Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 03:00 AM EDT

PDB ID	:	4K4B
Title	:	X-ray crystal structure of E. coli YdiI complexed with undeca-2-one-CoA
Authors	:	Ru, W.; Farelli, J.D.; Dunaway-Mariano, D.; Allen, K.N.
Deposited on	:	2013-04-12
Resolution	:	1.90 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 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:

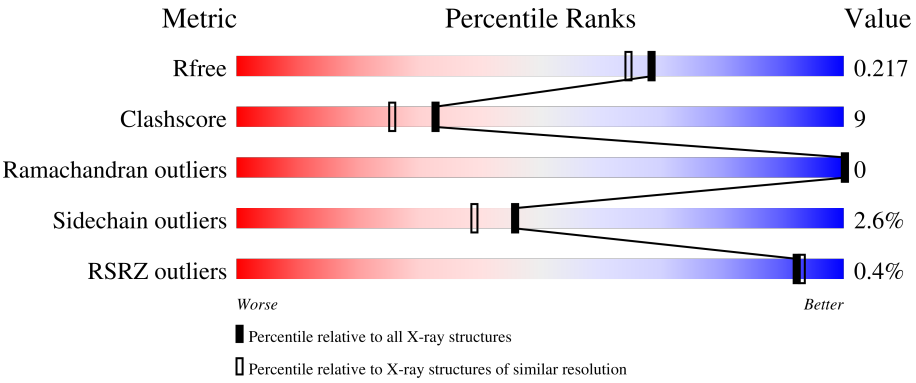
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	136	92% 8%
1	B	136	85% 15%
1	C	136	88% 12%
1	D	136	87% 12%
1	E	136	88% 12%

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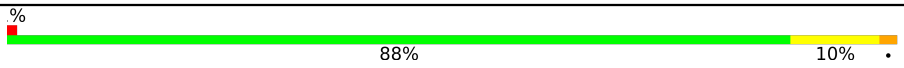
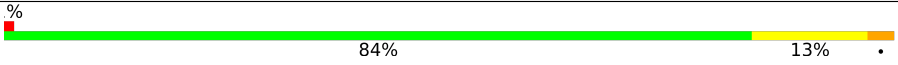
Mol	Chain	Length	Quality of chain
1	F	136	
1	G	136	
1	H	136	

2 Entry composition (i)

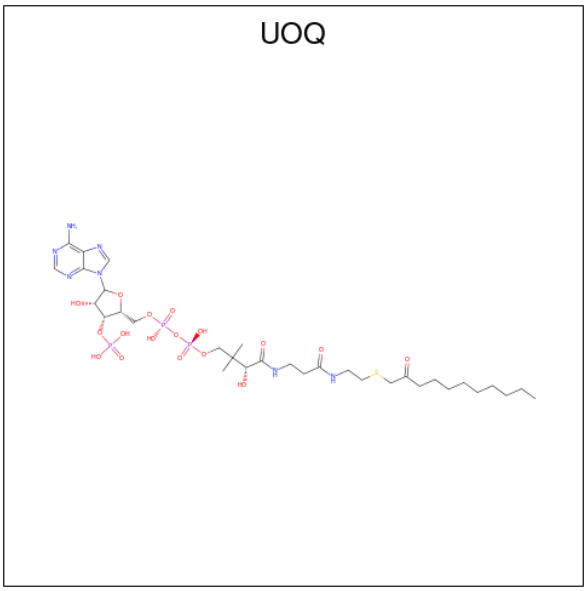
There are 4 unique types of molecules in this entry. The entry contains 10531 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Esterase YdiI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	9	0
			1116	694	207	206	9			
1	B	136	Total	C	N	O	S	0	8	0
			1103	685	205	203	10			
1	C	136	Total	C	N	O	S	0	10	0
			1125	699	211	205	10			
1	D	136	Total	C	N	O	S	0	10	0
			1122	699	206	208	9			
1	E	136	Total	C	N	O	S	0	9	0
			1112	692	206	205	9			
1	F	136	Total	C	N	O	S	0	7	0
			1098	685	202	203	8			
1	G	136	Total	C	N	O	S	0	6	0
			1084	677	199	199	9			
1	H	136	Total	C	N	O	S	0	8	0
			1114	690	207	208	9			

- Molecule 2 is undeca-2-one coenzyme A (three-letter code: UOQ) (formula: $C_{32}H_{56}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			60	32	7	17	3	1		
2	A	1	Total	C	N	O	P	S	2	0
			60	32	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			60	32	7	17	3	1		
2	B	1	Total	C	N	O	P	S	1	0
			60	32	7	17	3	1		
2	C	1	Total	C	N	O	P	S	1	0
			60	32	7	17	3	1		
2	D	1	Total	C	N	O	P	S	3	0
			60	32	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			60	32	7	17	3	1		
2	E	1	Total	C	N	O	P	S	1	0
			60	32	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			60	32	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			60	32	7	17	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			60	32	7	17	3	1		
2	H	1	Total	C	N	O	P	S	3	0
			60	32	7	17	3	1		
2	H	1	Total	C	N	O	P	S	1	0
			60	32	7	17	3	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

- Molecule 4 is water.

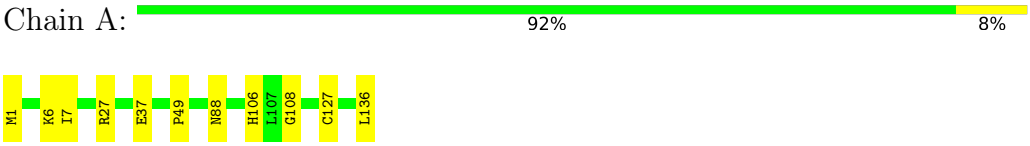
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	127	Total O 127 127	0	0
4	B	114	Total O 114 114	0	0
4	C	119	Total O 119 119	0	0
4	D	100	Total O 100 100	0	0
4	E	88	Total O 88 88	0	0
4	F	89	Total O 89 89	0	0
4	G	100	Total O 100 100	0	0
4	H	138	Total O 138 138	0	0

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.

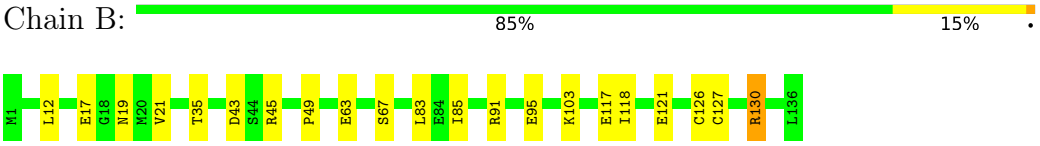
• Molecule 1: Esterase YdiI

Chain A:



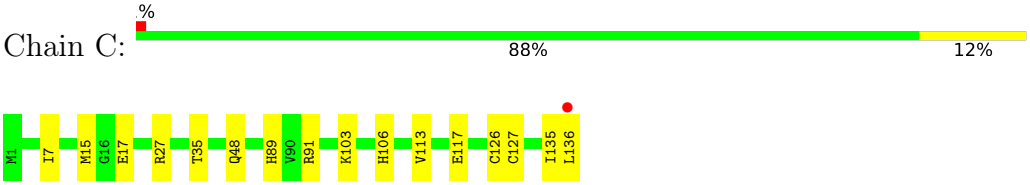
• Molecule 1: Esterase YdiI

Chain B:



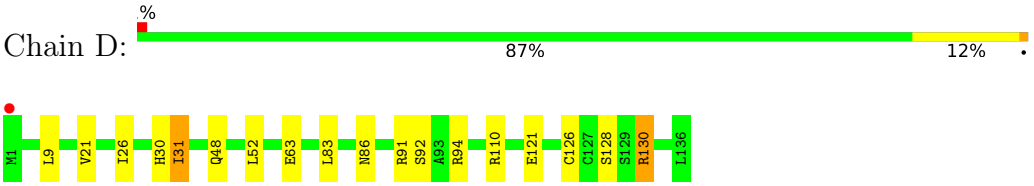
• Molecule 1: Esterase YdiI

Chain C:



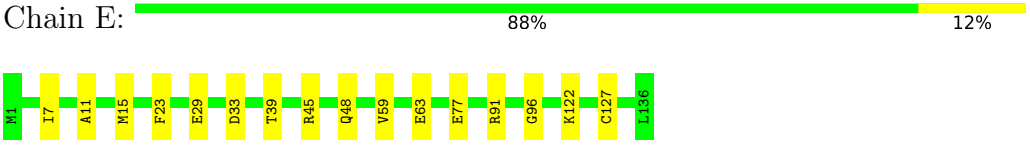
• Molecule 1: Esterase YdiI

Chain D:



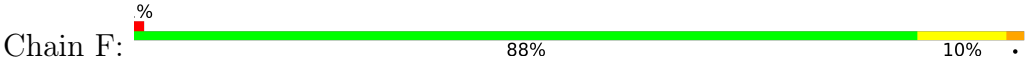
• Molecule 1: Esterase YdiI

Chain E:



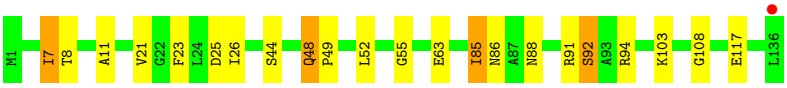
• Molecule 1: Esterase YdiI

Chain F:



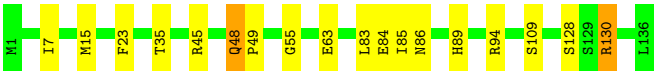
• Molecule 1: Esterase YdiI

Chain G:



• Molecule 1: Esterase YdiI

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.97Å 68.58Å 81.14Å 78.93° 84.69° 76.46°	Depositor
Resolution (Å)	33.89 – 1.90 35.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.3 (33.89-1.90) 87.9 (35.79-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.13 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.169 , 0.216 0.170 , 0.217	Depositor DCC
R_{free} test set	4421 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	11.4	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10531	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7081e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, UOQ

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	0.40	0/1136	0.57	0/1528
1	B	0.38	0/1122	0.55	0/1507
1	C	0.40	0/1145	0.55	0/1539
1	D	0.38	0/1145	0.55	0/1540
1	E	0.38	0/1132	0.56	0/1523
1	F	0.35	0/1118	0.54	0/1504
1	G	0.39	0/1106	0.56	0/1487
1	H	0.40	0/1130	0.56	0/1518
All	All	0.39	0/9034	0.55	0/12146

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

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	1116	0	1123	13	0
1	B	1103	0	1119	19	0
1	C	1125	0	1140	16	0
1	D	1122	0	1130	16	0
1	E	1112	0	1121	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1098	0	1112	13	0
1	G	1084	0	1105	18	0
1	H	1114	0	1115	21	0
2	A	120	0	104	22	0
2	B	120	0	104	5	0
2	C	60	0	52	9	0
2	D	60	0	52	8	0
2	E	180	0	156	18	0
2	F	60	0	52	10	0
2	H	180	0	155	9	0
3	A	1	0	0	0	0
3	E	1	0	0	0	0
4	A	127	0	0	11	0
4	B	114	0	0	6	0
4	C	119	0	0	6	0
4	D	100	0	0	6	0
4	E	88	0	0	9	0
4	F	89	0	0	4	0
4	G	100	0	0	5	0
4	H	138	0	0	10	0
All	All	10531	0	9640	168	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 9.

All (168) 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)
2:C:201:UOQ:S1P	4:D:693:HOH:O	2.02	1.14
2:H:202:UOQ:O8A	2:H:202:UOQ:H5B	1.38	1.12
1:E:127[B]:CYS:SG	4:E:749:HOH:O	2.23	0.96
2:A:203:UOQ:S1P	4:B:405:HOH:O	2.24	0.94
1:B:121:GLU:OE2	4:B:404:HOH:O	1.84	0.93
2:H:203:UOQ:O1A	4:H:372:HOH:O	1.85	0.93
1:H:84:GLU:OE1	4:H:413:HOH:O	1.86	0.93
1:H:94:ARG:NH2	4:H:321:HOH:O	2.00	0.90
1:A:127[B]:CYS:SG	4:A:346:HOH:O	2.31	0.89
2:E:204:UOQ:S1P	4:E:774:HOH:O	2.29	0.88
1:G:88:ASN:HB2	4:H:413:HOH:O	1.75	0.86
1:A:136:LEU:O	4:A:352:HOH:O	1.96	0.84
2:D:501:UOQ:CBX	2:D:501:UOQ:HCD	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:UOQ:C8A	4:A:416:HOH:O	2.30	0.79
1:A:88[B]:ASN:OD1	4:A:307:HOH:O	2.02	0.78
1:G:23:PHE:HB2	4:G:270:HOH:O	1.84	0.77
1:E:15:MET:SD	4:E:747:HOH:O	2.41	0.77
1:H:128:SER:OG	1:H:130:ARG:NH1	2.18	0.77
2:F:201:UOQ:H2P	1:G:63:GLU:OE2	1.84	0.77
2:E:201:UOQ:O9A	4:E:726:HOH:O	2.04	0.76
1:G:117:GLU:OE2	4:G:275:HOH:O	2.04	0.75
1:D:94:ARG:NH1	4:D:670:HOH:O	2.15	0.75
1:C:127[B]:CYS:SG	4:C:392:HOH:O	2.35	0.74
2:E:203:UOQ:O5P	4:E:786:HOH:O	2.06	0.73
1:C:35:THR:HG22	1:C:103[B]:LYS:HG2	1.69	0.72
2:E:204:UOQ:O5P	4:E:781:HOH:O	2.10	0.69
1:F:35[A]:THR:HG22	1:F:103[A]:LYS:HG2	1.75	0.68
1:C:17:GLU:OE2	4:C:362:HOH:O	2.11	0.68
2:F:201:UOQ:C2P	2:F:201:UOQ:HBY	2.24	0.67
2:F:201:UOQ:HBYA	1:H:55:GLY:H	1.59	0.67
1:A:108:GLY:HA3	2:C:201:UOQ:O4A	1.95	0.67
1:G:25:ASP:OD2	4:G:217:HOH:O	2.13	0.66
1:A:106:HIS:NE2	2:C:201:UOQ:O4A	2.24	0.65
1:D:30[B]:HIS:CE1	1:E:122:LYS:HE3	2.31	0.65
2:C:201:UOQ:H2P	1:D:63[B]:GLU:OE2	1.96	0.64
2:A:203:UOQ:O7A	2:A:203:UOQ:H5B	1.98	0.64
2:F:201:UOQ:H2P	2:F:201:UOQ:HBY	1.79	0.64
2:D:501:UOQ:P3B	2:D:501:UOQ:H5BA	2.38	0.63
1:B:35:THR:HG22	1:B:103:LYS:HG2	1.81	0.63
1:F:29:GLU:O	1:F:30[B]:HIS:ND1	2.31	0.62
2:B:202:UOQ:P3B	2:B:202:UOQ:H5BA	2.39	0.62
2:D:501:UOQ:H5BA	2:D:501:UOQ:O7A	2.00	0.62
1:F:117:GLU:OE1	4:F:329:HOH:O	2.15	0.61
2:A:203:UOQ:O4A	1:C:106:HIS:NE2	2.20	0.61
2:C:201:UOQ:O1A	2:C:201:UOQ:H4B	2.01	0.61
1:B:91:ARG:HD2	4:B:400:HOH:O	2.01	0.60
2:A:201:UOQ:O4B	4:A:403:HOH:O	2.16	0.60
2:A:201:UOQ:S1P	2:A:201:UOQ:HCAA	2.42	0.60
2:E:203:UOQ:HBWA	1:G:48:GLN:HG2	1.84	0.59
1:F:43:ASP:OD1	4:F:340:HOH:O	2.16	0.58
1:B:63:GLU:HG2	1:B:85:ILE:HD13	1.85	0.57
1:E:63:GLU:OE2	2:H:203:UOQ:HBWA	2.05	0.57
2:D:501:UOQ:H2B	2:D:501:UOQ:N3A	2.19	0.56
1:E:91:ARG:NH2	4:E:762:HOH:O	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:UOQ:H8A	4:A:416:HOH:O	1.99	0.56
2:A:201:UOQ:HCB	2:A:201:UOQ:HBW	1.87	0.56
2:A:203:UOQ:H56	1:B:21:VAL:HG11	1.88	0.55
1:C:91:ARG:O	1:C:126[B]:CYS:HB2	2.07	0.55
1:A:49:PRO:HG2	2:A:203:UOQ:HCD	1.89	0.55
2:E:203:UOQ:HBW	1:G:55:GLY:H	1.72	0.54
2:A:201:UOQ:H6P	1:B:17:GLU:O	2.07	0.54
1:E:96:GLY:N	2:E:201:UOQ:O9A	2.41	0.54
2:F:201:UOQ:CBY	1:H:55:GLY:H	2.21	0.54
1:F:103[B]:LYS:NZ	4:F:375:HOH:O	2.41	0.53
2:A:203:UOQ:CCG	1:B:21:VAL:HG11	2.37	0.53
1:D:121[A]:GLU:HG2	4:D:662:HOH:O	2.07	0.53
2:E:203:UOQ:OCH	2:E:203:UOQ:H2P	2.08	0.53
2:H:202:UOQ:O8A	2:H:202:UOQ:C5B	2.33	0.53
1:F:110:ARG:NH2	2:F:201:UOQ:H4B	2.25	0.52
1:B:49:PRO:HG2	2:B:202:UOQ:HCE	1.91	0.52
1:B:43:ASP:OD1	1:B:45[A]:ARG:NH1	2.32	0.52
1:G:44[B]:SER:HB3	1:H:23:PHE:HE1	1.74	0.52
2:E:204:UOQ:H2PA	1:F:82:GLY:HA3	1.93	0.51
1:D:86:ASN:OD1	1:D:130:ARG:HD2	2.11	0.51
1:A:1:MET:SD	1:A:6:LYS:HE3	2.50	0.51
2:A:201:UOQ:H5B	2:A:201:UOQ:O9A	2.11	0.51
1:D:30[B]:HIS:HE1	1:E:122:LYS:HE3	1.72	0.51
2:A:203:UOQ:O5P	4:A:421:HOH:O	2.18	0.50
1:D:110:ARG:HD3	4:D:618:HOH:O	2.11	0.50
1:D:9:LEU:HD21	1:D:31[A]:ILE:HG13	1.93	0.50
1:C:89:HIS:ND1	1:C:127[B]:CYS:SG	2.78	0.50
1:B:49:PRO:CG	2:B:202:UOQ:H53	2.41	0.49
2:D:501:UOQ:OCH	2:D:501:UOQ:H52	2.12	0.49
2:A:203:UOQ:CBW	4:B:405:HOH:O	2.55	0.49
1:C:17:GLU:HB2	4:D:695:HOH:O	2.13	0.49
1:E:48:GLN:NE2	2:E:204:UOQ:OCH	2.46	0.49
1:H:45[A]:ARG:CZ	4:H:402:HOH:O	2.60	0.49
1:H:109:SER:OG	2:H:203:UOQ:H5B	2.13	0.49
1:C:48[B]:GLN:NE2	2:C:201:UOQ:HBW	2.28	0.49
2:D:501:UOQ:HCD	2:D:501:UOQ:HBY	1.95	0.49
1:C:117:GLU:OE1	4:C:370:HOH:O	2.20	0.48
1:F:121:GLU:HG2	4:F:369:HOH:O	2.13	0.48
1:D:94:ARG:NH2	4:D:643:HOH:O	2.45	0.48
2:D:501:UOQ:HCD	2:D:501:UOQ:CBY	2.43	0.48
1:C:27:ARG:HD2	4:C:316:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:LEU:HD23	1:G:94:ARG:HG2	1.95	0.48
4:E:786:HOH:O	1:G:92:SER:HB2	2.14	0.48
2:A:203:UOQ:HCGA	1:B:12:LEU:O	2.13	0.47
2:B:202:UOQ:H8A	2:B:202:UOQ:H2B	1.55	0.47
1:H:94:ARG:NH1	4:H:415:HOH:O	2.35	0.47
4:B:359:HOH:O	1:D:92:SER:HA	2.15	0.47
1:C:48[A]:GLN:NE2	2:C:201:UOQ:HBW	2.30	0.47
1:F:130:ARG:NE	1:H:130:ARG:HD3	2.29	0.47
1:D:52:LEU:HD23	1:D:94:ARG:HG2	1.97	0.47
2:F:201:UOQ:OCH	2:F:201:UOQ:H3P	2.15	0.47
1:B:117:GLU:OE1	4:B:341:HOH:O	2.20	0.47
1:C:15:MET:HE2	1:C:15:MET:HB3	1.67	0.47
1:H:89:HIS:HB3	4:H:414:HOH:O	2.15	0.46
1:F:91:ARG:HB3	1:F:126:CYS:HA	1.95	0.46
1:H:7:ILE:HD11	1:H:15:MET:CE	2.44	0.46
1:E:11:ALA:O	1:E:15:MET:HG3	2.15	0.46
2:E:203:UOQ:H53	1:G:49:PRO:CD	2.45	0.46
2:E:201:UOQ:H7PA	2:E:201:UOQ:HAP	1.66	0.46
2:B:201:UOQ:O5A	2:B:201:UOQ:H5B	2.15	0.46
2:E:201:UOQ:O2A	4:E:776:HOH:O	2.21	0.45
1:D:21:VAL:HG13	1:D:26:ILE:HB	1.99	0.45
1:H:63[A]:GLU:HG2	1:H:85:ILE:HD13	1.98	0.45
1:B:91:ARG:O	1:B:126[B]:CYS:HB2	2.16	0.45
1:A:27[B]:ARG:HD3	4:A:398:HOH:O	2.16	0.45
1:G:7[A]:ILE:HD13	1:G:11:ALA:HB3	1.98	0.45
1:H:35[A]:THR:HG21	4:H:417:HOH:O	2.16	0.45
1:D:128:SER:OG	1:D:130:ARG:NH1	2.50	0.45
1:A:7:ILE:HA	4:A:311:HOH:O	2.16	0.45
1:F:6:LYS:HA	1:F:6:LYS:HD2	1.53	0.45
2:H:202:UOQ:HBZ	2:H:202:UOQ:H52	1.73	0.44
2:E:204:UOQ:H2P	1:F:63:GLU:OE1	2.17	0.44
1:H:45[A]:ARG:NE	4:H:402:HOH:O	2.51	0.44
1:A:49:PRO:HA	2:A:201:UOQ:O9P	2.18	0.44
2:F:201:UOQ:H51	1:H:48:GLN:HB3	2.00	0.43
1:A:27[B]:ARG:HD2	4:A:397:HOH:O	2.17	0.43
2:E:203:UOQ:O5A	2:E:203:UOQ:H5B	2.18	0.43
1:G:7[B]:ILE:HG13	4:G:255:HOH:O	2.18	0.43
1:B:118:ILE:HB	1:B:127[B]:CYS:SG	2.58	0.43
2:D:501:UOQ:HBY	2:D:501:UOQ:CCD	2.48	0.43
1:B:91:ARG:HB3	1:B:126[B]:CYS:HA	2.00	0.43
2:C:201:UOQ:P1A	2:C:201:UOQ:HCP	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:ASN:OD1	1:H:130:ARG:HD2	2.18	0.43
2:E:201:UOQ:O7A	2:E:201:UOQ:C5B	2.67	0.42
1:G:103:LYS:HE3	4:G:249:HOH:O	2.18	0.42
1:D:91:ARG:HB3	1:D:126[B]:CYS:HA	2.00	0.42
2:A:201:UOQ:HCAA	2:A:201:UOQ:CBW	2.50	0.42
2:F:201:UOQ:HCE	1:H:49:PRO:CD	2.50	0.42
1:G:85:ILE:HG13	1:G:86:ASN:N	2.34	0.42
2:H:203:UOQ:OCH	2:H:203:UOQ:H2PA	2.18	0.42
1:A:37:GLU:HG3	4:A:321:HOH:O	2.20	0.42
2:C:201:UOQ:H56	2:C:201:UOQ:HCD	1.82	0.42
1:E:29:GLU:OE2	1:E:39:THR:OG1	2.27	0.42
1:B:130:ARG:NE	1:D:130:ARG:HD3	2.34	0.42
2:A:203:UOQ:HBW	2:A:203:UOQ:HBZA	1.56	0.42
1:D:91:ARG:HB3	1:D:126[A]:CYS:HA	2.00	0.42
2:H:202:UOQ:C8A	4:H:428:HOH:O	2.68	0.42
2:A:201:UOQ:O9P	1:B:19:ASN:ND2	2.47	0.41
1:E:59:VAL:HG11	1:F:59:VAL:HG11	2.01	0.41
1:A:88[B]:ASN:OD1	1:C:113:VAL:HG21	2.21	0.41
2:F:201:UOQ:CBX	1:H:48:GLN:HE21	2.34	0.41
1:G:7[B]:ILE:HG22	1:G:8:THR:N	2.36	0.41
2:A:203:UOQ:H52	1:B:21:VAL:HG21	2.02	0.41
2:E:204:UOQ:O4A	1:G:108:GLY:HA3	2.21	0.41
1:H:7:ILE:HD11	1:H:15:MET:HE1	2.02	0.41
1:C:135:ILE:O	1:C:136:LEU:HD23	2.21	0.41
1:H:48:GLN:H	1:H:48:GLN:HG3	1.73	0.41
2:E:201:UOQ:H2P	2:E:201:UOQ:HBYA	2.03	0.40
1:G:21:VAL:HG13	1:G:26:ILE:HB	2.04	0.40
2:A:203:UOQ:HBWA	1:B:67:SER:OG	2.21	0.40
1:C:91:ARG:NH2	4:C:315:HOH:O	2.51	0.40
1:C:127[B]:CYS:SG	4:C:382:HOH:O	2.62	0.40
1:E:23:PHE:O	1:E:45[B]:ARG:NH2	2.54	0.40
2:H:201:UOQ:CCA	2:H:201:UOQ:HBW	2.52	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	143/136 (105%)	142 (99%)	1 (1%)	0	100	100
1	B	142/136 (104%)	142 (100%)	0	0	100	100
1	C	144/136 (106%)	143 (99%)	1 (1%)	0	100	100
1	D	144/136 (106%)	142 (99%)	2 (1%)	0	100	100
1	E	143/136 (105%)	140 (98%)	3 (2%)	0	100	100
1	F	141/136 (104%)	140 (99%)	1 (1%)	0	100	100
1	G	140/136 (103%)	138 (99%)	2 (1%)	0	100	100
1	H	142/136 (104%)	141 (99%)	1 (1%)	0	100	100
All	All	1139/1088 (105%)	1128 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	121/112 (108%)	121 (100%)	0	100	100
1	B	120/112 (107%)	117 (98%)	3 (2%)	47	41
1	C	122/112 (109%)	120 (98%)	2 (2%)	62	60
1	D	122/112 (109%)	117 (96%)	5 (4%)	30	21
1	E	121/112 (108%)	118 (98%)	3 (2%)	47	41
1	F	119/112 (106%)	115 (97%)	4 (3%)	37	28
1	G	118/112 (105%)	112 (95%)	6 (5%)	24	14
1	H	120/112 (107%)	117 (98%)	3 (2%)	47	41
All	All	963/896 (108%)	937 (97%)	26 (3%)	46	38

