wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 04:08 AM EDT

PDB ID	:	1Q23
Title	:	Crystal structure of Chloramphenicol acetyltransferase I complexed with Fusidic acid at 2.18 A resolution
Authors	:	Roidis, A.; Kokkinidis, M.
Deposited on	:	2003-07-23
Resolution	:	2.18 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:

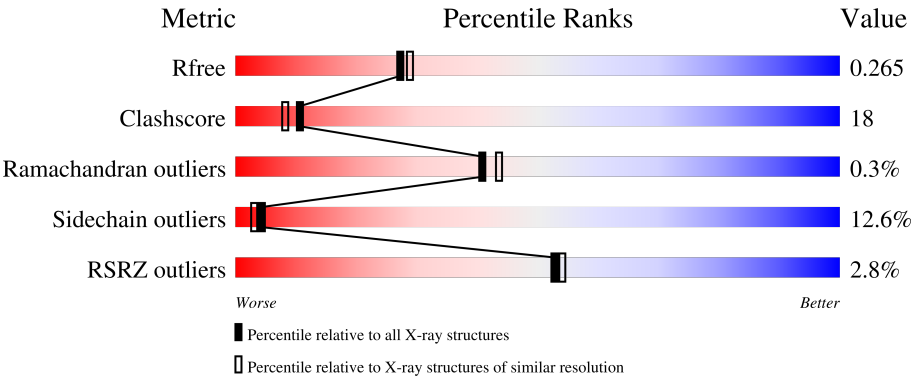
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.18 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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	219	57% 32% 8%
1	B	219	3% 68% 24% 6%
1	C	219	65% 22% 8%
1	D	219	56% 31% 10%
1	E	219	3% 61% 30% 7%

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Mol	Chain	Length	Quality of chain
1	F	219	61% 27% 7%
1	G	219	2% 63% 25% 7%
1	H	219	2% 58% 32% 6%
1	I	219	3% 55% 33% 8%
1	J	219	5% 60% 26% 9%
1	K	219	3% 62% 29% 5%
1	L	219	9% 53% 36% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUA	A	702	X	-	-	-
3	FUA	B	703	X	-	-	-
3	FUA	C	701	X	-	-	-
3	FUA	D	705	X	-	-	-
3	FUA	E	706	X	-	-	-
3	FUA	F	704	X	-	-	-
3	FUA	G	708	X	-	-	-
3	FUA	H	709	X	-	-	-
3	FUA	I	707	X	-	-	-
3	FUA	J	711	X	-	-	-
3	FUA	K	712	X	-	-	-
3	FUA	L	710	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22280 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.

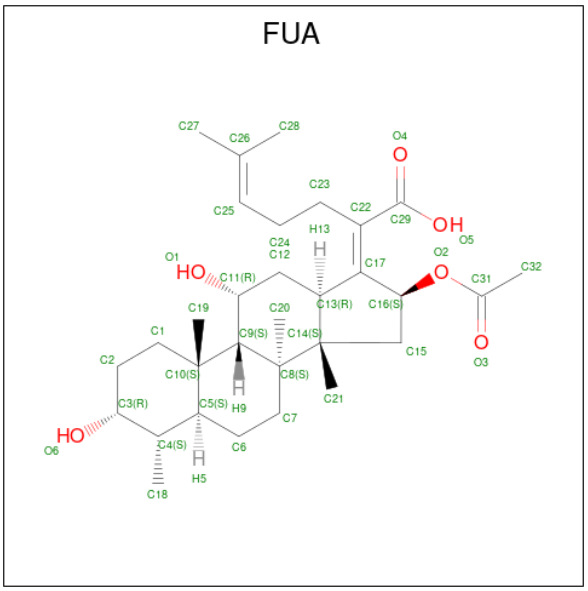
- Molecule 1 is a protein called Chloramphenicol acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1771	1150	291	317	13			
1	B	217	Total	C	N	O	S	0	0	0
			1798	1167	296	322	13			
1	C	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	D	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	E	215	Total	C	N	O	S	0	0	0
			1785	1160	294	318	13			
1	F	212	Total	C	N	O	S	0	0	0
			1759	1142	289	315	13			
1	G	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	H	216	Total	C	N	O	S	0	0	0
			1785	1159	294	319	13			
1	I	215	Total	C	N	O	S	0	0	0
			1785	1160	294	318	13			
1	J	212	Total	C	N	O	S	0	0	0
			1763	1146	289	315	13			
1	K	213	Total	C	N	O	S	0	0	0
			1772	1153	291	315	13			
1	L	210	Total	C	N	O	S	0	0	0
			1746	1135	286	312	13			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 37 31 6	0	0
3	B	1	Total C O 37 31 6	0	0
3	C	1	Total C O 37 31 6	0	0
3	D	1	Total C O 37 31 6	0	0
3	E	1	Total C O 37 31 6	0	0
3	F	1	Total C O 37 31 6	0	0
3	G	1	Total C O 37 31 6	0	0
3	H	1	Total C O 37 31 6	0	0
3	I	1	Total C O 37 31 6	0	0
3	J	1	Total C O 37 31 6	0	0
3	K	1	Total C O 37 31 6	0	0
3	L	1	Total C O 37 31 6	0	0

- Molecule 4 is water.

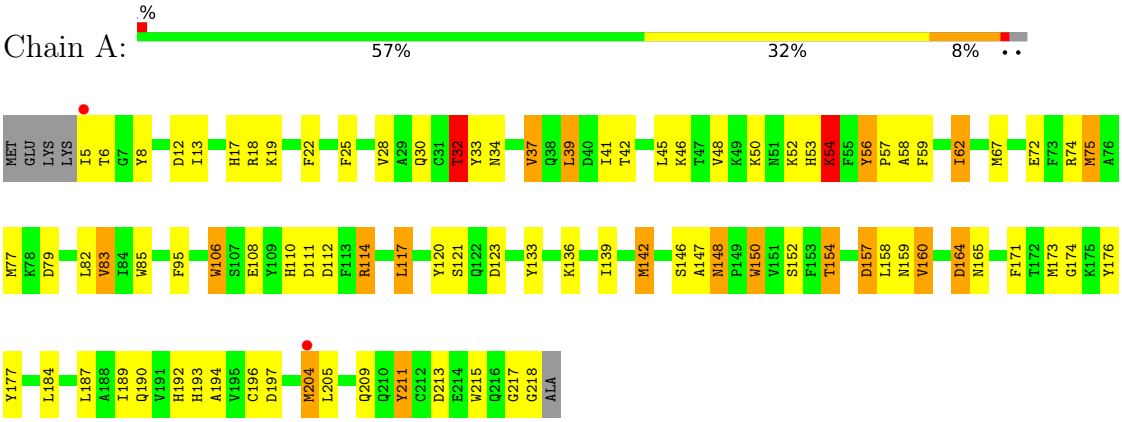
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	51	Total O 51 51	0	0
4	C	68	Total O 68 68	0	0
4	D	58	Total O 58 58	0	0
4	E	44	Total O 44 44	0	0
4	F	43	Total O 43 43	0	0
4	G	43	Total O 43 43	0	0
4	H	74	Total O 74 74	0	0
4	I	42	Total O 42 42	0	0
4	J	34	Total O 34 34	0	0
4	K	26	Total O 26 26	0	0
4	L	21	Total O 21 21	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.

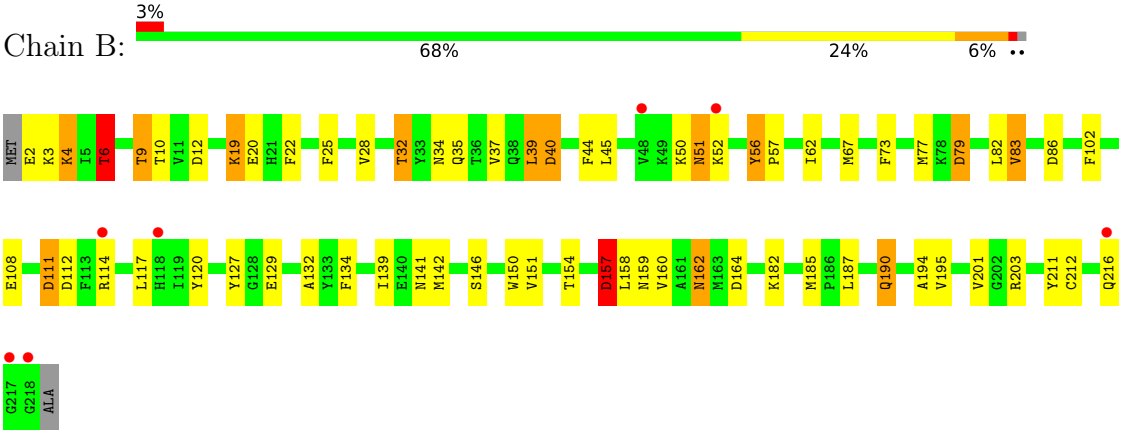
• Molecule 1: Chloramphenicol acetyltransferase

Chain A:



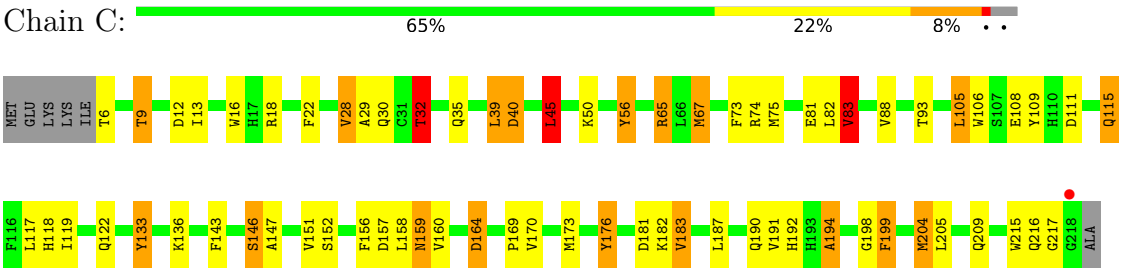
• Molecule 1: Chloramphenicol acetyltransferase

Chain B:



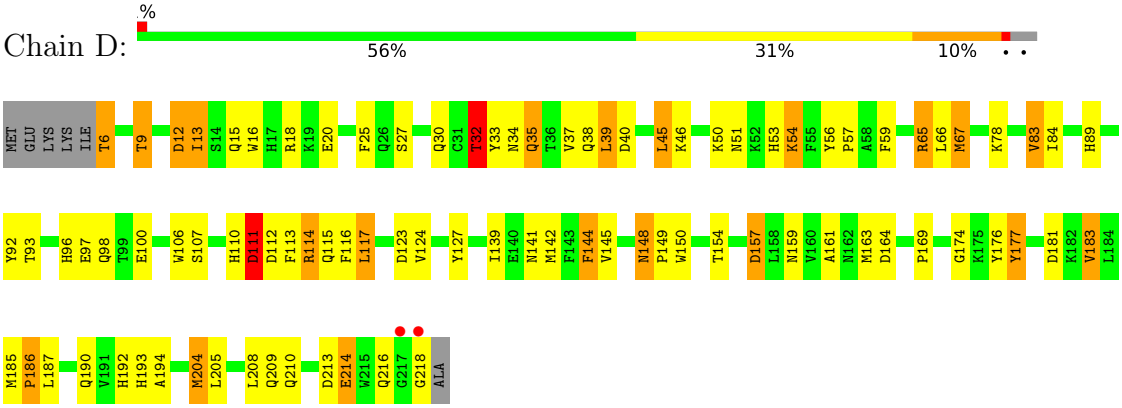
• Molecule 1: Chloramphenicol acetyltransferase

Chain C:



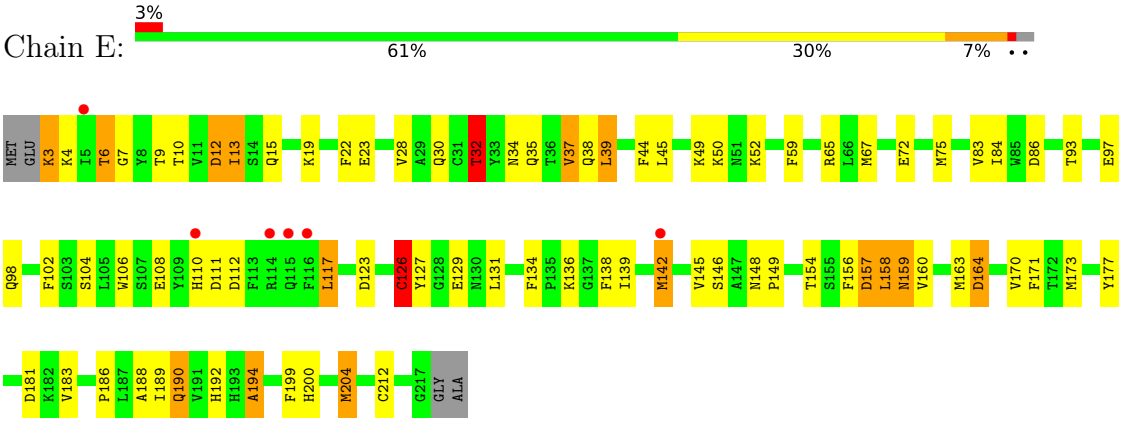
• Molecule 1: Chloramphenicol acetyltransferase

