Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 03:18 am BST

PDB ID	:	6Q9S
Title	:	HDMX (14-111; C17S) COMPLEXED WITH COMPOUND 14 AT 2.4A: Structural states of Hdm2 and HdmX: X-ray elucidation of adaptations and binding interactions for different chemical compound classes
Authors	:	Kallen, J.
Deposited on	:	2018-12-18
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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	:	2.11
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)	:	2.11

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 2.40 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.
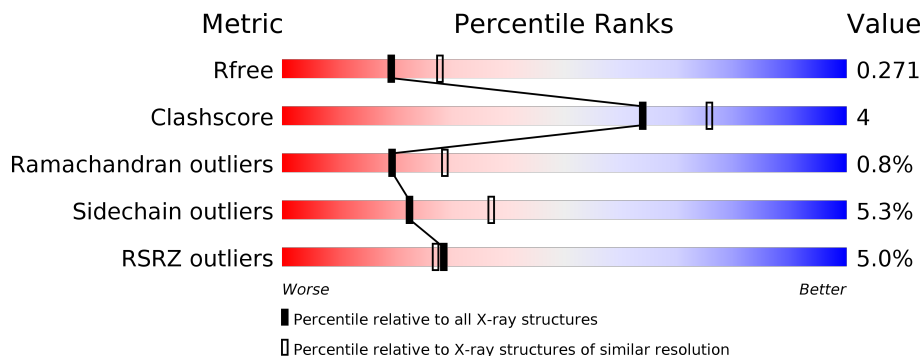
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	100	6% / 74% / 12% · 13%
1	B	100	5% / 71% / 15% / 14%
1	C	100	2% / 78% / 8% · 12%

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	O4B	C	207	-	-	-	X
4	SO4	A	205	-	-	-	X
5	NA	C	211	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2547 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.
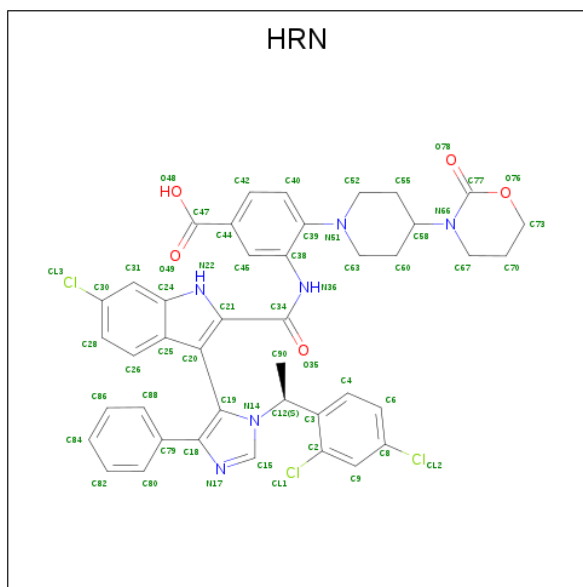
- Molecule 1 is a protein called Protein Mdm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	87	Total 694	C 445	N 119	O 124	S 6	0	0	0
1	C	88	Total 702	C 451	N 120	O 125	S 6	0	0	0
1	B	86	Total 686	C 441	N 117	O 122	S 6	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP O15151
A	14	PRO	-	expression tag	UNP O15151
A	18	SER	CYS	engineered mutation	UNP O15151
C	13	GLY	-	expression tag	UNP O15151
C	14	PRO	-	expression tag	UNP O15151
C	18	SER	CYS	engineered mutation	UNP O15151
B	13	GLY	-	expression tag	UNP O15151
B	14	PRO	-	expression tag	UNP O15151
B	18	SER	CYS	engineered mutation	UNP O15151

- Molecule 2 is 3-[[6-chloranyl-3-[3-[(1 {S})-1-(2,4-dichlorophenyl)ethyl]-5-phenyl-imidazol-4-yl]-1 {H}-indol-2-yl]carbonylamino]-4-[4-(2-oxidanylidene-1,3-oxazinan-3-yl)piperidin-1-yl]benzoic acid (three-letter code: HRN) (formula: $C_{42}H_{37}Cl_3N_6O_5$).
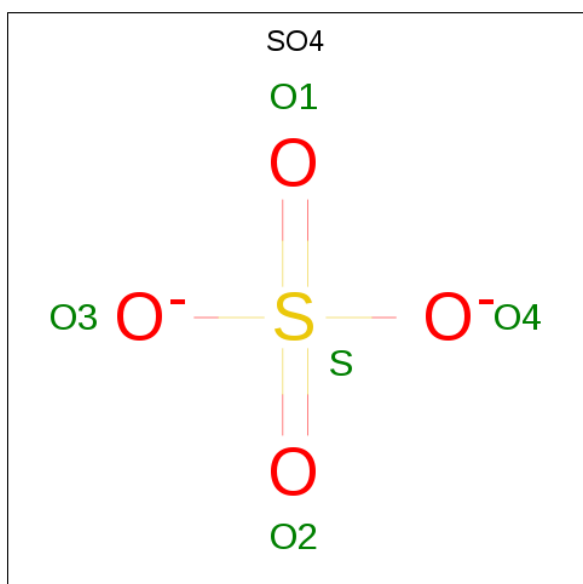
HRN

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			56	42	3	6	5		
2	C	1	Total	C	Cl	N	O	0	0
			56	42	3	6	5		
2	B	1	Total	C	Cl	N	O	0	0
			56	42	3	6	5		

- Molecule 3 is 1,4,7,10,13,16-HEXAOXACYCLOOCTADECANE (three-letter code: O4B) (formula: $C_{12}H_{24}O_6$).

O4B
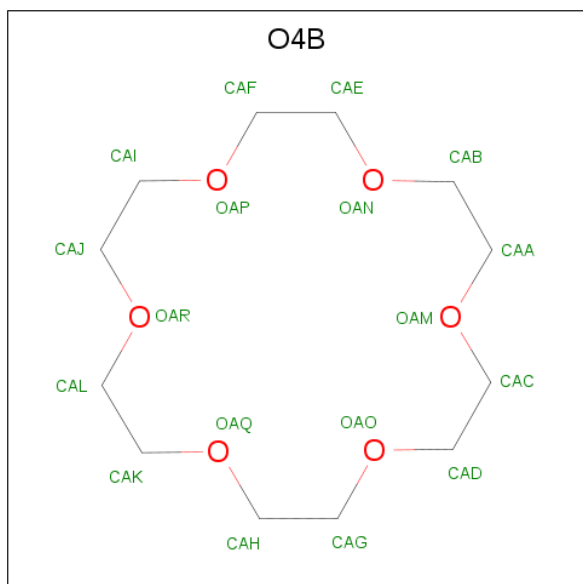
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 18	C 12	O 6	0	0
3	A	1	Total 18	C 12	O 6	0	0
3	A	1	Total 18	C 12	O 6	0	0
3	A	1	Total 18	C 12	O 6	0	0
3	C	1	Total 18	C 12	O 6	0	0
3	C	1	Total 18	C 12	O 6	0	0
3	C	1	Total 18	C 12	O 6	0	0
3	C	1	Total 18	C 12	O 6	0	0
3	C	1	Total 18	C 12	O 6	0	0
3	C	1	Total 18	C 12	O 6	0	0
3	C	1	Total 18	C 12	O 6	0	0
3	B	1	Total 18	C 12	O 6	0	0
3	B	1	Total 18	C 12	O 6	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Na 2	0	0
5	C	1	Total 1	Na 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	O 12	0	0
6	C	13	Total 13	O 13	0	0
6	B	10	Total 10	O 10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Protein Mdm4
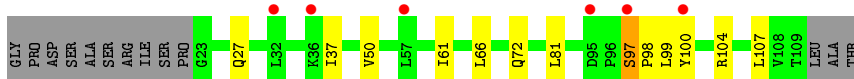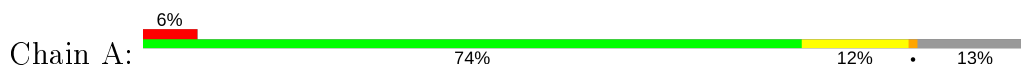
- Molecule 1: Protein Mdm4
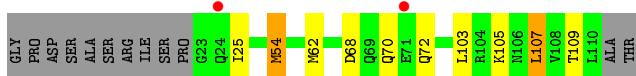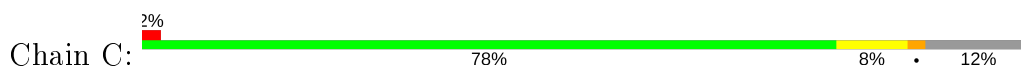
- Molecule 1: Protein Mdm4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.58Å 93.58Å 198.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.95-2.40) 99.9 (19.95-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.71 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.249 , 0.268 0.247 , 0.271	Depositor DCC
R_{free} test set	1043 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.1	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2547	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, O4B, HRN, SO4

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	0.43	0/707	0.56	0/951
1	B	0.46	0/699	0.62	0/941
1	C	0.50	0/715	0.62	0/962
All	All	0.47	0/2121	0.60	0/2854

There are no bond length outliers.