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

Mol	Chain	Res	Type
1	B	83	LEU
1	B	95	GLU
1	B	130	ARG
1	C	7[A]	ILE
1	C	7[B]	ILE
1	D	31[A]	ILE
1	D	31[B]	ILE
1	D	48	GLN
1	D	83	LEU
1	D	130	ARG
1	E	7	ILE
1	E	33	ASP
1	E	77	GLU
1	F	6	LYS
1	F	83	LEU
1	F	121	GLU
1	F	130	ARG
1	G	7[A]	ILE
1	G	7[B]	ILE
1	G	48	GLN
1	G	85	ILE
1	G	91	ARG
1	G	92	SER
1	H	48	GLN
1	H	83	LEU
1	H	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	112	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	UOQ	H	202	-	54,62,62	3.18	15 (27%)	66,88,88	1.95	17 (25%)
2	UOQ	C	201	-	54,62,62	1.99	12 (22%)	66,88,88	1.78	9 (13%)
2	UOQ	H	203	-	54,62,62	2.04	12 (22%)	66,88,88	1.90	14 (21%)
2	UOQ	D	501	-	54,62,62	2.10	13 (24%)	66,88,88	1.93	16 (24%)
2	UOQ	H	201	-	54,62,62	2.06	11 (20%)	66,88,88	1.97	15 (22%)
2	UOQ	E	203	-	54,62,62	2.10	13 (24%)	66,88,88	2.04	12 (18%)
2	UOQ	A	201	-	54,62,62	2.10	12 (22%)	66,88,88	2.95	21 (31%)
2	UOQ	B	202	-	54,62,62	2.04	14 (25%)	66,88,88	1.91	13 (19%)
2	UOQ	F	201	-	54,62,62	2.10	13 (24%)	66,88,88	1.98	16 (24%)
2	UOQ	E	204	-	54,62,62	2.01	14 (25%)	66,88,88	1.96	15 (22%)
2	UOQ	E	201	-	54,62,62	2.13	13 (24%)	66,88,88	2.27	16 (24%)
2	UOQ	B	201	-	54,62,62	2.09	13 (24%)	66,88,88	1.74	11 (16%)
2	UOQ	A	203	-	54,62,62	2.07	12 (22%)	66,88,88	1.97	14 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UOQ	H	202	-	-	18/57/77/77	0/3/3/3
2	UOQ	C	201	-	-	18/57/77/77	0/3/3/3
2	UOQ	H	203	-	-	12/57/77/77	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UOQ	D	501	-	-	22/57/77/77	0/3/3/3
2	UOQ	H	201	-	-	19/57/77/77	0/3/3/3
2	UOQ	E	203	-	-	15/57/77/77	0/3/3/3
2	UOQ	A	201	-	-	19/57/77/77	0/3/3/3
2	UOQ	B	202	-	-	13/57/77/77	0/3/3/3
2	UOQ	F	201	-	-	15/57/77/77	0/3/3/3
2	UOQ	E	204	-	-	20/57/77/77	0/3/3/3
2	UOQ	E	201	-	-	31/57/77/77	0/3/3/3
2	UOQ	B	201	-	-	14/57/77/77	0/3/3/3
2	UOQ	A	203	-	-	21/57/77/77	0/3/3/3

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	202	UOQ	P3B-O3B	-15.81	1.29	1.59
2	F	201	UOQ	OCH-CBX	8.81	1.36	1.21
2	E	201	UOQ	OCH-CBX	8.79	1.36	1.21
2	D	501	UOQ	OCH-CBX	8.72	1.36	1.21
2	A	203	UOQ	OCH-CBX	8.71	1.36	1.21
2	H	203	UOQ	OCH-CBX	8.64	1.36	1.21
2	H	201	UOQ	OCH-CBX	8.56	1.36	1.21
2	B	201	UOQ	OCH-CBX	8.53	1.36	1.21
2	E	203	UOQ	OCH-CBX	8.52	1.36	1.21
2	H	202	UOQ	OCH-CBX	8.43	1.36	1.21
2	B	202	UOQ	OCH-CBX	8.42	1.36	1.21
2	A	201	UOQ	OCH-CBX	8.23	1.35	1.21
2	H	202	UOQ	O3B-C3B	-8.15	1.14	1.44
2	E	204	UOQ	OCH-CBX	8.03	1.35	1.21
2	C	201	UOQ	OCH-CBX	7.54	1.34	1.21
2	A	201	UOQ	C9P-N8P	5.64	1.45	1.33
2	E	203	UOQ	C2B-C3B	-5.60	1.40	1.52
2	B	202	UOQ	C2B-C3B	-5.45	1.40	1.52
2	E	201	UOQ	C9P-N8P	5.29	1.45	1.33
2	B	201	UOQ	C2B-C3B	-5.23	1.41	1.52
2	D	501	UOQ	C2B-C3B	-5.11	1.41	1.52
2	C	201	UOQ	C2B-C3B	-5.09	1.41	1.52
2	H	201	UOQ	C9P-N8P	5.04	1.44	1.33
2	F	201	UOQ	C2B-C3B	-5.01	1.41	1.52
2	H	202	UOQ	C2B-C3B	-4.99	1.41	1.52
2	E	201	UOQ	C2B-C3B	-4.96	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	202	UOQ	C9P-N8P	4.93	1.44	1.33
2	B	201	UOQ	C9P-N8P	4.92	1.44	1.33
2	A	203	UOQ	C2B-C3B	-4.84	1.42	1.52
2	C	201	UOQ	C9P-N8P	4.83	1.44	1.33
2	E	203	UOQ	C9P-N8P	4.83	1.44	1.33
2	A	201	UOQ	C5P-N4P	4.82	1.44	1.33
2	H	201	UOQ	C2B-C3B	-4.82	1.42	1.52
2	A	201	UOQ	C2B-C3B	-4.82	1.42	1.52
2	E	204	UOQ	C2B-C3B	-4.68	1.42	1.52
2	H	201	UOQ	C5P-N4P	4.68	1.44	1.33
2	H	203	UOQ	C2B-C3B	-4.65	1.42	1.52
2	B	202	UOQ	C9P-N8P	4.61	1.43	1.33
2	D	501	UOQ	C9P-N8P	4.58	1.43	1.33
2	A	203	UOQ	C5P-N4P	4.57	1.43	1.33
2	E	204	UOQ	C9P-N8P	4.50	1.43	1.33
2	F	201	UOQ	C9P-N8P	4.47	1.43	1.33
2	H	203	UOQ	C9P-N8P	4.44	1.43	1.33
2	A	203	UOQ	C9P-N8P	4.43	1.43	1.33
2	B	201	UOQ	C5P-N4P	4.38	1.43	1.33
2	E	204	UOQ	C5P-N4P	4.35	1.43	1.33
2	D	501	UOQ	C5P-N4P	4.28	1.43	1.33
2	H	202	UOQ	C5P-N4P	4.24	1.43	1.33
2	E	201	UOQ	C5P-N4P	4.20	1.42	1.33
2	H	203	UOQ	C5P-N4P	4.19	1.42	1.33
2	C	201	UOQ	C5P-N4P	4.14	1.42	1.33
2	F	201	UOQ	C5P-N4P	3.99	1.42	1.33
2	E	203	UOQ	C3B-C4B	-3.89	1.42	1.52
2	E	203	UOQ	C5P-N4P	3.88	1.42	1.33
2	F	201	UOQ	C3B-C4B	-3.78	1.42	1.52
2	B	202	UOQ	C5P-N4P	3.65	1.41	1.33
2	H	203	UOQ	C3B-C4B	-3.56	1.43	1.52
2	B	201	UOQ	C3B-C4B	-3.50	1.43	1.52
2	E	201	UOQ	C3B-C4B	-3.46	1.43	1.52
2	B	202	UOQ	C3B-C4B	-3.40	1.43	1.52
2	H	202	UOQ	CEP-CBP	3.40	1.61	1.53
2	A	203	UOQ	C3B-C4B	-3.39	1.43	1.52
2	D	501	UOQ	CEP-CBP	3.32	1.61	1.53
2	E	204	UOQ	C3B-C4B	-3.30	1.44	1.52
2	F	201	UOQ	O4B-C1B	3.29	1.45	1.41
2	D	501	UOQ	C3B-C4B	-3.25	1.44	1.52
2	C	201	UOQ	C3B-C4B	-3.15	1.44	1.52
2	A	201	UOQ	C3B-C4B	-3.15	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	UOQ	CEP-CBP	3.14	1.60	1.53
2	A	203	UOQ	OAP-CAP	3.13	1.48	1.42
2	E	201	UOQ	CEP-CBP	3.11	1.60	1.53
2	H	201	UOQ	C3B-C4B	-3.11	1.44	1.52
2	C	201	UOQ	OAP-CAP	3.09	1.48	1.42
2	E	201	UOQ	OAP-CAP	3.07	1.47	1.42
2	H	202	UOQ	OAP-CAP	3.05	1.47	1.42
2	H	201	UOQ	CEP-CBP	3.04	1.60	1.53
2	H	202	UOQ	C3B-C4B	-3.04	1.44	1.52
2	E	203	UOQ	CBW-CBX	-3.01	1.45	1.51
2	A	201	UOQ	CEP-CBP	3.00	1.60	1.53
2	F	201	UOQ	CEP-CBP	2.93	1.60	1.53
2	A	201	UOQ	O9P-C9P	-2.90	1.17	1.23
2	D	501	UOQ	OAP-CAP	2.90	1.47	1.42
2	E	204	UOQ	OAP-CAP	2.88	1.47	1.42
2	C	201	UOQ	CEP-CBP	2.88	1.60	1.53
2	F	201	UOQ	OAP-CAP	2.84	1.47	1.42
2	E	204	UOQ	CBW-CBX	-2.84	1.46	1.51
2	E	204	UOQ	CEP-CBP	2.82	1.60	1.53
2	H	203	UOQ	O4B-C1B	2.81	1.45	1.41
2	H	201	UOQ	OAP-CAP	2.75	1.47	1.42
2	E	203	UOQ	CEP-CBP	2.75	1.59	1.53
2	A	203	UOQ	CEP-CBP	2.71	1.59	1.53
2	D	501	UOQ	CBW-CBX	-2.69	1.46	1.51
2	H	203	UOQ	OAP-CAP	2.65	1.47	1.42
2	B	202	UOQ	CEP-CBP	2.64	1.59	1.53
2	B	201	UOQ	OAP-CAP	2.64	1.47	1.42
2	H	203	UOQ	CEP-CBP	2.64	1.59	1.53
2	E	201	UOQ	O4B-C1B	2.63	1.44	1.41
2	E	201	UOQ	CBW-CBX	-2.60	1.46	1.51
2	A	201	UOQ	O4B-C1B	2.58	1.44	1.41
2	A	203	UOQ	CBW-CBX	-2.55	1.46	1.51
2	B	202	UOQ	O4B-C1B	2.54	1.44	1.41
2	A	203	UOQ	O4B-C4B	-2.53	1.39	1.45
2	A	203	UOQ	O9P-C9P	-2.52	1.18	1.23
2	H	202	UOQ	O4B-C1B	2.52	1.44	1.41
2	E	203	UOQ	OAP-CAP	2.52	1.46	1.42
2	H	201	UOQ	O4B-C4B	-2.49	1.39	1.45
2	E	203	UOQ	O4B-C4B	-2.49	1.39	1.45
2	B	201	UOQ	CBW-CBX	-2.49	1.46	1.51
2	E	201	UOQ	O9P-C9P	-2.49	1.18	1.23
2	C	201	UOQ	O4B-C4B	-2.47	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	203	UOQ	O9P-C9P	-2.46	1.18	1.23
2	B	202	UOQ	OAP-CAP	2.45	1.46	1.42
2	H	202	UOQ	O9P-C9P	-2.39	1.18	1.23
2	E	203	UOQ	O5B-C5B	-2.39	1.35	1.44
2	B	202	UOQ	O5B-C5B	-2.38	1.35	1.44
2	B	202	UOQ	O9P-C9P	-2.36	1.18	1.23
2	H	203	UOQ	CBW-CBX	-2.36	1.47	1.51
2	E	204	UOQ	O4B-C4B	-2.36	1.39	1.45
2	E	201	UOQ	O4B-C4B	-2.35	1.39	1.45
2	C	201	UOQ	O5B-C5B	-2.35	1.35	1.44
2	A	201	UOQ	CBW-CBX	-2.34	1.47	1.51
2	F	201	UOQ	C4A-N3A	2.32	1.38	1.35
2	B	202	UOQ	C4A-N3A	2.27	1.38	1.35
2	B	201	UOQ	O9P-C9P	-2.27	1.18	1.23
2	D	501	UOQ	O4B-C1B	2.26	1.44	1.41
2	D	501	UOQ	O9P-C9P	-2.26	1.18	1.23
2	B	201	UOQ	O4B-C1B	2.25	1.44	1.41
2	B	201	UOQ	O4B-C4B	-2.24	1.40	1.45
2	A	203	UOQ	O5B-C5B	-2.21	1.36	1.44
2	C	201	UOQ	CBW-CBX	-2.19	1.47	1.51
2	F	201	UOQ	CBW-CBX	-2.18	1.47	1.51
2	A	201	UOQ	OAP-CAP	-2.18	1.38	1.42
2	F	201	UOQ	O4B-C4B	-2.18	1.40	1.45
2	A	201	UOQ	O4B-C4B	-2.18	1.40	1.45
2	E	201	UOQ	C6A-N6A	2.16	1.41	1.34
2	E	204	UOQ	C6A-N6A	2.16	1.41	1.34
2	B	201	UOQ	C6A-N6A	2.15	1.41	1.34
2	F	201	UOQ	O9P-C9P	-2.15	1.19	1.23
2	A	201	UOQ	C6A-N6A	2.14	1.41	1.34
2	E	204	UOQ	O9P-C9P	-2.14	1.19	1.23
2	H	202	UOQ	O4B-C4B	-2.14	1.40	1.45
2	H	201	UOQ	C6A-N6A	2.13	1.41	1.34
2	E	203	UOQ	O4B-C1B	2.13	1.44	1.41
2	E	203	UOQ	O9P-C9P	-2.13	1.19	1.23
2	C	201	UOQ	C6A-N6A	2.12	1.41	1.34
2	A	203	UOQ	C6A-N6A	2.12	1.41	1.34
2	H	201	UOQ	O9P-C9P	-2.12	1.19	1.23
2	D	501	UOQ	C6A-N6A	2.11	1.41	1.34
2	E	204	UOQ	O5B-C5B	-2.11	1.36	1.44
2	H	202	UOQ	C6A-N6A	2.11	1.41	1.34
2	B	202	UOQ	C6A-N6A	2.10	1.41	1.34
2	B	201	UOQ	O5B-C5B	-2.10	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	203	UOQ	C6A-N6A	2.10	1.41	1.34
2	E	201	UOQ	C4A-N3A	2.09	1.38	1.35
2	D	501	UOQ	O4B-C4B	-2.09	1.40	1.45
2	C	201	UOQ	C4A-N3A	2.09	1.38	1.35
2	B	202	UOQ	O4B-C4B	-2.09	1.40	1.45
2	F	201	UOQ	C6A-N6A	2.08	1.41	1.34
2	H	203	UOQ	C6A-N6A	2.06	1.41	1.34
2	D	501	UOQ	O5B-C5B	-2.05	1.36	1.44
2	E	204	UOQ	C4A-N3A	2.05	1.38	1.35
2	H	202	UOQ	C4A-N3A	2.04	1.38	1.35
2	H	203	UOQ	C4A-N3A	2.04	1.38	1.35
2	E	204	UOQ	O4B-C1B	2.04	1.43	1.41
2	H	201	UOQ	C4A-N3A	2.04	1.38	1.35
2	H	202	UOQ	CDP-CBP	-2.03	1.49	1.53
2	B	202	UOQ	CBW-CBX	-2.00	1.47	1.51

