W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 05:10 pm GMT

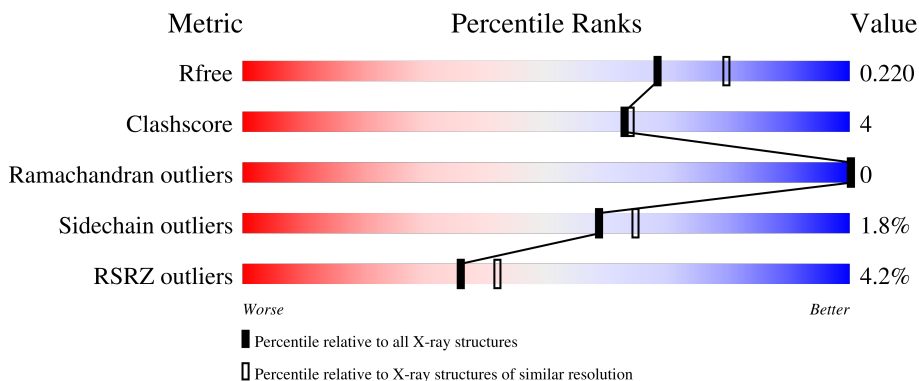|		
PDB ID	:	4BEM
Title	:	Crystal structure of the F-type ATP synthase c-ring from Acetobacterium woodii.
Authors	:	Matthies, D.; Meier, T.; Yildiz, O.
Deposited on	:	2013-03-11
Resolution	:	2.10 Å(reported)

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	Percentile Ranks	Value
Rfree		0.220
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.8%
RSRZ outliers		4.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	82	10% / 93% 7%
1	B	82	7% / 89% 10% ·
1	C	82	7% / 90% 7% ··
1	D	82	5% / 90% 9% ·
1	E	82	4% / 95% ··

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Mol	Chain	Length	Quality of chain
1	F	82	2% 94% 5%
1	G	82	5% 94% 6%
1	H	82	2% 91% 7%
1	I	82	91% 9%
2	J	182	2% 90% 10%

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
4	HTG	B	1084	-	-	-	X
4	HTG	E	1084	-	-	-	X
4	HTG	G	1084	-	-	-	X
4	HTG	G	1086	-	-	-	X
4	HTG	H	1083	-	-	-	X
4	HTG	H	1084	-	-	-	X
4	HTG	I	1086	-	-	-	X
4	HTG	I	1087	-	-	-	X
4	HTG	I	1088	-	-	-	X
4	HTG	J	1187	-	-	-	X
7	P6G	E	1083	-	-	-	X
8	ACT	G	1083	-	-	-	X

2 Entity composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 7053 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 F1FO ATPASE C2 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	S	0	0	0
			576	372	94	106	4			
1	B	82	Total	C	N	O	S	0	0	0
			576	372	94	106	4			
1	C	82	Total	C	N	O	S	0	0	0
			576	372	94	106	4			
1	D	82	Total	C	N	O	S	0	0	0
			576	372	94	106	4			
1	E	82	Total	C	N	O	S	0	0	0
			576	372	94	106	4			
1	F	82	Total	C	N	O	S	0	0	0
			576	372	94	106	4			
1	G	82	Total	C	N	O	S	0	0	0
			576	372	94	106	4			
1	H	82	Total	C	N	O	S	0	0	0
			576	372	94	106	4			
1	I	82	Total	C	N	O	S	0	0	0
			576	372	94	106	4			

- Molecule 2 is a protein called F1FO ATPASE C1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	182	Total	C	N	O	S	0	0	0
			1290	840	206	234	10			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	H	1	Total 1	Na 1	0	0
3	I	1	Total 1	Na 1	0	0
3	J	1	Total 1	Na 1	0	0

- Molecule 4 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).
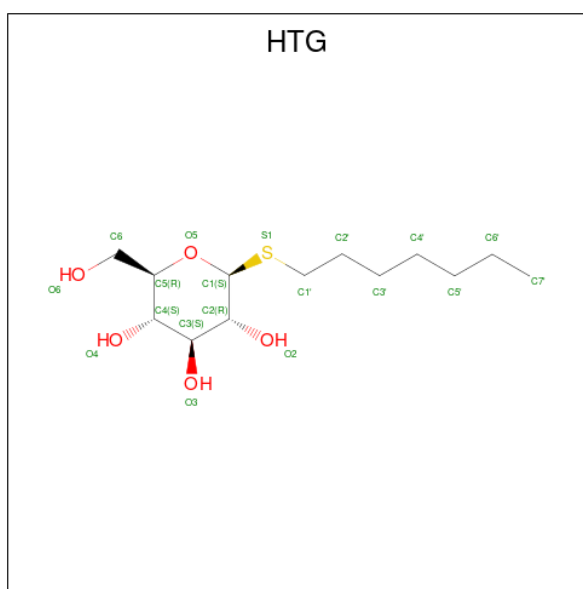
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 19	C 13	O 5	S 1	0	0
4	E	1	Total 19	C 13	O 5	S 1	0	0
4	E	1	Total 19	C 13	O 5	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	O	S	0	0
			19	13	5	1		
4	G	1	Total	C	O	S	0	0
			19	13	5	1		
4	G	1	Total	C	O	S	0	0
			19	13	5	1		
4	G	1	Total	C	O	S	0	0
			19	13	5	1		
4	H	1	Total	C	O	S	0	0
			19	13	5	1		
4	H	1	Total	C	O	S	0	0
			19	13	5	1		
4	I	1	Total	C	O	S	0	0
			19	13	5	1		
4	I	1	Total	C	O	S	0	0
			19	13	5	1		
4	I	1	Total	C	O	S	0	0
			19	13	5	1		
4	I	1	Total	C	O	S	0	0
			19	13	5	1		
4	J	1	Total	C	O	S	0	0
			19	13	5	1		
4	J	1	Total	C	O	S	0	0
			19	13	5	1		
4	J	1	Total	C	O	S	0	0
			19	13	5	1		
4	J	1	Total	C	O	S	0	0
			19	13	5	1		
4	J	1	Total	C	O	S	0	0
			19	13	5	1		
4	J	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mn	0	0
			1	1		

- Molecule 6 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).
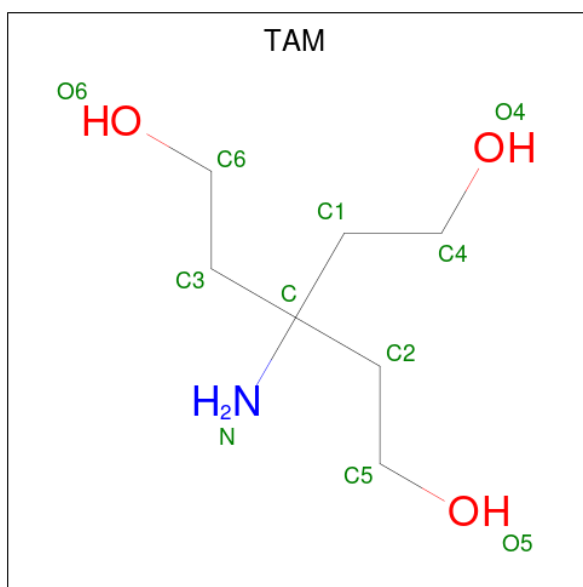
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	11	7	1	3	0	0

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).
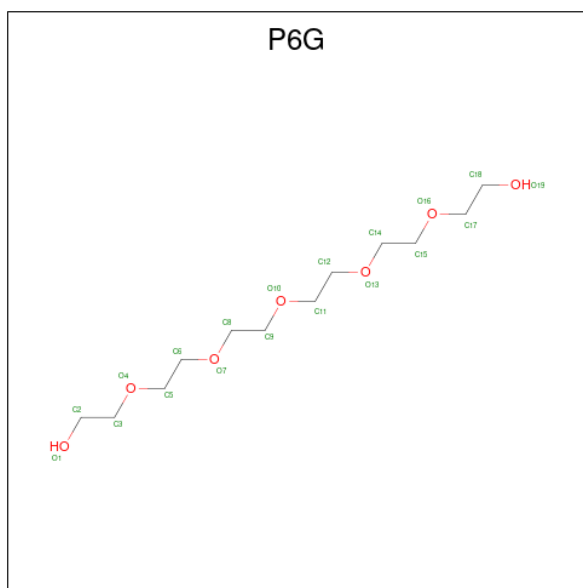
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	E	1	16	10	6	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O⁻