Chain D:



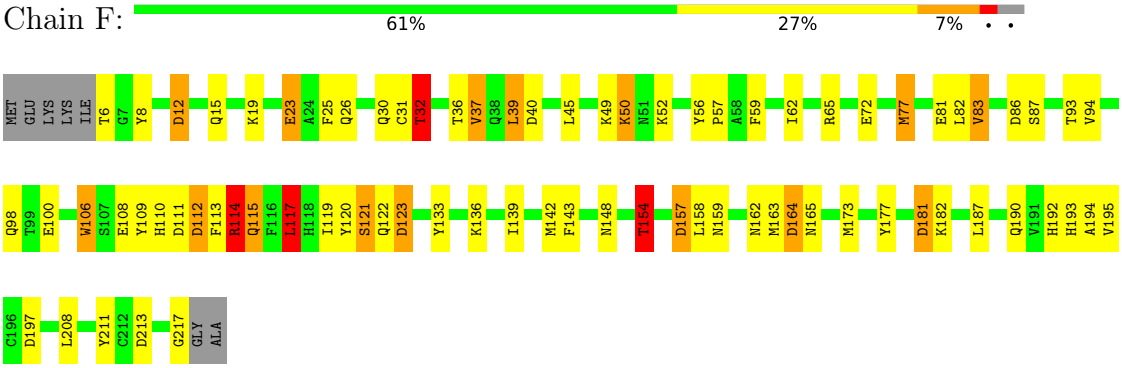
• Molecule 1: Chloramphenicol acetyltransferase

Chain E:



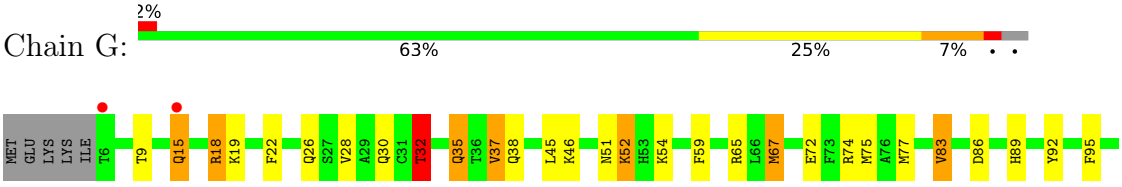
• Molecule 1: Chloramphenicol acetyltransferase

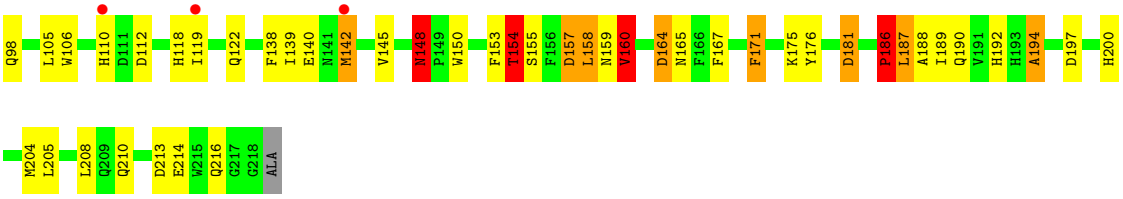
Chain F:



• Molecule 1: Chloramphenicol acetyltransferase

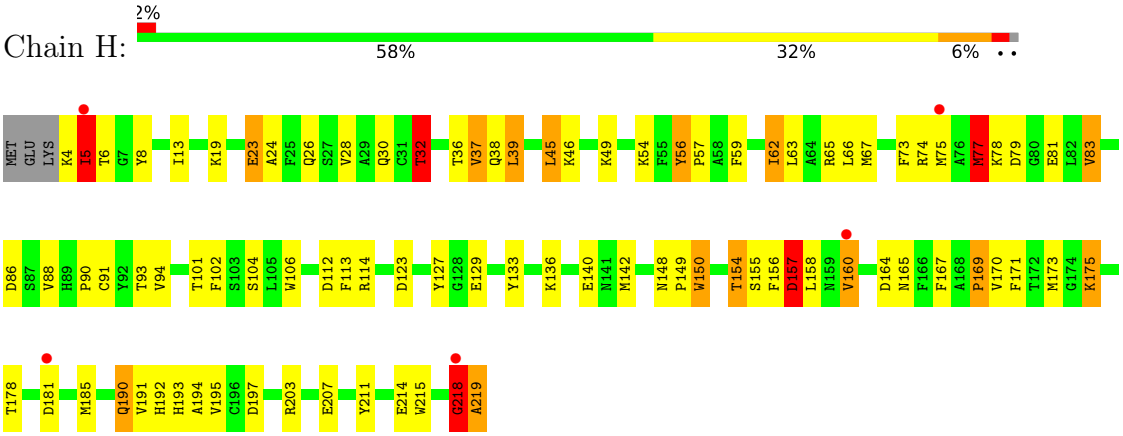
Chain G:





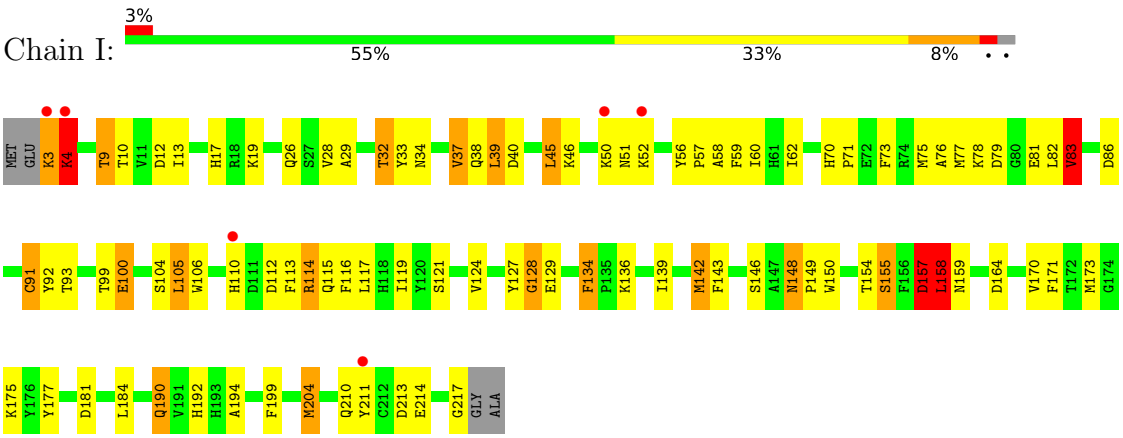
• Molecule 1: Chloramphenicol acetyltransferase

Chain H:



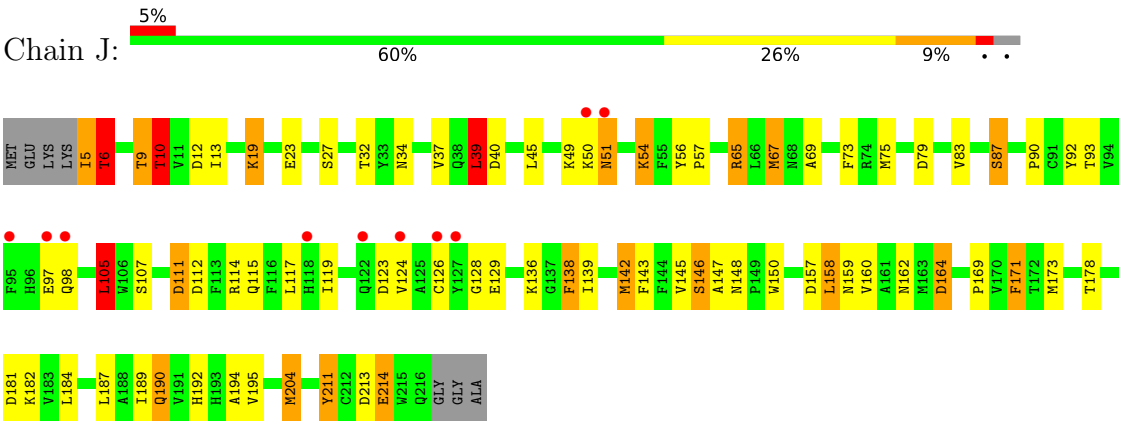
• Molecule 1: Chloramphenicol acetyltransferase

Chain I:



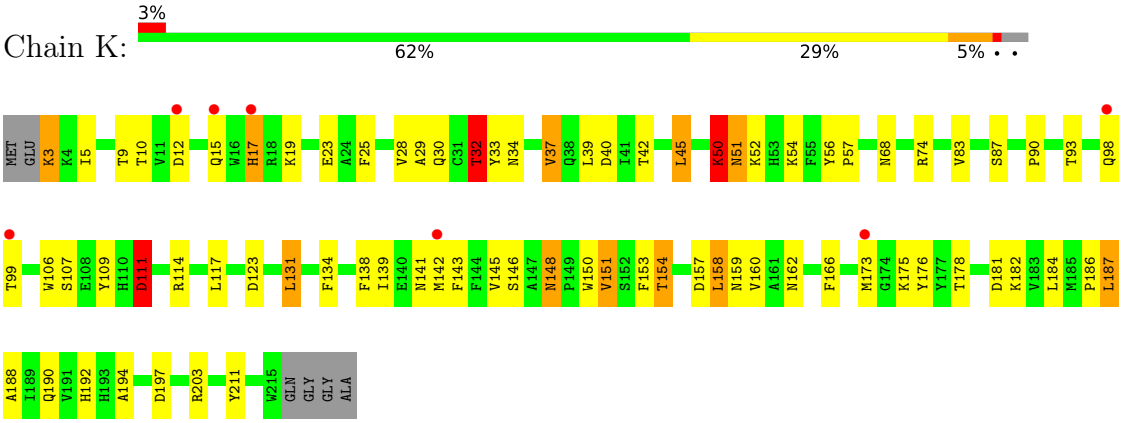
• Molecule 1: Chloramphenicol acetyltransferase

Chain J:



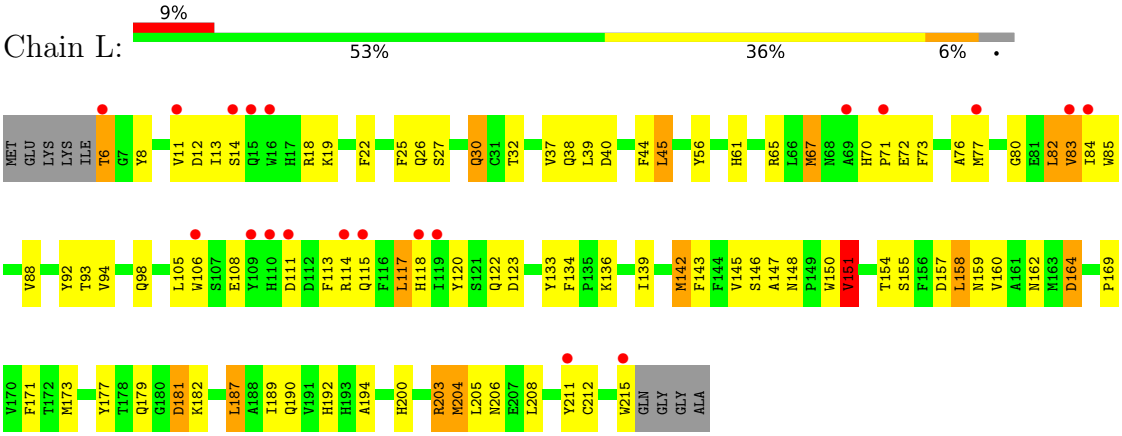
• Molecule 1: Chloramphenicol acetyltransferase

Chain K:



• Molecule 1: Chloramphenicol acetyltransferase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.35Å 129.20Å 118.07Å 90.00° 108.30° 90.00°	Depositor
Resolution (Å)	111.80 – 2.18 53.34 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.7 (111.80-2.18) 98.0 (53.34-2.12)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.192 , 0.263 0.200 , 0.265	Depositor DCC
R_{free} test set	9151 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22280	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FUA, CA

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	1.69	21/1830 (1.1%)	1.40	24/2484 (1.0%)
1	B	1.60	19/1857 (1.0%)	1.38	17/2518 (0.7%)
1	C	1.62	20/1822 (1.1%)	1.34	15/2473 (0.6%)
1	D	1.65	19/1822 (1.0%)	1.45	22/2473 (0.9%)
1	E	1.54	13/1844 (0.7%)	1.31	17/2501 (0.7%)
1	F	1.57	15/1818 (0.8%)	1.38	20/2468 (0.8%)
1	G	1.59	18/1822 (1.0%)	1.39	22/2473 (0.9%)
1	H	1.67	19/1844 (1.0%)	1.39	24/2502 (1.0%)
1	I	1.58	16/1844 (0.9%)	1.39	18/2501 (0.7%)
1	J	1.37	7/1822 (0.4%)	1.32	14/2474 (0.6%)
1	K	1.36	11/1831 (0.6%)	1.24	13/2484 (0.5%)
1	L	1.37	6/1805 (0.3%)	1.25	10/2451 (0.4%)
All	All	1.55	184/21961 (0.8%)	1.35	216/29802 (0.7%)

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	H	0	2
1	I	0	2
1	J	0	1
All	All	0	5