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	UOQ	C1B-N9A-C4A	-14.09	101.88	126.64
2	A	201	UOQ	OCH-CBX-CBW	-9.93	108.01	122.17
2	E	204	UOQ	OCH-CBX-CBW	-9.57	108.52	122.17
2	E	203	UOQ	OCH-CBX-CBW	-9.12	109.17	122.17
2	F	201	UOQ	OCH-CBX-CBW	-8.73	109.72	122.17
2	E	201	UOQ	OCH-CBX-CBW	-8.56	109.96	122.17
2	A	203	UOQ	OCH-CBX-CBW	-8.42	110.17	122.17
2	D	501	UOQ	OCH-CBX-CBW	-7.94	110.85	122.17
2	H	201	UOQ	OCH-CBX-CBW	-7.69	111.21	122.17
2	H	202	UOQ	OCH-CBX-CBW	-7.24	111.85	122.17
2	B	201	UOQ	OCH-CBX-CBW	-7.17	111.95	122.17
2	C	201	UOQ	OCH-CBX-CBW	-7.10	112.05	122.17
2	B	202	UOQ	OCH-CBX-CBW	-6.89	112.34	122.17
2	H	203	UOQ	OCH-CBX-CBW	-6.58	112.78	122.17
2	B	202	UOQ	OCH-CBX-CBY	-6.48	104.31	121.44
2	E	203	UOQ	O6A-CCP-CBP	5.99	120.17	110.55
2	E	203	UOQ	OCH-CBX-CBY	-5.92	105.77	121.44
2	H	203	UOQ	OCH-CBX-CBY	-5.83	106.02	121.44
2	H	201	UOQ	OCH-CBX-CBY	-5.75	106.22	121.44
2	H	201	UOQ	C2P-C3P-N4P	5.47	123.92	112.42
2	C	201	UOQ	OCH-CBX-CBY	-5.35	107.30	121.44
2	E	201	UOQ	O6A-CCP-CBP	5.25	118.99	110.55
2	E	201	UOQ	C2P-S1P-CBW	5.16	110.34	101.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	201	UOQ	OCH-CBX-CBY	-5.10	107.96	121.44
2	A	203	UOQ	OCH-CBX-CBY	-5.05	108.07	121.44
2	A	201	UOQ	O5B-C5B-C4B	5.04	126.35	108.99
2	A	201	UOQ	OCH-CBX-CBY	-4.90	108.48	121.44
2	D	501	UOQ	OCH-CBX-CBY	-4.89	108.49	121.44
2	E	204	UOQ	OCH-CBX-CBY	-4.89	108.50	121.44
2	A	201	UOQ	C7P-C6P-C5P	4.89	120.50	112.36
2	C	201	UOQ	O6A-CCP-CBP	4.85	118.35	110.55
2	E	201	UOQ	OCH-CBX-CBY	-4.85	108.61	121.44
2	E	201	UOQ	O5B-C5B-C4B	4.83	125.60	108.99
2	E	201	UOQ	C3P-N4P-C5P	-4.75	114.01	122.84
2	A	203	UOQ	O6A-CCP-CBP	4.70	118.10	110.55
2	B	201	UOQ	OCH-CBX-CBY	-4.68	109.07	121.44
2	E	203	UOQ	N3A-C2A-N1A	-4.60	121.49	128.68
2	B	202	UOQ	N3A-C2A-N1A	-4.58	121.51	128.68
2	B	201	UOQ	C3P-N4P-C5P	-4.48	114.52	122.84
2	H	202	UOQ	OCH-CBX-CBY	-4.46	109.65	121.44
2	H	202	UOQ	N3A-C2A-N1A	-4.44	121.73	128.68
2	E	203	UOQ	C2B-C3B-C4B	-4.43	95.38	103.22
2	E	201	UOQ	N3A-C2A-N1A	-4.42	121.77	128.68
2	C	201	UOQ	N3A-C2A-N1A	-4.38	121.83	128.68
2	B	201	UOQ	N3A-C2A-N1A	-4.38	121.84	128.68
2	A	201	UOQ	O6A-CCP-CBP	4.36	117.56	110.55
2	H	202	UOQ	C2P-S1P-CBW	4.32	108.94	101.71
2	A	203	UOQ	N3A-C2A-N1A	-4.32	121.92	128.68
2	F	201	UOQ	N3A-C2A-N1A	-4.32	121.93	128.68
2	A	201	UOQ	N3A-C2A-N1A	-4.29	121.97	128.68
2	E	201	UOQ	C7P-C6P-C5P	4.29	119.50	112.36
2	D	501	UOQ	N3A-C2A-N1A	-4.29	121.97	128.68
2	A	203	UOQ	C7P-C6P-C5P	4.27	119.47	112.36
2	H	203	UOQ	O6A-CCP-CBP	4.25	117.39	110.55
2	F	201	UOQ	C2P-S1P-CBW	4.25	108.81	101.71
2	H	202	UOQ	O5B-C5B-C4B	4.19	123.41	108.99
2	H	203	UOQ	N3A-C2A-N1A	-4.18	122.14	128.68
2	B	201	UOQ	P2A-O3A-P1A	-4.07	118.87	132.83
2	A	203	UOQ	C2P-S1P-CBW	4.05	108.48	101.71
2	E	204	UOQ	N3A-C2A-N1A	-3.99	122.44	128.68
2	A	201	UOQ	O4B-C4B-C3B	3.85	113.12	104.87
2	D	501	UOQ	P2A-O3A-P1A	-3.81	119.76	132.83
2	H	201	UOQ	C2P-S1P-CBW	3.79	108.05	101.71
2	H	201	UOQ	N3A-C2A-N1A	-3.78	122.77	128.68
2	H	203	UOQ	O5B-C5B-C4B	3.78	122.00	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	201	UOQ	C2P-C3P-N4P	3.76	120.32	112.42
2	F	201	UOQ	P2A-O3A-P1A	-3.75	119.96	132.83
2	D	501	UOQ	O5B-C5B-C4B	3.69	121.71	108.99
2	B	201	UOQ	O5B-C5B-C4B	3.65	121.56	108.99
2	B	202	UOQ	O6A-CCP-CBP	3.65	116.42	110.55
2	B	202	UOQ	C3B-C2B-C1B	3.63	107.93	99.89
2	A	201	UOQ	C2P-S1P-CBW	3.60	107.73	101.71
2	H	201	UOQ	C6P-C7P-N8P	3.58	119.11	111.90
2	A	201	UOQ	C6P-C7P-N8P	3.56	119.09	111.90
2	B	202	UOQ	C3P-N4P-C5P	-3.56	116.23	122.84
2	H	203	UOQ	C2P-S1P-CBW	3.52	107.60	101.71
2	F	201	UOQ	O4B-C4B-C5B	3.43	120.64	109.37
2	D	501	UOQ	C7P-C6P-C5P	3.42	118.05	112.36
2	A	201	UOQ	C4A-C5A-N7A	-3.41	105.84	109.40
2	E	204	UOQ	O6A-CCP-CBP	3.40	116.01	110.55
2	B	202	UOQ	P2A-O3A-P1A	-3.39	121.20	132.83
2	D	501	UOQ	C7P-N8P-C9P	-3.37	116.58	122.59
2	H	202	UOQ	O6A-CCP-CBP	3.31	115.87	110.55
2	C	201	UOQ	P2A-O3A-P1A	-3.29	121.53	132.83
2	H	203	UOQ	C3P-N4P-C5P	-3.28	116.75	122.84
2	A	201	UOQ	CEP-CBP-CAP	3.24	114.44	108.82
2	F	201	UOQ	O4B-C4B-C3B	3.23	111.79	104.87
2	C	201	UOQ	O4B-C4B-C3B	3.22	111.77	104.87
2	A	201	UOQ	P2A-O3A-P1A	-3.21	121.81	132.83
2	H	202	UOQ	C7P-N8P-C9P	-3.21	116.87	122.59
2	F	201	UOQ	C4A-C5A-N7A	-3.20	106.06	109.40
2	H	203	UOQ	C4A-C5A-N7A	-3.20	106.07	109.40
2	E	203	UOQ	CBW-CBX-CBY	-3.19	108.68	115.52
2	A	201	UOQ	OAP-CAP-CBP	3.18	117.75	110.25
2	E	204	UOQ	C7P-C6P-C5P	3.15	117.61	112.36
2	E	204	UOQ	P2A-O3A-P1A	-3.12	122.12	132.83
2	E	203	UOQ	P2A-O3A-P1A	-3.09	122.22	132.83
2	A	201	UOQ	O4B-C4B-C5B	3.08	119.51	109.37
2	C	201	UOQ	C4A-C5A-N7A	-3.05	106.22	109.40
2	B	201	UOQ	C4A-C5A-N7A	-3.03	106.24	109.40
2	A	203	UOQ	C3B-C2B-C1B	3.01	106.56	99.89
2	E	201	UOQ	C6P-C5P-N4P	3.01	121.48	116.42
2	H	203	UOQ	CBW-CBX-CBY	-3.00	109.08	115.52
2	A	201	UOQ	C6P-C5P-N4P	2.99	121.45	116.42
2	H	202	UOQ	O3B-P3B-O9A	-2.97	97.91	109.39
2	E	204	UOQ	CBW-CBX-CBY	-2.97	109.14	115.52
2	H	201	UOQ	C7P-C6P-C5P	2.94	117.25	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	201	UOQ	C4A-C5A-N7A	-2.92	106.35	109.40
2	F	201	UOQ	C3B-C2B-C1B	2.92	106.35	99.89
2	A	201	UOQ	C2P-C3P-N4P	2.91	118.53	112.42
2	H	201	UOQ	CBW-CBX-CBY	-2.90	109.30	115.52
2	D	501	UOQ	C4A-C5A-N7A	-2.88	106.39	109.40
2	H	203	UOQ	P2A-O3A-P1A	-2.88	122.95	132.83
2	A	203	UOQ	CBW-CBX-CBY	-2.87	109.36	115.52
2	B	202	UOQ	C2P-S1P-CBW	2.86	106.49	101.71
2	D	501	UOQ	C3B-C2B-C1B	2.85	106.21	99.89
2	A	203	UOQ	CDP-CBP-CCP	2.84	112.86	108.23
2	H	201	UOQ	P2A-O3A-P1A	-2.84	123.09	132.83
2	E	204	UOQ	C3B-C2B-C1B	2.82	106.14	99.89
2	E	201	UOQ	O5P-C5P-N4P	-2.81	117.72	123.01
2	H	202	UOQ	C4A-C5A-N7A	-2.80	106.48	109.40
2	B	202	UOQ	O4B-C4B-C3B	2.78	110.82	104.87
2	H	202	UOQ	P2A-O3A-P1A	-2.77	123.33	132.83
2	H	202	UOQ	CAP-C9P-N8P	2.77	122.09	116.58
2	F	201	UOQ	O3B-C3B-C2B	2.75	121.64	111.68
2	A	201	UOQ	C2B-C3B-C4B	2.73	108.06	103.22
2	E	201	UOQ	C1B-N9A-C4A	-2.72	121.87	126.64
2	H	203	UOQ	O3B-C3B-C2B	2.70	121.48	111.68
2	E	204	UOQ	C2P-S1P-CBW	2.70	106.22	101.71
2	D	501	UOQ	O4B-C4B-C3B	2.70	110.64	104.87
2	A	203	UOQ	C4A-C5A-N7A	-2.68	106.61	109.40
2	F	201	UOQ	O3B-C3B-C4B	2.63	119.58	110.08
2	E	203	UOQ	C7P-C6P-C5P	2.61	116.71	112.36
2	B	201	UOQ	CEP-CBP-CCP	2.61	112.49	108.23
2	E	203	UOQ	C4A-C5A-N7A	-2.61	106.68	109.40
2	E	201	UOQ	C6P-C7P-N8P	2.60	117.14	111.90
2	E	204	UOQ	C4A-C5A-N7A	-2.59	106.70	109.40
2	C	201	UOQ	O5B-C5B-C4B	2.59	117.89	108.99
2	B	202	UOQ	O5B-C5B-C4B	2.58	117.89	108.99
2	H	201	UOQ	C4A-C5A-N7A	-2.56	106.74	109.40
2	D	501	UOQ	C6P-C7P-N8P	2.55	117.04	111.90
2	H	201	UOQ	O4B-C4B-C3B	2.54	110.31	104.87
2	F	201	UOQ	C7P-N8P-C9P	-2.54	118.06	122.59
2	D	501	UOQ	C2P-S1P-CBW	2.52	105.93	101.71
2	A	201	UOQ	CBW-CBX-CBY	-2.50	110.14	115.52
2	H	203	UOQ	C2B-C3B-C4B	2.50	107.66	103.22
2	E	201	UOQ	P2A-O3A-P1A	-2.48	124.31	132.83
2	H	201	UOQ	O4B-C1B-C2B	-2.48	103.30	106.93
2	A	203	UOQ	P2A-O3A-P1A	-2.48	124.33	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	UOQ	O4B-C1B-C2B	2.48	110.54	106.93
2	E	203	UOQ	O4B-C1B-C2B	-2.47	103.32	106.93
2	F	201	UOQ	O6A-CCP-CBP	2.46	114.50	110.55
2	E	204	UOQ	O4B-C4B-C3B	2.45	110.12	104.87
2	E	204	UOQ	CDP-CBP-CCP	2.45	112.22	108.23
2	H	201	UOQ	C3P-N4P-C5P	2.42	127.34	122.84
2	D	501	UOQ	C3P-N4P-C5P	2.40	127.29	122.84
2	H	202	UOQ	O3B-C3B-C2B	2.39	120.36	111.68
2	E	201	UOQ	CBW-CBX-CBY	-2.39	110.39	115.52
2	H	201	UOQ	O5B-C5B-C4B	2.34	117.05	108.99
2	H	202	UOQ	O4B-C1B-C2B	-2.33	103.52	106.93
2	A	201	UOQ	O5P-C5P-N4P	-2.33	118.62	123.01
2	E	204	UOQ	O5B-C5B-C4B	2.31	116.93	108.99
2	E	204	UOQ	C6P-C5P-N4P	2.31	120.30	116.42
2	H	203	UOQ	C6P-C5P-N4P	2.29	120.28	116.42
2	H	202	UOQ	C6P-C7P-N8P	2.28	116.50	111.90
2	H	201	UOQ	O6A-CCP-CBP	2.27	114.20	110.55
2	D	501	UOQ	O6A-CCP-CBP	2.26	114.18	110.55
2	B	202	UOQ	O3B-C3B-C4B	2.25	118.22	110.08
2	B	201	UOQ	CBW-CBX-CBY	-2.25	110.69	115.52
2	D	501	UOQ	CBW-CBX-CBY	-2.24	110.70	115.52
2	B	202	UOQ	O2B-C2B-C3B	2.23	117.50	111.17
2	A	203	UOQ	O4B-C4B-C3B	2.21	109.60	104.87
2	E	204	UOQ	C2B-C3B-C4B	2.19	107.11	103.22
2	F	201	UOQ	CEP-CBP-CCP	2.19	111.80	108.23
2	H	202	UOQ	C7P-C6P-C5P	2.16	115.96	112.36
2	B	201	UOQ	C3B-C2B-C1B	2.13	104.61	99.89
2	A	203	UOQ	C2P-C3P-N4P	2.12	116.88	112.42
2	C	201	UOQ	C7P-N8P-C9P	-2.09	118.86	122.59
2	F	201	UOQ	CBZ-CBY-CBX	2.08	119.94	114.60
2	B	201	UOQ	C6P-C5P-N4P	2.07	119.90	116.42
2	H	202	UOQ	CBX-CBW-S1P	2.07	121.56	113.75
2	E	203	UOQ	CDP-CBP-CCP	2.05	111.57	108.23
2	H	203	UOQ	CDP-CBP-CCP	2.05	111.57	108.23
2	B	202	UOQ	C4A-C5A-N7A	-2.03	107.28	109.40
2	H	202	UOQ	O7A-P3B-O3B	2.02	115.04	105.99
2	A	203	UOQ	OAP-CAP-CBP	-2.02	105.50	110.25
2	F	201	UOQ	O5B-C5B-C4B	2.02	115.94	108.99
2	E	203	UOQ	C2P-S1P-CBW	2.02	105.08	101.71
2	D	501	UOQ	CBZ-CBY-CBX	2.01	119.77	114.60

There are no chirality outliers.

All (237) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	UOQ	C5B-O5B-P1A-O2A
2	A	201	UOQ	S1P-C2P-C3P-N4P
2	A	201	UOQ	C4B-C5B-O5B-P1A
2	A	201	UOQ	N8P-C9P-CAP-OAP
2	A	201	UOQ	O9P-C9P-CAP-OAP
2	A	201	UOQ	OAP-CAP-CBP-CCP
2	A	201	UOQ	OAP-CAP-CBP-CDP
2	A	201	UOQ	OAP-CAP-CBP-CEP
2	A	201	UOQ	S1P-CBW-CBX-CBY
2	A	201	UOQ	OCH-CBX-CBY-CBZ
2	A	203	UOQ	CCP-O6A-P2A-O4A
2	A	203	UOQ	CCP-O6A-P2A-O5A
2	A	203	UOQ	O4B-C4B-C5B-O5B
2	A	203	UOQ	CAP-CBP-CCP-O6A
2	A	203	UOQ	CDP-CBP-CCP-O6A
2	A	203	UOQ	CEP-CBP-CCP-O6A
2	A	203	UOQ	CBW-CBX-CBY-CBZ
2	B	201	UOQ	CCP-O6A-P2A-O4A
2	B	201	UOQ	CCP-O6A-P2A-O5A
2	B	202	UOQ	P2A-O3A-P1A-O5B
2	B	202	UOQ	C5B-O5B-P1A-O2A
2	C	201	UOQ	CCP-O6A-P2A-O3A
2	C	201	UOQ	CCP-O6A-P2A-O4A
2	C	201	UOQ	C3B-C4B-C5B-O5B
2	C	201	UOQ	C4B-C5B-O5B-P1A
2	C	201	UOQ	S1P-CBW-CBX-OCH
2	D	501	UOQ	C5B-O5B-P1A-O3A
2	D	501	UOQ	CCP-O6A-P2A-O3A
2	D	501	UOQ	CCP-O6A-P2A-O4A
2	D	501	UOQ	C4B-C5B-O5B-P1A
2	D	501	UOQ	CAP-CBP-CCP-O6A
2	D	501	UOQ	CDP-CBP-CCP-O6A
2	D	501	UOQ	S1P-CBW-CBX-OCH
2	E	201	UOQ	C5B-O5B-P1A-O2A
2	E	201	UOQ	C5B-O5B-P1A-O3A
2	E	201	UOQ	CBX-CBW-S1P-C2P
2	E	201	UOQ	S1P-C2P-C3P-N4P
2	E	201	UOQ	C3B-C4B-C5B-O5B
2	E	201	UOQ	C4B-C5B-O5B-P1A
2	E	201	UOQ	C5P-C6P-C7P-N8P
2	E	201	UOQ	CAP-C9P-N8P-C7P
2	E	201	UOQ	O9P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
2	E	201	UOQ	OAP-CAP-CBP-CCP
2	E	201	UOQ	OAP-CAP-CBP-CEP
2	E	201	UOQ	S1P-CBW-CBX-OCH
2	E	203	UOQ	P2A-O3A-P1A-O5B
2	E	203	UOQ	C5B-O5B-P1A-O2A
2	E	203	UOQ	CAP-CBP-CCP-O6A
2	E	203	UOQ	CDP-CBP-CCP-O6A
2	E	203	UOQ	CEP-CBP-CCP-O6A
2	E	203	UOQ	S1P-CBW-CBX-OCH
2	E	204	UOQ	CBX-CBW-S1P-C2P
2	E	204	UOQ	CCP-O6A-P2A-O4A
2	E	204	UOQ	CCP-O6A-P2A-O5A
2	E	204	UOQ	S1P-C2P-C3P-N4P
2	E	204	UOQ	C5P-C6P-C7P-N8P
2	F	201	UOQ	C3P-C2P-S1P-CBW
2	F	201	UOQ	P1A-O3A-P2A-O6A
2	F	201	UOQ	S1P-CBW-CBX-CBY
2	F	201	UOQ	OCH-CBX-CBY-CBZ
2	H	201	UOQ	C5B-O5B-P1A-O1A
2	H	201	UOQ	C5B-O5B-P1A-O2A
2	H	201	UOQ	CCP-O6A-P2A-O5A
2	H	201	UOQ	C2P-C3P-N4P-C5P
2	H	201	UOQ	C3B-C4B-C5B-O5B
2	H	201	UOQ	O4B-C4B-C5B-O5B
2	H	201	UOQ	S1P-CBW-CBX-OCH
2	H	201	UOQ	CBW-CBX-CBY-CBZ
2	H	202	UOQ	C5B-O5B-P1A-O3A
2	H	202	UOQ	CCP-O6A-P2A-O3A
2	H	202	UOQ	CCP-O6A-P2A-O4A
2	H	202	UOQ	C4B-C5B-O5B-P1A
2	H	202	UOQ	O9P-C9P-CAP-OAP
2	H	202	UOQ	CAP-CBP-CCP-O6A
2	H	203	UOQ	C5B-O5B-P1A-O2A
2	H	203	UOQ	C2B-C3B-O3B-P3B
2	E	201	UOQ	O9P-C9P-N8P-C7P
2	D	501	UOQ	CBY-CBZ-CCA-CCB
2	H	202	UOQ	CBZ-CCA-CCB-CCC
2	A	203	UOQ	C3B-C4B-C5B-O5B
2	B	202	UOQ	C3B-C4B-C5B-O5B
2	B	202	UOQ	O4B-C4B-C5B-O5B
2	D	501	UOQ	C3B-C4B-C5B-O5B
2	E	201	UOQ	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	F	201	UOQ	O4B-C4B-C5B-O5B
2	H	202	UOQ	C3B-C4B-C5B-O5B
2	H	202	UOQ	O4B-C4B-C5B-O5B
2	H	203	UOQ	C3B-C4B-C5B-O5B
2	H	203	UOQ	O4B-C4B-C5B-O5B
2	B	202	UOQ	C2B-C3B-O3B-P3B
2	E	201	UOQ	C4B-C3B-O3B-P3B
2	F	201	UOQ	C4B-C3B-O3B-P3B
2	C	201	UOQ	O4B-C4B-C5B-O5B
2	D	501	UOQ	CCC-CCD-CCE-CCF
2	E	201	UOQ	CBW-CBX-CBY-CBZ
2	B	202	UOQ	C4B-C3B-O3B-P3B
2	H	203	UOQ	CCD-CCE-CCF-CCG
2	A	203	UOQ	CBX-CBY-CBZ-CCA
2	B	201	UOQ	CBX-CBY-CBZ-CCA
2	F	201	UOQ	CBX-CBY-CBZ-CCA
2	B	201	UOQ	CCB-CCC-CCD-CCE
2	E	203	UOQ	CCA-CCB-CCC-CCD
2	D	501	UOQ	CEP-CBP-CCP-O6A
2	H	202	UOQ	CDP-CBP-CCP-O6A
2	H	202	UOQ	CEP-CBP-CCP-O6A
2	E	201	UOQ	CCA-CCB-CCC-CCD
2	D	501	UOQ	CCA-CCB-CCC-CCD
2	A	203	UOQ	CBY-CBZ-CCA-CCB
2	C	201	UOQ	CCC-CCD-CCE-CCF
2	E	201	UOQ	CCB-CCC-CCD-CCE
2	F	201	UOQ	CBY-CBZ-CCA-CCB
2	B	202	UOQ	CCA-CCB-CCC-CCD
2	H	203	UOQ	CCB-CCC-CCD-CCE
2	E	201	UOQ	OCH-CBX-CBY-CBZ
2	B	201	UOQ	CCA-CCB-CCC-CCD
2	H	201	UOQ	CCC-CCD-CCE-CCF
2	H	202	UOQ	CBY-CBZ-CCA-CCB
2	H	203	UOQ	CCC-CCD-CCE-CCF
2	E	204	UOQ	CCB-CCC-CCD-CCE
2	H	202	UOQ	CCA-CCB-CCC-CCD
2	F	201	UOQ	C2B-C3B-O3B-P3B
2	E	203	UOQ	CBX-CBY-CBZ-CCA
2	E	201	UOQ	CCC-CCD-CCE-CCF
2	C	201	UOQ	CCB-CCC-CCD-CCE
2	A	201	UOQ	C3B-C4B-C5B-O5B
2	C	201	UOQ	CCA-CCB-CCC-CCD