C

CH3

O

O

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total 4	C 2	O 2	0	0
8	G	1	Total 4	C 2	O 2	0	0
8	I	1	Total 4	C 2	O 2	0	0
8	I	1	Total 4	C 2	O 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	20	Total 20	O 20	0	0
9	B	12	Total 12	O 12	0	0
9	C	10	Total 10	O 10	0	0
9	D	12	Total 12	O 12	0	0
9	E	14	Total 14	O 14	0	0
9	F	12	Total 12	O 12	0	0
9	G	16	Total 16	O 16	0	0
9	H	20	Total 20	O 20	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	I	14	Total 14	O 14	0	0
9	J	34	Total 34	O 34	0	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: F1FO ATPASE C2 SUBUNIT
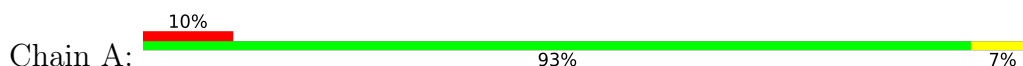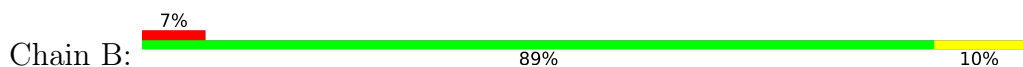
Chain A:

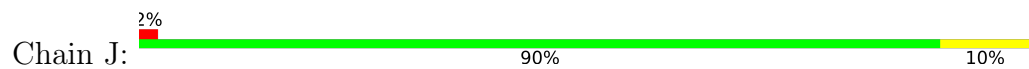
- Molecule 1: F1FO ATPASE C2 SUBUNIT

Chain B:

- Molecule 1: F1FO ATPASE C2 SUBUNIT

Chain C:

- Molecule 1: F1FO ATPASE C2 SUBUNIT

Chain D:

- Molecule 1: F1FO ATPASE C2 SUBUNIT

Chain E:

- Molecule 1: F1FO ATPASE C2 SUBUNIT

Chain F:

2%

94%　　5%

M1 E2 G3 L4 I20 Q43 L75 F82

• Molecule 1: F1FO ATPASE C2 SUBUNIT

Chain G:

5%

94%　　6%

M1 E2 G3 C10 I20 V23 G24 F31 E45 F82

• Molecule 1: F1FO ATPASE C2 SUBUNIT

Chain H:

2%

91%　　7%

M1 E2 G3 L4 D5 A9 I17 V23 F31 E45 A78 F82

• Molecule 1: F1FO ATPASE C2 SUBUNIT

Chain I:

91%　　9%

M1 L4 D5 F31 R42 I70 A78 F82
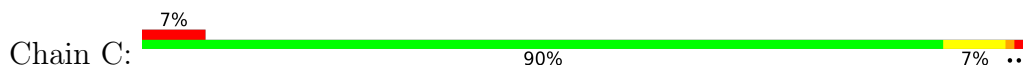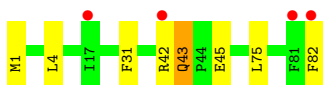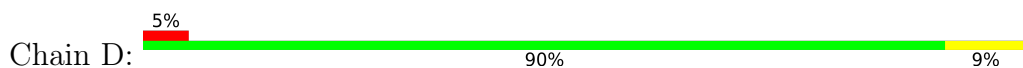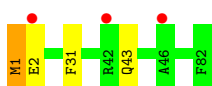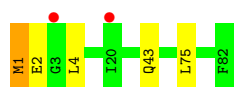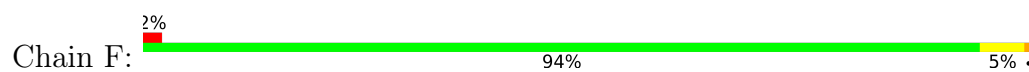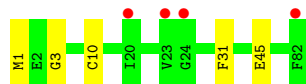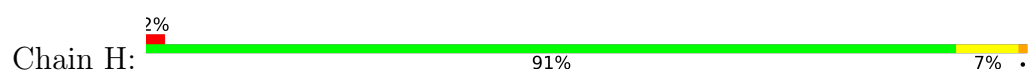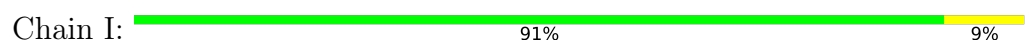
• Molecule 2: F1FO ATPASE C1 SUBUNIT

Chain J:

2%

90%　　10%

M1 M5 D9 F10 F18 F48 K59 N60 K63 V68 M69 L73 V87 T102 G124 R143 P144 V153 Y177 A178 N179 P180 F181 L182
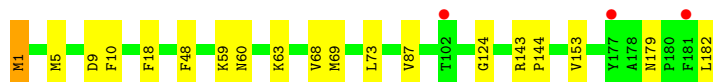
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.17Å 121.17Å 150.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 2.10 47.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.20-2.10) 99.3 (47.20-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.182 , 0.220 0.187 , 0.220	Depositor DCC
R_{free} test set	3270 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 73.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7053	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, P6G, FME, TAM, NA, ACT, HTG

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	0.36	0/574	0.48	0/774
1	B	0.34	0/574	0.45	0/774
1	C	0.34	0/574	0.51	1/774 (0.1%)
1	D	0.31	0/574	0.46	0/774
1	E	0.34	0/574	0.48	0/774
1	F	0.36	0/574	0.48	0/774
1	G	0.38	0/574	0.49	0/774
1	H	0.40	0/574	0.49	0/774
1	I	0.39	0/574	0.46	0/774
2	J	0.38	0/1300	0.46	0/1761
All	All	0.36	0/6466	0.47	1/8727 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4	LEU	CA-CB-CG	5.46	127.87	115.30

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	576	0	592	5	0
1	B	576	0	592	9	0
1	C	576	0	592	6	0
1	D	576	0	592	10	0
1	E	576	0	592	5	0
1	F	576	0	592	4	0
1	G	576	0	592	4	0
1	H	576	0	592	6	0
1	I	576	0	592	4	0
2	J	1290	0	1353	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	B	19	0	26	0	0
4	E	38	0	52	0	0
4	F	19	0	26	0	0
4	G	57	0	78	2	0
4	H	38	0	52	4	0
4	I	76	0	104	6	0
4	J	114	0	156	5	0
5	C	1	0	0	0	0
6	C	11	0	17	2	0
7	E	16	0	21	4	0
8	F	4	0	3	0	0
8	G	4	0	3	0	0
8	I	8	0	6	0	0
9	A	20	0	0	0	0
9	B	12	0	0	0	1
9	C	10	0	0	1	0
9	D	12	0	0	3	0
9	E	14	0	0	0	0
9	F	12	0	0	0	0
9	G	16	0	0	0	0
9	H	20	0	0	1	0
9	I	14	0	0	0	0
9	J	34	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7053	0	7225	60	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 60 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:D:43:GLN:HB3	7:E:1083:P6G:H141	1.63	0.79
1:B:43:GLN:NE2	1:B:45:GLU:OE2	2.11	0.79
1:A:40:VAL:HG21	2:J:153:VAL:HG21	1.66	0.76
4:H:1084:HTG:S1	4:I:1085:HTG:O2	2.43	0.75
1:D:45:GLU:OE2	9:D:2006:HOH:O	2.13	0.66

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:2006:HOH:O	9:B:2006:HOH:O[8_555]	2.06	0.14

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	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
1	B	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
1	C	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
1	D	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
1	E	80/82 (98%)	78 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
1	G	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
1	H	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
1	I	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
2	J	180/182 (99%)	175 (97%)	5 (3%)	0	100	100
All	All	900/920 (98%)	885 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	52/52 (100%)	52 (100%)	0	100	100
1	B	52/52 (100%)	52 (100%)	0	100	100
1	C	52/52 (100%)	50 (96%)	2 (4%)	33	34
1	D	52/52 (100%)	50 (96%)	2 (4%)	33	34
1	E	52/52 (100%)	51 (98%)	1 (2%)	57	63
1	F	52/52 (100%)	50 (96%)	2 (4%)	33	34
1	G	52/52 (100%)	52 (100%)	0	100	100
1	H	52/52 (100%)	51 (98%)	1 (2%)	57	63
1	I	52/52 (100%)	50 (96%)	2 (4%)	33	34
2	J	128/128 (100%)	127 (99%)	1 (1%)	81	86
All	All	596/596 (100%)	585 (98%)	11 (2%)	59	65

