wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 12:40 AM UTC

PDB ID	:	3MQG / pdb_00003mqg
Title	:	crystal structure of the 3-N-acetyl transferase WlbB from Bordetella petrii in complex with acetyl-CoA
Authors	:	Thoden, J.B.; Holden, H.M.
Deposited on	:	2010-04-28
Resolution	:	1.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

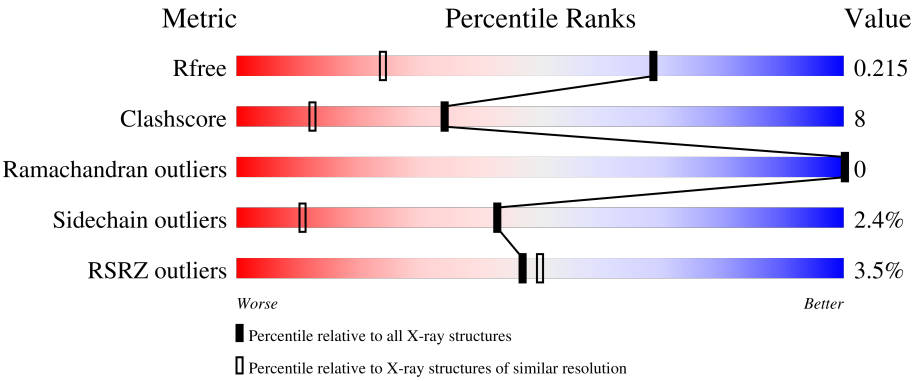
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.43 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	192	2% 91% 7% ••
1	B	192	5% 90% 8% ••
1	C	192	4% 93% 5% •
1	D	192	4% 94% 5% •
1	E	192	2% 92% 5% •••

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Mol	Chain	Length	Quality of chain
1	F	192	4% 93% 5%

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
7	EDO	B	194	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10694 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.

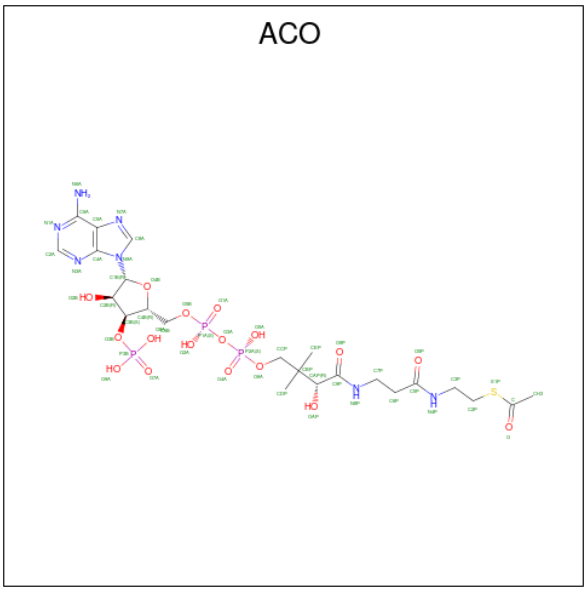
- Molecule 1 is a protein called Lipopolysaccharides biosynthesis acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	2	0
			1457	910	273	264	10			
1	B	190	Total	C	N	O	S	0	4	0
			1467	917	270	270	10			
1	C	192	Total	C	N	O	S	0	3	0
			1473	920	276	268	9			
1	D	192	Total	C	N	O	S	0	1	0
			1462	913	273	266	10			
1	E	190	Total	C	N	O	S	0	2	0
			1455	909	270	266	10			
1	F	189	Total	C	N	O	S	0	0	0
			1435	895	268	263	9			

There are 12 discrepancies between the modelled and reference sequences:

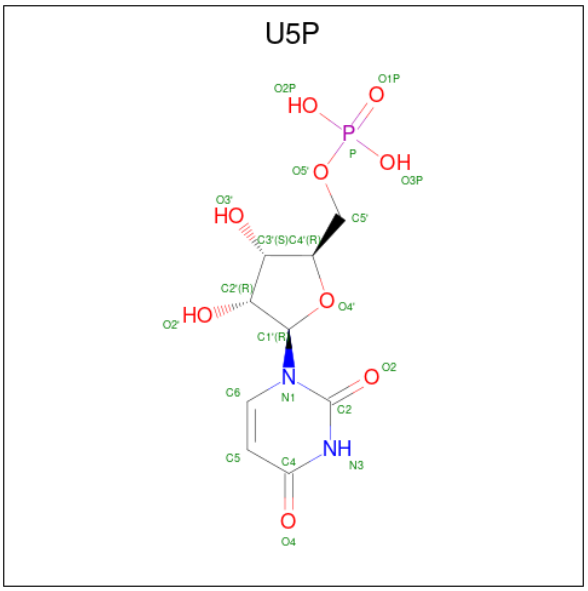
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A9IH93
A	0	HIS	-	expression tag	UNP A9IH93
B	-1	GLY	-	expression tag	UNP A9IH93
B	0	HIS	-	expression tag	UNP A9IH93
C	-1	GLY	-	expression tag	UNP A9IH93
C	0	HIS	-	expression tag	UNP A9IH93
D	-1	GLY	-	expression tag	UNP A9IH93
D	0	HIS	-	expression tag	UNP A9IH93
E	-1	GLY	-	expression tag	UNP A9IH93
E	0	HIS	-	expression tag	UNP A9IH93
F	-1	GLY	-	expression tag	UNP A9IH93
F	0	HIS	-	expression tag	UNP A9IH93

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



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

- Molecule 3 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: $C_9H_{13}N_2O_9P$).

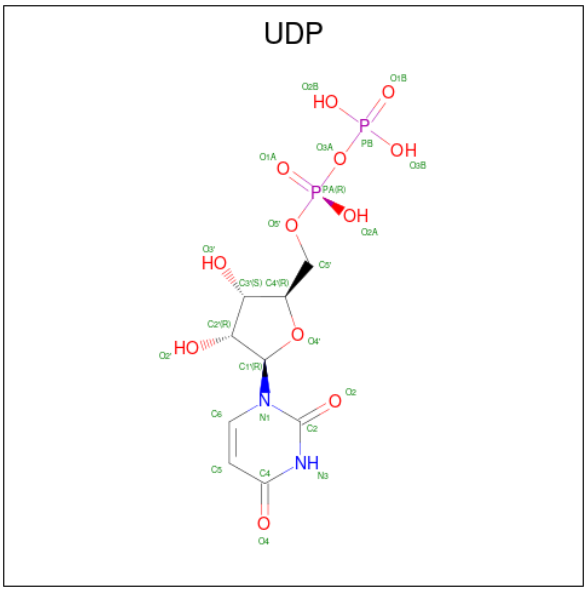


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 21 9 2 9 1	0	0
3	D	1	Total C N O P 21 9 2 9 1	0	0
3	E	1	Total C N O P 21 9 2 9 1	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

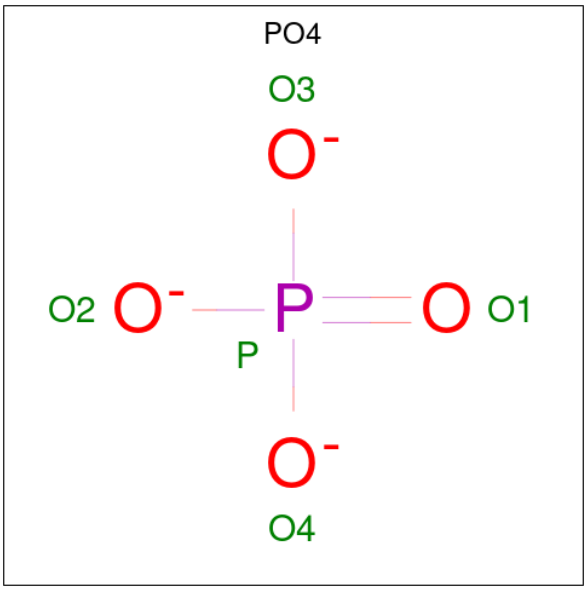
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



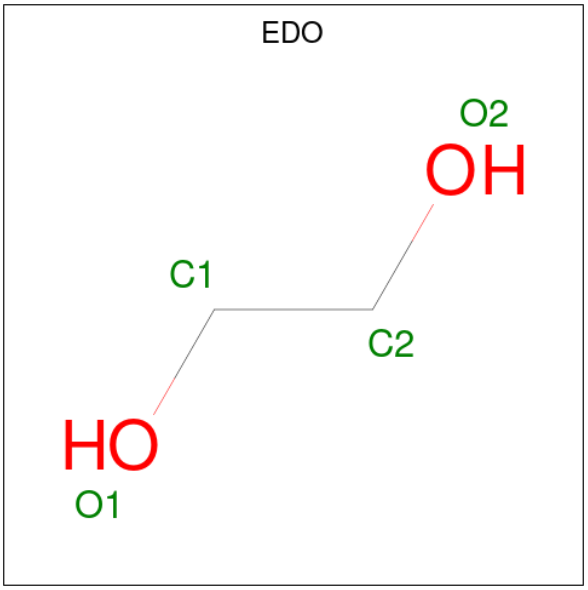
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O P 25 9 2 12 2	0	0
5	C	1	Total C N O P 25 9 2 12 2	0	0
5	F	1	Total O 1 1	0	0
5	F	1	Total C N O P 24 9 2 11 2	0	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



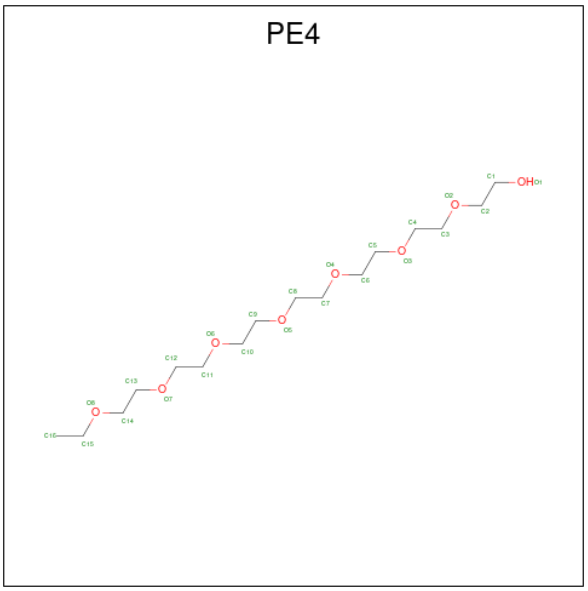
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 24 16 8	0	0

- Molecule 9 is water.

