Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 10:30 AM EDT

PDB ID	:	2A9W
Title	:	E. coli TS complexed with dUMP and inhibitor GA9
Authors	:	Finer-Moore, J.S.; Anderson, A.C.; O'Neil, R.H.; Costi, M.P.; Ferrari, S.; Krucinski, J.; Stroud, R.M.
Deposited on	:	2005-07-12
Resolution	:	1.65 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:

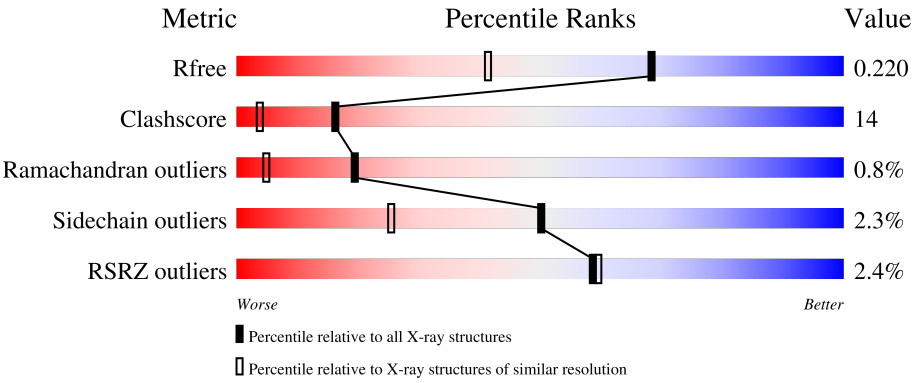
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	264	2% 75% 22% ·
1	B	264	2% 73% 25% ·
1	C	264	2% 77% 21% ·
1	D	264	3% 75% 23% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1266[A]	-	X	-	-
2	PO4	A	1270	-	X	-	-
2	PO4	B	1265[A]	-	X	-	-
2	PO4	B	1269	-	X	-	-
2	PO4	B	1273	-	X	-	-
2	PO4	B	1275	-	X	-	-
2	PO4	C	1267[A]	-	X	-	-
2	PO4	C	1271	-	X	-	-
2	PO4	C	1274	-	X	-	-
2	PO4	D	1268[A]	-	X	-	-
2	PO4	D	1272	-	X	-	-
2	PO4	D	1276	-	X	-	-
5	BME	A	1815[A]	-	-	X	-
5	BME	C	1816[A]	-	-	X	-
6	GOL	A	1804[A]	-	-	-	X
6	GOL	B	1802[A]	-	-	-	X
6	GOL	C	1808[A]	-	-	X	X
6	GOL	D	1807[A]	-	-	X	X
7	2BR	B	1819[A]	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9836 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.

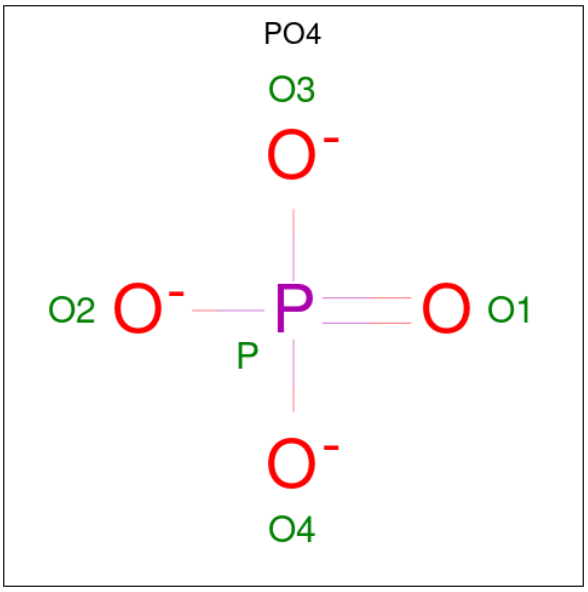
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	9	0
			2234	1427	387	405	15			
1	B	264	Total	C	N	O	S	0	8	0
			2216	1413	383	405	15			
1	C	264	Total	C	N	O	S	0	6	0
			2202	1405	381	402	14			
1	D	264	Total	C	N	O	S	0	8	0
			2217	1414	384	405	14			

There are 4 discrepancies between the modelled and reference sequences:

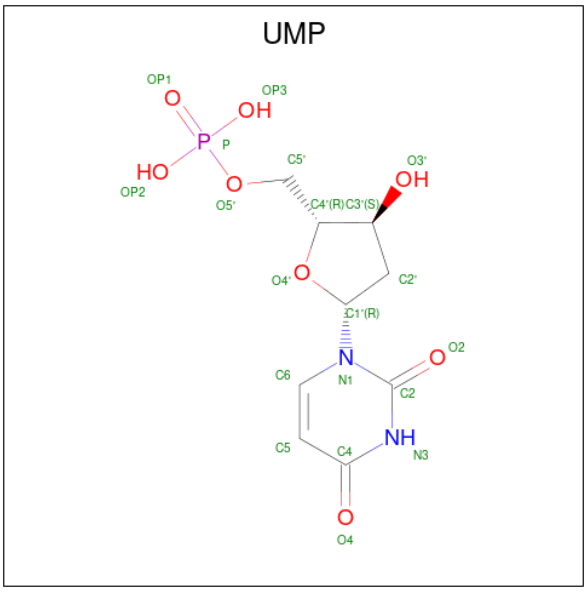
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	modified residue	UNP P0A884
B	1	CXM	MET	modified residue	UNP P0A884
C	1	CXM	MET	modified residue	UNP P0A884
D	1	CXM	MET	modified residue	UNP P0A884

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



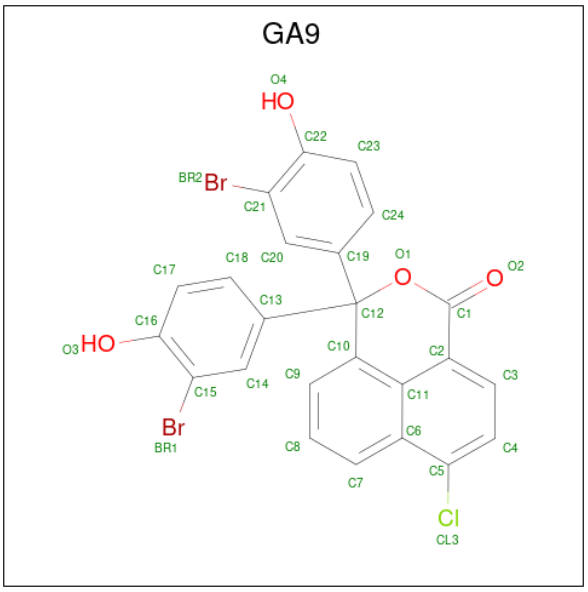
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	1
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	1
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	1
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	1
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



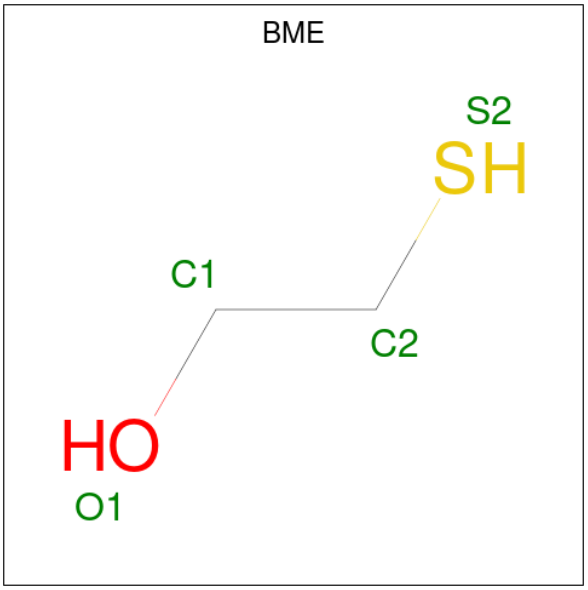
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
3	B	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
3	C	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
3	D	1	Total	C	N	O	P	0	1
			20	9	2	8	1		

- Molecule 4 is 3,3-BIS(3-BROMO-4-HYDROXYPHENYL)-7-CHLORO-1H,3H-BENZO[DE] ISOCHROMEN-1-ONE (three-letter code: GA9) (formula: $C_{24}H_{13}Br_2ClO_4$).



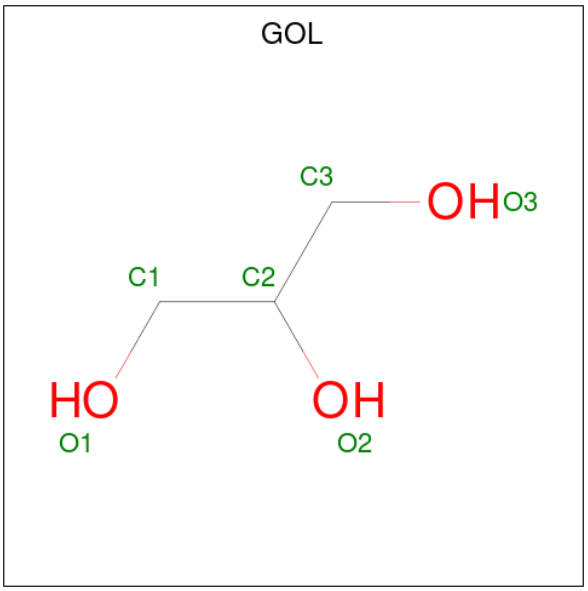
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Br	C	Cl	O	0	1
			62	4	48	2	8		
4	B	1	Total	Br	C	Cl	O	0	1
			62	4	48	2	8		
4	C	1	Total	Br	C	Cl	O	0	1
			62	4	48	2	8		
4	D	1	Total	Br	C	Cl	O	0	1
			62	4	48	2	8		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



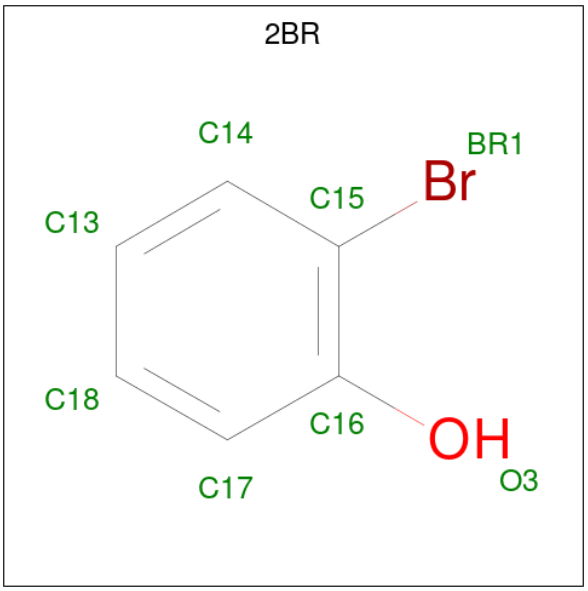
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	1
			4	2	1	1		
5	A	1	Total	C	O	S	0	1
			4	2	1	1		
5	C	1	Total	C	O	S	0	1
			4	2	1	1		
5	D	1	Total	C	O	S	0	1
			4	2	1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	1
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	1
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	1
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	1

- Molecule 7 is 2-BROMOPHENOL (three-letter code: 2BR) (formula: C_6H_5BrO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	Br	C	O	0	1
			16	2	12	2		

- Molecule 8 is water.

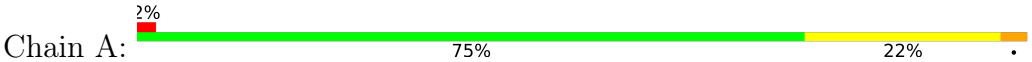
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	128	Total	O	0	3
			128	128		
8	B	115	Total	O	0	1
			115	115		
8	C	126	Total	O	0	3
			126	126		
8	D	118	Total	O	0	2
			118	118		

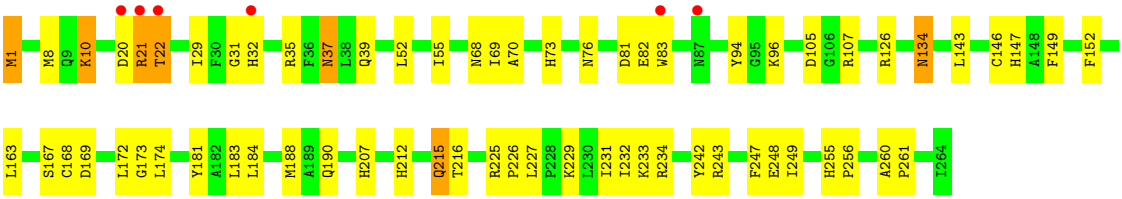
3 Residue-property plots (i)

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: Thymidylate synthase

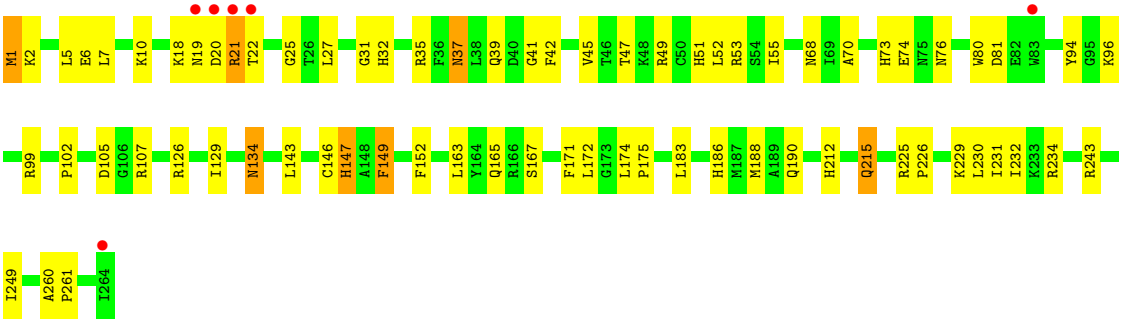
Chain A:





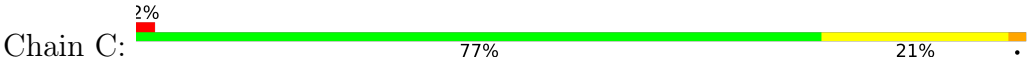
• Molecule 1: Thymidylate synthase

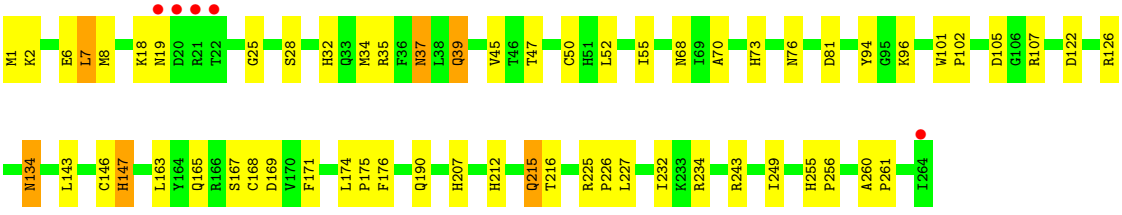
Chain B:



• Molecule 1: Thymidylate synthase

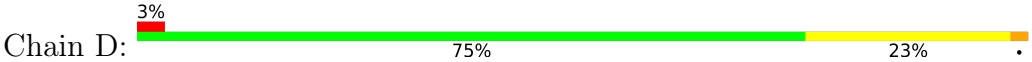
Chain C:

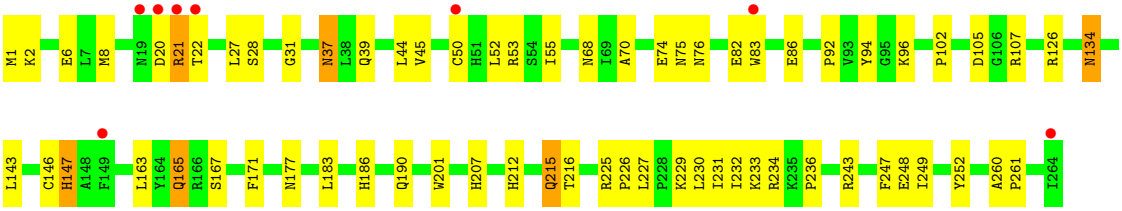




• Molecule 1: Thymidylate synthase

Chain D:




M1
K2
E6
L7
M8
N19
D20
R21
T22
L27
S28
G31
N37
L38
Q39
L44
V45
C50
H51
L52
R53
S54
I55
N68
I69
A70
E74
N75
N76
E82
W83
E86
P92
V93
Y94
G95
K96
P102
D105
G106
R107
R126
N134
L143
C146
H147
A148
F149
L163
Y164
Q165
R166
S167
F171
N177
L183
H186
Q190
W201
H207
H212
Q215
T216
R225
P226
L227
P228
K229
L230
I231
I232
K233
R234
K235
P236
R243
F247
E248
I249
Y252
A260
P261
I264

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	186.60Å 186.60Å 114.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.50 – 1.65 29.50 – 1.65	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.50-1.65) 89.3 (29.50-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.226 0.201 , 0.220	Depositor DCC
R_{free} test set	15874 reflections (9.50%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.017 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.017 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.477 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.469 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.470 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.019 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9836	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2BR, CXM, PO4, BME, UMP, GOL, GA9

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	0.31	0/2287	0.62	0/3105
1	B	0.31	0/2266	0.64	2/3075 (0.1%)
1	C	0.31	0/2252	0.62	1/3057 (0.0%)
1	D	0.31	0/2267	0.63	2/3076 (0.1%)
All	All	0.31	0/9072	0.63	5/12313 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	147	HIS	N-CA-C	-5.26	96.79	111.00
1	C	147	HIS	N-CA-C	-5.14	97.12	111.00
1	D	27	LEU	N-CA-C	-5.08	97.28	111.00
1	B	27	LEU	N-CA-C	-5.05	97.38	111.00
1	B	147	HIS	N-CA-C	-5.00	97.49	111.00

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	2234	0	2142	65	0
1	B	2216	0	2133	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2202	0	2120	64	0
1	D	2217	0	2135	65	0
2	A	10	0	0	0	0
2	B	20	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	20	0	11	2	0
3	B	20	0	11	1	0
3	C	20	0	11	1	0
3	D	20	0	11	1	0
4	A	62	0	26	2	0
4	B	62	0	26	2	0
4	C	62	0	26	2	0
4	D	62	0	26	3	0
5	A	8	0	10	7	0
5	C	4	0	5	5	0
5	D	4	0	5	0	0
6	A	18	0	24	0	0
6	B	18	0	24	3	0
6	C	12	0	16	8	0
6	D	12	0	15	6	0
7	B	16	0	10	8	0
8	A	128	0	0	4	0
8	B	115	0	0	4	0
8	C	126	0	0	2	0
8	D	118	0	0	8	0
All	All	9836	0	8787	261	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 14.

