



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:20 PM UTC

PDB ID : 4XNH / pdb_00004xnh
Title : Crystal structure of yeast N-terminal acetyltransferase NatE (IP6) in complex with a bisubstrate
Authors : Dong, J.; Wang, S.; York, J.D.
Deposited on : 2015-01-15
Resolution : 2.10 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

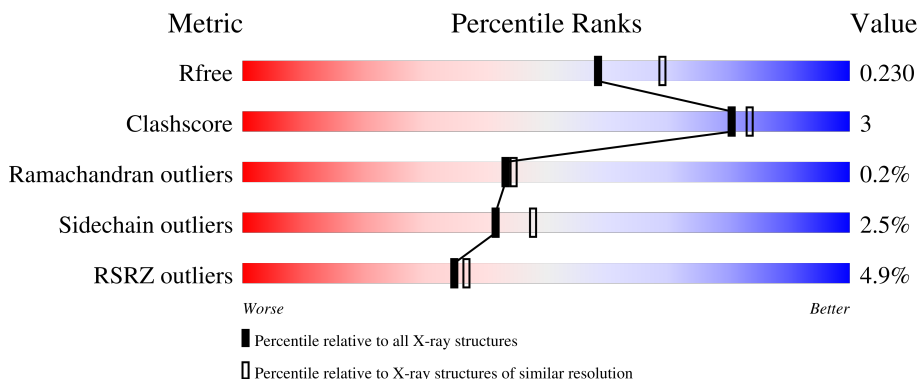
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	854	5% 85% 7% 8%
2	B	238	2% 75% 7% 17%
3	C	176	3% 84% 5% 10%
4	F	8	12% 50% 25% 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19404 atoms, of which 9272 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 N-terminal acetyltransferase A complex subunit NAT1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	786	Total	C	H	N	O	S	0	4	0
			12725	4121	6324	1064	1194	22			

- Molecule 2 is a protein called N-terminal acetyltransferase A complex catalytic subunit ARD1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	197	Total	C	H	N	O	S	0	1	0
			3213	1022	1595	280	305	11			

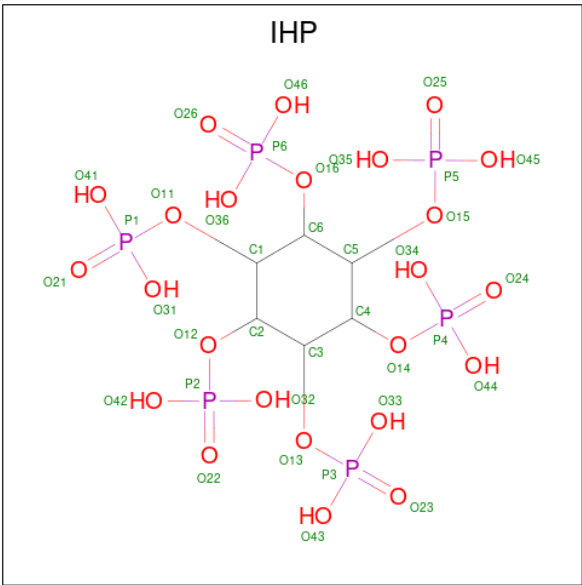
- Molecule 3 is a protein called N-terminal acetyltransferase A complex subunit NAT5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	159	Total	C	H	N	O	S	0	1	0
			2493	812	1241	208	226	6			

- Molecule 4 is a protein called ACYH8.

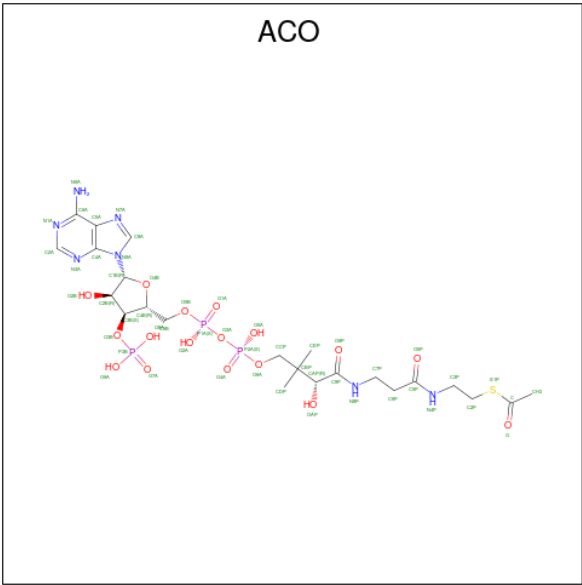
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	6	Total	C	H	N	O	S	0	0	0
			92	31	41	8	11	1			