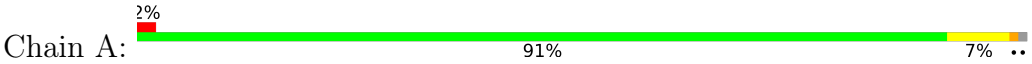
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	246	Total O 246 246	0	0
9	B	243	Total O 243 243	0	0
9	C	238	Total O 238 238	0	0
9	D	230	Total O 230 230	0	0
9	E	250	Total O 250 250	0	0
9	F	242	Total O 242 242	0	0

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: Lipopolysaccharides biosynthesis acetyltransferase

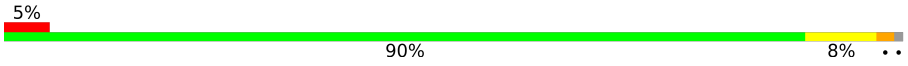
Chain A:

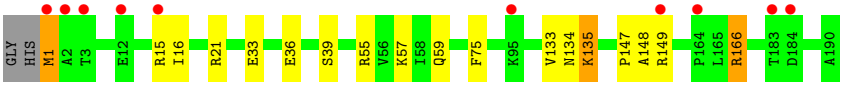




• Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase

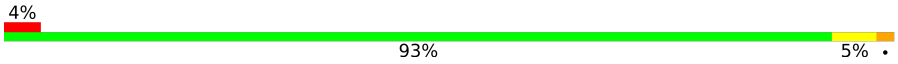
Chain B:

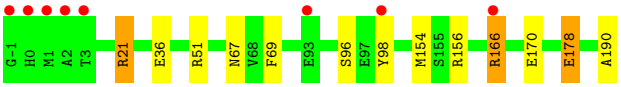




• Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase

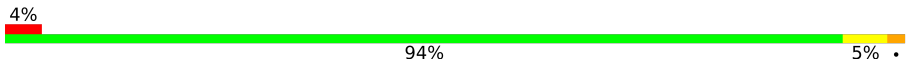
Chain C:

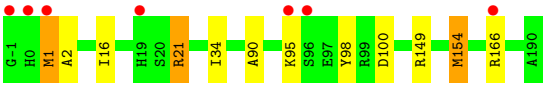




• Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase

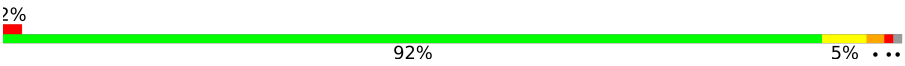
Chain D:

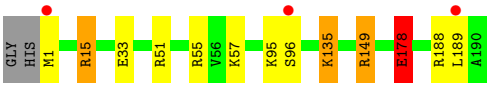




• Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase

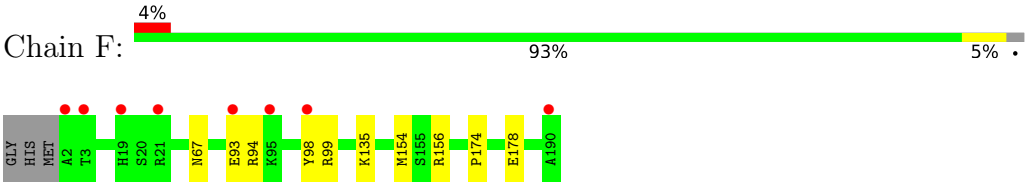
Chain E:





• Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase

Chain F:


4%
93%
5%
GLY
HIS
MET
A2
T3
H19
S20
R21
N67
E93
R94
K95
Y98
R99
K135
M154
S155
R156
P174
E178
A190

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.49Å 107.82Å 90.97Å 90.00° 102.49° 90.00°	Depositor
Resolution (Å)	30.00 – 1.43 30.00 – 1.43	Depositor EDS
% Data completeness (in resolution range)	95.6 (30.00-1.43) 92.1 (30.00-1.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	6.76 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.190 , 0.217 (Not available) , 0.215	Depositor DCC
R_{free} test set	11376 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	9.6	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10694	wwPDB-VP
Average B, all atoms (Å^2)	14.0	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 36.55 % 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 4.9142e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PO4, ACO, PE4, UDP, NA, U5P, 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	0.66	0/1492	1.08	0/2024
1	B	0.65	0/1508	1.10	0/2046
1	C	0.71	0/1512	1.16	2/2053 (0.1%)
1	D	0.64	0/1495	1.09	1/2030 (0.0%)
1	E	0.65	0/1490	1.11	1/2022 (0.0%)
1	F	0.73	0/1464	1.21	3/1989 (0.2%)
All	All	0.68	0/8961	1.12	7/12164 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	154	MET	CA-CB-CG	6.59	127.29	114.10
1	F	93	GLU	CA-C-N	-6.18	112.91	122.49
1	F	93	GLU	C-N-CA	-6.18	112.91	122.49
1	F	94	ARG	N-CA-C	5.78	121.05	113.30
1	E	178	GLU	CB-CA-C	-5.44	101.69	109.84

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	1457	0	1445	23	0
1	B	1467	0	1450	40	0
1	C	1473	0	1452	30	1
1	D	1462	0	1440	10	0
1	E	1455	0	1438	23	0
1	F	1435	0	1407	8	0
2	A	51	0	34	1	0
2	B	51	0	34	0	0
2	C	51	0	34	0	0
2	D	51	0	34	0	0
2	E	51	0	34	0	0
2	F	51	0	34	0	0
3	A	21	0	11	2	0
3	D	21	0	11	1	0
3	E	21	0	11	1	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	B	25	0	11	1	0
5	C	25	0	11	2	0
5	F	25	0	11	0	0
6	B	5	0	0	0	0
6	D	5	0	0	0	0
7	B	4	0	6	15	0
7	C	4	0	6	0	0
7	D	8	0	12	0	0
8	C	24	0	34	6	0
9	A	246	0	0	9	2
9	B	243	0	0	10	1
9	C	238	0	0	4	4
9	D	230	0	0	3	1
9	E	250	0	0	8	0
9	F	242	0	0	2	1
All	All	10694	0	8960	139	5

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 8.

The worst 5 of 139 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LYS:HZ2	1:B:135:LYS:CB	1.17	1.25
1:B:135:LYS:HB3	1:B:135:LYS:NZ	1.15	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:LYS:HB3	1:E:135:LYS:NZ	1.39	1.18
1:C:67:ASN:ND2	1:C:98:TYR:CD2	2.11	1.17
1:C:67:ASN:ND2	1:C:98:TYR:HD2	1.44	1.15

All (5) 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)
9:A:1965:HOH:O	9:C:1875:HOH:O[2_454]	1.63	0.57
9:C:1725:HOH:O	9:F:1805:HOH:O[1_454]	1.64	0.56
9:A:1944:HOH:O	9:C:1835:HOH:O[2_454]	1.97	0.23
1:C:190:ALA:O	9:D:1964:HOH:O[2_545]	2.02	0.18
9:B:1064:HOH:O	9:C:1712:HOH:O[2_554]	2.16	0.04

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	190/192 (99%)	187 (98%)	3 (2%)	0	100	100
1	B	192/192 (100%)	188 (98%)	4 (2%)	0	100	100
1	C	193/192 (100%)	189 (98%)	4 (2%)	0	100	100
1	D	191/192 (100%)	188 (98%)	3 (2%)	0	100	100
1	E	190/192 (99%)	187 (98%)	3 (2%)	0	100	100
1	F	187/192 (97%)	184 (98%)	3 (2%)	0	100	100
All	All	1143/1152 (99%)	1123 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	152/151 (101%)	151 (99%)	1 (1%)	76 53
1	B	154/151 (102%)	151 (98%)	3 (2%)	50 16
1	C	153/151 (101%)	148 (97%)	5 (3%)	33 5
1	D	152/151 (101%)	148 (97%)	4 (3%)	40 9
1	E	152/151 (101%)	144 (95%)	8 (5%)	20 1
1	F	149/151 (99%)	147 (99%)	2 (1%)	61 29
All	All	912/906 (101%)	889 (98%)	23 (2%)	43 10

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	15	ARG
1	E	96	SER
1	E	95	LYS
1	E	135	LYS
1	C	96	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	42	GLN
1	F	42	GLN
1	E	160	GLN
1	F	43	ASN
1	B	59	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACO	E	191	-	51,53,53	0.96	3 (5%)	73,79,79	1.66	11 (15%)
6	PO4	D	195	-	4,4,4	1.39	1 (25%)	6,6,6	1.14	0
5	UDP	C	192	-	25,26,26	1.21	3 (12%)	38,40,40	1.79	9 (23%)
7	EDO	B	194	-	3,3,3	0.35	0	2,2,2	0.45	0
5	UDP	B	192	-	25,26,26	1.24	3 (12%)	38,40,40	1.91	10 (26%)
3	U5P	D	192	-	22,22,22	1.12	2 (9%)	32,33,33	2.47	13 (40%)
8	PE4	C	193	-	23,23,23	0.47	0	22,22,22	1.00	0
3	U5P	E	192	-	22,22,22	1.15	2 (9%)	32,33,33	1.90	7 (21%)
2	ACO	A	191	-	51,53,53	1.00	3 (5%)	73,79,79	1.51	12 (16%)
2	ACO	B	191	-	51,53,53	0.96	2 (3%)	73,79,79	1.38	9 (12%)
7	EDO	C	194	-	3,3,3	0.53	0	2,2,2	0.50	0
7	EDO	D	196	-	3,3,3	0.42	0	2,2,2	0.71	0
6	PO4	B	193	-	4,4,4	1.33	0	6,6,6	1.97	2 (33%)
2	ACO	D	191	-	51,53,53	1.01	3 (5%)	73,79,79	1.52	12 (16%)
3	U5P	A	192	-	22,22,22	1.16	2 (9%)	32,33,33	2.11	12 (37%)
7	EDO	D	194	-	3,3,3	0.44	0	2,2,2	0.37	0
2	ACO	F	191	-	51,53,53	1.00	4 (7%)	73,79,79	1.49	10 (13%)
2	ACO	C	191	-	51,53,53	0.94	3 (5%)	73,79,79	1.56	15 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	UDP	F	193	-	21,25,26	1.17	2 (9%)	32,37,40	2.07	10 (31%)

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	E	191	-	-	4/51/67/67	0/3/3/3
5	UDP	C	192	-	-	5/16/32/32	0/2/2/2
7	EDO	D	196	-	-	0/1/1/1	-
8	PE4	C	193	-	-	13/21/21/21	-
2	ACO	D	191	-	-	3/51/67/67	0/3/3/3
3	U5P	A	192	-	-	0/10/26/26	0/2/2/2
7	EDO	D	194	-	-	1/1/1/1	-
2	ACO	F	191	-	-	3/51/67/67	0/3/3/3
2	ACO	C	191	-	-	2/51/67/67	0/3/3/3
5	UDP	F	193	-	-	3/13/31/32	0/2/2/2
5	UDP	B	192	-	-	5/16/32/32	0/2/2/2
3	U5P	D	192	-	-	5/10/26/26	0/2/2/2
3	U5P	E	192	-	-	0/10/26/26	0/2/2/2
2	ACO	A	191	-	-	3/51/67/67	0/3/3/3
2	ACO	B	191	-	-	4/51/67/67	0/3/3/3
7	EDO	B	194	-	-	1/1/1/1	-
7	EDO	C	194	-	-	0/1/1/1	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	191	ACO	P3B-O3B	3.48	1.65	1.59
2	A	191	ACO	P2A-O3A	3.29	1.63	1.59
5	B	192	UDP	PA-O3A	3.24	1.63	1.59
3	E	192	U5P	C2-N1	-3.07	1.33	1.38
2	A	191	ACO	P3B-O3B	2.98	1.64	1.59

