Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 01:04 am GMT

PDB ID	:	2VI5
Title	:	LUMAZINE SYNTHASE FROM MYCOBACTERIUM TUBERCULOSIS BOUND TO N-6-(ribitylamino)pyrimidine-2,4(1H,3H)-dione-5-yl-propionamide
Authors	:	Morgunova, E.; Zhang, Y.; Jin, G.; Illarionov, B.; Bacher, A.; Fischer, M.; Cushman, M.; Ladenstein, R.
Deposited on	:	2007-11-27
Resolution	:	2.30 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

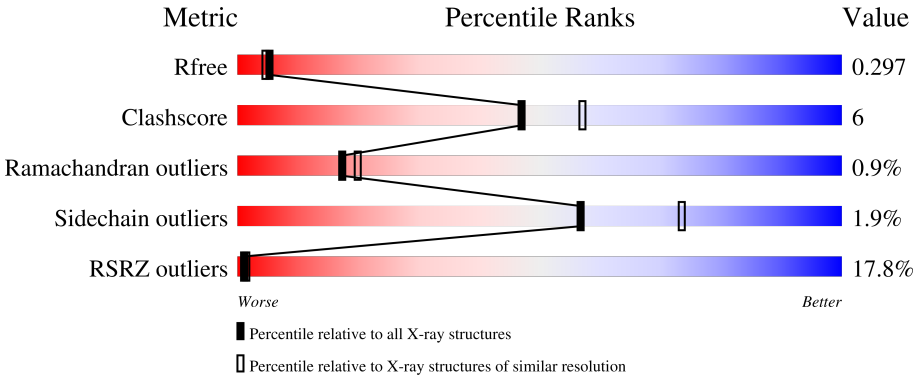
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	160	14% 78% 15% • 6%
1	B	160	16% 80% 12% 8%
1	C	160	21% 81% 11% 9%
1	D	160	14% 78% 14% • 8%
1	E	160	16% 76% 18% • 6%

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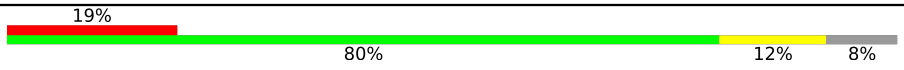
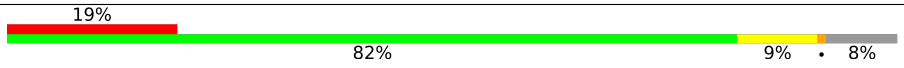
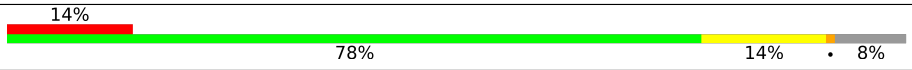
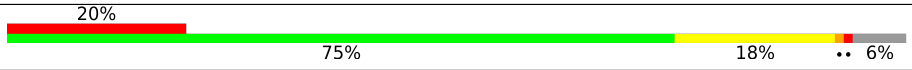
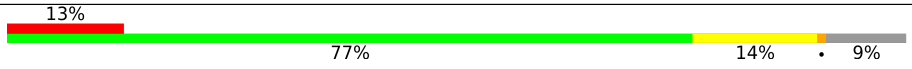
Mol	Chain	Length	Quality of chain
1	F	160	
1	G	160	
1	H	160	
1	I	160	
1	J	160	

2 Entry composition (i)

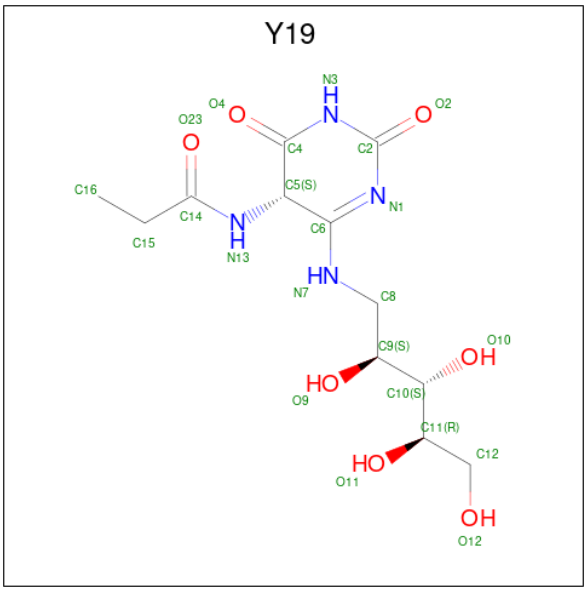
There are 5 unique types of molecules in this entry. The entry contains 11766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1084	669	197	215	3			
1	B	147	Total	C	N	O	S	0	0	0
			1063	655	194	211	3			
1	C	146	Total	C	N	O	S	0	0	0
			1055	651	193	208	3			
1	D	148	Total	C	N	O	S	0	0	0
			1071	661	195	212	3			
1	E	151	Total	C	N	O	S	0	0	0
			1092	675	198	216	3			
1	F	147	Total	C	N	O	S	0	0	0
			1063	655	194	211	3			
1	G	147	Total	C	N	O	S	0	0	0
			1063	655	194	211	3			
1	H	148	Total	C	N	O	S	0	0	0
			1071	661	195	212	3			
1	I	150	Total	C	N	O	S	0	0	0
			1084	669	197	215	3			
1	J	146	Total	C	N	O	S	0	0	0
			1055	651	193	208	3			

- Molecule 2 is 1-deoxy-1-{[(5S)-2,6-dioxo-5-(propanoylamino)-1,2,5,6-tetrahydropyrimidin-4-yl]amino}-D-ribitol (three-letter code: Y19) (formula: $C_{12}H_{20}N_4O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 23 12 4 7	0	0
2	B	1	Total C N O 23 12 4 7	0	0
2	C	1	Total C N O 23 12 4 7	0	0
2	D	1	Total C N O 23 12 4 7	0	0
2	E	1	Total C N O 23 12 4 7	0	0
2	F	1	Total C N O 23 12 4 7	0	0
2	G	1	Total C N O 23 12 4 7	0	0
2	H	1	Total C N O 23 12 4 7	0	0
2	I	1	Total C N O 23 12 4 7	0	0
2	J	1	Total C N O 23 12 4 7	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0

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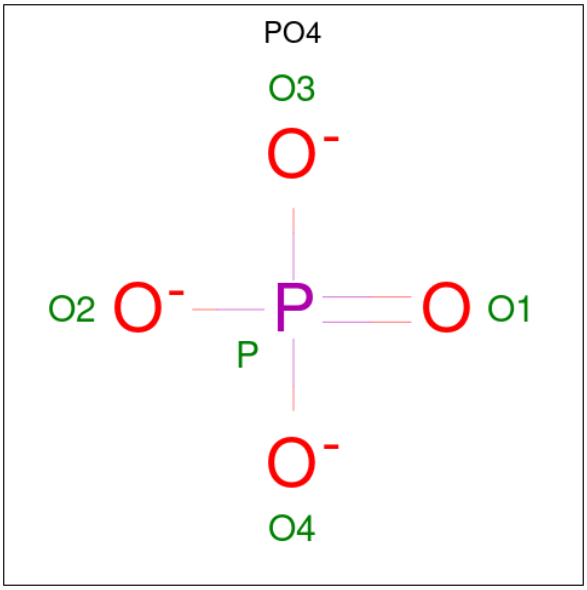
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0
3	E	2	Total K 2 2	0	0
3	F	1	Total K 1 1	0	0
3	G	1	Total K 1 1	0	0
3	H	1	Total K 1 1	0	0
3	I	1	Total K 1 1	0	0
3	J	1	Total K 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0
4	I	1	Total O P 5 4 1	0	0
4	J	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

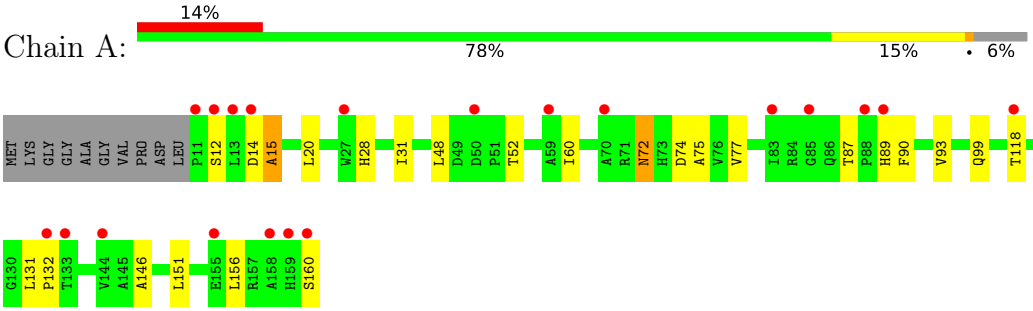
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	87	Total O 87 87	0	0
5	B	85	Total O 85 85	0	0
5	C	59	Total O 59 59	0	0
5	D	70	Total O 70 70	0	0
5	E	84	Total O 84 84	0	0
5	F	76	Total O 76 76	0	0
5	G	53	Total O 53 53	0	0
5	H	80	Total O 80 80	0	0
5	I	77	Total O 77 77	0	0
5	J	99	Total O 99 99	0	0

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.

