Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:17 PM UTC

PDB ID	:	7M15 / pdb_00007m15
Title	:	crystal structure of cj1430 in the presence of GDP-D-glycero-L-gluco-heptose , a GDP-D-glycero-4-keto-D-lyxo-heptose-3,5-epimerase from campylobacter jejuni
Authors	:	Girardi, N.M.; Thoden, J.B.; Raushel, F.M.; Holden, H.M.
Deposited on	:	2021-03-12
Resolution	:	1.85 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

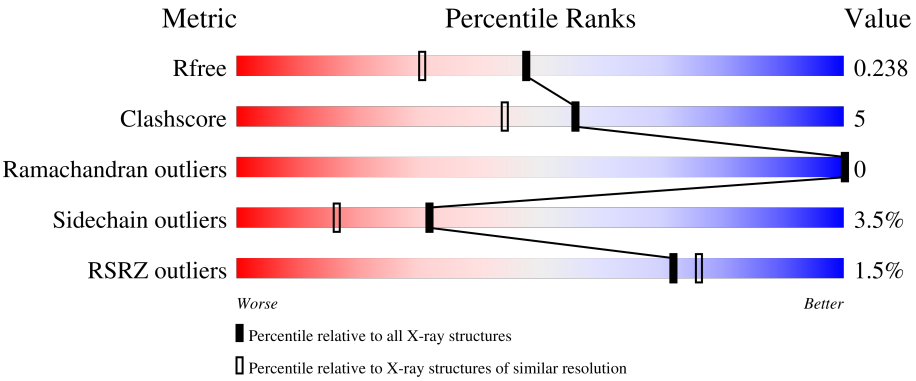
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	185	2% 89% 8%
1	B	185	% 84% 12%
1	C	185	% 84% 12%
1	D	185	3% 83% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	185	2% 86% 10%
1	F	185	% 81% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9944 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 GDP-D-glycero-L-gluco-heptose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1476	960	241	270	5			
1	B	179	Total	C	N	O	S	0	0	0
			1476	960	241	270	5			
1	C	178	Total	C	N	O	S	0	0	0
			1467	954	239	269	5			
1	D	181	Total	C	N	O	S	0	0	0
			1488	966	243	274	5			
1	E	179	Total	C	N	O	S	0	1	0
			1482	964	242	271	5			
1	F	179	Total	C	N	O	S	0	0	0
			1476	960	241	270	5			

There are 36 discrepancies between the modelled and reference sequences:

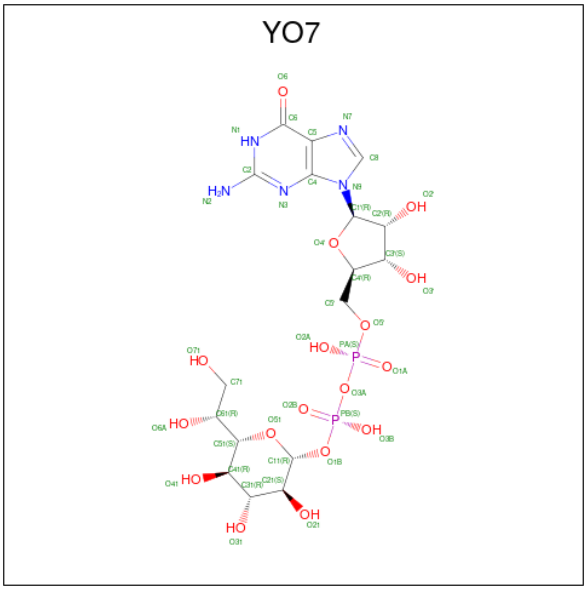
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q0P8I4
A	-2	GLY	-	expression tag	UNP Q0P8I4
A	-1	GLY	-	expression tag	UNP Q0P8I4
A	0	HIS	-	expression tag	UNP Q0P8I4
A	128	ALA	LYS	engineered mutation	UNP Q0P8I4
A	129	ALA	GLU	engineered mutation	UNP Q0P8I4
B	-3	GLY	-	expression tag	UNP Q0P8I4
B	-2	GLY	-	expression tag	UNP Q0P8I4
B	-1	GLY	-	expression tag	UNP Q0P8I4
B	0	HIS	-	expression tag	UNP Q0P8I4
B	128	ALA	LYS	engineered mutation	UNP Q0P8I4
B	129	ALA	GLU	engineered mutation	UNP Q0P8I4
C	-3	GLY	-	expression tag	UNP Q0P8I4
C	-2	GLY	-	expression tag	UNP Q0P8I4
C	-1	GLY	-	expression tag	UNP Q0P8I4
C	0	HIS	-	expression tag	UNP Q0P8I4
C	128	ALA	LYS	engineered mutation	UNP Q0P8I4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	129	ALA	GLU	engineered mutation	UNP Q0P8I4
D	-3	GLY	-	expression tag	UNP Q0P8I4
D	-2	GLY	-	expression tag	UNP Q0P8I4
D	-1	GLY	-	expression tag	UNP Q0P8I4
D	0	HIS	-	expression tag	UNP Q0P8I4
D	128	ALA	LYS	engineered mutation	UNP Q0P8I4
D	129	ALA	GLU	engineered mutation	UNP Q0P8I4
E	-3	GLY	-	expression tag	UNP Q0P8I4
E	-2	GLY	-	expression tag	UNP Q0P8I4
E	-1	GLY	-	expression tag	UNP Q0P8I4
E	0	HIS	-	expression tag	UNP Q0P8I4
E	128	ALA	LYS	engineered mutation	UNP Q0P8I4
E	129	ALA	GLU	engineered mutation	UNP Q0P8I4
F	-3	GLY	-	expression tag	UNP Q0P8I4
F	-2	GLY	-	expression tag	UNP Q0P8I4
F	-1	GLY	-	expression tag	UNP Q0P8I4
F	0	HIS	-	expression tag	UNP Q0P8I4
F	128	ALA	LYS	engineered mutation	UNP Q0P8I4
F	129	ALA	GLU	engineered mutation	UNP Q0P8I4

- Molecule 2 is [(2R,3S,4R,5R)-5-(2-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl (2R,3S,4R,5R,6S)-6-[(1R)-1,2-dihydroxyethyl]-3,4,5-trihydroxyoxan-2-yl dihydrogen diphosphate (non-preferred name) (CCD ID: YO7) (formula: $C_{17}H_{27}N_5O_{17}P_2$).



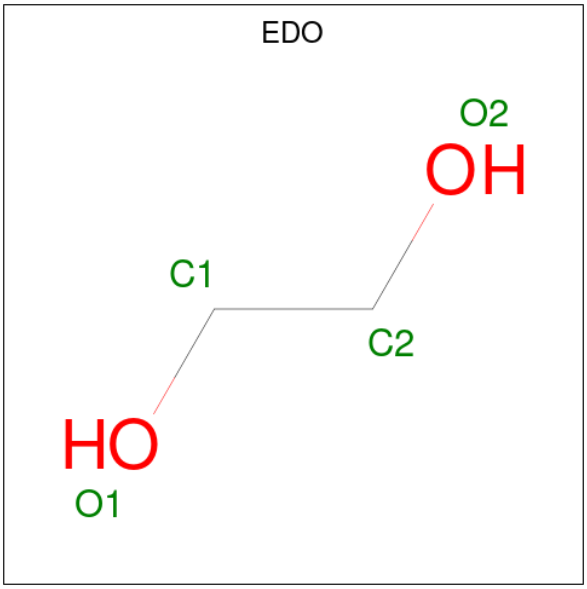
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			41	17	5	17	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			41	17	5	17	2		
2	C	1	Total	C	N	O	P	0	0
			41	17	5	17	2		
2	D	1	Total	C	N	O	P	0	0
			41	17	5	17	2		
2	E	1	Total	C	N	O	P	0	0
			41	17	5	17	2		
2	F	1	Total	C	N	O	P	0	0
			41	17	5	17	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O		0	0
			4	2	2			
3	C	1	Total	C	O		0	0
			4	2	2			
3	E	1	Total	C	O		0	0
			4	2	2			
3	E	1	Total	C	O		0	0
			4	2	2			
3	F	1	Total	C	O		0	0
			4	2	2			

- Molecule 4 is water.

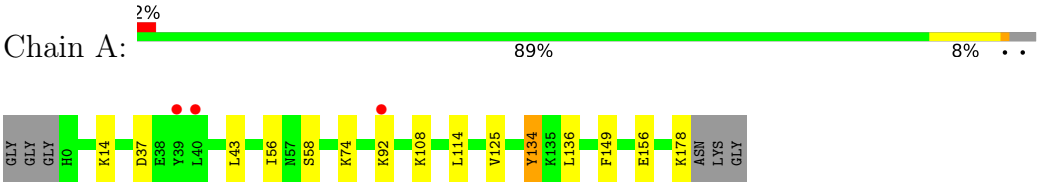
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	115	Total O 115 115	0	0
4	B	166	Total O 166 166	0	0
4	C	135	Total O 135 135	0	0
4	D	130	Total O 130 130	0	0
4	E	137	Total O 137 137	0	0
4	F	130	Total O 130 130	0	0

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.