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50[A]:CYS:SG	6:D:1807[A]:GOL:O3	1.92	1.27
1:C:55:ILE:HD11	6:C:1808[A]:GOL:H31	1.51	0.92
1:A:169:ASP:H	5:A:1815[A]:BME:H12	1.36	0.88
1:C:215:GLN:H	1:C:215:GLN:HE21	1.21	0.86
1:B:215:GLN:H	1:B:215:GLN:HE21	1.26	0.83
1:B:147:HIS:HB3	1:B:165:GLN:HE22	1.42	0.82
1:B:80:TRP:HZ3	1:B:143:LEU:HD21	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:HD2	7:B:1819[B]:2BR:BR1	2.37	0.80
1:D:215:GLN:H	1:D:215:GLN:HE21	1.25	0.79
1:A:73:HIS:HE1	1:A:81:ASP:OD1	1.66	0.78
1:D:44:LEU:HG	1:D:50[B]:CYS:SG	2.24	0.78
1:A:169:ASP:N	5:A:1815[A]:BME:H12	2.00	0.77
1:A:215:GLN:H	1:A:215:GLN:HE21	1.27	0.77
1:D:147:HIS:HB3	1:D:165:GLN:HE22	1.50	0.76
1:D:50[A]:CYS:HB3	6:D:1807[A]:GOL:O2	1.87	0.74
1:C:215:GLN:H	1:C:215:GLN:NE2	1.86	0.74
1:A:29:ILE:HD12	1:A:32[A]:HIS:CD2	2.23	0.73
1:A:168:CYS:HA	5:A:1815[A]:BME:H12	1.69	0.72
1:B:249:ILE:H	6:B:1809:GOL:C1	2.01	0.72
1:C:168:CYS:HA	5:C:1816[A]:BME:H11	1.71	0.71
1:C:50[A]:CYS:HG	6:C:1808[A]:GOL:HO2	1.39	0.70
1:B:215:GLN:H	1:B:215:GLN:NE2	1.89	0.70
1:D:102:PRO:HG2	8:D:1895:HOH:O	1.92	0.70
1:D:215:GLN:H	1:D:215:GLN:NE2	1.89	0.70
1:A:52:LEU:HD12	1:A:249:ILE:HG13	1.74	0.69
1:C:52:LEU:HD12	1:C:249:ILE:HG13	1.73	0.68
1:C:50[A]:CYS:SG	6:C:1808[A]:GOL:O2	2.50	0.68
1:D:52:LEU:HD12	1:D:249:ILE:HG13	1.76	0.68
1:D:105:ASP:OD2	1:D:107:ARG:HD3	1.94	0.68
1:B:249:ILE:H	6:B:1809:GOL:H11	1.59	0.67
1:B:52:LEU:HD12	1:B:249:ILE:HG13	1.76	0.67
1:D:50[A]:CYS:HB3	6:D:1807[A]:GOL:C2	2.24	0.67
1:B:18:LYS:HG2	8:B:1898:HOH:O	1.94	0.67
1:B:68:ASN:HD22	1:B:70:ALA:H	1.41	0.67
1:C:18:LYS:CD	8:D:1936:HOH:O	2.41	0.67
1:A:215:GLN:H	1:A:215:GLN:NE2	1.92	0.67
1:B:70:ALA:O	1:B:74:GLU:HG3	1.96	0.66
1:C:50[A]:CYS:HB3	6:C:1808[A]:GOL:C3	2.26	0.66
1:D:86:GLU:H	1:D:86:GLU:CD	1.98	0.66
1:B:80:TRP:CZ3	1:B:143:LEU:HD21	2.28	0.65
1:B:21:ARG:HG3	1:B:21:ARG:O	1.96	0.65
1:B:102:PRO:HG2	8:B:1932:HOH:O	1.97	0.65
1:A:10:LYS:HB2	1:A:10:LYS:NZ	2.12	0.65
1:D:50[A]:CYS:HB3	6:D:1807[A]:GOL:H2	1.78	0.65
4:A:1320[B]:GA9:H18	4:A:1320[B]:GA9:C9	2.27	0.64
1:A:168:CYS:HA	5:A:1815[A]:BME:C1	2.27	0.63
1:A:52:LEU:CD1	1:A:249:ILE:HG13	2.28	0.63
1:A:225:ARG:HB3	1:A:226:PRO:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:THR:HA	8:A:1905:HOH:O	1.98	0.63
1:C:168:CYS:HA	5:C:1816[A]:BME:C1	2.29	0.62
1:D:146[B]:CYS:SG	1:D:167:SER:O	2.58	0.62
4:C:1318[A]:GA9:H14	4:C:1318[A]:GA9:C9	2.27	0.62
1:A:212:HIS:HE1	1:A:261:PRO:O	1.83	0.62
1:A:234:ARG:NE	1:A:243:ARG:HH21	1.98	0.62
1:A:143:LEU:O	1:A:143:LEU:HD12	2.00	0.61
4:A:1320[A]:GA9:H14	4:A:1320[A]:GA9:C9	2.29	0.61
4:D:1319[A]:GA9:H14	4:D:1319[A]:GA9:C9	2.31	0.61
1:B:229:LYS:HE2	1:B:231:ILE:HD11	1.82	0.61
1:C:68:ASN:HD22	1:C:70:ALA:H	1.48	0.61
4:B:1321[A]:GA9:H14	4:B:1321[A]:GA9:C9	2.29	0.61
4:C:1318[B]:GA9:C9	4:C:1318[B]:GA9:H18	2.30	0.61
1:D:212:HIS:HE1	1:D:261:PRO:O	1.83	0.61
4:B:1321[B]:GA9:C9	4:B:1321[B]:GA9:H18	2.30	0.61
1:C:212:HIS:HE1	1:C:261:PRO:O	1.83	0.60
1:A:174:LEU:N	5:A:1815[A]:BME:H22	2.16	0.60
4:D:1319[B]:GA9:C9	4:D:1319[B]:GA9:H18	2.32	0.60
1:A:1:CXM:HG3	1:A:227:LEU:HD21	1.83	0.60
1:A:152:PHE:CZ	1:A:188[B]:MET:SD	2.94	0.60
1:B:225:ARG:HB3	1:B:226:PRO:HD2	1.83	0.60
1:D:52:LEU:CD1	1:D:249:ILE:HG13	2.31	0.59
1:C:225:ARG:HB3	1:C:226:PRO:HD2	1.84	0.59
1:B:212:HIS:HE1	1:B:261:PRO:O	1.85	0.59
1:D:225:ARG:HB3	1:D:226:PRO:HD2	1.84	0.59
1:A:37:ASN:ND2	1:A:39:GLN:H	2.01	0.59
1:B:143:LEU:HD23	1:B:143:LEU:N	2.17	0.59
1:D:68:ASN:HD22	1:D:70:ALA:H	1.50	0.58
1:A:146[B]:CYS:SG	1:A:167:SER:O	2.61	0.58
1:C:146[B]:CYS:SG	1:C:167:SER:O	2.61	0.58
1:D:50[B]:CYS:SG	1:D:252:TYR:OH	2.60	0.58
1:C:143:LEU:HD12	1:C:143:LEU:O	2.04	0.58
1:D:53[B]:ARG:NH2	1:D:75:ASN:O	2.35	0.58
1:B:147:HIS:HB3	1:B:165:GLN:NE2	2.16	0.57
1:C:1:CXM:HG3	1:C:227:LEU:HD21	1.87	0.57
1:D:1:CXM:HG3	1:D:227:LEU:HD21	1.85	0.57
1:C:1:CXM:ON2	1:C:45[A]:VAL:HG23	2.04	0.57
1:A:21:ARG:O	1:A:22:THR:C	2.42	0.57
1:C:50[A]:CYS:HB3	6:C:1808[A]:GOL:H32	1.87	0.57
1:C:52:LEU:CD1	1:C:249:ILE:HG13	2.35	0.57
1:C:169:ASP:H	5:C:1816[A]:BME:H12	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASN:HD22	1:A:70:ALA:H	1.53	0.56
1:B:249:ILE:N	6:B:1809:GOL:H11	2.19	0.56
1:D:92:PRO:CB	1:D:96[A]:LYS:HD3	2.35	0.56
1:A:107:ARG:NH1	8:A:1944:HOH:O	2.27	0.56
1:B:152:PHE:CZ	1:B:188[B]:MET:SD	2.99	0.56
1:C:50[A]:CYS:HB3	6:C:1808[A]:GOL:O3	2.05	0.56
1:D:143:LEU:HD12	1:D:143:LEU:O	2.05	0.56
1:D:147:HIS:HB3	1:D:165:GLN:NE2	2.18	0.55
1:B:96:LYS:HE2	1:B:102:PRO:HD3	1.88	0.55
1:C:45[A]:VAL:CG1	1:C:50[A]:CYS:SG	2.95	0.55
1:C:190:GLN:HE22	1:C:232:ILE:HG21	1.72	0.55
1:D:21:ARG:N	1:D:21:ARG:HE	2.04	0.55
1:B:146[B]:CYS:SG	1:B:167:SER:O	2.64	0.55
1:C:96:LYS:HE3	1:C:96:LYS:HA	1.88	0.55
1:C:176:PHE:HD2	6:C:1808[A]:GOL:H12	1.71	0.55
1:A:126:ARG:NH2	1:B:20:ASP:HB3	2.23	0.54
1:C:126:ARG:NH2	1:D:20:ASP:HB3	2.22	0.54
1:D:92:PRO:HB3	1:D:96[B]:LYS:HD2	1.88	0.54
1:A:31:GLY:O	1:B:35:ARG:NH2	2.41	0.54
1:B:52:LEU:H	7:B:1819[B]:2BR:C18	2.21	0.54
1:D:92:PRO:CB	1:D:96[B]:LYS:HD2	2.38	0.54
1:D:2:LYS:HG2	1:D:6:GLU:OE2	2.08	0.54
1:C:19:ASN:HA	1:C:25:GLY:HA2	1.90	0.53
1:D:37:ASN:ND2	1:D:39:GLN:H	2.05	0.53
1:D:107:ARG:NH1	8:D:1931:HOH:O	2.42	0.53
4:D:1319[A]:GA9:BR1	6:D:1807[A]:GOL:O1	2.76	0.53
1:C:37:ASN:ND2	1:C:39:GLN:H	2.07	0.53
1:A:147:HIS:HB2	1:A:163:LEU:HD11	1.91	0.52
1:B:73:HIS:HE1	1:B:81:ASP:OD1	1.92	0.52
1:C:52:LEU:HD23	1:C:55:ILE:HD12	1.90	0.52
1:A:69:ILE:HD12	1:A:73:HIS:CE1	2.45	0.52
1:A:37:ASN:HD22	1:A:39:GLN:H	1.56	0.52
1:A:183:LEU:HD11	1:A:247:PHE:CE1	2.45	0.52
1:C:215:GLN:HE21	1:C:215:GLN:N	2.01	0.52
1:C:73:HIS:HE1	1:C:81:ASP:OD1	1.92	0.52
1:A:52:LEU:HD23	1:A:55:ILE:HD12	1.92	0.51
1:A:134:ASN:C	1:A:134:ASN:HD22	2.13	0.51
1:B:52:LEU:CD1	1:B:249:ILE:HG13	2.40	0.51
1:B:229:LYS:HE2	1:B:231:ILE:CD1	2.40	0.51
1:C:105:ASP:OD2	1:C:107:ARG:HD3	2.10	0.51
1:D:190:GLN:HE22	1:D:232:ILE:HG21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD13	1:B:32:HIS:CD2	2.46	0.51
1:B:53[A]:ARG:N	7:B:1819[A]:2BR:BR1	2.91	0.51
1:A:20:ASP:HB2	1:B:126:ARG:NH2	2.25	0.51
1:C:18:LYS:HD3	8:D:1936:HOH:O	2.07	0.51
1:A:168:CYS:CA	5:A:1815[A]:BME:H12	2.39	0.51
1:B:52:LEU:HD23	1:B:55:ILE:HD12	1.91	0.51
1:B:1:CXM:ON2	1:B:45[A]:VAL:HG13	2.11	0.51
1:C:32:HIS:HE1	1:C:34:MET:HG2	1.75	0.51
1:D:134:ASN:C	1:D:134:ASN:HD22	2.15	0.51
1:D:212:HIS:HD2	8:D:1901:HOH:O	1.94	0.50
1:D:243:ARG:HD2	8:D:1917:HOH:O	2.10	0.50
1:A:233:LYS:HE3	1:A:248:GLU:HB2	1.92	0.50
1:A:37:ASN:HD22	1:A:37:ASN:C	2.14	0.50
1:A:184:LEU:O	1:A:188[B]:MET:HG3	2.11	0.50
1:C:2:LYS:O	1:C:6:GLU:HG3	2.12	0.49
1:D:37:ASN:HD22	1:D:39:GLN:H	1.60	0.49
1:A:20:ASP:CB	1:B:126:ARG:NH2	2.76	0.49
1:B:5:LEU:HD11	1:B:47:THR:HG21	1.94	0.49
1:B:134:ASN:C	1:B:134:ASN:HD22	2.16	0.49
1:C:147:HIS:HB2	1:C:163:LEU:HD11	1.95	0.49
1:A:212:HIS:HD2	8:A:1834:HOH:O	1.94	0.49
1:B:19:ASN:HA	1:B:25:GLY:HA2	1.95	0.49
1:B:41:GLY:HA2	8:B:1923:HOH:O	2.13	0.49
1:C:37:ASN:C	1:C:37:ASN:HD22	2.16	0.49
1:C:134:ASN:C	1:C:134:ASN:HD22	2.16	0.49
1:C:176:PHE:CD2	6:C:1808[A]:GOL:H12	2.48	0.49
1:B:52:LEU:H	7:B:1819[A]:2BR:C14	2.26	0.48
3:C:1279[B]:UMP:OP3	1:D:126:ARG:HD2	2.13	0.48
1:D:92:PRO:HB3	1:D:96[A]:LYS:HD3	1.94	0.48
1:B:105:ASP:OD2	1:B:107:ARG:HD3	2.13	0.48
1:C:18:LYS:HD2	8:D:1936:HOH:O	2.10	0.48
1:A:229:LYS:HE3	1:A:231:ILE:HD11	1.96	0.48
1:B:190:GLN:HE22	1:B:232:ILE:HG21	1.79	0.48
1:B:172:LEU:HD21	1:B:260:ALA:HB3	1.95	0.48
1:B:21:ARG:O	1:B:22:THR:C	2.51	0.48
1:B:2:LYS:HG2	1:B:6:GLU:OE2	2.14	0.48
1:A:105:ASP:OD2	1:A:107:ARG:HD3	2.14	0.47
1:C:37:ASN:HD21	1:C:39:GLN:HB2	1.79	0.47
1:D:21:ARG:NE	1:D:21:ARG:CA	2.77	0.47
1:A:96:LYS:HE3	1:A:96:LYS:HA	1.97	0.47
1:A:173:GLY:C	5:A:1815[A]:BME:H22	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ALA:O	1:D:74:GLU:HG3	2.14	0.47
1:D:37:ASN:HD21	1:D:39:GLN:HB2	1.79	0.47
1:D:233:LYS:HE3	1:D:248:GLU:HB2	1.96	0.47
1:A:20:ASP:O	1:A:22:THR:N	2.48	0.47
1:C:18:LYS:NZ	8:D:1936:HOH:O	2.47	0.47
1:D:20:ASP:O	1:D:22:THR:N	2.48	0.47
1:D:82:GLU:HG3	1:D:83:TRP:CD1	2.50	0.47
1:D:52:LEU:HD23	1:D:55:ILE:HD12	1.97	0.46
1:A:255:HIS:HB3	1:A:256:PRO:HD2	1.98	0.46
1:B:37:ASN:C	1:B:37:ASN:HD22	2.19	0.46
1:C:45[A]:VAL:HG13	1:C:50[A]:CYS:SG	2.55	0.46
1:A:190:GLN:HE22	1:A:232:ILE:HG21	1.80	0.46
1:D:147:HIS:HB2	1:D:163:LEU:HD11	1.98	0.46
1:D:229:LYS:HE3	1:D:231:ILE:HD11	1.97	0.46
1:D:177[A]:ASN:ND2	1:D:201:TRP:HE1	2.13	0.46
1:D:183:LEU:HD11	1:D:247:PHE:CD1	2.51	0.46
1:C:126:ARG:HD2	3:D:1280[B]:UMP:OP3	2.16	0.46
1:A:10:LYS:HB2	1:A:10:LYS:HZ3	1.81	0.46
1:B:51:HIS:HB3	7:B:1819[A]:2BR:BR1	2.71	0.46
1:B:53[A]:ARG:HB2	7:B:1819[A]:2BR:BR1	2.71	0.45
1:C:35:ARG:NH2	1:D:31:GLY:O	2.49	0.45
1:A:68:ASN:ND2	1:A:70:ALA:H	2.13	0.45
1:D:37:ASN:HD22	1:D:37:ASN:C	2.18	0.45
1:D:50[A]:CYS:CB	6:D:1807[A]:GOL:H2	2.45	0.45
1:A:229:LYS:HE3	1:A:231:ILE:CD1	2.46	0.45
1:C:234:ARG:NE	1:C:243:ARG:HH21	2.14	0.45
1:B:37:ASN:ND2	1:B:39:GLN:H	2.15	0.45
1:B:147:HIS:HB2	1:B:163:LEU:HD11	1.98	0.45
1:D:229:LYS:HE3	1:D:231:ILE:CD1	2.47	0.45
1:D:21:ARG:NE	1:D:21:ARG:HA	2.31	0.45
1:A:31:GLY:O	1:A:32[A]:HIS:CG	2.70	0.45
1:B:52:LEU:HB2	7:B:1819[A]:2BR:H14	1.99	0.44
1:D:183:LEU:HD11	1:D:247:PHE:CE1	2.52	0.44
1:B:10:LYS:HE2	8:B:1894:HOH:O	2.17	0.44
1:A:147:HIS:HD2	1:A:181:TYR:OH	2.01	0.44
1:C:122:ASP:CG	1:D:21:ARG:HH12	2.20	0.44
1:C:212:HIS:HD2	8:C:1827:HOH:O	2.01	0.44
1:D:8:MET:CG	1:D:216:THR:HG23	2.47	0.44
1:A:207:HIS:HE1	8:A:1942[A]:HOH:O	2.00	0.43
1:B:174:LEU:HB3	1:B:175:PRO:HD3	2.01	0.43
1:B:186:HIS:CG	1:B:230:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:HD11	1:A:247:PHE:CD1	2.53	0.43
1:B:129:ILE:HG21	1:B:149[A]:PHE:CE2	2.53	0.43
1:A:31:GLY:O	1:A:32[A]:HIS:CD2	2.72	0.43
1:B:215:GLN:HE21	1:B:215:GLN:N	2.05	0.43
1:A:8:MET:CG	1:A:216:THR:HG23	2.48	0.43
1:A:172:LEU:HD21	1:A:260:ALA:HB3	2.00	0.43
1:B:234:ARG:NE	1:B:243:ARG:HH21	2.17	0.43
1:C:7:LEU:HG	1:C:32:HIS:CE1	2.54	0.43
1:C:165:GLN:HE21	5:C:1816[A]:BME:H11	1.84	0.43
1:C:207:HIS:HE1	8:C:1941[A]:HOH:O	2.02	0.43
1:C:174:LEU:HB3	1:C:175:PRO:HD3	2.01	0.43
1:C:28:SER:HB3	1:C:207:HIS:HB3	2.01	0.43
1:D:28[B]:SER:HB2	1:D:207:HIS:HB3	2.01	0.43
1:C:73:HIS:CE1	1:C:81:ASP:OD1	2.72	0.42
1:B:52:LEU:N	7:B:1819[A]:2BR:BR1	3.06	0.42
1:B:143:LEU:N	1:B:143:LEU:CD2	2.82	0.42
1:A:126:ARG:HD2	3:B:1278[B]:UMP:OP3	2.20	0.42
3:A:1277[B]:UMP:OP3	1:B:126:ARG:HD2	2.19	0.42
1:A:35:ARG:NH2	1:B:31:GLY:O	2.53	0.42
1:C:165:GLN:NE2	5:C:1816[A]:BME:S2	2.93	0.42
1:A:126:ARG:NH2	1:B:20:ASP:CB	2.83	0.42
1:B:20:ASP:O	1:B:21:ARG:C	2.58	0.42
1:C:255:HIS:HB3	1:C:256:PRO:HD2	2.02	0.42
1:D:44:LEU:CG	1:D:50[B]:CYS:SG	3.02	0.42
1:D:143:LEU:HD12	1:D:143:LEU:C	2.41	0.42
1:D:234:ARG:O	1:D:236:PRO:HD3	2.19	0.42
1:A:149[B]:PHE:CD1	1:A:149[B]:PHE:C	2.94	0.42
1:D:186:HIS:CG	1:D:230:LEU:HD23	2.55	0.41
1:A:207:HIS:HE1	3:A:1277[B]:UMP:O3'	2.03	0.41
1:B:96:LYS:O	1:B:96:LYS:HD3	2.20	0.41
1:C:171:PHE:CZ	1:C:215:GLN:HB3	2.55	0.41
1:B:171:PHE:CZ	1:B:215:GLN:HB3	2.56	0.41
1:C:8:MET:CG	1:C:216:THR:HG23	2.50	0.41
1:C:47:THR:HA	1:C:255:HIS:HD2	1.84	0.41
1:D:1:CXM:ON2	1:D:45[A]:VAL:HG13	2.20	0.41
1:D:171:PHE:CE1	1:D:260:ALA:HB2	2.55	0.41
1:A:10:LYS:HB2	1:A:10:LYS:HZ2	1.83	0.41
1:A:82:GLU:HG3	1:A:83[A]:TRP:CD1	2.55	0.41
1:B:20:ASP:O	1:B:22:THR:N	2.53	0.41
1:B:99:ARG:HH11	1:B:99:ARG:HG3	1.86	0.41
1:C:37:ASN:HD22	1:C:39:GLN:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:PHE:CE1	1:C:260:ALA:HB2	2.55	0.41
1:A:190:GLN:NE2	1:A:242:TYR:OH	2.54	0.40
1:A:215:GLN:HE21	1:A:215:GLN:N	2.08	0.40
1:D:215:GLN:HE21	1:D:215:GLN:N	2.05	0.40
1:C:101:TRP:HA	1:C:102:PRO:HD3	1.90	0.40
1:B:42:PHE:HZ	1:B:183:LEU:HG	1.86	0.40
1:C:126:ARG:HD3	1:D:167:SER:OG	2.22	0.40
1:C:215:GLN:NE2	1:C:215:GLN:N	2.64	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	271/264 (103%)	260 (96%)	8 (3%)	3 (1%)	14 2
1	B	270/264 (102%)	260 (96%)	8 (3%)	2 (1%)	22 6
1	C	268/264 (102%)	259 (97%)	8 (3%)	1 (0%)	34 16
1	D	270/264 (102%)	260 (96%)	8 (3%)	2 (1%)	22 6
All	All	1079/1056 (102%)	1039 (96%)	32 (3%)	8 (1%)	19 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	94	TYR
1	D	21	ARG
1	A	21	ARG
1	A	22	THR
1	A	94	TYR
1	B	21	ARG
1	B	94	TYR