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	45	GLU
1	I	4	LEU

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Mol	Chain	Res	Type
2	J	69	MET
1	I	42	ARG
1	E	43	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	47	GLN
1	H	47	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	FME	A	1	1	8,9,10	0.71	0	7,9,11	3.65	2 (28%)
1	FME	D	1	1,5	8,9,10	0.68	0	7,9,11	3.82	3 (42%)
1	FME	G	1	1	8,9,10	0.72	0	7,9,11	3.68	2 (28%)
1	FME	H	1	1	8,9,10	0.76	0	7,9,11	4.33	3 (42%)
1	FME	I	1	1	8,9,10	0.67	0	7,9,11	4.05	3 (42%)
1	FME	C	1	1	8,9,10	0.70	0	7,9,11	3.83	3 (42%)
1	FME	E	1	1	8,9,10	0.68	0	7,9,11	3.71	3 (42%)
2	FME	J	1	2	8,9,10	0.76	0	7,9,11	3.16	2 (28%)
1	FME	B	1	1	8,9,10	0.70	0	7,9,11	3.95	3 (42%)
1	FME	F	1	1	8,9,10	0.71	0	7,9,11	3.43	2 (28%)

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
1	FME	A	1	1	-	5/7/9/11	-
1	FME	D	1	1,5	-	2/7/9/11	-
1	FME	G	1	1	-	5/7/9/11	-
1	FME	H	1	1	-	4/7/9/11	-
1	FME	I	1	1	-	2/7/9/11	-
1	FME	C	1	1	-	3/7/9/11	-
1	FME	E	1	1	-	5/7/9/11	-
2	FME	J	1	2	-	4/7/9/11	-
1	FME	B	1	1	-	4/7/9/11	-
1	FME	F	1	1	-	2/7/9/11	-

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	1	FME	CA-N-CN	-10.67	106.41	122.82
1	I	1	FME	CA-N-CN	-10.02	107.41	122.82
1	B	1	FME	CA-N-CN	-9.59	108.08	122.82
1	D	1	FME	CA-N-CN	-9.39	108.38	122.82
1	C	1	FME	CA-N-CN	-9.28	108.55	122.82

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	O-C-CA-CB
1	B	1	FME	O1-CN-N-CA
1	B	1	FME	N-CA-CB-CG
1	B	1	FME	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	1	FME	1	0
2	J	1	FME	1	0
1	B	1	FME	1	0
1	F	1	FME	3	0

5.5　Carbohydrates　ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry　ⓘ

Of 36 ligands modelled in this entry, 11 are monoatomic - leaving 25 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	$\#|Z| > 2$
4	HTG	I	1086	-	19,19,19	1.01	2 (10%)	23,24,24	0.58	0
4	HTG	J	1185	-	19,19,19	1.01	2 (10%)	23,24,24	0.99	2 (8%)
4	HTG	H	1083	-	19,19,19	1.05	2 (10%)	23,24,24	0.67	0
4	HTG	J	1186	-	19,19,19	1.01	2 (10%)	23,24,24	0.68	0
7	P6G	E	1083	-	15,15,18	0.40	0	14,14,17	0.70	0
4	HTG	E	1085	-	19,19,19	1.07	2 (10%)	23,24,24	0.87	1 (4%)
4	HTG	I	1087	-	19,19,19	1.11	2 (10%)	23,24,24	0.70	0
8	ACT	I	1084	-	3,3,3	0.82	0	3,3,3	1.25	0
4	HTG	J	1184	-	19,19,19	1.12	2 (10%)	23,24,24	0.69	0
4	HTG	H	1084	-	19,19,19	1.12	2 (10%)	23,24,24	1.53	3 (13%)
4	HTG	G	1086	-	19,19,19	1.07	2 (10%)	23,24,24	1.51	3 (13%)
8	ACT	I	1083	-	3,3,3	0.78	0	3,3,3	1.28	0
4	HTG	J	1187	-	19,19,19	1.07	2 (10%)	23,24,24	0.52	0
4	HTG	G	1084	-	19,19,19	1.07	2 (10%)	23,24,24	0.58	0
4	HTG	I	1085	-	19,19,19	1.12	2 (10%)	23,24,24	1.12	3 (13%)
4	HTG	E	1084	-	19,19,19	1.09	2 (10%)	23,24,24	1.29	3 (13%)
4	HTG	I	1088	-	19,19,19	1.05	2 (10%)	23,24,24	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	HTG	F	1083	-	19,19,19	1.04	2 (10%)	23,24,24	0.95	0
8	ACT	G	1083	-	3,3,3	0.77	0	3,3,3	1.35	0
4	HTG	J	1188	-	19,19,19	1.04	2 (10%)	23,24,24	0.85	0
4	HTG	G	1085	-	19,19,19	1.07	2 (10%)	23,24,24	1.02	3 (13%)
6	TAM	C	1084	-	7,10,10	0.48	0	9,12,12	0.76	0
8	ACT	F	1084	-	3,3,3	0.76	0	3,3,3	1.28	0
4	HTG	J	1183	-	19,19,19	0.94	2 (10%)	23,24,24	1.44	3 (13%)
4	HTG	B	1084	-	19,19,19	1.06	2 (10%)	23,24,24	0.69	0

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
4	HTG	I	1086	-	-	4/10/30/30	0/1/1/1
4	HTG	J	1185	-	-	4/10/30/30	0/1/1/1
4	HTG	H	1083	-	-	6/10/30/30	0/1/1/1
4	HTG	J	1186	-	-	3/10/30/30	0/1/1/1
7	P6G	E	1083	-	-	7/13/13/16	-
4	HTG	E	1085	-	-	2/10/30/30	0/1/1/1
4	HTG	I	1087	-	-	3/10/30/30	0/1/1/1
4	HTG	J	1184	-	-	3/10/30/30	0/1/1/1
4	HTG	H	1084	-	-	4/10/30/30	0/1/1/1
4	HTG	G	1086	-	-	5/10/30/30	0/1/1/1
4	HTG	J	1187	-	-	1/10/30/30	0/1/1/1
4	HTG	G	1084	-	-	1/10/30/30	0/1/1/1
4	HTG	I	1085	-	-	5/10/30/30	0/1/1/1
4	HTG	E	1084	-	-	5/10/30/30	0/1/1/1
4	HTG	I	1088	-	-	3/10/30/30	0/1/1/1
4	HTG	F	1083	-	-	3/10/30/30	0/1/1/1
4	HTG	J	1188	-	-	7/10/30/30	0/1/1/1
4	HTG	G	1085	-	-	4/10/30/30	0/1/1/1
6	TAM	C	1084	-	-	5/12/12/12	-
4	HTG	J	1183	-	-	6/10/30/30	0/1/1/1
4	HTG	B	1084	-	-	4/10/30/30	0/1/1/1

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1184	HTG	C1'-S1	-4.22	1.76	1.81
4	I	1085	HTG	C1'-S1	-3.99	1.76	1.81
4	I	1087	HTG	C1'-S1	-3.87	1.76	1.81
4	J	1187	HTG	C1'-S1	-3.81	1.76	1.81
4	G	1084	HTG	C1'-S1	-3.79	1.76	1.81

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1086	HTG	O5-C1-C2	5.38	117.09	110.31
4	J	1183	HTG	O5-C1-C2	-4.12	105.13	110.31
4	H	1084	HTG	C1-C2-C3	-4.03	102.63	110.59
4	E	1084	HTG	O5-C1-C2	-3.60	105.79	110.31
4	J	1183	HTG	C3-C4-C5	3.58	116.62	110.24

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1084	HTG	O5-C1-S1-C1'
4	E	1084	HTG	O5-C1-S1-C1'
4	E	1085	HTG	O5-C1-S1-C1'
4	G	1085	HTG	C2'-C1'-S1-C1
4	H	1083	HTG	O5-C1-S1-C1'

There are no ring outliers.