There are no bond angle outliers.

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	694	0	709	6	0
1	B	686	0	703	7	0
1	C	702	0	720	8	0
2	A	56	0	0	0	0
2	B	56	0	0	0	0
2	C	56	0	0	1	0
3	A	72	0	96	0	0
3	B	36	0	48	1	0
3	C	126	0	168	7	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	0	0	0
4	C	10	0	0	0	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
6	A	12	0	0	0	0
6	B	10	0	0	0	0
6	C	13	0	0	0	0
All	All	2547	0	2444	21	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 4.

All (21) 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)
3:C:205:O4B:HAJ2	1:B:84:GLU:HA	1.51	0.92
1:B:97:SER:HB3	1:B:98:PRO:HD3	1.74	0.69
1:C:62:MET:SD	3:C:207:O4B:HAI1	2.33	0.67
1:C:105:LYS:HE2	3:C:205:O4B:HAB1	1.84	0.60
1:A:97:SER:HB2	1:A:98:PRO:HD3	1.86	0.57
1:C:103:LEU:O	1:C:107:LEU:HB2	2.08	0.54
1:A:27:GLN:NE2	1:A:50:VAL:H	2.06	0.54
1:C:105:LYS:HG2	3:C:205:O4B:HAA1	1.90	0.52
1:A:100:TYR:HB3	1:A:104:ARG:NH1	2.24	0.52
1:A:27:GLN:HE21	1:A:50:VAL:H	1.57	0.52
1:C:105:LYS:HD2	3:C:208:O4B:HAB1	1.94	0.49
1:B:74:MET:CE	1:B:90:SER:HB2	2.46	0.45
1:C:25:ILE:H	1:C:25:ILE:HG13	1.67	0.45
1:C:68:ASP:O	1:C:72:GLN:HA	2.17	0.44
1:A:61:ILE:HG23	1:A:66:LEU:HB2	2.00	0.44
1:A:37:ILE:HD11	1:A:81:LEU:HG	2.01	0.42
1:B:30:PRO:HG2	1:B:35:LEU:HD13	2.01	0.42
1:C:54:MET:HG2	2:C:201:HRN:CL1	2.57	0.41
3:C:204:O4B:HAG1	1:B:31:LYS:HZ3	1.86	0.41
3:C:205:O4B:HAJ2	1:B:84:GLU:CA	2.35	0.40
1:B:62:MET:SD	3:B:203:O4B:HAF2	2.61	0.40

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	85/100 (85%)	82 (96%)	2 (2%)	1 (1%)	13	19
1	B	84/100 (84%)	81 (96%)	2 (2%)	1 (1%)	13	19
1	C	86/100 (86%)	82 (95%)	4 (5%)	0	100	100
All	All	255/300 (85%)	245 (96%)	8 (3%)	2 (1%)	19	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	GLN
1	A	97	SER

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	76/86 (88%)	73 (96%)	3 (4%)	32	50
1	B	75/86 (87%)	70 (93%)	5 (7%)	16	26
1	C	77/86 (90%)	73 (95%)	4 (5%)	23	38
All	All	228/258 (88%)	216 (95%)	12 (5%)	22	37

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	107	LEU
1	C	54	MET
1	C	70	GLN
1	C	107	LEU
1	C	109	THR
1	B	65	GLN
1	B	69	GLN
1	B	99	LEU
1	B	102	MET
1	B	107	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	C	69	GLN
1	B	26	ASN
1	B	65	GLN
1	B	69	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	SO4	C	210	-	4,4,4	0.17	0	6,6,6	0.09	0
3	O4B	C	206	5	18,18,18	0.96	0	18,18,18	0.19	0
3	O4B	C	205	-	18,18,18	0.87	0	18,18,18	0.27	0
4	SO4	B	204	-	4,4,4	0.55	0	6,6,6	0.50	0
3	O4B	A	203	-	18,18,18	0.86	0	18,18,18	0.27	0
2	HRN	C	201	-	56,63,63	1.74	8 (14%)	71,92,92	1.77	15 (21%)
3	O4B	C	207	-	18,18,18	0.90	0	18,18,18	0.22	0
3	O4B	C	202	-	18,18,18	0.85	0	18,18,18	0.34	0
3	O4B	C	208	-	18,18,18	0.91	0	18,18,18	0.18	0
3	O4B	C	203	-	18,18,18	0.85	0	18,18,18	0.18	0
4	SO4	A	205	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	205	-	4,4,4	0.14	0	6,6,6	0.16	0
3	O4B	A	204	-	18,18,18	0.87	0	18,18,18	0.23	0
3	O4B	A	202	5	18,18,18	0.88	0	18,18,18	0.21	0
3	O4B	B	203	-	18,18,18	0.84	0	18,18,18	0.25	0
3	O4B	B	202	-	18,18,18	0.78	0	18,18,18	0.34	0
3	O4B	A	208	5	18,18,18	0.92	0	18,18,18	0.42	0
4	SO4	C	209	-	4,4,4	0.14	0	6,6,6	0.08	0
3	O4B	C	204	-	18,18,18	0.88	0	18,18,18	0.17	0
2	HRN	A	201	-	56,63,63	1.70	6 (10%)	71,92,92	1.56	13 (18%)
2	HRN	B	201	-	56,63,63	1.77	8 (14%)	71,92,92	1.78	19 (26%)