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



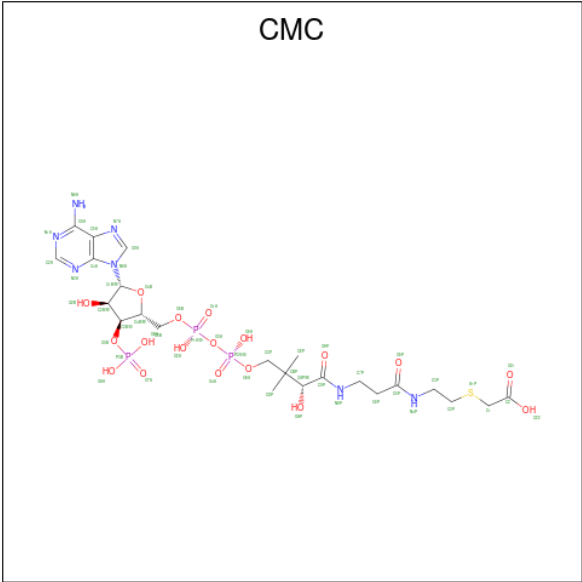
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	P	0	0
			42	6	6	24	6		

- Molecule 6 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	P	S	0	0
			85	23	34	7	17	3	1		

- Molecule 7 is CARBOXYMETHYL COENZYME *A (CCD ID: CMC) (formula: C₂₃H₃₈N₇O₁₈P₃S).

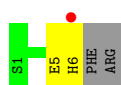


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	H	N	O	P	S		
7	F	1	82	23	31	7	17	3	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	464	Total	O	0	0
			464	464		
8	B	130	Total	O	0	0
			130	130		
8	C	62	Total	O	0	0
			62	62		
8	F	16	Total	O	0	0
			16	16		

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.47Å 114.52Å 146.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.59 – 2.10 40.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	85.8 (40.59-2.10) 85.8 (40.59-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.168 , 0.228 0.173 , 0.230	Depositor DCC
R_{free} test set	3623 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19404	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, CMC, 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	0.73	0/6552	0.87	6/8840 (0.1%)
2	B	0.78	0/1651	0.86	0/2230
3	C	0.68	0/1282	0.83	0/1733
4	F	0.62	0/52	0.83	0/68
All	All	0.73	0/9537	0.86	6/12871 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ILE	N-CA-C	5.80	117.07	111.91
1	A	310	PRO	N-CA-C	5.19	117.03	110.70
1	A	349	LYS	CA-C-N	-5.10	114.41	119.56
1	A	349	LYS	C-N-CA	-5.10	114.41	119.56
1	A	400	PHE	CA-C-N	-5.09	113.40	119.05
1	A	400	PHE	C-N-CA	-5.09	113.40	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6401	6324	6319	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1618	1595	1594	12	0
3	C	1252	1241	1235	4	0
4	F	51	41	40	0	0
5	A	36	6	6	1	0
6	C	51	34	34	1	0
7	F	51	31	32	2	0
8	A	464	0	0	8	0
8	B	130	0	0	2	0
8	C	62	0	0	2	0
8	F	16	0	0	1	0
All	All	10132	9272	9260	48	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 3.

All (48) 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:617[A]:GLN:NE2	1:A:621:ASP:OD2	2.11	0.82
3:C:6[A]:CYS:SG	8:C:353:HOH:O	2.45	0.73
2:B:143:GLU:OE2	8:B:301:HOH:O	2.14	0.64
1:A:593:GLU:OE1	8:A:1001:HOH:O	2.15	0.64
5:A:901:IHP:O34	8:A:1002:HOH:O	2.15	0.63
6:C:201:ACO:N3A	8:C:301:HOH:O	2.30	0.60
1:A:23:GLN:HB3	1:A:26:GLU:HG2	1.84	0.59
1:A:398:LYS:NZ	1:A:842:GLU:OE1	2.36	0.56
1:A:789:GLU:HG2	1:A:795:PHE:CD1	2.44	0.52
2:B:166:ARG:NH1	8:B:304:HOH:O	2.32	0.52
1:A:45:ALA:O	8:A:1004:HOH:O	2.19	0.52
1:A:536:ILE:O	1:A:540:ILE:HG23	2.11	0.51
3:C:85:GLU:HG3	3:C:88:LEU:HD13	1.93	0.50
1:A:346[B]:SER:OG	8:A:1003:HOH:O	2.18	0.49
1:A:693:GLU:OE1	8:A:1005:HOH:O	2.19	0.49
1:A:769:LEU:HA	1:A:772:VAL:HG12	1.96	0.48
1:A:757:HIS:CG	1:A:823:VAL:HG13	2.49	0.47
1:A:760:ARG:NH1	8:A:1020:HOH:O	2.39	0.47
1:A:54:VAL:HG22	1:A:83:LYS:HB3	1.97	0.46
1:A:227:LEU:HB2	1:A:250:ILE:HG21	1.98	0.46
2:B:206:HIS:CE1	2:B:215:LYS:HG3	2.50	0.46
1:A:89:ALA:O	1:A:120:ASN:ND2	2.46	0.45
1:A:617[B]:GLN:NE2	1:A:621:ASP:OD1	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:MET:SD	1:A:257:LEU:HD22	2.56	0.45
2:B:95:TYR:C	2:B:95:TYR:CD1	2.95	0.45
2:B:110:PRO:HB2	2:B:148:GLU:HG3	1.99	0.45
2:B:103:ASP:N	2:B:103:ASP:OD1	2.48	0.45
2:B:103:ASP:HB3	2:B:104:PRO:HD2	1.99	0.45
3:C:21:LYS:O	3:C:25:VAL:HG13	2.16	0.44
2:B:207:ARG:HB3	2:B:208:ARG:HE	1.81	0.44
1:A:291:ASN:ND2	8:A:1037:HOH:O	2.50	0.44
1:A:355:ARG:HE	2:B:56:ASP:CG	2.26	0.44
2:B:152:LEU:C	2:B:152:LEU:HD12	2.42	0.44
2:B:163:HIS:NE2	7:F:301:CMC:O7A	2.41	0.44
1:A:23:GLN:HG3	1:A:25:LEU:H	1.83	0.44
1:A:839:SER:N	1:A:840:PRO:CD	2.81	0.44
1:A:801:TYR:OH	1:A:812:GLY:HA3	2.18	0.43
7:F:301:CMC:O8A	8:F:401:HOH:O	2.21	0.43
1:A:108:LYS:NZ	8:A:1046:HOH:O	2.51	0.43
1:A:31:TYR:CE1	1:A:62:LEU:HG	2.54	0.42
1:A:314:ILE:N	1:A:315:PRO:CD	2.83	0.42
1:A:849:ILE:HA	1:A:853:TYR:CD1	2.55	0.42
3:C:65:TYR:HA	3:C:69:ILE:O	2.20	0.41
1:A:411:LEU:HG	1:A:420:PHE:HB3	2.03	0.41
1:A:561:ILE:HB	1:A:562:PRO:HD3	2.02	0.41
1:A:234:GLU:HB3	1:A:235:PRO:HD3	2.03	0.41
2:B:208:ARG:H	2:B:208:ARG:NE	2.19	0.41
1:A:54:VAL:CG2	1:A:83:LYS:HB3	2.51	0.40