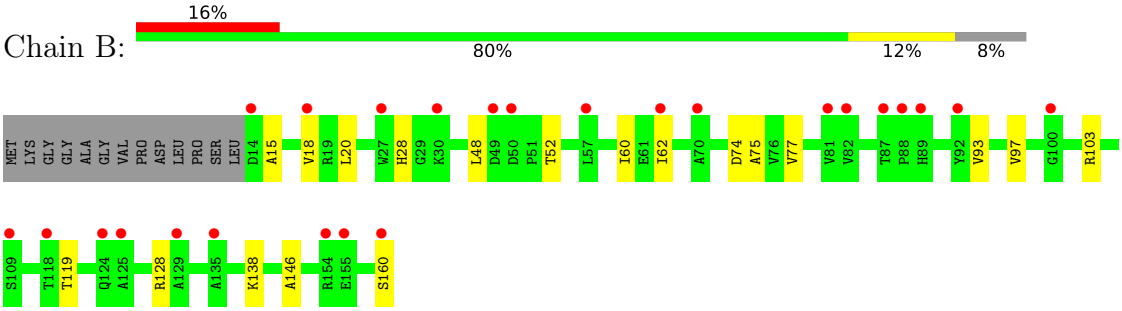
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE

Chain A:



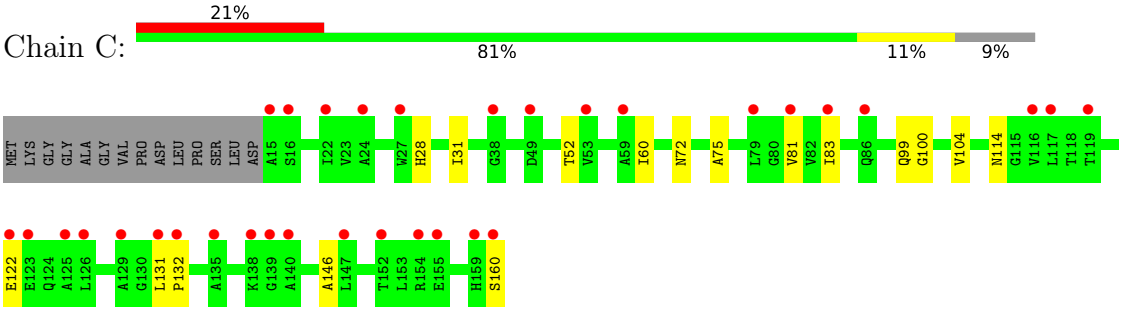
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE

Chain B:



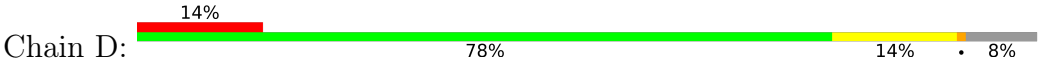
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE

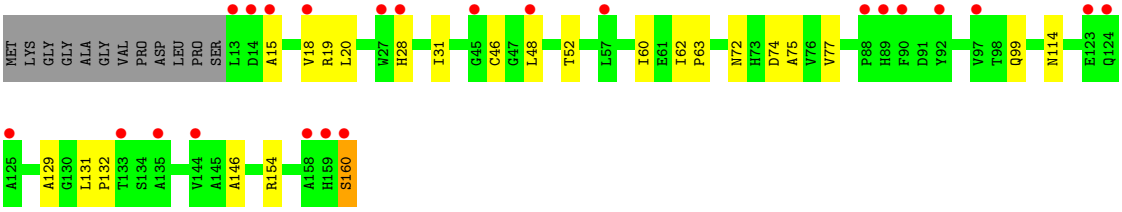
Chain C:



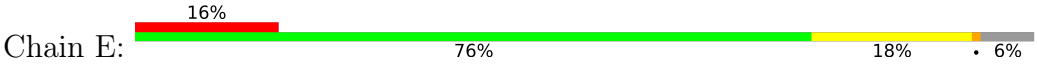
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE

Chain D:

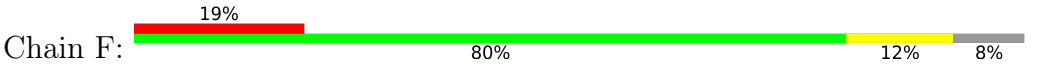


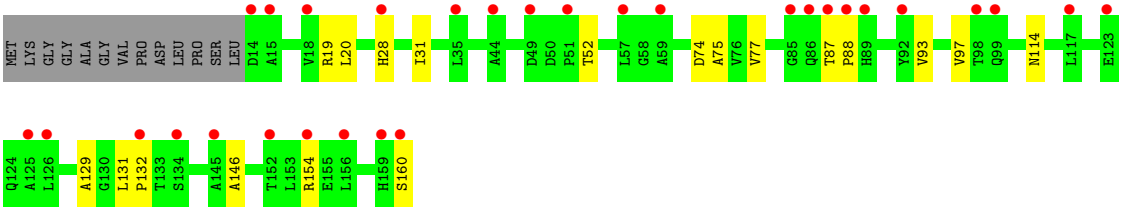


• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE

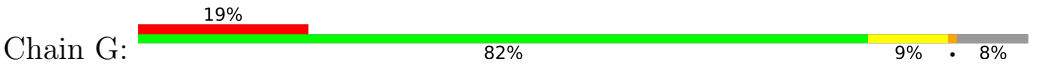


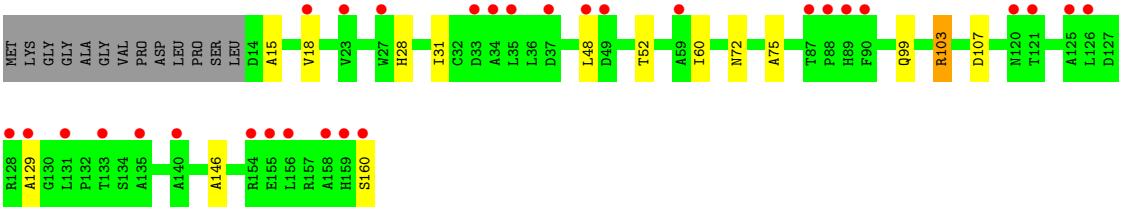
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



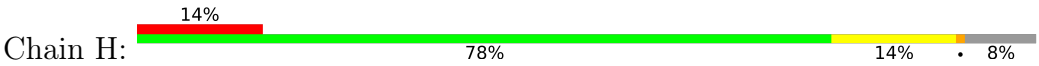


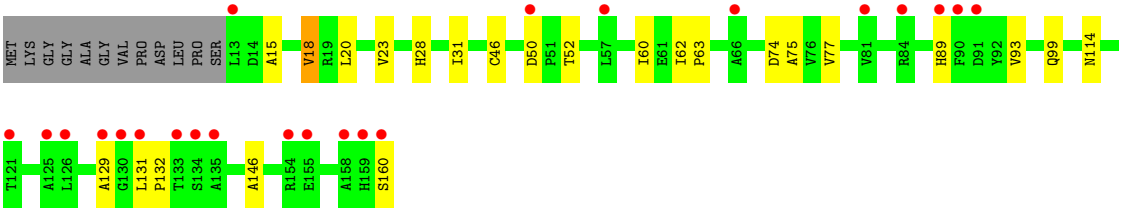
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE





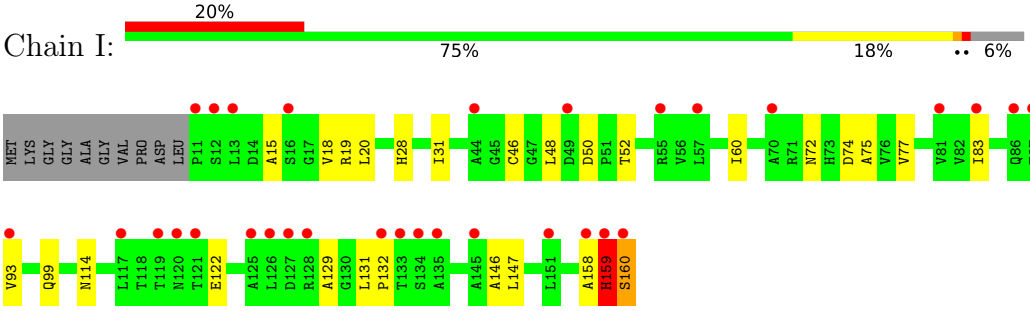
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE





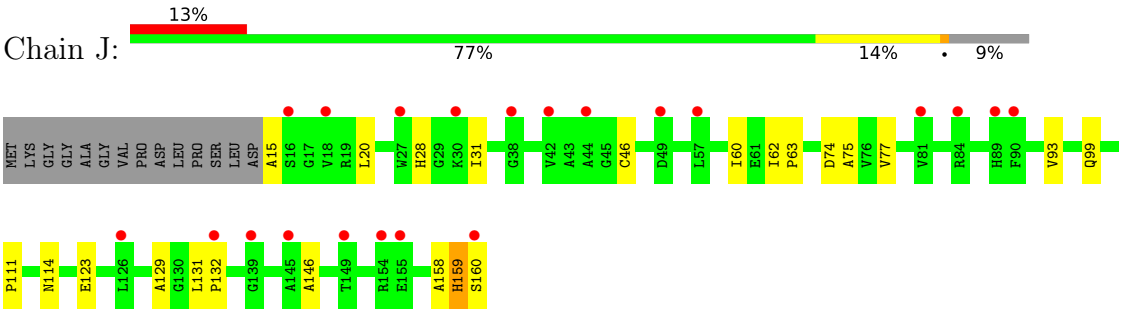
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE

Chain I:



• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.03Å 76.69Å 86.25Å 64.32° 64.41° 63.60°	Depositor
Resolution (Å)	30.00 – 2.30 28.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.30) 96.2 (28.89-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.260 , 0.299 0.259 , 0.297	Depositor DCC
R_{free} test set	3352 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 29.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.387 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11766	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.06% 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: Y19, K, PO4

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	0.30	0/1097	0.51	0/1497
1	B	0.30	0/1075	0.50	0/1467
1	C	0.29	0/1067	0.49	0/1456
1	D	0.30	0/1083	0.50	0/1478
1	E	0.32	0/1105	0.55	1/1509 (0.1%)
1	F	0.29	0/1075	0.50	0/1467
1	G	0.29	0/1075	0.50	0/1467
1	H	0.30	0/1083	0.51	0/1478
1	I	0.40	1/1097 (0.1%)	0.56	2/1497 (0.1%)
1	J	0.35	0/1067	0.55	0/1456
All	All	0.32	1/10824 (0.0%)	0.52	3/14772 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	I	0	1
1	J	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	159	HIS	CE1-NE2	5.31	1.44	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	160	SER	N-CA-C	6.81	129.38	111.00
1	E	160	SER	N-CA-C	6.66	128.97	111.00
1	I	160	SER	CA-C-O	5.92	132.53	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	159	HIS	Peptide
1	I	159	HIS	Peptide
1	J	159	HIS	Peptide