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Mol	Chain	Res	Type
1	D	94	TYR

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	241/232 (104%)	236 (98%)	5 (2%)	53	29
1	B	240/232 (103%)	234 (98%)	6 (2%)	47	22
1	C	238/232 (103%)	232 (98%)	6 (2%)	47	22
1	D	240/232 (103%)	235 (98%)	5 (2%)	53	29
All	All	959/928 (103%)	937 (98%)	22 (2%)	50	25

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	37	ASN
1	A	76	ASN
1	A	134	ASN
1	A	215	GLN
1	B	37	ASN
1	B	76	ASN
1	B	134	ASN
1	B	149[A]	PHE
1	B	149[B]	PHE
1	B	215	GLN
1	C	7	LEU
1	C	37	ASN
1	C	39	GLN
1	C	76	ASN
1	C	134	ASN
1	C	215	GLN
1	D	37	ASN
1	D	76	ASN
1	D	134	ASN

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Mol	Chain	Res	Type
1	D	165	GLN
1	D	215	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	37	ASN
1	A	39	GLN
1	A	68	ASN
1	A	73	HIS
1	A	76	ASN
1	A	117	ASN
1	A	134	ASN
1	A	147	HIS
1	A	162	GLN
1	A	190	GLN
1	A	207	HIS
1	A	212	HIS
1	A	215	GLN
1	A	219	GLN
1	B	33	GLN
1	B	37	ASN
1	B	39	GLN
1	B	68	ASN
1	B	73	HIS
1	B	76	ASN
1	B	117	ASN
1	B	134	ASN
1	B	147	HIS
1	B	162	GLN
1	B	165	GLN
1	B	190	GLN
1	B	207	HIS
1	B	212	HIS
1	B	215	GLN
1	B	219	GLN
1	C	32	HIS
1	C	33	GLN
1	C	37	ASN
1	C	68	ASN
1	C	73	HIS

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Mol	Chain	Res	Type
1	C	76	ASN
1	C	108	HIS
1	C	117	ASN
1	C	134	ASN
1	C	147	HIS
1	C	162	GLN
1	C	190	GLN
1	C	207	HIS
1	C	212	HIS
1	C	215	GLN
1	C	219	GLN
1	D	32	HIS
1	D	33	GLN
1	D	37	ASN
1	D	68	ASN
1	D	76	ASN
1	D	117	ASN
1	D	134	ASN
1	D	147	HIS
1	D	162	GLN
1	D	190	GLN
1	D	207	HIS
1	D	212	HIS
1	D	215	GLN
1	D	219	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CXM	C	1	1	8,10,11	0.81	0	7,11,13	0.70	0
1	CXM	A	1	1	8,10,11	0.92	1 (12%)	7,11,13	4.70	1 (14%)
1	CXM	B	1	1	8,10,11	0.89	1 (12%)	7,11,13	1.75	1 (14%)
1	CXM	D	1	1	8,10,11	0.82	0	7,11,13	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	C	1	1	-	0/9/10/12	-
1	CXM	A	1	1	-	2/9/10/12	-
1	CXM	B	1	1	-	2/9/10/12	-
1	CXM	D	1	1	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	CXM	ON1-CN	2.26	1.25	1.21
1	B	1	CXM	ON1-CN	2.10	1.25	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	CXM	ON1-CN-N	-12.32	104.64	124.85
1	B	1	CXM	ON1-CN-N	-3.95	118.37	124.85

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CXM	O-C-CA-CB
1	B	1	CXM	ON1-CN-N-CA
1	B	1	CXM	CB-CG-SD-CE
1	A	1	CXM	ON1-CN-N-CA

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1	CXM	2	0
1	A	1	CXM	1	0
1	B	1	CXM	1	0
1	D	1	CXM	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

40 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	$\#\|Z\| > 2$
2	PO4	C	1274	-	4,4,4	2.87	4 (100%)	6,6,6	2.21	6 (100%)
4	GA9	C	1318[B]	-	35,35,35	2.64	14 (40%)	50,54,54	1.07	4 (8%)
3	UMP	A	1277[B]	-	21,21,21	1.52	3 (14%)	31,31,31	2.08	4 (12%)
4	GA9	A	1320[A]	-	35,35,35	2.65	13 (37%)	50,54,54	1.17	5 (10%)
3	UMP	B	1278[B]	-	21,21,21	1.54	3 (14%)	31,31,31	2.08	4 (12%)
5	BME	C	1816[A]	1	3,3,3	0.46	0	1,2,2	0.17	0
7	2BR	B	1819[B]	-	8,8,8	2.25	4 (50%)	10,10,10	1.03	0
5	BME	A	1815[A]	1	3,3,3	0.33	0	1,2,2	0.11	0
4	GA9	B	1321[A]	-	35,35,35	2.65	12 (34%)	50,54,54	1.16	4 (8%)
4	GA9	D	1319[B]	-	35,35,35	2.62	14 (40%)	50,54,54	1.05	4 (8%)
6	GOL	A	1804[A]	-	5,5,5	0.36	0	5,5,5	0.67	0
2	PO4	A	1266[A]	-	4,4,4	2.83	4 (100%)	6,6,6	2.19	5 (83%)
2	PO4	D	1272	-	4,4,4	2.94	3 (75%)	6,6,6	2.21	5 (83%)
6	GOL	B	1809	-	5,5,5	0.16	0	5,5,5	0.69	0
2	PO4	B	1269	-	4,4,4	2.93	4 (100%)	6,6,6	2.18	5 (83%)
6	GOL	A	1810	-	5,5,5	0.42	0	5,5,5	0.52	0
4	GA9	C	1318[A]	-	35,35,35	2.65	14 (40%)	50,54,54	1.14	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	B	1801	-	5,5,5	0.17	0	5,5,5	0.57	0
7	2BR	B	1819[A]	-	8,8,8	1.97	3 (37%)	10,10,10	1.39	1 (10%)
2	PO4	C	1271	-	4,4,4	2.92	4 (100%)	6,6,6	2.18	5 (83%)
4	GA9	D	1319[A]	-	35,35,35	2.64	14 (40%)	50,54,54	1.19	6 (12%)
6	GOL	A	1803	-	5,5,5	0.14	0	5,5,5	0.85	0
6	GOL	D	1805	-	5,5,5	0.14	0	5,5,5	0.78	0
2	PO4	B	1275	-	4,4,4	2.84	4 (100%)	6,6,6	2.23	6 (100%)
2	PO4	D	1268[A]	-	4,4,4	2.86	4 (100%)	6,6,6	2.14	6 (100%)
6	GOL	B	1802[A]	-	5,5,5	0.30	0	5,5,5	0.65	0
4	GA9	A	1320[B]	-	35,35,35	2.65	13 (37%)	50,54,54	1.04	4 (8%)
2	PO4	B	1265[A]	-	4,4,4	2.79	4 (100%)	6,6,6	2.17	5 (83%)
5	BME	A	1817[A]	1	3,3,3	0.27	0	1,2,2	0.06	0
2	PO4	D	1276	-	4,4,4	2.87	4 (100%)	6,6,6	2.19	6 (100%)
4	GA9	B	1321[B]	-	35,35,35	2.65	13 (37%)	50,54,54	1.04	4 (8%)
6	GOL	D	1807[A]	-	5,5,5	0.19	0	5,5,5	0.82	0
5	BME	D	1818[A]	1	3,3,3	0.28	0	1,2,2	0.14	0
3	UMP	D	1280[B]	-	21,21,21	1.52	3 (14%)	31,31,31	2.06	4 (12%)
2	PO4	A	1270	-	4,4,4	2.88	3 (75%)	6,6,6	2.21	5 (83%)
3	UMP	C	1279[B]	-	21,21,21	1.53	3 (14%)	31,31,31	2.09	4 (12%)
2	PO4	C	1267[A]	-	4,4,4	2.82	4 (100%)	6,6,6	2.19	5 (83%)
6	GOL	C	1806	-	5,5,5	0.19	0	5,5,5	0.91	0
6	GOL	C	1808[A]	-	5,5,5	0.24	0	5,5,5	0.52	0
2	PO4	B	1273	-	4,4,4	2.92	4 (100%)	6,6,6	2.17	6 (100%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GA9	C	1318[B]	-	-	0/12/27/27	0/5/5/5
4	GA9	A	1320[A]	-	-	0/12/27/27	0/5/5/5
3	UMP	A	1277[B]	-	-	1/10/22/22	0/2/2/2
3	UMP	B	1278[B]	-	-	1/10/22/22	0/2/2/2
5	BME	C	1816[A]	1	-	1/1/1/1	-
7	2BR	B	1819[B]	-	-	-	0/1/1/1
5	BME	A	1815[A]	1	-	0/1/1/1	-
4	GA9	B	1321[A]	-	-	0/12/27/27	0/5/5/5
4	GA9	D	1319[B]	-	-	0/12/27/27	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1804[A]	-	-	0/4/4/4	-
6	GOL	B	1809	-	-	0/4/4/4	-
6	GOL	A	1810	-	-	0/4/4/4	-
4	GA9	C	1318[A]	-	-	0/12/27/27	0/5/5/5
6	GOL	B	1801	-	-	0/4/4/4	-
7	2BR	B	1819[A]	-	-	-	0/1/1/1
4	GA9	D	1319[A]	-	-	0/12/27/27	0/5/5/5
6	GOL	A	1803	-	-	0/4/4/4	-
6	GOL	D	1805	-	-	0/4/4/4	-
6	GOL	B	1802[A]	-	-	0/4/4/4	-
5	BME	A	1817[A]	1	-	0/1/1/1	-
4	GA9	A	1320[B]	-	-	0/12/27/27	0/5/5/5
4	GA9	B	1321[B]	-	-	0/12/27/27	0/5/5/5
6	GOL	D	1807[A]	-	-	0/4/4/4	-
5	BME	D	1818[A]	1	-	0/1/1/1	-
3	UMP	D	1280[B]	-	-	1/10/22/22	0/2/2/2
3	UMP	C	1279[B]	-	-	2/10/22/22	0/2/2/2
6	GOL	C	1806	-	-	0/4/4/4	-
6	GOL	C	1808[A]	-	-	0/4/4/4	-