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	782/854 (92%)	758 (97%)	24 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	190/238 (80%)	184 (97%)	4 (2%)	2 (1%)	11	8
3	C	154/176 (88%)	149 (97%)	5 (3%)	0	100	100
4	F	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
All	All	1130/1276 (89%)	1094 (97%)	34 (3%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	222	SER
2	B	109	GLU

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	684/759 (90%)	671 (98%)	13 (2%)	50	58
2	B	178/216 (82%)	173 (97%)	5 (3%)	38	43
3	C	134/153 (88%)	128 (96%)	6 (4%)	24	25
4	F	6/8 (75%)	4 (67%)	2 (33%)	0	0
All	All	1002/1136 (88%)	976 (97%)	26 (3%)	42	46

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	37	LYS
1	A	133	THR
1	A	323[A]	GLU
1	A	323[B]	GLU
1	A	333	VAL
1	A	341	VAL
1	A	440	ILE
1	A	441	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	540	ILE
1	A	693	GLU
1	A	790	ILE
1	A	818	ARG
2	B	200	GLN
2	B	207	ARG
2	B	208	ARG
2	B	221	GLU
2	B	223	ASP
3	C	25	VAL
3	C	86	LEU
3	C	88	LEU
3	C	134	VAL
3	C	159	LYS
3	C	172	LYS
4	F	5	GLU
4	F	6	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	176	GLN
1	A	320	GLN
1	A	544	GLN
1	A	844	HIS
3	C	155	ASN
3	C	156	ASN
3	C	174	HIS

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](#)

3 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
6	ACO	C	201	-	51,53,53	1.21	7 (13%)	73,79,79	1.64	14 (19%)
7	CMC	F	301	-	51,53,54	1.22	5 (9%)	72,78,80	1.92	15 (20%)
5	IHP	A	901	-	36,36,36	1.18	3 (8%)	60,60,60	1.23	7 (11%)