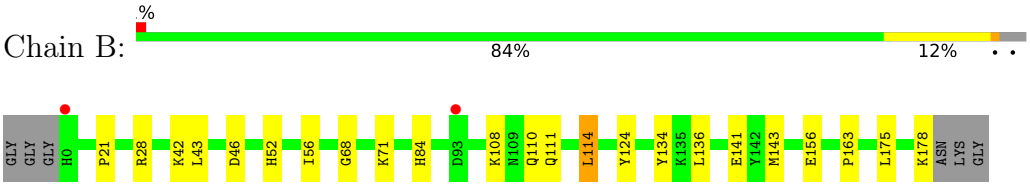
• Molecule 1: GDP-D-glycero-L-gluco-heptose

Chain A:



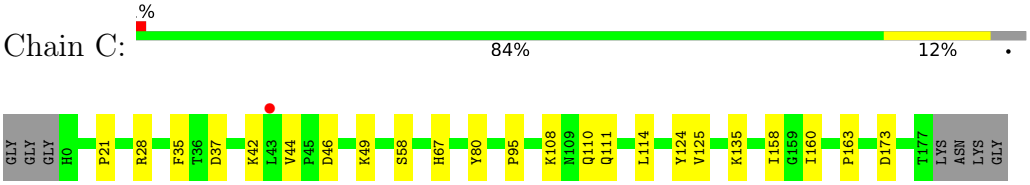
• Molecule 1: GDP-D-glycero-L-gluco-heptose

Chain B:



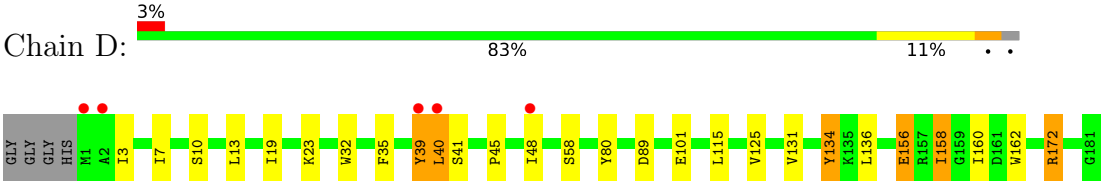
• Molecule 1: GDP-D-glycero-L-gluco-heptose

Chain C:



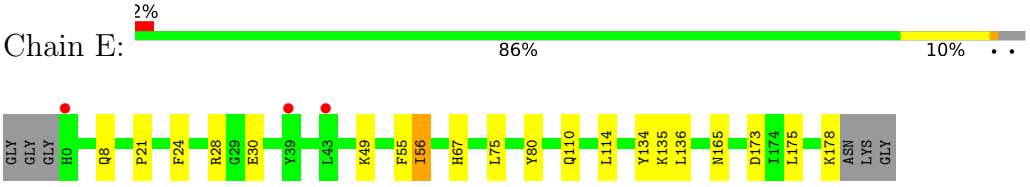
• Molecule 1: GDP-D-glycero-L-gluco-heptose

Chain D:



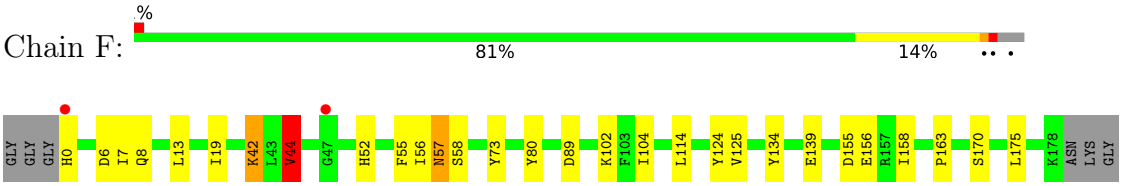
• Molecule 1: GDP-D-glycero-L-gluco-heptose

Chain E:



• Molecule 1: GDP-D-glycero-L-gluco-heptose

Chain F:


%
81%
14%
GLY GLY GLY HO D6 I7 Q8 L13 I19 K42 L43 V44 G47 H52 F55 I56 N57 S58 Y73 Y80 D89 K102 F103 I104 L114 Y124 V125 Y134 E139 D155 E156 R157 I158 P163 S170 L175 K178 ASN LYS GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.41Å 81.57Å 109.45Å 90.00° 94.38° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-1.85) 97.7 (30.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.190 , 0.234 0.197 , 0.238	Depositor DCC
R_{free} test set	5212 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.6	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	0.94	EDS
Total number of atoms	9944	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, YO7