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1321[A]	GA9	C9-C10	8.37	1.48	1.37
4	C	1318[A]	GA9	C9-C10	8.36	1.48	1.37
4	A	1320[A]	GA9	C9-C10	8.35	1.48	1.37
4	D	1319[A]	GA9	C9-C10	8.33	1.48	1.37
4	C	1318[B]	GA9	C9-C10	8.21	1.48	1.37
4	B	1321[B]	GA9	C9-C10	8.21	1.48	1.37
4	A	1320[B]	GA9	C9-C10	8.20	1.48	1.37
4	D	1319[B]	GA9	C9-C10	8.16	1.48	1.37
4	A	1320[A]	GA9	C12-C19	-5.32	1.44	1.53
4	B	1321[A]	GA9	C12-C19	-5.30	1.44	1.53
4	B	1321[B]	GA9	C12-C19	-5.26	1.44	1.53
4	D	1319[A]	GA9	C12-C19	-5.21	1.45	1.53
4	D	1319[B]	GA9	C12-C19	-5.19	1.45	1.53
4	C	1318[A]	GA9	C12-C19	-5.11	1.45	1.53
4	A	1320[B]	GA9	C12-C19	-5.02	1.45	1.53
4	C	1318[B]	GA9	C12-C19	-4.97	1.45	1.53
4	D	1319[A]	GA9	C12-C13	-4.88	1.45	1.53
4	A	1320[A]	GA9	C12-C13	-4.86	1.45	1.53
4	B	1321[A]	GA9	C12-C13	-4.81	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1321[B]	GA9	C12-C13	-4.79	1.45	1.53
4	D	1319[B]	GA9	C12-C13	-4.77	1.45	1.53
4	A	1320[B]	GA9	C12-C13	-4.76	1.45	1.53
4	C	1318[A]	GA9	C12-C13	-4.75	1.45	1.53
2	D	1272	PO4	P-O1	4.71	1.61	1.50
2	B	1269	PO4	P-O1	4.68	1.61	1.50
4	C	1318[B]	GA9	C12-C13	-4.68	1.45	1.53
2	C	1271	PO4	P-O1	4.65	1.61	1.50
2	A	1270	PO4	P-O1	4.60	1.61	1.50
4	A	1320[A]	GA9	C3-C2	4.54	1.46	1.38
3	C	1279[B]	UMP	O4'-C1'	4.54	1.52	1.42
3	B	1278[B]	UMP	O4'-C1'	4.51	1.52	1.42
4	A	1320[B]	GA9	C3-C2	4.49	1.46	1.38
4	C	1318[A]	GA9	C3-C2	4.49	1.46	1.38
3	A	1277[B]	UMP	O4'-C1'	4.48	1.52	1.42
4	B	1321[B]	GA9	C3-C2	4.46	1.46	1.38
3	D	1280[B]	UMP	O4'-C1'	4.46	1.52	1.42
4	B	1321[A]	GA9	C3-C2	4.46	1.46	1.38
2	D	1268[A]	PO4	P-O1	4.44	1.61	1.50
2	C	1274	PO4	P-O1	4.43	1.61	1.50
2	B	1275	PO4	P-O1	4.43	1.61	1.50
4	D	1319[A]	GA9	C3-C2	4.42	1.46	1.38
4	C	1318[B]	GA9	C3-C2	4.42	1.46	1.38
2	B	1273	PO4	P-O1	4.41	1.61	1.50
4	D	1319[B]	GA9	C3-C2	4.38	1.46	1.38
2	A	1266[A]	PO4	P-O1	4.31	1.61	1.50
2	D	1276	PO4	P-O1	4.30	1.61	1.50
2	C	1267[A]	PO4	P-O1	4.28	1.60	1.50
7	B	1819[B]	2BR	O3-C16	4.22	1.45	1.36
2	B	1265[A]	PO4	P-O1	4.16	1.60	1.50
4	C	1318[A]	GA9	C20-C19	3.55	1.45	1.39
4	D	1319[A]	GA9	C20-C19	3.44	1.45	1.39
4	A	1320[A]	GA9	O4-C22	3.37	1.43	1.36
4	B	1321[A]	GA9	C20-C19	3.37	1.45	1.39
4	C	1318[B]	GA9	O3-C16	3.36	1.43	1.36
4	D	1319[B]	GA9	C24-C19	3.35	1.44	1.39
4	A	1320[B]	GA9	O4-C22	3.35	1.43	1.36
4	C	1318[A]	GA9	O3-C16	3.30	1.43	1.36
4	C	1318[B]	GA9	C24-C19	3.29	1.44	1.39
4	A	1320[A]	GA9	C20-C19	3.29	1.44	1.39
4	B	1321[B]	GA9	C24-C19	3.29	1.44	1.39
4	B	1321[A]	GA9	O4-C22	3.29	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1321[A]	GA9	O3-C16	3.27	1.43	1.36
4	D	1319[B]	GA9	O3-C16	3.26	1.43	1.36
4	A	1320[B]	GA9	O3-C16	3.25	1.43	1.36
4	C	1318[B]	GA9	O4-C22	3.25	1.43	1.36
4	C	1318[A]	GA9	O4-C22	3.22	1.42	1.36
4	B	1321[B]	GA9	O4-C22	3.21	1.42	1.36
7	B	1819[A]	2BR	O3-C16	3.20	1.42	1.36
4	A	1320[B]	GA9	C24-C19	3.20	1.44	1.39
4	B	1321[B]	GA9	O3-C16	3.19	1.42	1.36
4	D	1319[A]	GA9	O4-C22	3.17	1.42	1.36
4	A	1320[A]	GA9	O3-C16	3.11	1.42	1.36
4	A	1320[A]	GA9	C18-C13	3.11	1.44	1.39
4	B	1321[A]	GA9	C18-C13	3.10	1.44	1.39
4	D	1319[A]	GA9	O3-C16	3.10	1.42	1.36
4	D	1319[B]	GA9	O4-C22	3.09	1.42	1.36
4	C	1318[A]	GA9	C18-C13	3.09	1.44	1.39
4	D	1319[A]	GA9	C18-C13	2.96	1.44	1.39
7	B	1819[A]	2BR	BR1-C15	-2.96	1.83	1.89
4	B	1321[B]	GA9	C18-C13	2.95	1.44	1.39
4	C	1318[B]	GA9	C18-C13	2.92	1.43	1.39
4	A	1320[B]	GA9	C20-C21	2.91	1.44	1.38
4	A	1320[B]	GA9	C18-C13	2.88	1.43	1.39
4	C	1318[B]	GA9	C20-C21	2.83	1.44	1.38
4	D	1319[B]	GA9	C18-C13	2.83	1.43	1.39
3	B	1278[B]	UMP	O4'-C4'	2.81	1.51	1.45
4	A	1320[B]	GA9	C20-C19	2.80	1.44	1.39
3	A	1277[B]	UMP	O4'-C4'	2.78	1.51	1.45
7	B	1819[B]	2BR	BR1-C15	-2.77	1.83	1.89
3	C	1279[B]	UMP	O4'-C4'	2.75	1.51	1.45
4	C	1318[B]	GA9	C20-C19	2.72	1.43	1.39
3	D	1280[B]	UMP	O4'-C4'	2.71	1.51	1.45
4	D	1319[B]	GA9	BR1-C15	-2.68	1.83	1.89
4	B	1321[B]	GA9	BR1-C15	-2.66	1.83	1.89
4	C	1318[B]	GA9	C14-C13	2.65	1.43	1.39
4	A	1320[B]	GA9	C14-C13	2.62	1.43	1.39
4	B	1321[B]	GA9	C14-C13	2.60	1.43	1.39
4	D	1319[B]	GA9	C20-C21	2.58	1.43	1.38
4	A	1320[B]	GA9	BR1-C15	-2.56	1.84	1.89
4	B	1321[B]	GA9	C20-C21	2.55	1.43	1.38
4	D	1319[B]	GA9	C20-C19	2.52	1.43	1.39
4	C	1318[B]	GA9	BR1-C15	-2.51	1.84	1.89
4	D	1319[B]	GA9	C14-C13	2.51	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1319[A]	GA9	C14-C13	2.47	1.43	1.39
4	C	1318[A]	GA9	C14-C13	2.45	1.43	1.39
4	B	1321[B]	GA9	C20-C19	2.45	1.43	1.39
3	B	1278[B]	UMP	C6-C5	2.42	1.40	1.35
3	D	1280[B]	UMP	C6-C5	2.38	1.40	1.35
3	A	1277[B]	UMP	C6-C5	2.37	1.40	1.35
4	A	1320[A]	GA9	C14-C13	2.34	1.43	1.39
3	C	1279[B]	UMP	C6-C5	2.33	1.40	1.35
4	B	1321[A]	GA9	BR1-C15	-2.30	1.84	1.89
2	B	1273	PO4	P-O4	-2.30	1.47	1.54
4	D	1319[A]	GA9	C22-C21	2.28	1.42	1.39
4	C	1318[A]	GA9	C22-C21	2.26	1.42	1.39
2	D	1276	PO4	P-O2	-2.25	1.47	1.54
2	D	1276	PO4	P-O4	-2.24	1.47	1.54
2	B	1273	PO4	P-O2	-2.23	1.47	1.54
4	B	1321[A]	GA9	C14-C13	2.22	1.43	1.39
4	C	1318[A]	GA9	C20-C21	2.21	1.43	1.38
4	B	1321[A]	GA9	C22-C21	2.20	1.42	1.39
2	C	1274	PO4	P-O3	-2.20	1.48	1.54
4	D	1319[A]	GA9	C16-C15	2.19	1.42	1.39
4	D	1319[B]	GA9	BR2-C21	-2.19	1.84	1.89
4	D	1319[A]	GA9	C20-C21	2.19	1.43	1.38
2	B	1265[A]	PO4	P-O3	-2.19	1.48	1.54
2	C	1267[A]	PO4	P-O2	-2.17	1.48	1.54
2	B	1265[A]	PO4	P-O2	-2.17	1.48	1.54
4	A	1320[A]	GA9	C22-C21	2.17	1.42	1.39
2	A	1266[A]	PO4	P-O4	-2.16	1.48	1.54
4	A	1320[A]	GA9	C24-C19	2.15	1.42	1.39
4	D	1319[A]	GA9	C24-C19	2.15	1.42	1.39
7	B	1819[B]	2BR	C17-C16	2.14	1.43	1.39
4	A	1320[A]	GA9	BR1-C15	-2.14	1.85	1.89
7	B	1819[B]	2BR	C16-C15	2.13	1.42	1.39
2	D	1268[A]	PO4	P-O3	-2.13	1.48	1.54
2	C	1267[A]	PO4	P-O4	-2.13	1.48	1.54
4	D	1319[A]	GA9	C5-C6	2.12	1.45	1.42
2	D	1276	PO4	P-O3	-2.11	1.48	1.54
4	C	1318[A]	GA9	C24-C19	2.10	1.42	1.39
2	A	1266[A]	PO4	P-O3	-2.10	1.48	1.54
2	A	1266[A]	PO4	P-O2	-2.10	1.48	1.54
2	D	1268[A]	PO4	P-O4	-2.09	1.48	1.54
2	B	1269	PO4	P-O4	-2.09	1.48	1.54
2	B	1273	PO4	P-O3	-2.09	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1275	PO4	P-O2	-2.08	1.48	1.54
4	A	1320[B]	GA9	C14-C15	2.08	1.42	1.38
4	B	1321[A]	GA9	C24-C19	2.08	1.42	1.39
2	C	1267[A]	PO4	P-O3	-2.08	1.48	1.54
2	C	1271	PO4	P-O3	-2.07	1.48	1.54
2	C	1274	PO4	P-O2	-2.07	1.48	1.54
2	B	1265[A]	PO4	P-O4	-2.06	1.48	1.54
4	C	1318[B]	GA9	C5-C6	2.06	1.45	1.42
2	C	1274	PO4	P-O4	-2.06	1.48	1.54
2	D	1272	PO4	P-O3	-2.06	1.48	1.54
4	C	1318[A]	GA9	BR1-C15	-2.06	1.85	1.89
4	D	1319[B]	GA9	C5-C6	2.05	1.45	1.42
4	C	1318[A]	GA9	C5-C6	2.05	1.45	1.42
2	A	1270	PO4	P-O3	-2.05	1.48	1.54
2	B	1275	PO4	P-O4	-2.04	1.48	1.54
2	A	1270	PO4	P-O2	-2.04	1.48	1.54
4	A	1320[A]	GA9	C5-C6	2.04	1.45	1.42
2	D	1272	PO4	P-O4	-2.04	1.48	1.54
4	C	1318[B]	GA9	C14-C15	2.03	1.42	1.38
2	D	1268[A]	PO4	P-O2	-2.03	1.48	1.54
2	C	1271	PO4	P-O4	-2.02	1.48	1.54
4	B	1321[B]	GA9	BR2-C21	-2.02	1.85	1.89
2	C	1271	PO4	P-O2	-2.02	1.48	1.54
2	B	1275	PO4	P-O3	-2.01	1.48	1.54
2	B	1269	PO4	P-O2	-2.01	1.48	1.54
2	B	1269	PO4	P-O3	-2.01	1.48	1.54
7	B	1819[A]	2BR	C17-C16	2.00	1.43	1.39

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1277[B]	UMP	O4'-C1'-N1	9.24	124.38	107.86
3	B	1278[B]	UMP	O4'-C1'-N1	9.23	124.36	107.86
3	C	1279[B]	UMP	O4'-C1'-N1	9.22	124.34	107.86
3	D	1280[B]	UMP	O4'-C1'-N1	9.09	124.10	107.86
7	B	1819[A]	2BR	BR1-C15-C16	-3.19	116.69	119.31
3	B	1278[B]	UMP	O4'-C4'-C3'	-3.12	98.40	105.67
3	A	1277[B]	UMP	O4'-C4'-C3'	-3.10	98.44	105.67
3	C	1279[B]	UMP	O4'-C4'-C3'	-3.08	98.48	105.67
3	D	1280[B]	UMP	O4'-C4'-C3'	-3.04	98.58	105.67
3	A	1277[B]	UMP	C6-N1-C2	2.86	124.66	120.99
4	D	1319[A]	GA9	O1-C1-O2	2.80	120.16	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1318[B]	GA9	O1-C1-O2	2.77	120.13	117.20
3	D	1280[B]	UMP	C6-N1-C2	2.76	124.52	120.99
4	A	1320[A]	GA9	O1-C1-O2	2.75	120.11	117.20
4	C	1318[A]	GA9	O1-C1-O2	2.75	120.11	117.20
3	C	1279[B]	UMP	C6-N1-C2	2.75	124.51	120.99
4	B	1321[B]	GA9	O1-C1-O2	2.73	120.09	117.20
4	D	1319[B]	GA9	O1-C1-O2	2.73	120.08	117.20
3	B	1278[B]	UMP	C6-N1-C2	2.70	124.44	120.99
4	B	1321[A]	GA9	O1-C1-O2	2.68	120.03	117.20
4	A	1320[B]	GA9	O1-C1-O2	2.68	120.03	117.20
4	C	1318[B]	GA9	C13-C12-C10	-2.54	106.27	111.84
2	D	1272	PO4	O4-P-O1	-2.45	101.92	110.89
3	B	1278[B]	UMP	O4'-C1'-C2'	-2.45	101.63	106.25
4	C	1318[A]	GA9	C7-C6-C5	-2.44	120.71	125.06
3	D	1280[B]	UMP	O4'-C1'-C2'	-2.44	101.64	106.25
4	B	1321[A]	GA9	C7-C6-C5	-2.43	120.74	125.06
3	C	1279[B]	UMP	O4'-C1'-C2'	-2.43	101.67	106.25
4	A	1320[A]	GA9	C7-C6-C5	-2.43	120.74	125.06
4	B	1321[B]	GA9	C7-C6-C5	-2.42	120.74	125.06
2	A	1266[A]	PO4	O4-P-O1	-2.39	102.16	110.89
4	C	1318[B]	GA9	C7-C6-C5	-2.38	120.82	125.06
4	A	1320[B]	GA9	C7-C6-C5	-2.37	120.84	125.06
4	D	1319[A]	GA9	C7-C6-C5	-2.37	120.84	125.06
2	B	1269	PO4	O3-P-O1	-2.35	102.31	110.89
2	D	1272	PO4	O4-P-O3	2.35	115.50	107.97
2	B	1269	PO4	O3-P-O2	2.34	115.49	107.97
4	C	1318[B]	GA9	O1-C12-C13	-2.33	102.05	106.17
2	A	1270	PO4	O3-P-O1	-2.33	102.36	110.89
2	B	1275	PO4	O2-P-O1	-2.33	102.37	110.89
2	A	1270	PO4	O4-P-O1	-2.32	102.42	110.89
2	D	1276	PO4	O4-P-O3	2.32	115.41	107.97
2	C	1271	PO4	O3-P-O2	2.31	115.38	107.97
4	D	1319[B]	GA9	C13-C12-C10	-2.30	106.79	111.84
3	A	1277[B]	UMP	O4'-C1'-C2'	-2.30	101.90	106.25
4	B	1321[B]	GA9	C13-C12-C10	-2.30	106.80	111.84
2	D	1276	PO4	O3-P-O2	2.30	115.34	107.97
4	D	1319[B]	GA9	C7-C6-C5	-2.29	120.98	125.06
2	B	1275	PO4	O4-P-O3	2.29	115.32	107.97
2	C	1274	PO4	O3-P-O1	-2.29	102.53	110.89
2	B	1275	PO4	O4-P-O2	2.29	115.31	107.97
2	C	1274	PO4	O3-P-O2	2.28	115.30	107.97
2	A	1266[A]	PO4	O4-P-O3	2.28	115.28	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1272	PO4	O3-P-O1	-2.28	102.57	110.89
2	C	1274	PO4	O4-P-O2	2.28	115.27	107.97
2	A	1270	PO4	O3-P-O2	2.27	115.27	107.97
2	B	1275	PO4	O4-P-O1	-2.27	102.58	110.89
2	B	1273	PO4	O3-P-O2	2.27	115.26	107.97
2	B	1273	PO4	O4-P-O3	2.26	115.23	107.97
4	D	1319[B]	GA9	O1-C12-C13	-2.26	102.18	106.17
2	A	1266[A]	PO4	O3-P-O1	-2.25	102.65	110.89
2	C	1267[A]	PO4	O4-P-O1	-2.25	102.65	110.89
2	B	1265[A]	PO4	O4-P-O3	2.25	115.19	107.97
2	C	1271	PO4	O4-P-O1	-2.25	102.67	110.89
2	C	1267[A]	PO4	O3-P-O1	-2.25	102.67	110.89
2	C	1267[A]	PO4	O3-P-O2	2.24	115.16	107.97
2	A	1270	PO4	O4-P-O3	2.24	115.15	107.97
2	A	1266[A]	PO4	O3-P-O2	2.23	115.14	107.97
2	B	1265[A]	PO4	O2-P-O1	-2.23	102.74	110.89
2	D	1268[A]	PO4	O4-P-O3	2.22	115.11	107.97
2	C	1267[A]	PO4	O4-P-O2	2.22	115.08	107.97
2	C	1267[A]	PO4	O4-P-O3	2.21	115.06	107.97
2	D	1268[A]	PO4	O3-P-O2	2.20	115.04	107.97
2	C	1271	PO4	O3-P-O1	-2.20	102.83	110.89
2	B	1273	PO4	O4-P-O1	-2.20	102.84	110.89
2	B	1269	PO4	O4-P-O2	2.20	115.02	107.97
2	D	1276	PO4	O4-P-O1	-2.20	102.86	110.89
2	B	1265[A]	PO4	O4-P-O1	-2.19	102.86	110.89
2	B	1275	PO4	O3-P-O2	2.19	115.01	107.97
4	A	1320[B]	GA9	C13-C12-C10	-2.19	107.04	111.84
2	C	1271	PO4	O4-P-O2	2.19	115.00	107.97
2	B	1265[A]	PO4	O4-P-O2	2.19	114.99	107.97
2	A	1270	PO4	O4-P-O2	2.18	114.98	107.97
4	B	1321[A]	GA9	BR1-C15-C16	2.17	121.09	119.31
2	D	1272	PO4	O4-P-O2	2.17	114.94	107.97
4	A	1320[A]	GA9	C13-C12-C10	-2.17	107.08	111.84
4	B	1321[A]	GA9	C13-C12-C10	-2.17	107.09	111.84
2	B	1265[A]	PO4	O3-P-O2	2.17	114.92	107.97
4	A	1320[B]	GA9	O1-C12-C13	-2.16	102.35	106.17
2	D	1272	PO4	O3-P-O2	2.16	114.90	107.97
2	D	1276	PO4	O2-P-O1	-2.16	102.99	110.89
4	D	1319[A]	GA9	O1-C12-C13	-2.16	102.36	106.17
2	D	1268[A]	PO4	O4-P-O1	-2.15	103.02	110.89
2	D	1268[A]	PO4	O2-P-O1	-2.14	103.05	110.89
2	C	1274	PO4	O4-P-O3	2.14	114.85	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1274	PO4	O2-P-O1	-2.14	103.05	110.89
2	B	1269	PO4	O2-P-O1	-2.14	103.07	110.89
4	B	1321[B]	GA9	O1-C12-C13	-2.14	102.39	106.17
2	C	1271	PO4	O4-P-O3	2.14	114.82	107.97
4	A	1320[A]	GA9	O1-C12-C13	-2.13	102.40	106.17
2	A	1266[A]	PO4	O4-P-O2	2.13	114.81	107.97
2	B	1273	PO4	O3-P-O1	-2.12	103.14	110.89
2	D	1276	PO4	O3-P-O1	-2.12	103.15	110.89
2	D	1268[A]	PO4	O4-P-O2	2.10	114.72	107.97
2	B	1269	PO4	O4-P-O3	2.10	114.70	107.97
2	C	1274	PO4	O4-P-O1	-2.10	103.22	110.89
4	A	1320[A]	GA9	BR2-C21-C22	2.09	121.02	119.31
2	B	1273	PO4	O2-P-O1	-2.09	103.26	110.89
2	B	1273	PO4	O4-P-O2	2.07	114.62	107.97
4	D	1319[A]	GA9	C13-C12-C10	-2.05	107.34	111.84
2	D	1276	PO4	O4-P-O2	2.04	114.53	107.97
2	D	1268[A]	PO4	O3-P-O1	-2.02	103.49	110.89
4	D	1319[A]	GA9	C20-C21-C22	-2.01	119.35	121.00
2	B	1275	PO4	O3-P-O1	-2.01	103.54	110.89
4	C	1318[A]	GA9	C20-C21-C22	-2.01	119.35	121.00
4	D	1319[A]	GA9	BR1-C15-C16	2.01	120.96	119.31

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1816[A]	BME	O1-C1-C2-S2
3	C	1279[B]	UMP	C5'-O5'-P-OP1
3	A	1277[B]	UMP	O4'-C4'-C5'-O5'
3	B	1278[B]	UMP	O4'-C4'-C5'-O5'
3	C	1279[B]	UMP	O4'-C4'-C5'-O5'
3	D	1280[B]	UMP	O4'-C4'-C5'-O5'

There are no ring outliers.

19 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1318[B]	GA9	1	0
3	A	1277[B]	UMP	2	0
4	A	1320[A]	GA9	1	0
3	B	1278[B]	UMP	1	0

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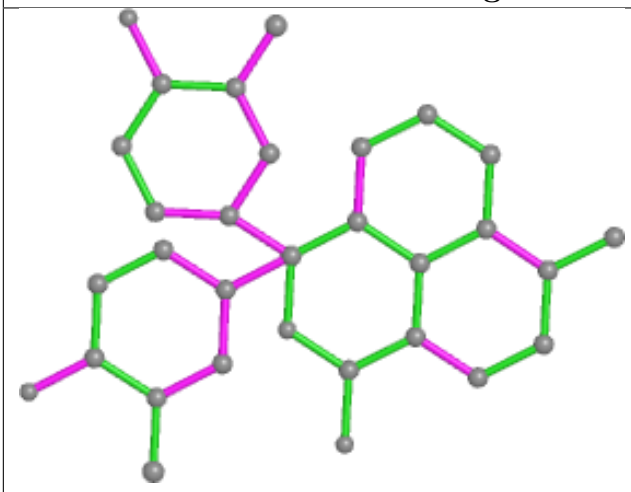
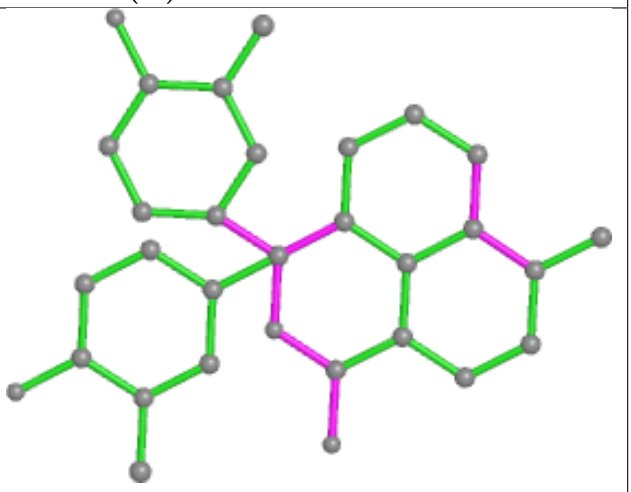
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1816[A]	BME	5	0
7	B	1819[B]	2BR	2	0
5	A	1815[A]	BME	7	0
4	B	1321[A]	GA9	1	0
4	D	1319[B]	GA9	1	0
6	B	1809	GOL	3	0
4	C	1318[A]	GA9	1	0
7	B	1819[A]	2BR	6	0
4	D	1319[A]	GA9	2	0
4	A	1320[B]	GA9	1	0
4	B	1321[B]	GA9	1	0
6	D	1807[A]	GOL	6	0
3	D	1280[B]	UMP	1	0
3	C	1279[B]	UMP	1	0
6	C	1808[A]	GOL	8	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.