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Mol	Chain	Res	Type	Atoms
2	E	201	UOQ	CBY-CBZ-CCA-CCB
2	B	202	UOQ	CCD-CCE-CCF-CCG
2	H	202	UOQ	CCB-CCC-CCD-CCE
2	C	201	UOQ	CCD-CCE-CCF-CCG
2	E	204	UOQ	CCD-CCE-CCF-CCG
2	B	202	UOQ	CCC-CCD-CCE-CCF
2	B	201	UOQ	CCD-CCE-CCF-CCG
2	F	201	UOQ	C3B-C4B-C5B-O5B
2	E	204	UOQ	CCC-CCD-CCE-CCF
2	E	204	UOQ	CBZ-CCA-CCB-CCC
2	E	203	UOQ	CBZ-CCA-CCB-CCC
2	E	201	UOQ	OAP-CAP-CBP-CDP
2	A	201	UOQ	CCD-CCE-CCF-CCG
2	E	201	UOQ	CCD-CCE-CCF-CCG
2	E	203	UOQ	CCC-CCD-CCE-CCF
2	B	202	UOQ	CCB-CCC-CCD-CCE
2	A	201	UOQ	CBY-CBZ-CCA-CCB
2	A	203	UOQ	CCC-CCD-CCE-CCF
2	D	501	UOQ	O4B-C4B-C5B-O5B
2	E	204	UOQ	CCA-CCB-CCC-CCD
2	H	201	UOQ	C4B-C5B-O5B-P1A
2	A	203	UOQ	CCA-CCB-CCC-CCD
2	E	201	UOQ	N8P-C9P-CAP-CBP
2	E	201	UOQ	C2B-C3B-O3B-P3B
2	B	201	UOQ	P2A-O3A-P1A-O5B
2	E	204	UOQ	P1A-O3A-P2A-O6A
2	F	201	UOQ	C3B-O3B-P3B-O9A
2	E	204	UOQ	S1P-CBW-CBX-OCH
2	B	202	UOQ	C5B-O5B-P1A-O3A
2	C	201	UOQ	C5B-O5B-P1A-O3A
2	E	203	UOQ	C5B-O5B-P1A-O3A
2	H	201	UOQ	CCP-O6A-P2A-O3A
2	H	202	UOQ	C3B-O3B-P3B-O8A
2	H	203	UOQ	C5B-O5B-P1A-O3A
2	E	201	UOQ	CBZ-CCA-CCB-CCC
2	B	202	UOQ	C5B-O5B-P1A-O1A
2	C	201	UOQ	C5B-O5B-P1A-O2A
2	C	201	UOQ	CCP-O6A-P2A-O5A
2	D	501	UOQ	C5B-O5B-P1A-O1A
2	D	501	UOQ	C5B-O5B-P1A-O2A
2	D	501	UOQ	CCP-O6A-P2A-O5A
2	E	203	UOQ	C5B-O5B-P1A-O1A

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Mol	Chain	Res	Type	Atoms
2	H	201	UOQ	CCP-O6A-P2A-O4A
2	H	202	UOQ	C5B-O5B-P1A-O2A
2	H	202	UOQ	CCP-O6A-P2A-O5A
2	H	203	UOQ	CCA-CCB-CCC-CCD
2	H	201	UOQ	O5P-C5P-C6P-C7P
2	H	201	UOQ	N4P-C5P-C6P-C7P
2	A	201	UOQ	CBX-CBY-CBZ-CCA
2	D	501	UOQ	O9P-C9P-CAP-OAP
2	A	203	UOQ	CCD-CCE-CCF-CCG
2	C	201	UOQ	OCH-CBX-CBY-CBZ
2	H	203	UOQ	OCH-CBX-CBY-CBZ
2	C	201	UOQ	CEP-CBP-CCP-O6A
2	H	203	UOQ	CBY-CBZ-CCA-CCB
2	H	203	UOQ	CBZ-CCA-CCB-CCC
2	C	201	UOQ	CBX-CBY-CBZ-CCA
2	A	203	UOQ	P1A-O3A-P2A-O4A
2	C	201	UOQ	P1A-O3A-P2A-O5A
2	H	201	UOQ	P2A-O3A-P1A-O1A
2	E	204	UOQ	CBX-CBY-CBZ-CCA
2	H	201	UOQ	CCB-CCC-CCD-CCE
2	A	201	UOQ	O9P-C9P-CAP-CBP
2	A	201	UOQ	N8P-C9P-CAP-CBP
2	B	202	UOQ	OCH-CBX-CBY-CBZ
2	D	501	UOQ	CBW-CBX-CBY-CBZ
2	H	201	UOQ	CBY-CBZ-CCA-CCB
2	A	203	UOQ	C3P-C2P-S1P-CBW
2	B	201	UOQ	OCH-CBX-CBY-CBZ
2	E	201	UOQ	O5P-C5P-C6P-C7P
2	A	201	UOQ	CBX-CBW-S1P-C2P
2	A	203	UOQ	CBX-CBW-S1P-C2P
2	E	201	UOQ	P2A-O3A-P1A-O2A
2	H	202	UOQ	CCD-CCE-CCF-CCG
2	E	203	UOQ	O4B-C4B-C5B-O5B
2	E	204	UOQ	O4B-C4B-C5B-O5B
2	E	204	UOQ	OCH-CBX-CBY-CBZ
2	E	204	UOQ	C3B-C4B-C5B-O5B
2	D	501	UOQ	C3B-O3B-P3B-O9A
2	E	201	UOQ	N8P-C9P-CAP-OAP
2	C	201	UOQ	CDP-CBP-CCP-O6A
2	F	201	UOQ	CCB-CCC-CCD-CCE
2	D	501	UOQ	S1P-C2P-C3P-N4P
2	E	203	UOQ	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
2	F	201	UOQ	CCC-CCD-CCE-CCF
2	B	201	UOQ	S1P-CBW-CBX-CBY
2	E	204	UOQ	CBY-CBZ-CCA-CCB
2	A	201	UOQ	C5B-O5B-P1A-O3A
2	A	201	UOQ	C3B-O3B-P3B-O7A
2	A	203	UOQ	CCP-O6A-P2A-O3A
2	A	203	UOQ	C3B-O3B-P3B-O8A
2	B	201	UOQ	CCP-O6A-P2A-O3A
2	B	201	UOQ	C3B-O3B-P3B-O8A
2	E	204	UOQ	CCP-O6A-P2A-O3A
2	E	204	UOQ	C3B-O3B-P3B-O8A
2	F	201	UOQ	C5B-O5B-P1A-O3A
2	F	201	UOQ	C3B-O3B-P3B-O8A
2	H	201	UOQ	C5B-O5B-P1A-O3A
2	B	201	UOQ	CBY-CBZ-CCA-CCB
2	B	201	UOQ	O4B-C4B-C5B-O5B
2	A	203	UOQ	P1A-O3A-P2A-O5A
2	D	501	UOQ	P2A-O3A-P1A-O1A
2	D	501	UOQ	P2A-O3A-P1A-O2A
2	E	203	UOQ	P2A-O3A-P1A-O2A
2	E	204	UOQ	P2A-O3A-P1A-O1A
2	H	201	UOQ	P2A-O3A-P1A-O2A
2	A	203	UOQ	CBP-CCP-O6A-P2A
2	A	203	UOQ	C5B-O5B-P1A-O2A
2	B	201	UOQ	C5B-O5B-P1A-O1A
2	E	201	UOQ	O9P-C9P-CAP-CBP
2	E	201	UOQ	N4P-C5P-C6P-C7P

There are no ring outliers.

13 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	202	UOQ	4	0
2	C	201	UOQ	9	0
2	H	203	UOQ	4	0
2	D	501	UOQ	8	0
2	H	201	UOQ	1	0
2	E	203	UOQ	6	0
2	A	201	UOQ	10	0
2	B	202	UOQ	4	0
2	F	201	UOQ	10	0
2	E	204	UOQ	6	0

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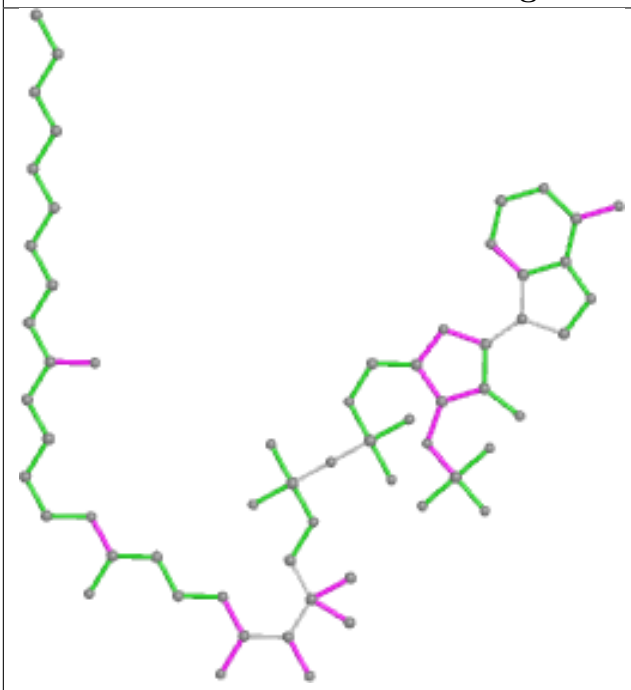
Continued from previous page...

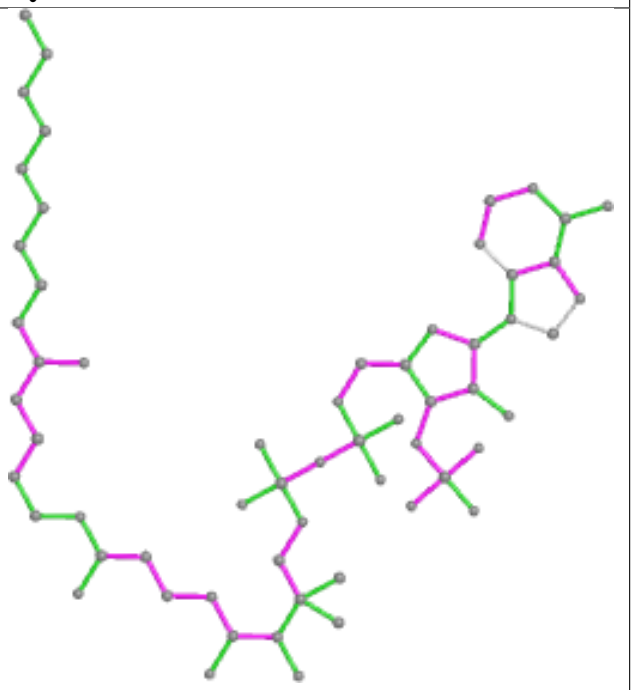
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	UOQ	6	0
2	B	201	UOQ	1	0
2	A	203	UOQ	12	0

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.