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	PHE	CE2-CZ	9.96	1.56	1.37
1	G	37	VAL	CB-CG2	-9.18	1.33	1.52
1	D	183	VAL	CB-CG2	9.01	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	59	PHE	CE1-CZ	8.92	1.54	1.37
1	D	157	ASP	CB-CG	8.88	1.70	1.51

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	4	LYS	O-C-N	-17.03	95.45	122.70
1	D	157	ASP	CB-CG-OD2	13.29	130.26	118.30
1	D	65	ARG	NE-CZ-NH2	-13.11	113.75	120.30
1	G	213	ASP	CB-CG-OD2	12.42	129.48	118.30
1	B	164	ASP	CB-CG-OD2	11.94	129.05	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	218	GLY	Peptide
1	H	5	ILE	Peptide
1	I	3	LYS	Peptide
1	I	4	LYS	Mainchain
1	J	6	THR	Peptide

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	1771	0	1658	59	0
1	B	1798	0	1690	46	0
1	C	1763	0	1647	45	0
1	D	1763	0	1647	71	0
1	E	1785	0	1681	70	0
1	F	1759	0	1644	55	0
1	G	1763	0	1647	61	0
1	H	1785	0	1676	78	0
1	I	1785	0	1681	79	0
1	J	1763	0	1652	88	0
1	K	1772	0	1670	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1746	0	1633	75	0
2	A	1	0	0	0	0
3	A	37	0	44	8	0
3	B	37	0	44	9	0
3	C	37	0	44	5	0
3	D	37	0	44	10	0
3	E	37	0	44	3	0
3	F	37	0	44	8	0
3	G	37	0	43	6	0
3	H	37	0	43	5	0
3	I	37	0	44	16	0
3	J	37	0	44	10	0
3	K	37	0	44	10	0
3	L	37	0	44	4	0
4	A	78	0	0	6	0
4	B	51	0	0	7	0
4	C	68	0	0	10	0
4	D	58	0	0	7	0
4	E	44	0	0	8	0
4	F	43	0	0	5	0
4	G	43	0	0	6	0
4	H	74	0	0	10	0
4	I	42	0	0	8	0
4	J	34	0	0	9	0
4	K	26	0	0	7	0
4	L	21	0	0	7	0
All	All	22280	0	20452	774	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 18.

The worst 5 of 774 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:E:139:ILE:H	1:E:142:MET:CE	1.31	1.37
1:E:139:ILE:N	1:E:142:MET:HE3	1.39	1.36
1:H:218:GLY:HA2	1:H:219:ALA:O	1.36	1.24
1:E:67:MET:CE	1:E:171:PHE:HE1	1.49	1.24
1:J:67:MET:HA	1:J:67:MET:CE	1.71	1.20

There are no symmetry-related clashes.

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	212/219 (97%)	205 (97%)	6 (3%)	1 (0%)	29	28
1	B	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	29	28
1	C	211/219 (96%)	202 (96%)	9 (4%)	0	100	100
1	D	211/219 (96%)	207 (98%)	4 (2%)	0	100	100
1	E	213/219 (97%)	202 (95%)	11 (5%)	0	100	100
1	F	210/219 (96%)	201 (96%)	8 (4%)	1 (0%)	29	28
1	G	211/219 (96%)	206 (98%)	5 (2%)	0	100	100
1	H	214/219 (98%)	208 (97%)	6 (3%)	0	100	100
1	I	213/219 (97%)	206 (97%)	6 (3%)	1 (0%)	29	28
1	J	210/219 (96%)	202 (96%)	6 (3%)	2 (1%)	15	12
1	K	211/219 (96%)	202 (96%)	8 (4%)	1 (0%)	29	28
1	L	208/219 (95%)	200 (96%)	8 (4%)	0	100	100
All	All	2539/2628 (97%)	2447 (96%)	85 (3%)	7 (0%)	41	43

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	50	LYS
1	I	128	GLY
1	J	51	ASN
1	F	52	LYS
1	A	165	ASN

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	190/194 (98%)	171 (90%)	19 (10%)	7	6
1	B	193/194 (100%)	171 (89%)	22 (11%)	5	4
1	C	189/194 (97%)	166 (88%)	23 (12%)	5	3
1	D	189/194 (97%)	165 (87%)	24 (13%)	4	3
1	E	192/194 (99%)	173 (90%)	19 (10%)	8	6
1	F	189/194 (97%)	164 (87%)	25 (13%)	4	2
1	G	189/194 (97%)	171 (90%)	18 (10%)	8	7
1	H	191/194 (98%)	167 (87%)	24 (13%)	4	3
1	I	192/194 (99%)	170 (88%)	22 (12%)	5	4
1	J	190/194 (98%)	161 (85%)	29 (15%)	2	2
1	K	191/194 (98%)	157 (82%)	34 (18%)	2	1
1	L	188/194 (97%)	160 (85%)	28 (15%)	3	2
All	All	2283/2328 (98%)	1996 (87%)	287 (13%)	4	3

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	19	LYS
1	L	215	TRP
1	K	45	LEU
1	L	13	ILE
1	E	52	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	15	GLN
1	L	179	GLN
1	J	34	ASN
1	K	98	GLN
1	E	38	GLN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\#\|Z\| > 2$
3	FUA	E	706	-	39,40,40	1.82	7 (17%)	49,64,64	5.09	34 (69%)
3	FUA	F	704	-	39,40,40	1.90	8 (20%)	49,64,64	4.88	30 (61%)
3	FUA	J	711	-	39,40,40	1.70	8 (20%)	49,64,64	5.74	36 (73%)
3	FUA	B	703	-	39,40,40	2.12	12 (30%)	49,64,64	5.52	33 (67%)
3	FUA	G	708	-	39,40,40	1.64	6 (15%)	49,64,64	5.18	36 (73%)
3	FUA	K	712	-	39,40,40	1.77	5 (12%)	49,64,64	5.28	28 (57%)
3	FUA	H	709	-	39,40,40	2.04	11 (28%)	49,64,64	5.77	37 (75%)
3	FUA	L	710	-	39,40,40	1.77	7 (17%)	49,64,64	5.10	30 (61%)
3	FUA	A	702	-	39,40,40	2.21	11 (28%)	49,64,64	5.16	37 (75%)
3	FUA	C	701	-	39,40,40	2.10	11 (28%)	49,64,64	5.73	34 (69%)
3	FUA	D	705	-	39,40,40	1.97	9 (23%)	49,64,64	5.39	32 (65%)
3	FUA	I	707	-	39,40,40	1.64	8 (20%)	49,64,64	4.99	34 (69%)

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
3	FUA	E	706	-	4/4/15/16	8/15/92/92	0/4/4/4
3	FUA	F	704	-	3/3/15/16	5/15/92/92	0/4/4/4
3	FUA	J	711	-	2/2/15/16	6/15/92/92	0/4/4/4
3	FUA	B	703	-	4/4/15/16	8/15/92/92	0/4/4/4
3	FUA	G	708	-	4/4/15/16	1/15/92/92	0/4/4/4
3	FUA	K	712	-	3/3/15/16	7/15/92/92	0/4/4/4
3	FUA	H	709	-	3/3/15/16	9/15/92/92	0/4/4/4
3	FUA	L	710	-	3/3/15/16	6/15/92/92	0/4/4/4
3	FUA	A	702	-	3/3/15/16	5/15/92/92	0/4/4/4
3	FUA	C	701	-	3/3/15/16	7/15/92/92	0/4/4/4
3	FUA	D	705	-	2/2/15/16	7/15/92/92	0/4/4/4
3	FUA	I	707	-	2/2/15/16	6/15/92/92	0/4/4/4

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	705	FUA	C14-C8	-7.37	1.46	1.59
3	A	702	FUA	C14-C8	-6.66	1.47	1.59
3	B	703	FUA	C14-C8	-6.53	1.47	1.59
3	L	710	FUA	O2-C31	6.23	1.49	1.35
3	C	701	FUA	C14-C8	-6.04	1.48	1.59

The worst 5 of 401 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	709	FUA	C21-C14-C8	-18.91	94.81	112.27
3	J	711	FUA	C21-C14-C8	-17.22	96.38	112.27
3	B	703	FUA	C19-C10-C1	-15.06	83.99	108.26
3	K	712	FUA	C21-C14-C8	-14.35	99.03	112.27
3	D	705	FUA	C19-C10-C5	-13.94	91.97	111.18

5 of 36 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	702	FUA	C10
3	A	702	FUA	C13
3	A	702	FUA	C9
3	B	703	FUA	C4
3	B	703	FUA	C13

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	FUA	C23-C22-C29-O4
3	A	702	FUA	C23-C22-C29-O5
3	B	703	FUA	C17-C22-C23-C24
3	B	703	FUA	C23-C22-C29-O4
3	C	701	FUA	C15-C16-O2-C31

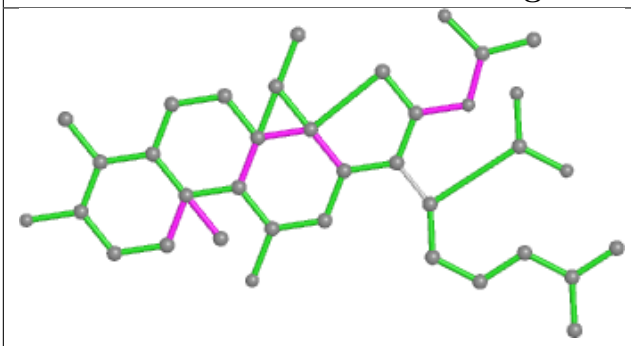
There are no ring outliers.

12 monomers are involved in 94 short contacts:

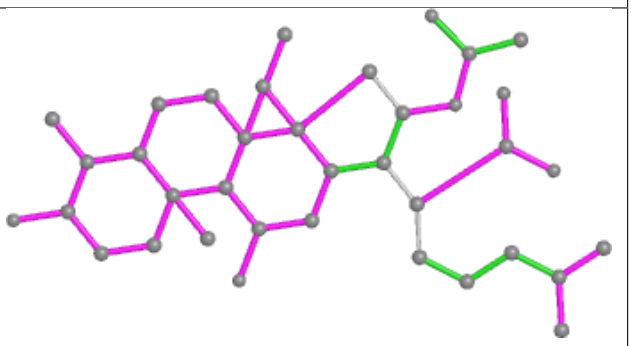
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	706	FUA	3	0
3	F	704	FUA	8	0
3	J	711	FUA	10	0
3	B	703	FUA	9	0
3	G	708	FUA	6	0
3	K	712	FUA	10	0
3	H	709	FUA	5	0
3	L	710	FUA	4	0
3	A	702	FUA	8	0
3	C	701	FUA	5	0
3	D	705	FUA	10	0
3	I	707	FUA	16	0

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.

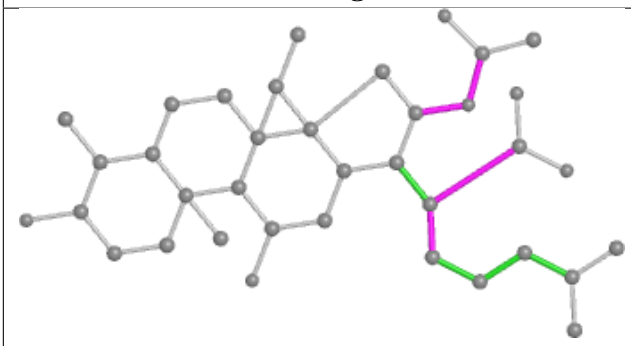
Ligand FUA E 706



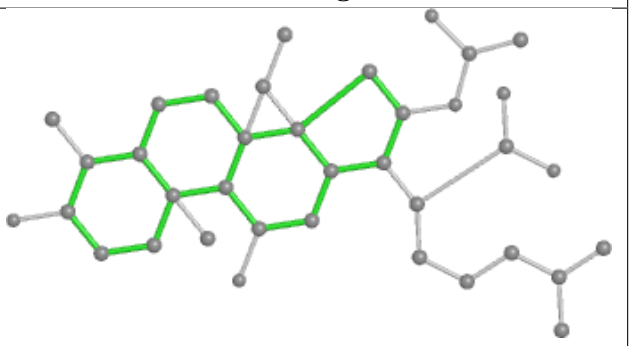
Bond lengths



Bond angles

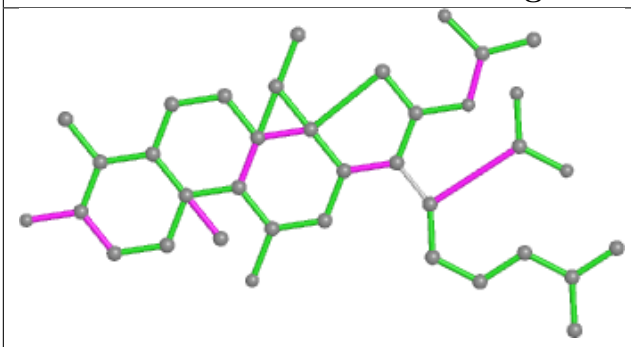


Torsions



Rings

Ligand FUA F 704



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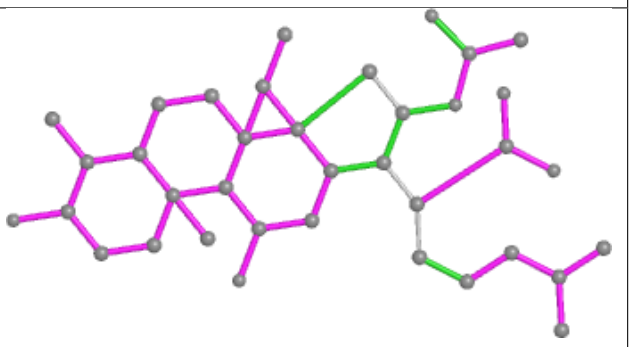