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
6	ACO	C	201	-	-	9/51/67/67	0/3/3/3
7	CMC	F	301	-	-	2/50/67/68	0/3/3/3
5	IHP	A	901	-	-	2/30/54/54	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	301	CMC	P1A-O3A	4.35	1.64	1.59
6	C	201	ACO	C5A-C4A	3.90	1.46	1.39
5	A	901	IHP	P2-O12	3.19	1.65	1.59
5	A	901	IHP	P6-O16	3.04	1.64	1.59
5	A	901	IHP	P4-O14	2.97	1.64	1.59
6	C	201	ACO	P1A-O3A	2.84	1.62	1.59
7	F	301	CMC	C5A-C6A	2.67	1.48	1.41
6	C	201	ACO	P2A-O3A	2.66	1.62	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	301	CMC	C9P-N8P	-2.61	1.27	1.33
7	F	301	CMC	P2A-O3A	2.56	1.62	1.59
6	C	201	ACO	C8A-N7A	2.52	1.36	1.31
6	C	201	ACO	C5A-N7A	-2.42	1.34	1.39
6	C	201	ACO	C4A-N9A	-2.30	1.32	1.37
6	C	201	ACO	C5A-C6A	2.18	1.47	1.41
7	F	301	CMC	C5P-N4P	-2.08	1.28	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	301	CMC	C2P-S1P-C1	6.63	112.66	101.72
7	F	301	CMC	C3P-N4P-C5P	5.57	133.20	122.82
7	F	301	CMC	C5A-C4A-N3A	-5.54	119.09	126.72
6	C	201	ACO	C4A-N9A-C8A	4.46	110.42	105.74
6	C	201	ACO	N3A-C2A-N1A	-4.45	121.84	128.58
6	C	201	ACO	C5A-C4A-N3A	-4.44	120.61	126.72
7	F	301	CMC	N3A-C2A-N1A	-4.23	122.17	128.58
7	F	301	CMC	N3A-C4A-N9A	4.17	134.25	127.17
7	F	301	CMC	C2A-N3A-C4A	4.11	121.88	111.83
6	C	201	ACO	N3A-C4A-N9A	4.11	134.15	127.17
6	C	201	ACO	C2A-N3A-C4A	3.53	120.45	111.83
7	F	301	CMC	N9A-C8A-N7A	-3.38	109.15	113.94
7	F	301	CMC	O3B-P3B-O7A	-3.33	97.45	109.33
6	C	201	ACO	N9A-C8A-N7A	-3.27	109.30	113.94
7	F	301	CMC	C4A-N9A-C8A	2.98	108.87	105.74
6	C	201	ACO	C4A-C5A-N7A	-2.76	107.43	110.58
6	C	201	ACO	C2A-N1A-C6A	2.70	123.17	118.73
5	A	901	IHP	O12-P2-O22	-2.69	99.75	109.33
6	C	201	ACO	O-C-S1P	-2.67	111.85	122.65
6	C	201	ACO	C5A-N7A-C8A	2.64	107.60	103.45
7	F	301	CMC	CEP-CBP-CAP	2.59	113.18	108.77
5	A	901	IHP	O43-P3-O33	2.58	117.48	107.80
6	C	201	ACO	C4A-N9A-C1B	-2.53	120.72	126.63
5	A	901	IHP	P3-O13-C3	2.48	130.04	123.43
6	C	201	ACO	N6A-C6A-N1A	2.43	123.80	118.38
7	F	301	CMC	O5A-P2A-O4A	2.25	122.93	112.44
7	F	301	CMC	O2A-P1A-O1A	2.24	122.87	112.44
7	F	301	CMC	O5P-C5P-C6P	-2.23	117.98	122.02
7	F	301	CMC	O5P-C5P-N4P	2.16	127.28	123.03
5	A	901	IHP	O33-P3-O13	-2.11	97.63	105.85
6	C	201	ACO	C6A-C5A-N7A	2.10	136.14	132.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	IHP	O13-P3-O23	-2.10	101.86	109.33
6	C	201	ACO	O5A-P2A-O4A	2.08	122.12	112.44
5	A	901	IHP	O35-P5-O15	-2.05	97.84	105.85
5	A	901	IHP	O13-C3-C2	-2.05	104.40	108.76
7	F	301	CMC	C5A-N7A-C8A	2.01	106.61	103.45

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	201	ACO	C3P-C2P-S1P-C
6	C	201	ACO	O-C-S1P-C2P
6	C	201	ACO	CH3-C-S1P-C2P
5	A	901	IHP	C6-O16-P6-O26
6	C	201	ACO	C2B-C1B-N9A-C8A
7	F	301	CMC	C2-C1-S1P-C2P
6	C	201	ACO	P2A-O3A-P1A-O1A
7	F	301	CMC	CCP-O6A-P2A-O4A
6	C	201	ACO	C2B-C1B-N9A-C4A
5	A	901	IHP	C1-O11-P1-O31
6	C	201	ACO	P2A-O3A-P1A-O2A
6	C	201	ACO	O4B-C1B-N9A-C8A
6	C	201	ACO	C3B-O3B-P3B-O8A