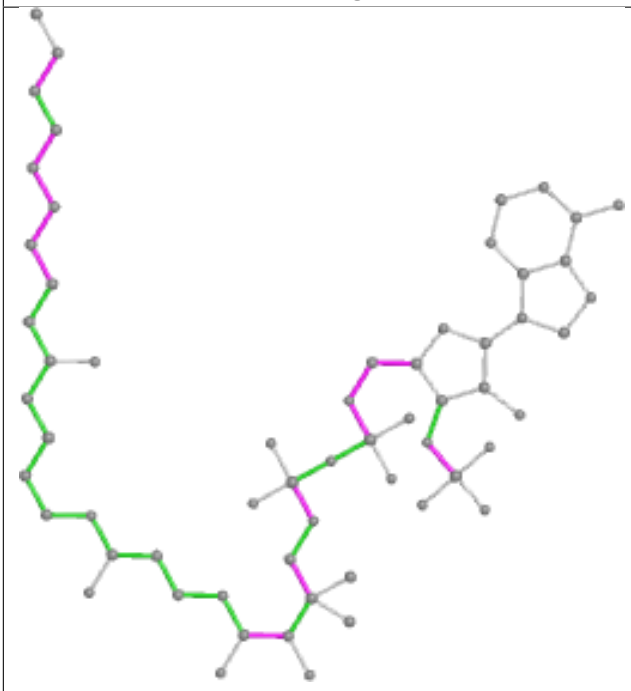
Ligand UOQ H 202



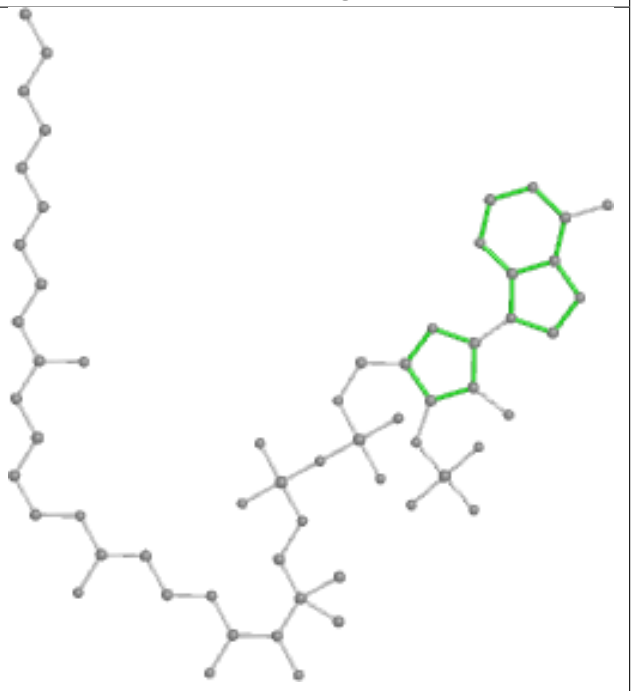
Bond lengths



Bond angles

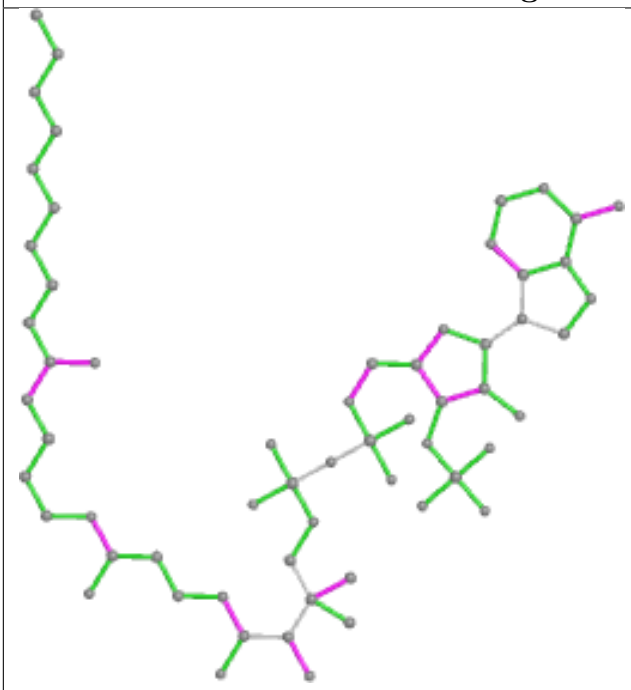


Torsions

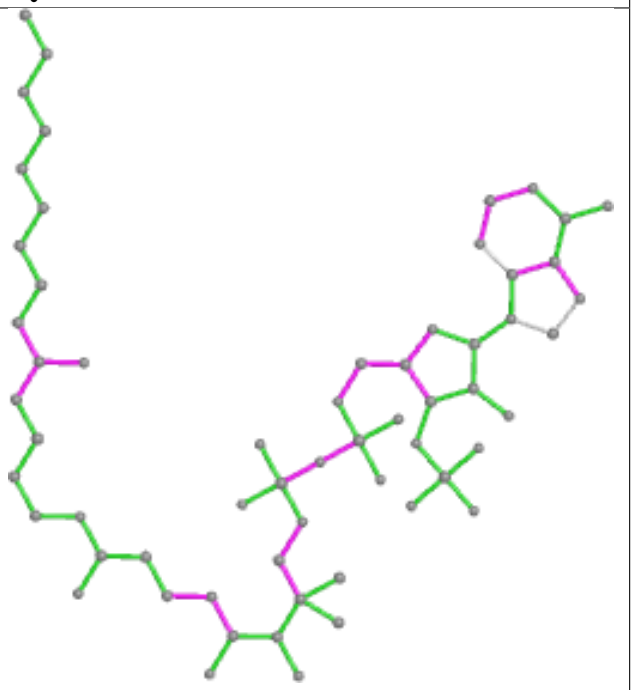


Rings

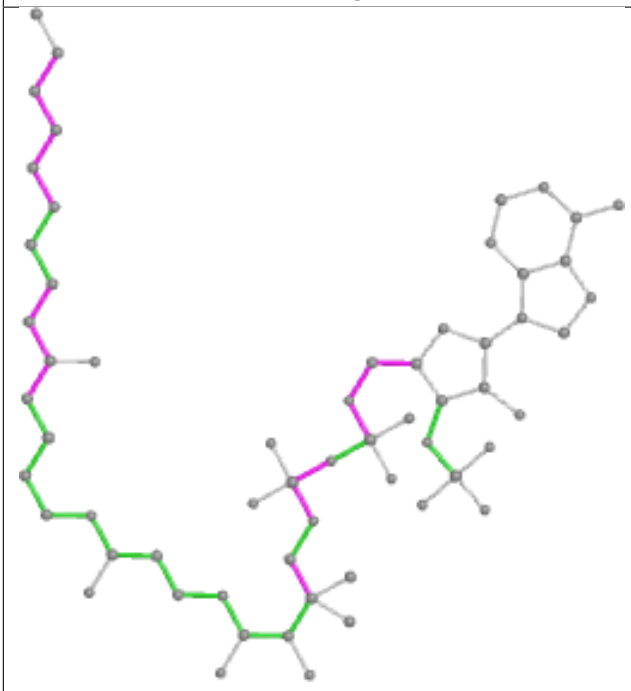
Ligand UOQ C 201



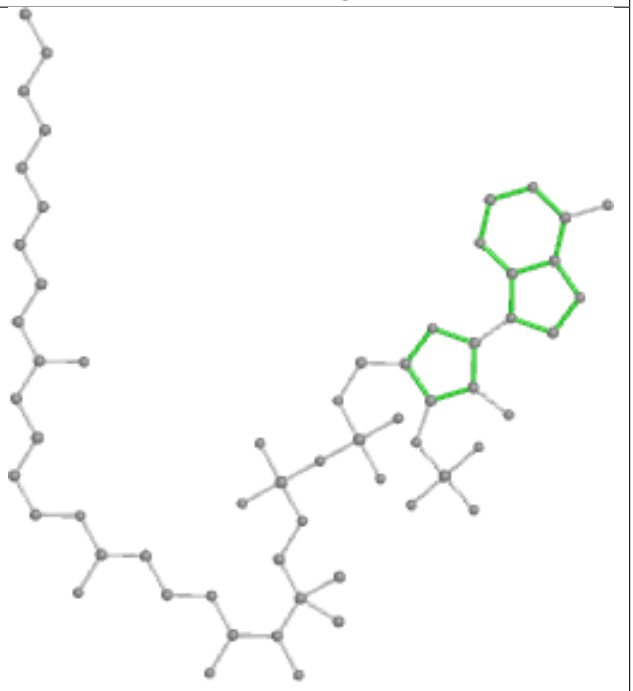
Bond lengths



Bond angles

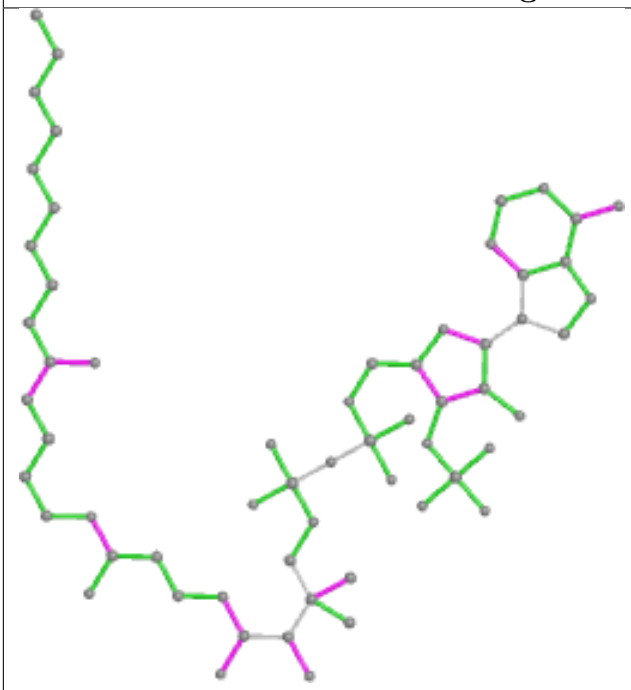


Torsions

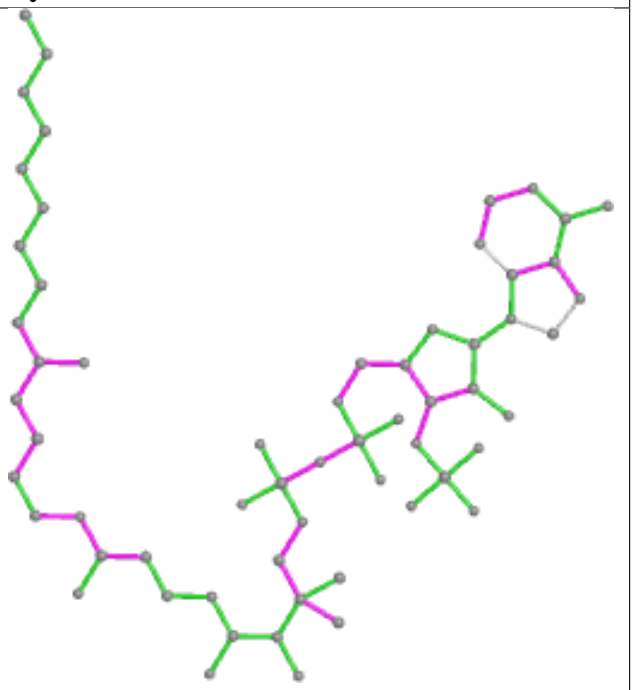


Rings

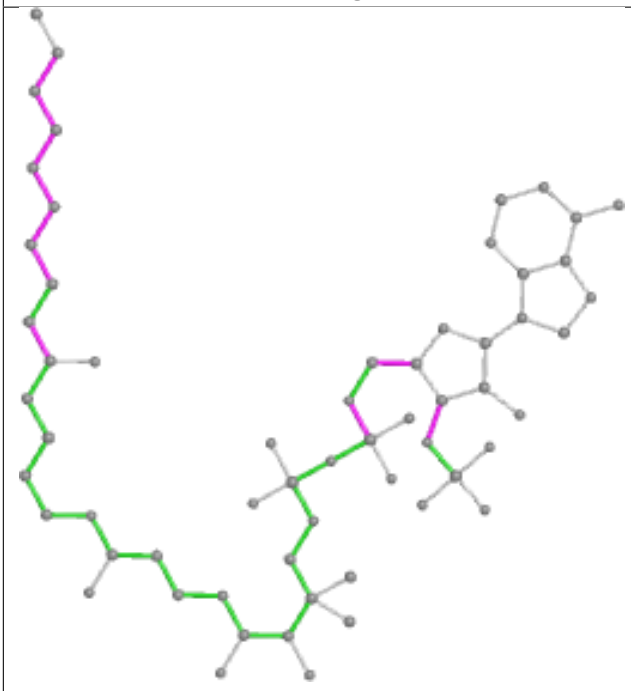
Ligand UOQ H 203



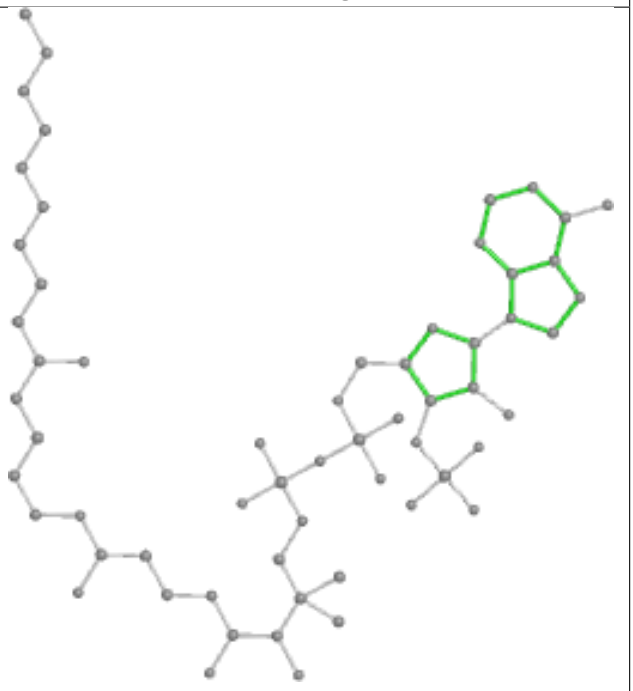
Bond lengths



Bond angles

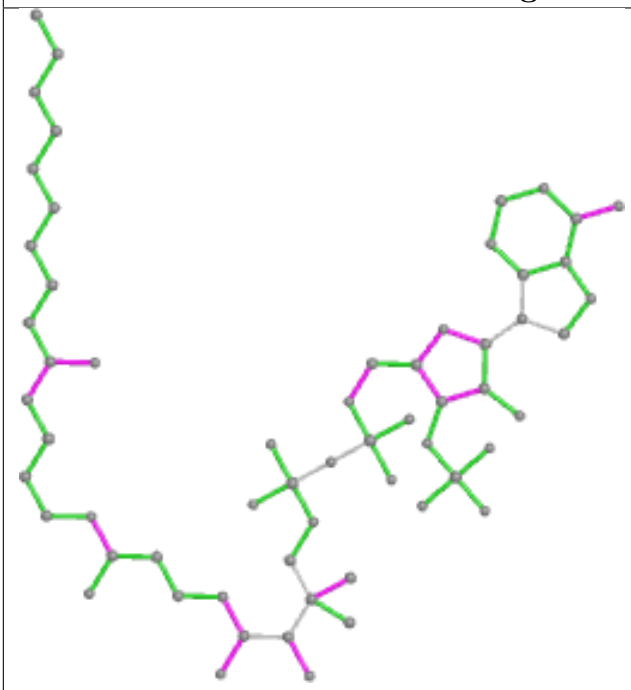


Torsions

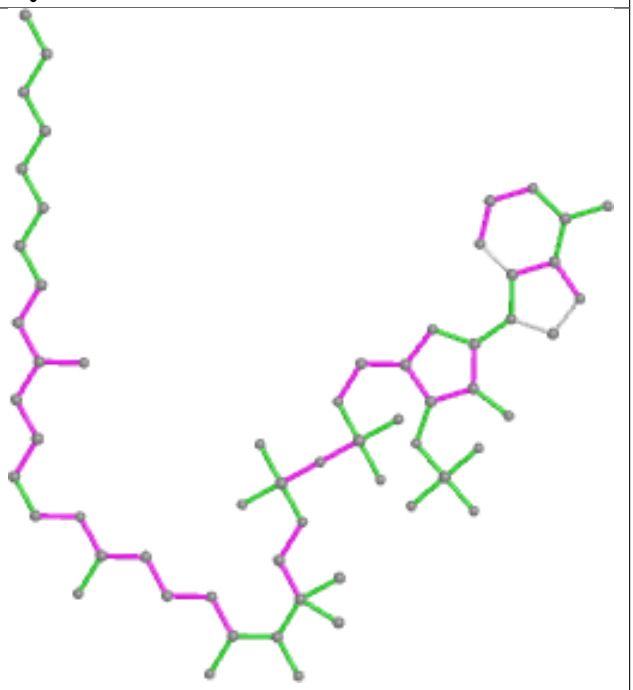


Rings

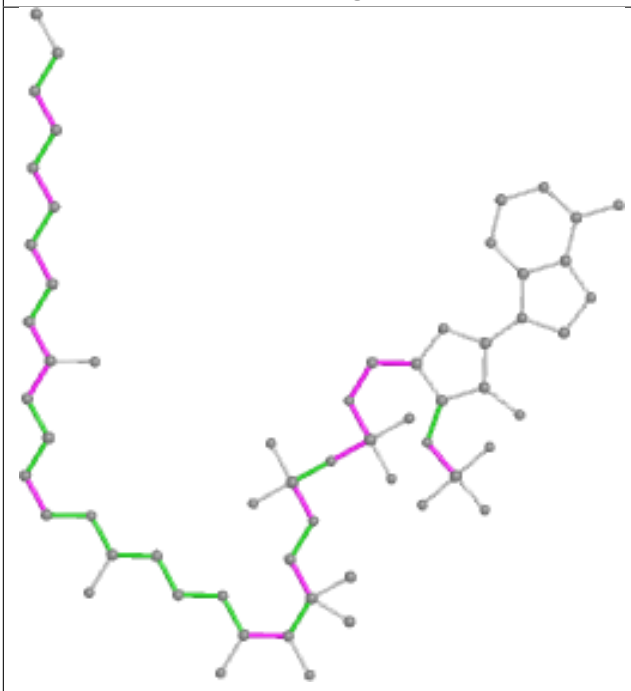
Ligand UOQ D 501



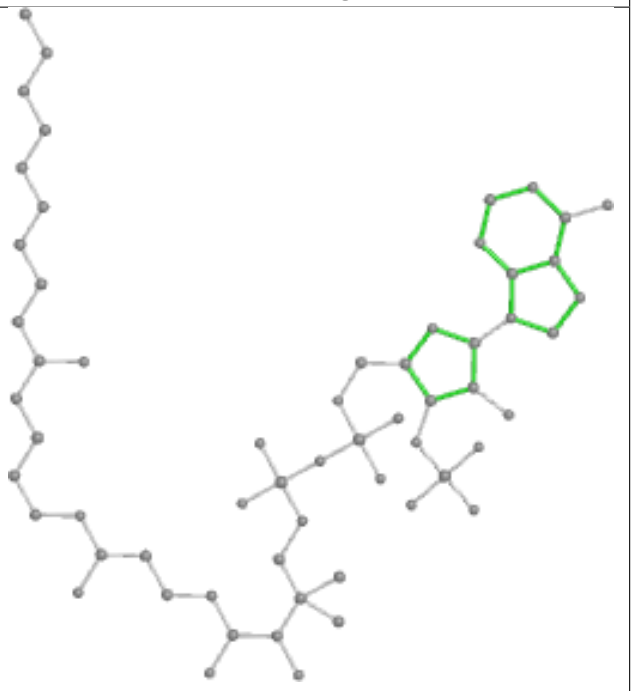
Bond lengths



Bond angles

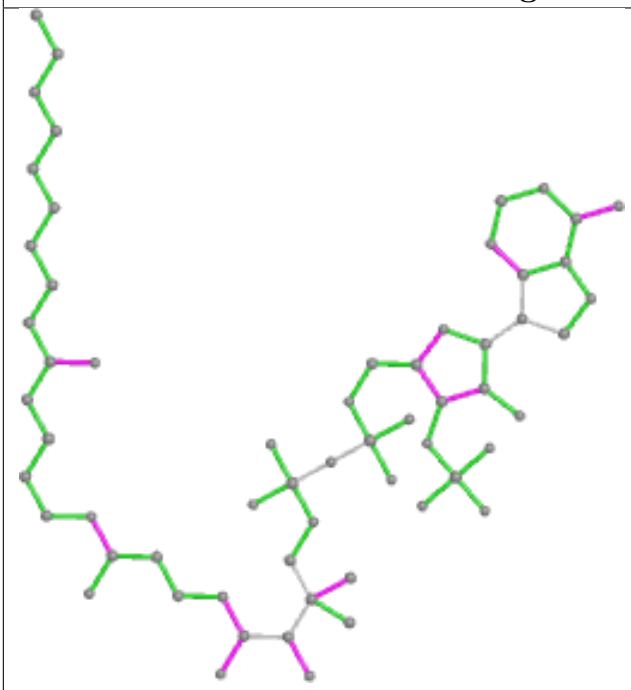


Torsions

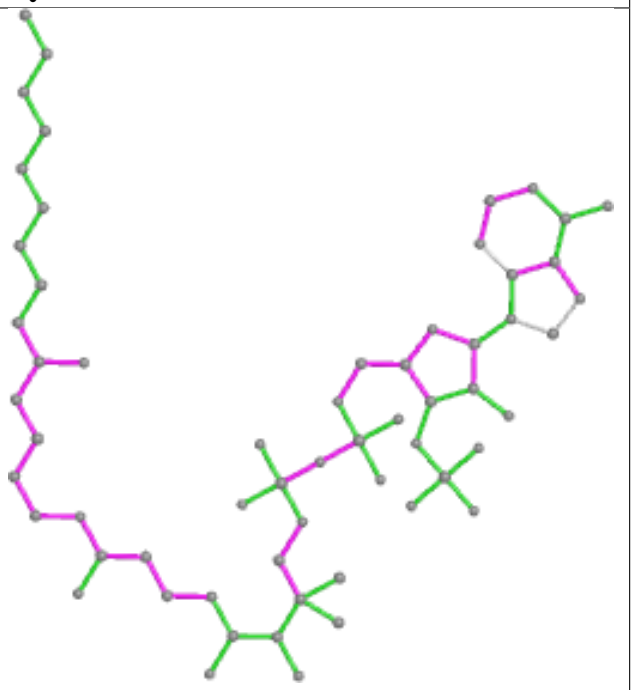


Rings

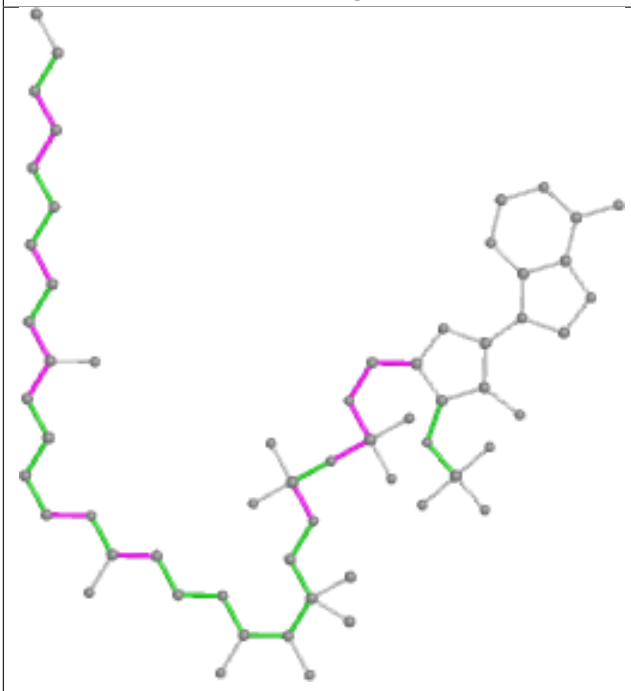
Ligand UOQ H 201



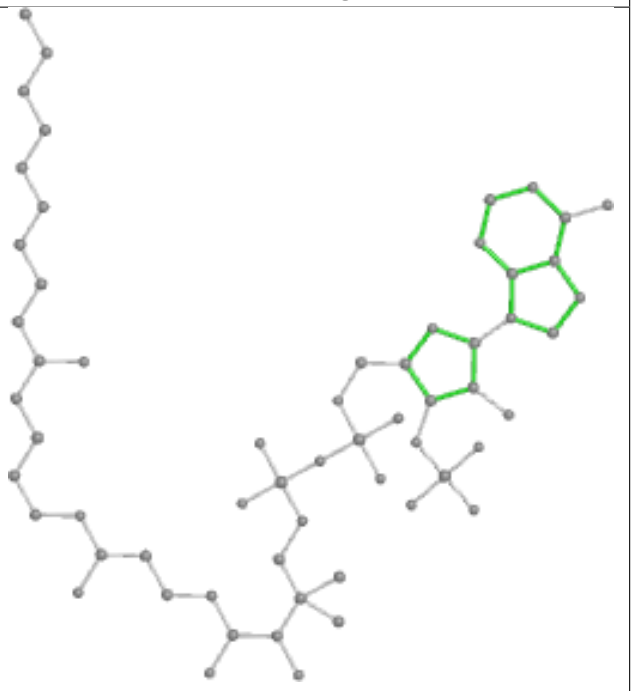
Bond lengths



Bond angles

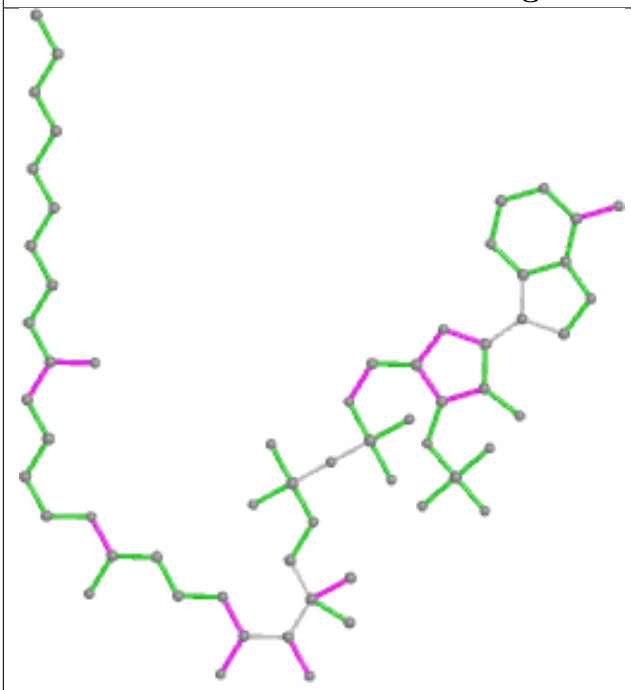


Torsions



Rings

Ligand UOQ E 203



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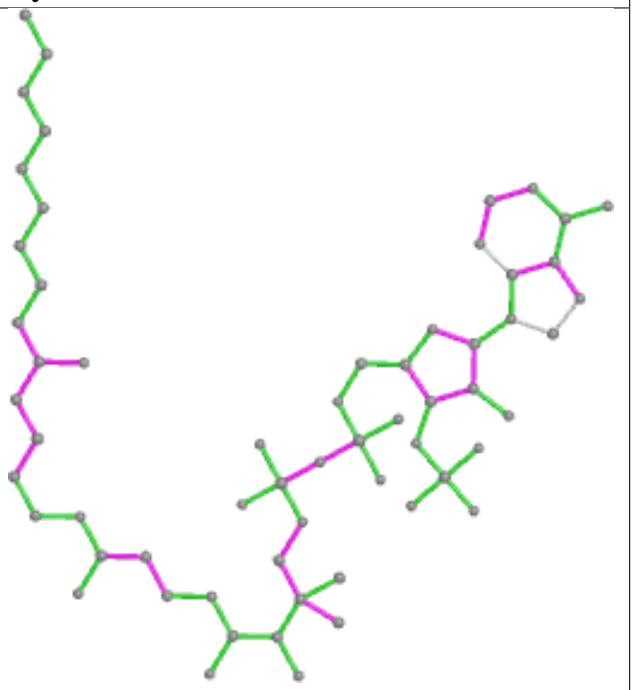
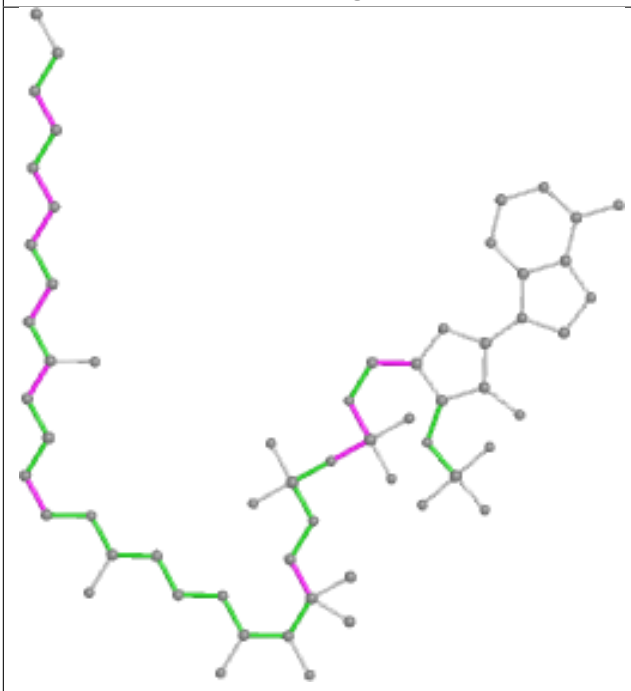


Bond angles



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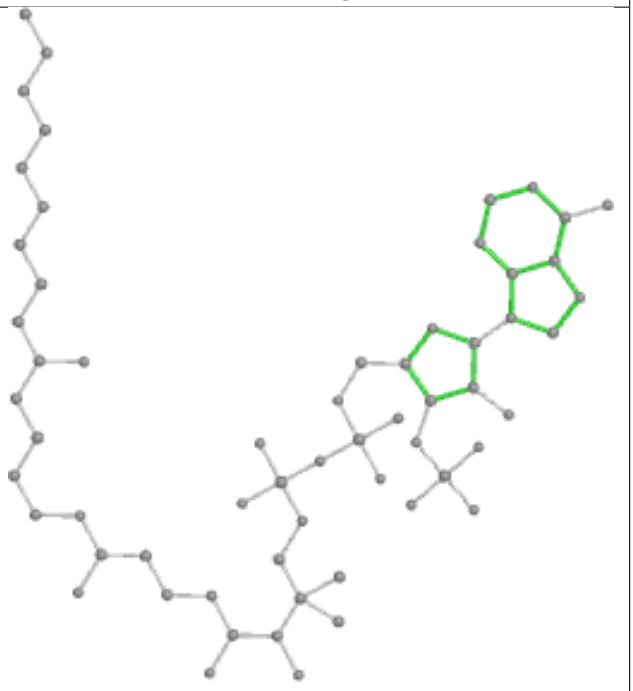
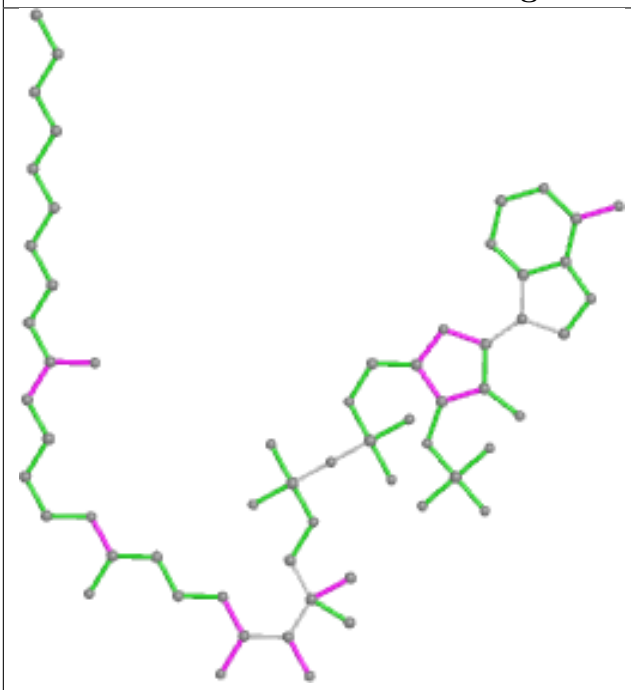