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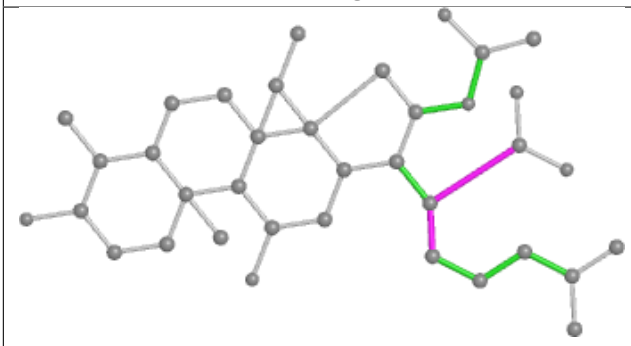

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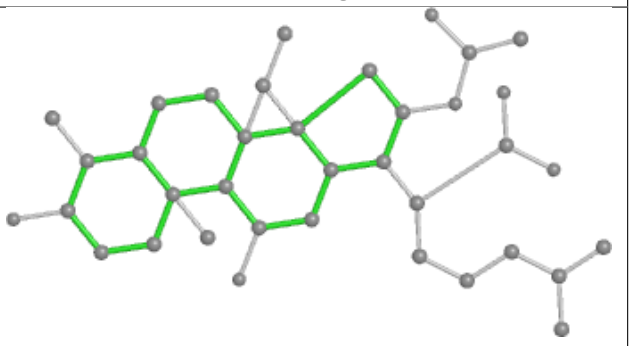
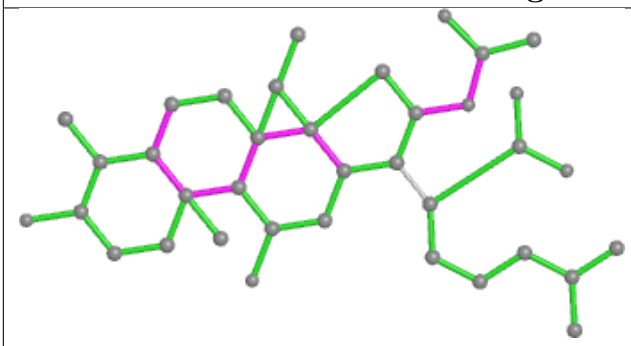


Rings

Ligand FUA J 711



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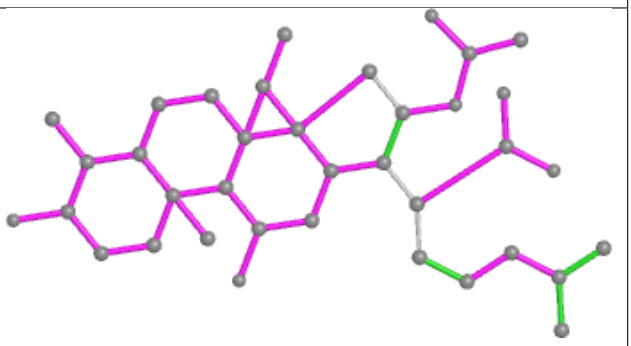

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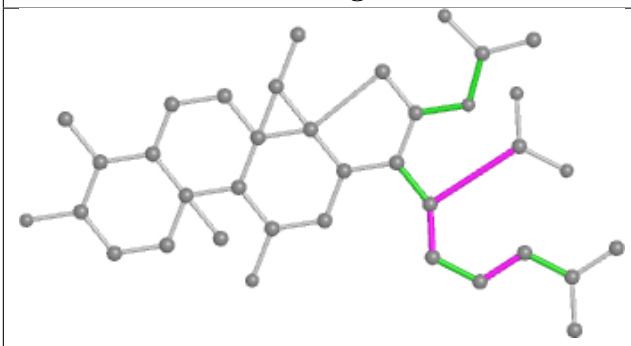
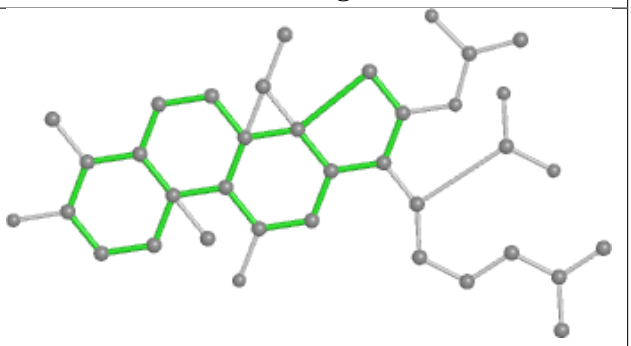
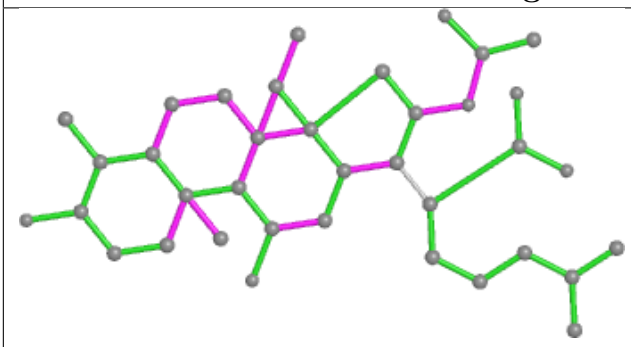


Torsions



Rings

Ligand FUA B 703



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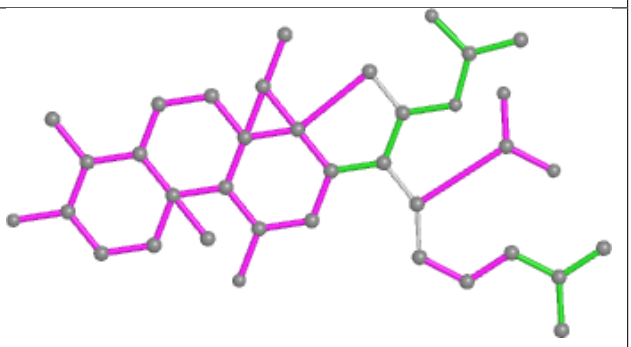
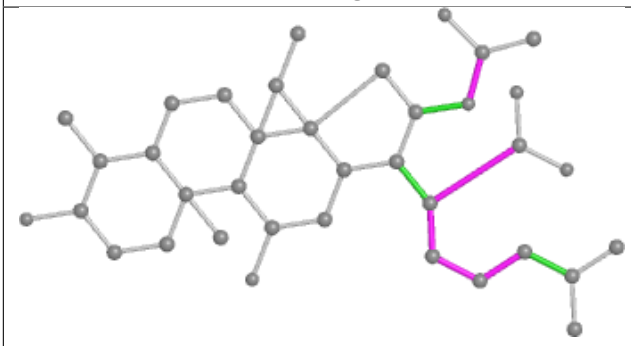


Bond angles



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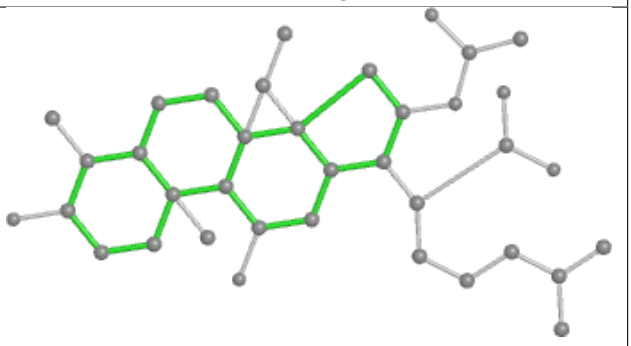
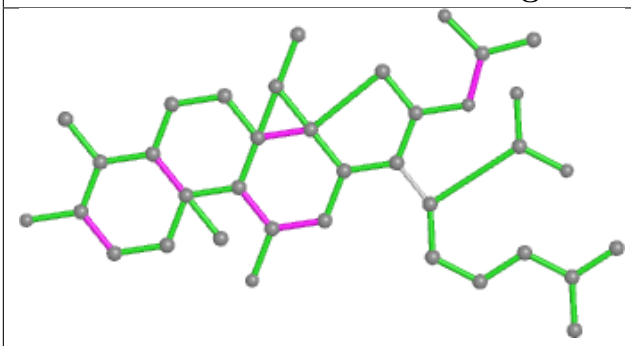


Rings

Ligand FUA G 708



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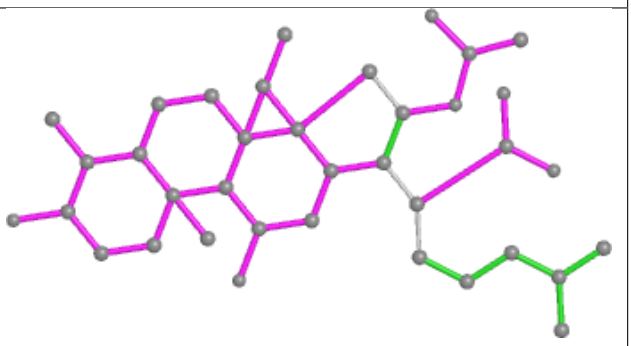

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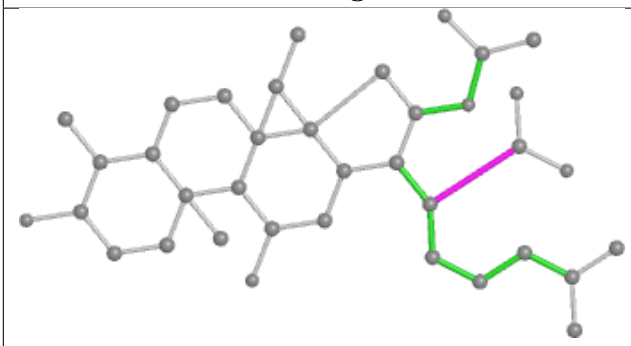

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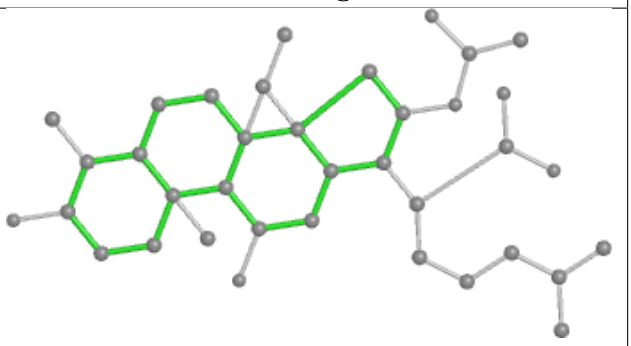
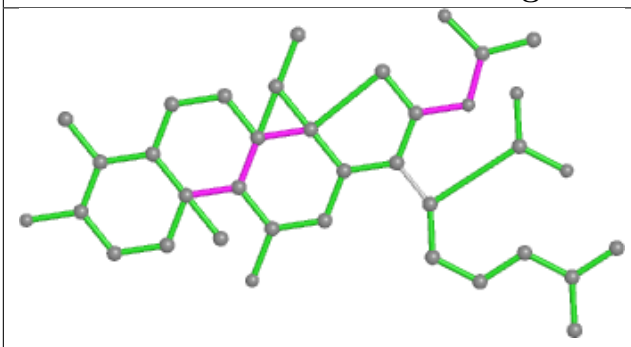


Rings

Ligand FUA K 712



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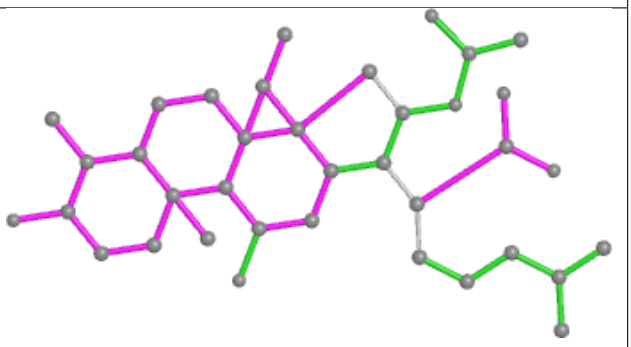
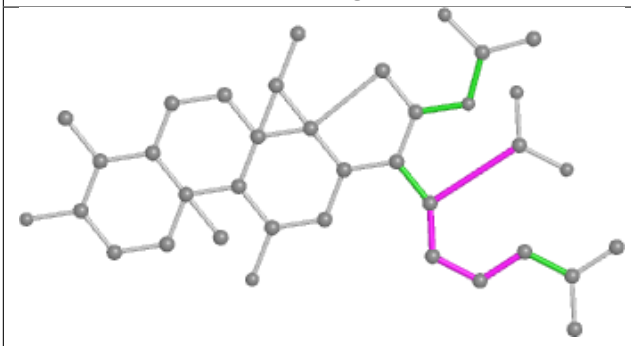