13 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1086	HTG	3	0
4	H	1083	HTG	1	0
4	J	1186	HTG	1	0
7	E	1083	P6G	4	0
4	J	1184	HTG	1	0
4	H	1084	HTG	3	0
4	J	1187	HTG	1	0
4	G	1084	HTG	2	0
4	I	1085	HTG	3	0
4	I	1088	HTG	1	0
4	J	1188	HTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1084	TAM	2	0
4	J	1183	HTG	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 HTG I 1086

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG J 1185

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG H 1083

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG J 1186

Bond lengths

Bond angles

Torsions

Rings

Ligand P6G E 1083

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG E 1085

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG I 1087

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG J 1184

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG H 1084

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG G 1086

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG J 1187

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG G 1084

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG I 1085

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG E 1084

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG I 1088

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG F 1083

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG J 1188

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG G 1085

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG J 1183

Bond lengths

Bond angles

Torsions

Rings

Ligand HTG B 1084

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	81/82 (98%)	0.38	8 (9%)	7	9	35, 52, 74, 106	0
1	B	81/82 (98%)	0.24	6 (7%)	14	18	36, 55, 78, 89	1 (1%)
1	C	81/82 (98%)	0.17	6 (7%)	14	18	36, 56, 82, 103	0
1	D	81/82 (98%)	0.16	4 (4%)	29	35	37, 56, 80, 99	0
1	E	81/82 (98%)	0.11	3 (3%)	41	48	36, 52, 80, 124	0
1	F	81/82 (98%)	0.04	2 (2%)	57	62	34, 47, 70, 87	0
1	G	81/82 (98%)	0.07	4 (4%)	29	35	32, 44, 69, 93	1 (1%)
1	H	81/82 (98%)	-0.11	2 (2%)	57	62	30, 42, 62, 79	0
1	I	81/82 (98%)	-0.21	0	100	100	30, 41, 61, 72	0
2	J	181/182 (99%)	-0.05	3 (1%)	70	74	31, 47, 85, 132	0
All	All	910/920 (98%)	0.07	38 (4%)	36	42	30, 49, 80, 132	2 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	GLU	6.1
1	B	82	PHE	5.6
1	C	4	LEU	5.0
1	D	82	PHE	5.0
2	J	181	PHE	4.7