Rings

Ligand UOQ A 201



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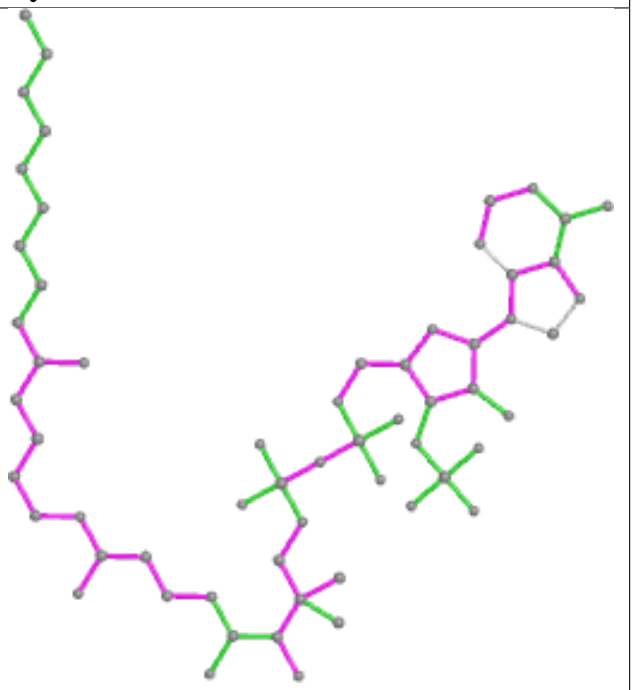
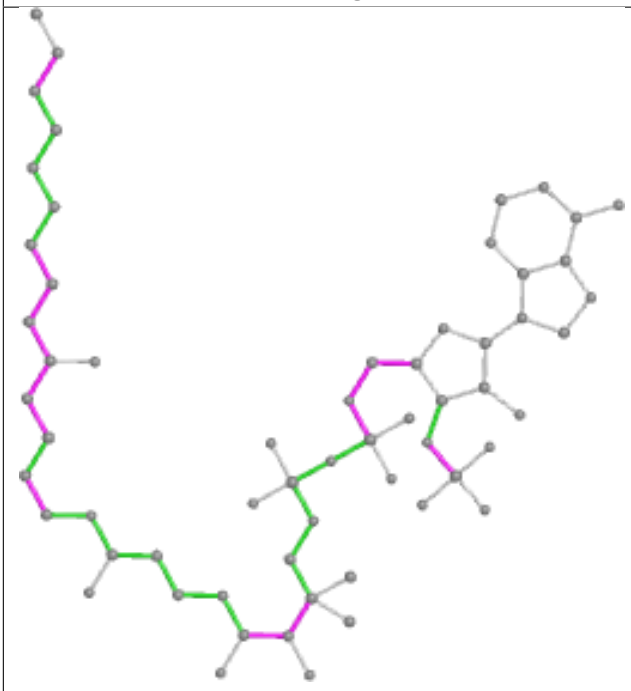
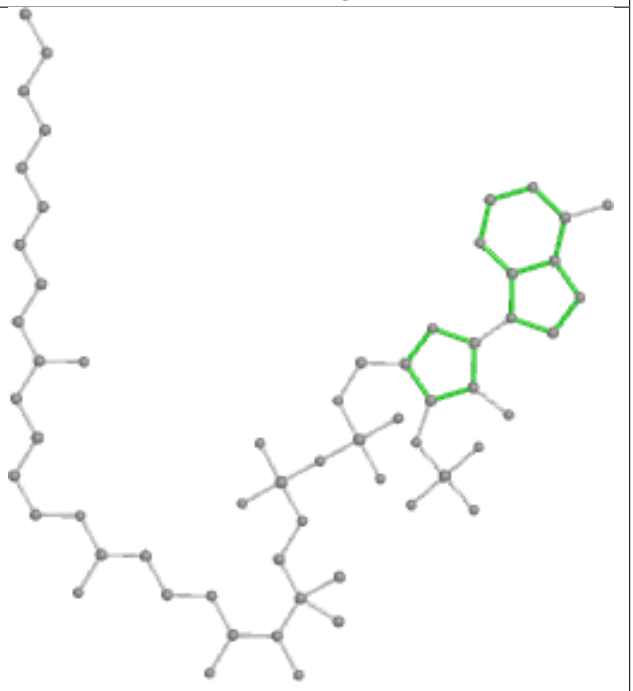


Bond angles

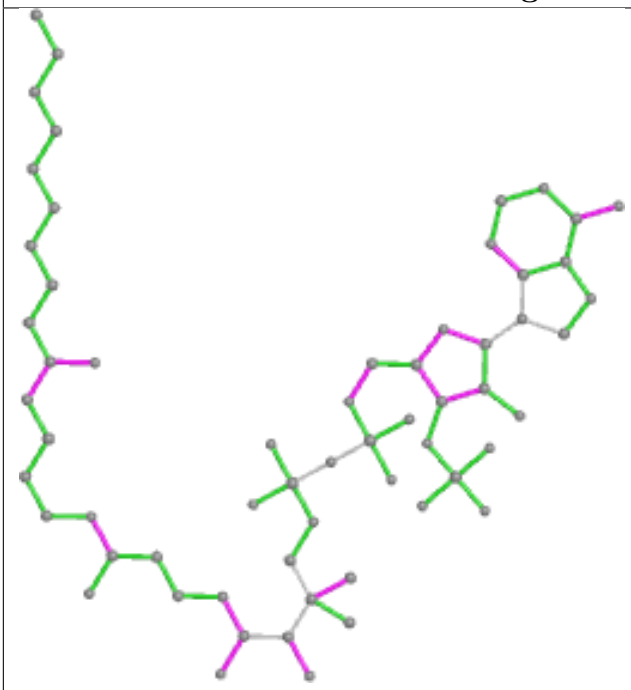


Torsions

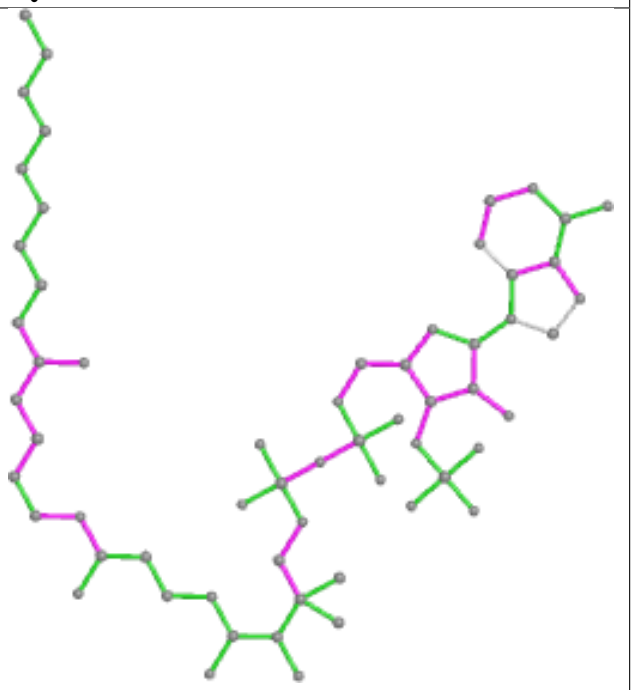


Rings

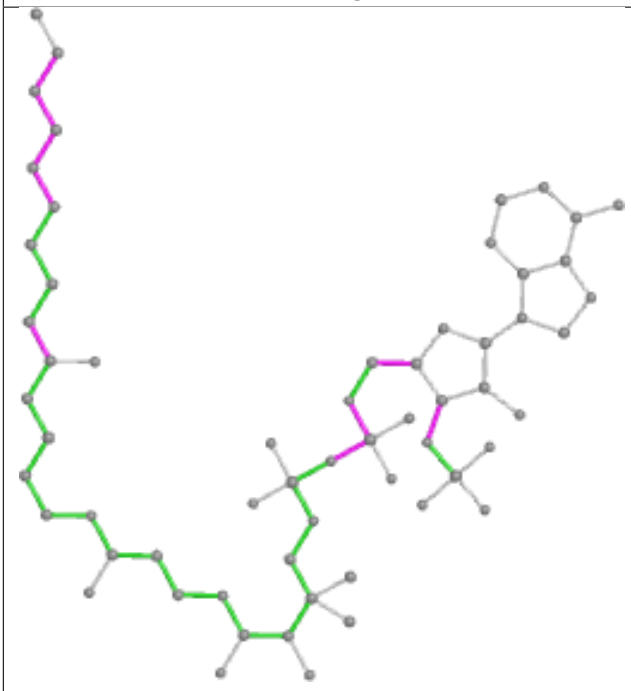
Ligand UOQ B 202



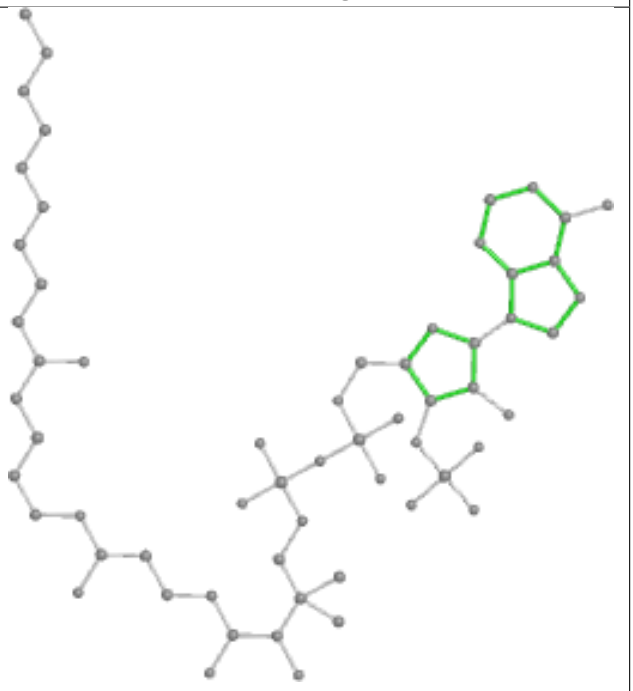
Bond lengths



Bond angles

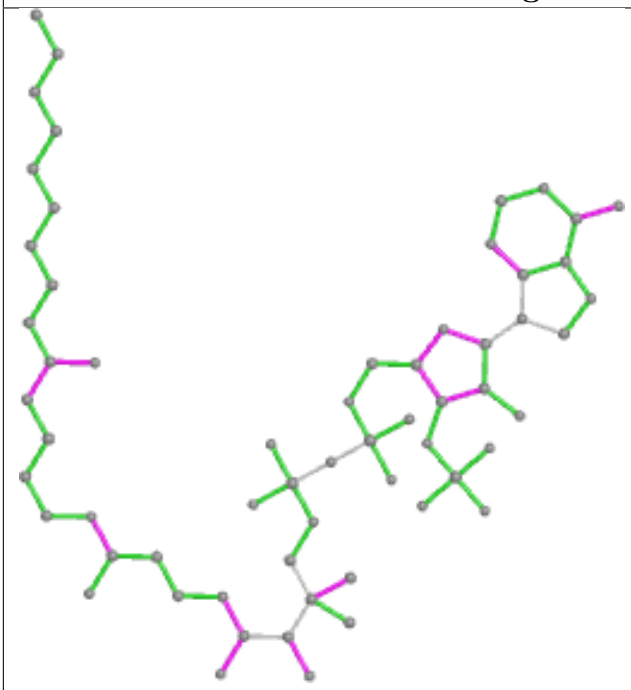


Torsions

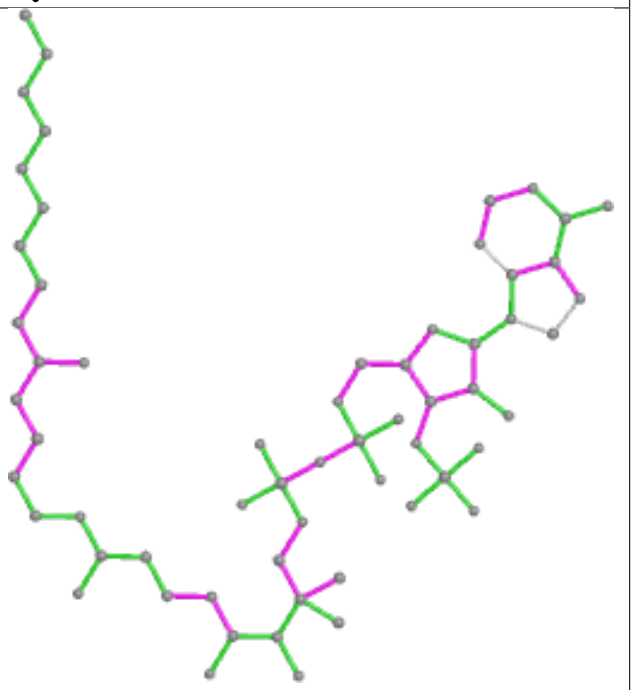


Rings

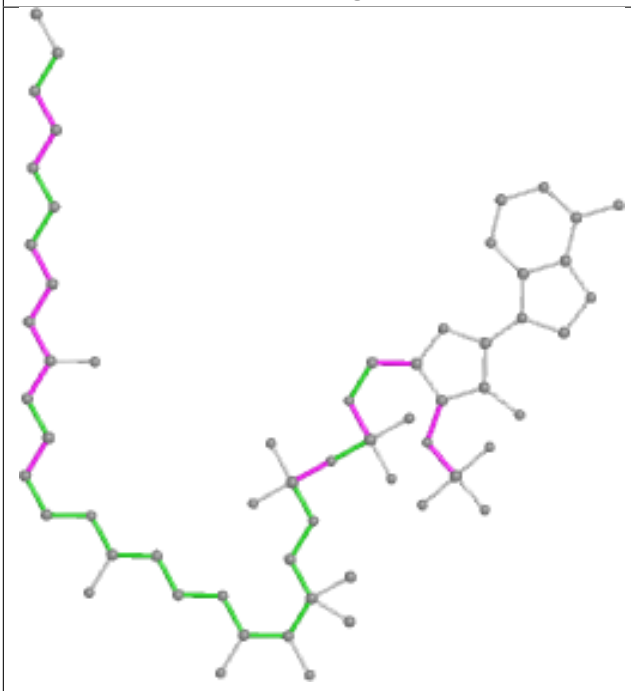
Ligand UOQ F 201



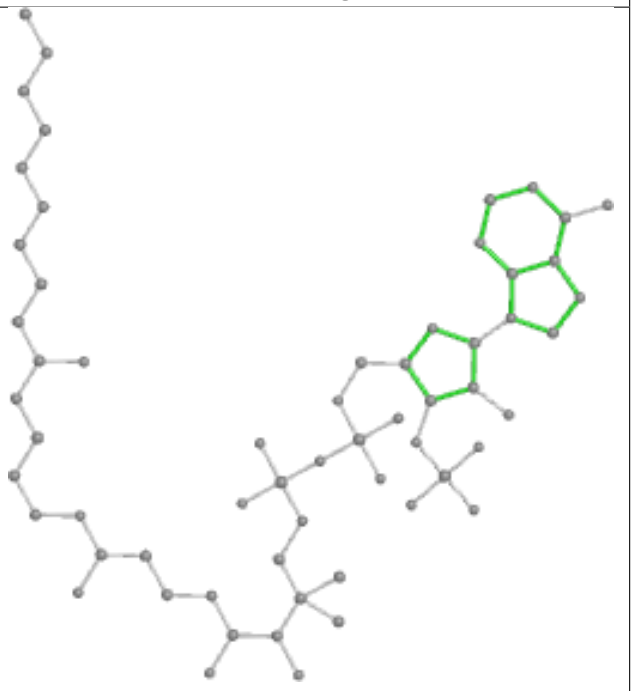
Bond lengths



Bond angles

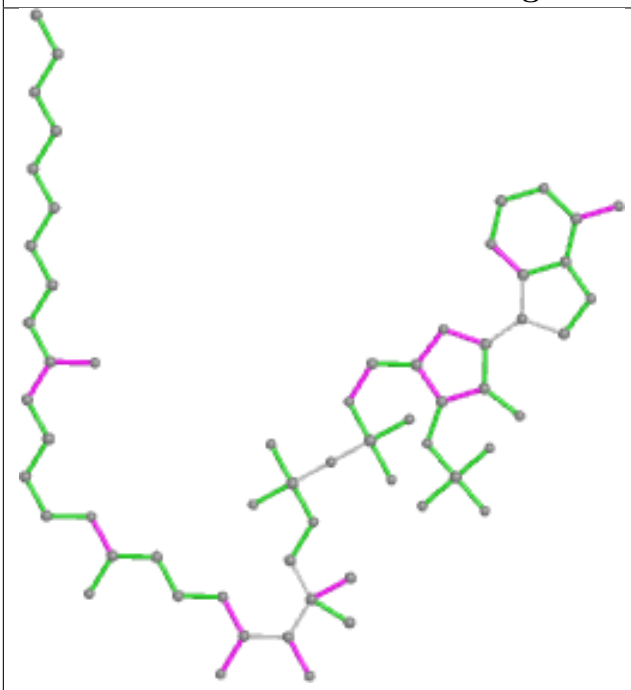


Torsions



Rings

Ligand UOQ E 204



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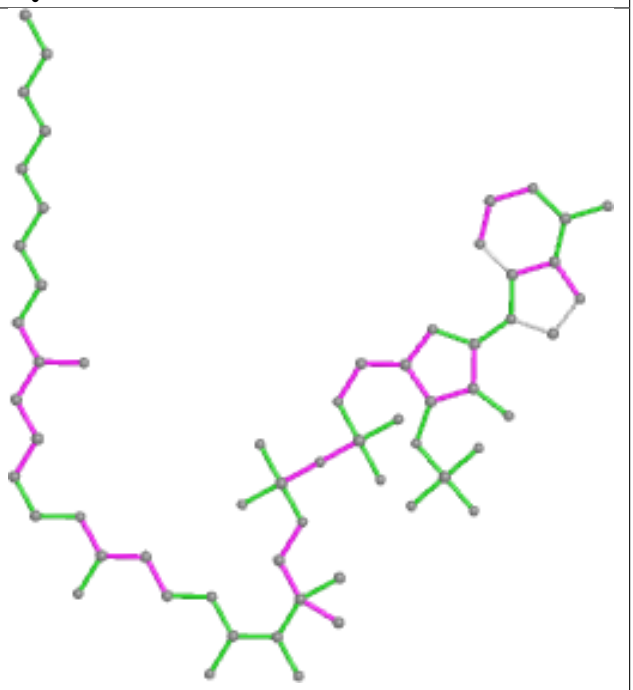
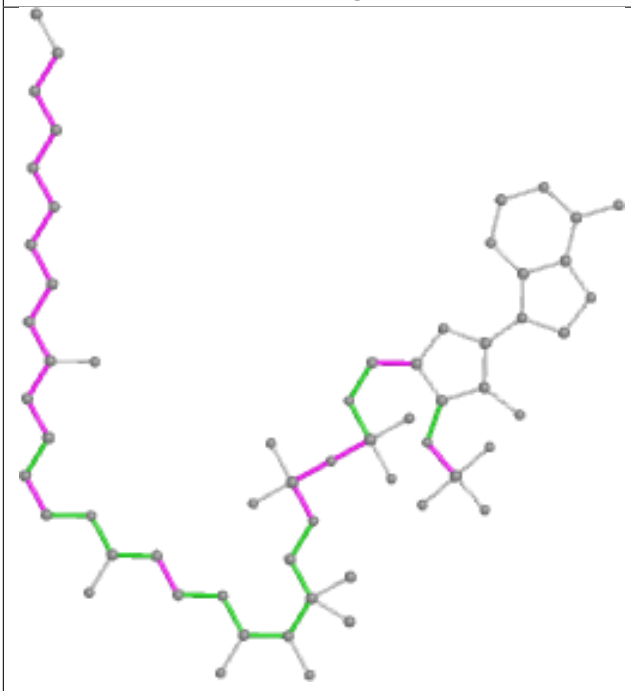
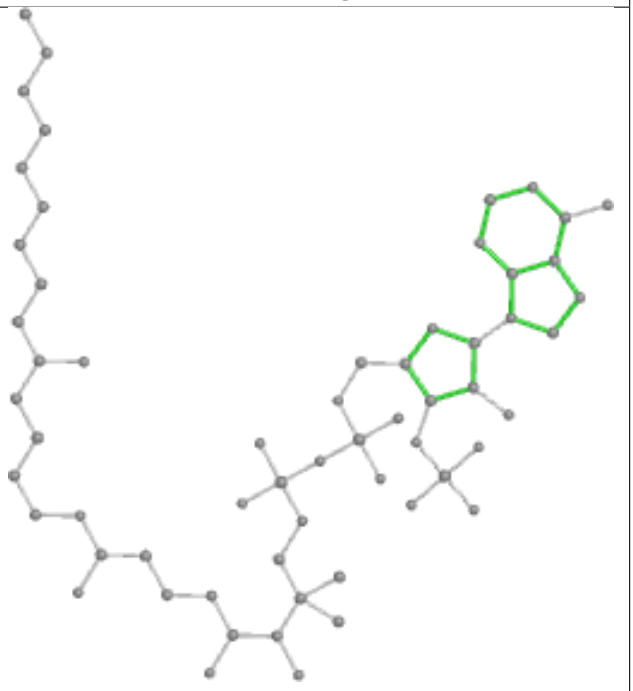