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.03	0/1518	1.20	2/2061 (0.1%)
1	B	1.03	1/1518 (0.1%)	1.19	1/2061 (0.0%)
1	C	1.00	0/1509	1.19	0/2050
1	D	0.97	0/1529	1.25	4/2073 (0.2%)
1	E	1.01	0/1527	1.23	2/2073 (0.1%)
1	F	1.00	0/1518	1.22	3/2061 (0.1%)
All	All	1.01	1/9119 (0.0%)	1.21	12/12379 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	GLY	C-O	5.19	1.28	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	134	TYR	CB-CA-C	8.70	123.33	110.62
1	F	52	HIS	CB-CA-C	6.14	119.21	110.24
1	F	44	VAL	CB-CA-C	5.78	114.99	109.33
1	E	134	TYR	N-CA-CB	-5.70	102.00	110.90
1	D	156	GLU	CB-CA-C	-5.62	100.22	110.63
1	B	134	TYR	CB-CA-C	5.60	118.80	110.62
1	D	134	TYR	CB-CA-C	5.47	118.60	110.62
1	A	134	TYR	CB-CA-C	5.44	118.57	110.62
1	D	158	ILE	N-CA-C	-5.21	106.60	111.45
1	A	149	PHE	CA-CB-CG	5.05	118.85	113.80
1	F	134	TYR	CB-CA-C	5.03	118.21	110.62
1	D	172	ARG	CB-CG-CD	5.00	122.81	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1476	0	1451	6	0
1	B	1476	0	1451	17	0
1	C	1467	0	1438	18	0
1	D	1488	0	1466	22	0
1	E	1482	0	1459	15	0
1	F	1476	0	1451	16	0
2	A	41	0	0	0	0
2	B	41	0	0	0	0
2	C	41	0	0	1	0
2	D	41	0	0	0	0
2	E	41	0	0	0	0
2	F	41	0	0	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	E	8	0	12	0	0
3	F	4	0	6	0	0
4	A	115	0	0	0	0
4	B	166	0	0	2	0
4	C	135	0	0	1	0
4	D	130	0	0	1	0
4	E	137	0	0	2	0
4	F	130	0	0	0	0
All	All	9944	0	8746	84	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 5.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:HIS:HE1	1:E:173:ASP:OD1	1.67	0.78
1:B:71:LYS:HD2	1:B:143:MET:SD	2.25	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:HIS:HE1	1:C:173:ASP:OD1	1.73	0.71
1:B:111:GLN:NE2	1:C:108:LYS:O	2.24	0.71
1:E:56:ILE:HD12	1:E:56:ILE:N	2.09	0.67
1:B:114:LEU:C	1:B:114:LEU:HD13	2.20	0.67
1:E:55:PHE:C	1:E:56:ILE:HD12	2.21	0.66
1:E:67:HIS:CE1	1:E:173:ASP:OD1	2.49	0.65
1:D:19:ILE:CG2	1:D:39:TYR:OH	2.46	0.63
1:E:165:ASN:ND2	4:E:303:HOH:O	2.33	0.61
1:C:114:LEU:C	1:C:114:LEU:HD13	2.25	0.60
1:D:19:ILE:HG21	1:D:39:TYR:OH	2.03	0.59
1:E:114:LEU:C	1:E:114:LEU:HD13	2.29	0.57
1:D:7:ILE:HD11	1:D:39:TYR:HE1	1.70	0.56
1:D:35:PHE:HD2	1:D:40:LEU:HD13	1.70	0.56
1:A:74:LYS:HE2	1:A:134:TYR:OH	2.05	0.56
1:D:13:LEU:HD22	1:D:89:ASP:HB2	1.88	0.56
1:C:67:HIS:CE1	1:C:173:ASP:OD1	2.57	0.56
1:B:143:MET:HE2	1:B:143:MET:HA	1.88	0.55
1:D:7:ILE:HG23	1:D:19:ILE:CD1	2.39	0.52
1:D:41:SER:O	4:D:301:HOH:O	2.19	0.52
1:F:114:LEU:C	1:F:114:LEU:HD13	2.35	0.52
1:E:56:ILE:HG12	4:E:407:HOH:O	2.09	0.51
1:B:71:LYS:HD2	1:B:143:MET:CG	2.40	0.51
1:B:108:LYS:O	1:C:111:GLN:NE2	2.44	0.50
1:D:23:LYS:HG2	1:D:32:TRP:HB3	1.94	0.50
1:C:58:SER:HB2	1:C:125:VAL:HG21	1.93	0.50
1:D:19:ILE:HG13	1:D:39:TYR:HH	1.75	0.50
1:D:158:ILE:HG22	1:D:160:ILE:HG13	1.95	0.49
1:D:35:PHE:CD2	1:D:40:LEU:HD13	2.49	0.48
1:D:58:SER:HB2	1:D:125:VAL:HG21	1.96	0.48
1:F:6:ASP:OD2	1:F:8:GLN:NE2	2.47	0.48
1:D:115:LEU:HD12	1:D:115:LEU:N	2.29	0.47
1:B:71:LYS:NZ	1:B:141:GLU:O	2.48	0.47
1:F:124:TYR:CE2	1:F:163:PRO:HG2	2.50	0.47
1:A:58:SER:HB2	1:A:125:VAL:HG21	1.97	0.47
1:B:114:LEU:C	1:B:114:LEU:CD1	2.87	0.46
1:E:24:PHE:O	1:E:30:GLU:HA	2.16	0.46
1:E:80:TYR:CE2	1:F:80:TYR:CZ	3.04	0.46
1:C:21:PRO:HD2	1:C:110:GLN:O	2.16	0.46
1:F:7:ILE:HG23	1:F:19:ILE:CD1	2.46	0.45
1:C:67:HIS:HD2	2:C:201:YO7:O51	2.00	0.45
1:C:95:PRO:HA	1:F:163:PRO:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLU:HB2	4:B:337:HOH:O	2.16	0.45
1:C:124:TYR:CE2	1:C:163:PRO:HG2	2.52	0.45
1:D:10:SER:OG	1:D:101:GLU:OE2	2.28	0.45
1:C:108:LYS:NZ	4:C:309:HOH:O	2.47	0.45
1:B:84:HIS:CE1	1:B:163:PRO:HG3	2.52	0.45
1:C:80:TYR:HB2	1:D:131:VAL:HG21	1.98	0.45
1:A:58:SER:HA	1:B:28:ARG:O	2.17	0.44
1:B:124:TYR:CE2	1:B:163:PRO:HG2	2.52	0.44
1:B:21:PRO:HD2	1:B:110:GLN:O	2.16	0.44
1:C:35:PHE:CG	1:C:135:LYS:HE2	2.52	0.44
1:F:7:ILE:HG23	1:F:19:ILE:HD12	2.00	0.44
1:F:155:ASP:HB3	1:F:158:ILE:HD12	2.00	0.44
1:C:158:ILE:HG22	1:C:160:ILE:HG13	2.00	0.44
1:D:136:LEU:N	1:D:136:LEU:HD12	2.33	0.43
1:D:7:ILE:CD1	1:D:39:TYR:HE1	2.30	0.43
1:F:57:ASN:HD22	1:F:57:ASN:N	2.15	0.43
1:F:44:VAL:HG22	1:F:73:TYR:CD1	2.53	0.43
1:E:56:ILE:N	1:E:56:ILE:CD1	2.79	0.43
1:B:56:ILE:HG12	4:B:383:HOH:O	2.18	0.43
1:F:55:PHE:C	1:F:56:ILE:HD12	2.43	0.43
1:B:52:HIS:HB3	1:B:136:LEU:HB2	2.00	0.43
1:F:42:LYS:O	1:F:42:LYS:HG2	2.18	0.42
1:C:28:ARG:O	1:D:58:SER:HA	2.19	0.42
1:B:43:LEU:HB3	1:B:114:LEU:HG	2.02	0.42
1:C:49:LYS:HD2	1:C:49:LYS:HA	1.90	0.42
1:E:28:ARG:CZ	1:F:170:SER:HB3	2.50	0.41
1:D:134:TYR:CE1	1:D:136:LEU:HG	2.55	0.41
1:C:114:LEU:C	1:C:114:LEU:CD1	2.93	0.41
1:E:21:PRO:HD2	1:E:110:GLN:O	2.21	0.41
1:F:58:SER:HB2	1:F:125:VAL:HG21	2.02	0.41
1:D:160:ILE:HG21	1:D:162:TRP:CE2	2.55	0.41
1:F:13:LEU:HD22	1:F:89:ASP:HB2	2.02	0.41
1:A:56:ILE:HD12	1:A:56:ILE:N	2.36	0.41
1:A:136:LEU:N	1:A:136:LEU:HD12	2.36	0.41
1:B:56:ILE:N	1:B:56:ILE:HD12	2.36	0.41
1:C:80:TYR:CE2	1:D:80:TYR:CE2	3.08	0.40
1:E:75:LEU:HB3	1:E:135:LYS:HB2	2.04	0.40
1:D:45:PRO:HB2	1:D:48:ILE:HD12	2.04	0.40
1:E:136:LEU:N	1:E:136:LEU:HD12	2.37	0.40
1:A:43:LEU:HB3	1:A:114:LEU:CD2	2.52	0.40
1:E:80:TYR:CE2	1:F:80:TYR:CE2	3.10	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	177/185 (96%)	170 (96%)	7 (4%)	0	100	100
1	B	177/185 (96%)	174 (98%)	3 (2%)	0	100	100
1	C	176/185 (95%)	173 (98%)	3 (2%)	0	100	100
1	D	179/185 (97%)	174 (97%)	5 (3%)	0	100	100
1	E	178/185 (96%)	174 (98%)	4 (2%)	0	100	100
1	F	177/185 (96%)	173 (98%)	4 (2%)	0	100	100
All	All	1064/1110 (96%)	1038 (98%)	26 (2%)	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	161/163 (99%)	155 (96%)	6 (4%)	30	15
1	B	161/163 (99%)	156 (97%)	5 (3%)	35	20
1	C	160/163 (98%)	156 (98%)	4 (2%)	42	27
1	D	162/163 (99%)	157 (97%)	5 (3%)	35	20
1	E	162/163 (99%)	156 (96%)	6 (4%)	30	15
1	F	161/163 (99%)	152 (94%)	9 (6%)	19	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	967/978 (99%)	932 (96%)	35 (4%)	32 16

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	37	ASP
1	A	92	LYS
1	A	108	LYS
1	A	156	GLU
1	A	178	LYS
1	B	42	LYS
1	B	46	ASP
1	B	114	LEU
1	B	175	LEU
1	B	178	LYS
1	C	37	ASP
1	C	42	LYS
1	C	44	VAL
1	C	46	ASP
1	D	3	ILE
1	D	39	TYR
1	D	40	LEU
1	D	156	GLU
1	D	172	ARG
1	E	8[A]	GLN
1	E	8[B]	GLN
1	E	49	LYS
1	E	56	ILE
1	E	175	LEU
1	E	178	LYS
1	F	0	HIS
1	F	42	LYS
1	F	44	VAL
1	F	57	ASN
1	F	102	LYS
1	F	104	ILE
1	F	139	GLU
1	F	156	GLU
1	F	175	LEU

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

sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	GLN
1	C	67	HIS
1	C	165	ASN
1	D	165	ASN
1	E	0	HIS
1	E	67	HIS
1	F	57	ASN
1	F	165	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	B	202	-	3,3,3	0.07	0	2,2,2	0.06	0
2	YO7	D	201	-	43,44,44	0.87	1 (2%)	64,68,68	1.45	8 (12%)
3	EDO	F	202	-	3,3,3	0.07	0	2,2,2	0.10	0
2	YO7	E	201	-	43,44,44	1.08	3 (6%)	64,68,68	1.74	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	YO7	C	201	-	43,44,44	0.95	2 (4%)	64,68,68	1.58	11 (17%)
3	EDO	C	202	-	3,3,3	0.26	0	2,2,2	0.24	0
3	EDO	E	202	-	3,3,3	0.22	0	2,2,2	0.32	0
2	YO7	B	201	-	43,44,44	1.11	3 (6%)	64,68,68	1.60	7 (10%)
2	YO7	A	201	-	43,44,44	1.08	2 (4%)	64,68,68	1.88	14 (21%)
3	EDO	E	203	-	3,3,3	0.11	0	2,2,2	0.12	0
2	YO7	F	201	-	43,44,44	0.92	1 (2%)	64,68,68	1.67	8 (12%)