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

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(Å²)	Q<0.9
1	FME	E	1	10/11	-0.03	0.39	123,135,138,158	0
2	FME	J	1	10/11	0.80	0.15	87,101,110,137	0
1	FME	B	1	10/11	0.81	0.26	72,84,107,164	0
1	FME	A	1	10/11	0.86	0.27	76,107,120,169	0
1	FME	I	1	10/11	0.87	0.17	50,70,78,122	0
1	FME	G	1	10/11	0.89	0.25	80,93,115,120	0
1	FME	F	1	10/11	0.90	0.24	86,91,111,114	0
1	FME	D	1	10/11	0.91	0.16	70,96,107,119	0
1	FME	C	1	10/11	0.91	0.15	73,79,84,84	0
1	FME	H	1	10/11	0.93	0.10	61,68,88,95	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	MN	C	1083	1/1	0.18	0.25	213,213,213,213	0
4	HTG	H	1083	19/19	0.48	0.54	71,135,144,173	0
4	HTG	E	1084	19/19	0.50	0.41	87,144,148,204	0
4	HTG	H	1084	19/19	0.56	0.49	108,133,144,177	0
8	ACT	G	1083	4/4	0.56	0.44	96,100,103,107	0
8	ACT	I	1083	4/4	0.56	0.38	75,85,87,87	0
4	HTG	I	1088	19/19	0.58	0.40	98,116,126,152	0
4	HTG	B	1084	19/19	0.59	0.57	116,159,164,167	0
4	HTG	G	1085	19/19	0.62	0.40	84,132,141,185	0
4	HTG	J	1185	19/19	0.63	0.20	74,131,143,178	0
4	HTG	G	1084	19/19	0.64	0.56	103,140,148,164	0
4	HTG	G	1086	19/19	0.67	0.71	85,128,132,186	0
4	HTG	E	1085	19/19	0.67	0.30	94,124,140,202	0
4	HTG	J	1187	19/19	0.68	0.43	110,121,127,160	0
7	P6G	E	1083	16/19	0.68	0.53	74,105,116,117	0
6	TAM	C	1084	11/11	0.69	0.27	99,103,107,107	0
4	HTG	I	1086	19/19	0.70	0.66	91,131,136,137	0
4	HTG	I	1087	19/19	0.70	0.55	87,130,145,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HTG	J	1188	19/19	0.71	0.30	94,124,134,165	0
8	ACT	I	1084	4/4	0.72	0.26	73,78,80,81	0
4	HTG	J	1186	19/19	0.75	0.34	65,134,138,183	0
4	HTG	F	1083	19/19	0.77	0.35	80,114,128,193	0