Bond angles

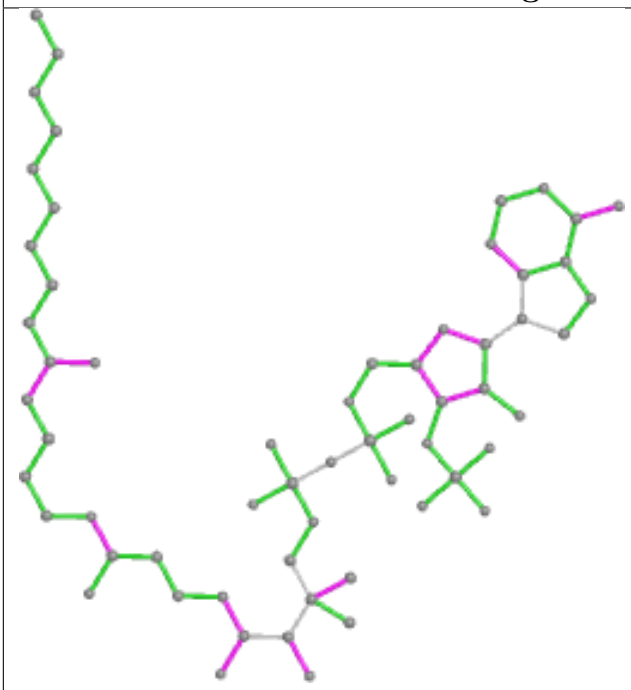


Torsions

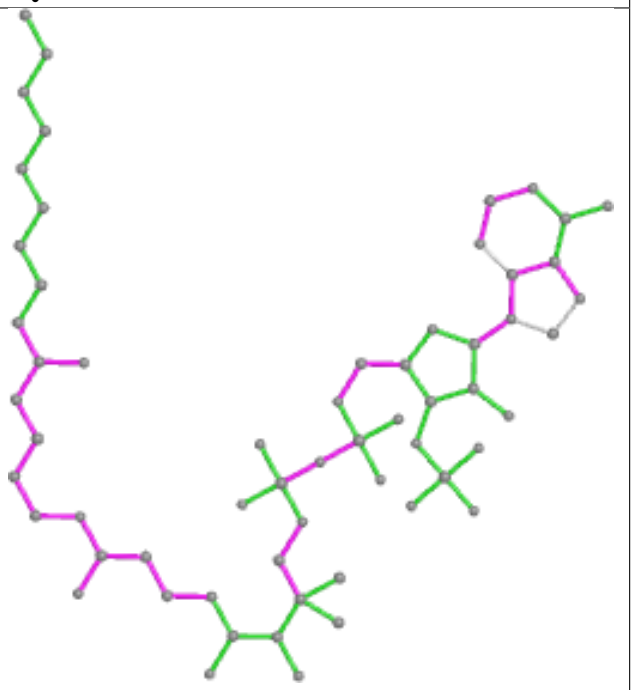


Rings

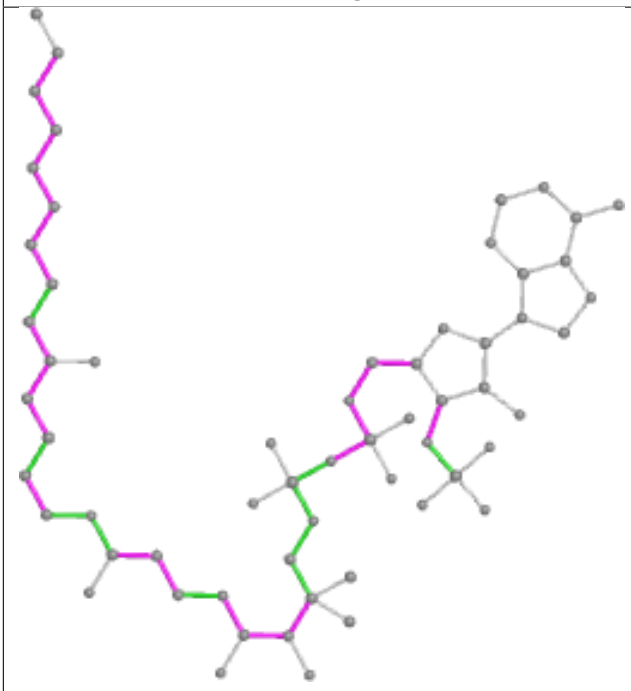
Ligand UOQ E 201



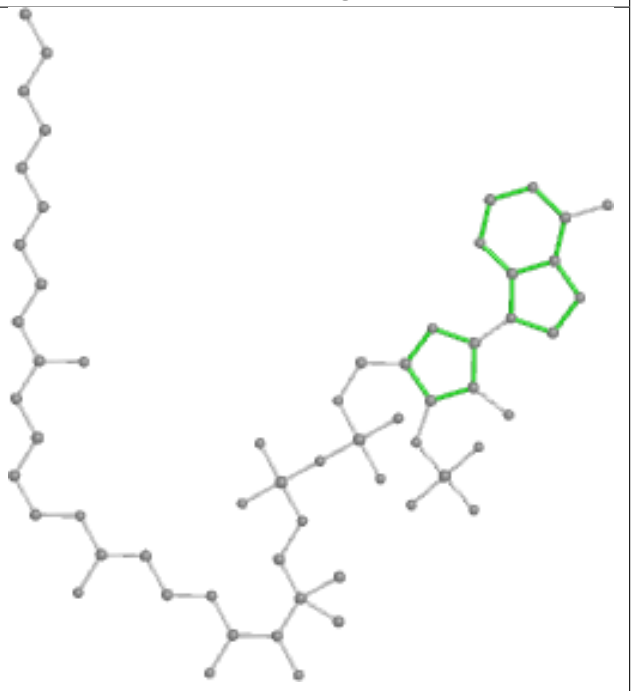
Bond lengths



Bond angles

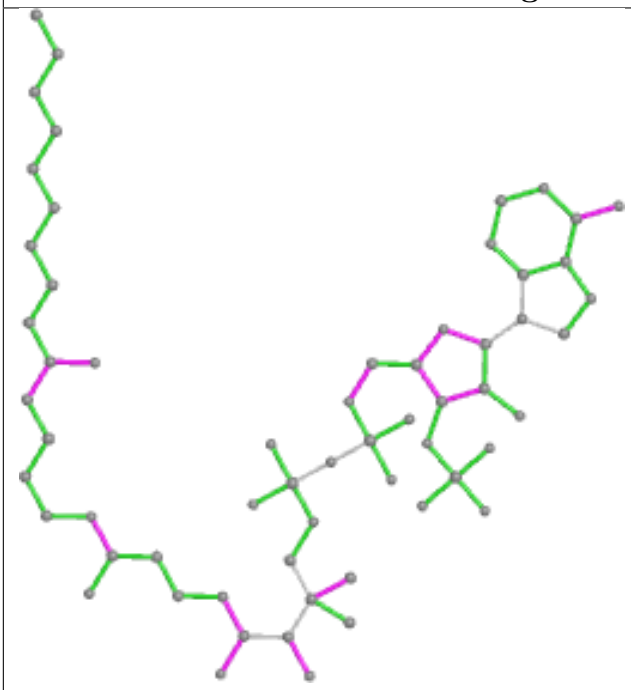


Torsions

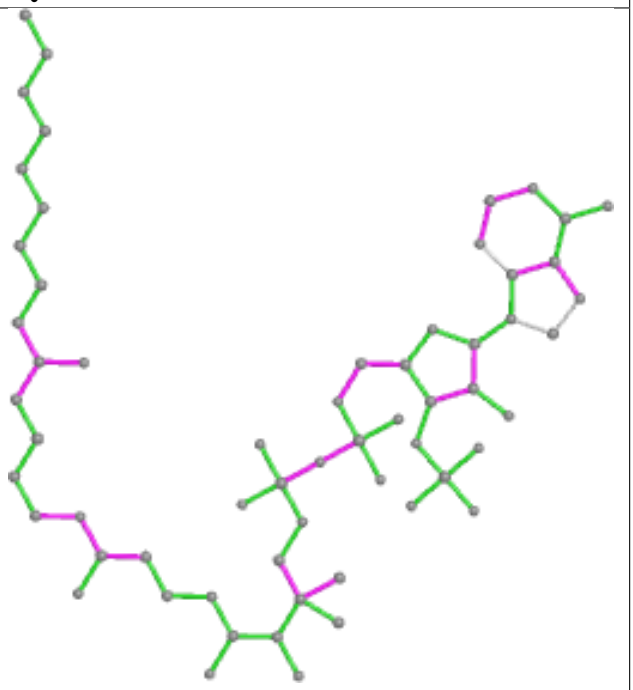


Rings

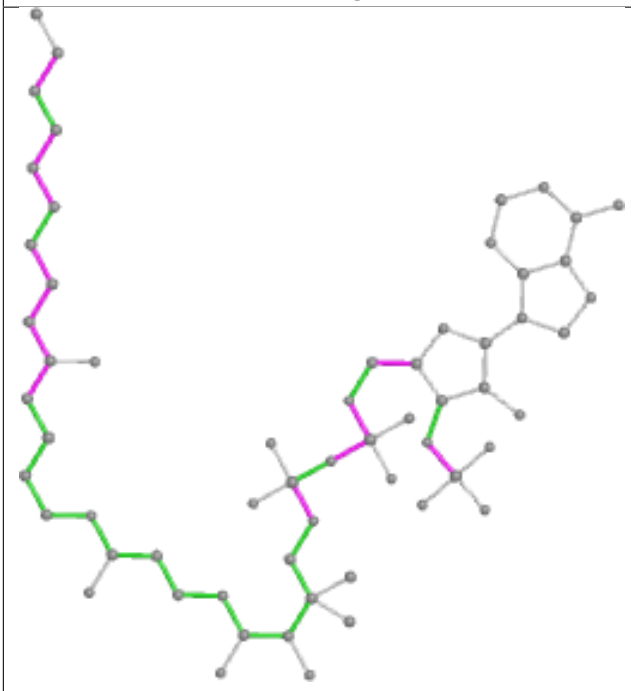
Ligand UOQ B 201



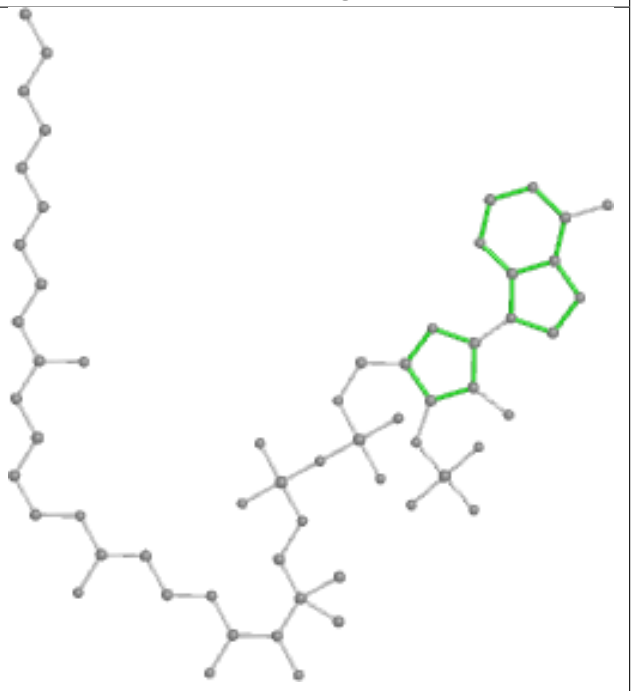
Bond lengths



Bond angles

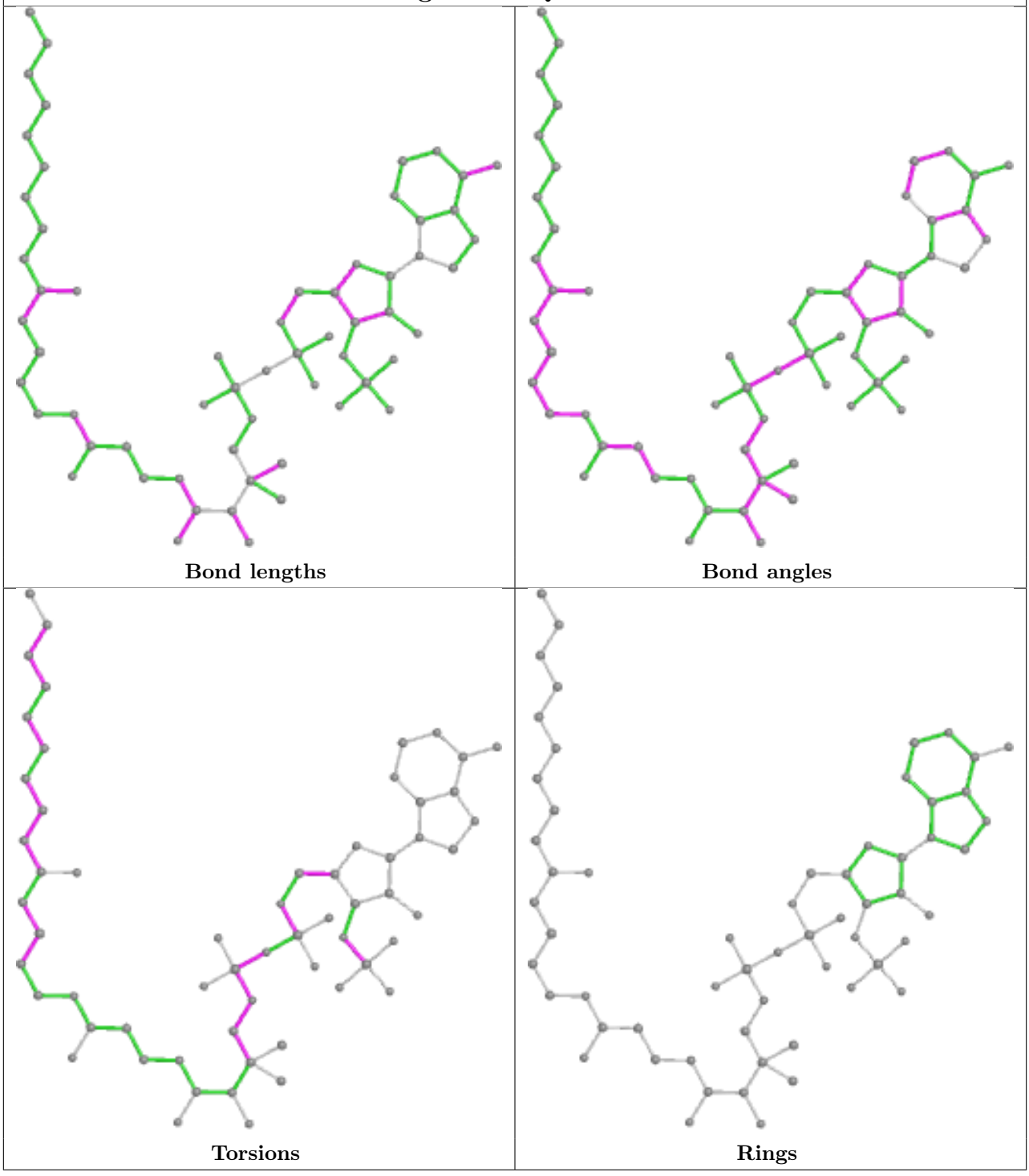


Torsions



Rings

Ligand UOQ A 203



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	136/136 (100%)	-0.46	0 100 100	4, 10, 27, 40	0
1	B	136/136 (100%)	-0.51	0 100 100	4, 13, 34, 47	0
1	C	136/136 (100%)	-0.34	1 (0%) 87 88	5, 12, 28, 44	0
1	D	136/136 (100%)	-0.41	1 (0%) 87 88	5, 12, 31, 35	0
1	E	136/136 (100%)	-0.29	0 100 100	7, 15, 36, 48	0
1	F	136/136 (100%)	-0.40	1 (0%) 87 88	6, 14, 34, 47	0
1	G	136/136 (100%)	-0.42	1 (0%) 87 88	5, 13, 30, 42	0
1	H	136/136 (100%)	-0.52	0 100 100	5, 11, 27, 34	0
All	All	1088/1088 (100%)	-0.42	4 (0%) 92 93	4, 13, 31, 48	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	LEU	2.6
1	F	1	MET	2.5
1	G	136	LEU	2.5
1	D	1	MET	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

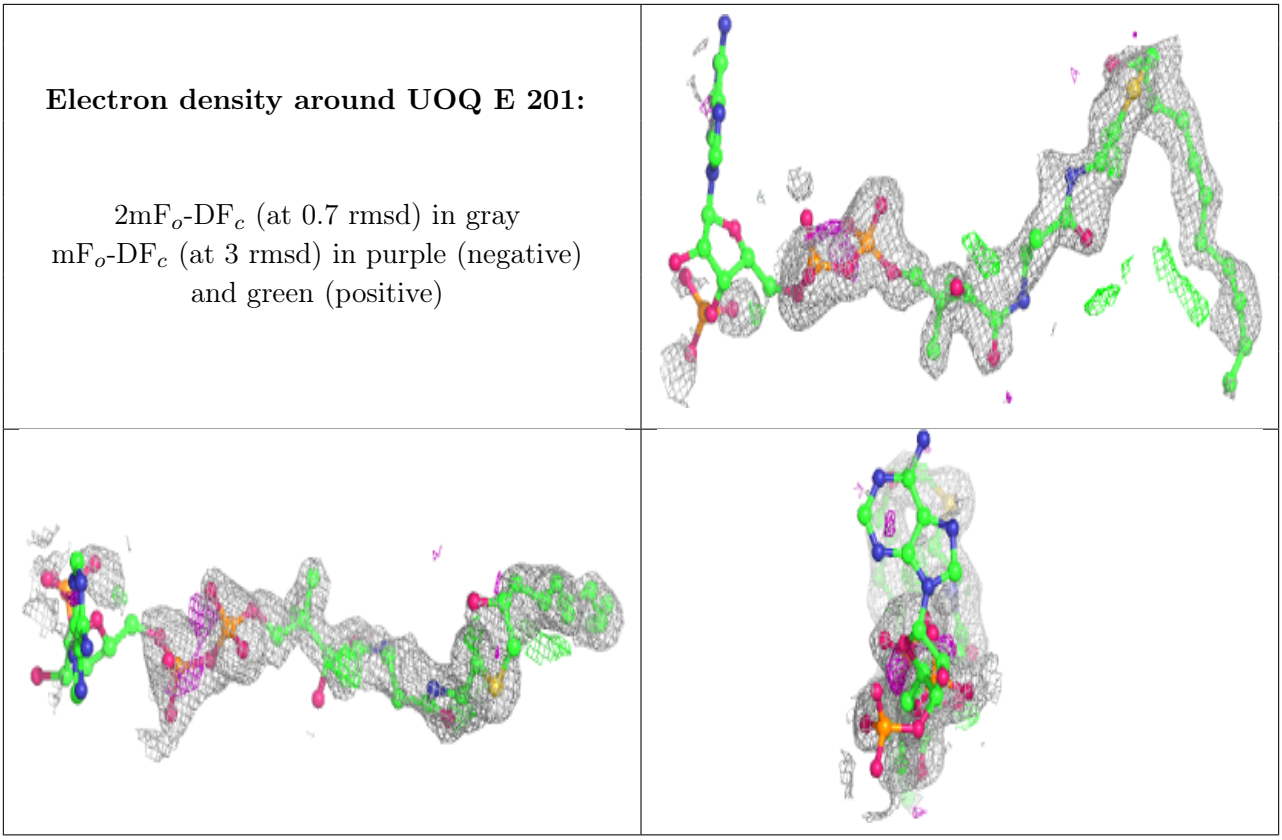
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	UOQ	E	201	60/60	0.84	0.25	16,47,65,76	24
2	UOQ	E	203	60/60	0.85	0.21	10,48,72,83	22
2	UOQ	D	501	60/60	0.86	0.25	6,43,61,73	28
2	UOQ	A	201	60/60	0.86	0.26	15,46,80,89	24
2	UOQ	C	201	60/60	0.86	0.22	9,49,77,90	21
2	UOQ	H	201	60/60	0.88	0.21	11,45,79,81	23
2	UOQ	F	201	60/60	0.89	0.19	15,33,71,79	24
2	UOQ	B	201	60/60	0.89	0.21	15,38,80,88	23
2	UOQ	H	202	60/60	0.89	0.23	7,43,65,76	25
2	UOQ	E	204	60/60	0.90	0.19	10,37,97,97	19
2	UOQ	A	203	60/60	0.90	0.20	11,41,79,81	21
2	UOQ	B	202	60/60	0.93	0.16	8,26,69,84	21
2	UOQ	H	203	60/60	0.94	0.16	11,27,70,76	21
3	CL	A	202	1/1	0.99	0.04	25,25,25,25	0
3	CL	E	202	1/1	0.99	0.08	27,27,27,27	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.

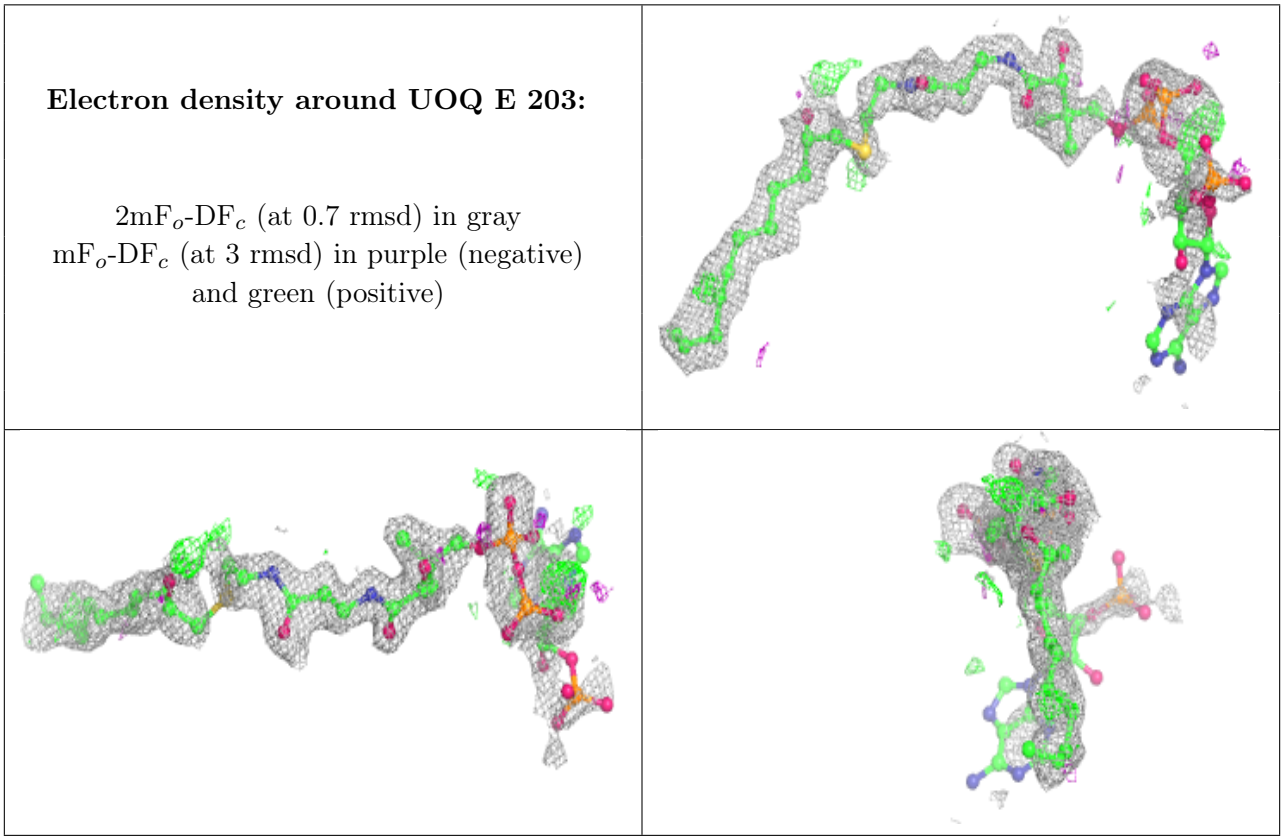
Electron density around UOQ E 201:

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



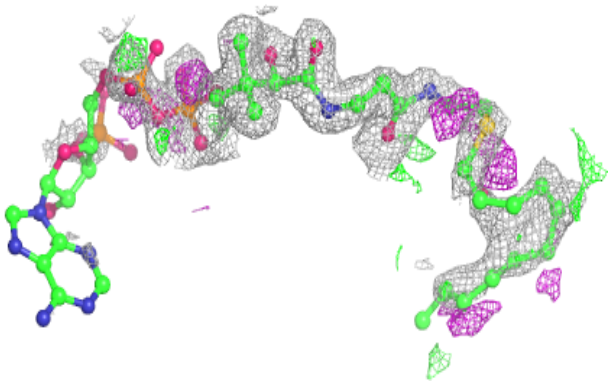
Electron density around UOQ E 203:

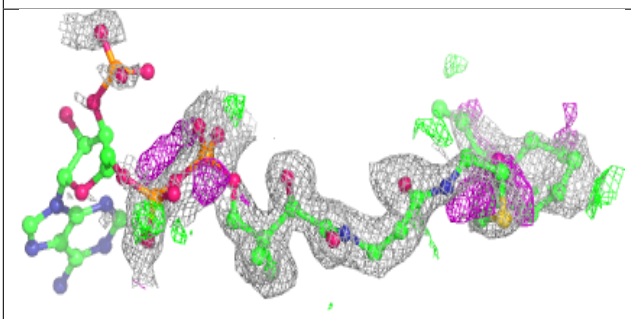
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