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	O4B	C	206	5	-	5/18/18/18	0/1/1/1
2	HRN	C	201	-	-	7/24/57/57	0/8/8/8
3	O4B	C	205	-	-	7/18/18/18	0/1/1/1
3	O4B	A	202	5	-	5/18/18/18	0/1/1/1
3	O4B	C	202	-	-	6/18/18/18	0/1/1/1
3	O4B	C	208	-	-	8/18/18/18	0/1/1/1
3	O4B	C	203	-	-	3/18/18/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	O4B	A	204	-	-	5/18/18/18	0/1/1/1
3	O4B	A	203	-	-	5/18/18/18	0/1/1/1
3	O4B	C	207	-	-	9/18/18/18	0/1/1/1
3	O4B	B	203	-	-	6/18/18/18	0/1/1/1
3	O4B	B	202	-	-	5/18/18/18	0/1/1/1
3	O4B	A	208	5	-	4/18/18/18	0/1/1/1
3	O4B	C	204	-	-	8/18/18/18	0/1/1/1
2	HRN	A	201	-	-	5/24/57/57	0/8/8/8
2	HRN	B	201	-	-	4/24/57/57	0/8/8/8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	HRN	C15-N17	-6.18	1.24	1.35
2	B	201	HRN	C15-N17	-5.97	1.24	1.35
2	B	201	HRN	C44-C47	5.55	1.52	1.47
2	C	201	HRN	C15-N17	-5.50	1.25	1.35
2	C	201	HRN	C44-C47	5.35	1.52	1.47
2	A	201	HRN	C20-C21	-4.73	1.36	1.41
2	B	201	HRN	C20-C21	-4.70	1.36	1.41
2	C	201	HRN	C20-C21	-4.69	1.36	1.41
2	A	201	HRN	C44-C47	4.54	1.51	1.47
2	A	201	HRN	C19-C18	-3.71	1.34	1.43
2	B	201	HRN	C19-C18	-3.42	1.35	1.43
2	C	201	HRN	C19-C18	-3.25	1.35	1.43
2	C	201	HRN	C79-C18	2.53	1.52	1.49
2	A	201	HRN	C31-C30	2.49	1.41	1.36
2	A	201	HRN	C79-C18	2.38	1.51	1.49
2	C	201	HRN	C77-N66	2.28	1.38	1.35
2	B	201	HRN	C31-C30	2.22	1.40	1.36
2	B	201	HRN	C2-C3	2.13	1.42	1.39
2	B	201	HRN	C28-C30	2.13	1.42	1.38
2	C	201	HRN	C3-C12	2.11	1.56	1.53
2	C	201	HRN	C31-C30	2.04	1.40	1.36
2	B	201	HRN	C79-C18	2.02	1.51	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	HRN	C30-C31-C24	-4.82	115.43	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	HRN	O76-C77-N66	4.54	125.00	118.77
2	C	201	HRN	C15-N17-C18	4.06	110.72	102.99
2	B	201	HRN	O76-C77-N66	4.05	124.33	118.77
2	B	201	HRN	C26-C25-C24	3.98	123.45	118.17
2	A	201	HRN	C21-N22-C24	3.96	112.03	103.90
2	C	201	HRN	C21-N22-C24	3.92	111.96	103.90
2	B	201	HRN	C28-C26-C25	-3.87	115.75	121.13
2	B	201	HRN	C15-N17-C18	3.86	110.35	102.99
2	A	201	HRN	C15-N17-C18	3.85	110.32	102.99
2	B	201	HRN	C21-N22-C24	3.82	111.75	103.90
2	C	201	HRN	C28-C26-C25	-3.81	115.84	121.13
2	C	201	HRN	C26-C25-C24	3.59	122.94	118.17
2	B	201	HRN	C30-C31-C24	-3.54	116.51	119.50
2	C	201	HRN	O76-C77-O78	-3.52	113.23	118.64
2	A	201	HRN	C63-N51-C52	3.46	119.15	111.52
2	A	201	HRN	C26-C25-C24	3.43	122.72	118.17
2	C	201	HRN	C60-C58-N66	3.33	116.61	111.85
2	B	201	HRN	C60-C58-N66	3.26	116.50	111.85
2	A	201	HRN	C28-C26-C25	-3.26	116.60	121.13
2	B	201	HRN	C67-C70-C73	-3.20	105.88	111.08
2	A	201	HRN	C30-C31-C24	-3.14	116.85	119.50
2	C	201	HRN	C80-C79-C18	-3.11	115.67	120.61
2	A	201	HRN	O76-C77-N66	3.11	123.04	118.77
2	B	201	HRN	C55-C58-N66	-3.11	107.41	111.85
2	B	201	HRN	O76-C77-O78	-3.06	113.94	118.64
2	C	201	HRN	C88-C79-C18	2.96	125.30	120.61
2	A	201	HRN	C4-C3-C2	2.96	119.76	116.81
2	A	201	HRN	C67-C70-C73	-2.77	106.59	111.08
2	B	201	HRN	C3-C2-CL1	2.70	123.21	120.41
2	B	201	HRN	C80-C79-C18	-2.55	116.57	120.61
2	A	201	HRN	O78-C77-N66	-2.53	121.61	124.54
2	C	201	HRN	C67-C70-C73	-2.50	107.03	111.08
2	C	201	HRN	O35-C34-C21	-2.46	116.91	120.59
2	A	201	HRN	C70-C67-N66	2.46	114.52	110.67
2	B	201	HRN	O78-C77-N66	-2.44	121.72	124.54
2	A	201	HRN	C73-O76-C77	-2.44	115.72	119.33
2	B	201	HRN	O35-C34-C21	-2.44	116.95	120.59
2	B	201	HRN	C73-O76-C77	-2.42	115.76	119.33
2	C	201	HRN	O78-C77-N66	-2.40	121.77	124.54
2	B	201	HRN	C20-C21-C34	-2.38	126.32	130.97
2	B	201	HRN	C26-C28-C30	2.17	121.74	119.21
2	A	201	HRN	O76-C77-O78	-2.14	115.35	118.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	HRN	C63-N51-C52	2.12	116.21	111.52
2	B	201	HRN	C19-N14-C12	-2.08	122.60	126.72
2	B	201	HRN	C88-C79-C18	2.05	123.86	120.61
2	C	201	HRN	C18-C19-N14	2.01	109.19	108.14

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	HRN	C60-C58-N66-C67
2	C	201	HRN	C90-C12-N14-C19
3	C	208	O4B	OAP-CAI-CAJ-OAR
3	C	205	O4B	OAP-CAI-CAJ-OAR
3	C	208	O4B	OAN-CAE-CAF-OAP
3	B	203	O4B	OAO-CAG-CAH-OAQ
3	C	207	O4B	OAO-CAG-CAH-OAQ
3	C	208	O4B	OAM-CAA-CAB-OAN
3	C	207	O4B	OAM-CAC-CAD-OAO
3	C	207	O4B	OAP-CAI-CAJ-OAR
3	C	206	O4B	OAQ-CAK-CAL-OAR
3	C	206	O4B	OAP-CAI-CAJ-OAR
3	C	204	O4B	OAM-CAC-CAD-OAO
3	C	205	O4B	OAO-CAG-CAH-OAQ
3	A	208	O4B	OAO-CAG-CAH-OAQ
3	A	204	O4B	OAO-CAG-CAH-OAQ
3	C	204	O4B	OAP-CAI-CAJ-OAR
3	C	205	O4B	OAN-CAE-CAF-OAP
3	A	208	O4B	OAM-CAA-CAB-OAN
2	A	201	HRN	C40-C39-N51-C63
3	C	202	O4B	OAM-CAC-CAD-OAO
3	C	202	O4B	OAN-CAE-CAF-OAP
2	B	201	HRN	C40-C39-N51-C63
2	C	201	HRN	C40-C39-N51-C63
2	A	201	HRN	C90-C12-N14-C19
2	C	201	HRN	C90-C12-N14-C15
3	A	203	O4B	OAN-CAE-CAF-OAP
3	C	205	O4B	OAM-CAC-CAD-OAO
2	A	201	HRN	C40-C39-N51-C52
3	B	202	O4B	OAQ-CAK-CAL-OAR
3	C	208	O4B	CAL-CAK-OAQ-CAH
3	B	202	O4B	CAB-CAA-OAM-CAC
3	A	204	O4B	CAE-CAF-OAP-CAI

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Mol	Chain	Res	Type	Atoms
3	C	205	O4B	CAD-CAC-OAM-CAA
3	C	208	O4B	OAM-CAC-CAD-OAO
3	C	207	O4B	CAF-CAE-OAN-CAB
2	A	201	HRN	C90-C12-N14-C15
3	C	208	O4B	CAE-CAF-OAP-CAI
3	B	202	O4B	CAK-CAL-OAR-CAJ
3	C	205	O4B	CAB-CAA-OAM-CAC
2	C	201	HRN	C40-C39-N51-C52
3	A	203	O4B	CAF-CAE-OAN-CAB
3	C	207	O4B	CAH-CAG-OAO-CAD
3	A	202	O4B	CAA-CAB-OAN-CAE
3	C	207	O4B	CAB-CAA-OAM-CAC
3	C	204	O4B	CAC-CAD-OAO-CAG
3	B	203	O4B	CAE-CAF-OAP-CAI
3	C	204	O4B	CAF-CAE-OAN-CAB
3	C	206	O4B	CAA-CAB-OAN-CAE
3	C	207	O4B	CAK-CAL-OAR-CAJ
3	C	206	O4B	CAE-CAF-OAP-CAI
3	A	204	O4B	CAI-CAJ-OAR-CAL
3	C	204	O4B	OAO-CAG-CAH-OAQ
2	B	201	HRN	C40-C39-N51-C52
3	A	203	O4B	OAP-CAI-CAJ-OAR
3	A	204	O4B	CAK-CAL-OAR-CAJ
3	C	207	O4B	OAM-CAA-CAB-OAN
3	C	204	O4B	CAL-CAK-OAQ-CAH
2	C	201	HRN	C55-C58-N66-C67
3	C	203	O4B	CAE-CAF-OAP-CAI
3	B	202	O4B	CAE-CAF-OAP-CAI
3	C	205	O4B	CAK-CAL-OAR-CAJ
3	C	202	O4B	OAP-CAI-CAJ-OAR
3	A	204	O4B	CAA-CAB-OAN-CAE
3	A	208	O4B	OAQ-CAK-CAL-OAR
3	A	202	O4B	OAN-CAE-CAF-OAP
3	B	203	O4B	CAC-CAD-OAO-CAG
3	A	202	O4B	CAE-CAF-OAP-CAI
3	A	208	O4B	OAP-CAI-CAJ-OAR
2	B	201	HRN	C90-C12-N14-C15
3	B	203	O4B	CAK-CAL-OAR-CAJ
3	B	203	O4B	OAN-CAE-CAF-OAP
3	C	203	O4B	CAD-CAC-OAM-CAA
2	C	201	HRN	C38-C39-N51-C63
2	A	201	HRN	C38-C39-N51-C63