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	191	ACO	C4A-N9A-C8A	6.11	112.15	105.74

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	193	UDP	C4-N3-C2	-5.71	119.52	126.61
5	B	192	UDP	N3-C2-N1	5.48	122.02	114.89
3	D	192	U5P	O4'-C4'-C3'	-5.29	94.65	105.15
3	A	192	U5P	C4-N3-C2	-5.15	120.22	126.61

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	192	U5P	C5'-O5'-P-O2P
3	D	192	U5P	C5'-O5'-P-O3P
5	B	192	UDP	PA-O3A-PB-O2B
5	C	192	UDP	PA-O3A-PB-O2B
3	D	192	U5P	C3'-C4'-C5'-O5'

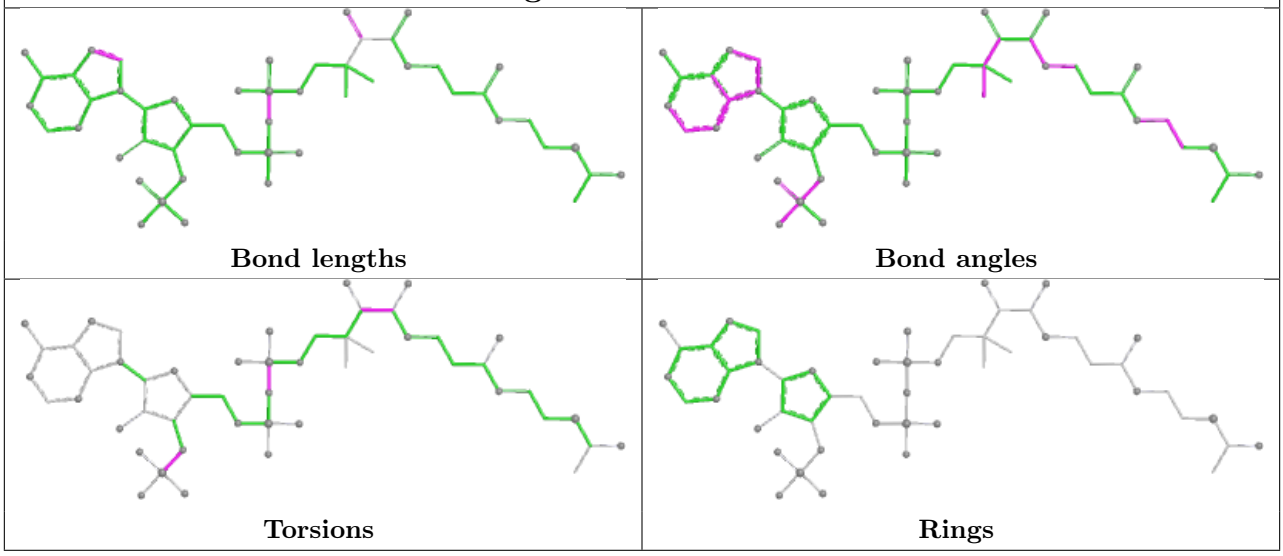
There are no ring outliers.

8 monomers are involved in 29 short contacts:

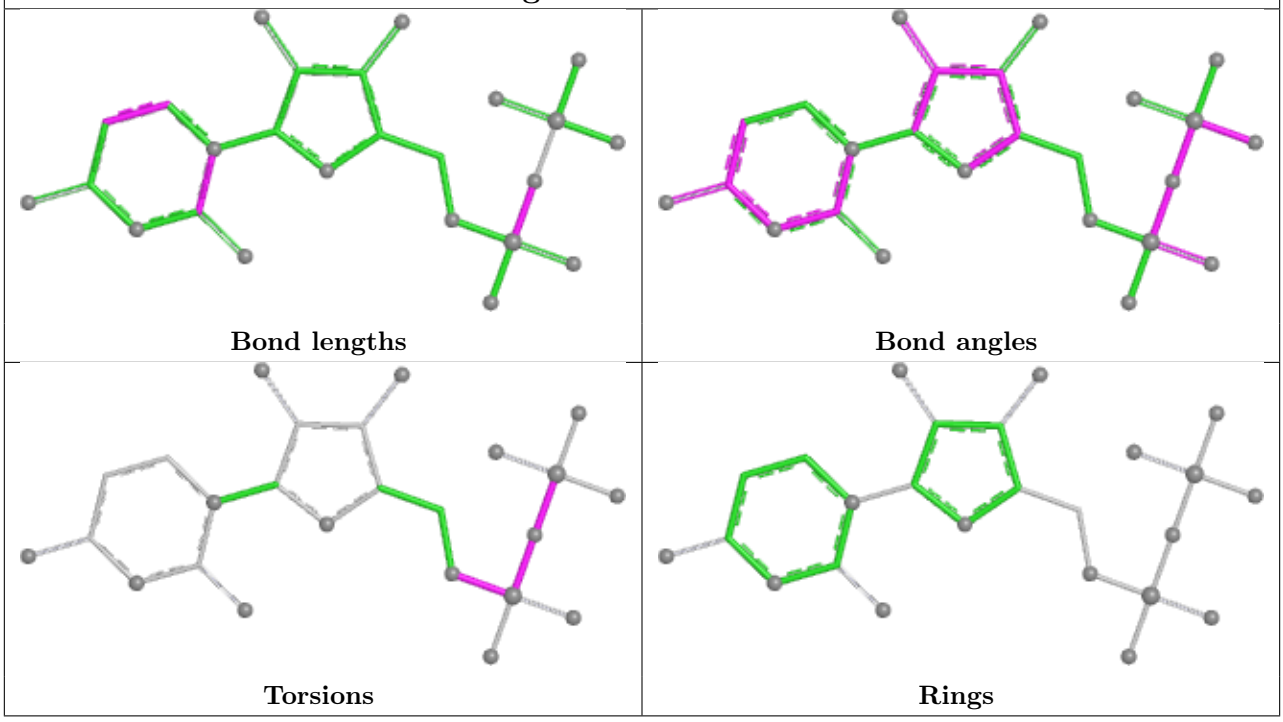
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	192	UDP	2	0
7	B	194	EDO	15	0
5	B	192	UDP	1	0
3	D	192	U5P	1	0
8	C	193	PE4	6	0
3	E	192	U5P	1	0
2	A	191	ACO	1	0
3	A	192	U5P	2	0

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.