8	ACT	F	1084	4/4	0.81	0.17	96,98,100,100	0
4	HTG	I	1085	19/19	0.81	0.37	109,136,143,185	0
4	HTG	J	1183	19/19	0.83	0.42	81,123,128,129	0
4	HTG	J	1184	19/19	0.91	0.21	56,67,82,84	0
3	NA	H	201	1/1	0.94	0.07	38,38,38,38	0
3	NA	F	201	1/1	0.95	0.07	43,43,43,43	0
3	NA	B	201	1/1	0.97	0.05	52,52,52,52	0
3	NA	A	201	1/1	0.97	0.07	45,45,45,45	0
3	NA	G	201	1/1	0.97	0.06	38,38,38,38	0
3	NA	E	201	1/1	0.99	0.03	48,48,48,48	0
3	NA	I	201	1/1	0.99	0.08	39,39,39,39	0
3	NA	C	201	1/1	0.99	0.09	48,48,48,48	0
3	NA	D	201	1/1	0.99	0.05	52,52,52,52	0
3	NA	J	201	1/1	1.00	0.08	38,38,38,38	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.
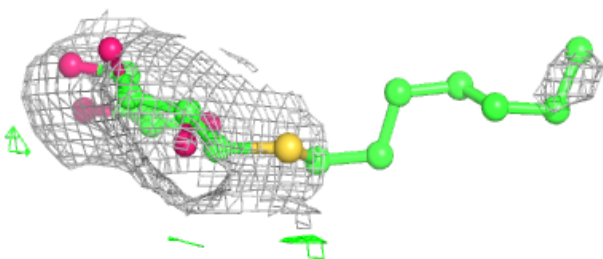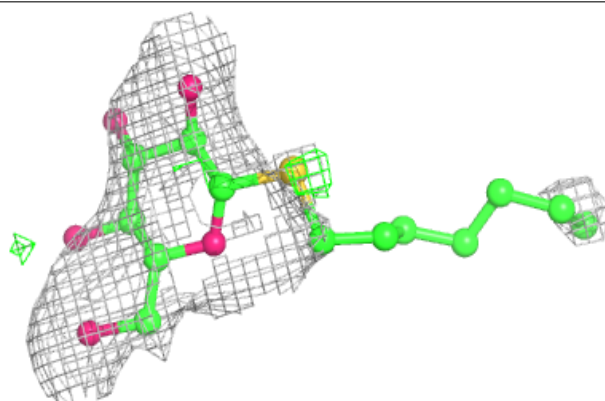
Electron density around HTG H 1083:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
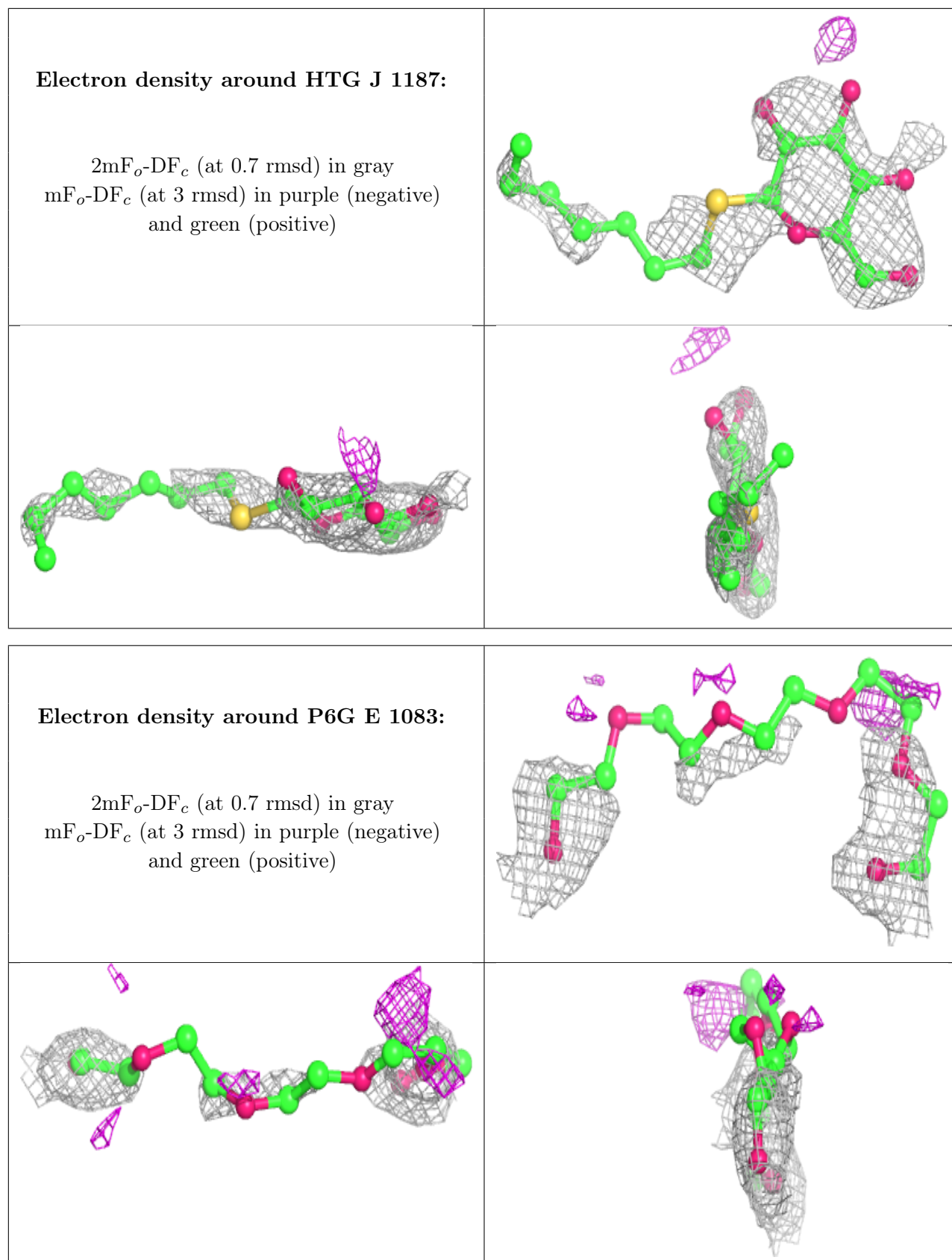mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
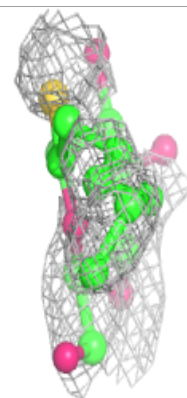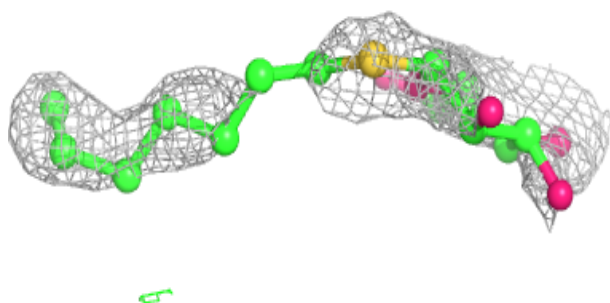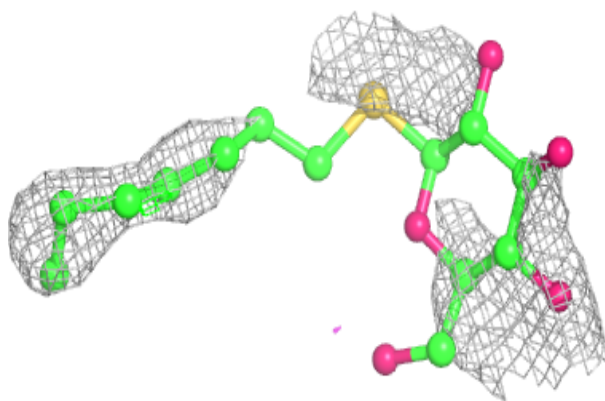
Electron density around HTG E 1084:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
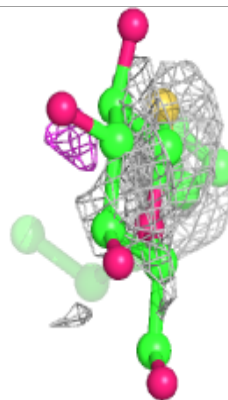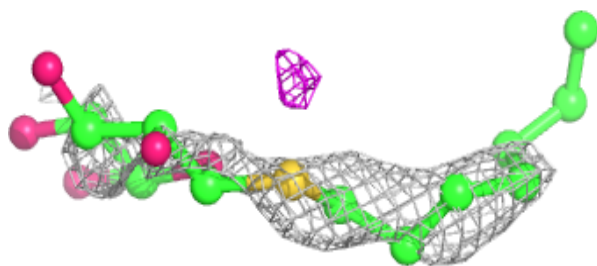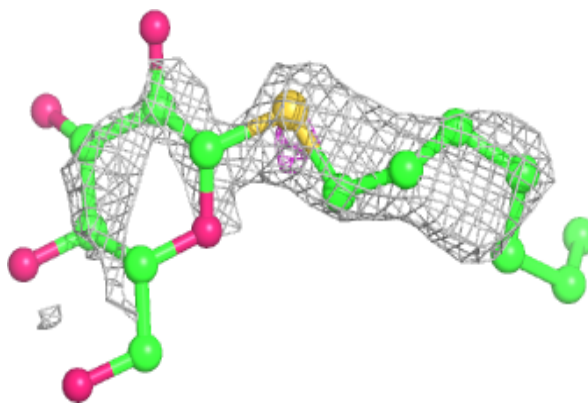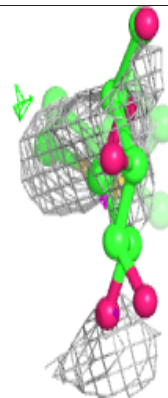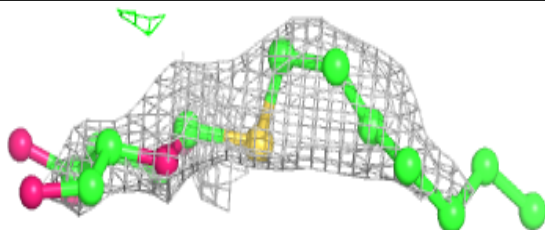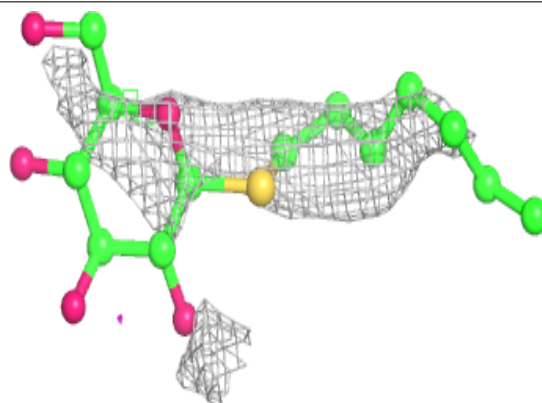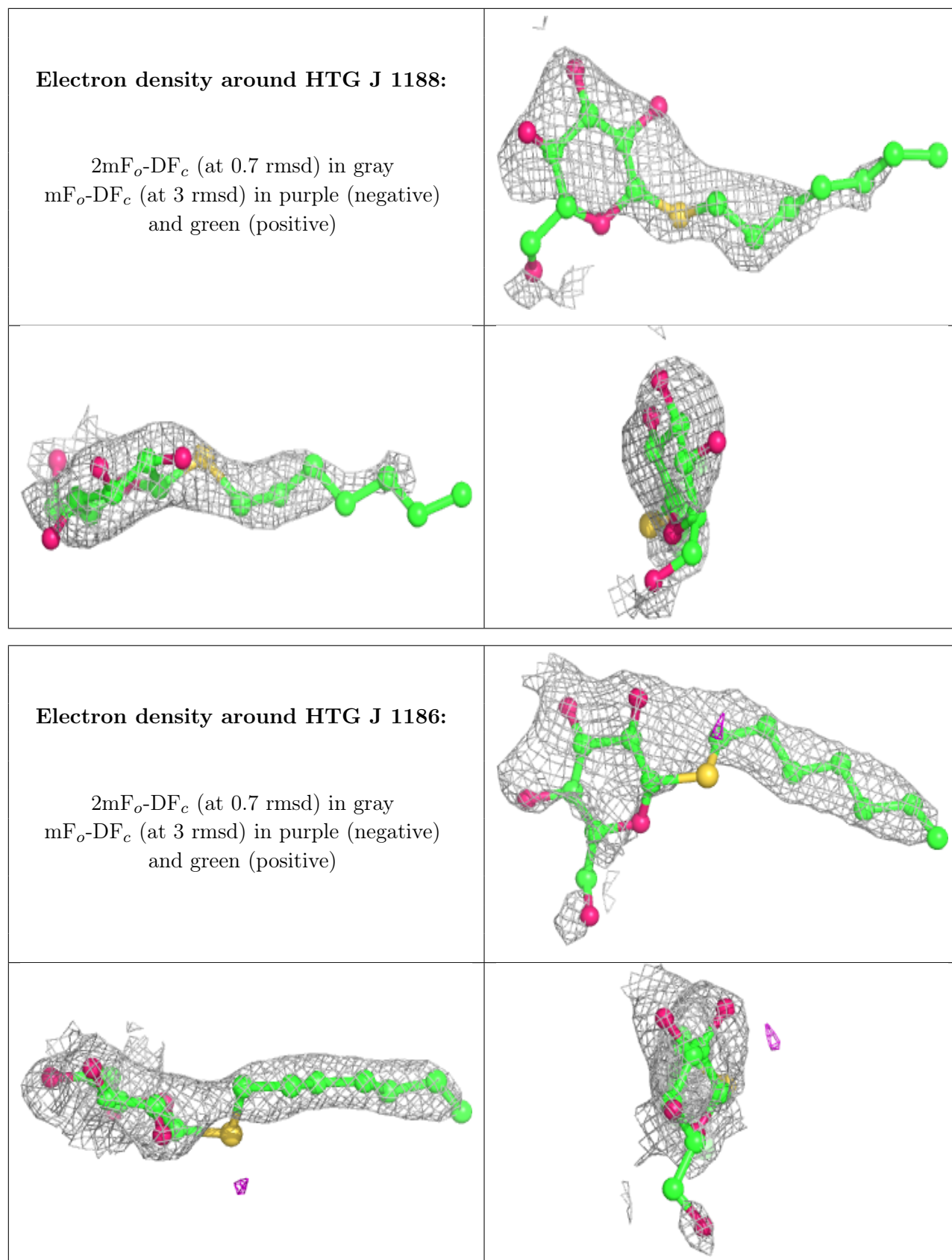mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
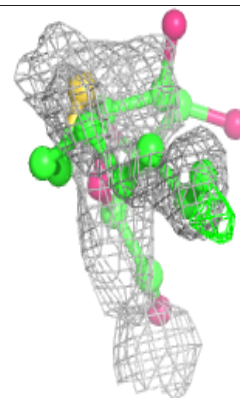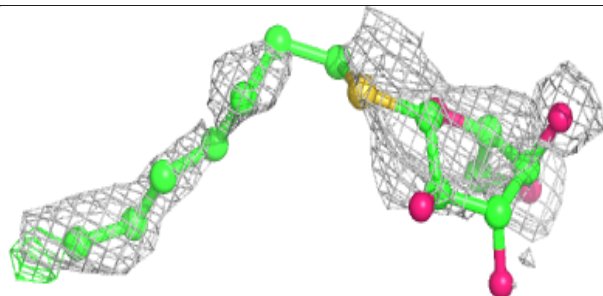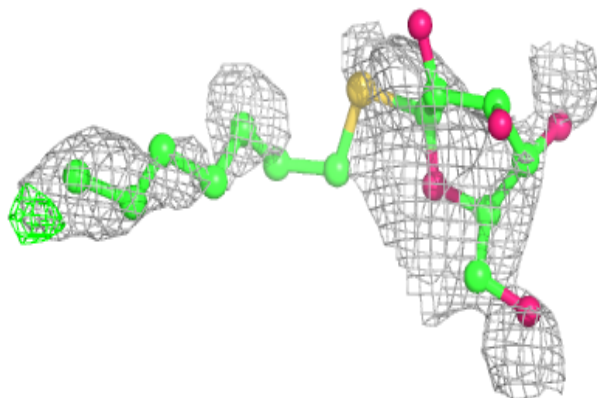
Electron density around HTG H 1084:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