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Mol	Chain	Res	Type	Atoms
3	A	202	O4B	OAQ-CAK-CAL-OAR
3	C	208	O4B	CAA-CAB-OAN-CAE
3	C	202	O4B	CAA-CAB-OAN-CAE
3	C	204	O4B	CAG-CAH-OAQ-CAK
3	C	208	O4B	CAD-CAC-OAM-CAA
3	A	203	O4B	OAO-CAG-CAH-OAQ
3	C	204	O4B	CAA-CAB-OAN-CAE
3	C	206	O4B	CAI-CAJ-OAR-CAL
3	B	202	O4B	OAM-CAA-CAB-OAN
3	C	202	O4B	CAB-CAA-OAM-CAC
3	A	203	O4B	CAE-CAF-OAP-CAI
3	C	202	O4B	CAK-CAL-OAR-CAJ
3	B	203	O4B	CAB-CAA-OAM-CAC
3	C	203	O4B	CAB-CAA-OAM-CAC
3	A	202	O4B	OAM-CAA-CAB-OAN
3	C	207	O4B	CAE-CAF-OAP-CAI
2	B	201	HRN	C38-C39-N51-C63

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	205	O4B	4	0
2	C	201	HRN	1	0
3	C	207	O4B	1	0
3	C	208	O4B	1	0
3	B	203	O4B	1	0
3	C	204	O4B	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

Full wwPDB X-ray Structure Validation Report

Ligand O4B C 206

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B C 205

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Ligand O4B A 203

Bond lengths

Bond angles

Torsions

Rings

Ligand HRN C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B C 207

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B C 202

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B C 208

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B C 203

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B A 204

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B A 202

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B B 203

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B B 202

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B A 208

Bond lengths

Bond angles

Torsions

Rings

Ligand O4B C 204

Bond lengths

Bond angles

Torsions

Rings

Ligand HRN A 201

Bond lengths

Bond angles

Torsions

Rings

Ligand HRN B 201

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	87/100 (87%)	0.30	6 (6%)	16	15	41, 57, 69, 72	0
1	B	86/100 (86%)	0.09	5 (5%)	23	22	36, 43, 61, 70	0
1	C	88/100 (88%)	0.02	2 (2%)	60	58	36, 44, 60, 64	0
All	All	261/300 (87%)	0.14	13 (4%)	28	27	36, 47, 67, 72	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	24	GLN	3.4
1	B	104	ARG	3.1
1	A	57	LEU	3.0
1	B	70	GLN	2.9
1	B	26	ASN	2.5
1	C	71	GLU	2.5
1	A	100	TYR	2.5
1	B	73	HIS	2.5
1	B	71	GLU	2.4
1	A	97	SER	2.3
1	A	95	ASP	2.1
1	A	36	LYS	2.1
1	A	32	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