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	1084	0	1097	18	0
1	B	1063	0	1073	12	0
1	C	1055	0	1069	9	0
1	D	1071	0	1084	16	0
1	E	1092	0	1107	22	0
1	F	1063	0	1073	10	0
1	G	1063	0	1073	9	0
1	H	1071	0	1084	16	0
1	I	1084	0	1097	24	0
1	J	1055	0	1069	15	0
2	A	23	0	20	4	0
2	B	23	0	20	1	0
2	C	23	0	20	2	0
2	D	23	0	20	1	0
2	E	23	0	20	4	0
2	F	23	0	20	0	0
2	G	23	0	20	1	0
2	H	23	0	20	4	0
2	I	23	0	20	6	0
2	J	23	0	20	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	0	0
5	A	87	0	0	0	0
5	B	85	0	0	2	0
5	C	59	0	0	0	0
5	D	70	0	0	1	0
5	E	84	0	0	0	0
5	F	76	0	0	0	0
5	G	53	0	0	0	0
5	H	80	0	0	0	0
5	I	77	0	0	0	0
5	J	99	0	0	3	0
All	All	11766	0	11026	137	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 6.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:201:Y19:H5	2:I:201:Y19:H162	1.50	0.92
1:E:52:THR:HG23	1:J:160:SER:HB3	1.64	0.79
1:I:89:HIS:CD2	2:I:201:Y19:H163	2.28	0.69
1:D:18:VAL:HG23	1:D:74:ASP:HB2	1.74	0.68
1:B:52:THR:HG23	1:H:160:SER:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:HIS:CD2	1:I:159:HIS:O	2.48	0.67
1:H:18:VAL:HG23	1:H:74:ASP:HB2	1.77	0.66
1:E:18:VAL:HG23	1:E:74:ASP:HB2	1.79	0.65
1:I:18:VAL:HG23	1:I:74:ASP:HB2	1.79	0.64
1:D:160:SER:H	1:F:52:THR:HG23	1.61	0.64
1:B:18:VAL:HG23	1:B:74:ASP:HB2	1.78	0.64
1:A:72:ASN:HD21	1:I:158:ALA:HB3	1.62	0.64
1:J:77:VAL:HG23	5:J:2055:HOH:O	1.98	0.62
1:D:52:THR:HG23	1:F:160:SER:H	1.64	0.62
1:G:99:GLN:HE22	1:H:99:GLN:HA	1.65	0.62
1:J:20:LEU:CD1	5:J:2055:HOH:O	2.48	0.61
1:D:99:GLN:HE22	1:E:99:GLN:HA	1.66	0.60
1:E:15:ALA:HB3	1:E:46:CYS:HB3	1.82	0.60
1:D:60:ILE:HB	2:D:201:Y19:H10	1.83	0.60
1:A:89:HIS:HD2	2:A:201:Y19:H152	1.67	0.59
1:J:60:ILE:HD11	1:J:93:VAL:HA	1.84	0.58
1:B:160:SER:H	1:H:52:THR:HG23	1.70	0.56
1:E:60:ILE:HB	2:E:201:Y19:H10	1.87	0.56
1:G:60:ILE:HB	2:G:201:Y19:H10	1.87	0.56
1:I:20:LEU:HD11	1:I:77:VAL:HG23	1.88	0.56
1:H:99:GLN:HE22	1:I:99:GLN:HA	1.70	0.55
2:I:201:Y19:H5	2:I:201:Y19:C16	2.27	0.55
1:I:15:ALA:HB3	1:I:46:CYS:HB3	1.88	0.55
1:H:31:ILE:HG23	1:H:129:ALA:HB2	1.89	0.55
1:I:89:HIS:HD2	2:I:201:Y19:H163	1.71	0.54
1:A:14:ASP:O	1:A:15:ALA:HB2	2.08	0.54
1:E:89:HIS:HD2	2:E:201:Y19:H163	1.71	0.54
1:C:60:ILE:HB	2:C:201:Y19:H10	1.90	0.54
1:H:89:HIS:HD2	2:H:201:Y19:H152	1.72	0.53
1:A:60:ILE:HD11	1:A:93:VAL:HA	1.92	0.52
1:B:20:LEU:HD11	1:B:77:VAL:HG23	1.90	0.52
2:E:201:Y19:H5	2:E:201:Y19:H162	1.91	0.52
1:I:159:HIS:O	1:I:159:HIS:CG	2.63	0.52
1:H:20:LEU:HD11	1:H:77:VAL:HG23	1.92	0.51
1:A:99:GLN:HA	1:E:99:GLN:HE22	1.74	0.51
1:A:160:SER:H	1:I:52:THR:HG23	1.76	0.51
1:I:99:GLN:HE22	1:J:99:GLN:HA	1.74	0.51
1:D:20:LEU:HD11	1:D:77:VAL:HG23	1.93	0.51
1:D:15:ALA:HB3	1:D:46:CYS:HB3	1.92	0.51
1:E:15:ALA:O	1:E:18:VAL:HG12	2.10	0.51
1:E:10:LEU:N	1:E:144:VAL:HG22	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ARG:HB3	1:B:138:LYS:HG3	1.93	0.50
1:C:99:GLN:HE22	1:D:99:GLN:HA	1.77	0.50
1:H:15:ALA:HB3	1:H:46:CYS:HB3	1.95	0.49
1:I:15:ALA:O	1:I:18:VAL:HG12	2.12	0.49
1:J:31:ILE:HG23	1:J:129:ALA:HB2	1.94	0.49
1:C:160:SER:H	1:G:52:THR:HG23	1.78	0.49
1:I:20:LEU:HD22	1:I:147:LEU:HD21	1.94	0.49
1:G:103:ARG:HD3	1:G:107:ASP:OD1	2.13	0.49
1:B:97:VAL:HG13	5:B:2038:HOH:O	2.12	0.48
1:E:14:ASP:O	1:E:46:CYS:O	2.31	0.48
1:J:20:LEU:HD12	5:J:2055:HOH:O	2.10	0.48
1:B:18:VAL:HG13	1:B:48:LEU:HD11	1.96	0.48
1:E:14:ASP:O	1:E:16:SER:N	2.47	0.48
1:H:23:VAL:HG22	1:H:62:ILE:HD13	1.96	0.48
1:I:18:VAL:HG13	1:I:48:LEU:HD11	1.96	0.47
1:D:75:ALA:HB1	1:D:146:ALA:HB1	1.97	0.46
1:E:18:VAL:HG13	1:E:48:LEU:HD11	1.97	0.46
1:J:62:ILE:HB	1:J:63:PRO:HD3	1.97	0.46
1:A:14:ASP:O	1:A:151:LEU:HD11	2.15	0.46
1:A:131:LEU:HB3	1:A:132:PRO:HD2	1.98	0.46
1:I:31:ILE:HG23	1:I:129:ALA:HB2	1.97	0.46
1:J:75:ALA:HB1	1:J:146:ALA:HB1	1.98	0.46
1:D:62:ILE:HB	1:D:63:PRO:HD3	1.98	0.46
1:A:74:ASP:OD1	1:I:19:ARG:NH2	2.48	0.46
1:A:75:ALA:HB1	1:A:146:ALA:HB1	1.98	0.45
1:A:31:ILE:HG23	1:A:129:ALA:HB2	1.98	0.45
1:C:31:ILE:HB	1:C:81:VAL:HG21	1.98	0.45
1:C:131:LEU:HB3	1:C:132:PRO:HD2	1.97	0.45
1:H:75:ALA:HB1	1:H:146:ALA:HB1	1.98	0.45
1:H:89:HIS:CD2	2:H:201:Y19:H152	2.51	0.45
1:E:31:ILE:HG23	1:E:129:ALA:HB2	1.98	0.45
1:G:31:ILE:HG23	1:G:129:ALA:HB2	1.98	0.45
1:D:31:ILE:HG23	1:D:129:ALA:HB2	1.99	0.45
1:E:89:HIS:CD2	2:E:201:Y19:H163	2.52	0.45
1:E:140:ALA:O	1:E:144:VAL:HG23	2.17	0.45
1:I:75:ALA:HB1	1:I:146:ALA:HB1	1.99	0.45
1:E:20:LEU:HD11	1:E:77:VAL:HG23	1.99	0.44
2:J:201:Y19:H151	2:J:201:Y19:H5	1.62	0.44
1:A:89:HIS:CD2	2:A:201:Y19:H152	2.50	0.44
1:C:52:THR:HG23	1:G:160:SER:H	1.82	0.44
1:C:75:ALA:HB1	1:C:146:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:LEU:HB3	1:J:132:PRO:HD2	2.00	0.44
1:B:62:ILE:HB	5:B:2038:HOH:O	2.17	0.44
1:B:75:ALA:HB1	1:B:146:ALA:HB1	2.00	0.44
1:A:87:THR:HG21	1:B:119:THR:HG22	2.00	0.43
1:B:15:ALA:O	1:B:18:VAL:HG12	2.18	0.43
1:F:87:THR:HB	1:F:88:PRO:HD2	2.00	0.43
1:H:131:LEU:HB3	1:H:132:PRO:HD2	2.00	0.43
2:B:201:Y19:H5	2:B:201:Y19:H151	1.63	0.43
1:G:15:ALA:O	1:G:18:VAL:HG22	2.18	0.43
1:A:20:LEU:HD11	1:A:77:VAL:HG23	1.99	0.43
1:A:90:PHE:CZ	1:A:118:THR:HG23	2.53	0.43
1:F:31:ILE:HG23	1:F:129:ALA:HB2	2.00	0.43
1:D:19:ARG:NH2	1:F:74:ASP:OD1	2.52	0.43
2:H:201:Y19:H151	2:H:201:Y19:H5	1.45	0.43
1:I:90:PHE:HA	2:I:201:Y19:H161	1.99	0.43
1:F:75:ALA:HB1	1:F:146:ALA:HB1	2.00	0.43
1:F:131:LEU:HB3	1:F:132:PRO:HD2	2.00	0.43
1:G:75:ALA:HB1	1:G:146:ALA:HB1	2.00	0.43
1:I:131:LEU:HB3	1:I:132:PRO:HD2	2.00	0.43
1:H:60:ILE:HB	2:H:201:Y19:H10	2.00	0.43
1:E:75:ALA:HB1	1:E:146:ALA:HB1	2.00	0.43
1:A:52:THR:HG23	1:I:160:SER:H	1.84	0.42
1:B:60:ILE:HD11	1:B:93:VAL:HG22	2.00	0.42
1:E:131:LEU:HB3	1:E:132:PRO:HD2	2.01	0.42
1:I:83:ILE:HD12	1:I:122:GLU:HA	2.02	0.42
1:J:159:HIS:O	1:J:159:HIS:CD2	2.73	0.42
1:H:60:ILE:HD11	1:H:93:VAL:HA	2.02	0.41
1:D:18:VAL:HG13	1:D:48:LEU:HD11	2.02	0.41
1:D:74:ASP:OD1	1:F:19:ARG:NH2	2.53	0.41
1:D:154:ARG:HG3	5:D:2062:HOH:O	2.20	0.41
1:G:18:VAL:HG23	1:G:48:LEU:HD11	2.02	0.41
1:I:60:ILE:HD11	1:I:93:VAL:HG22	2.02	0.41
1:C:83:ILE:HD12	1:C:122:GLU:HA	2.02	0.41
2:C:201:Y19:H151	2:C:201:Y19:H5	1.61	0.41
1:F:93:VAL:O	1:F:97:VAL:HG23	2.21	0.41
1:I:31:ILE:HD12	1:I:31:ILE:H	1.85	0.41
1:D:131:LEU:HB3	1:D:132:PRO:HD2	2.02	0.41
1:E:83:ILE:HD12	1:E:122:GLU:HA	2.02	0.41
1:H:62:ILE:HB	1:H:63:PRO:HD3	2.03	0.41
1:A:60:ILE:HB	2:A:201:Y19:H10	2.03	0.41
1:E:11:PRO:HG3	1:E:45:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:LEU:HD11	1:F:77:VAL:HG23	2.01	0.41
1:I:60:ILE:HB	2:I:201:Y19:H10	2.03	0.41
1:J:15:ALA:HB3	1:J:46:CYS:HB3	2.02	0.41
2:A:201:Y19:H151	2:A:201:Y19:H5	1.54	0.40
1:A:156:LEU:HD22	1:J:158:ALA:HB1	2.03	0.40
1:E:52:THR:HA	1:J:160:SER:CB	2.52	0.40
1:E:27:TRP:O	1:E:28:HIS:HB2	2.22	0.40
1:C:100:GLY:O	1:C:104:VAL:HG23	2.21	0.40
1:J:74:ASP:O	1:J:111:PRO:HD2	2.22	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	148/160 (92%)	142 (96%)	3 (2%)	3 (2%)	7	6
1	B	145/160 (91%)	141 (97%)	3 (2%)	1 (1%)	22	26
1	C	144/160 (90%)	140 (97%)	3 (2%)	1 (1%)	22	26
1	D	146/160 (91%)	140 (96%)	5 (3%)	1 (1%)	22	26
1	E	149/160 (93%)	142 (95%)	5 (3%)	2 (1%)	12	12
1	F	145/160 (91%)	139 (96%)	5 (3%)	1 (1%)	22	26
1	G	145/160 (91%)	141 (97%)	3 (2%)	1 (1%)	22	26
1	H	146/160 (91%)	142 (97%)	3 (2%)	1 (1%)	22	26
1	I	148/160 (92%)	142 (96%)	5 (3%)	1 (1%)	22	26
1	J	144/160 (90%)	139 (96%)	4 (3%)	1 (1%)	22	26
All	All	1460/1600 (91%)	1408 (96%)	39 (3%)	13 (1%)	17	20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ALA
1	E	15	ALA
1	A	28	HIS
1	B	28	HIS
1	C	28	HIS
1	D	28	HIS
1	E	28	HIS
1	F	28	HIS
1	G	28	HIS
1	H	28	HIS
1	I	28	HIS
1	J	28	HIS
1	A	12	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/120 (95%)	112 (98%)	2 (2%)	59	75
1	B	111/120 (92%)	110 (99%)	1 (1%)	78	89
1	C	110/120 (92%)	108 (98%)	2 (2%)	59	75
1	D	112/120 (93%)	109 (97%)	3 (3%)	44	61
1	E	115/120 (96%)	115 (100%)	0	100	100
1	F	111/120 (92%)	109 (98%)	2 (2%)	59	75
1	G	111/120 (92%)	109 (98%)	2 (2%)	59	75
1	H	112/120 (93%)	109 (97%)	3 (3%)	44	61
1	I	114/120 (95%)	110 (96%)	4 (4%)	36	50
1	J	110/120 (92%)	108 (98%)	2 (2%)	59	75
All	All	1120/1200 (93%)	1099 (98%)	21 (2%)	57	73