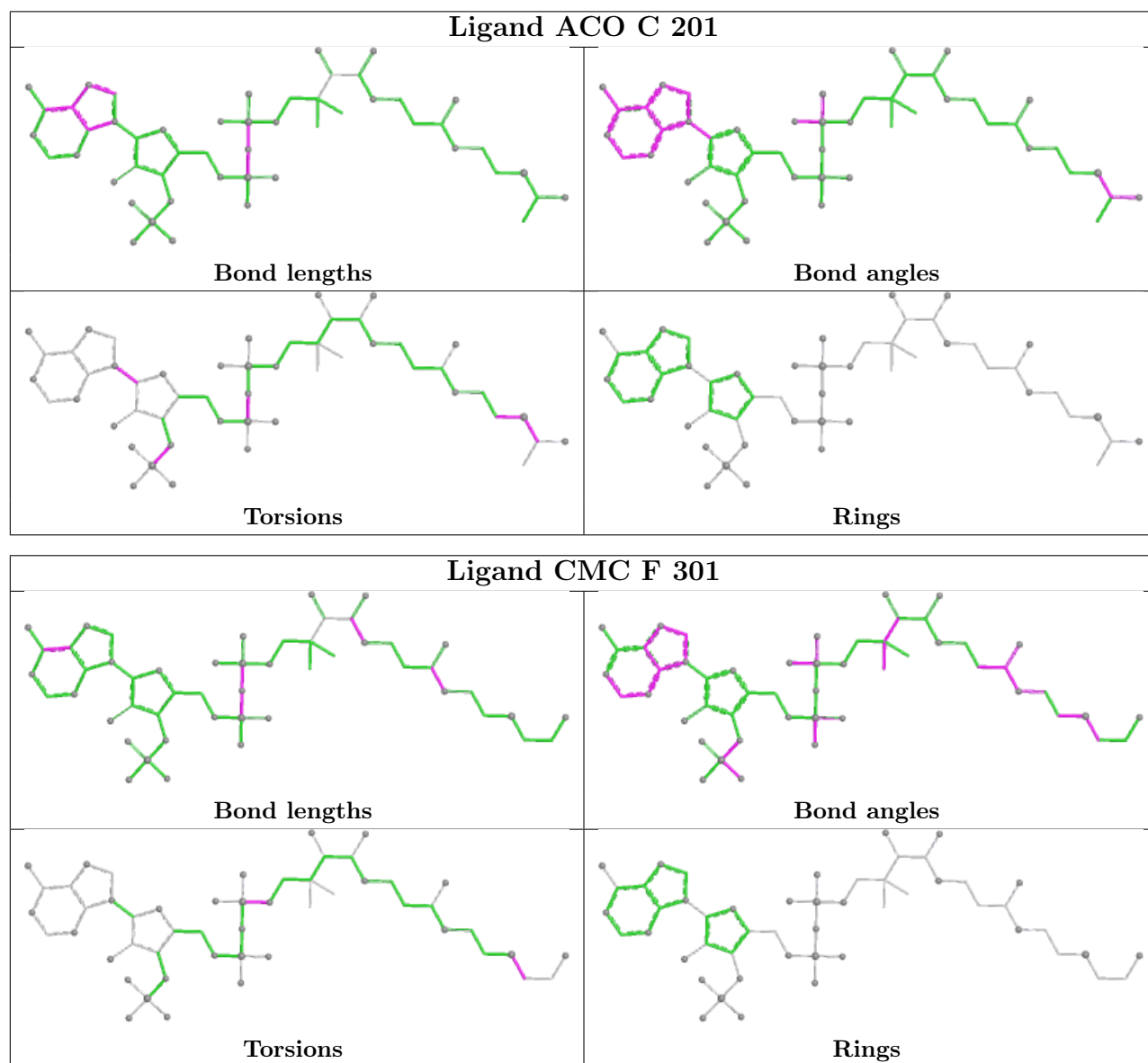
There are no ring outliers.

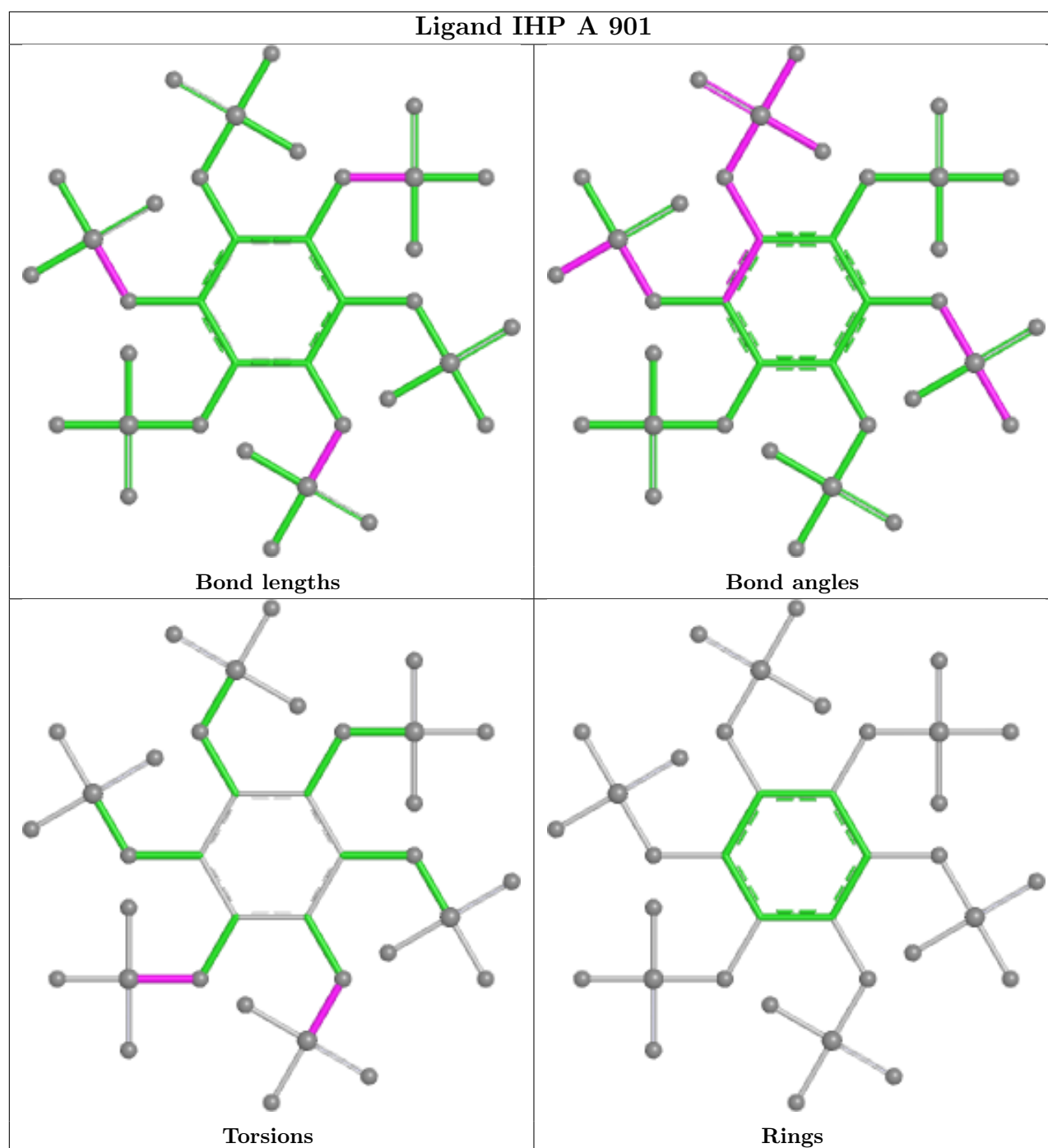
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	201	ACO	1	0
7	F	301	CMC	2	0
5	A	901	IHP	1	0