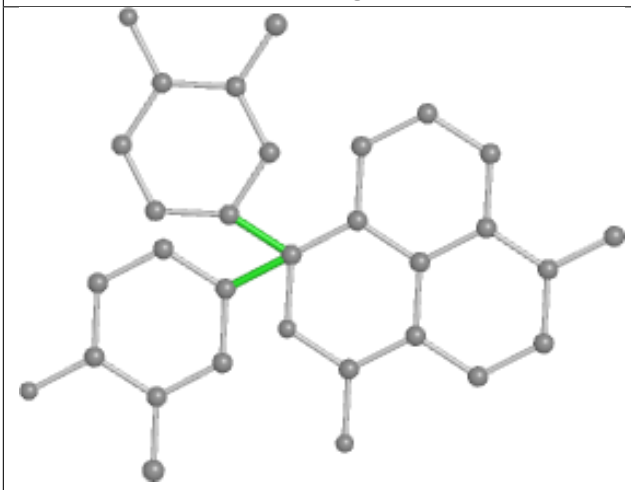
Ligand GA9 C 1318 (B)



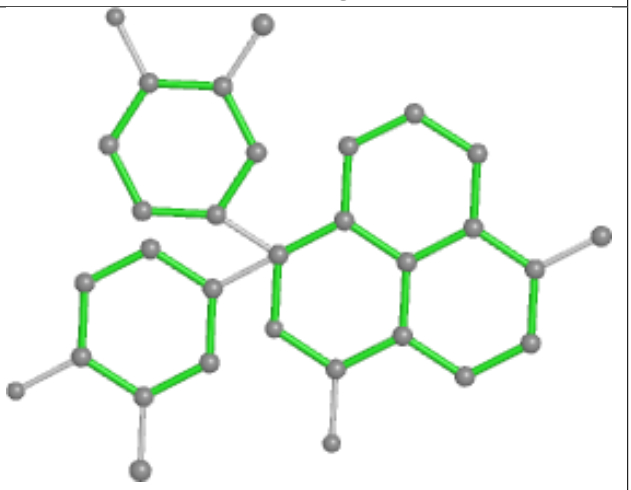
Bond lengths



Bond angles

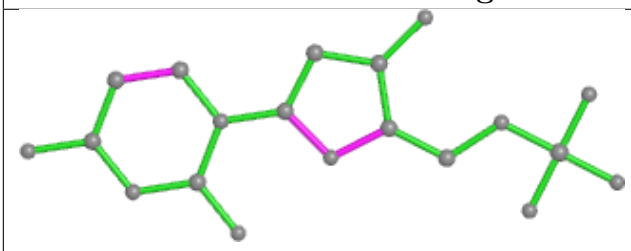


Torsions

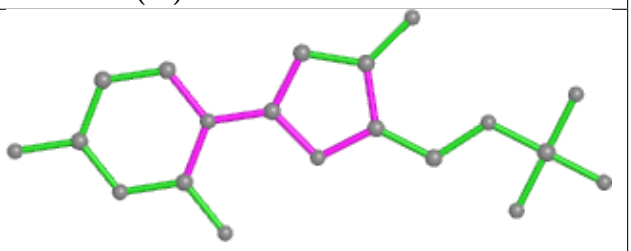


Rings

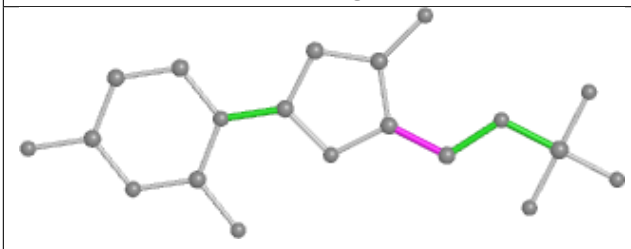
Ligand UMP A 1277 (B)



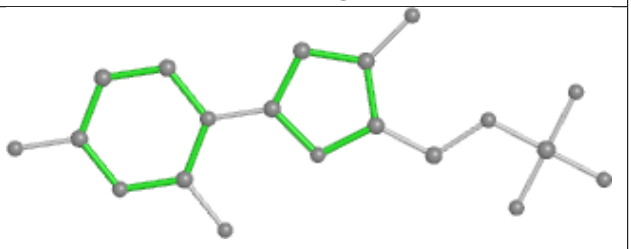
Bond lengths



Bond angles

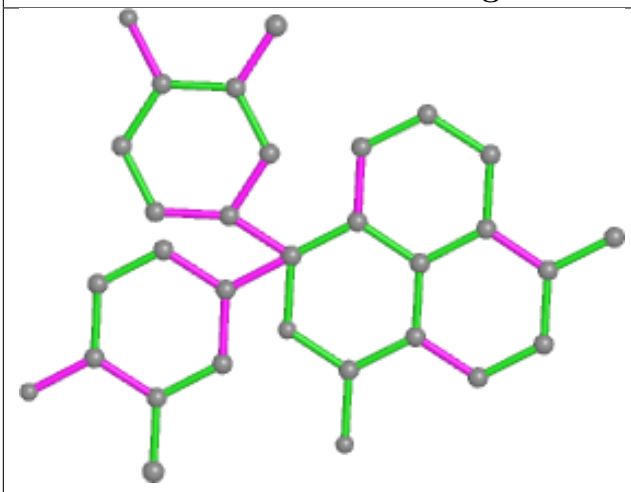


Torsions

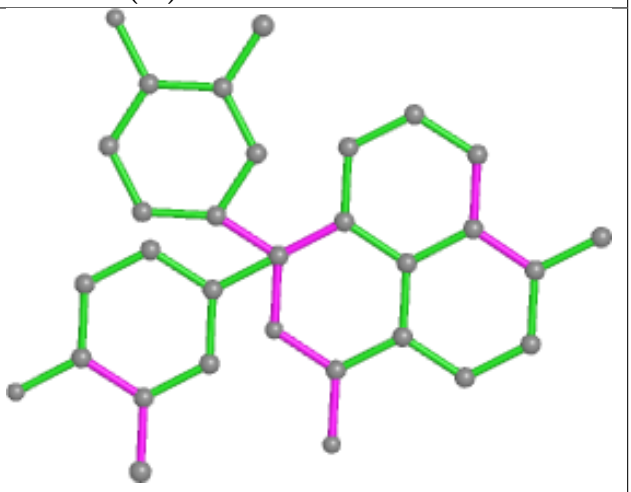


Rings

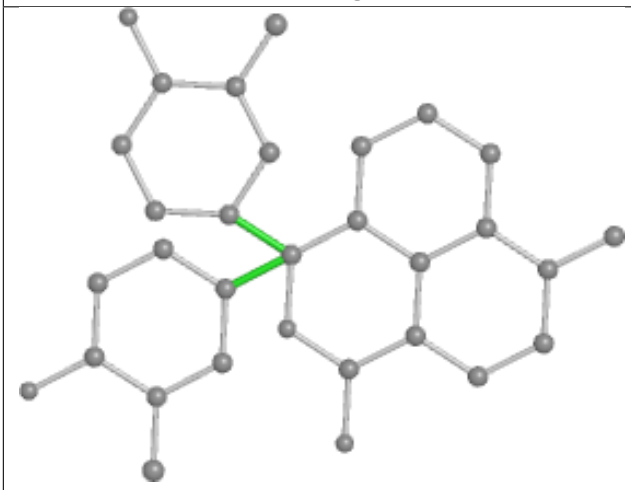
Ligand GA9 A 1320 (A)



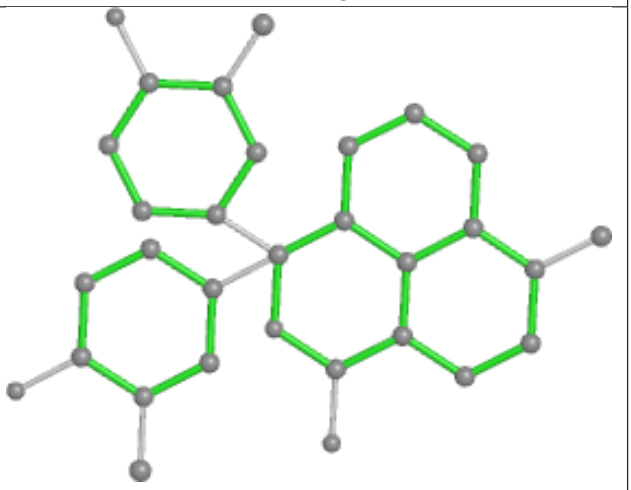
Bond lengths



Bond angles

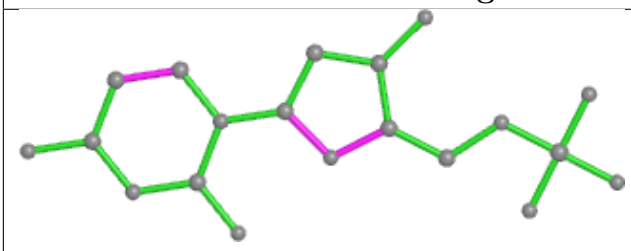


Torsions

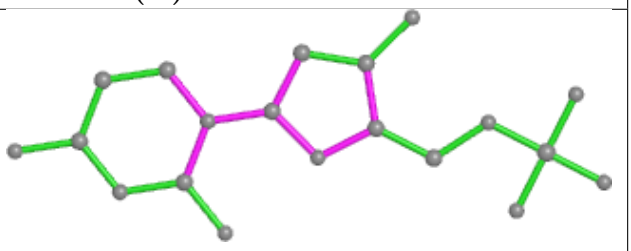


Rings

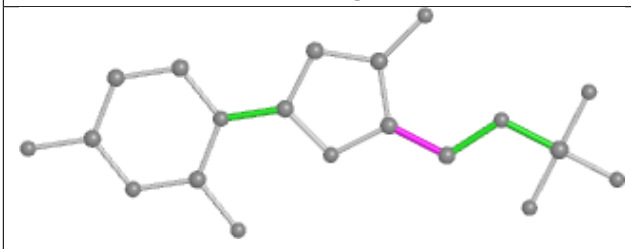
Ligand UMP B 1278 (B)



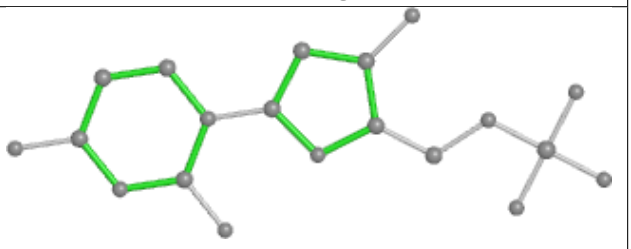
Bond lengths



Bond angles

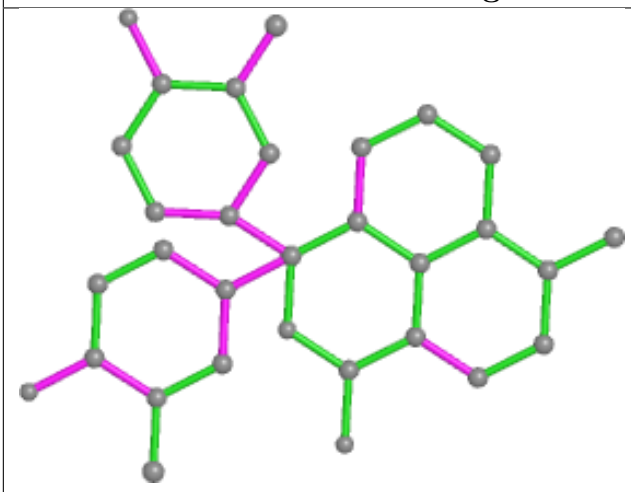


Torsions

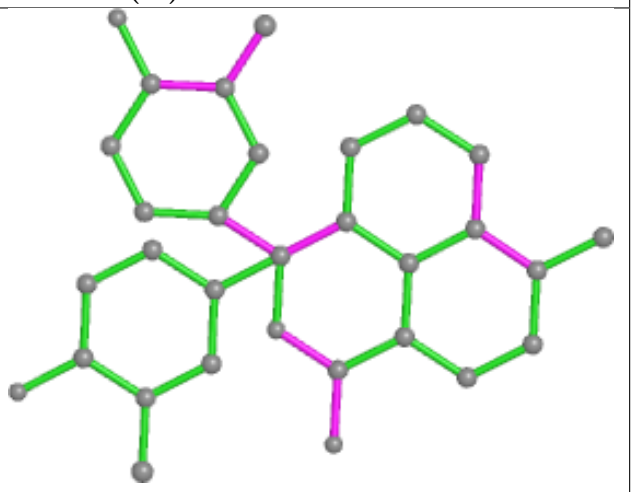


Rings

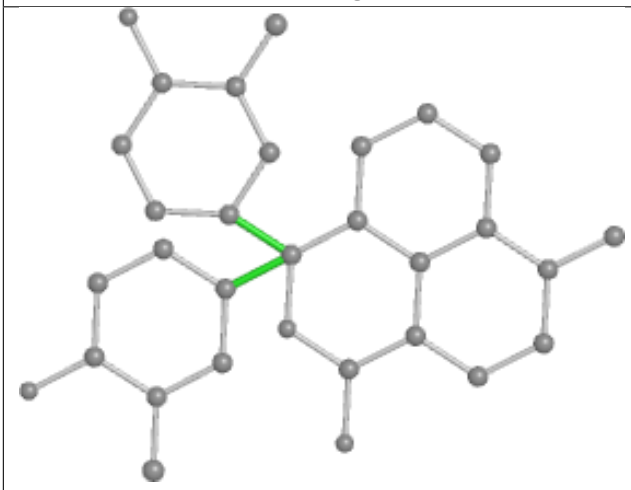
Ligand GA9 B 1321 (A)



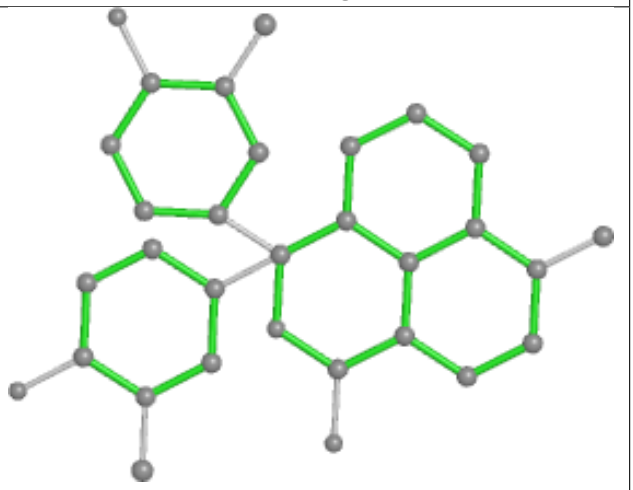
Bond lengths



Bond angles

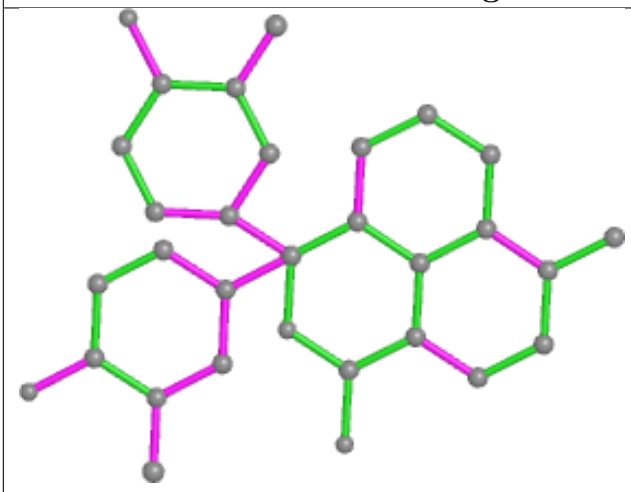


Torsions

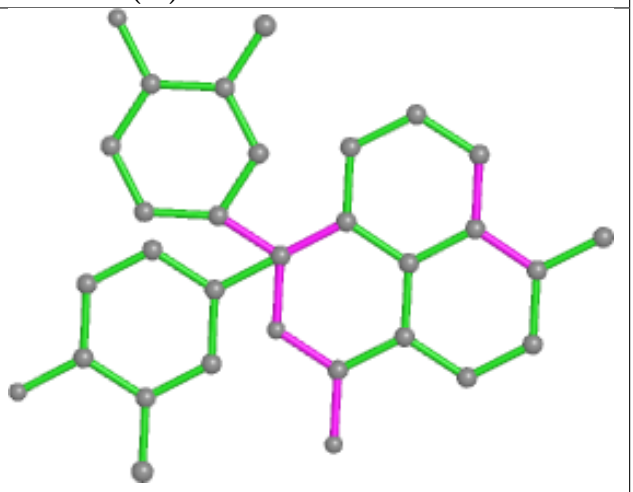


Rings

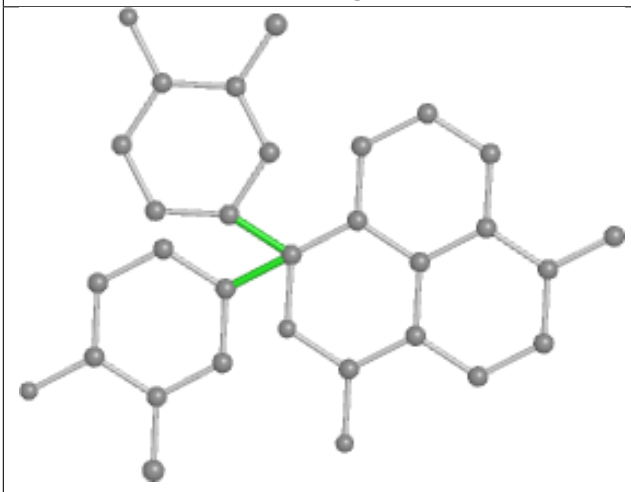
Ligand GA9 D 1319 (B)