Full wwPDB X-ray Structure Validation Report

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	O4B	C	207	18/18	0.38	0.40	76,82,85,86	0
4	SO4	A	205	5/5	0.59	0.66	158,159,159,159	0
3	O4B	B	203	18/18	0.65	0.36	74,77,81,82	0
3	O4B	C	208	18/18	0.65	0.34	72,76,77,78	0
5	NA	A	207	1/1	0.72	0.25	68,68,68,68	0
3	O4B	C	206	18/18	0.73	0.30	81,82,85,85	0
5	NA	C	211	1/1	0.73	0.52	89,89,89,89	0
3	O4B	A	204	18/18	0.73	0.27	66,70,73,74	0
3	O4B	C	204	18/18	0.73	0.27	78,80,81,81	0
5	NA	A	206	1/1	0.83	0.41	73,73,73,73	0
2	HRN	B	201	56/56	0.86	0.18	43,50,60,61	0
2	HRN	C	201	56/56	0.88	0.15	44,57,62,64	0
3	O4B	C	205	18/18	0.89	0.18	68,71,73,74	0
4	SO4	B	205	5/5	0.90	0.24	94,94,94,95	0
3	O4B	A	203	18/18	0.90	0.13	54,58,59,60	0
3	O4B	A	208	18/18	0.91	0.16	43,47,50,51	0
4	SO4	B	204	5/5	0.92	0.16	54,54,55,55	5
4	SO4	C	210	5/5	0.93	0.21	95,95,95,95	0
3	O4B	A	202	18/18	0.93	0.11	53,55,57,57	0
4	SO4	C	209	5/5	0.94	0.14	114,114,114,114	0
3	O4B	C	203	18/18	0.94	0.13	52,56,57,58	0
2	HRN	A	201	56/56	0.94	0.13	36,41,55,63	0
3	O4B	C	202	18/18	0.95	0.11	48,51,54,56	0
3	O4B	B	202	18/18	0.96	0.12	39,43,45,46	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.