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

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	786/854 (92%)	-0.01	44 (5%) 30 32	17, 38, 74, 93	4 (0%)
2	B	197/238 (82%)	-0.34	5 (2%) 58 61	17, 32, 70, 93	1 (0%)
3	C	159/176 (90%)	0.14	6 (3%) 44 46	23, 44, 83, 99	2 (1%)
4	F	6/8 (75%)	0.48	1 (16%) 4 4	27, 36, 75, 90	0
All	All	1148/1276 (89%)	-0.04	56 (4%) 35 37	17, 38, 75, 99	7 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	104	PRO	5.1
1	A	42	LEU	4.7
3	C	87	SER	4.6
1	A	46	ILE	4.4
1	A	661	ARG	4.3
1	A	57	LEU	4.2
1	A	27	ALA	4.1
1	A	30	LEU	4.1
1	A	31	TYR	4.0
1	A	526	LYS	3.8
1	A	40	LEU	3.7
1	A	24	PHE	3.5
1	A	662	LYS	3.5
1	A	660	LYS	3.4
1	A	58	ALA	3.4
1	A	534	GLU	3.2
1	A	36	TYR	3.1
1	A	25	LEU	3.0
1	A	47	LEU	3.0
3	C	84	ASN	3.0
3	C	80	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	663	GLU	2.9
1	A	524	LEU	2.9
1	A	28	LEU	2.8
2	B	78	THR	2.7
1	A	89	ALA	2.7
3	C	86	LEU	2.7
4	F	6	HIS	2.7
2	B	77	ARG	2.6
1	A	91	PRO	2.6
1	A	790	ILE	2.5
1	A	67	VAL	2.5
3	C	88	LEU	2.5
1	A	54	VAL	2.4
1	A	537	ALA	2.4
1	A	43	LEU	2.4
1	A	536	ILE	2.4
3	C	81	LYS	2.4
1	A	64	LEU	2.4
1	A	84	ILE	2.4
1	A	540	ILE	2.4
1	A	93	CYS	2.3
1	A	38	LYS	2.3
1	A	50	ASP	2.3
1	A	92	ILE	2.2
2	B	56	ASP	2.2
1	A	33	GLY	2.2
1	A	68	GLY	2.2
1	A	49	LYS	2.2
1	A	59	LEU	2.1
1	A	76	TYR	2.1
1	A	63	ASP	2.1
1	A	82	ARG	2.1
1	A	521	LEU	2.0
2	B	208	ARG	2.0
1	A	41	LYS	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 [i](#)