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	EDO	B	202	-	-	0/1/1/1	-
2	YO7	D	201	-	-	3/27/63/63	0/4/4/4
3	EDO	F	202	-	-	0/1/1/1	-
2	YO7	E	201	-	-	3/27/63/63	0/4/4/4
2	YO7	C	201	-	-	5/27/63/63	0/4/4/4
3	EDO	C	202	-	-	0/1/1/1	-
3	EDO	E	202	-	-	1/1/1/1	-
2	YO7	B	201	-	-	3/27/63/63	0/4/4/4
2	YO7	A	201	-	-	2/27/63/63	0/4/4/4
3	EDO	E	203	-	-	1/1/1/1	-
2	YO7	F	201	-	-	6/27/63/63	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	YO7	PA-O3A	4.22	1.64	1.59
2	A	201	YO7	PA-O3A	3.71	1.63	1.59
2	F	201	YO7	PA-O3A	3.46	1.63	1.59
2	B	201	YO7	C5-N7	-2.56	1.33	1.39
2	B	201	YO7	PA-O3A	2.55	1.62	1.59
2	B	201	YO7	C6-N1	-2.46	1.34	1.38
2	D	201	YO7	C6-N1	-2.36	1.34	1.38
2	C	201	YO7	PA-O3A	2.27	1.61	1.59
2	E	201	YO7	C5-N7	-2.12	1.34	1.39
2	C	201	YO7	PB-O3A	2.07	1.61	1.59
2	A	201	YO7	C5-N7	-2.06	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	YO7	C6-N1	-2.02	1.35	1.38

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	YO7	O51-C11-O1B	-7.56	101.48	111.36
2	E	201	YO7	O51-C11-O1B	-6.31	103.11	111.36
2	A	201	YO7	C2-N3-C4	6.20	122.98	112.30
2	E	201	YO7	C5-C4-N3	-5.78	119.19	128.39
2	F	201	YO7	C5-C4-N3	-5.37	119.84	128.39
2	F	201	YO7	C2-N3-C4	5.36	121.54	112.30
2	C	201	YO7	C2-N3-C4	5.36	121.54	112.30
2	F	201	YO7	O51-C11-O1B	-5.19	104.58	111.36
2	C	201	YO7	C5-C4-N3	-5.16	120.17	128.39
2	A	201	YO7	C5-C4-N3	-5.15	120.20	128.39
2	A	201	YO7	C11-O51-C51	4.60	120.44	113.07
2	D	201	YO7	C5-C4-N3	-4.47	121.28	128.39
2	E	201	YO7	C2-N3-C4	4.46	119.99	112.30
2	A	201	YO7	O51-C11-O1B	-4.32	105.71	111.36
2	B	201	YO7	C5-C4-N3	-4.25	121.63	128.39
2	D	201	YO7	O51-C11-O1B	-3.99	106.15	111.36
2	F	201	YO7	N9-C4-N3	3.82	133.59	125.95
2	D	201	YO7	C11-O51-C51	3.81	119.17	113.07
2	D	201	YO7	C2-N3-C4	3.72	118.71	112.30
2	F	201	YO7	C2-N1-C6	-3.42	118.90	125.11
2	E	201	YO7	C2-N1-C6	-3.28	119.16	125.11
2	C	201	YO7	O51-C51-C41	3.28	112.58	107.94
2	A	201	YO7	N9-C4-N3	3.23	132.41	125.95
2	F	201	YO7	O6-C6-C5	-3.21	118.05	126.53
2	A	201	YO7	N2-C2-N1	3.18	123.48	116.76
2	A	201	YO7	O71-C71-C61	-3.15	104.53	111.16
2	E	201	YO7	N9-C4-N3	3.09	132.14	125.95
2	A	201	YO7	O6-C6-C5	-3.07	118.42	126.53
2	D	201	YO7	N9-C4-N3	2.90	131.75	125.95
2	B	201	YO7	N9-C4-N3	2.90	131.75	125.95
2	A	201	YO7	C2-N1-C6	-2.79	120.05	125.11
2	E	201	YO7	O3B-PB-O3A	2.75	114.70	107.27
2	B	201	YO7	C2-N3-C4	2.74	117.02	112.30
2	C	201	YO7	N9-C4-N3	2.71	131.37	125.95
2	A	201	YO7	N9-C8-N7	-2.67	108.45	113.40
2	F	201	YO7	N9-C8-N7	-2.64	108.51	113.40
2	F	201	YO7	C5-C6-N1	2.64	119.97	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	201	YO7	O71-C71-C61	-2.61	105.68	111.16
2	D	201	YO7	N9-C8-N7	-2.56	108.65	113.40
2	A	201	YO7	O3A-PB-O2B	-2.53	103.08	110.70
2	C	201	YO7	C4-C5-N7	-2.53	106.66	110.67
2	D	201	YO7	O3B-PB-O3A	2.53	114.11	107.27
2	E	201	YO7	O3A-PB-O2B	-2.53	103.10	110.70
2	B	201	YO7	O3'-C3'-C4'	-2.53	103.83	111.08
2	E	201	YO7	O2A-PA-O3A	2.52	114.08	107.27
2	C	201	YO7	N2-C2-N1	2.46	121.95	116.76
2	E	201	YO7	C11-O51-C51	2.45	117.00	113.07
2	C	201	YO7	N9-C8-N7	-2.36	109.02	113.40
2	C	201	YO7	C6-C5-N7	2.32	134.51	130.29
2	C	201	YO7	O51-C11-O1B	-2.26	108.41	111.36
2	B	201	YO7	O51-C51-C41	2.23	111.09	107.94
2	C	201	YO7	C8-N7-C5	2.22	108.21	104.26
2	E	201	YO7	N2-C2-N3	-2.21	115.35	119.67
2	A	201	YO7	O3B-PB-O3A	2.20	113.21	107.27
2	E	201	YO7	C4-C5-N7	-2.17	107.23	110.67
2	A	201	YO7	O41-C41-C31	2.14	115.43	110.38
2	B	201	YO7	O41-C41-C31	-2.11	105.40	110.38
2	A	201	YO7	C5-C6-N1	2.11	118.62	113.25
2	C	201	YO7	O3'-C3'-C4'	-2.09	105.08	111.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	YO7	PA-O3A-PB-O1B
2	C	201	YO7	C11-O1B-PB-O2B
2	C	201	YO7	C11-O1B-PB-O3A
2	E	201	YO7	PA-O3A-PB-O1B
2	C	201	YO7	C51-C61-C71-O71
2	B	201	YO7	O6A-C61-C71-O71
2	C	201	YO7	O6A-C61-C71-O71
2	D	201	YO7	O6A-C61-C71-O71
2	B	201	YO7	PA-O3A-PB-O1B
2	C	201	YO7	PA-O3A-PB-O1B
2	D	201	YO7	PA-O3A-PB-O1B
2	F	201	YO7	PA-O3A-PB-O1B
2	D	201	YO7	C51-C61-C71-O71
2	F	201	YO7	O6A-C61-C71-O71
2	E	201	YO7	O6A-C61-C71-O71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	201	YO7	C51-C61-C71-O71
2	F	201	YO7	C41-C51-C61-C71
2	A	201	YO7	O51-C51-C61-O6A
2	E	201	YO7	O51-C51-C61-O6A
2	F	201	YO7	C41-C51-C61-O6A
2	F	201	YO7	O51-C51-C61-C71
2	F	201	YO7	O51-C51-C61-O6A
3	E	202	EDO	O1-C1-C2-O2
3	E	203	EDO	O1-C1-C2-O2

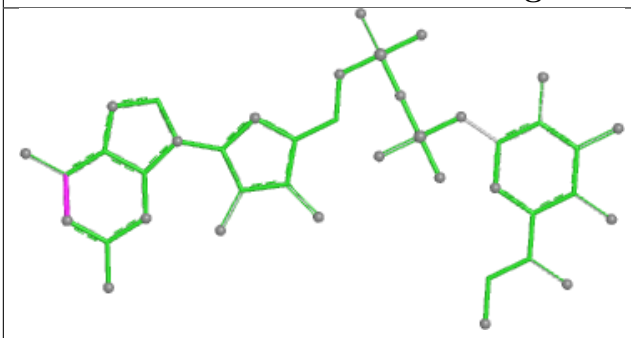
There are no ring outliers.