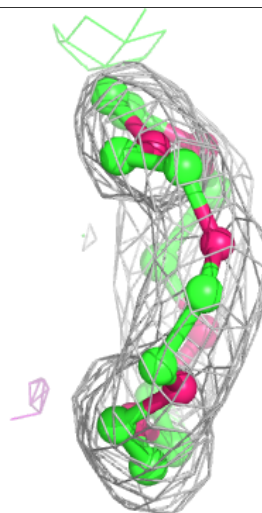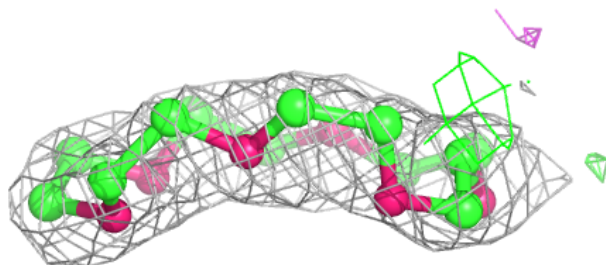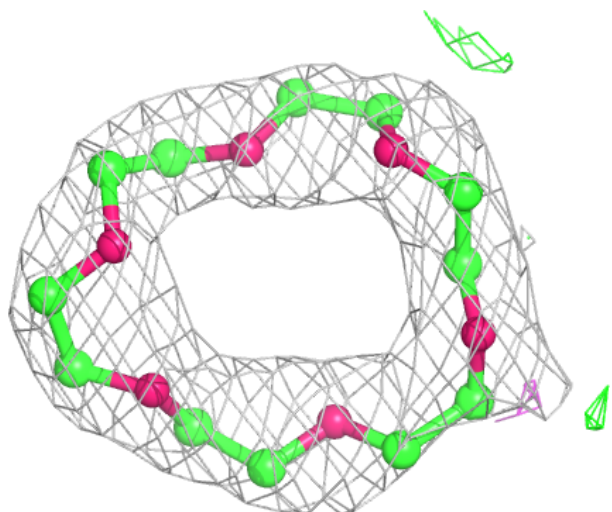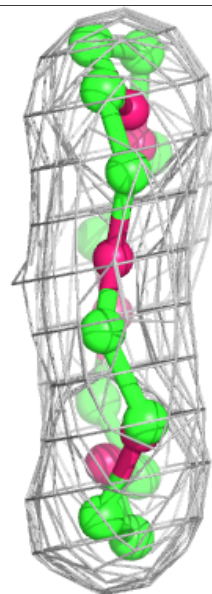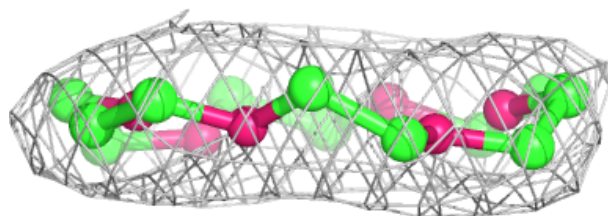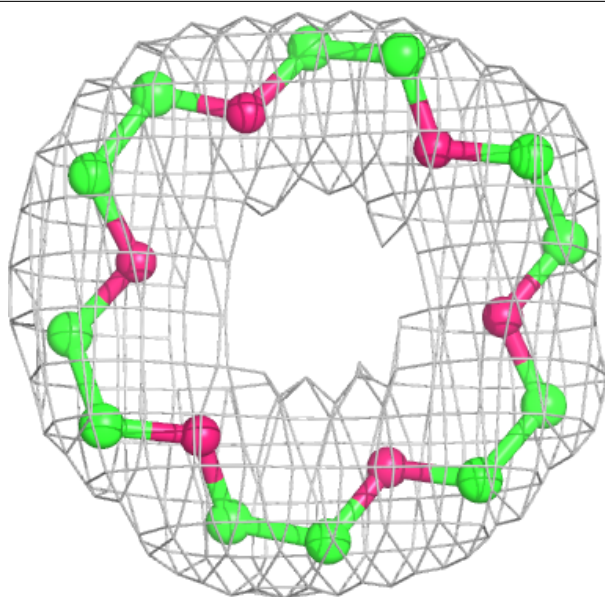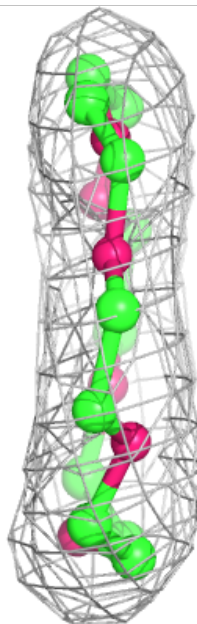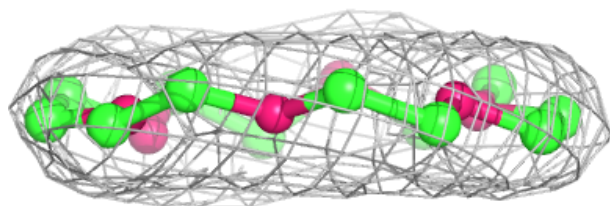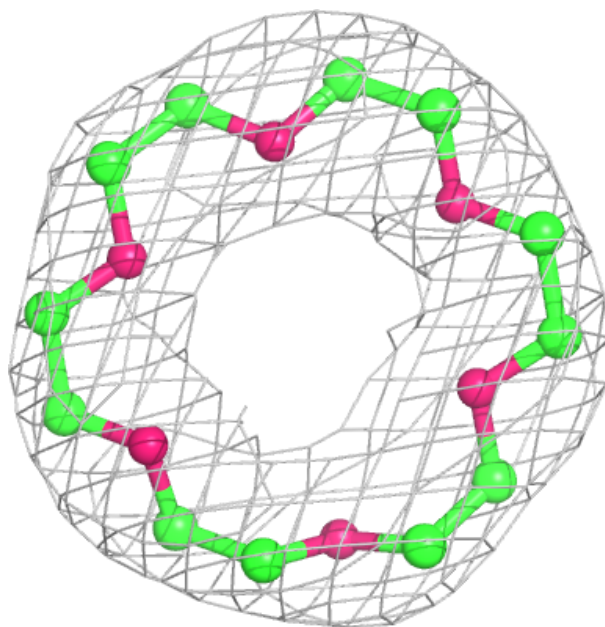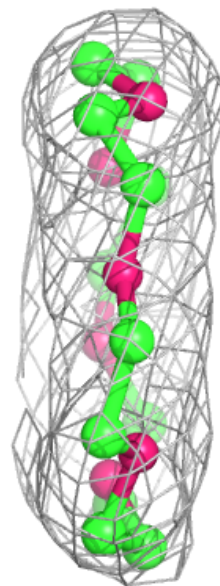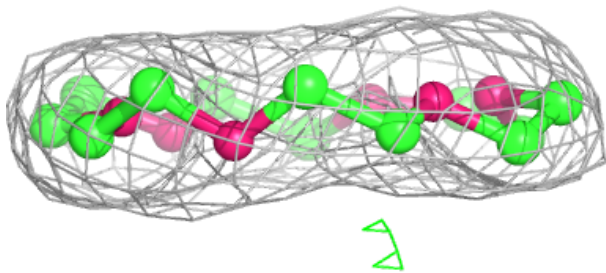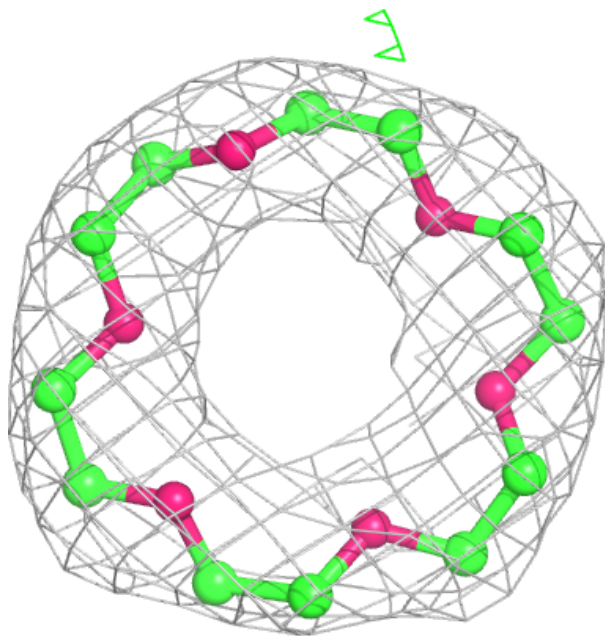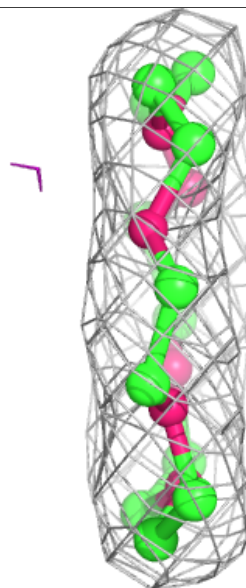
Electron density around O4B C 207:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
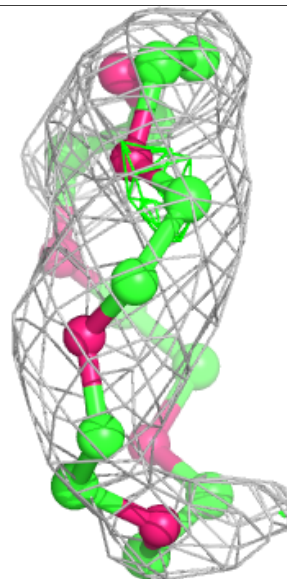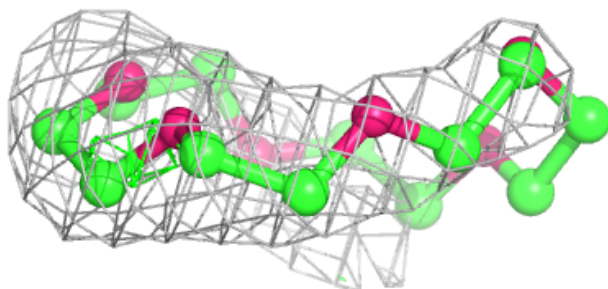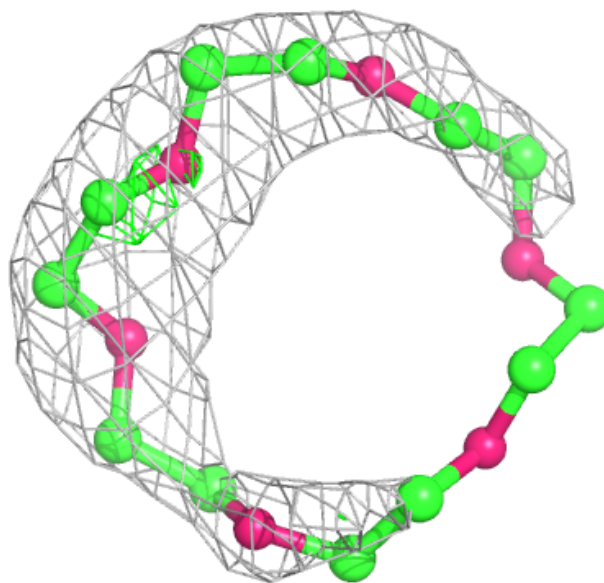
Electron density around O4B B 203:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
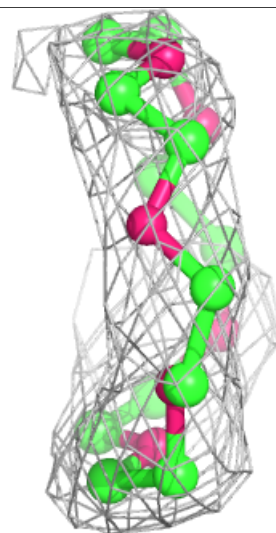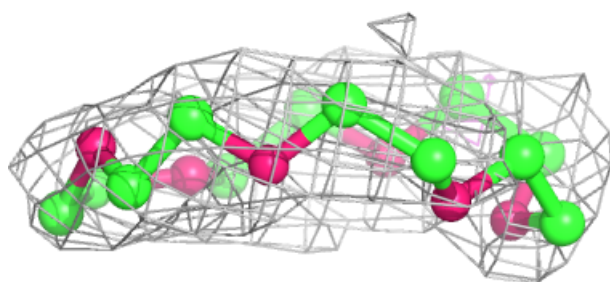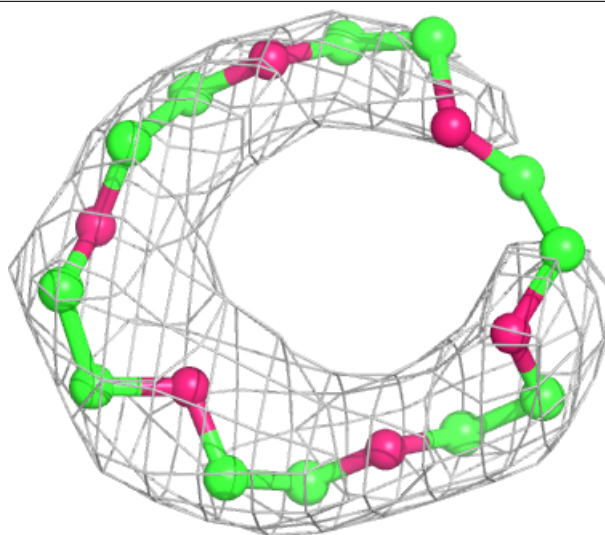
Electron density around O4B C 208:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
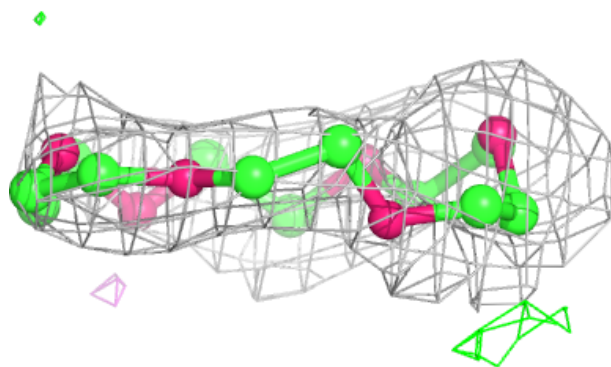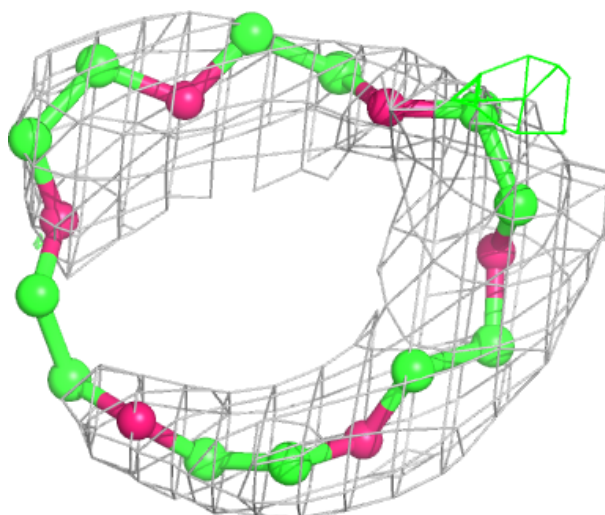
Electron density around O4B C 206:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
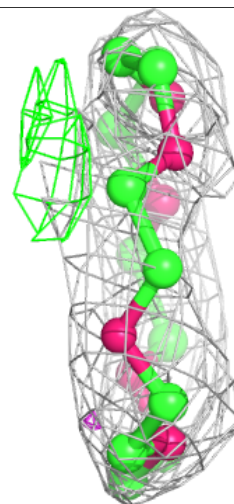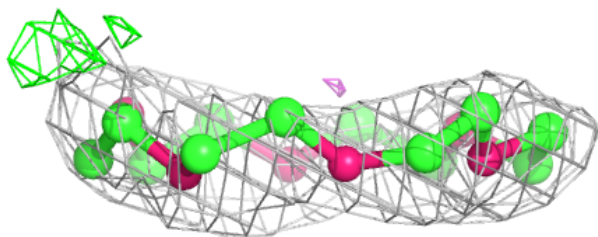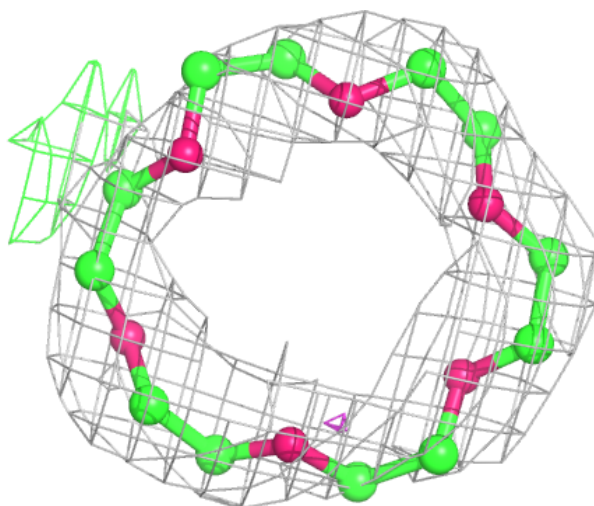