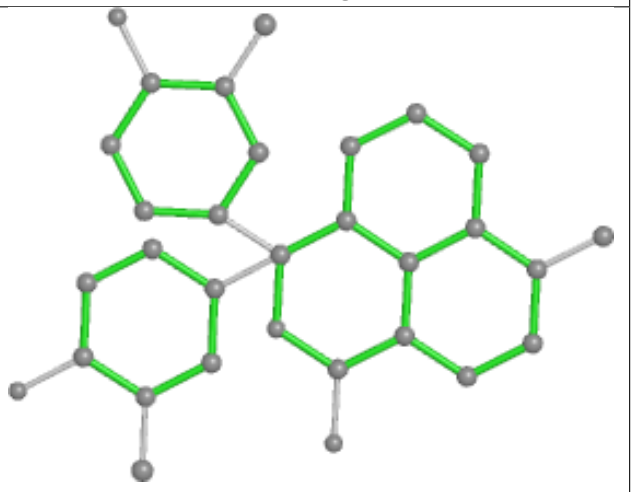
Bond lengths



Bond angles

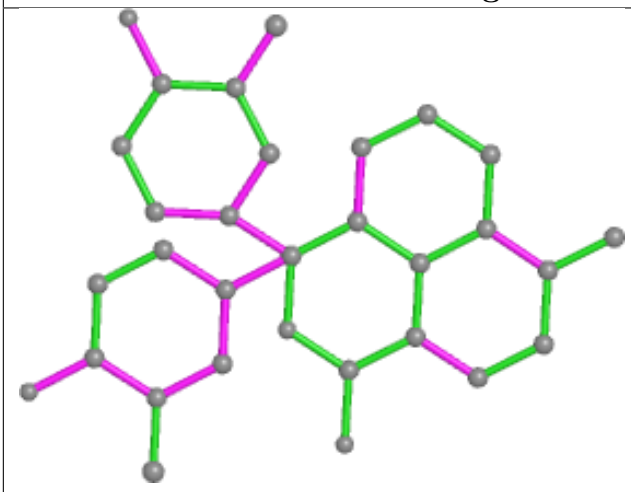


Torsions

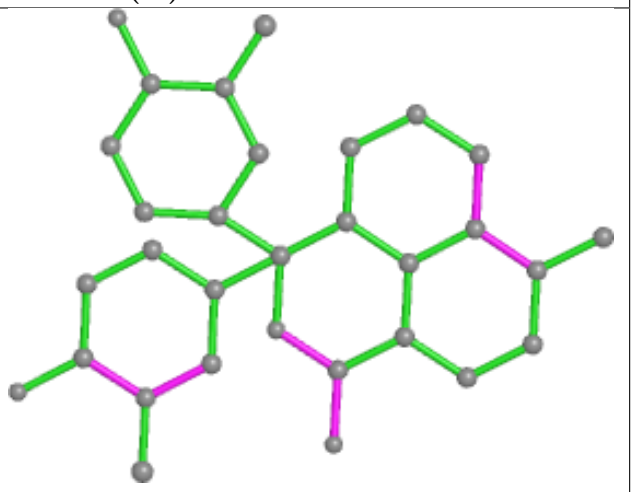


Rings

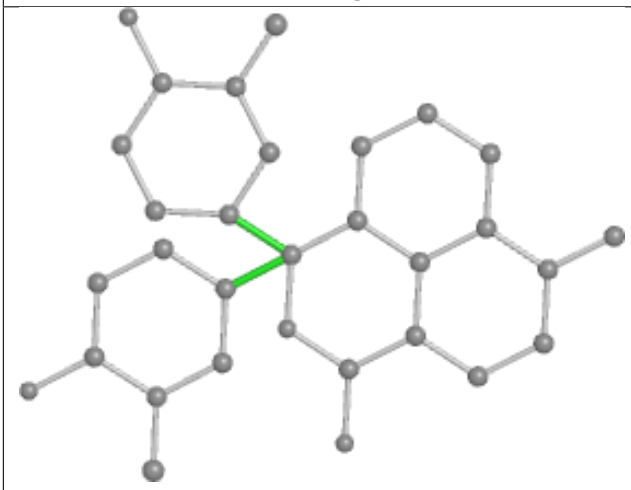
Ligand GA9 C 1318 (A)



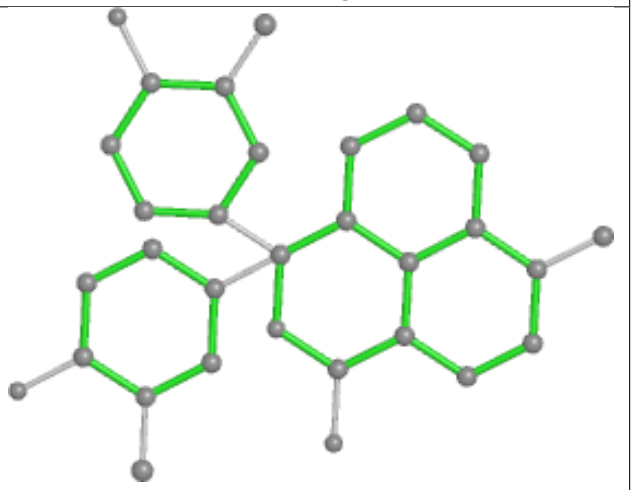
Bond lengths



Bond angles

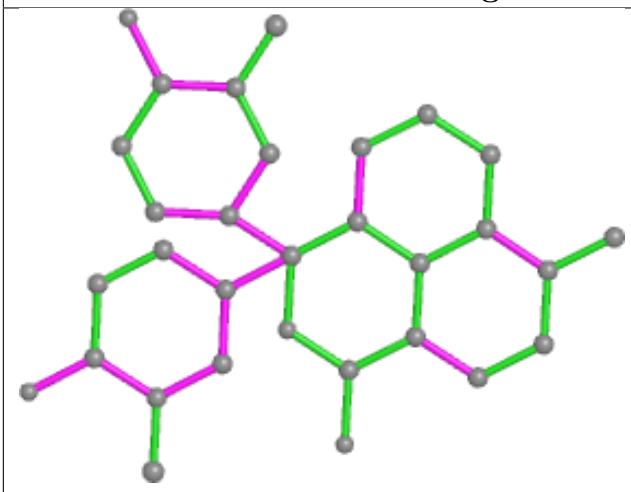


Torsions

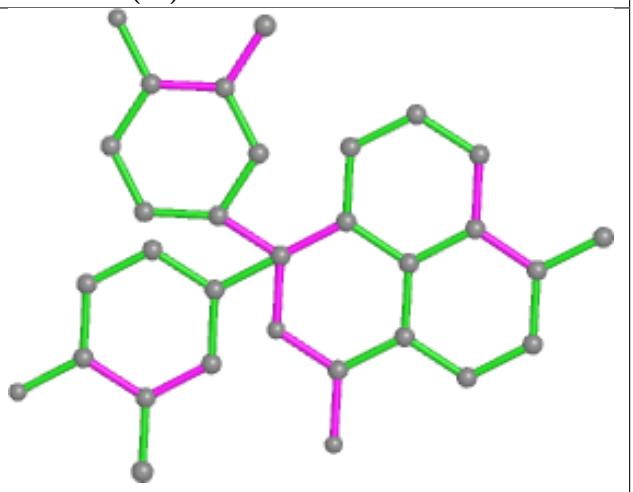


Rings

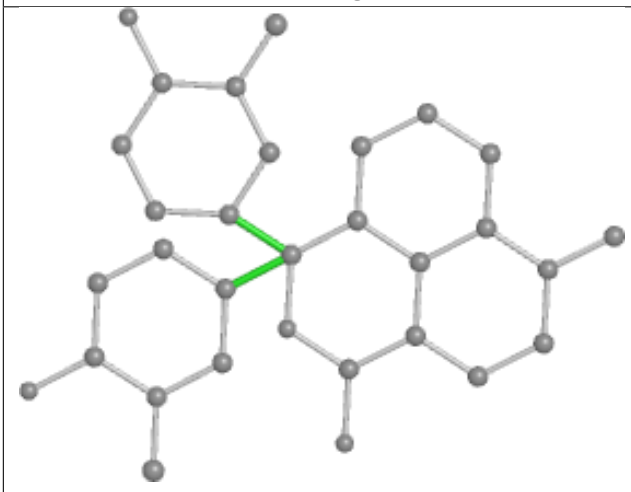
Ligand GA9 D 1319 (A)



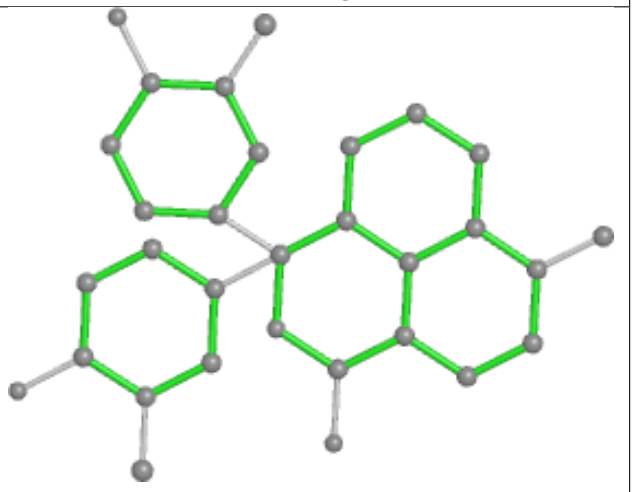
Bond lengths



Bond angles

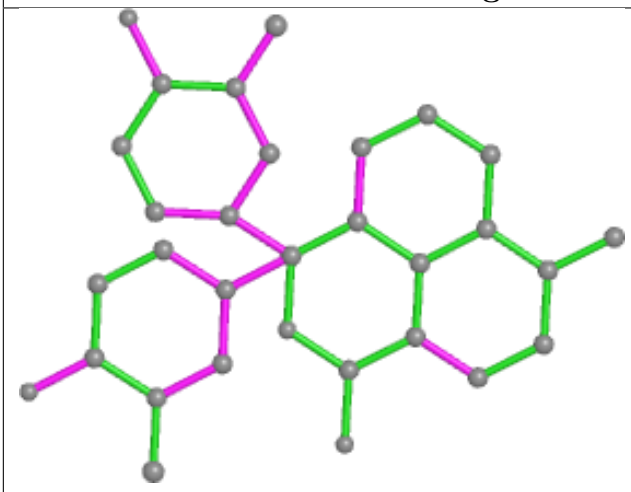


Torsions

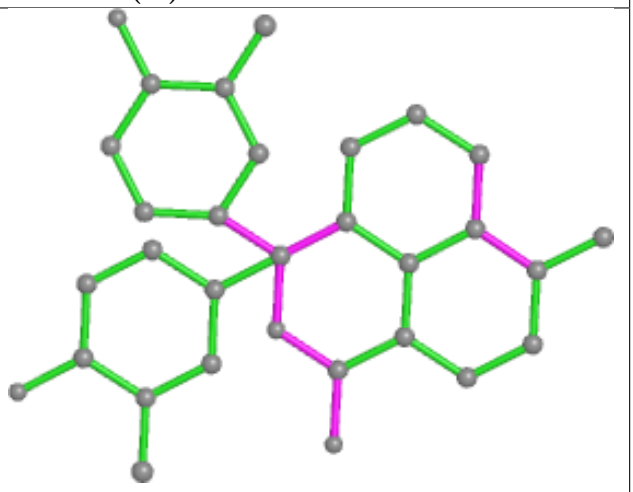


Rings

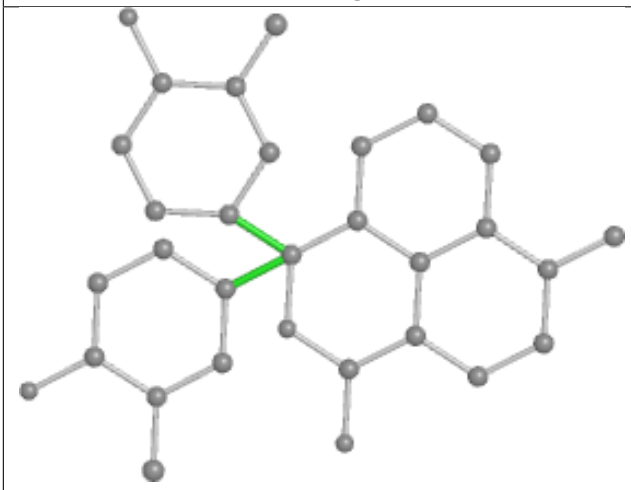
Ligand GA9 A 1320 (B)



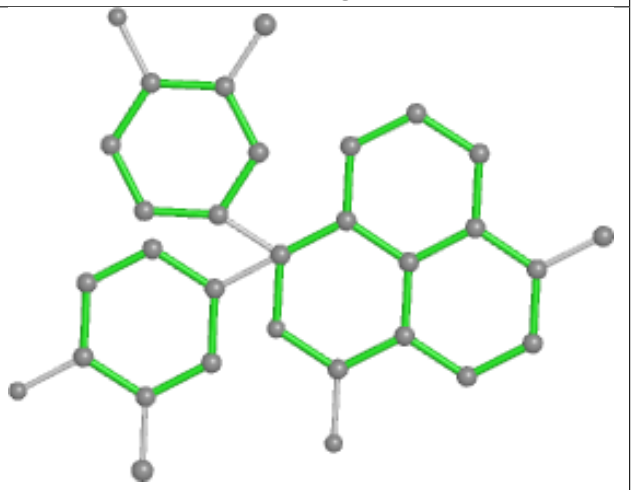
Bond lengths



Bond angles

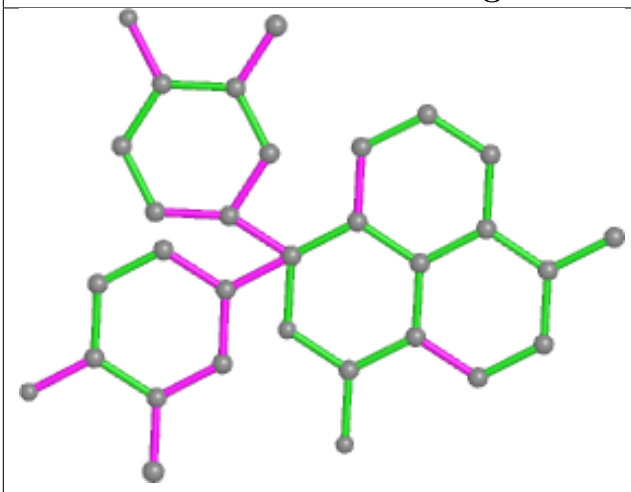


Torsions

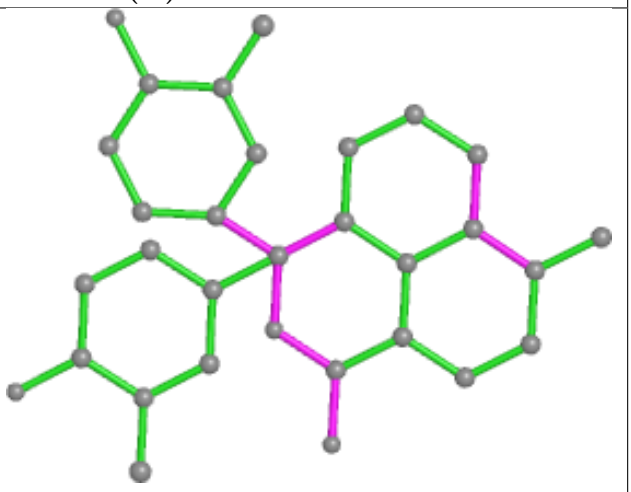


Rings

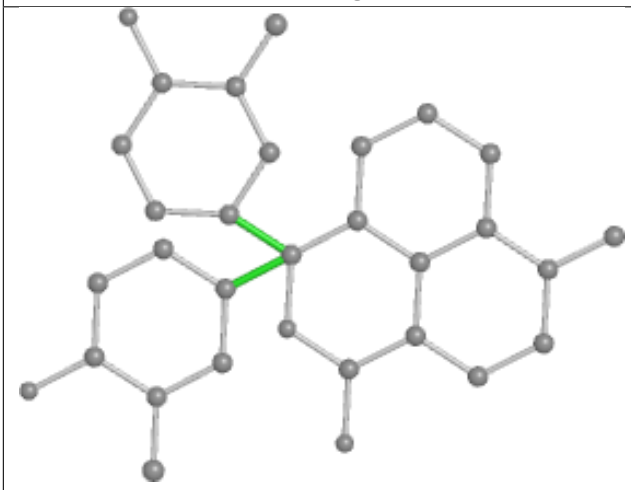
Ligand GA9 B 1321 (B)



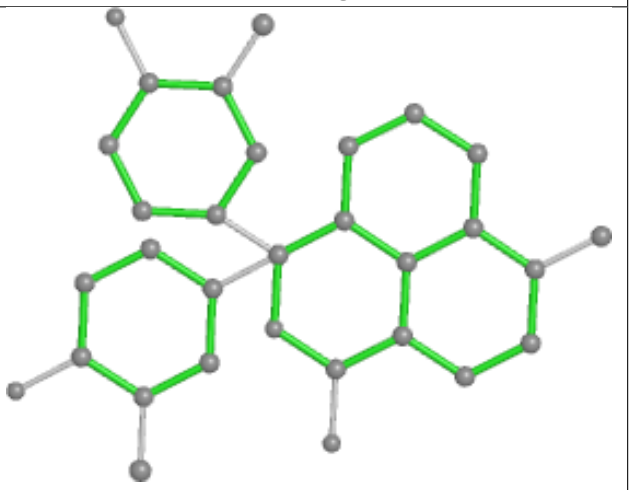
Bond lengths



Bond angles

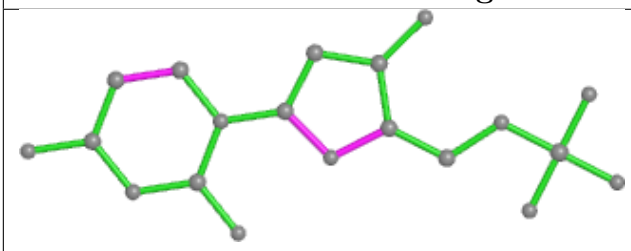


Torsions

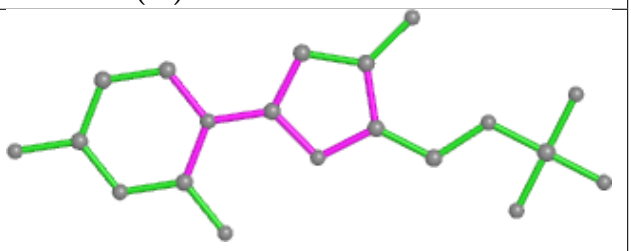


Rings

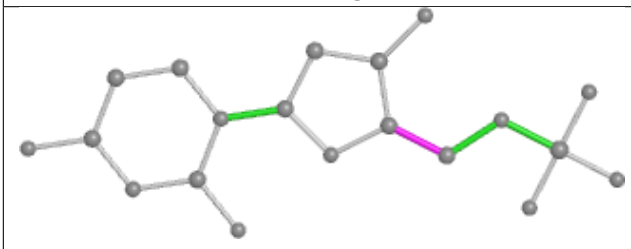
Ligand UMP D 1280 (B)