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	72	ASN
1	B	103	ARG
1	C	72	ASN
1	C	114	ASN
1	D	72	ASN
1	D	114	ASN
1	D	160	SER
1	F	114	ASN
1	F	154	ARG
1	G	72	ASN
1	G	103	ARG
1	H	18	VAL
1	H	50	ASP
1	H	114	ASN
1	I	50	ASP
1	I	72	ASN
1	I	114	ASN
1	I	159	HIS
1	J	114	ASN
1	J	123	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	72	ASN
1	A	86	GLN
1	A	89	HIS
1	A	159	HIS
1	B	28	HIS
1	B	72	ASN
1	B	99	GLN
1	B	159	HIS
1	C	72	ASN
1	C	99	GLN
1	C	114	ASN
1	C	159	HIS
1	D	72	ASN
1	D	99	GLN
1	D	114	ASN
1	D	159	HIS
1	E	89	HIS

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Mol	Chain	Res	Type
1	E	99	GLN
1	F	89	HIS
1	F	159	HIS
1	G	72	ASN
1	G	99	GLN
1	H	89	HIS
1	H	99	GLN
1	H	159	HIS
1	I	72	ASN
1	I	99	GLN
1	I	159	HIS
1	J	99	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 35 ligands modelled in this entry, 15 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	B	702	-	4,4,4	0.93	0	6,6,6	0.44	0
4	PO4	J	702	-	4,4,4	0.89	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PO4	A	702	-	4,4,4	0.90	0	6,6,6	0.41	0
2	Y19	F	201	-	19,23,23	0.62	0	22,31,31	1.24	2 (9%)
4	PO4	D	702	-	4,4,4	0.92	0	6,6,6	0.44	0
2	Y19	H	201	-	19,23,23	0.54	0	22,31,31	0.90	1 (4%)
4	PO4	I	702	-	4,4,4	0.96	0	6,6,6	0.40	0
2	Y19	J	201	-	19,23,23	0.56	0	22,31,31	0.84	0
2	Y19	G	201	-	19,23,23	0.63	0	22,31,31	1.20	2 (9%)
2	Y19	I	201	-	19,23,23	0.61	0	22,31,31	1.58	3 (13%)
4	PO4	F	702	-	4,4,4	0.91	0	6,6,6	0.42	0
2	Y19	E	201	-	19,23,23	0.63	0	22,31,31	1.24	3 (13%)
2	Y19	B	201	-	19,23,23	0.56	0	22,31,31	0.93	2 (9%)
2	Y19	D	201	-	19,23,23	0.61	0	22,31,31	1.32	3 (13%)
4	PO4	C	702	-	4,4,4	0.89	0	6,6,6	0.45	0
4	PO4	G	702	-	4,4,4	0.94	0	6,6,6	0.43	0
4	PO4	H	702	-	4,4,4	0.89	0	6,6,6	0.53	0
4	PO4	E	702	-	4,4,4	0.97	0	6,6,6	0.45	0
2	Y19	C	201	-	19,23,23	0.60	0	22,31,31	0.88	2 (9%)
2	Y19	A	201	-	19,23,23	0.58	0	22,31,31	0.88	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y19	H	201	-	-	2/21/37/37	0/1/1/1
2	Y19	E	201	-	-	3/21/37/37	0/1/1/1
2	Y19	F	201	-	-	2/21/37/37	0/1/1/1
2	Y19	B	201	-	-	4/21/37/37	0/1/1/1
2	Y19	J	201	-	-	5/21/37/37	0/1/1/1
2	Y19	G	201	-	-	7/21/37/37	0/1/1/1
2	Y19	I	201	-	-	5/21/37/37	0/1/1/1
2	Y19	D	201	-	-	2/21/37/37	0/1/1/1
2	Y19	C	201	-	-	5/21/37/37	0/1/1/1
2	Y19	A	201	-	-	2/21/37/37	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	201	Y19	C15-C14-N13	5.17	122.43	115.77
2	E	201	Y19	C15-C14-N13	4.01	120.93	115.77
2	D	201	Y19	C15-C14-N13	3.96	120.86	115.77
2	G	201	Y19	C15-C14-N13	3.44	120.20	115.77
2	F	201	Y19	C15-C14-N13	3.39	120.13	115.77
2	I	201	Y19	C5-N13-C14	3.34	124.96	121.39
2	F	201	Y19	C5-N13-C14	3.08	124.67	121.39
2	G	201	Y19	C5-N13-C14	2.74	124.31	121.39
2	D	201	Y19	C5-N13-C14	2.73	124.31	121.39
2	C	201	Y19	C15-C14-N13	2.35	118.80	115.77
2	B	201	Y19	C4-N3-C2	-2.15	122.18	125.42
2	A	201	Y19	C4-N3-C2	-2.14	122.19	125.42
2	D	201	Y19	C4-N3-C2	-2.13	122.21	125.42
2	E	201	Y19	C4-N3-C2	-2.12	122.23	125.42
2	E	201	Y19	C5-N13-C14	2.10	123.64	121.39
2	H	201	Y19	C4-N3-C2	-2.10	122.25	125.42
2	B	201	Y19	C15-C14-N13	2.10	118.47	115.77
2	C	201	Y19	C4-N3-C2	-2.09	122.28	125.42
2	I	201	Y19	C4-N3-C2	-2.01	122.39	125.42
2	A	201	Y19	C15-C14-N13	2.00	118.35	115.77