Electron density around O4B A 204:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
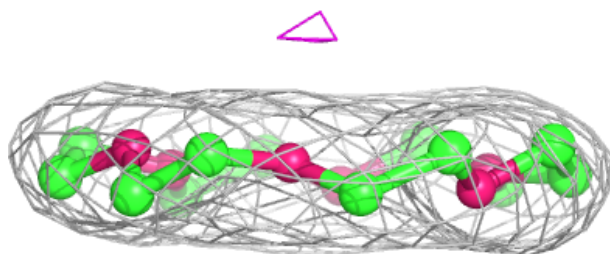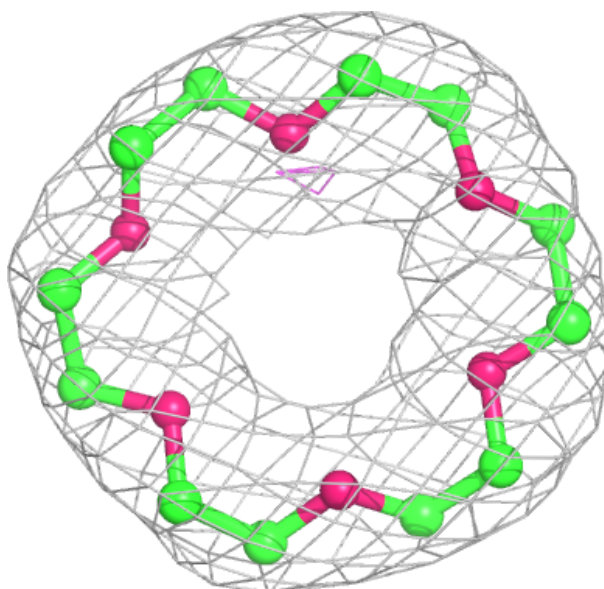$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
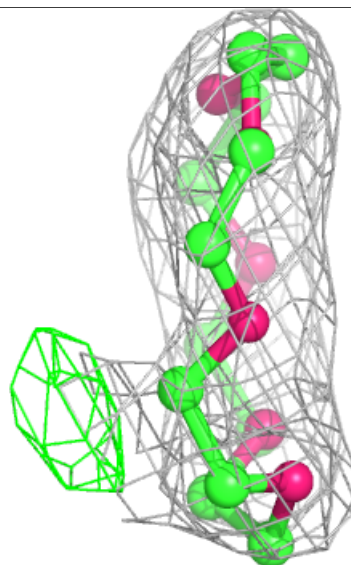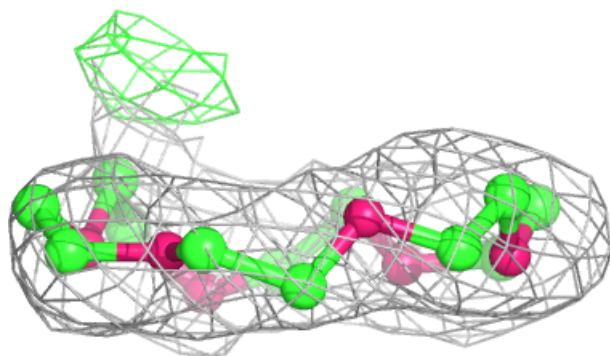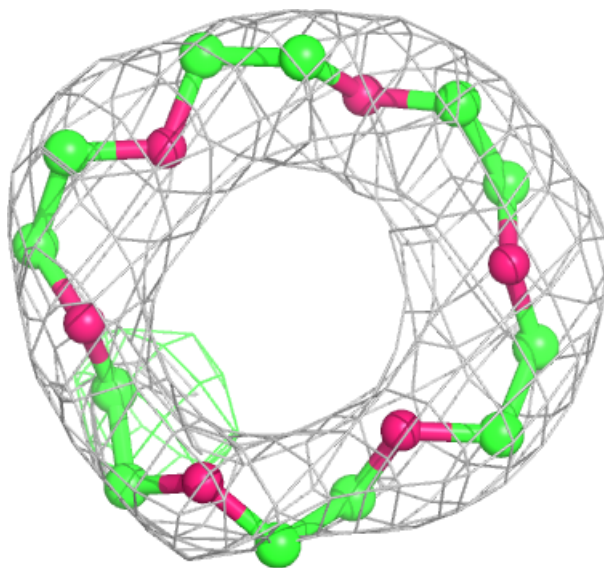
Electron density around O4B C 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
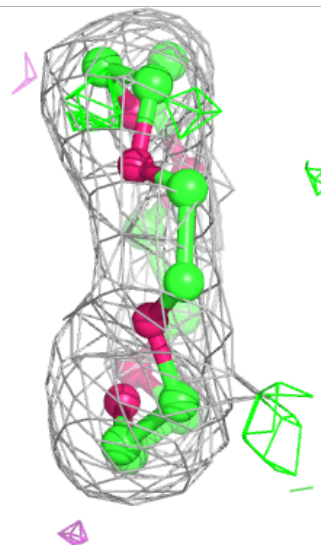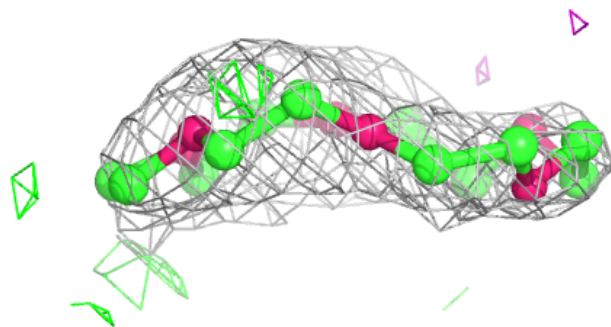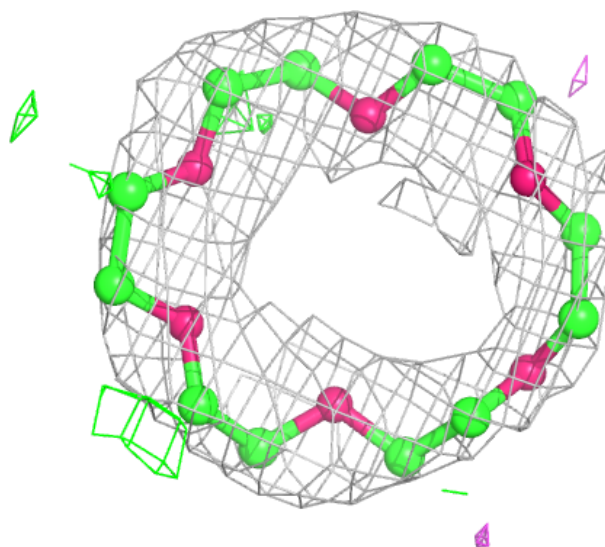
Electron density around HRN B 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
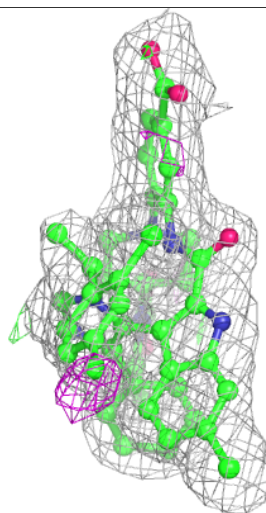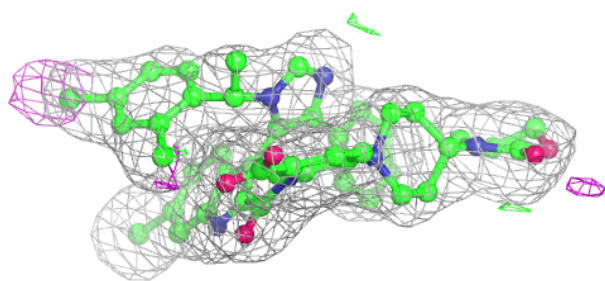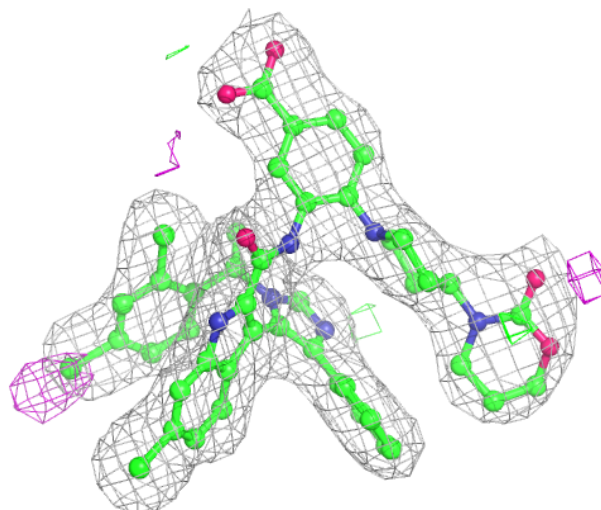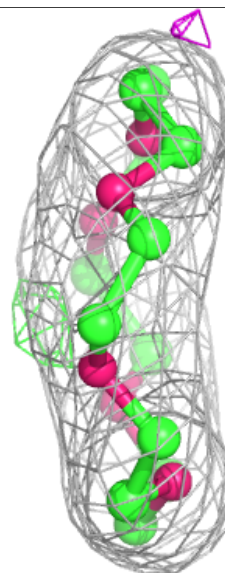and green (positive)
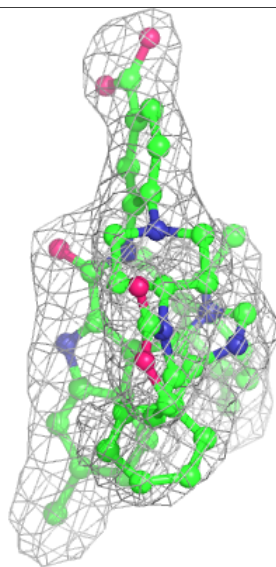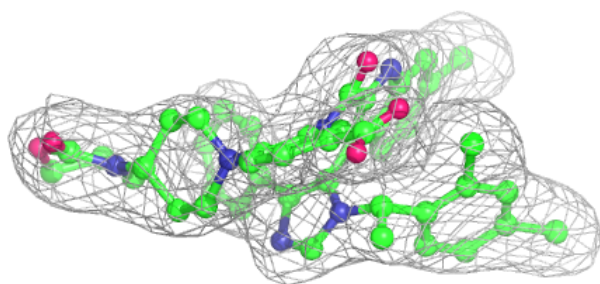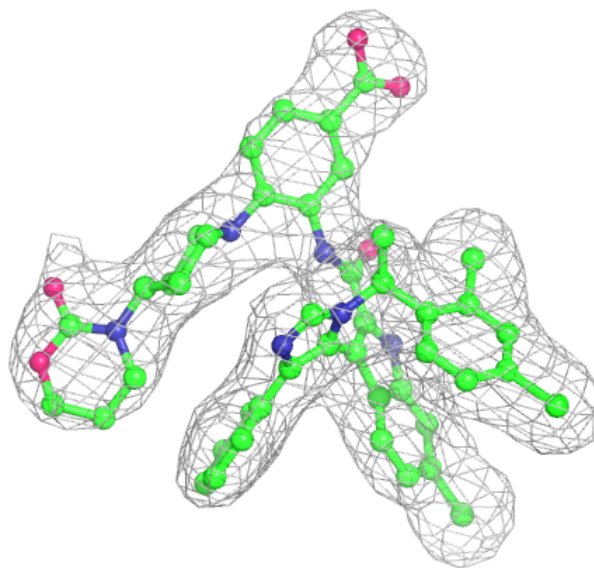
Electron density around HRN C 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
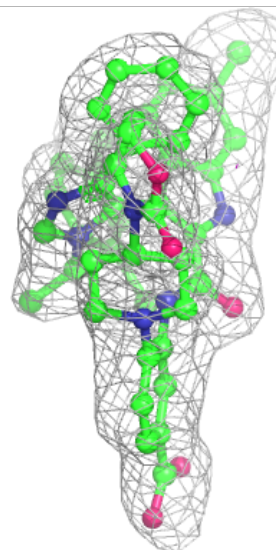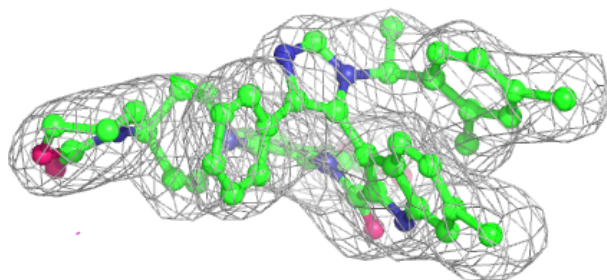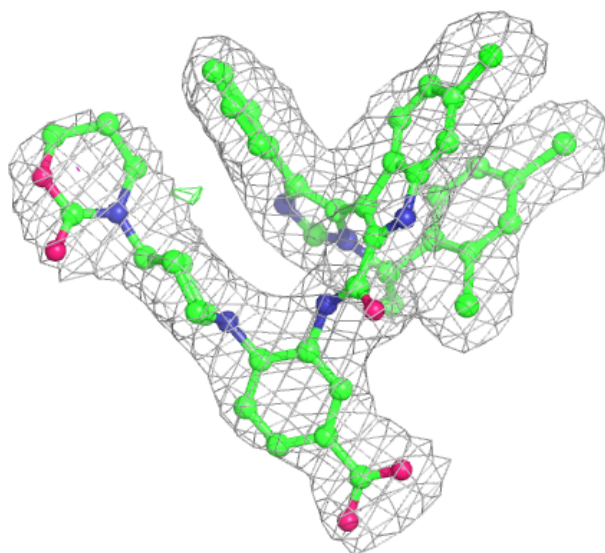
Electron density around O4B C 205:

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

Electron density around O4B A 203:

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

Electron density around O4B A 208:

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

Electron density around O4B A 202:

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

Electron density around O4B C 203:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
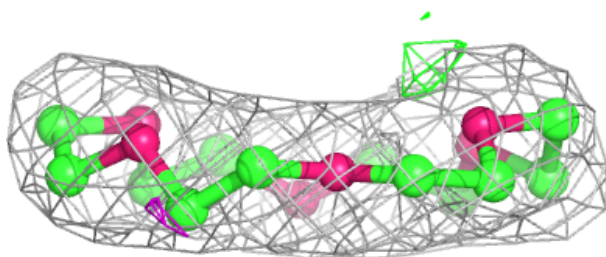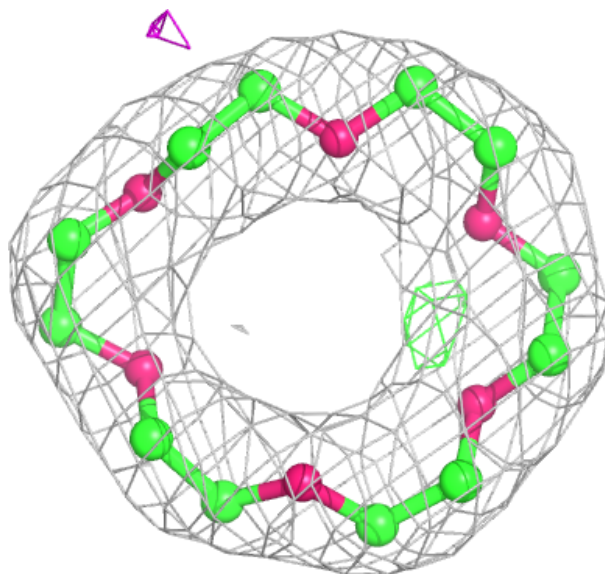and green (positive)
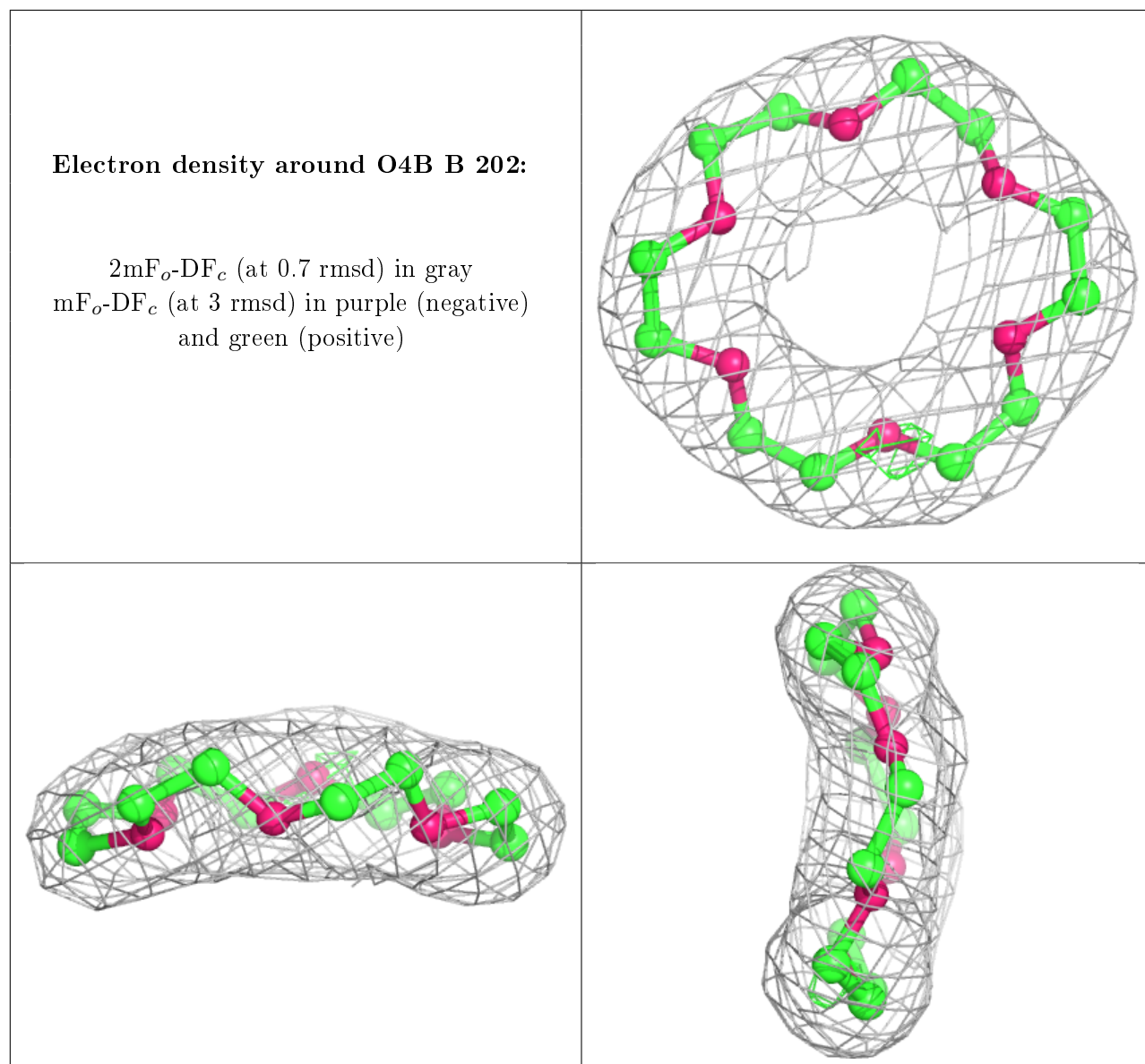
Electron density around HRN A 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around O4B C 202:

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

Electron density around O4B B 202:

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

6.5 Other polymers (i)

There are no such residues in this entry.