1 monomer is involved in 1 short contact:

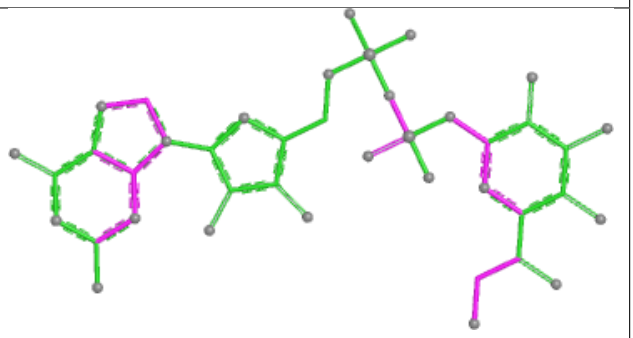
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	YO7	1	0

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.

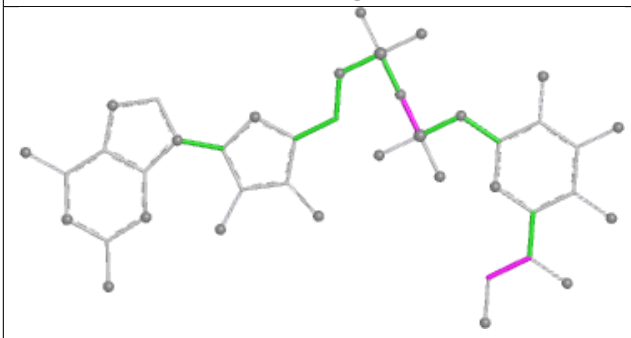
Ligand YO7 D 201



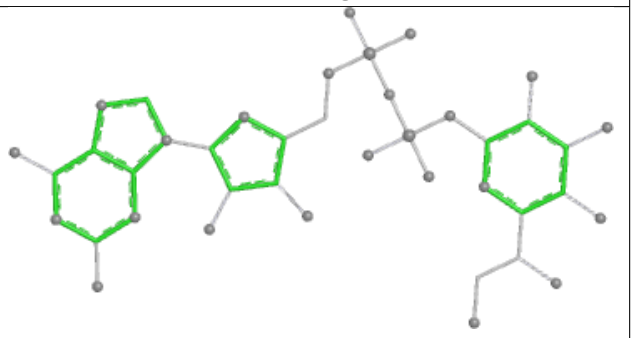
Bond lengths



Bond angles

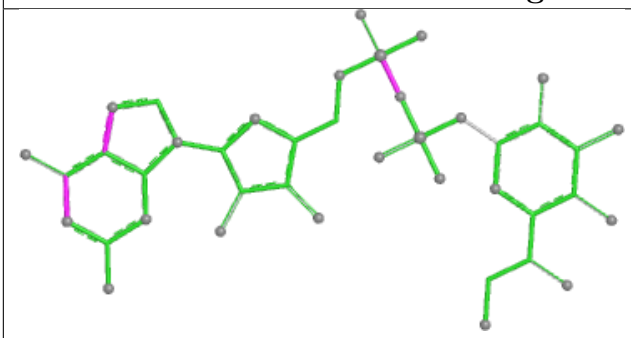


Torsions

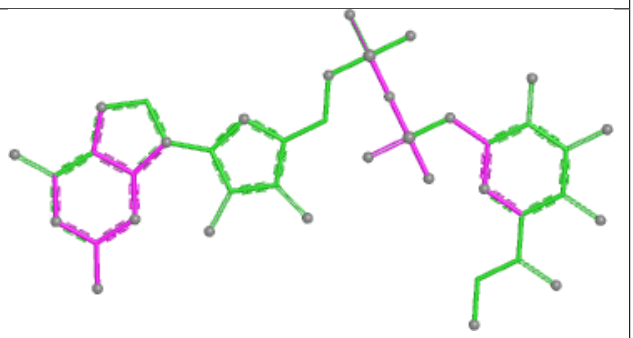


Rings

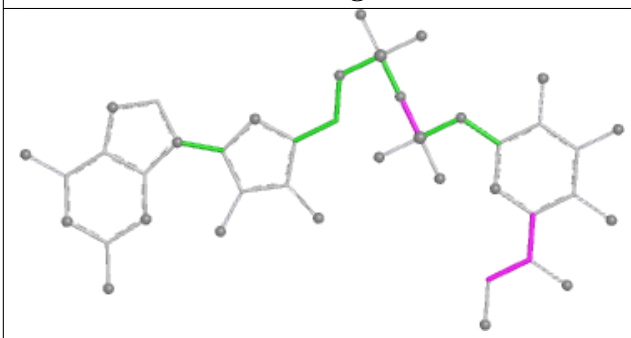
Ligand YO7 E 201



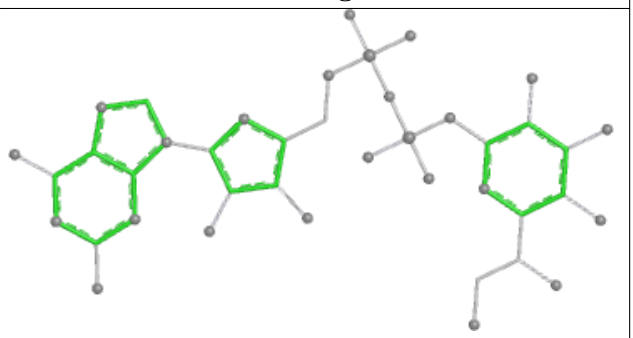
Bond lengths



Bond angles

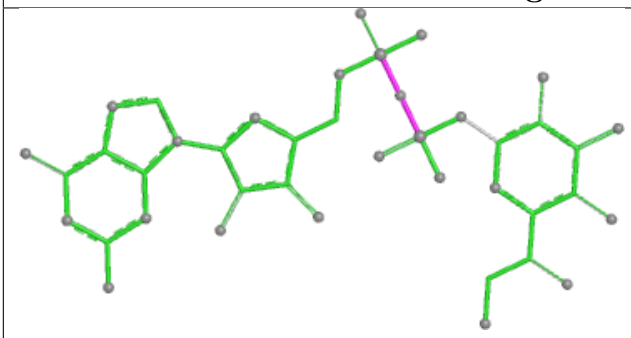


Torsions

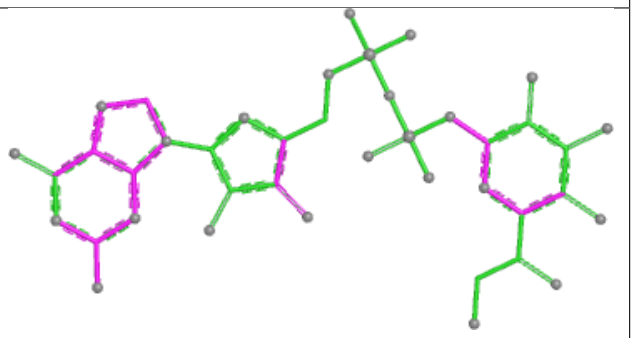


Rings

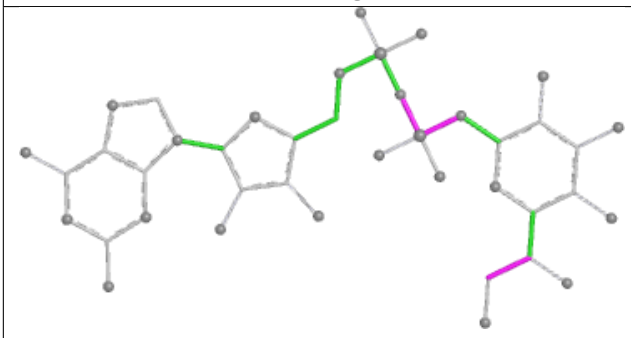
Ligand YO7 C 201



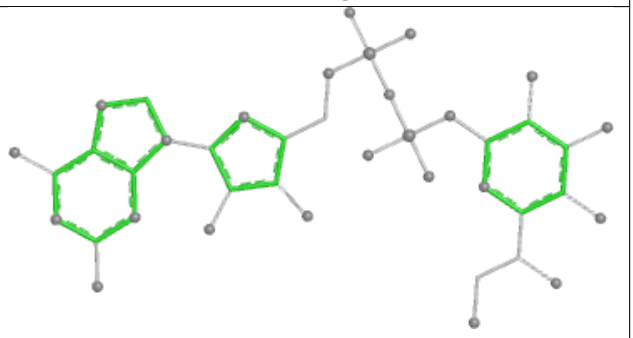
Bond lengths



Bond angles

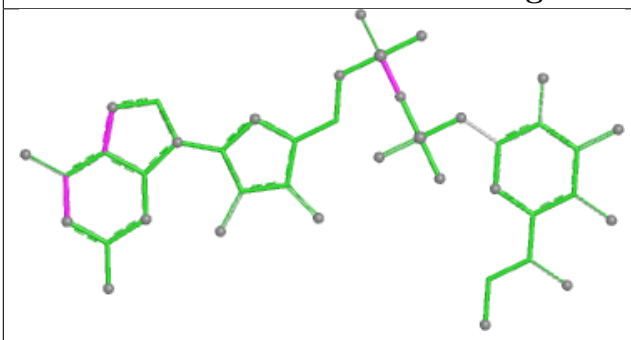


Torsions

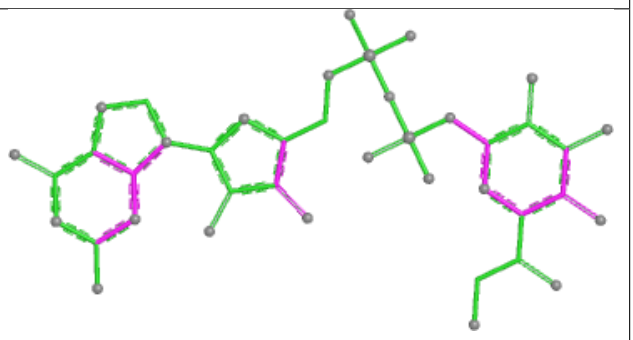


