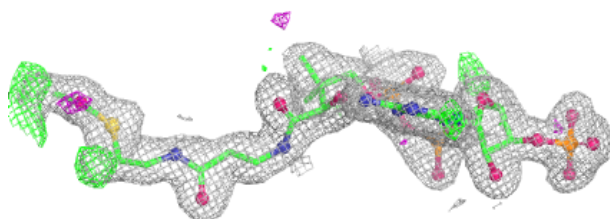
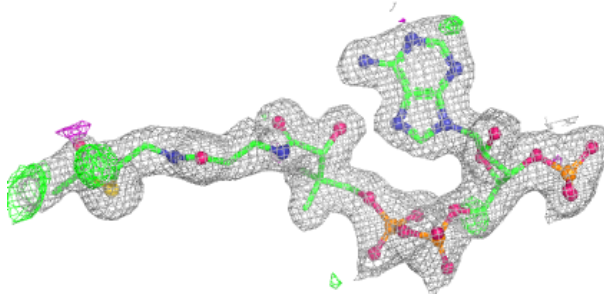


Electron density around COA F 201:

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

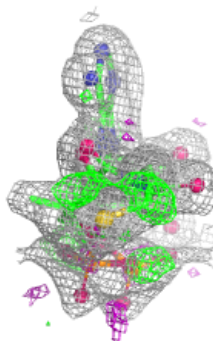
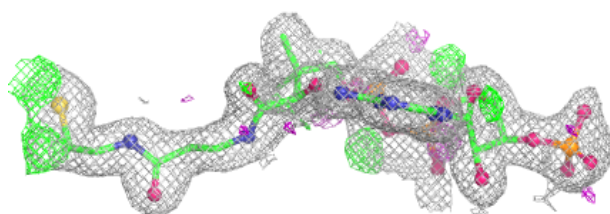
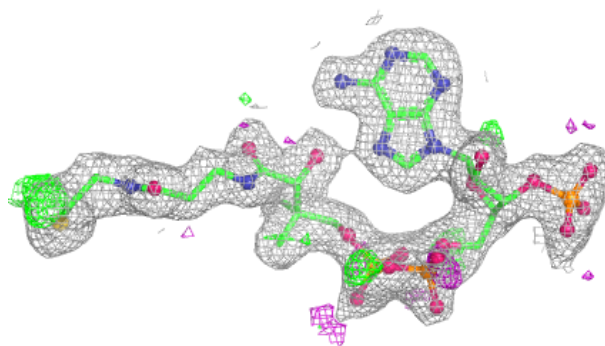
**Electron density around ACO E 201:**

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

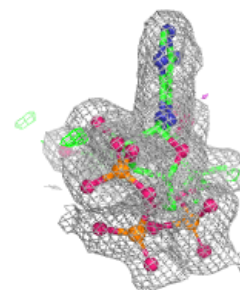
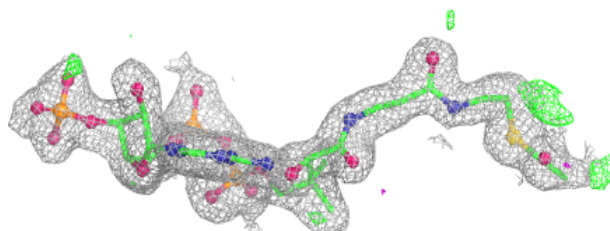
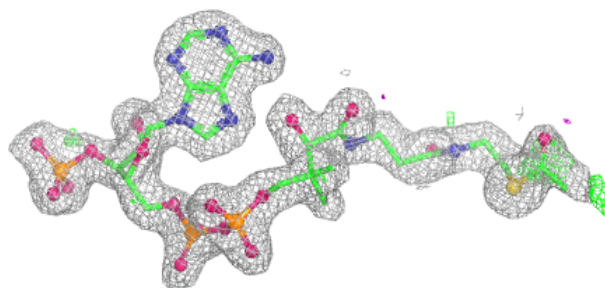


Electron density around COA B 201:

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

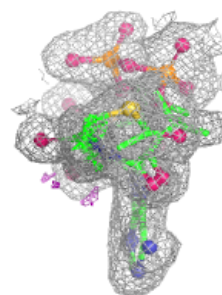
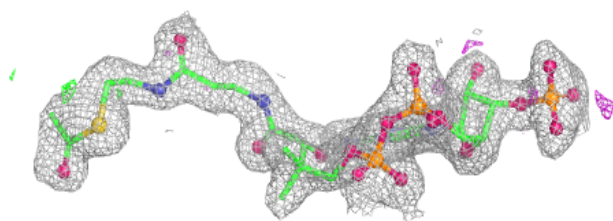
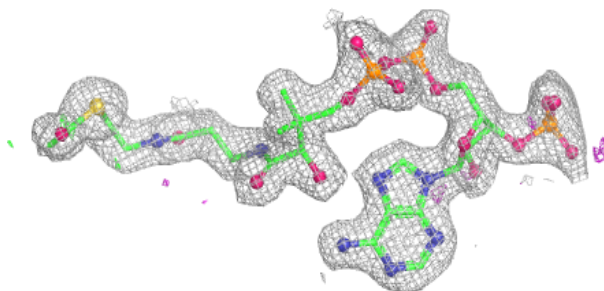
**Electron density around ACO C 201:**

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

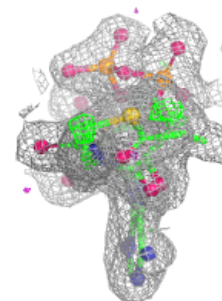
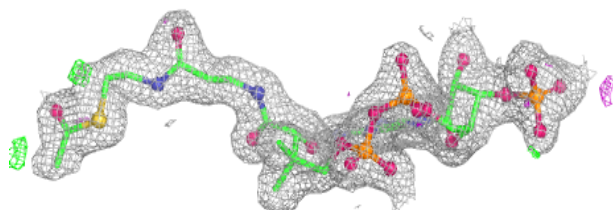
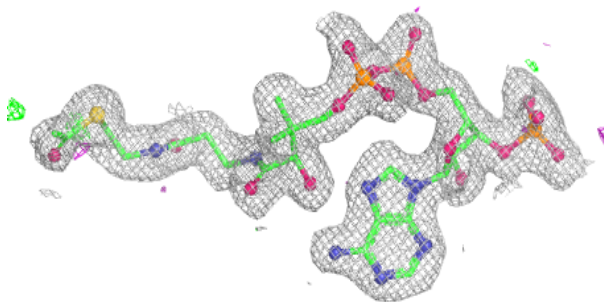


Electron density around ACO D 201:

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

**Electron density around ACO A 201:**

$2mF_o-DF_c$ (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.