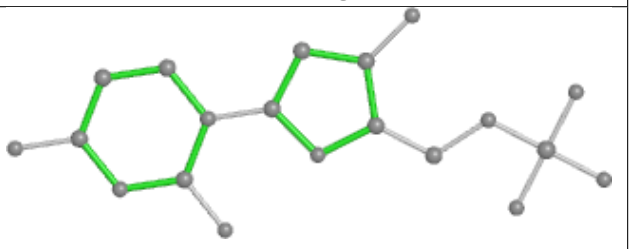
Bond lengths



Bond angles

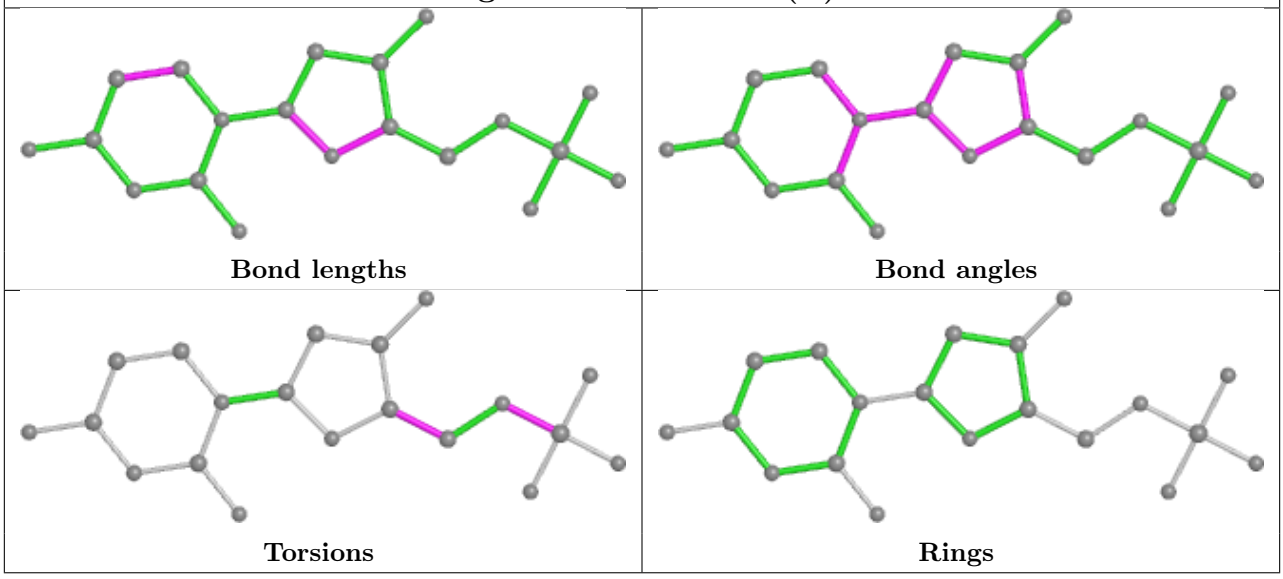


Torsions



Rings

Ligand UMP C 1279 (B)



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	263/264 (99%)	0.07	6 (2%)	60	61	13, 24, 37, 68	6 (2%)
1	B	263/264 (99%)	-0.01	6 (2%)	60	61	13, 24, 37, 66	7 (2%)
1	C	263/264 (99%)	-0.05	5 (1%)	66	69	13, 24, 37, 65	5 (1%)
1	D	263/264 (99%)	-0.05	8 (3%)	50	51	13, 24, 37, 65	5 (1%)
All	All	1052/1056 (99%)	-0.01	25 (2%)	59	59	13, 24, 37, 68	23 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	THR	7.7
1	B	21	ARG	7.2
1	A	21	ARG	7.0
1	C	22	THR	6.8
1	A	22	THR	6.5
1	D	21	ARG	5.6
1	D	22	THR	5.5
1	C	21	ARG	5.3
1	D	20	ASP	4.8
1	D	19	ASN	4.2
1	C	20	ASP	4.1
1	B	264	ILE	3.5
1	A	20	ASP	3.3
1	B	20	ASP	3.0
1	A	83[A]	TRP	2.9
1	A	32[A]	HIS	2.7
1	B	19	ASN	2.6
1	D	83	TRP	2.5
1	B	83	TRP	2.4
1	C	264	ILE	2.3
1	D	50[A]	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	19	ASN	2.2
1	D	264	ILE	2.1
1	A	87	ASN	2.1
1	D	149[A]	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CXM	D	1	11/12	0.93	0.07	24,25,30,31	0
1	CXM	B	1	11/12	0.94	0.07	25,27,33,34	0
1	CXM	C	1	11/12	0.95	0.08	24,25,30,32	0
1	CXM	A	1	11/12	0.95	0.08	23,25,30,31	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UMP	D	1280[B]	20/20	0.52	0.37	57,58,60,60	20
6	GOL	A	1804[A]	6/6	0.52	0.41	48,51,52,52	6
5	BME	D	1818[A]	4/4	0.56	0.30	62,63,63,65	4
6	GOL	B	1802[A]	6/6	0.57	0.43	49,52,52,53	6
3	UMP	B	1278[B]	20/20	0.66	0.37	57,59,60,60	20
2	PO4	D	1268[A]	5/5	0.68	0.21	59,59,59,60	5
5	BME	A	1817[A]	4/4	0.75	0.23	61,61,62,62	4
6	GOL	C	1808[A]	6/6	0.77	0.56	59,59,60,60	6
6	GOL	D	1807[A]	6/6	0.79	0.48	54,55,56,56	6
6	GOL	A	1810	6/6	0.80	0.12	46,49,50,51	0

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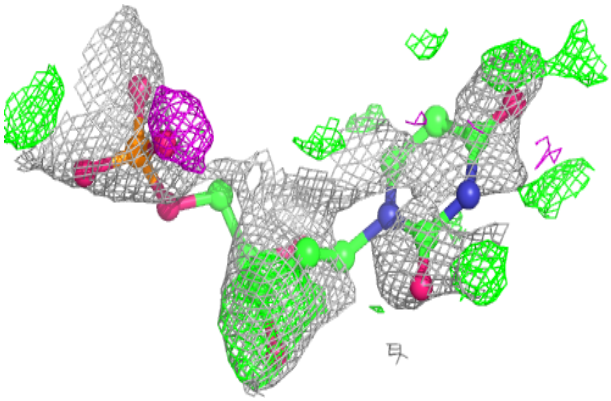
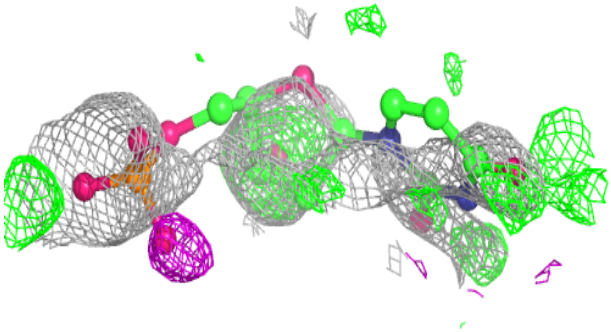
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	C	1267[A]	5/5	0.81	0.20	62,62,62,62	5
3	UMP	C	1279[B]	20/20	0.81	0.32	60,60,61,61	20
6	GOL	B	1809	6/6	0.82	0.17	52,53,54,54	0
2	PO4	A	1266[A]	5/5	0.82	0.25	60,60,61,61	5
3	UMP	A	1277[B]	20/20	0.82	0.34	59,60,61,61	20
5	BME	C	1816[A]	4/4	0.83	0.14	32,33,34,36	4
6	GOL	D	1805	6/6	0.83	0.16	32,34,36,38	0
6	GOL	B	1801	6/6	0.83	0.15	34,35,38,41	0
7	2BR	B	1819[A]	8/8	0.83	0.25	46,46,47,47	8
7	2BR	B	1819[B]	8/8	0.83	0.25	48,49,50,52	8
6	GOL	C	1806	6/6	0.85	0.17	32,33,34,36	0
2	PO4	B	1265[A]	5/5	0.85	0.23	59,59,60,60	5
5	BME	A	1815[A]	4/4	0.85	0.11	30,31,31,33	4
6	GOL	A	1803	6/6	0.86	0.15	30,33,33,36	0
4	GA9	A	1320[A]	31/31	0.87	0.22	38,49,53,54	31
4	GA9	A	1320[B]	31/31	0.87	0.22	34,44,48,48	31
2	PO4	B	1273	5/5	0.87	0.18	61,61,62,62	5
2	PO4	A	1270	5/5	0.88	0.15	59,59,60,60	0
2	PO4	B	1275	5/5	0.88	0.12	63,63,64,64	5
4	GA9	C	1318[A]	31/31	0.89	0.28	39,50,57,58	31
4	GA9	C	1318[B]	31/31	0.89	0.28	32,42,44,44	31
4	GA9	D	1319[A]	31/31	0.90	0.22	39,48,53,54	31
4	GA9	D	1319[B]	31/31	0.90	0.22	35,45,49,49	31
2	PO4	C	1274	5/5	0.90	0.19	62,62,62,62	5
4	GA9	B	1321[A]	31/31	0.91	0.22	38,47,53,53	31
4	GA9	B	1321[B]	31/31	0.91	0.22	33,42,45,46	31
2	PO4	D	1272	5/5	0.93	0.13	58,58,59,59	0
2	PO4	D	1276	5/5	0.93	0.18	64,64,64,64	5
2	PO4	B	1269	5/5	0.94	0.13	61,62,62,62	0
2	PO4	C	1271	5/5	0.97	0.09	55,55,55,56	5

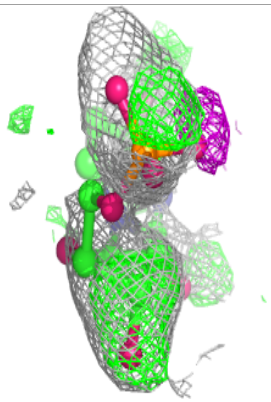
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UMP D 1280 (B):

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

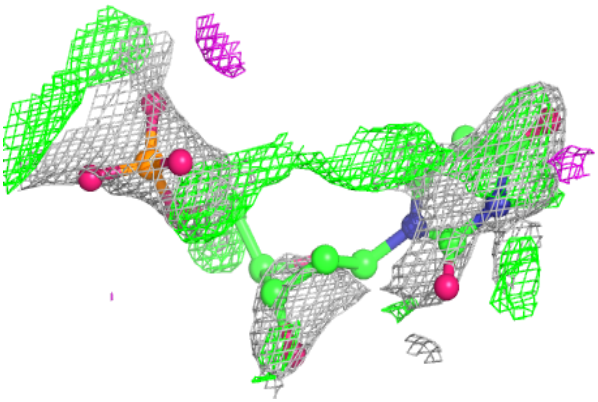


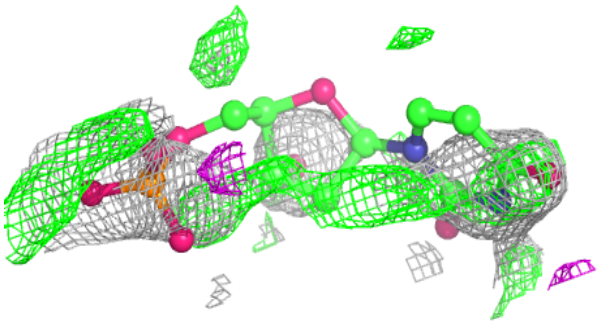


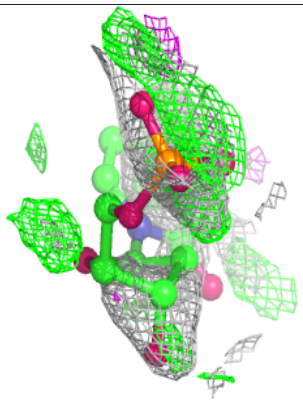


Electron density around UMP B 1278 (B):

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

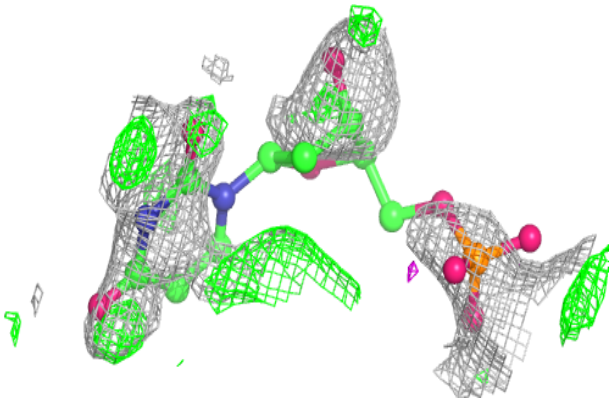


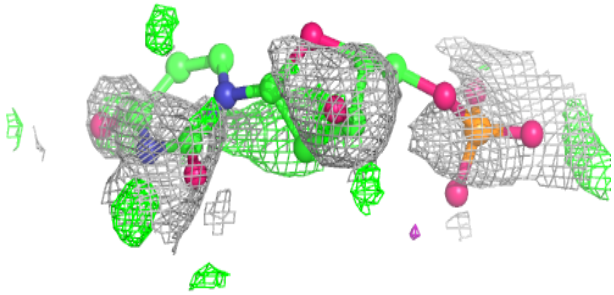


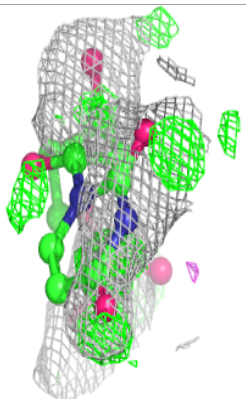


Electron density around UMP C 1279 (B):

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

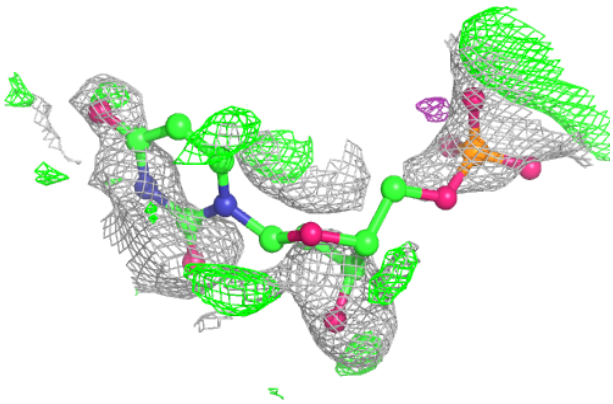


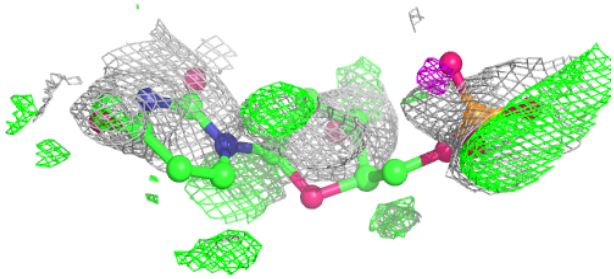


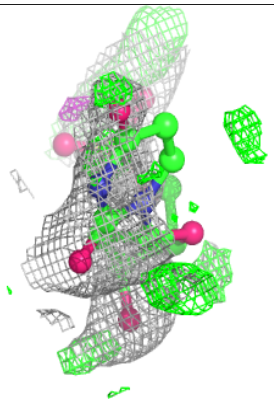


Electron density around UMP A 1277 (B):

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

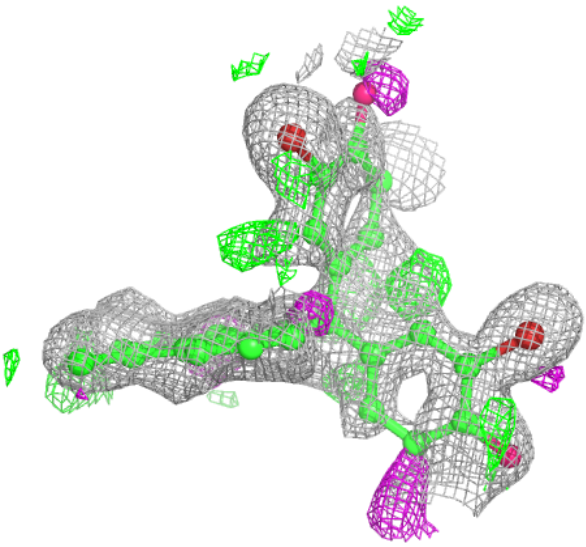


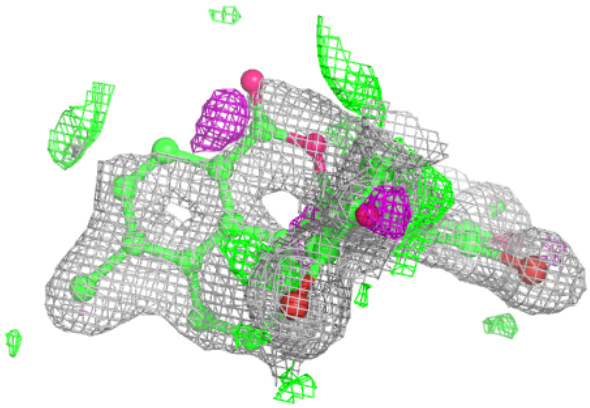


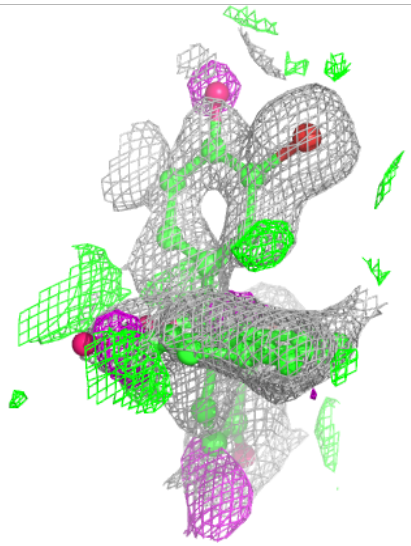


Electron density around GA9 A 1320 (A):

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

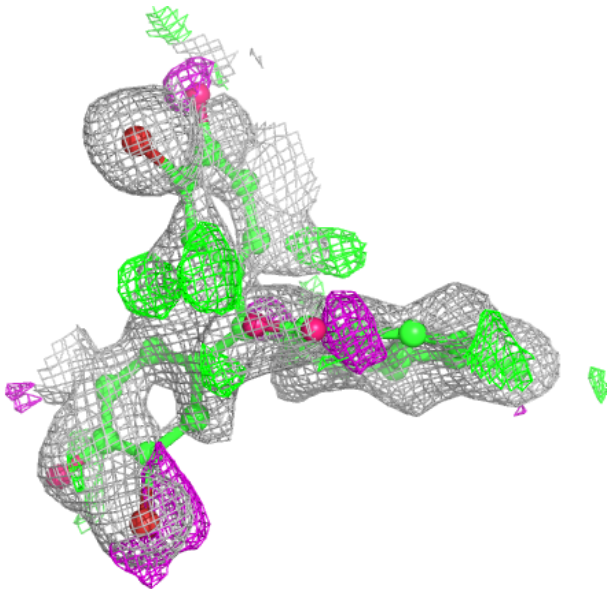


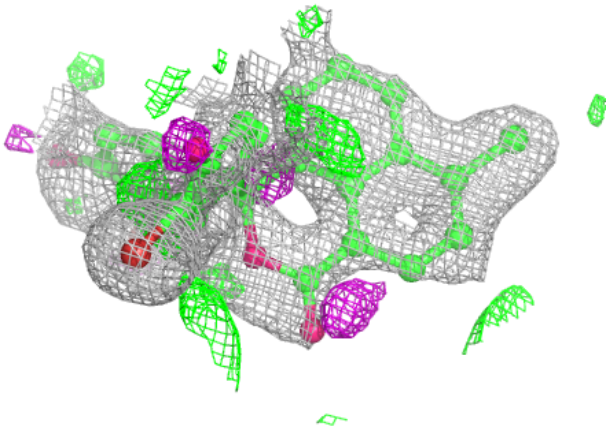


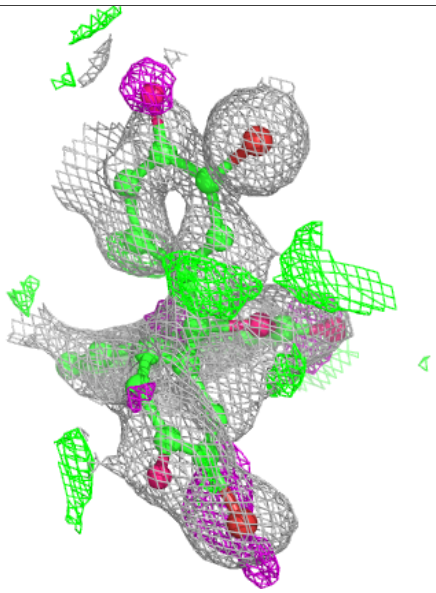


Electron density around GA9 A 1320 (B):