Bond angles



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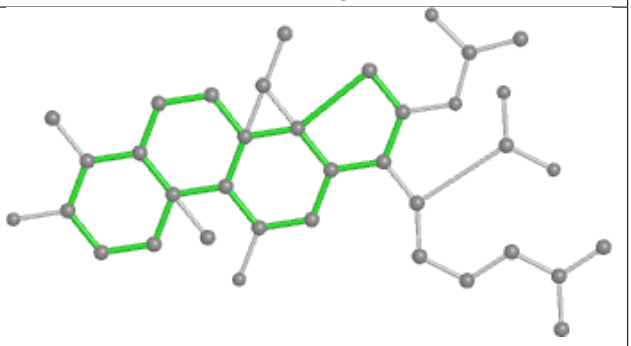
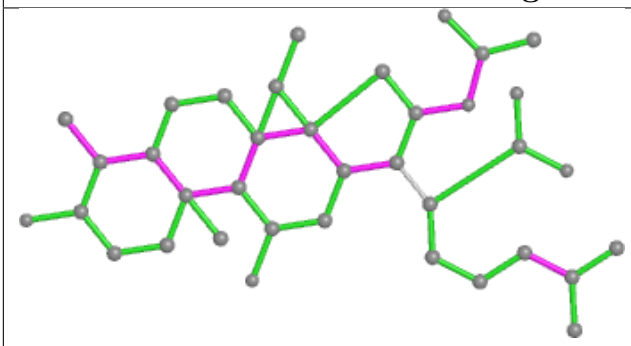


Rings

Ligand FUA H 709



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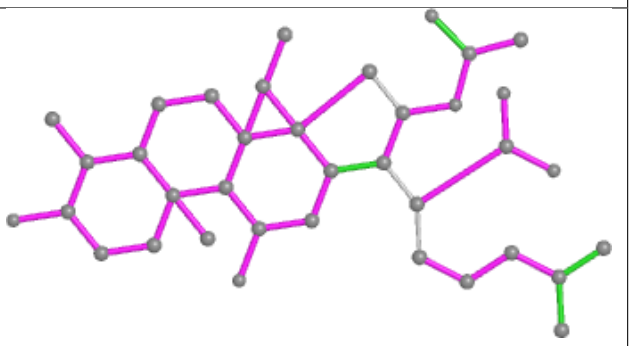

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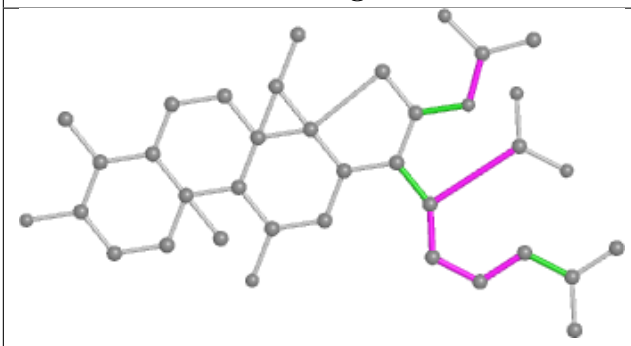

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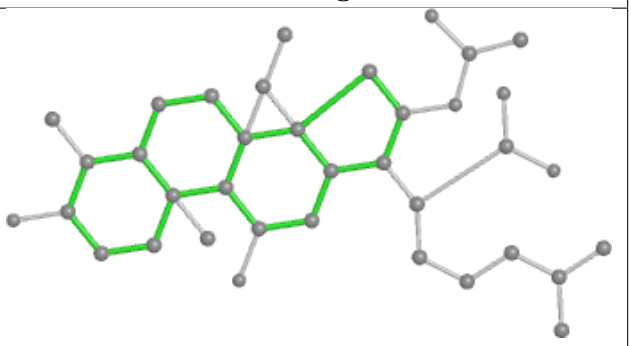
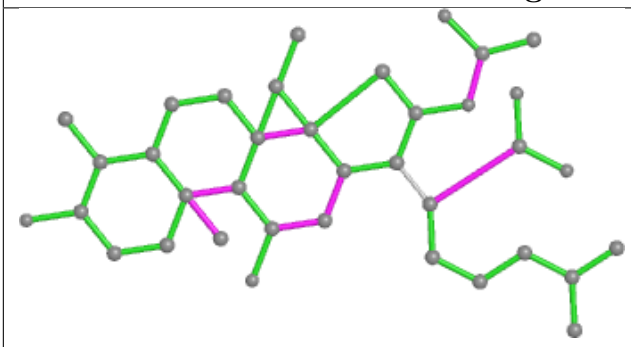
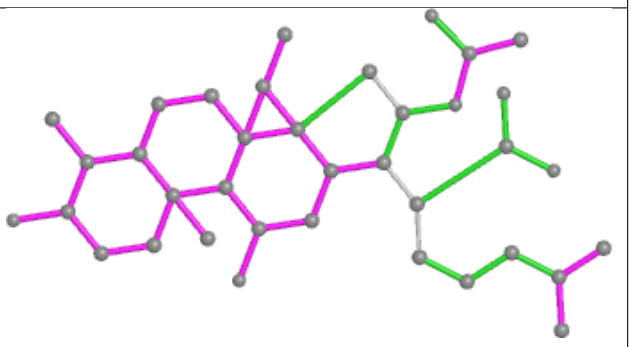


Rings

Ligand FUA L 710



Bond lengths



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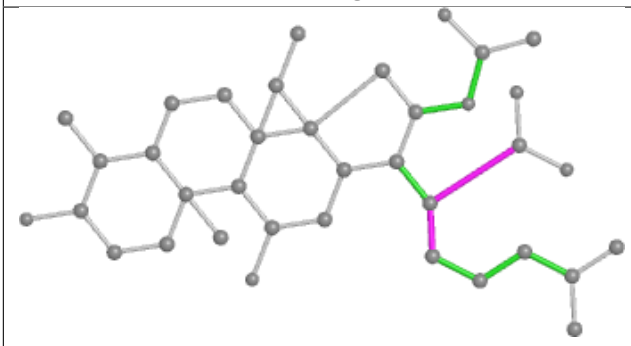

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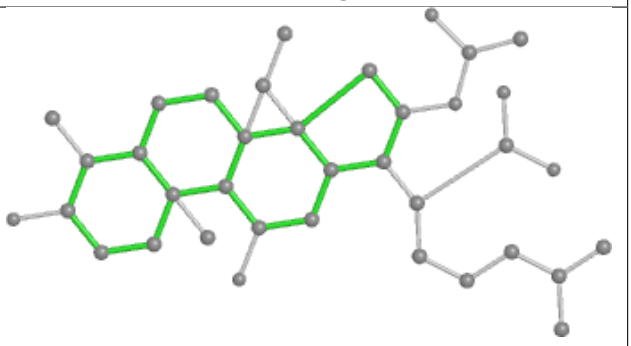
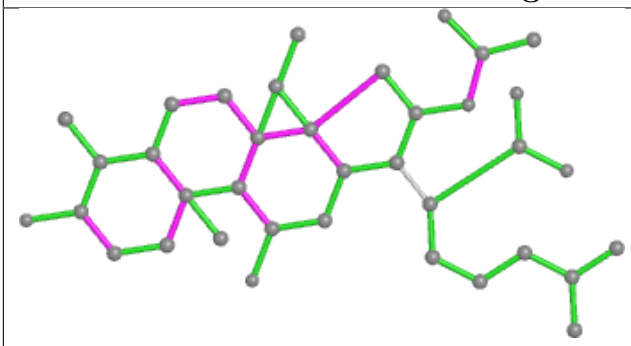
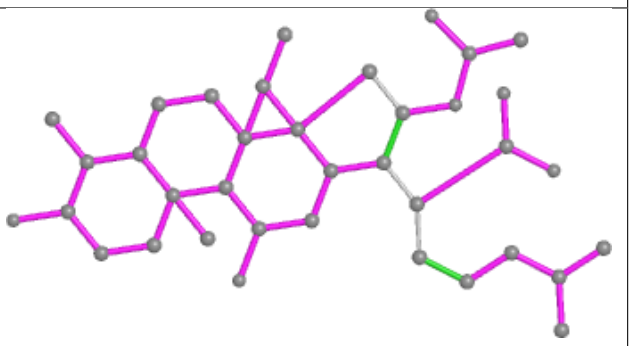