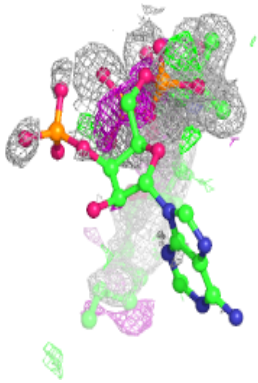


Electron density around UOQ D 501:

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

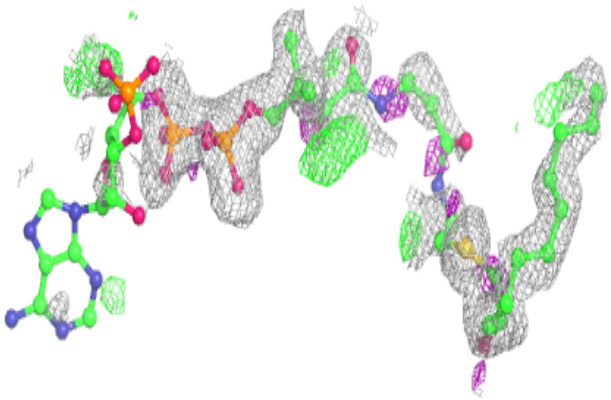


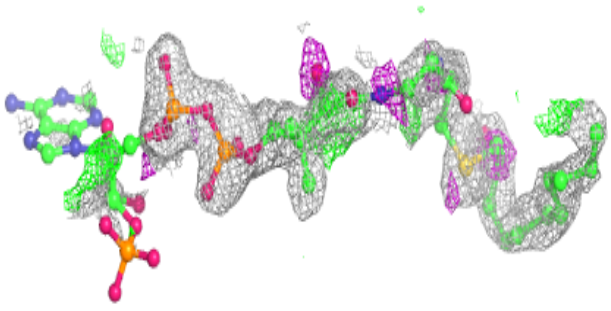


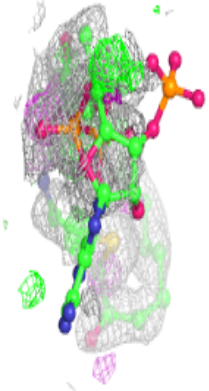


Electron density around UOQ A 201:

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

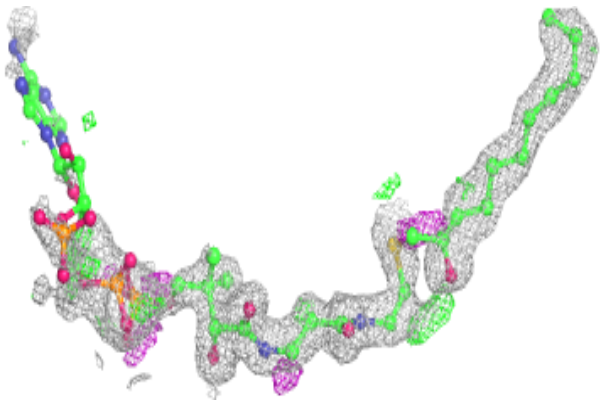


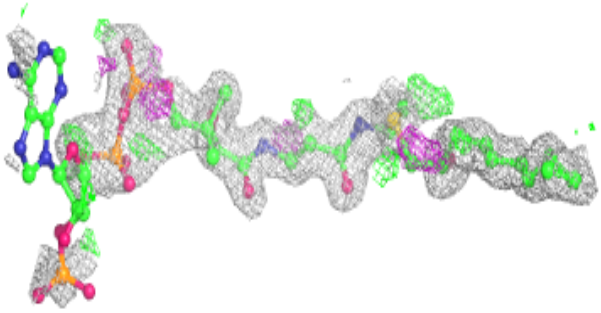


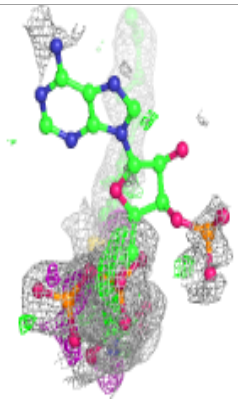


Electron density around UOQ C 201:

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

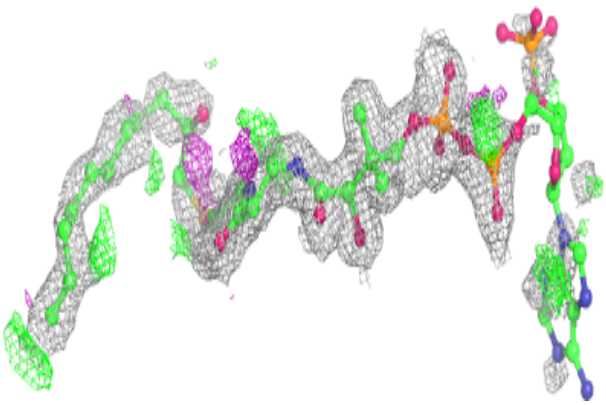


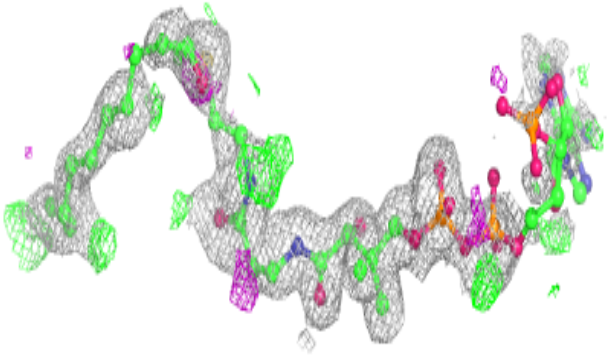


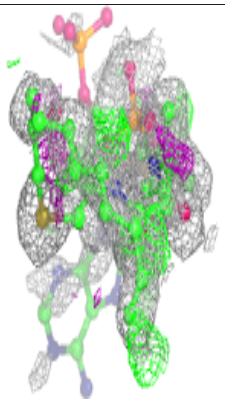


Electron density around UOQ H 201:

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

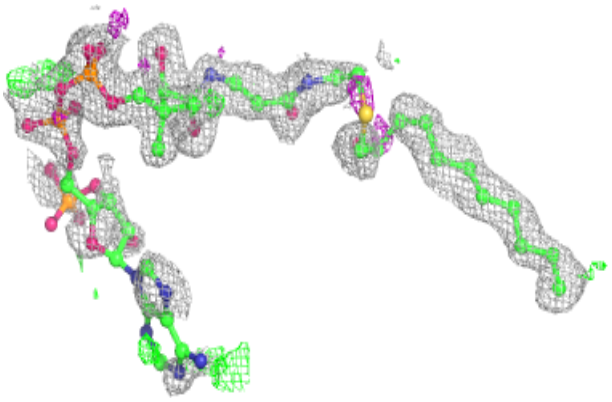


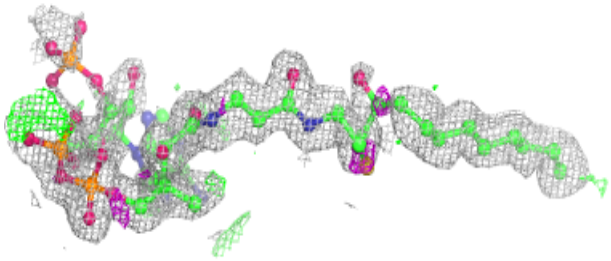


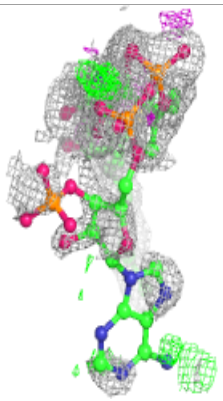


Electron density around UOQ F 201:

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

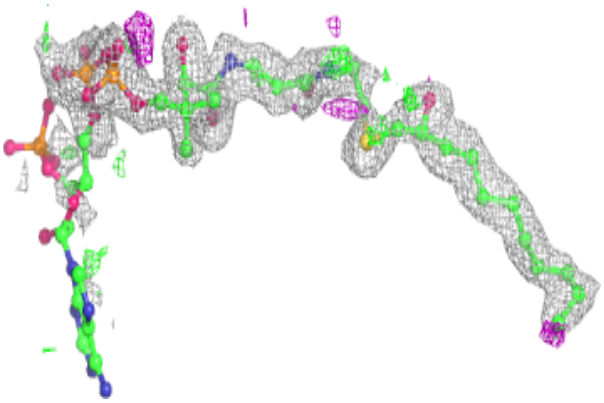


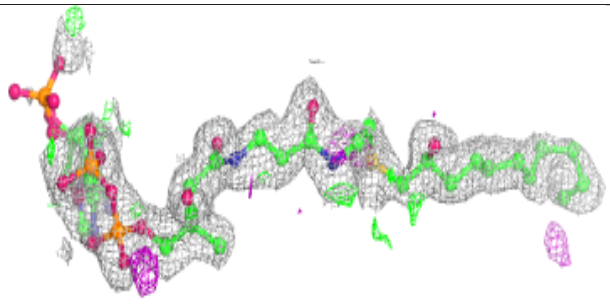


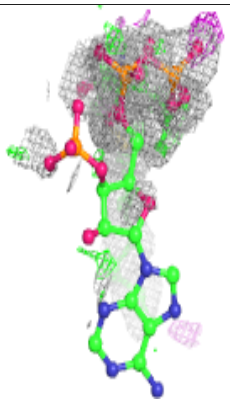


Electron density around UOQ B 201:

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

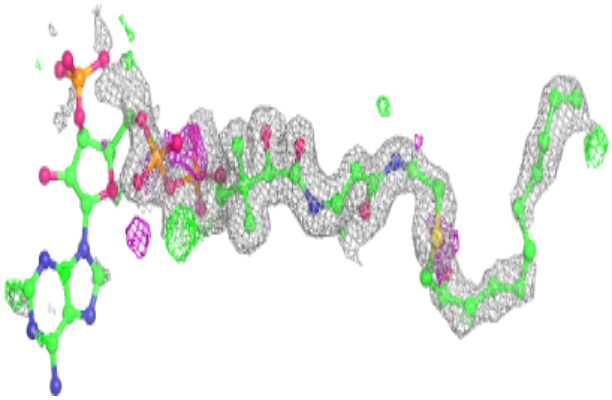


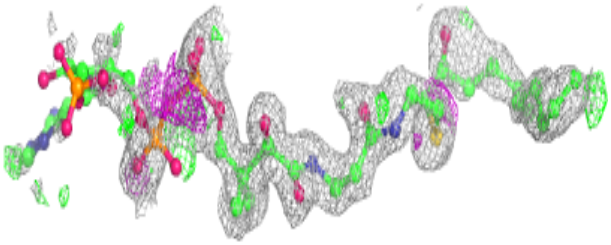


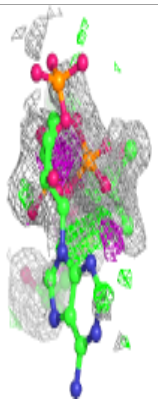


Electron density around UOQ H 202:

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

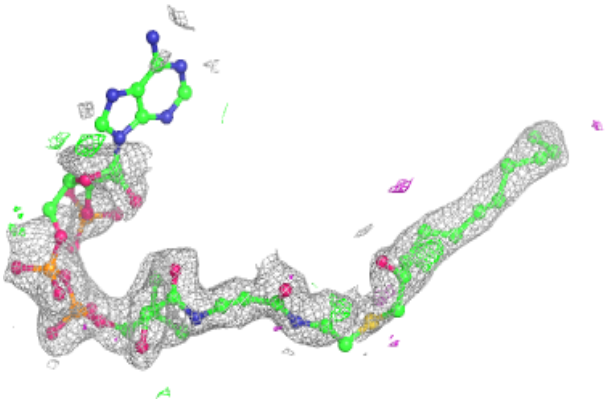


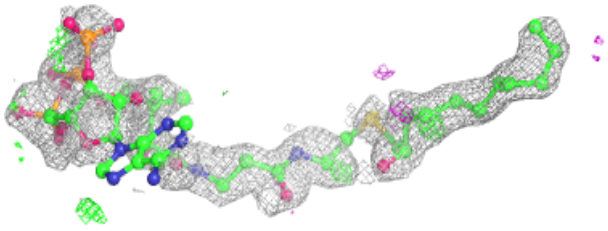


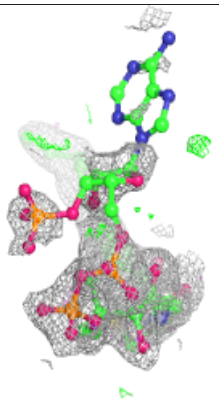


Electron density around UOQ E 204:

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

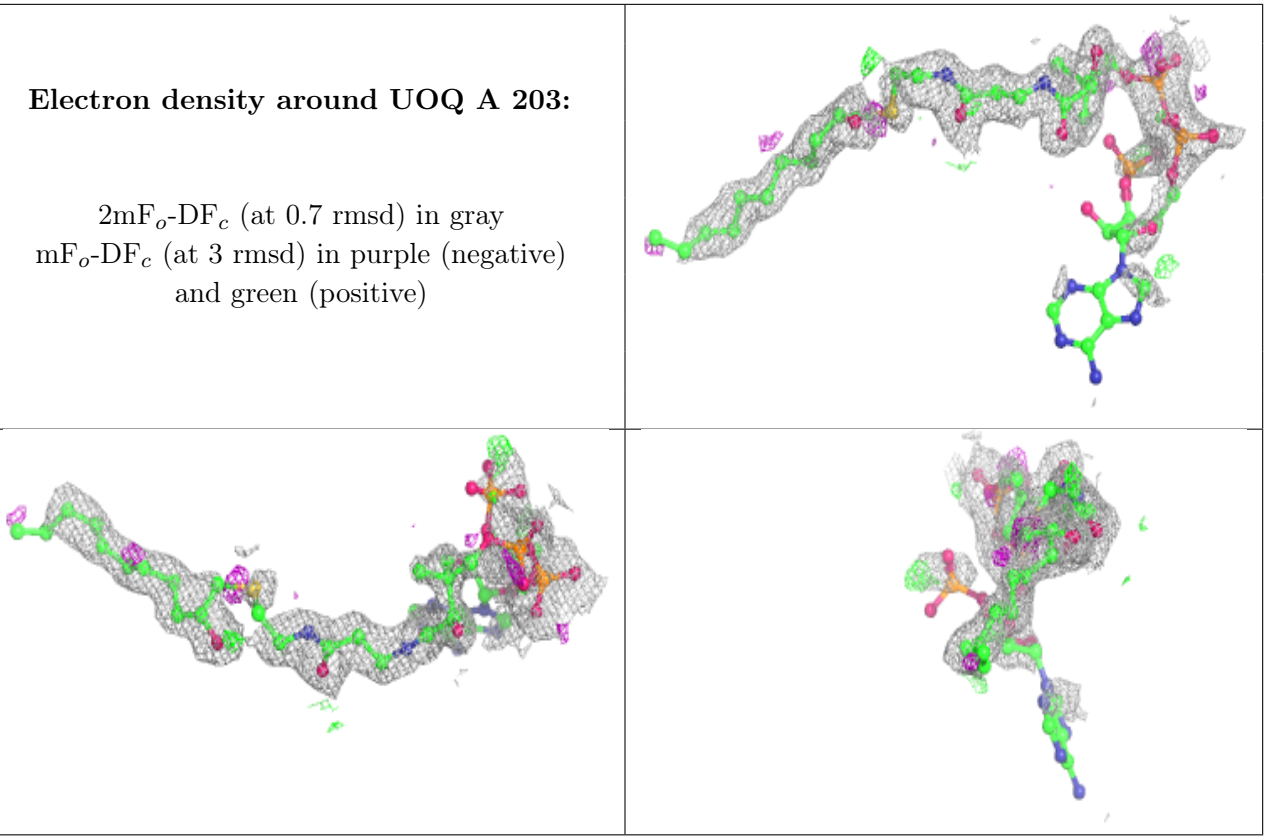






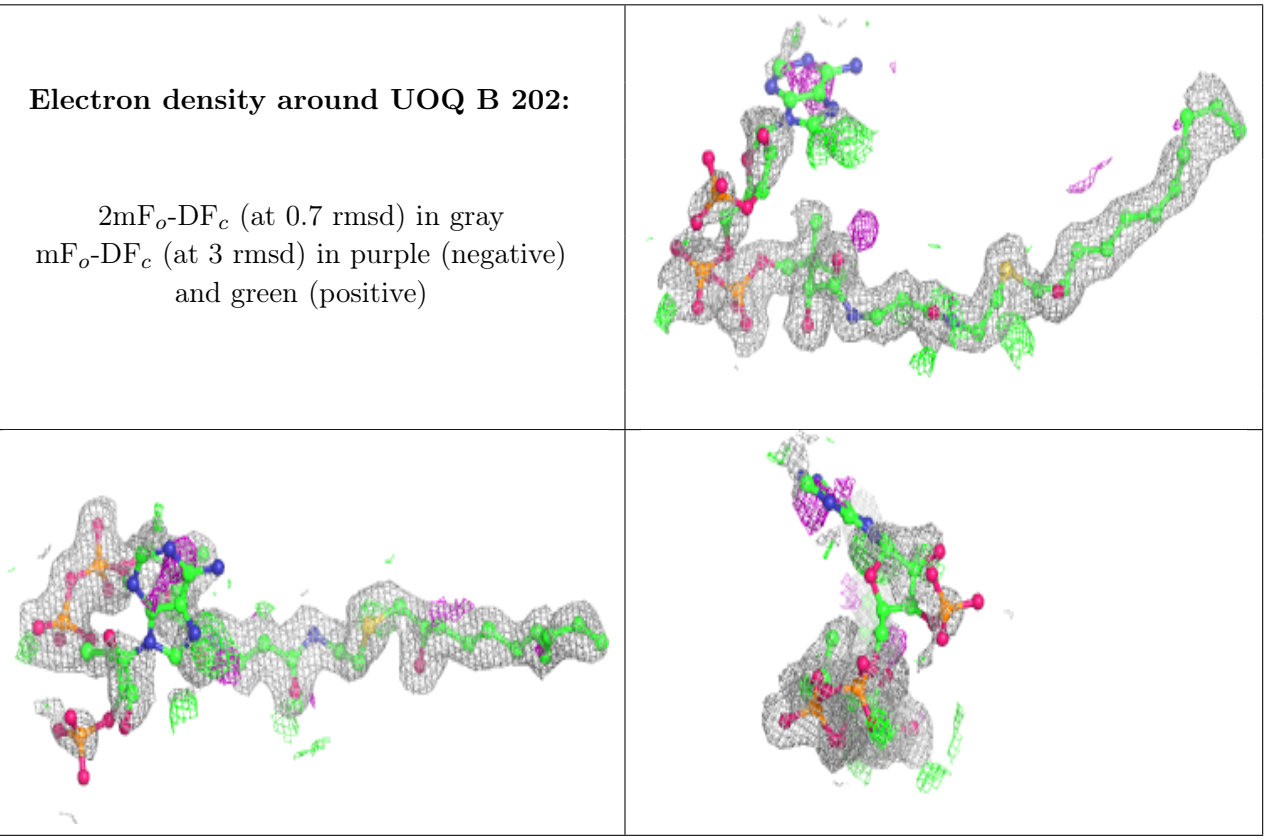
Electron density around UOQ A 203:

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



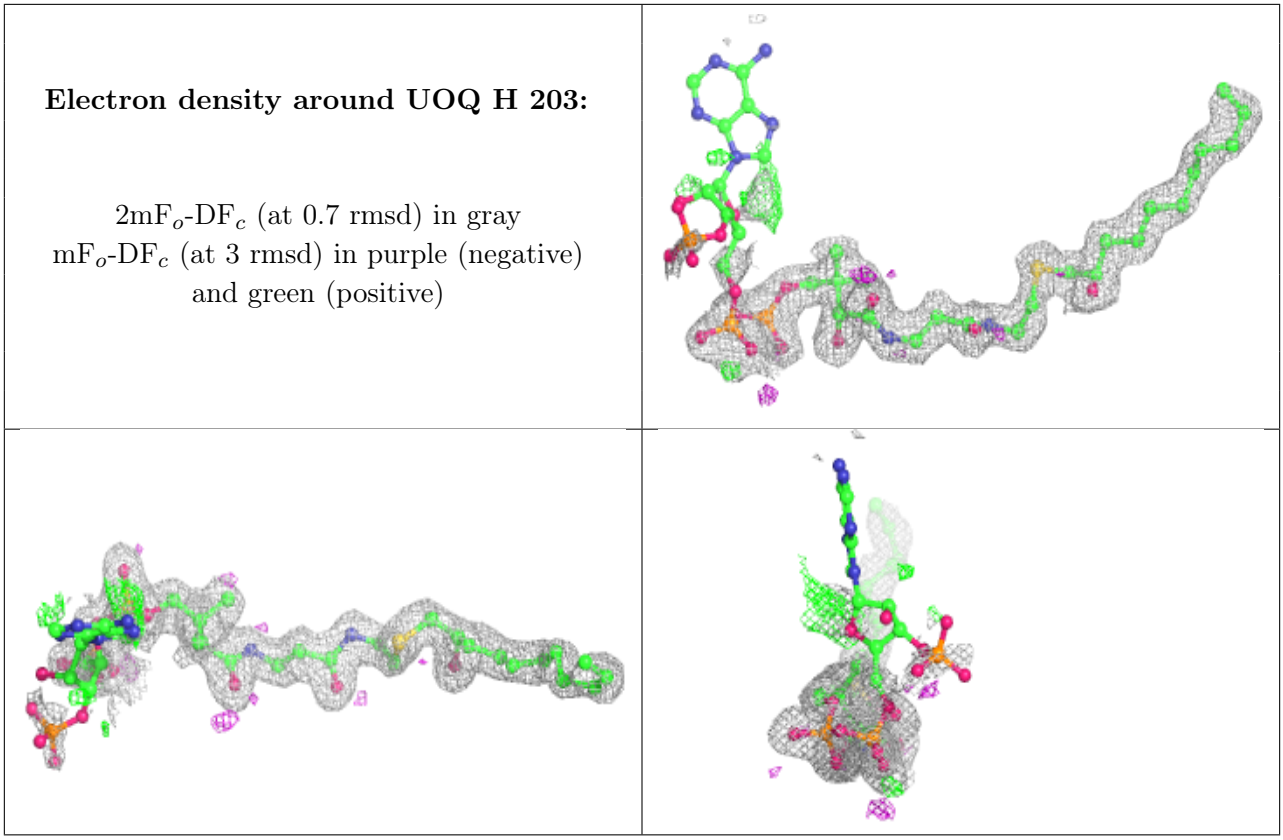
Electron density around UOQ B 202:

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



Electron density around UOQ H 203:

$2mF_o$-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.