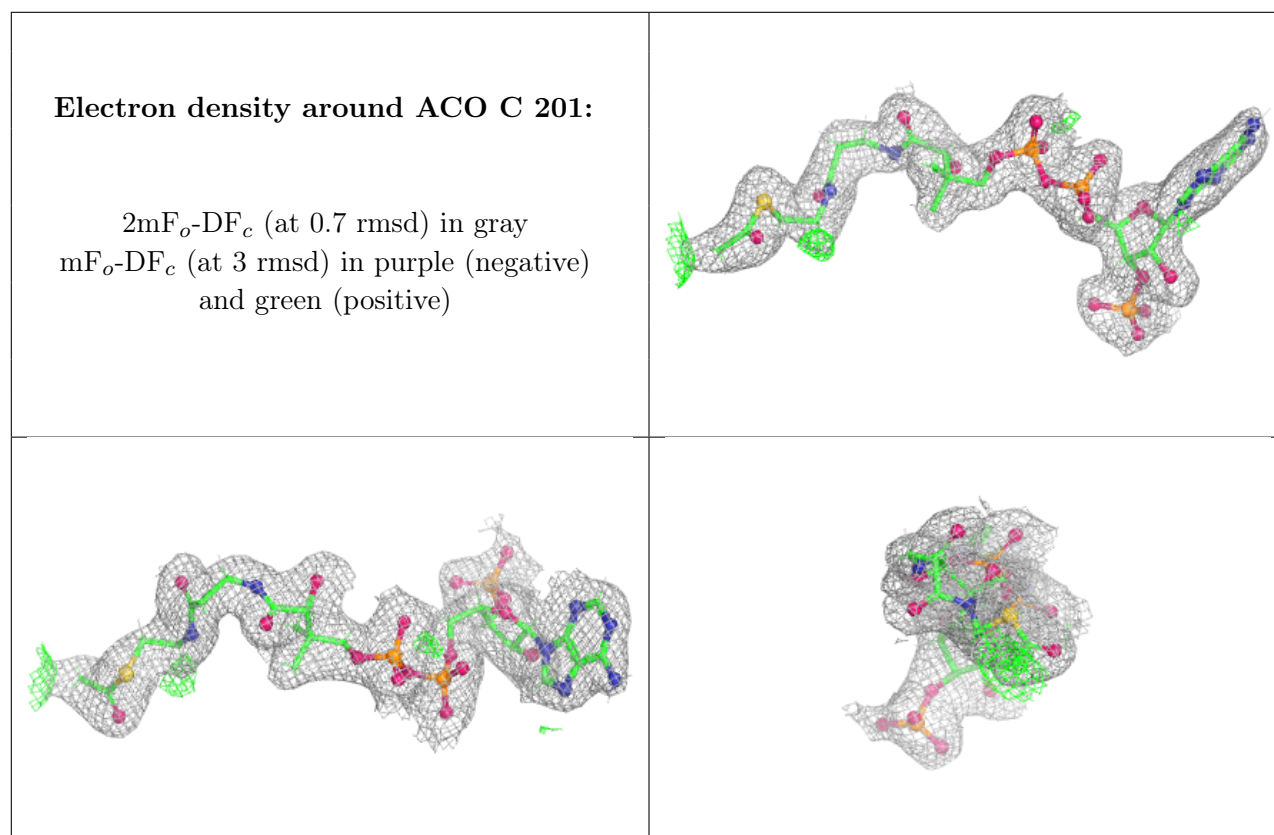
There are no oligosaccharides in this entry.

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.

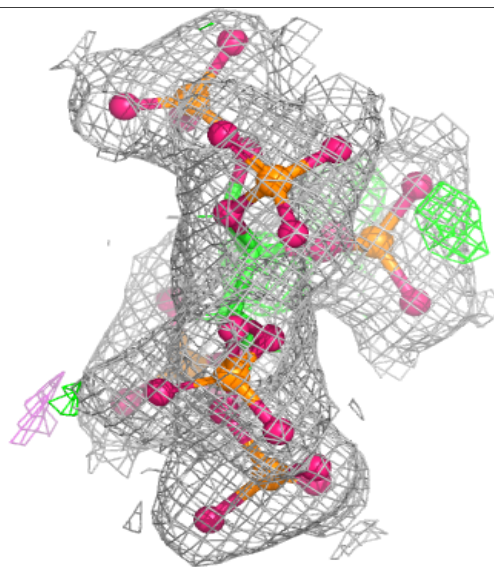
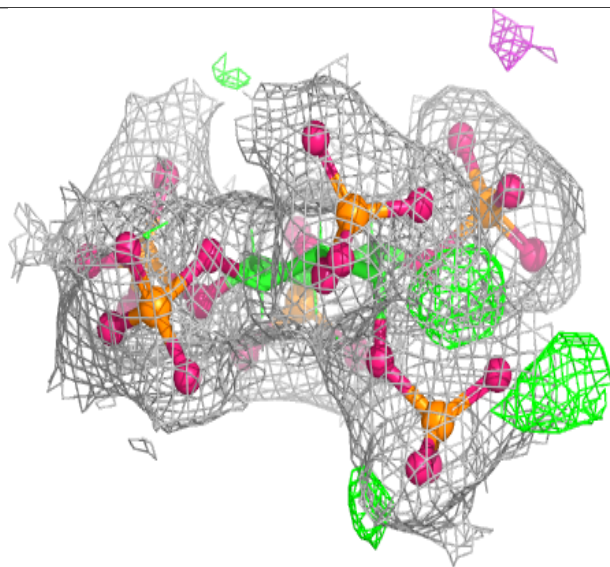
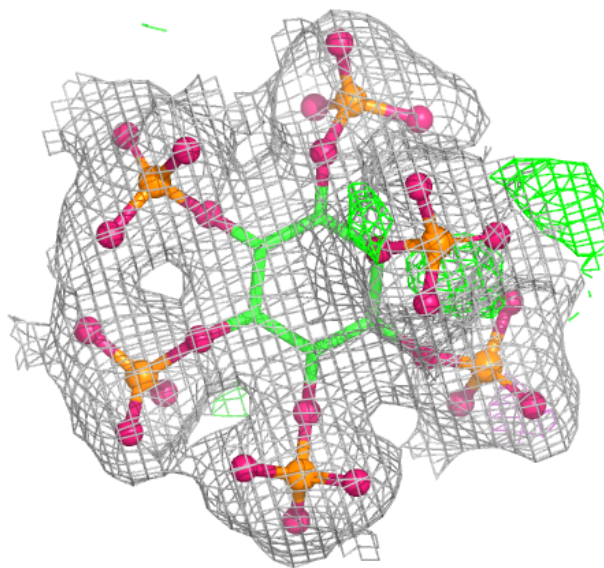
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACO	C	201	51/51	0.96	0.07	26,37,62,92	0
5	IHP	A	901	36/36	0.97	0.06	22,31,37,43	0
7	CMC	F	301	51/52	0.97	0.06	19,30,46,57	0