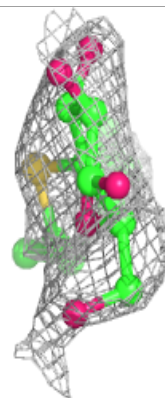and green (positive)
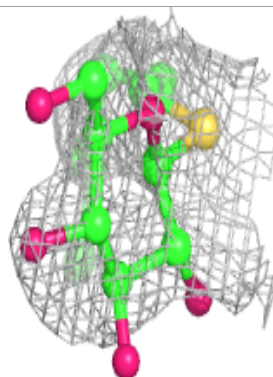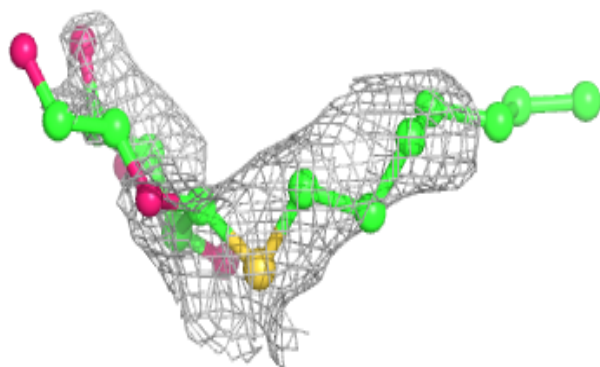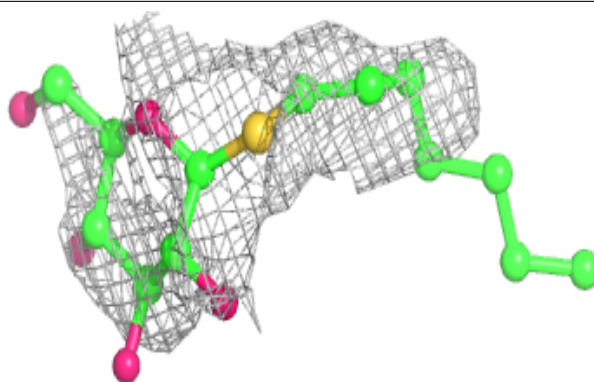
Electron density around HTG I 1088:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
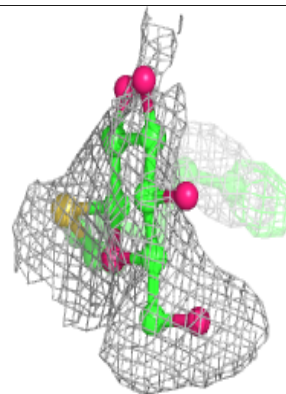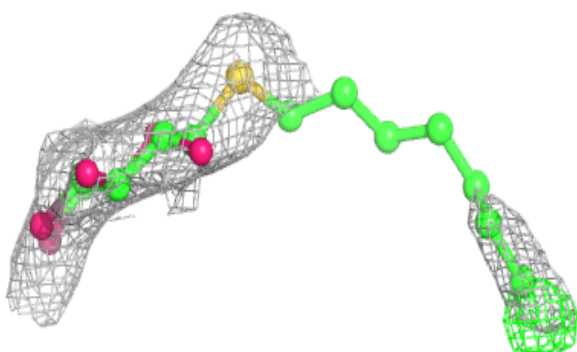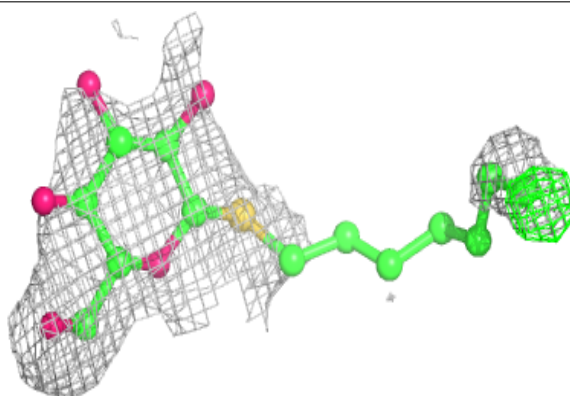
Electron density around HTG B 1084:
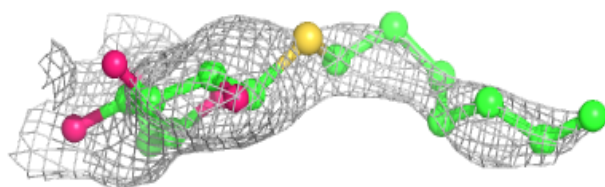
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
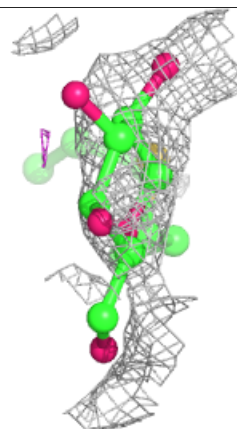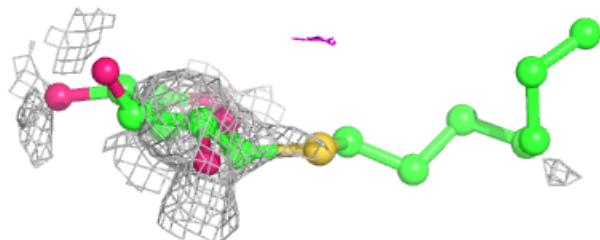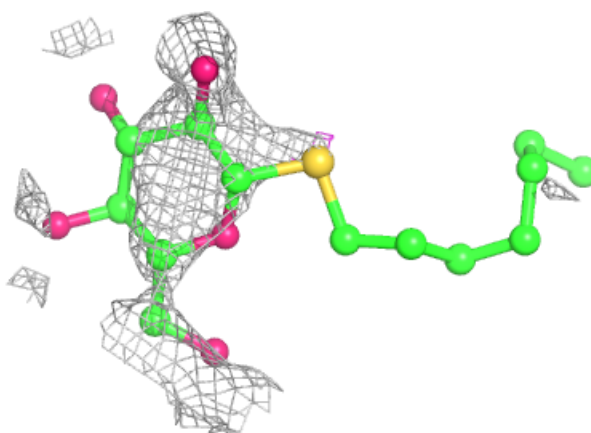
Electron density around HTG G 1085:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
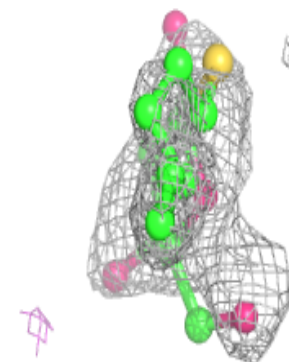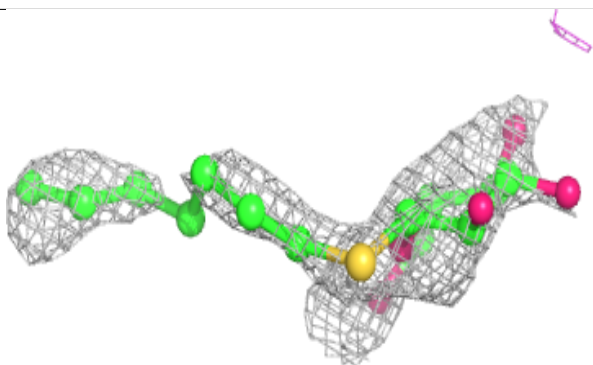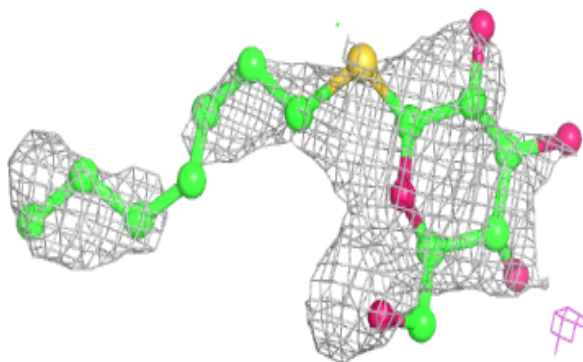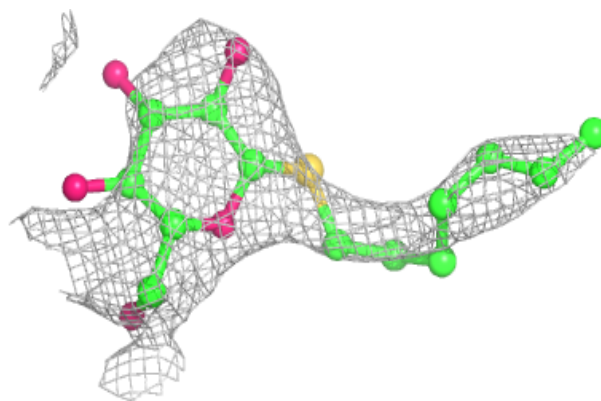
Electron density around HTG J 1185:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
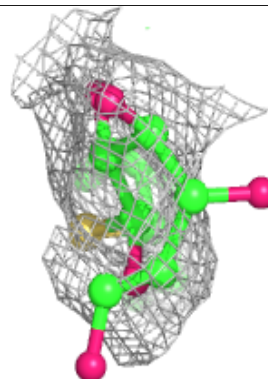and green (positive)
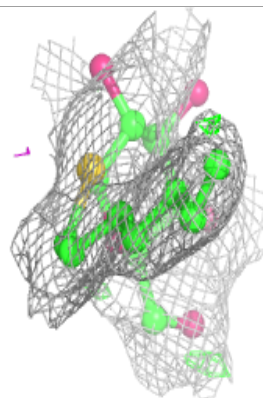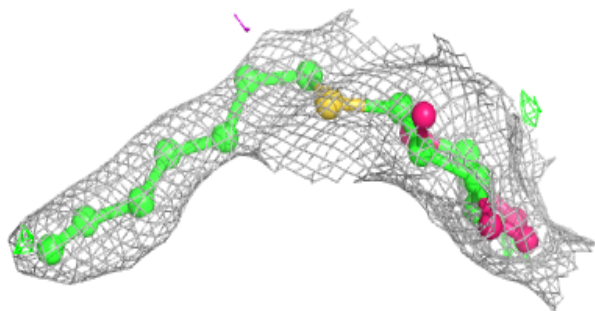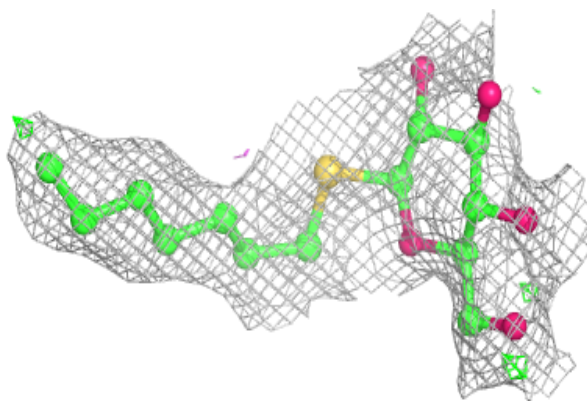
Electron density around HTG G 1084:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
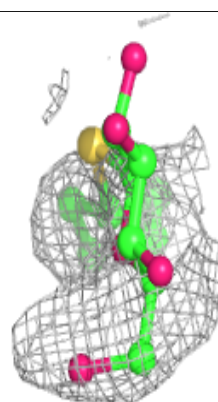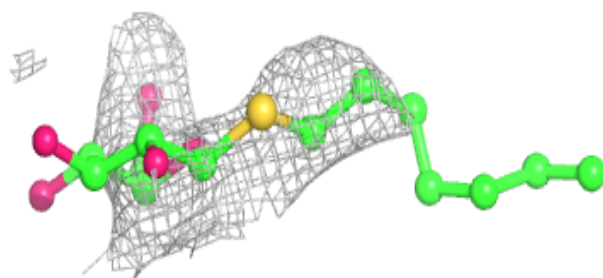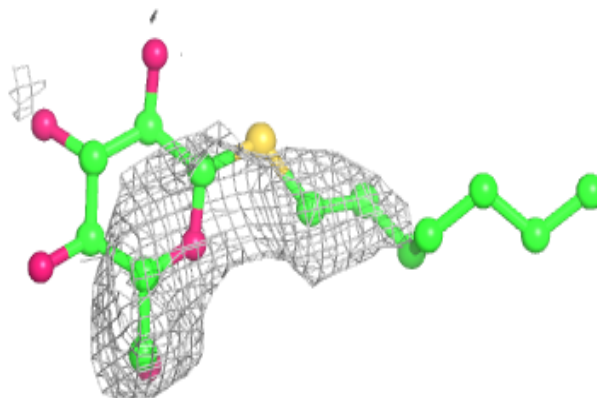
Electron density around HTG G 1086:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
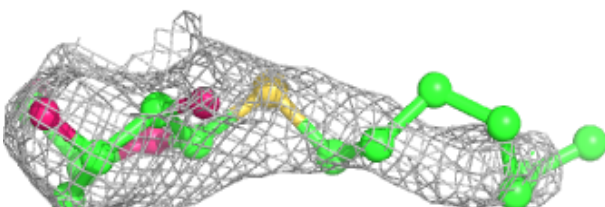and green (positive)
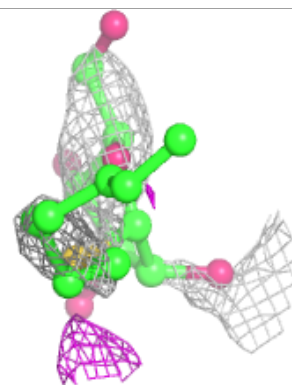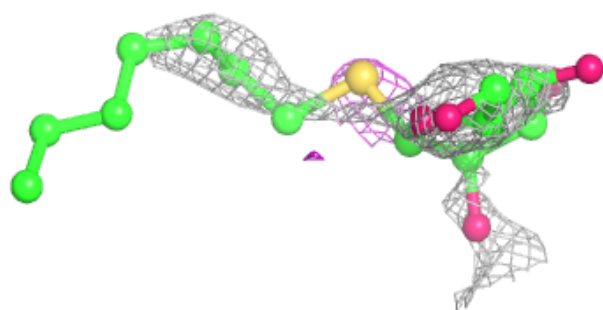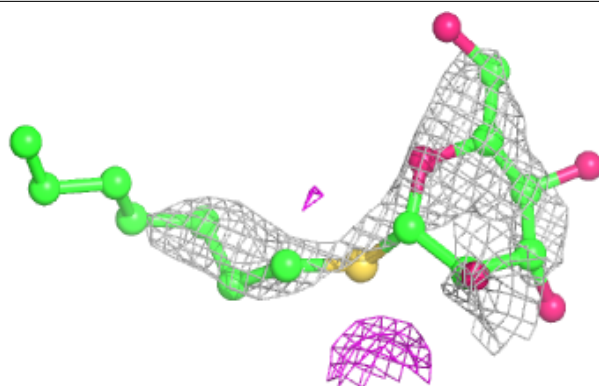
Electron density around HTG E 1085:

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 HTG J 1187:

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

Electron density around P6G E 1083:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
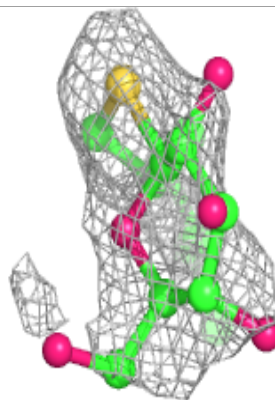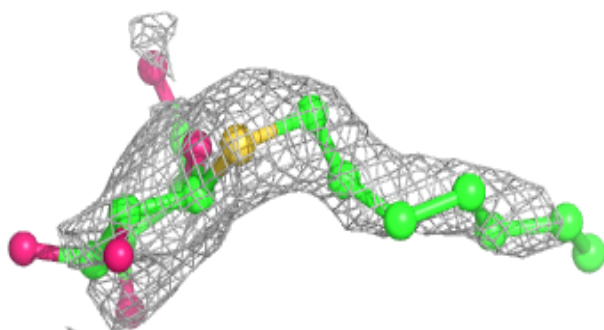$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
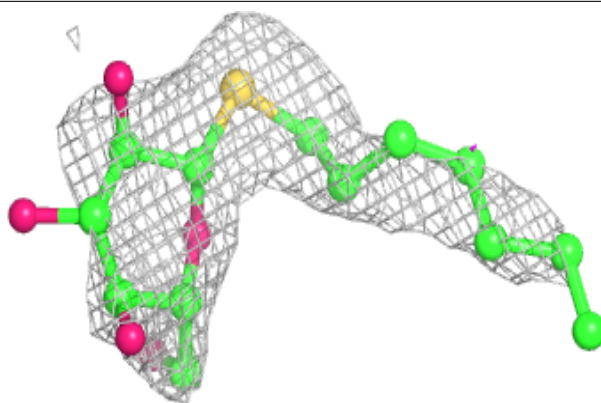and green (positive)
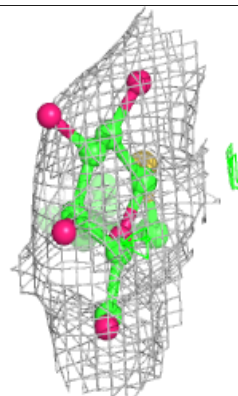
Electron density around HTG I 1086:

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 HTG I 1087:

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 HTG J 1188:

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

Electron density around HTG J 1186:

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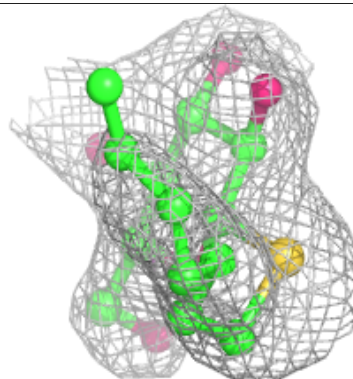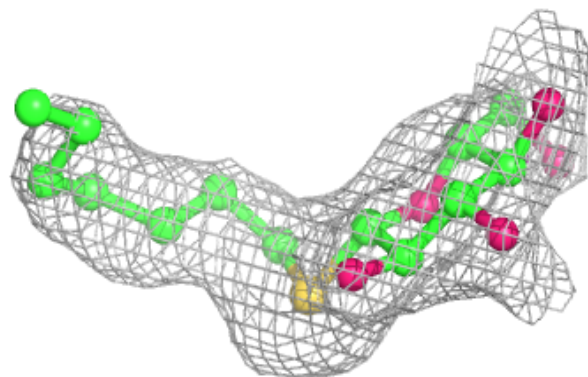$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
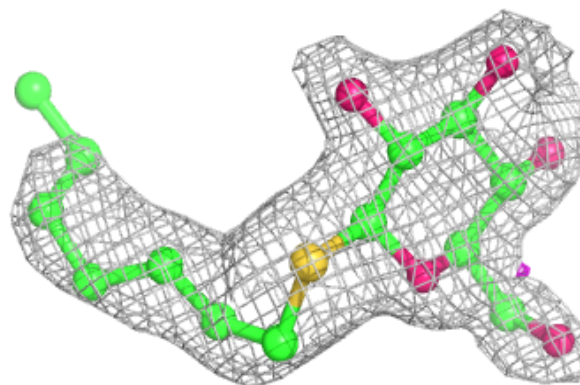and green (positive)

Electron density around HTG F 1083:

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

Electron density around HTG I 1085:

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

Electron density around HTG J 1183:

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

Electron density around HTG J 1184:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.