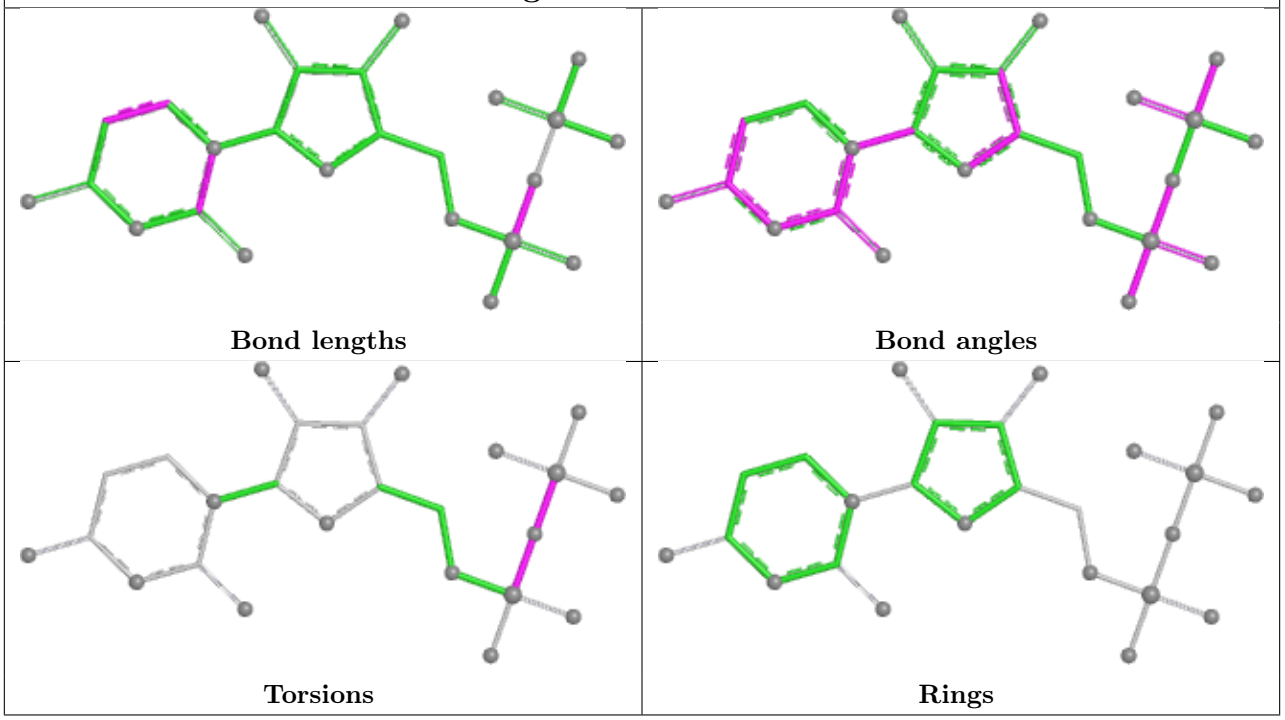
Ligand ACO E 191



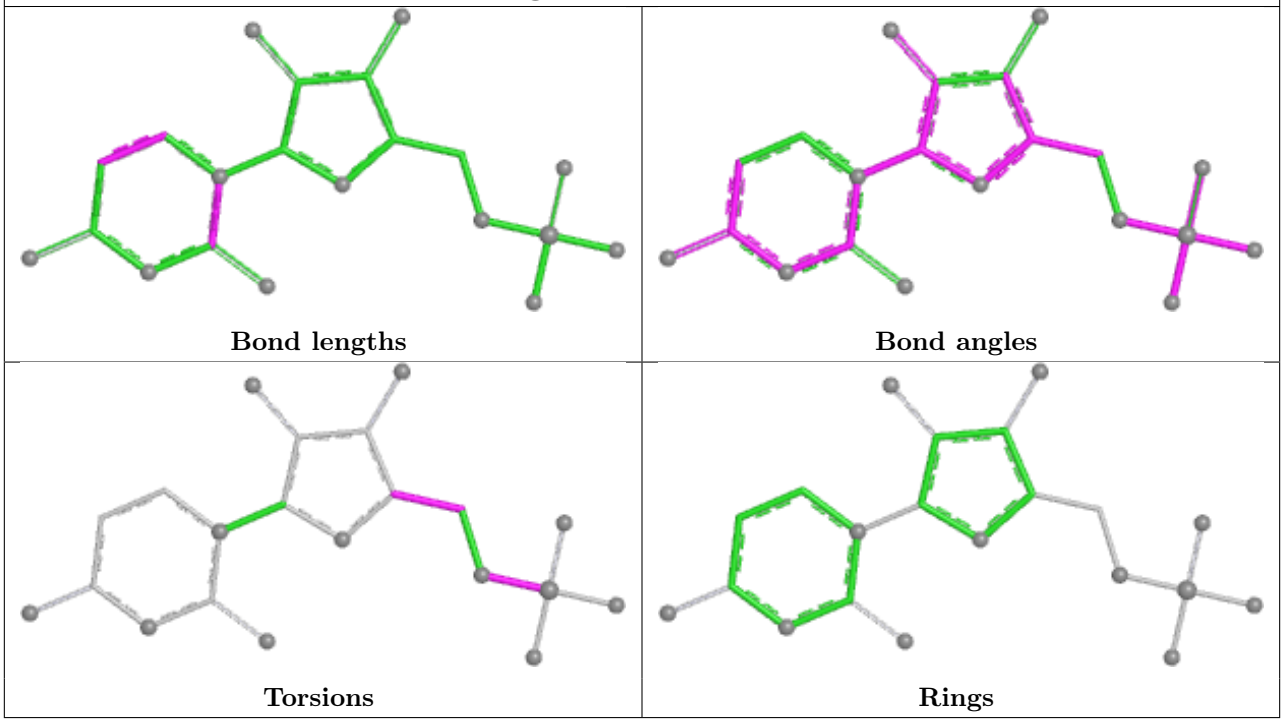
Ligand UDP C 192



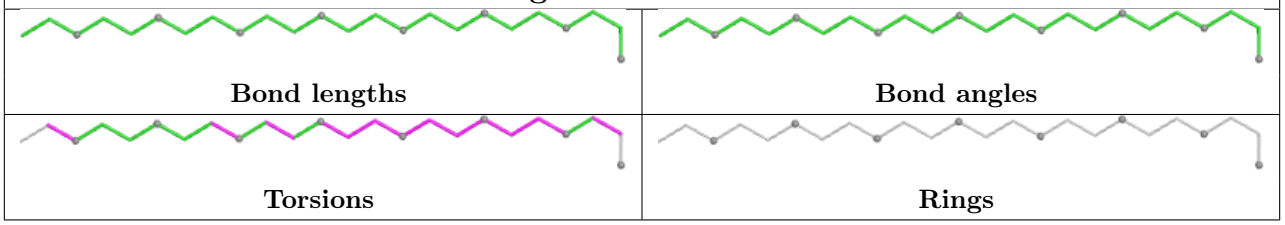
Ligand UDP B 192



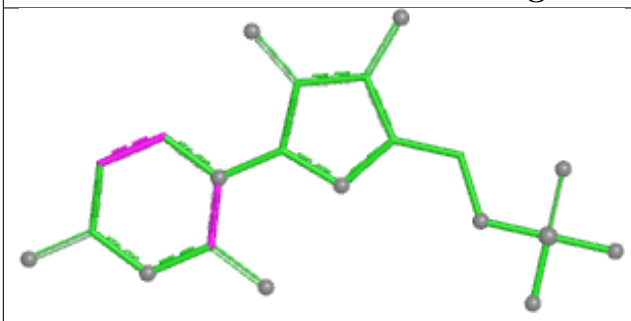
Ligand U5P D 192



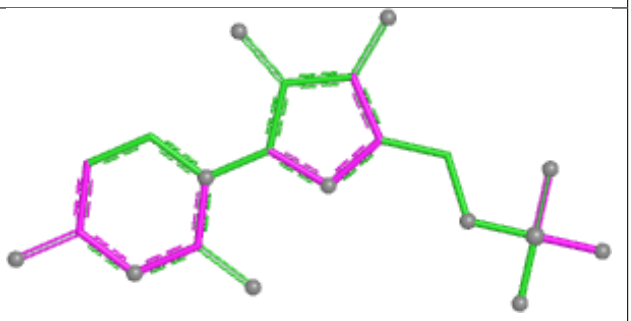
Ligand PE4 C 193



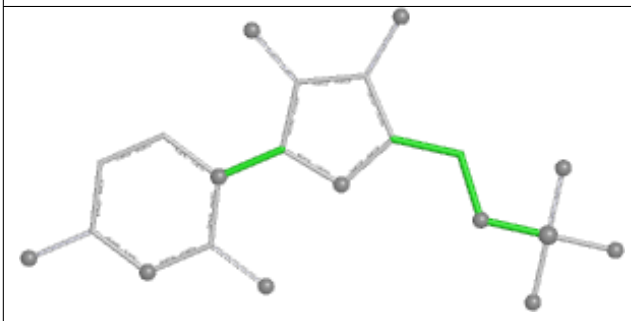
Ligand U5P E 192



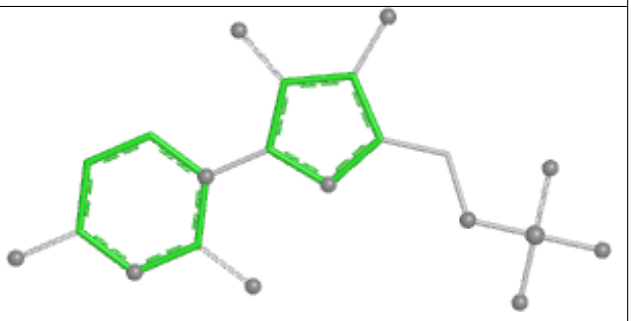
Bond lengths



Bond angles

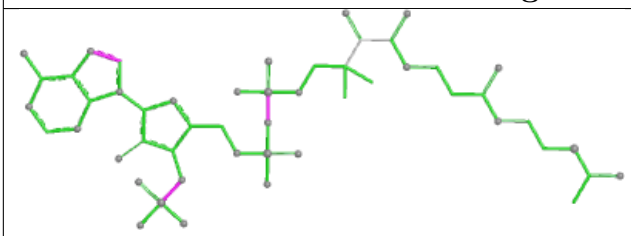


Torsions

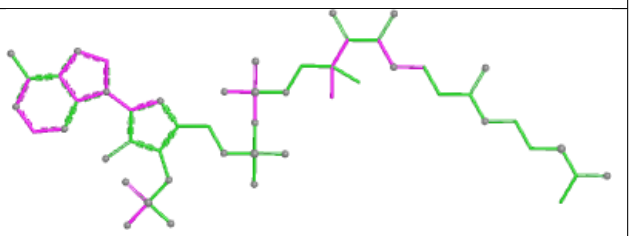


Rings

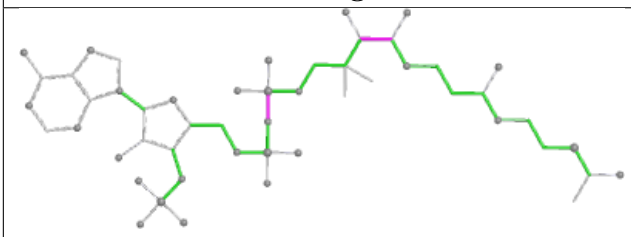
Ligand ACO A 191



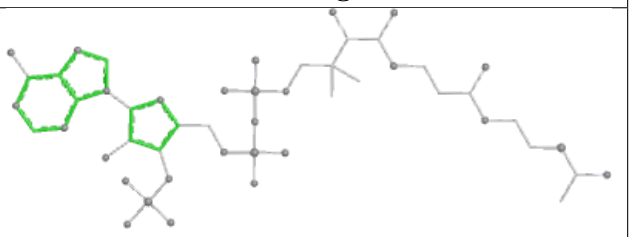
Bond lengths



Bond angles

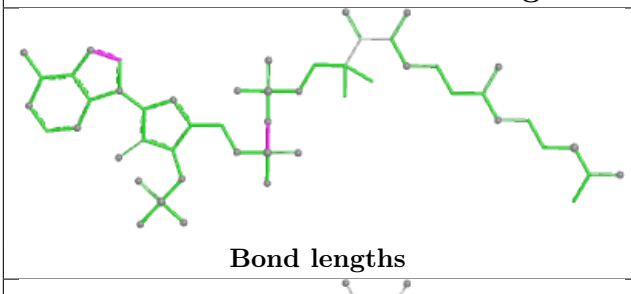


Torsions

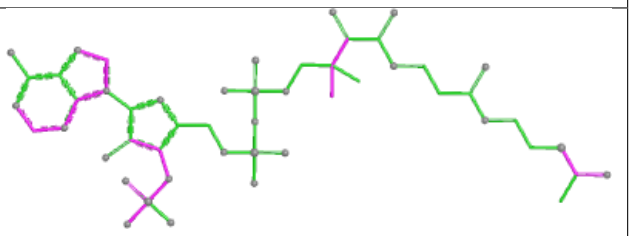


Rings

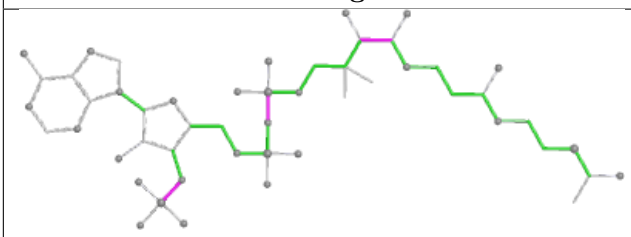
Ligand ACO B 191



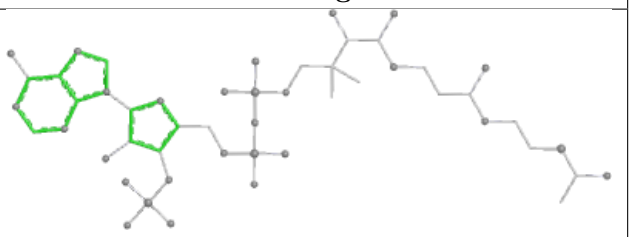
Bond lengths



Bond angles

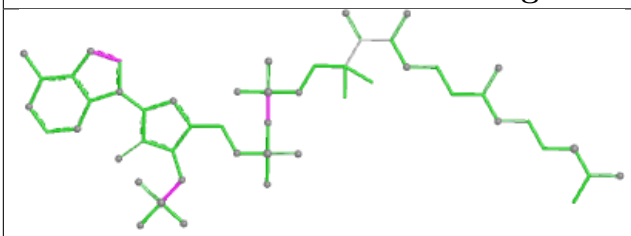


Torsions

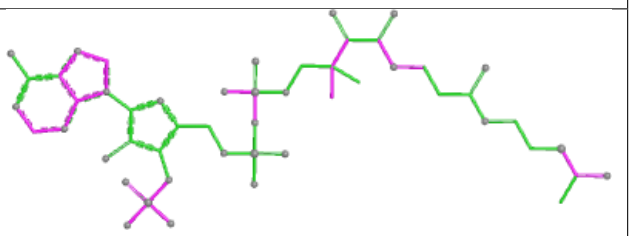


Rings

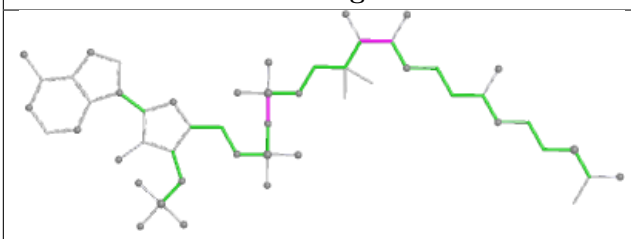
Ligand ACO D 191



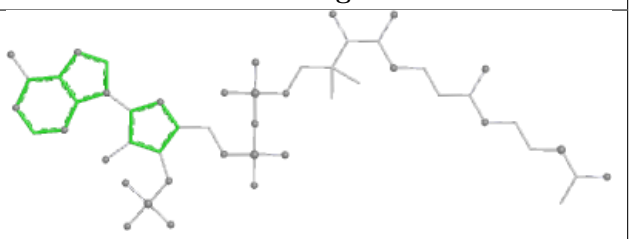
Bond lengths



Bond angles

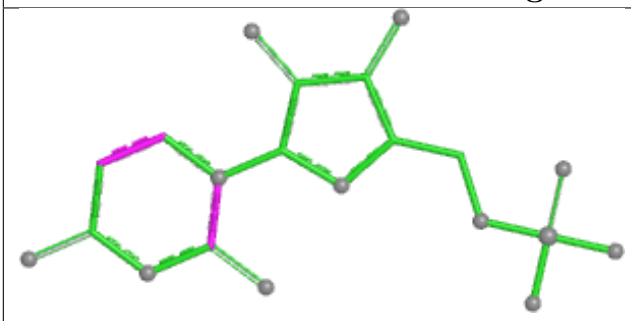


Torsions

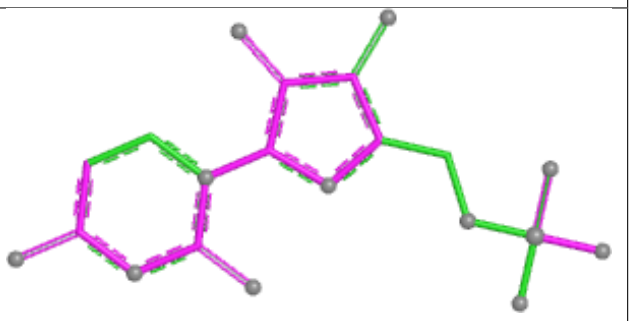


Rings