Rings

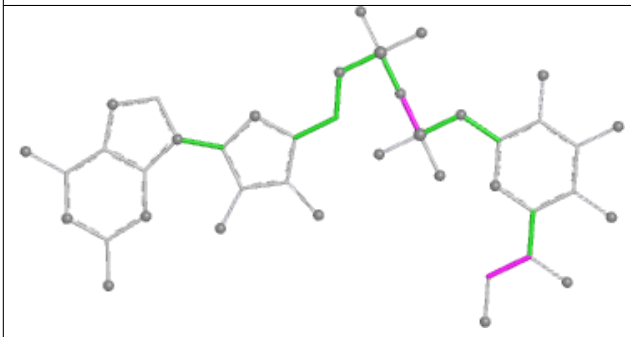
Ligand YO7 B 201



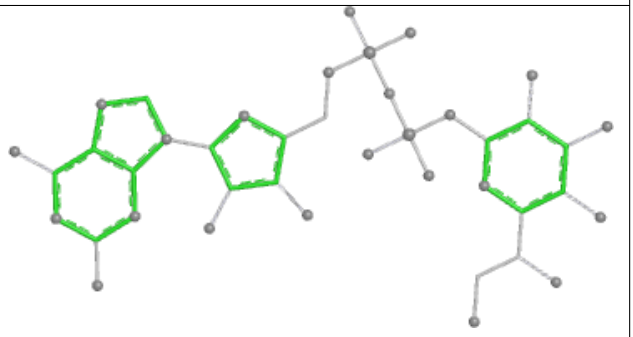
Bond lengths



Bond angles

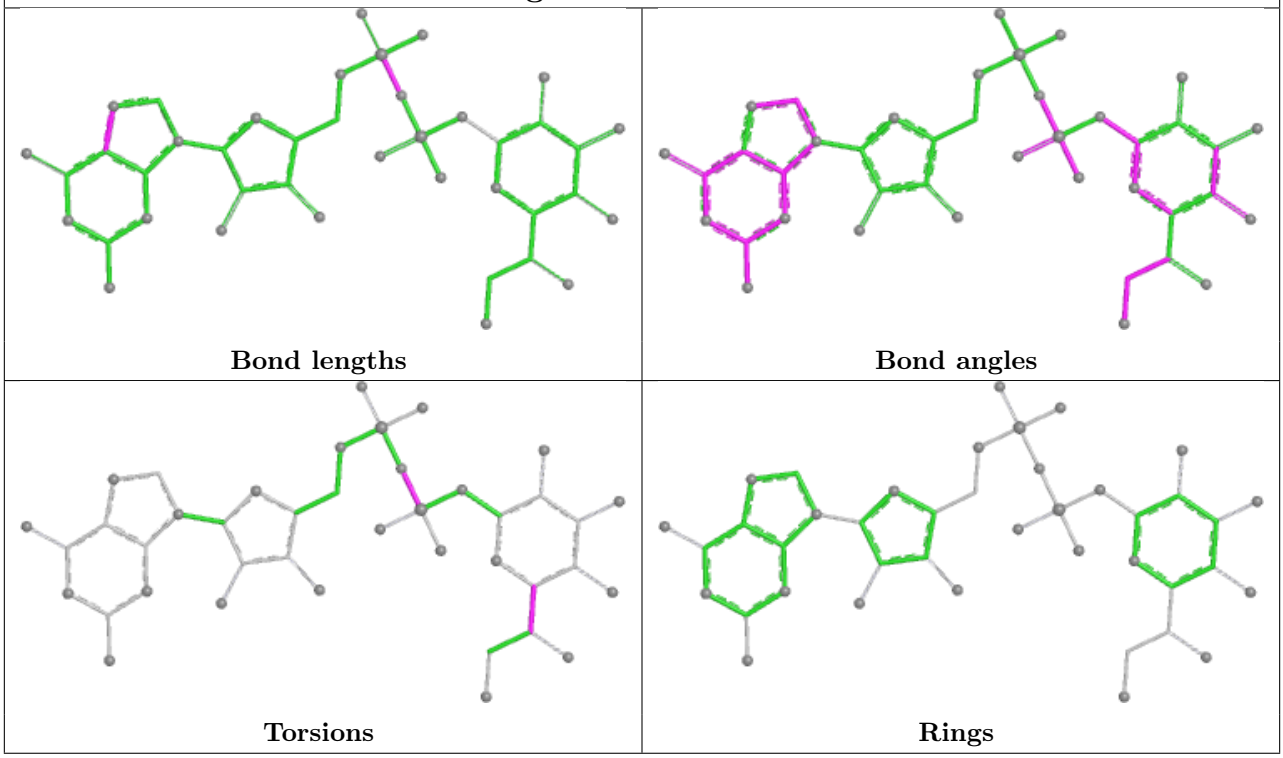


Torsions

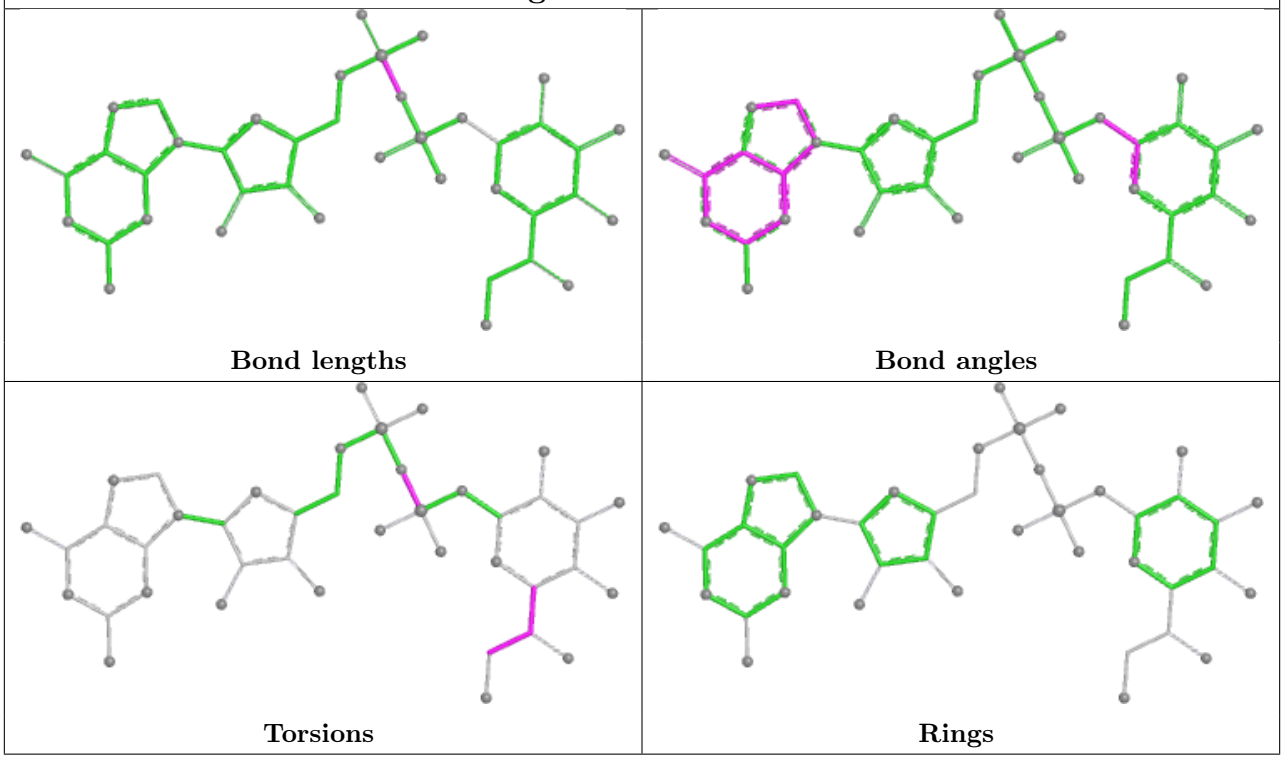


Rings

Ligand YO7 A 201



Ligand YO7 F 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	179/185 (96%)	-0.10	3 (1%)	69	73	7, 17, 36, 54	0
1	B	179/185 (96%)	-0.39	2 (1%)	78	81	8, 13, 30, 50	0
1	C	178/185 (96%)	-0.28	1 (0%)	85	88	9, 15, 33, 43	0
1	D	181/185 (97%)	-0.14	5 (2%)	55	58	9, 15, 37, 53	0
1	E	179/185 (96%)	-0.18	3 (1%)	69	73	8, 16, 34, 64	1 (0%)
1	F	179/185 (96%)	-0.26	2 (1%)	78	81	9, 16, 33, 48	0
All	All	1075/1110 (96%)	-0.23	16 (1%)	72	76	7, 15, 34, 64	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	39	TYR	5.8
1	E	0	HIS	4.1
1	A	39	TYR	3.7
1	E	39	TYR	3.6
1	F	47	GLY	3.1
1	D	48	ILE	2.8
1	B	0	HIS	2.8
1	D	2	ALA	2.7