Rings

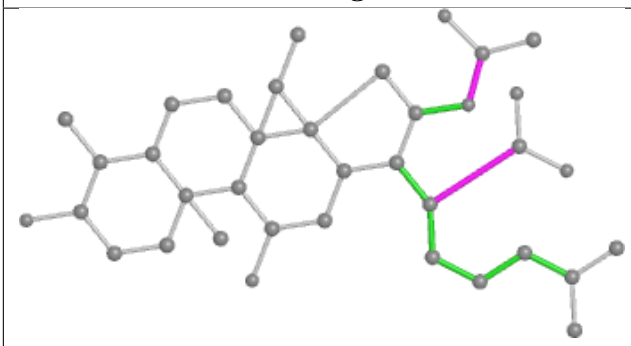
Ligand FUA A 702



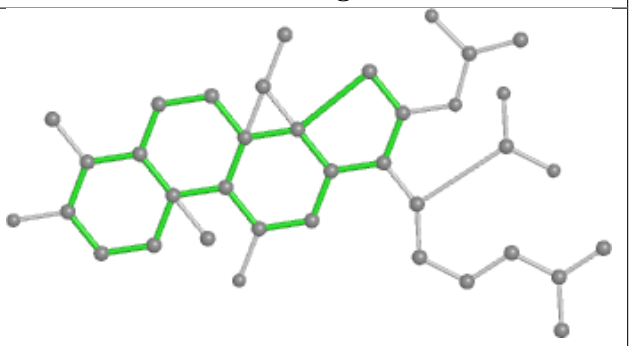
Bond lengths



Bond angles

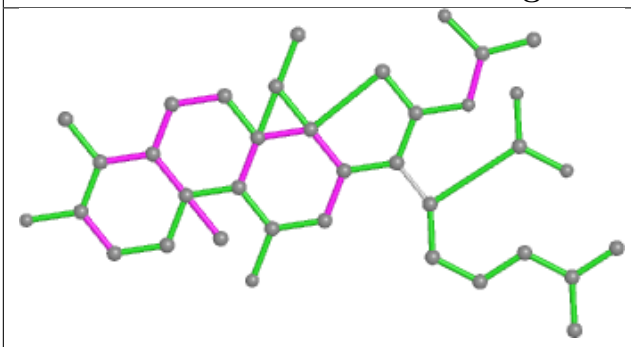


Torsions

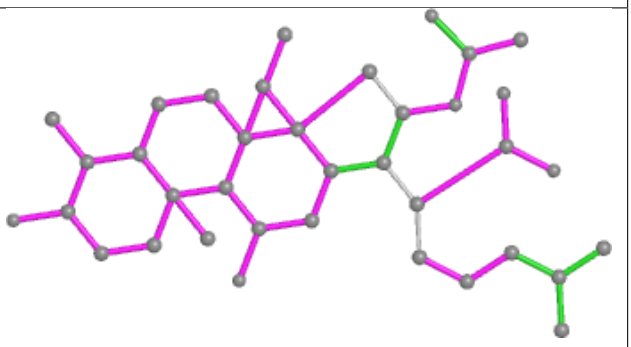


Rings

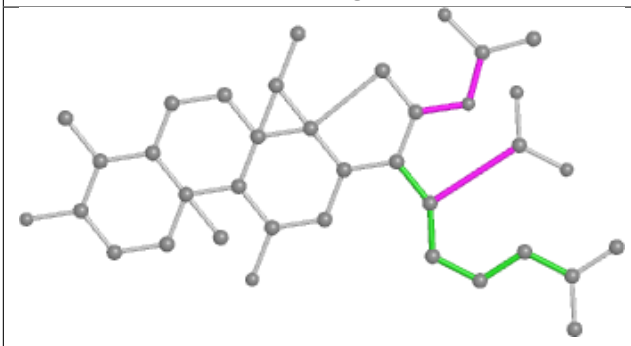
Ligand FUA C 701



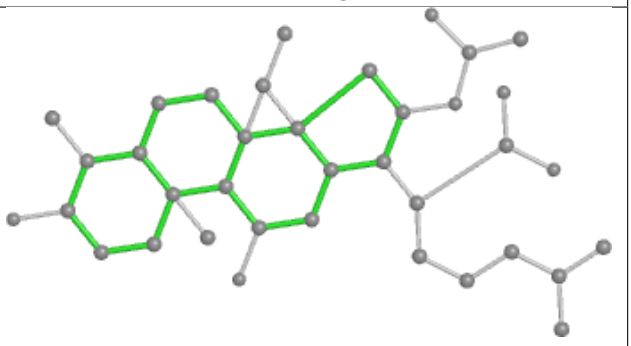
Bond lengths



Bond angles

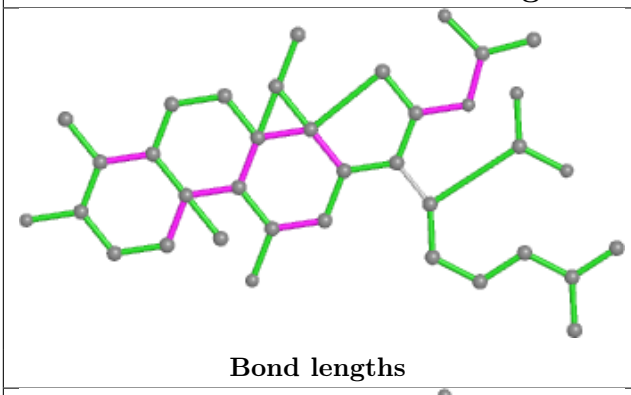


Torsions

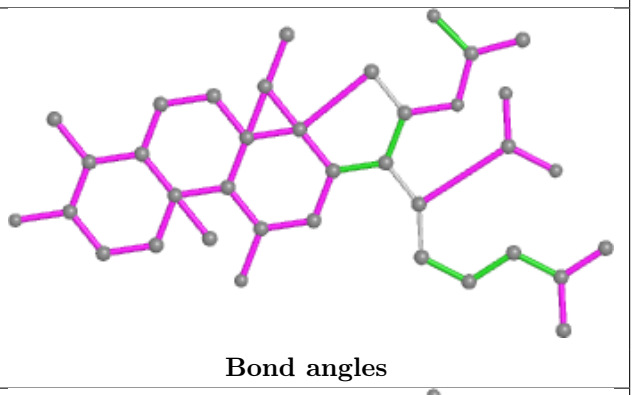


Rings

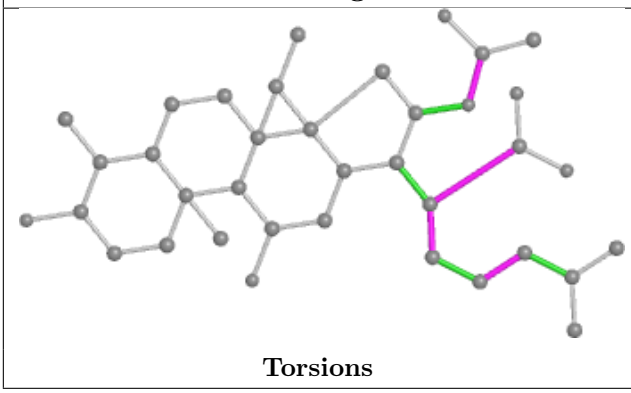
Ligand FUA D 705



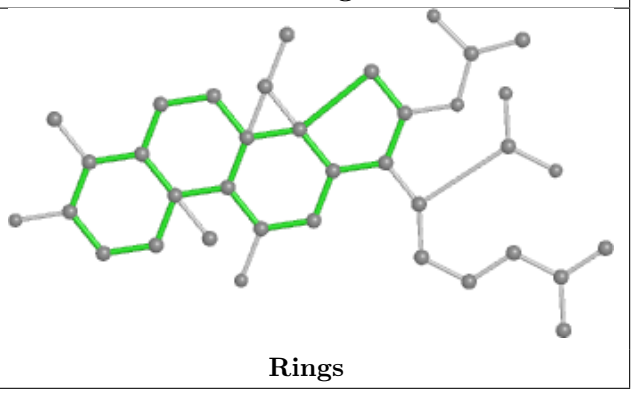
Bond lengths



Bond angles

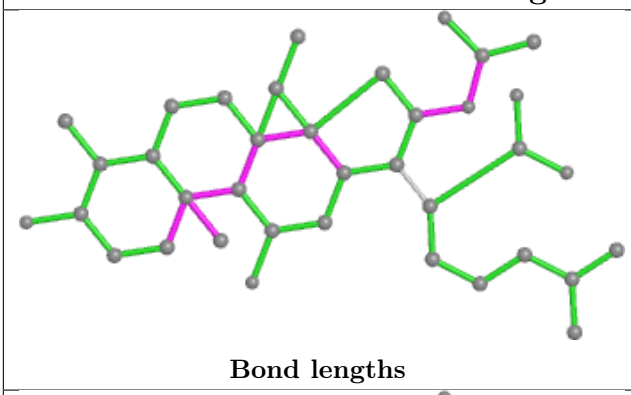


Torsions

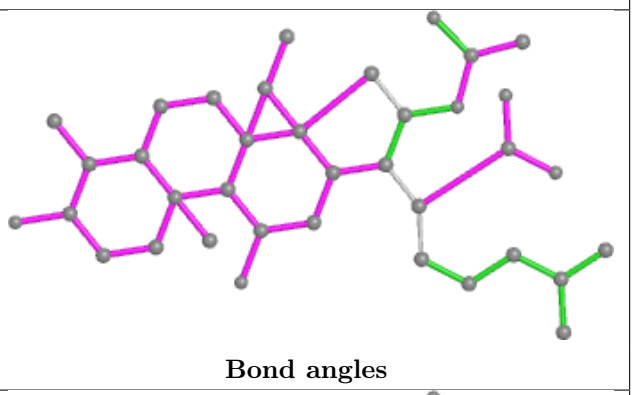


Rings

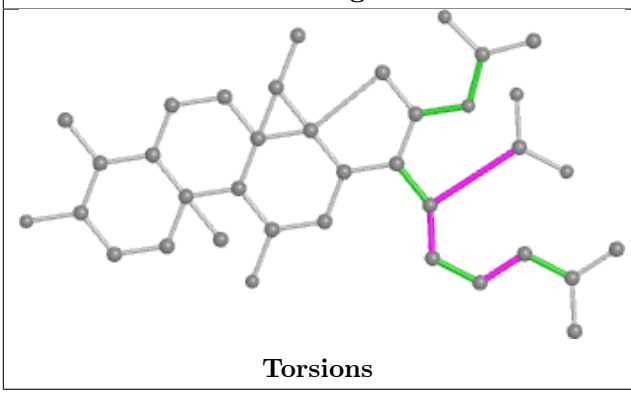
Ligand FUA I 707



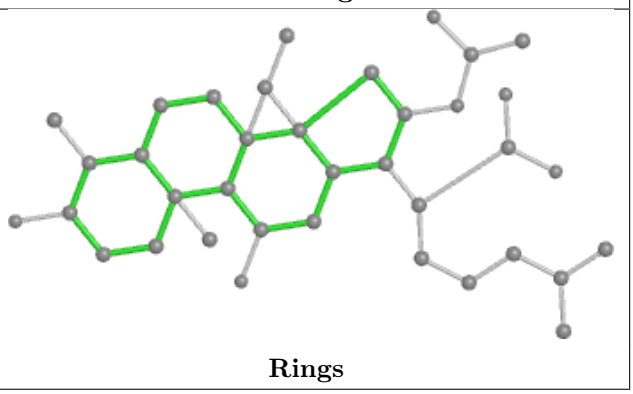
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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	214/219 (97%)	0.12	2 (0%) 84 84	14, 24, 41, 64	0
1	B	217/219 (99%)	0.19	7 (3%) 47 48	17, 28, 50, 71	0
1	C	213/219 (97%)	0.06	1 (0%) 91 91	16, 27, 48, 63	0
1	D	213/219 (97%)	0.25	2 (0%) 84 84	18, 26, 44, 70	0
1	E	215/219 (98%)	0.17	6 (2%) 53 54	19, 30, 47, 66	0
1	F	212/219 (96%)	0.02	0 100 100	19, 29, 49, 56	0
1	G	213/219 (97%)	0.14	5 (2%) 60 61	21, 30, 47, 57	0
1	H	216/219 (98%)	0.26	5 (2%) 60 61	14, 26, 40, 63	0
1	I	215/219 (98%)	0.22	6 (2%) 53 54	19, 32, 51, 68	0
1	J	212/219 (96%)	0.42	10 (4%) 31 32	25, 36, 55, 60	0
1	K	213/219 (97%)	0.24	7 (3%) 46 47	28, 39, 57, 64	0
1	L	210/219 (95%)	0.56	20 (9%) 8 8	26, 42, 63, 75	0
All	All	2563/2628 (97%)	0.22	71 (2%) 53 54	14, 31, 52, 75	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	217	GLY	7.3
1	D	218	GLY	6.0
1	H	5	ILE	4.7
1	L	114	ARG	4.2
1	L	11	VAL	4.2

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 monosaccharides in this entry.

6.4 Ligands (i)

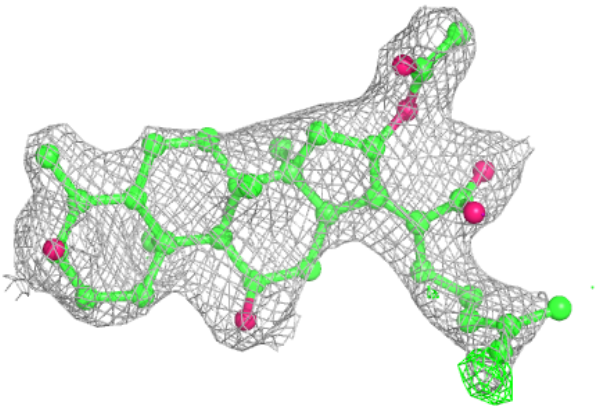
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

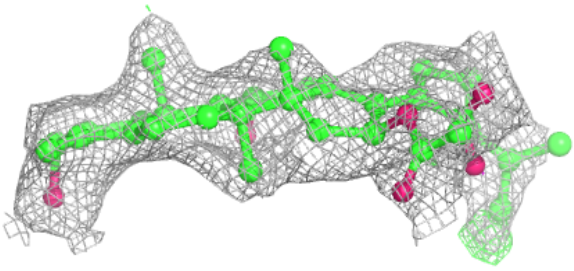
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUA	L	710	37/37	0.84	0.18	33,59,71,72	0
3	FUA	G	708	37/37	0.85	0.17	43,55,68,70	0
3	FUA	K	712	37/37	0.86	0.16	42,55,72,74	0
3	FUA	H	709	37/37	0.88	0.20	28,38,60,60	0
3	FUA	I	707	37/37	0.88	0.15	36,42,51,55	0
3	FUA	J	711	37/37	0.89	0.16	43,50,60,64	0
3	FUA	F	704	37/37	0.89	0.14	27,40,55,55	0
3	FUA	D	705	37/37	0.89	0.19	31,37,58,62	0
3	FUA	E	706	37/37	0.90	0.14	33,42,51,57	0
3	FUA	C	701	37/37	0.90	0.15	31,41,52,55	0
3	FUA	A	702	37/37	0.92	0.16	19,34,40,44	0
3	FUA	B	703	37/37	0.93	0.13	25,35,57,59	0
2	CA	A	801	1/1	0.99	0.29	5,5,5,5	1

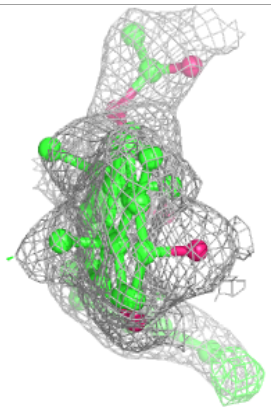
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FUA L 710:

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

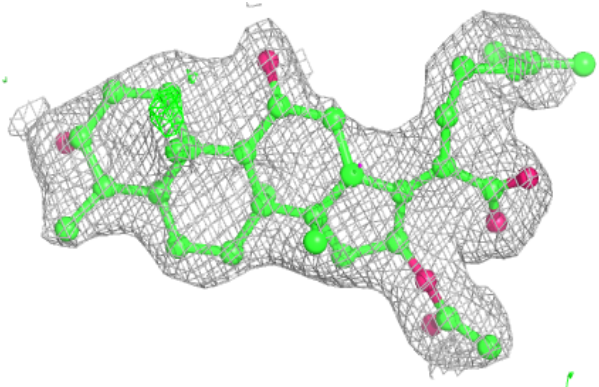


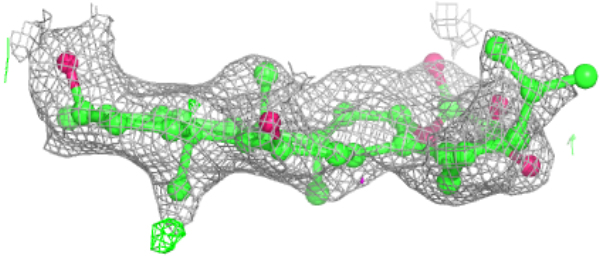


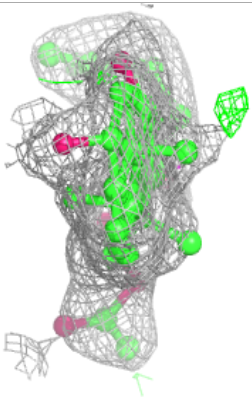


Electron density around FUA G 708:

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

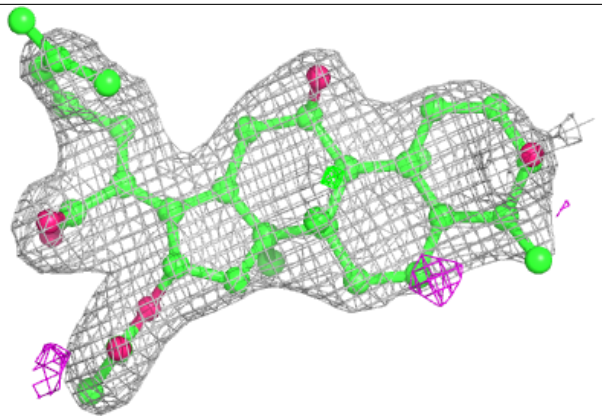


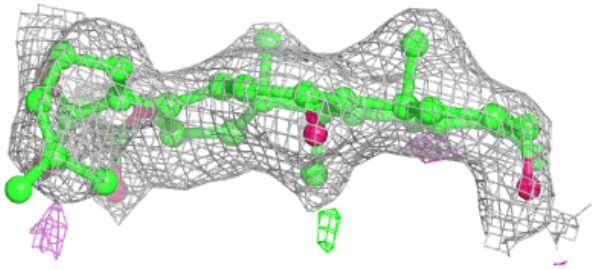


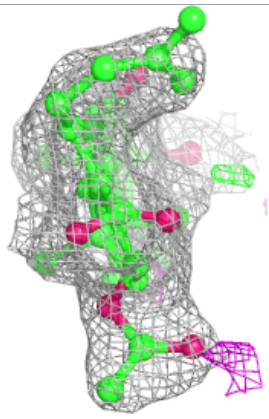


Electron density around FUA K 712:

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

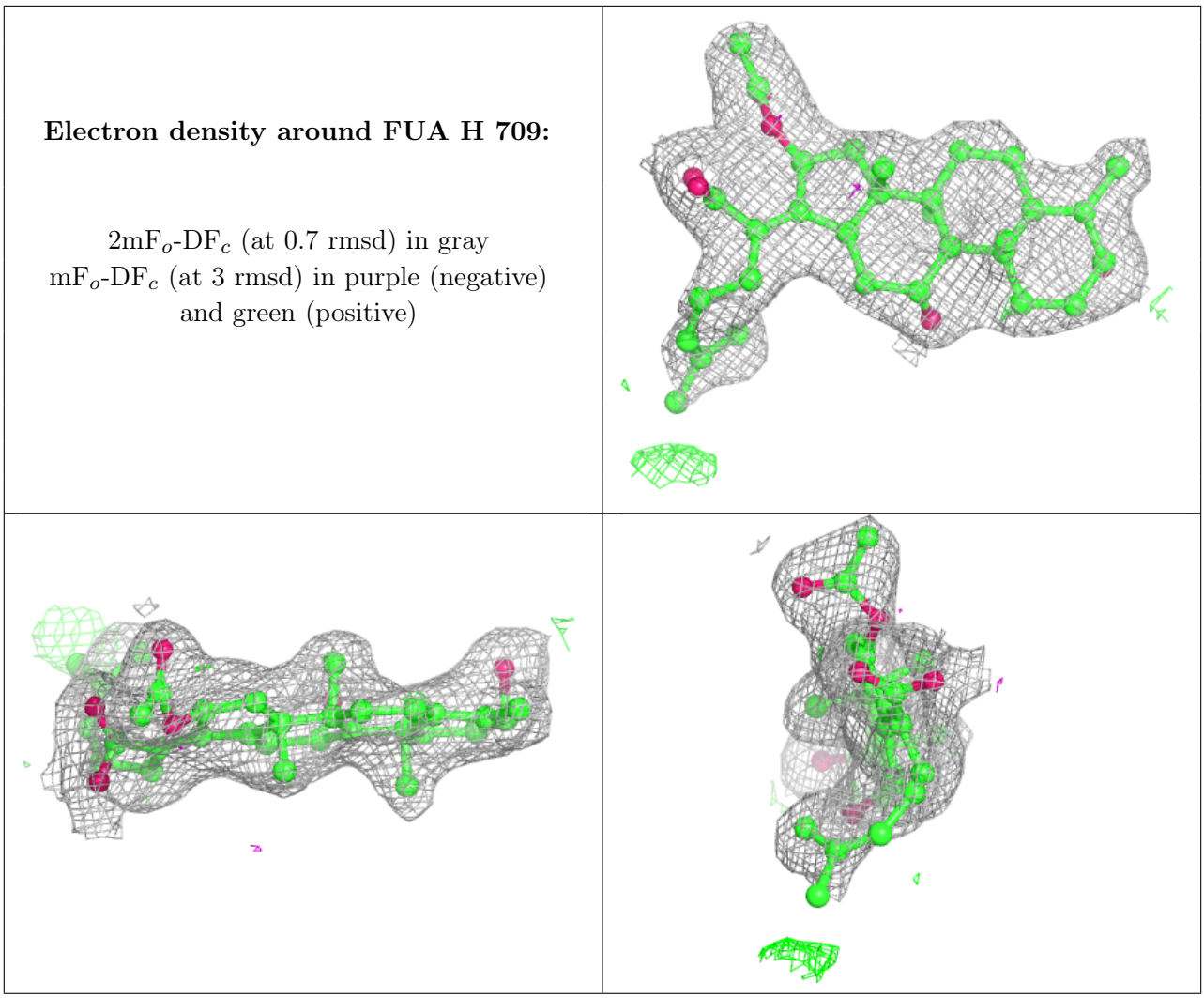






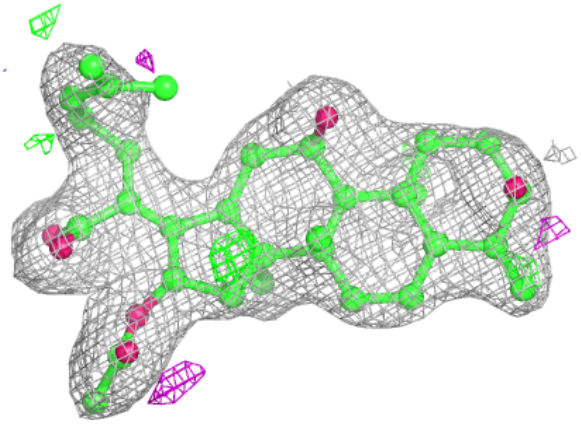
Electron density around FUA H 709:

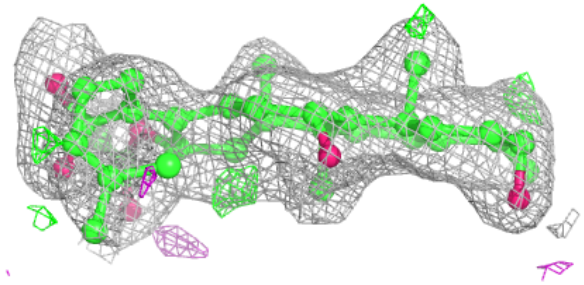
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

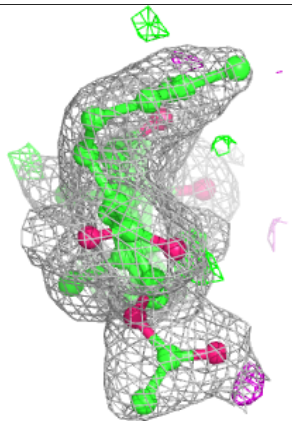


Electron density around FUA I 707:

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

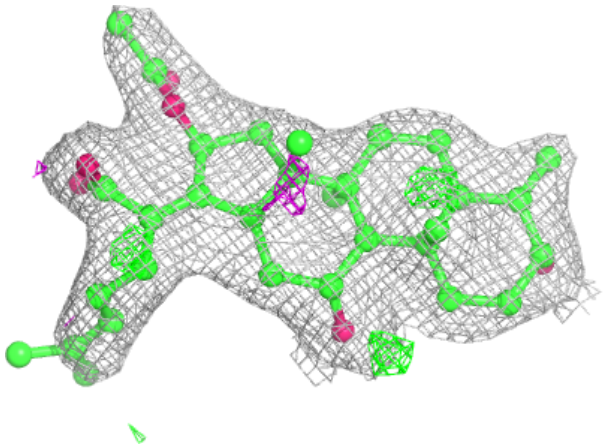


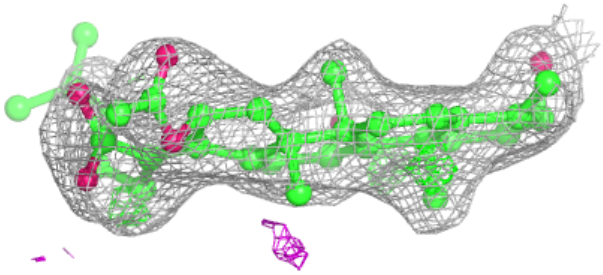


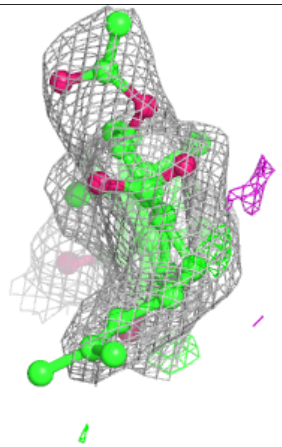


Electron density around FUA J 711:

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

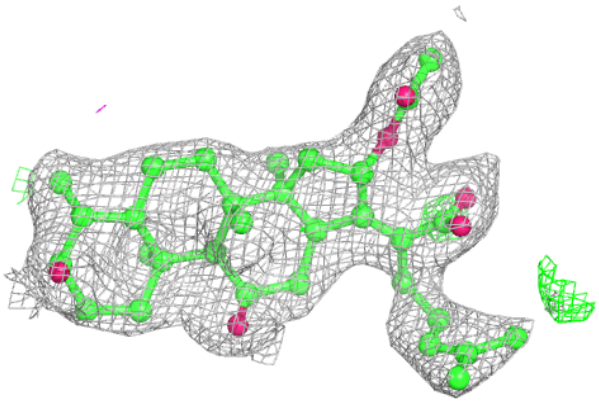


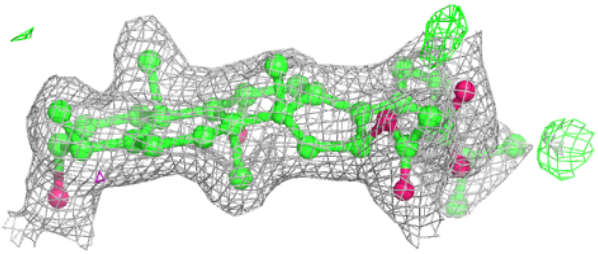


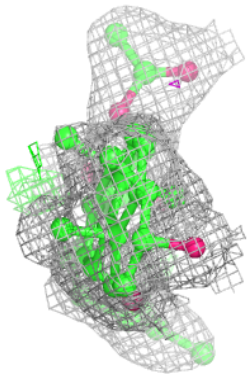


Electron density around FUA F 704:

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

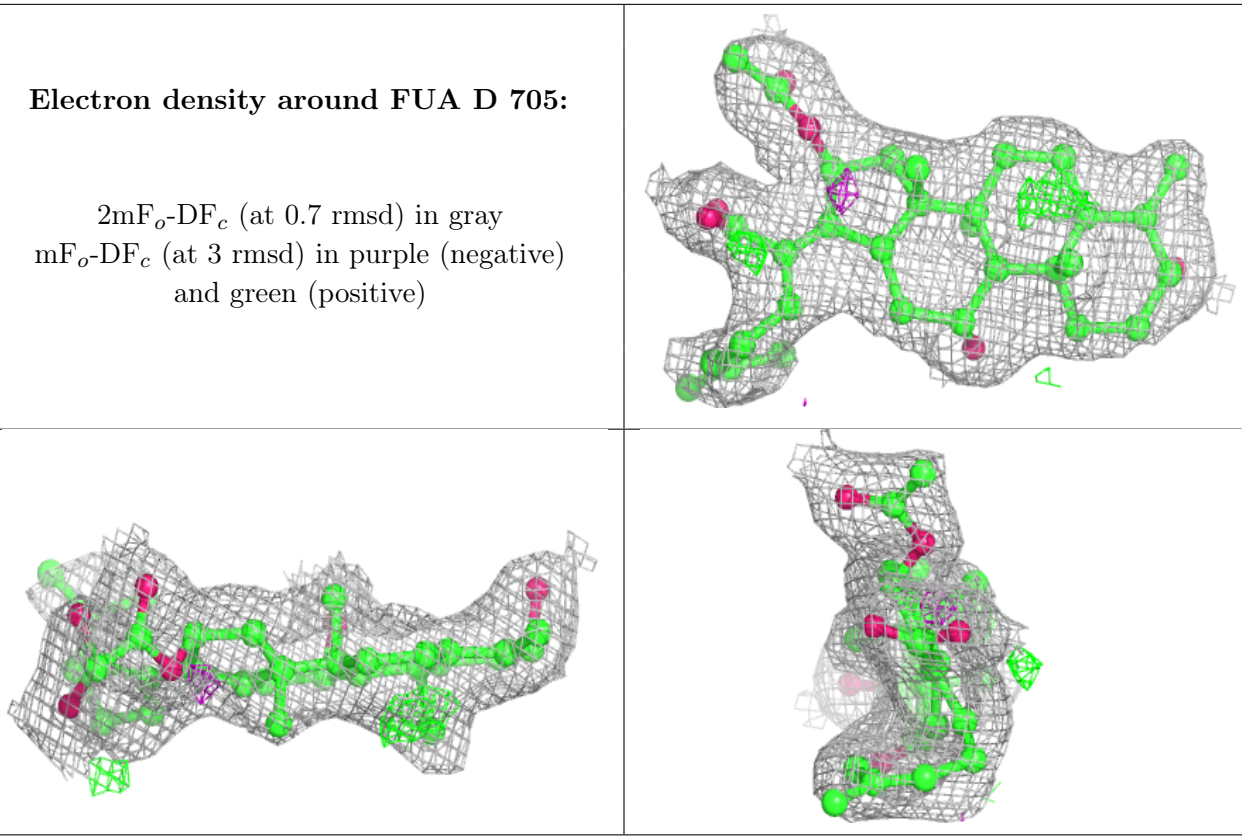






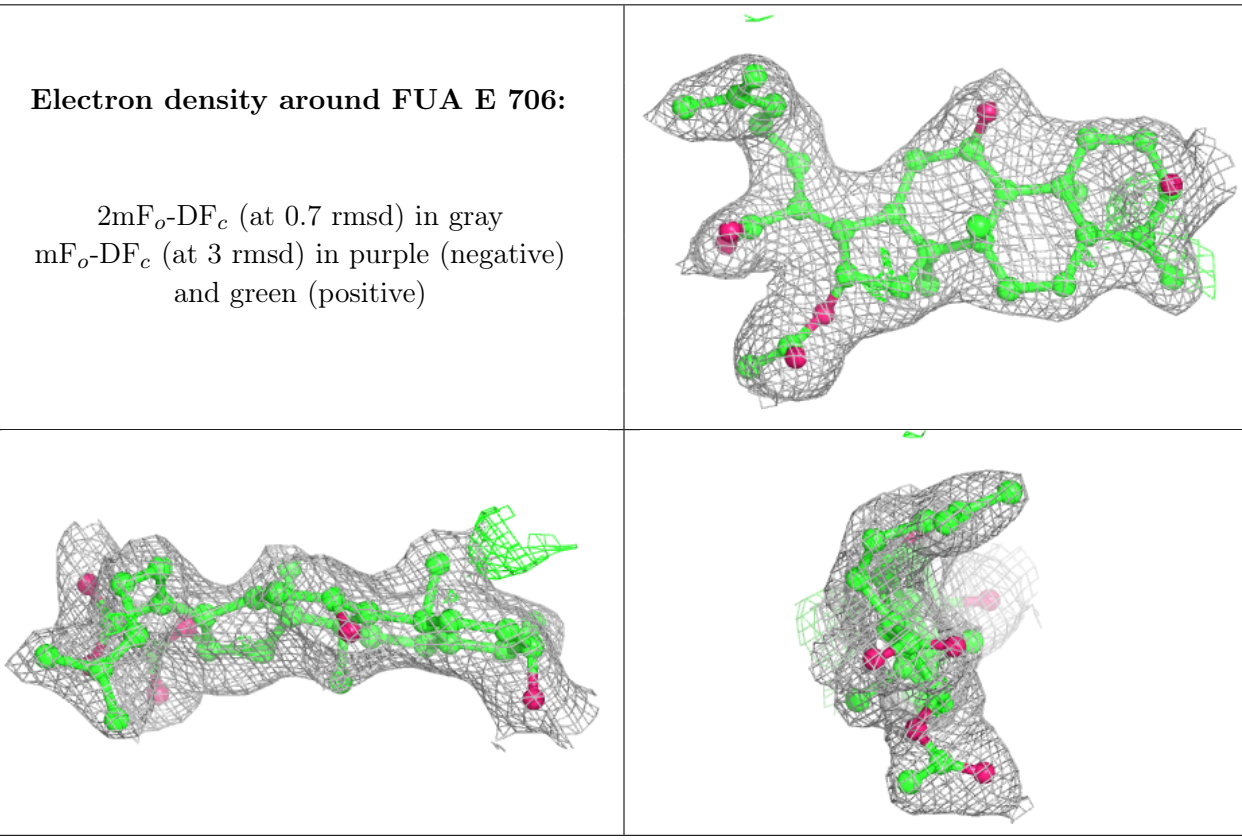
Electron density around FUA D 705:

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



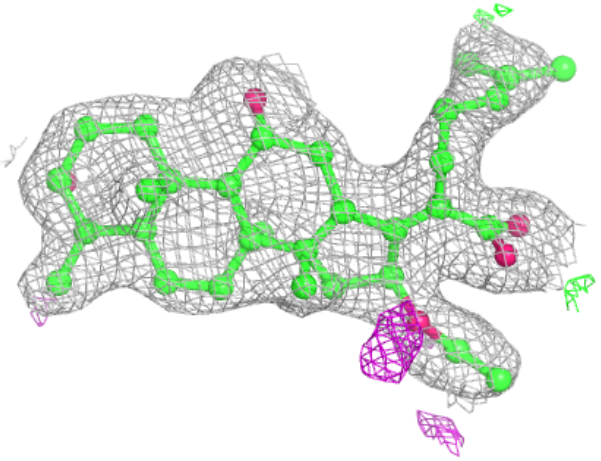
Electron density around FUA E 706:

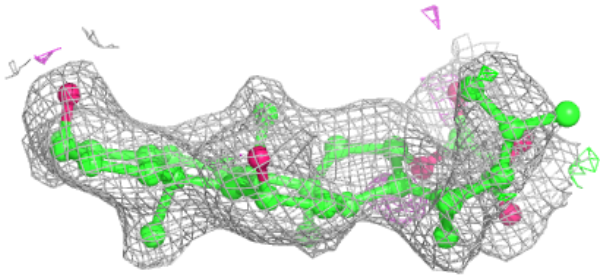
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

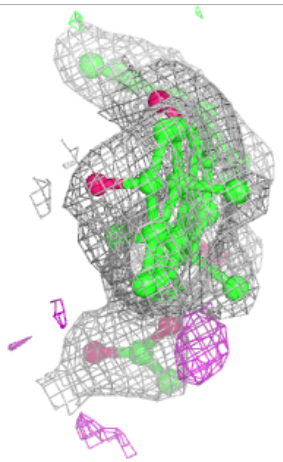


Electron density around FUA C 701:

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

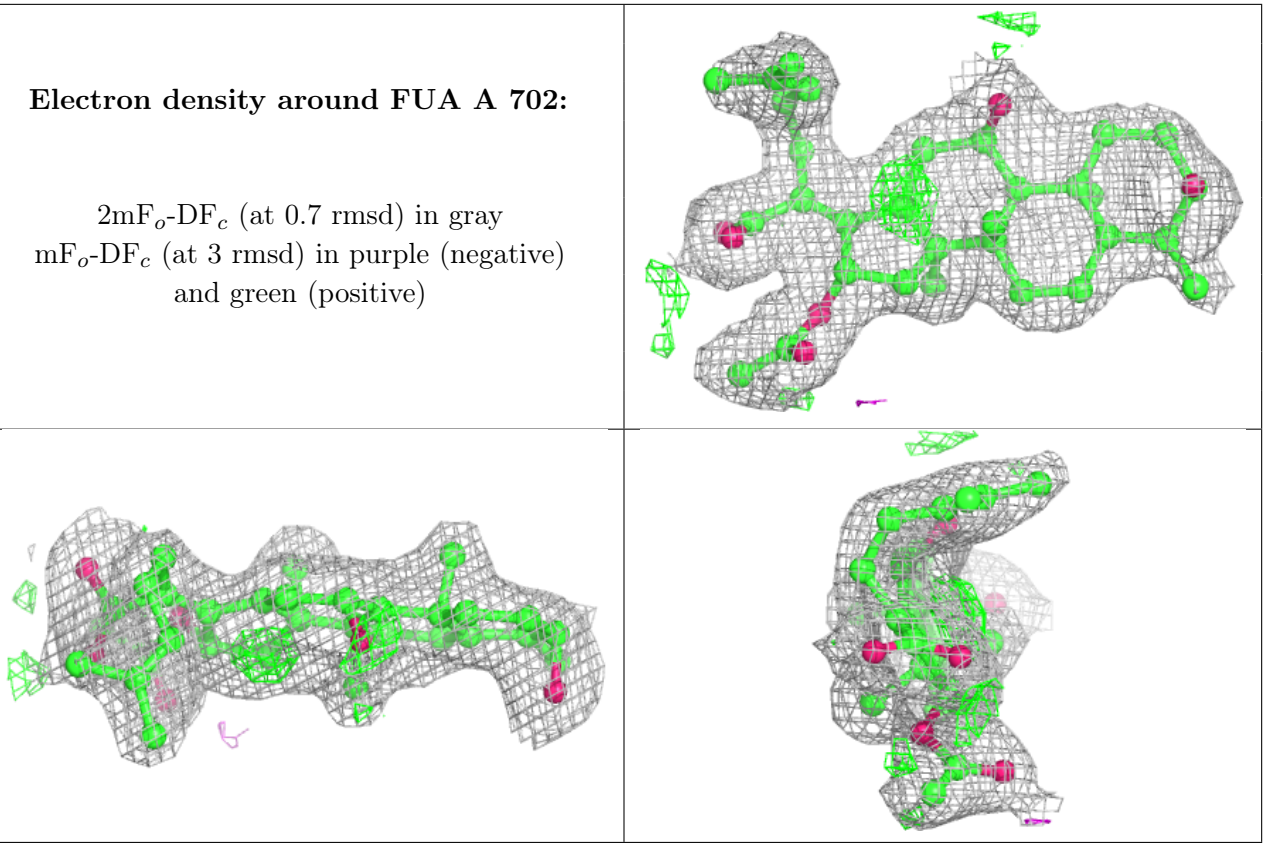






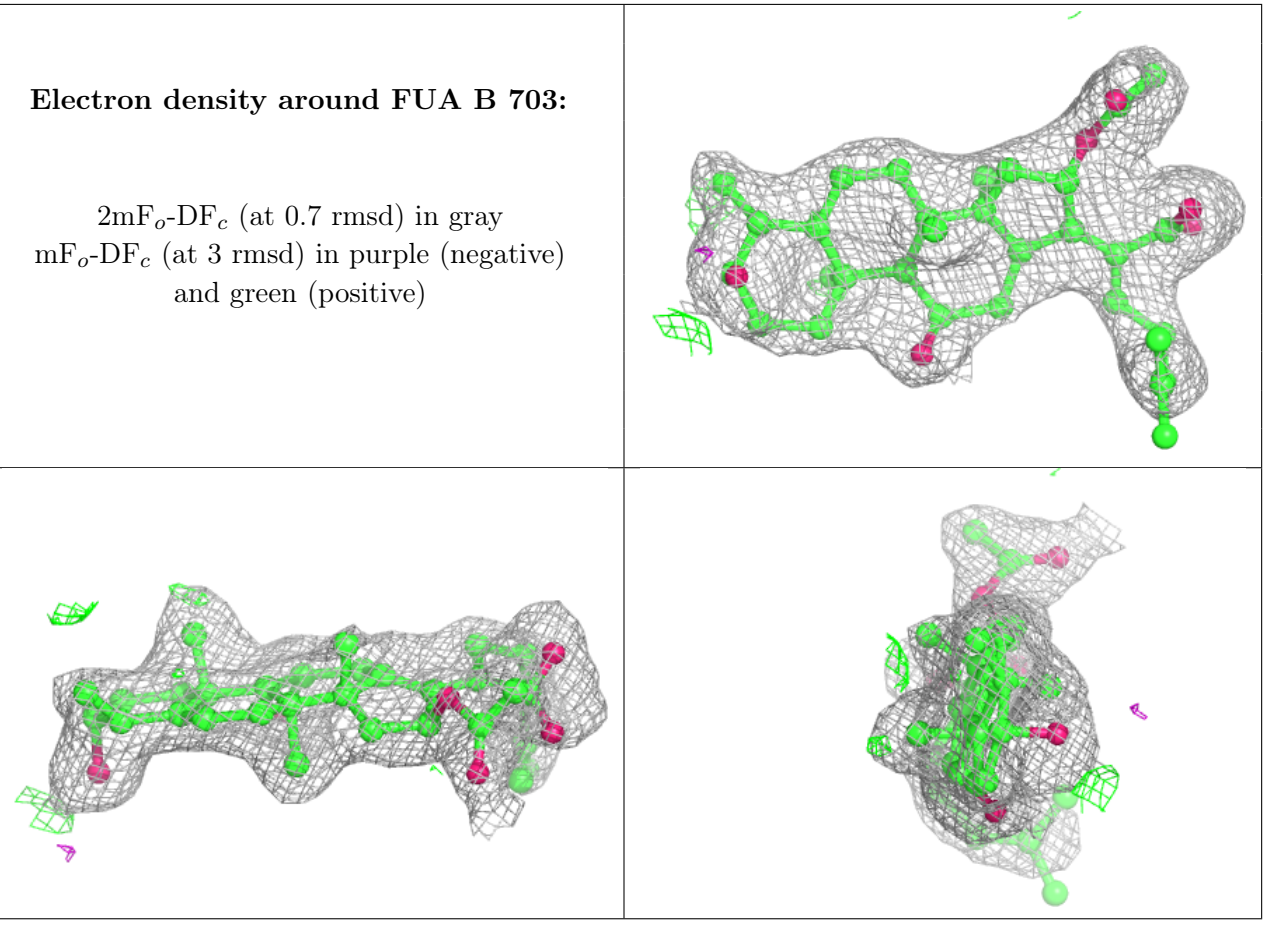
Electron density around FUA A 702:

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



Electron density around FUA B 703:

$2mF_o$-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.