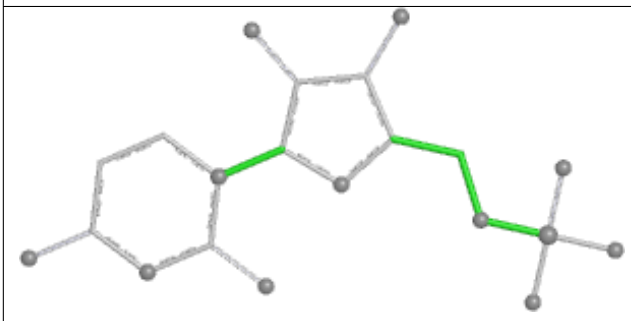
Ligand U5P A 192



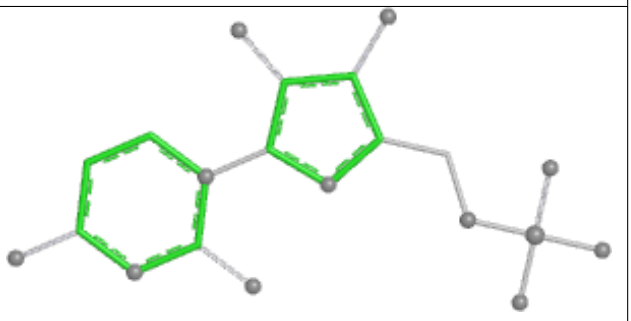
Bond lengths



Bond angles

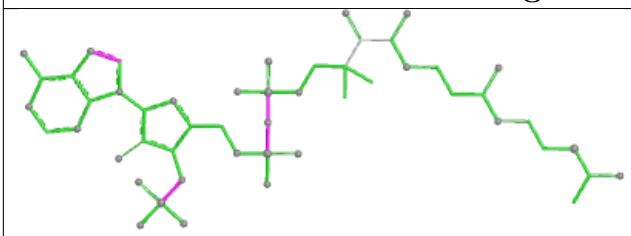


Torsions

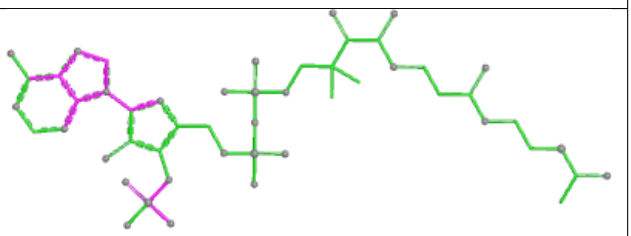


Rings

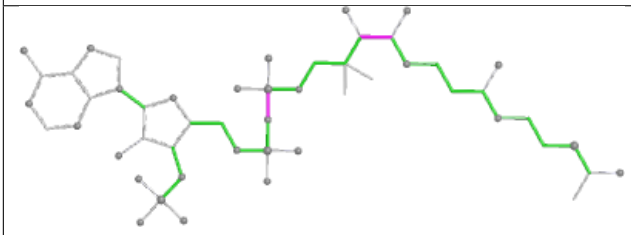
Ligand ACO F 191



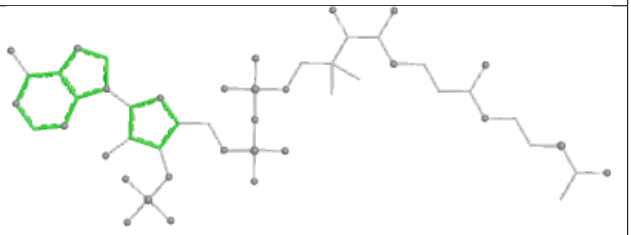
Bond lengths



Bond angles

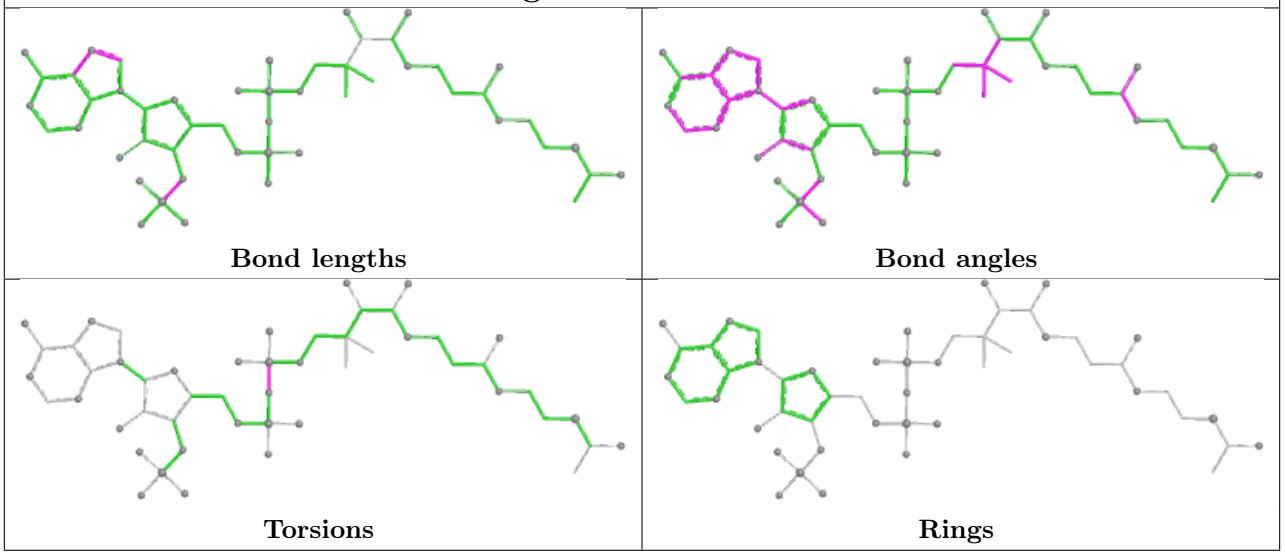


Torsions

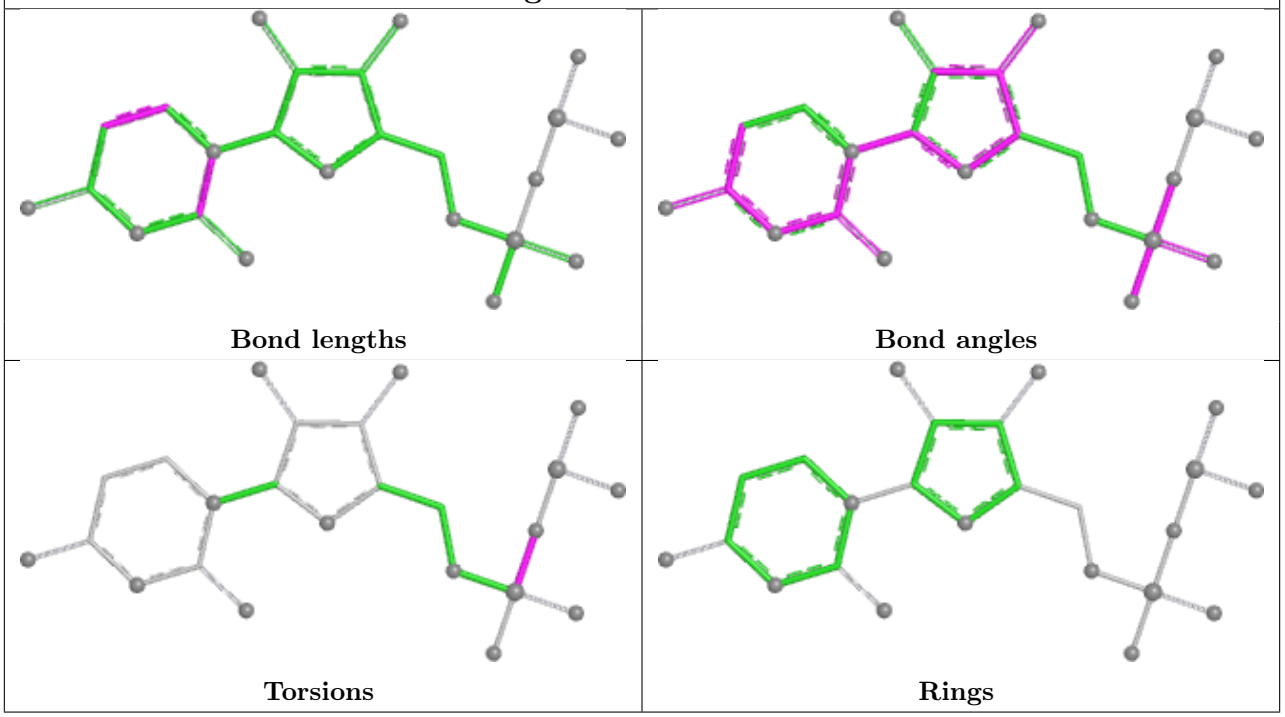


Rings

Ligand ACO C 191



Ligand UDP F 193



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, 95^{th} 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	190/192 (98%)	0.17	4 (2%) 63 67	5, 11, 23, 35	2 (1%)
1	B	190/192 (98%)	0.24	10 (5%) 32 33	5, 10, 24, 36	4 (2%)
1	C	192/192 (100%)	0.06	8 (4%) 40 44	4, 9, 25, 44	3 (1%)
1	D	192/192 (100%)	-0.01	7 (3%) 46 49	5, 10, 22, 34	1 (0%)
1	E	190/192 (98%)	0.10	3 (1%) 70 75	5, 10, 22, 32	2 (1%)
1	F	189/192 (98%)	0.19	8 (4%) 40 44	5, 10, 23, 45	0
All	All	1143/1152 (99%)	0.13	40 (3%) 47 50	4, 10, 23, 45	12 (1%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	98	TYR	4.4
1	B	2	ALA	4.1
1	C	-1	GLY	3.8
1	C	98	TYR	3.7
1	B	1	MET	3.7

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 oligosaccharides in this entry.