1	A	40	LEU	2.6
1	D	1	MET	2.5
1	D	40	LEU	2.5
1	C	43	LEU	2.3
1	F	0	HIS	2.1
1	A	92	LYS	2.1
1	E	43	LEU	2.1
1	B	93	ASP	2.0

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 oligosaccharides in this entry.

6.4 Ligands (i)

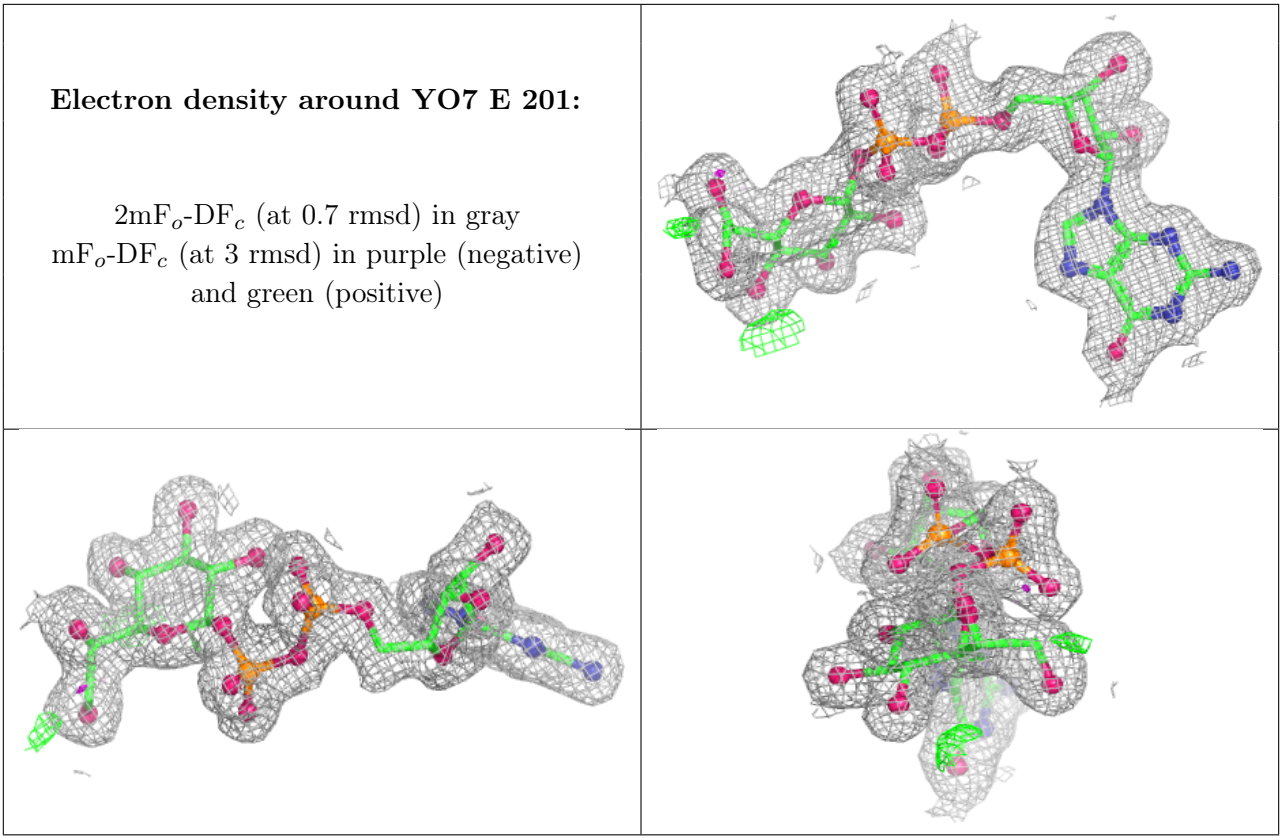
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	E	202	4/4	0.85	0.13	32,32,34,34	0
3	EDO	E	203	4/4	0.92	0.11	36,38,40,40	0
3	EDO	F	202	4/4	0.93	0.08	22,23,25,26	0
3	EDO	B	202	4/4	0.95	0.06	21,22,22,22	0
2	YO7	E	201	41/41	0.98	0.04	11,12,14,15	0
2	YO7	F	201	41/41	0.98	0.05	10,12,14,14	0
2	YO7	A	201	41/41	0.98	0.04	10,11,13,13	0
3	EDO	C	202	4/4	0.98	0.04	19,19,20,20	0
2	YO7	B	201	41/41	0.98	0.04	8,8,9,12	0
2	YO7	C	201	41/41	0.98	0.05	10,13,14,16	0
2	YO7	D	201	41/41	0.98	0.04	9,11,12,14	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.

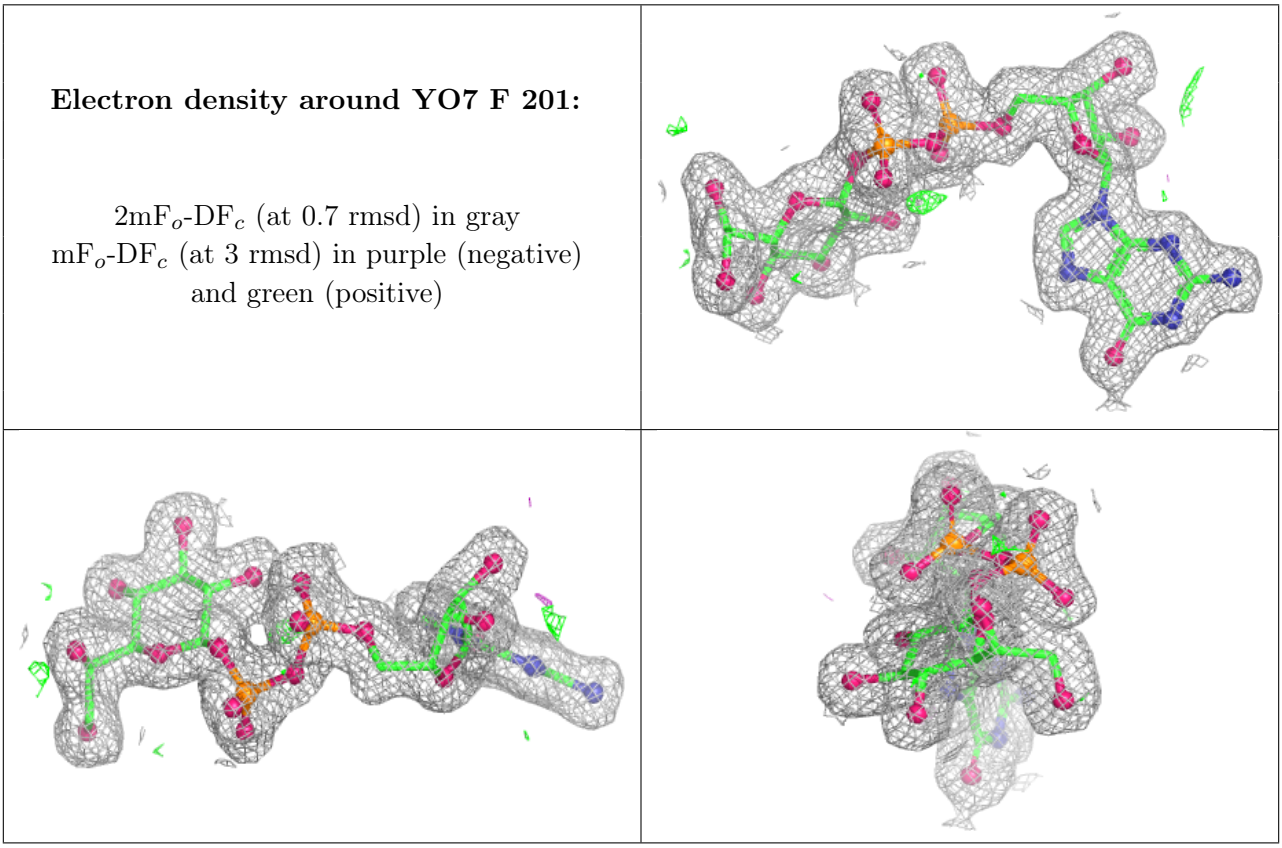
Electron density around YO7 E 201:

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



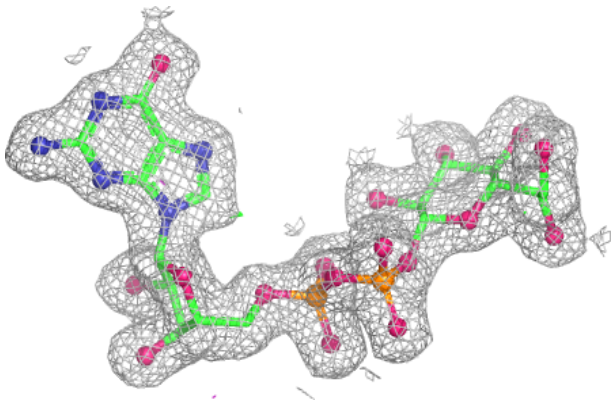
Electron density around YO7 F 201:

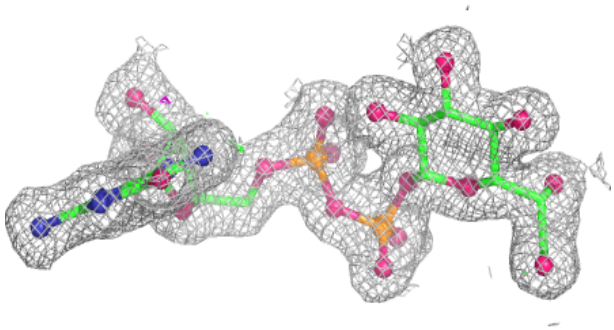
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

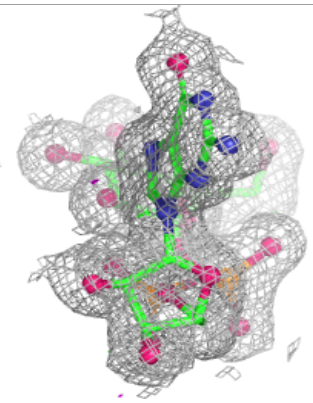


Electron density around YO7 A 201:

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

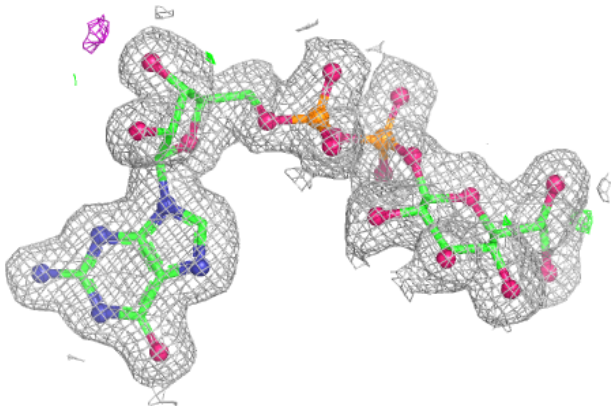


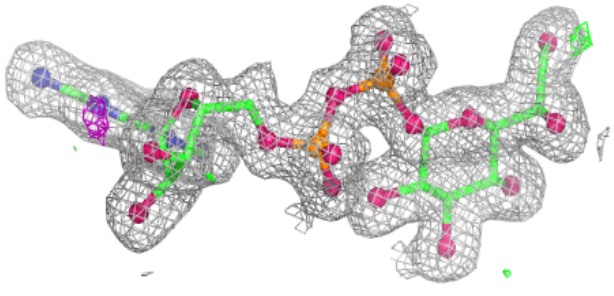


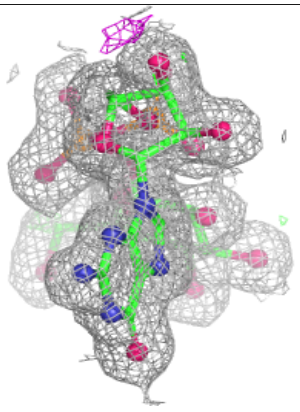


Electron density around YO7 B 201:

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

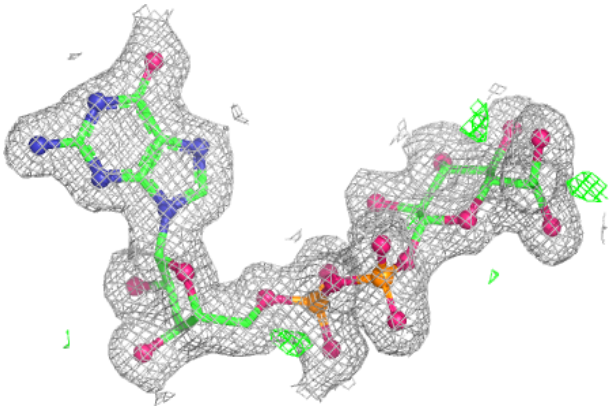


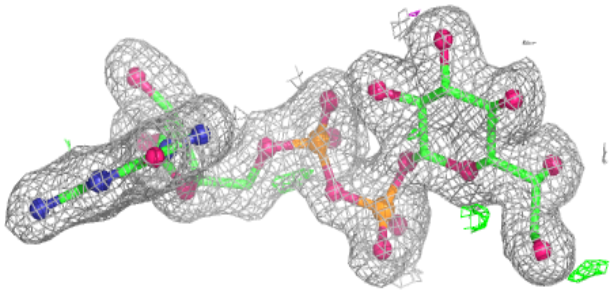


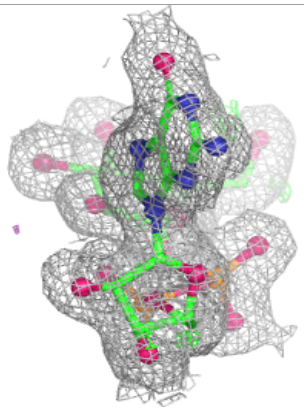


Electron density around YO7 C 201:

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

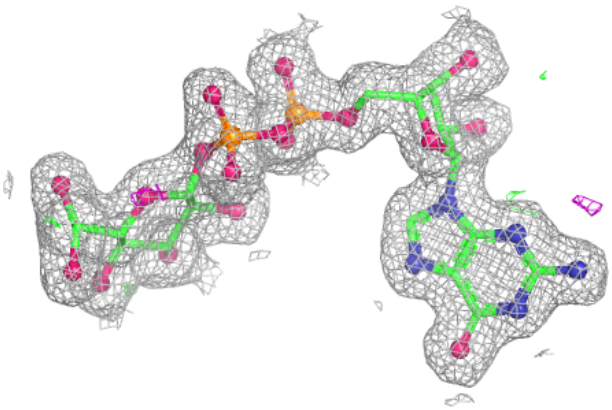


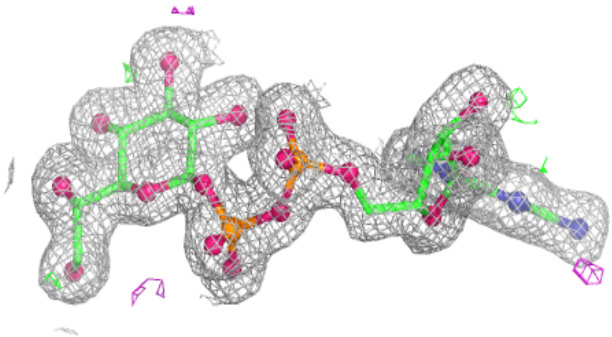


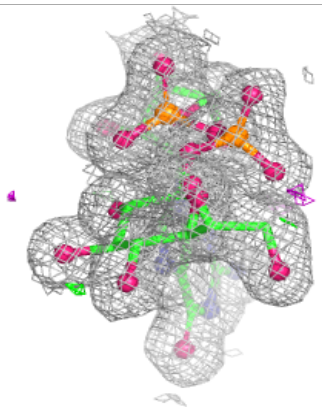


Electron density around YO7 D 201:

$2mF_o$-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.