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	Y19	N7-C8-C9-O9
2	G	201	Y19	N7-C8-C9-O9
2	G	201	Y19	C11-C10-C9-C8
2	J	201	Y19	N7-C8-C9-O9
2	A	201	Y19	C15-C14-N13-C5
2	B	201	Y19	C15-C14-N13-C5
2	C	201	Y19	C15-C14-N13-C5
2	D	201	Y19	C15-C14-N13-C5
2	E	201	Y19	C15-C14-N13-C5
2	F	201	Y19	C15-C14-N13-C5
2	G	201	Y19	C15-C14-N13-C5
2	H	201	Y19	C15-C14-N13-C5
2	I	201	Y19	C15-C14-N13-C5
2	J	201	Y19	C15-C14-N13-C5
2	A	201	Y19	O23-C14-N13-C5
2	B	201	Y19	O23-C14-N13-C5
2	C	201	Y19	O23-C14-N13-C5
2	D	201	Y19	O23-C14-N13-C5

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Mol	Chain	Res	Type	Atoms
2	E	201	Y19	O23-C14-N13-C5
2	F	201	Y19	O23-C14-N13-C5
2	G	201	Y19	O23-C14-N13-C5
2	H	201	Y19	O23-C14-N13-C5
2	I	201	Y19	O23-C14-N13-C5
2	J	201	Y19	O23-C14-N13-C5
2	G	201	Y19	C11-C10-C9-O9
2	I	201	Y19	O23-C14-C15-C16
2	C	201	Y19	C11-C10-C9-O9
2	B	201	Y19	N7-C8-C9-O9
2	I	201	Y19	N7-C8-C9-O9
2	C	201	Y19	N7-C8-C9-C10
2	J	201	Y19	N7-C8-C9-C10
2	I	201	Y19	N13-C14-C15-C16
2	G	201	Y19	O10-C10-C9-O9
2	G	201	Y19	N7-C8-C9-C10
2	J	201	Y19	C11-C10-C9-O9
2	B	201	Y19	C4-C5-N13-C14
2	E	201	Y19	N7-C8-C9-O9

There are no ring outliers.

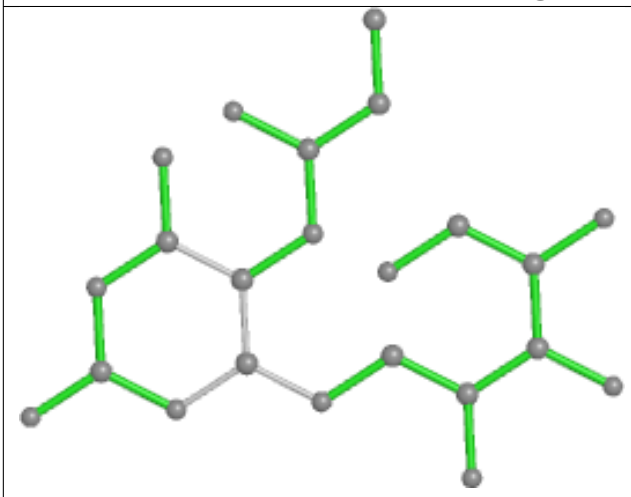
9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	201	Y19	4	0
2	J	201	Y19	1	0
2	G	201	Y19	1	0
2	I	201	Y19	6	0
2	E	201	Y19	4	0
2	B	201	Y19	1	0
2	D	201	Y19	1	0
2	C	201	Y19	2	0
2	A	201	Y19	4	0

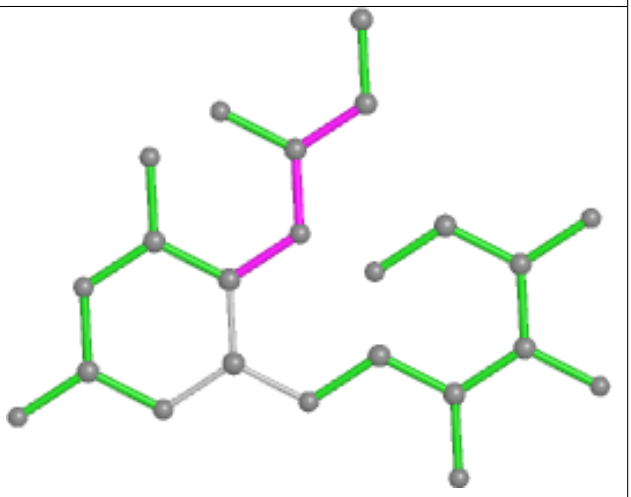
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