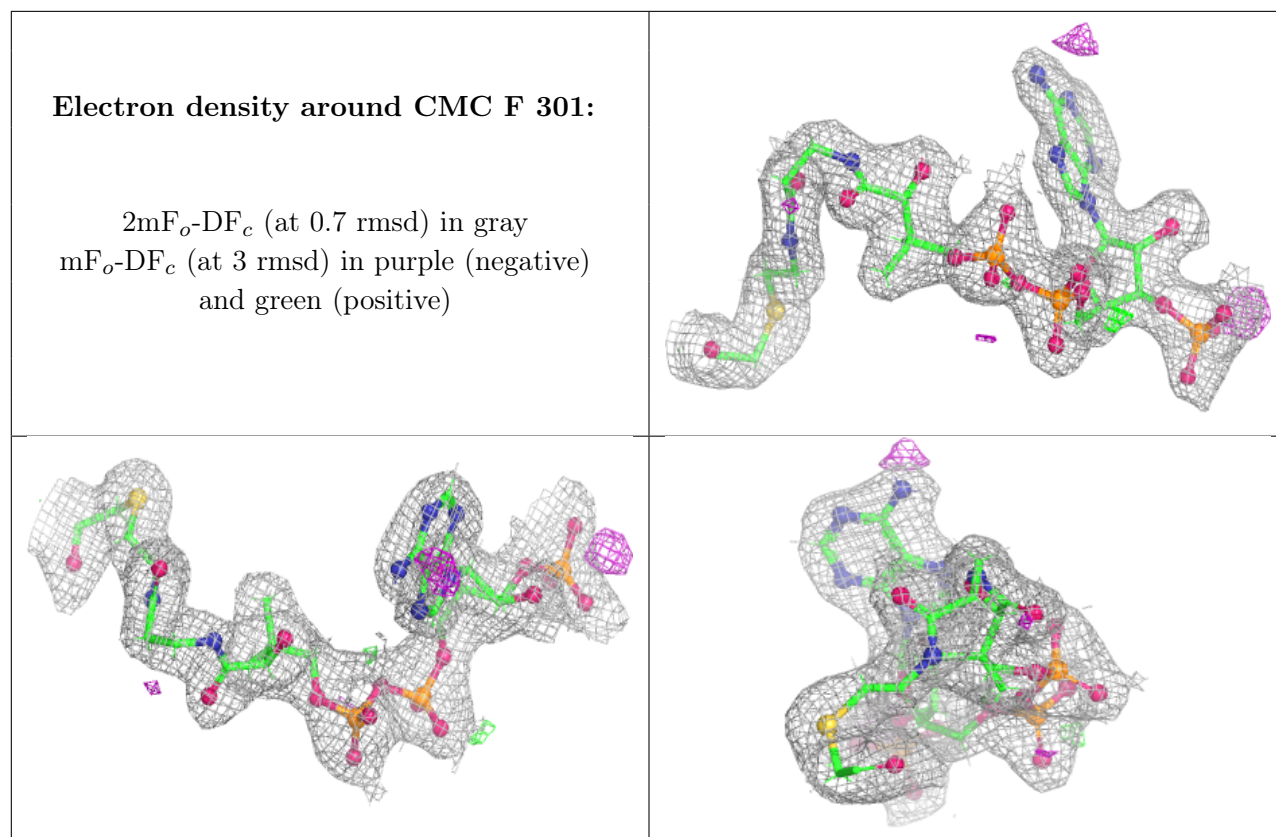
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around IHP A 901:

$2mF_o-DF_c$ (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.