6.4 Ligands (i)

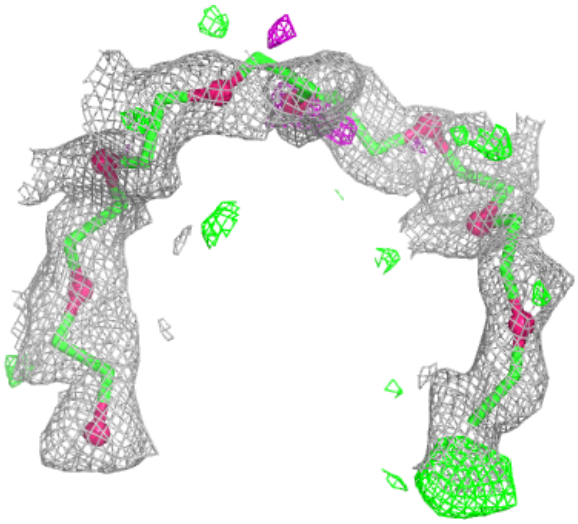
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

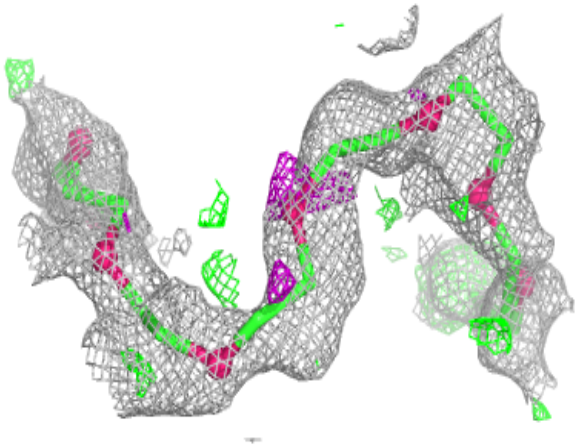
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PE4	C	193	24/24	0.82	0.14	22,28,33,39	0
5	UDP	C	192	25/25	0.83	0.15	16,29,43,47	0
5	UDP	B	192	25/25	0.83	0.16	19,29,41,46	0
3	U5P	A	192	21/21	0.84	0.16	15,29,38,43	0
6	PO4	D	195	5/5	0.85	0.16	21,23,25,37	0
5	UDP	F	192	1/25	0.85	0.14	21,21,21,21	0
3	U5P	D	192	21/21	0.86	0.15	13,27,37,42	0
7	EDO	C	194	4/4	0.87	0.13	22,22,23,25	0
5	UDP	F	193	24/25	0.87	0.14	16,25,35,37	0
6	PO4	B	193	5/5	0.88	0.20	21,22,24,29	0
3	U5P	E	192	21/21	0.88	0.14	17,29,39,43	0
7	EDO	B	194	4/4	0.91	0.14	17,21,23,27	0
7	EDO	D	196	4/4	0.92	0.11	21,22,22,25	0
2	ACO	C	191	51/51	0.96	0.07	6,11,22,26	0
2	ACO	A	191	51/51	0.97	0.07	5,10,22,26	0
2	ACO	E	191	51/51	0.97	0.07	4,8,27,34	0
7	EDO	D	194	4/4	0.97	0.07	12,14,14,18	0
2	ACO	F	191	51/51	0.97	0.07	6,11,28,31	0
2	ACO	B	191	51/51	0.97	0.06	5,8,30,34	0
2	ACO	D	191	51/51	0.98	0.05	6,9,21,24	0
4	NA	D	193	1/1	0.99	0.04	6,6,6,6	0
4	NA	A	193	1/1	1.00	0.03	6,6,6,6	0

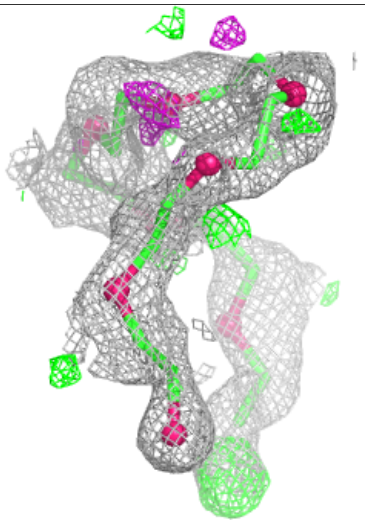
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PE4 C 193:

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

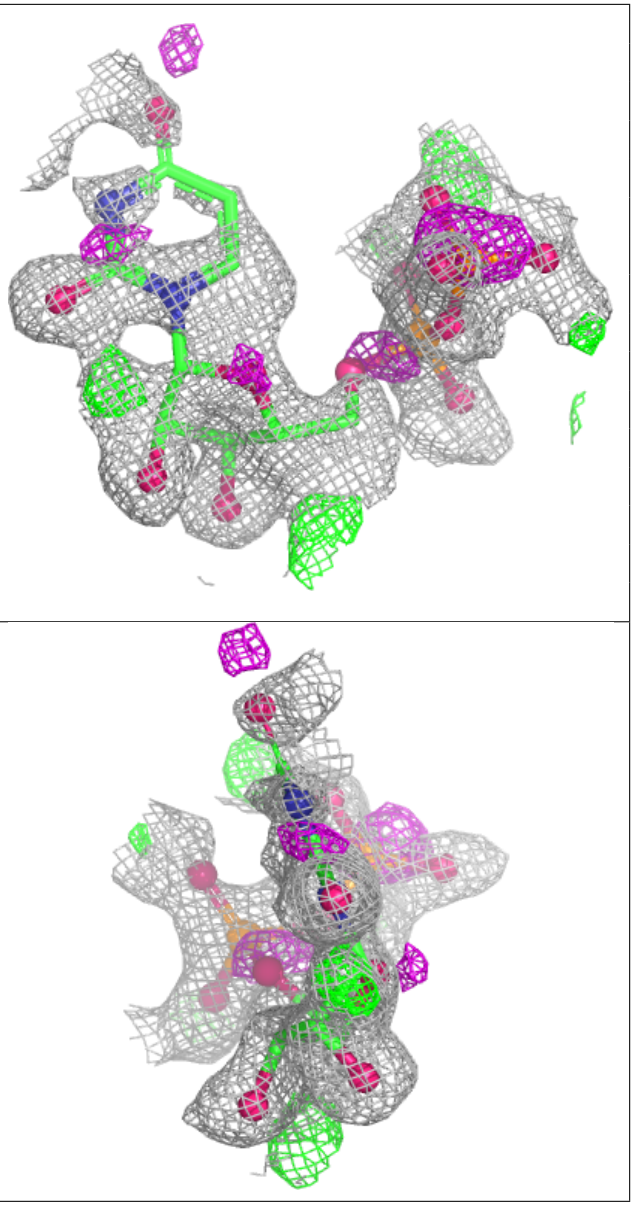






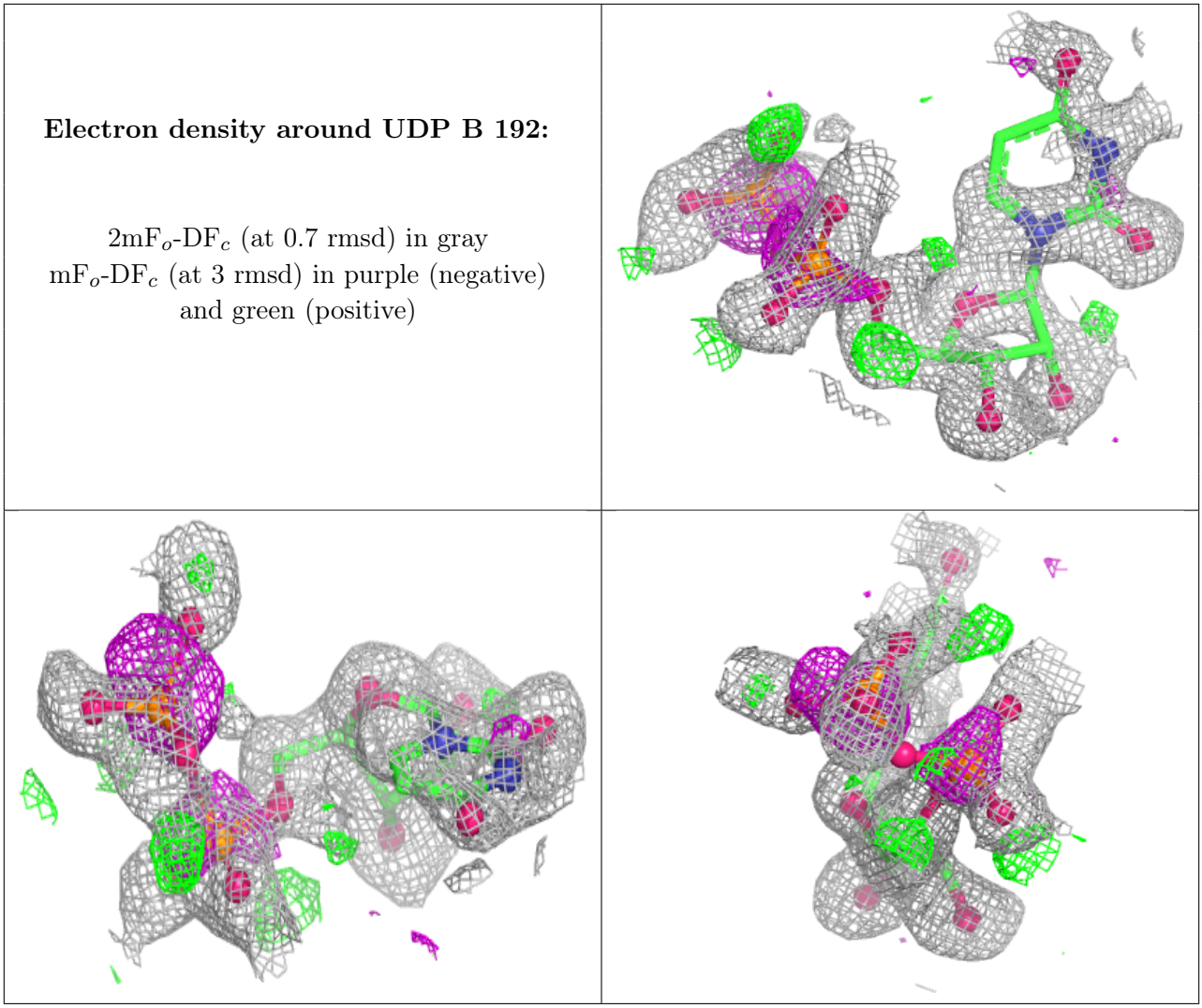
Electron density around UDP C 192:

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



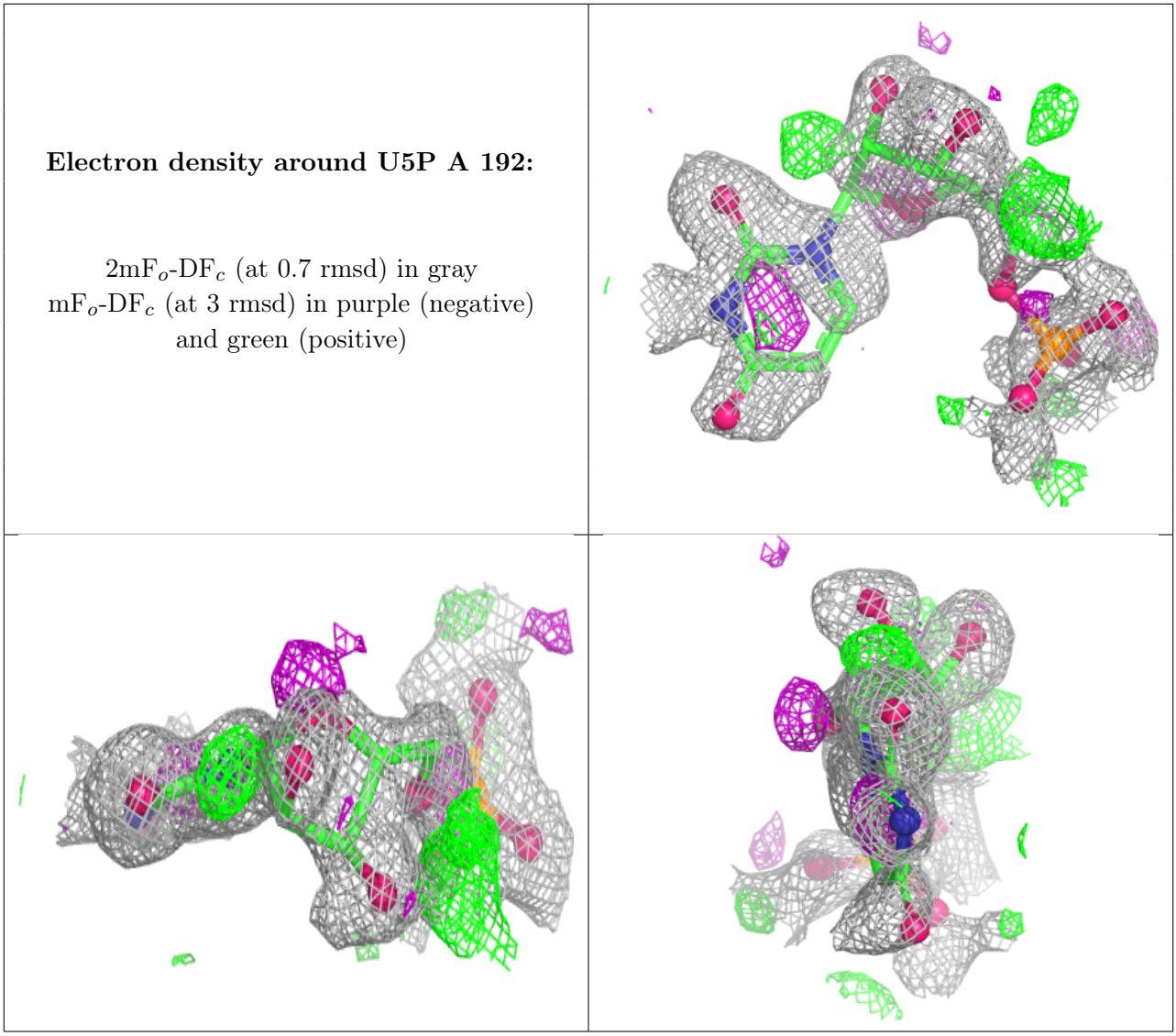
Electron density around UDP B 192:

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



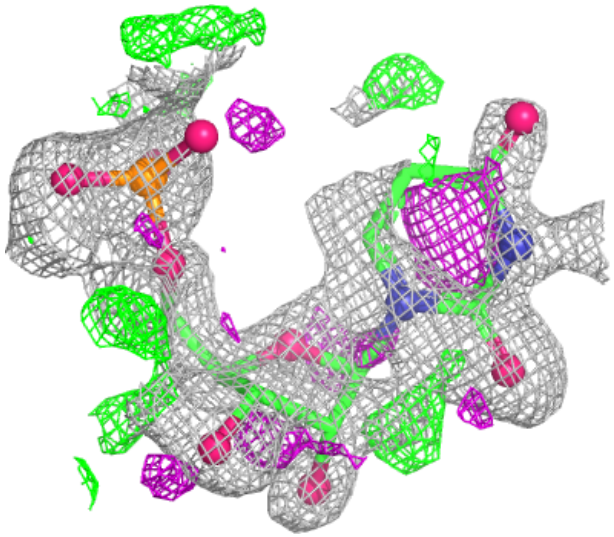
Electron density around U5P A 192:

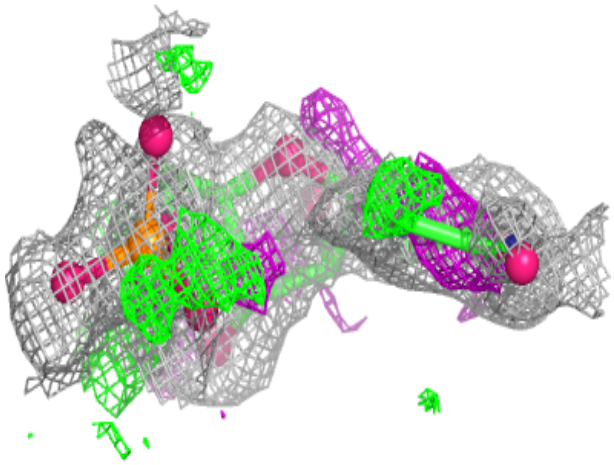
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

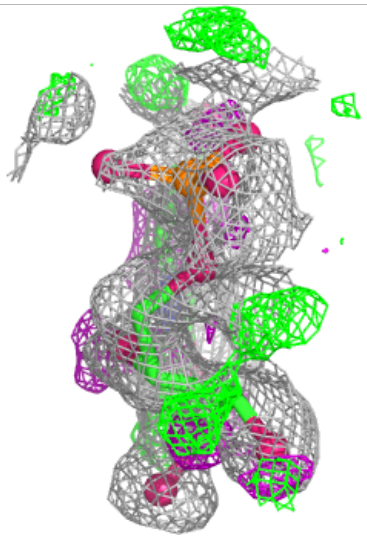


Electron density around U5P D 192:

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

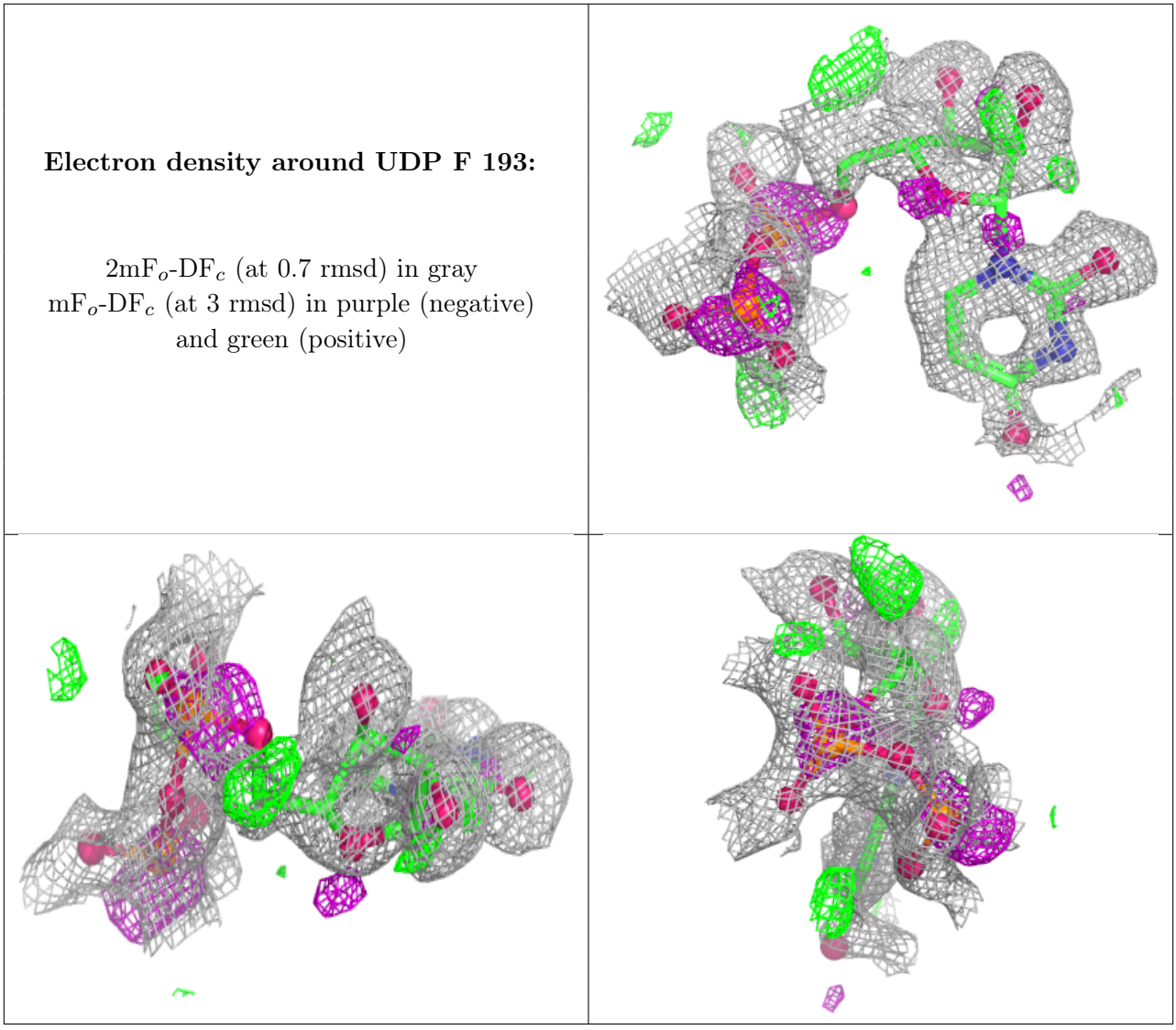






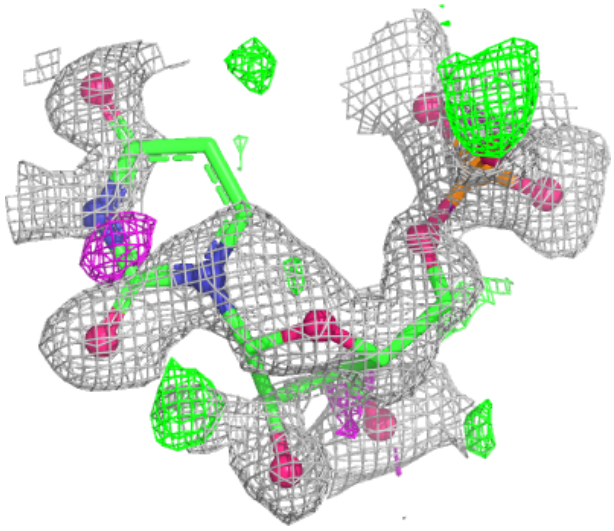
Electron density around UDP F 193:

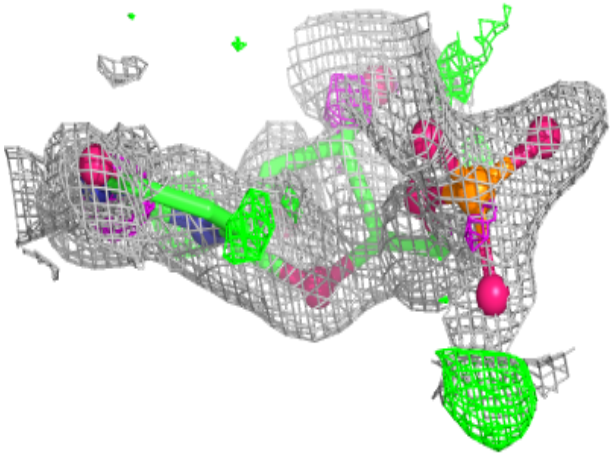
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

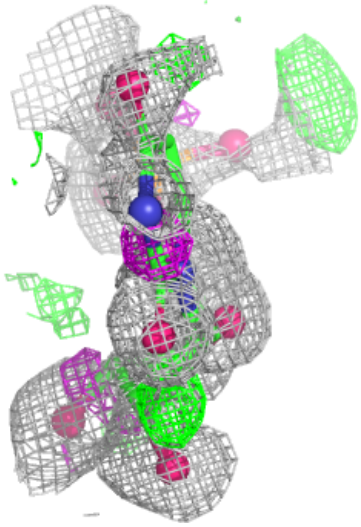


Electron density around U5P E 192:

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

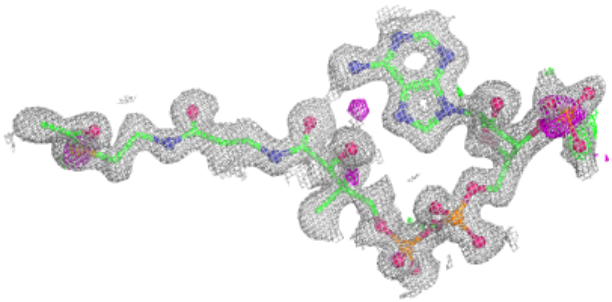


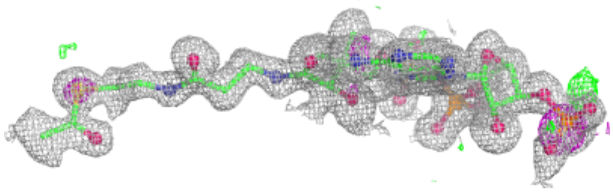


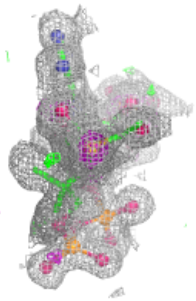


Electron density around ACO C 191:

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

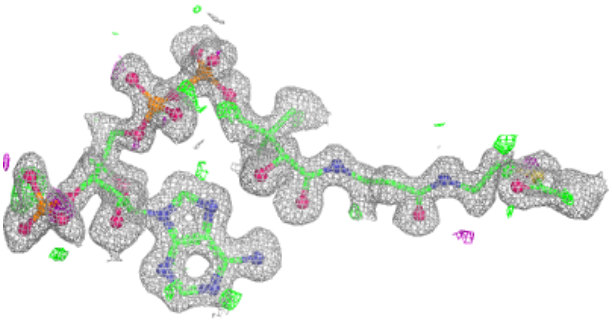


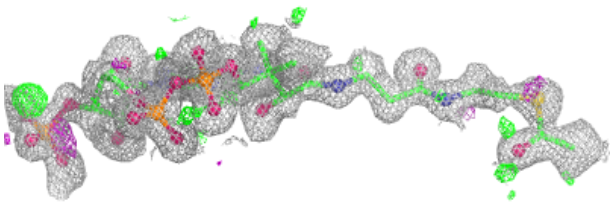


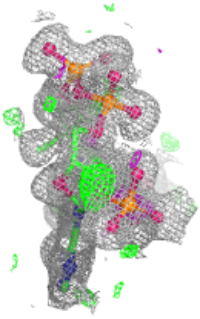


Electron density around ACO A 191:

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

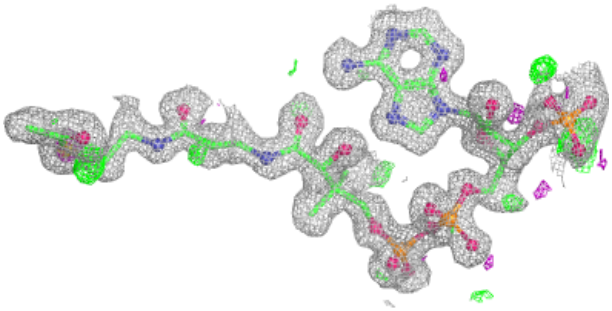


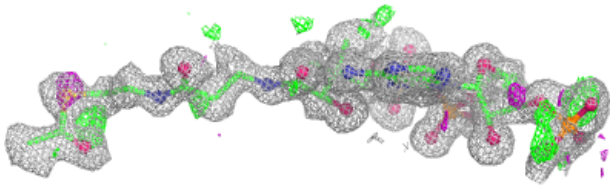


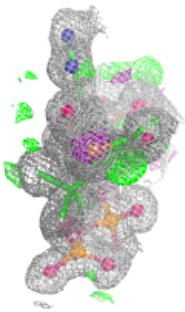


Electron density around ACO E 191:

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

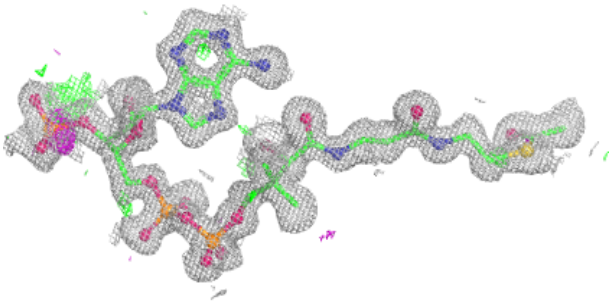


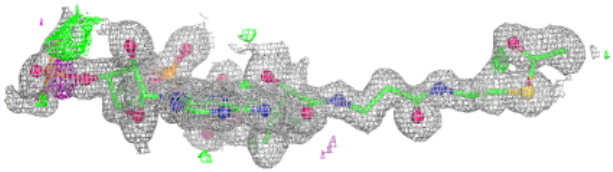


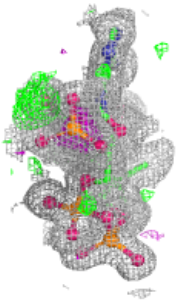


Electron density around ACO F 191:

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

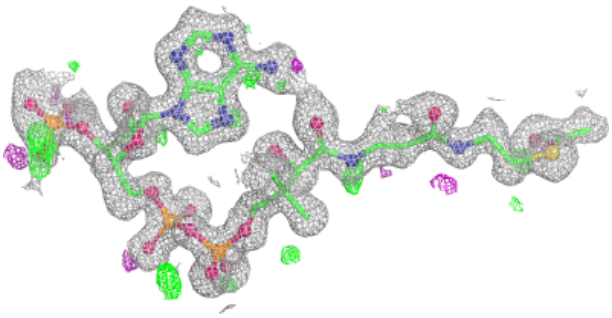


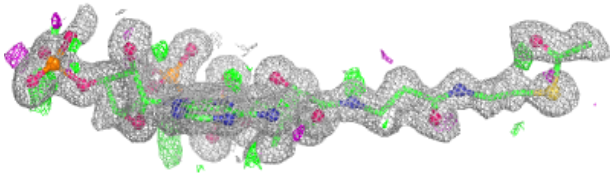


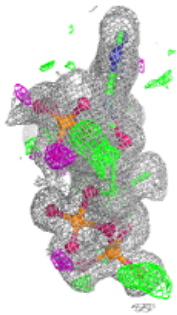


Electron density around ACO B 191:

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

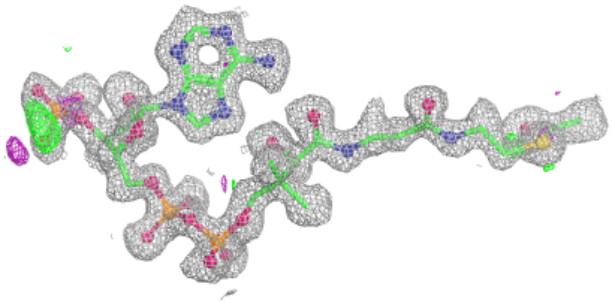


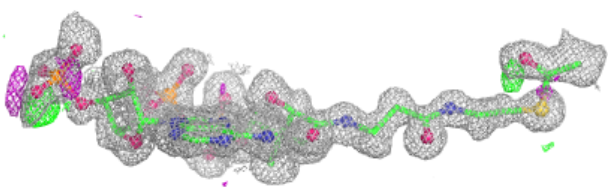


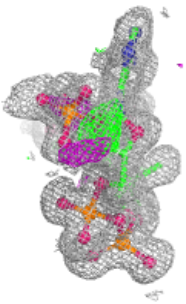


Electron density around ACO D 191:

$2mF_o$-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.