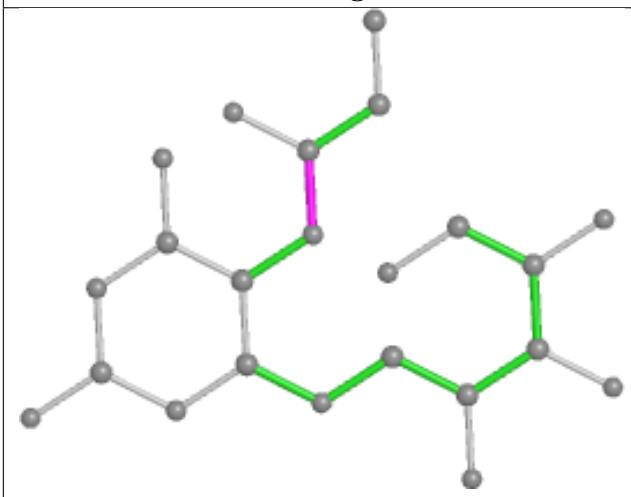
Ligand Y19 F 201



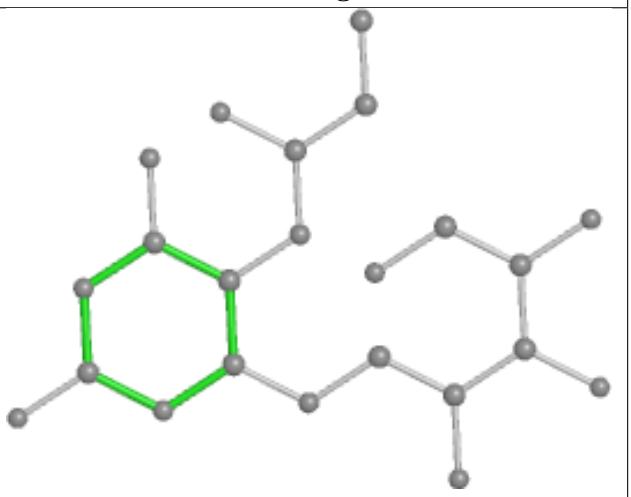
Bond lengths



Bond angles

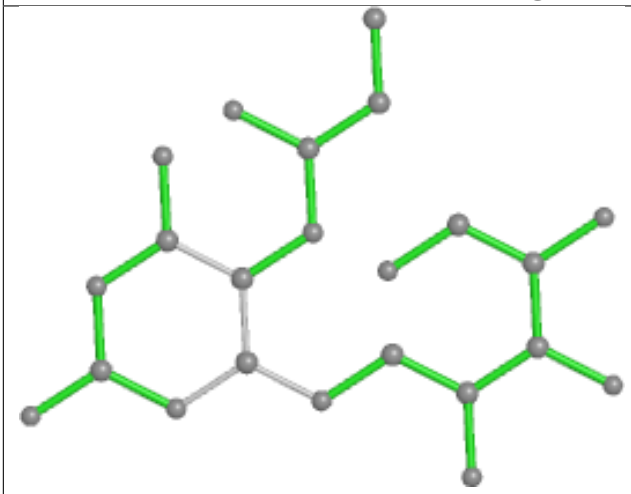


Torsions

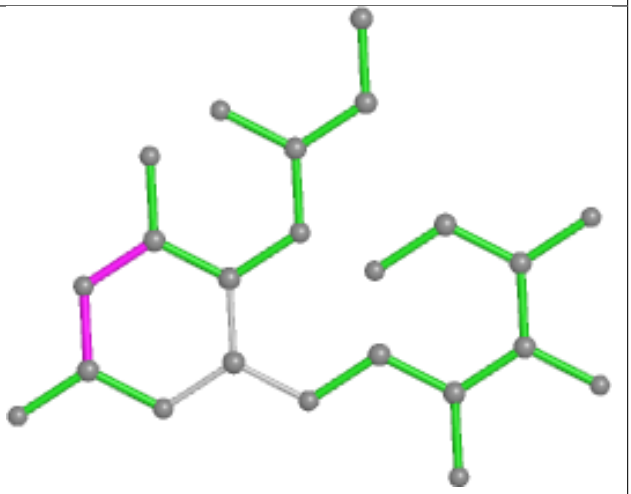


Rings

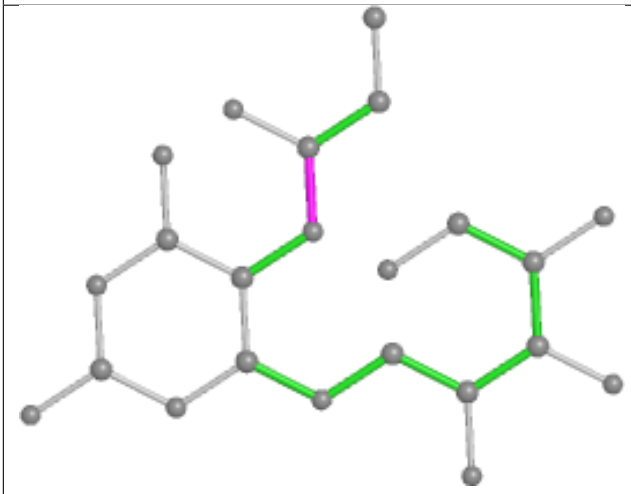
Ligand Y19 H 201



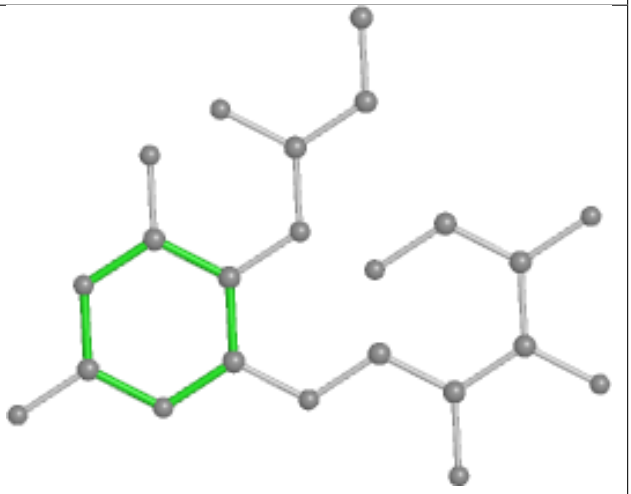
Bond lengths



Bond angles

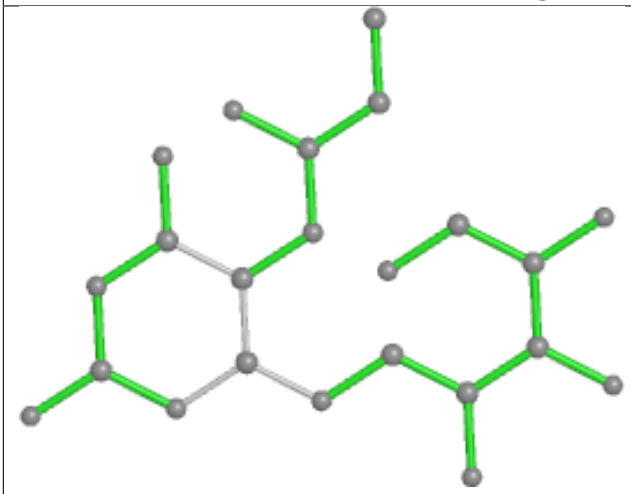


Torsions

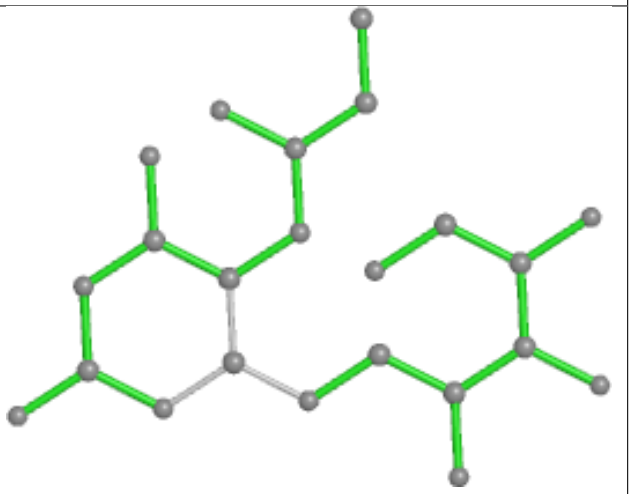


Rings

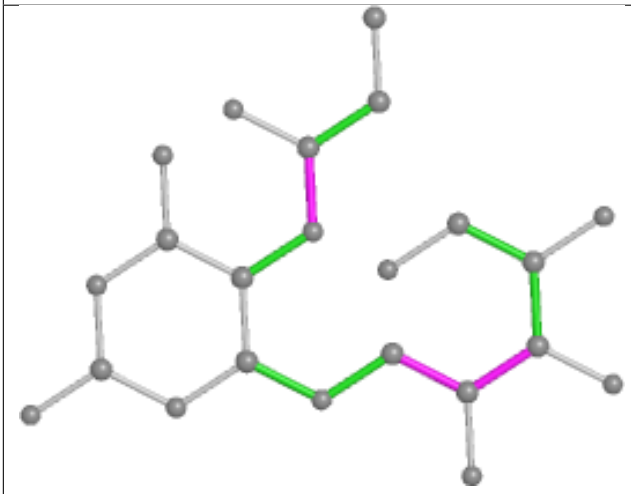
Ligand Y19 J 201



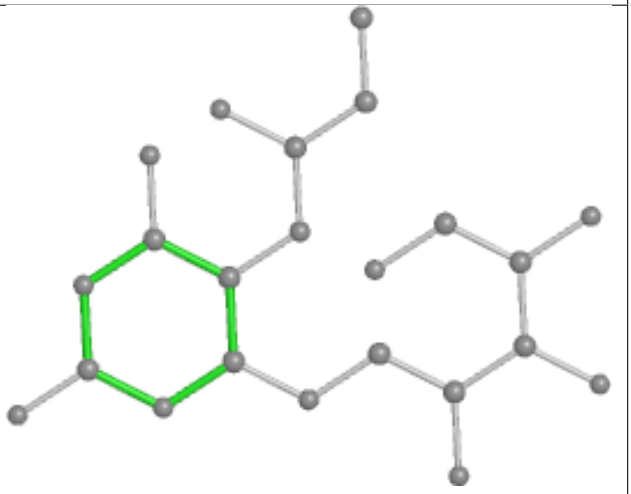
Bond lengths



Bond angles

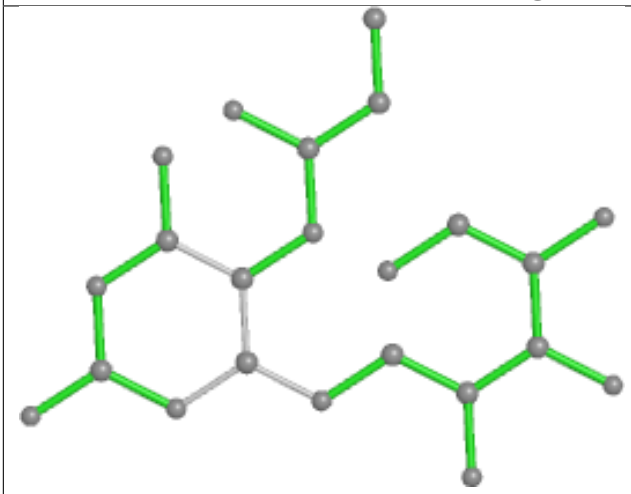


Torsions



Rings