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

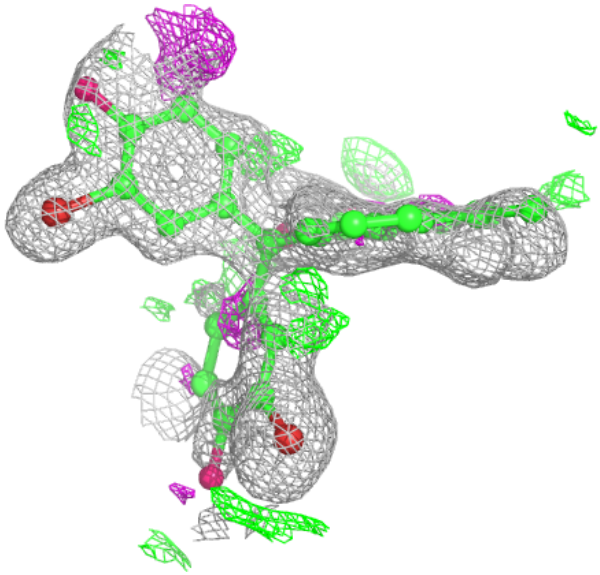


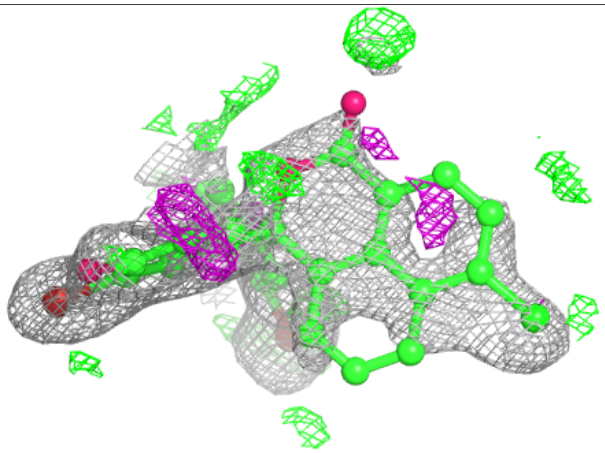


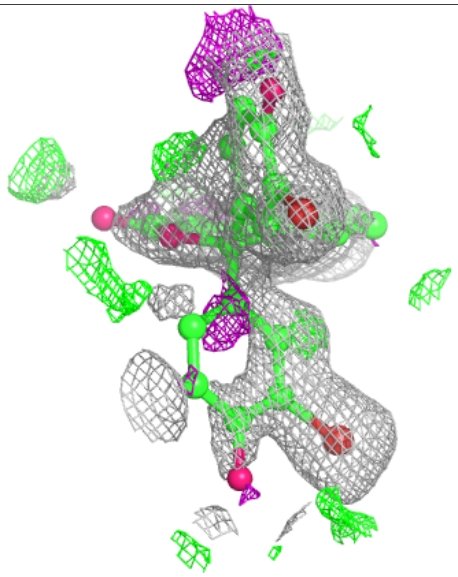


Electron density around GA9 C 1318 (A):

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

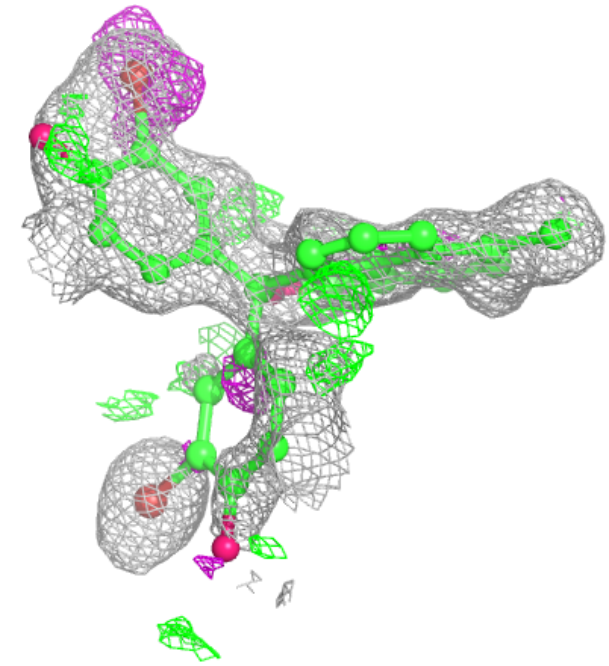


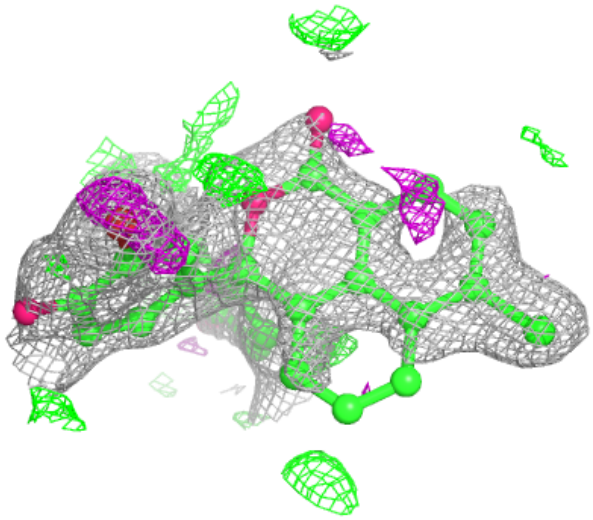


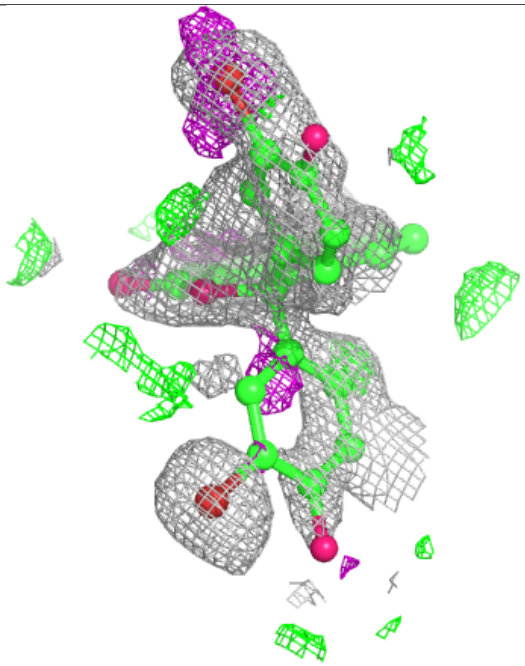


Electron density around GA9 C 1318 (B):

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

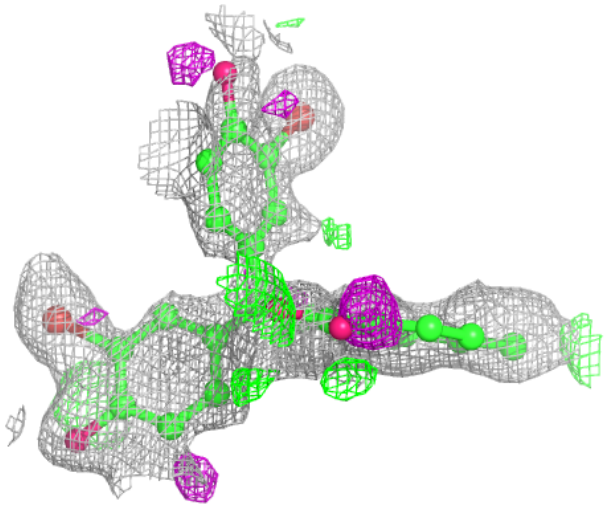


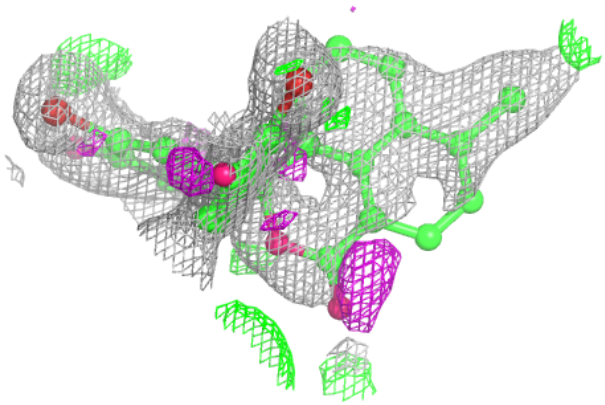


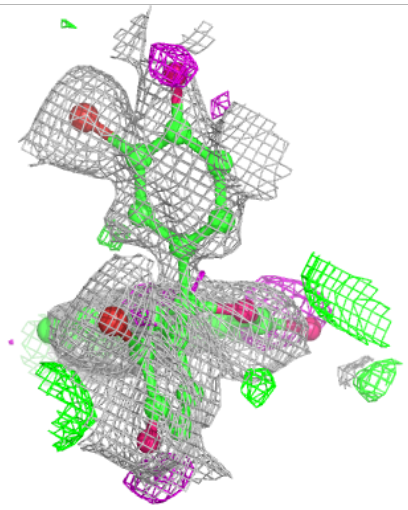


Electron density around GA9 D 1319 (A):

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

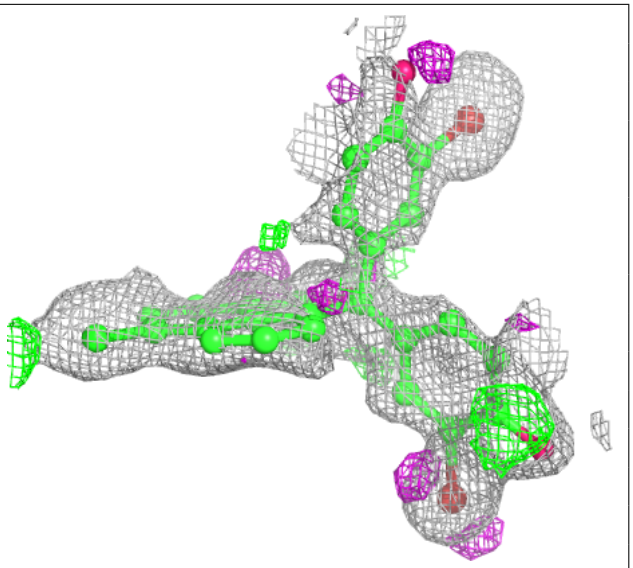


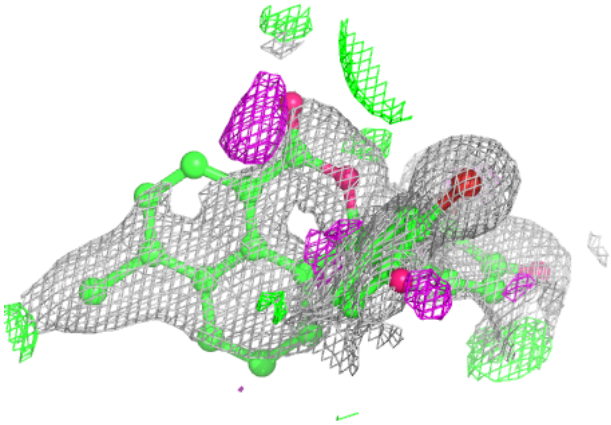


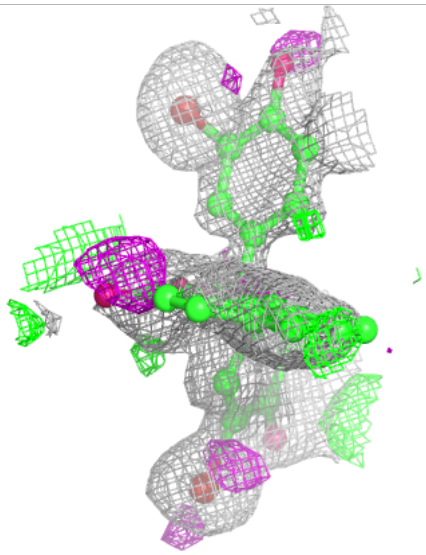


Electron density around GA9 D 1319 (B):

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

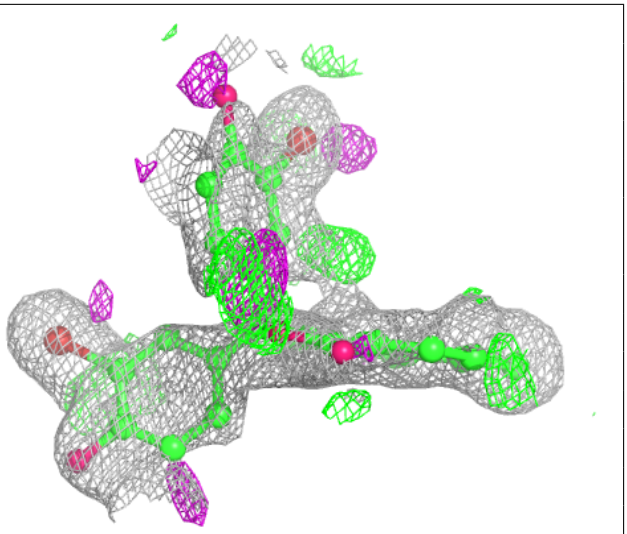


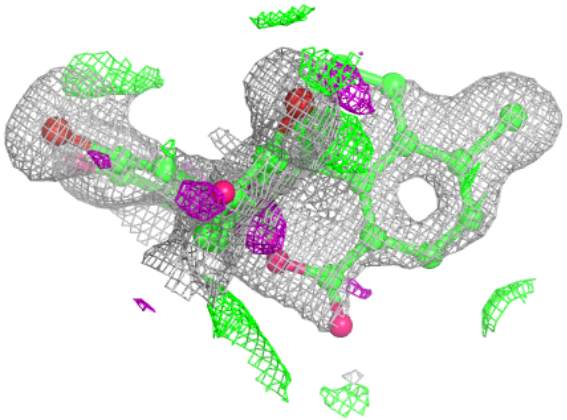


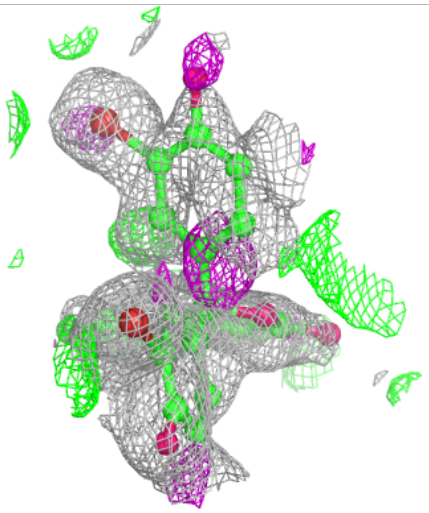


Electron density around GA9 B 1321 (A):

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

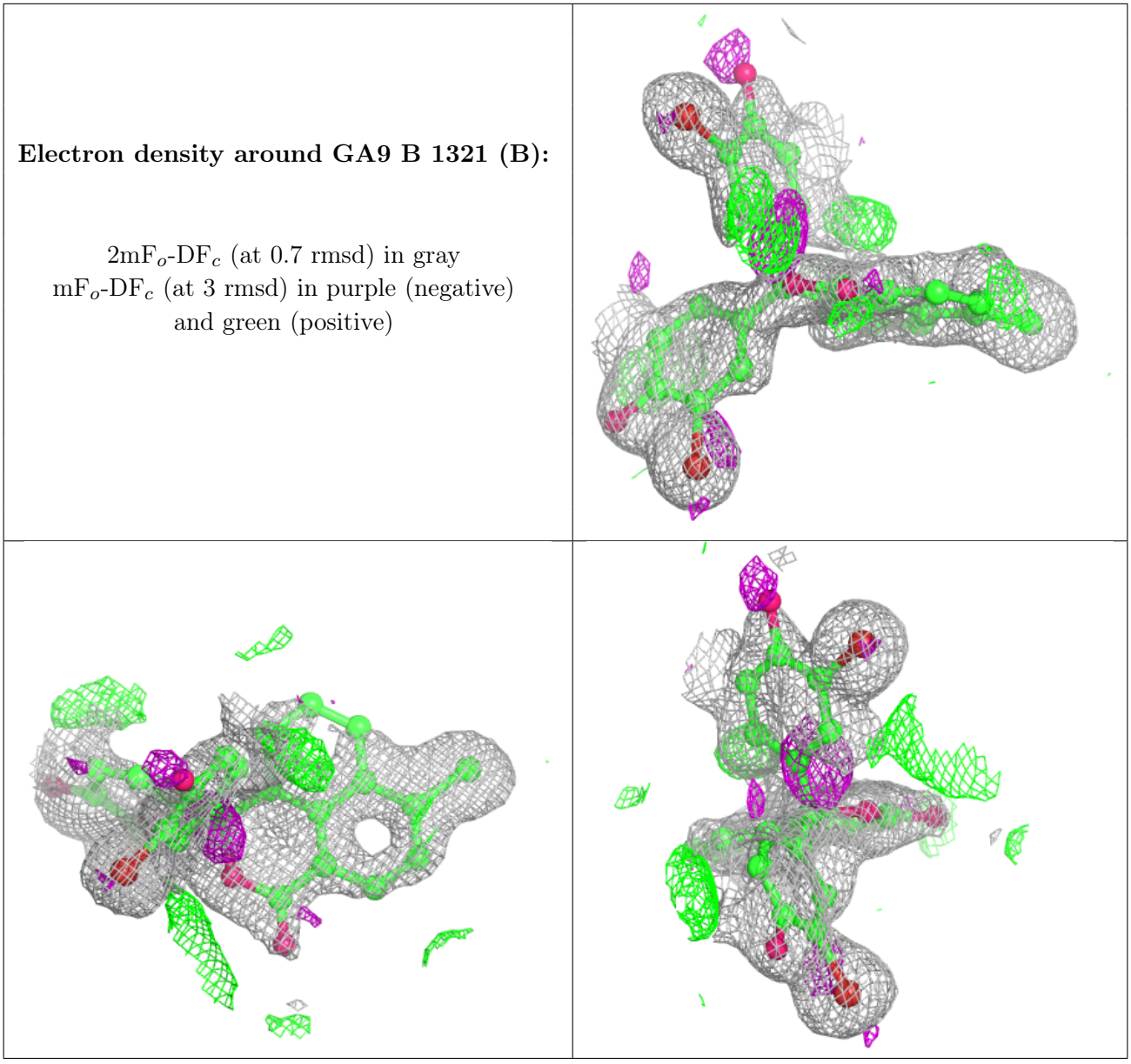






Electron density around GA9 B 1321 (B):

$2mF_o$-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.