Ligand Y19 G 201



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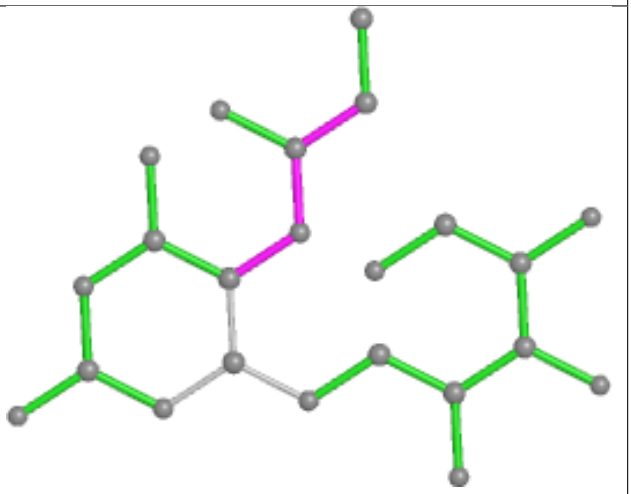
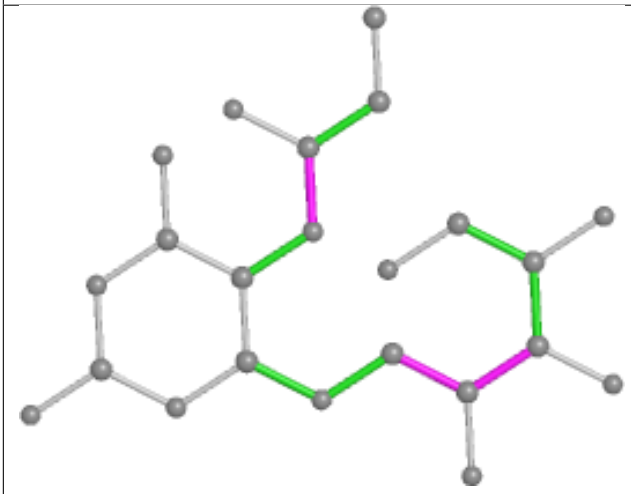


Bond angles



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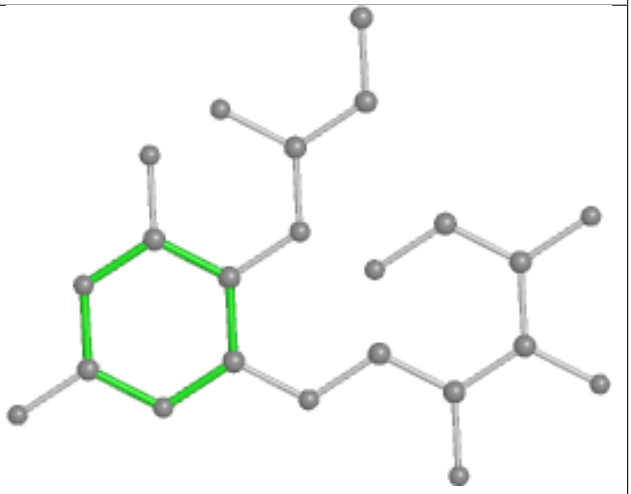
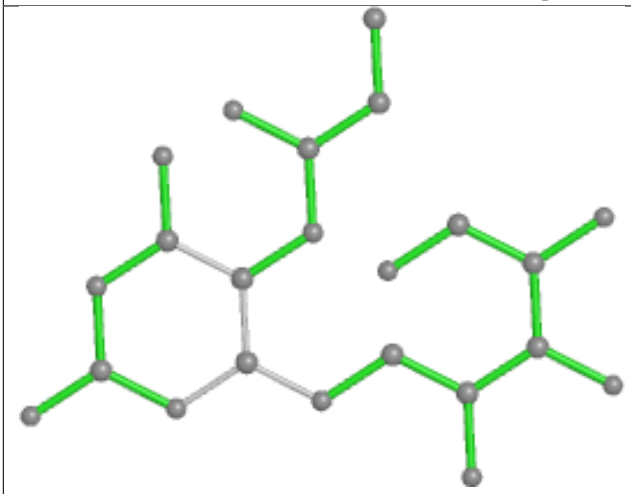


Rings

Ligand Y19 I 201



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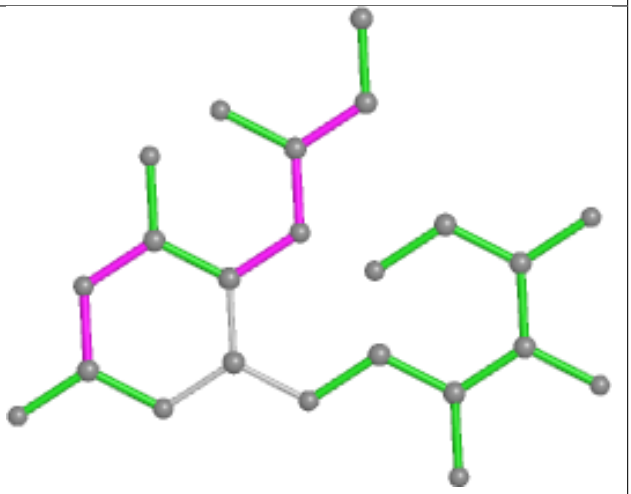
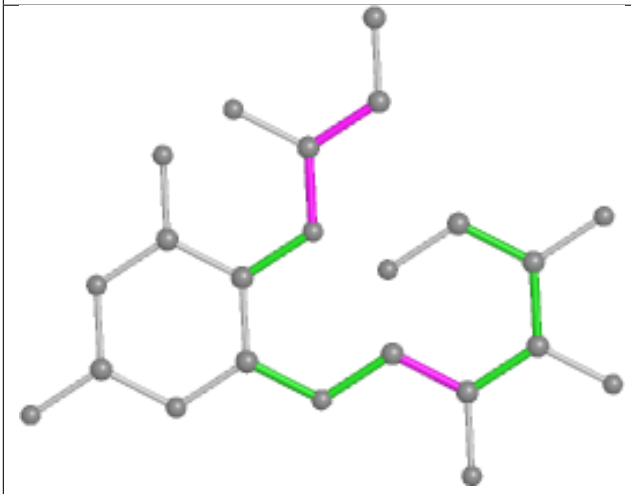
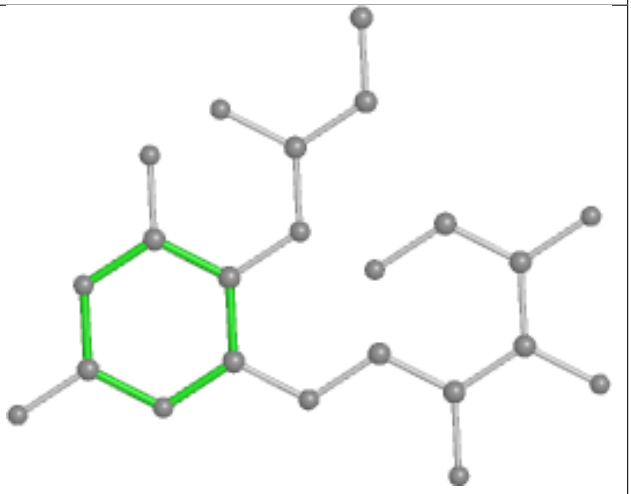


Bond angles

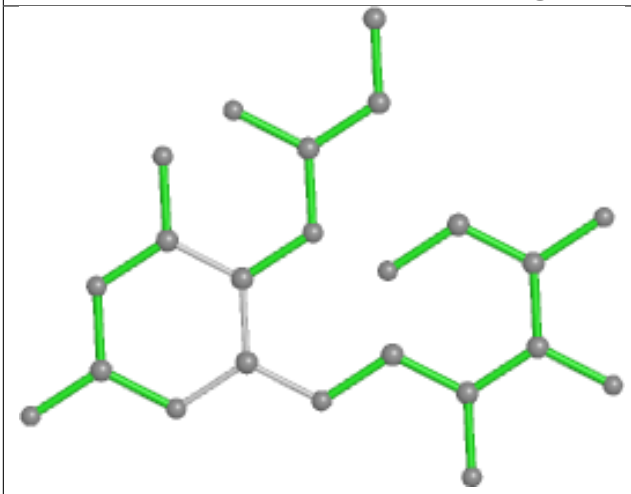


Torsions



Rings

Ligand Y19 E 201



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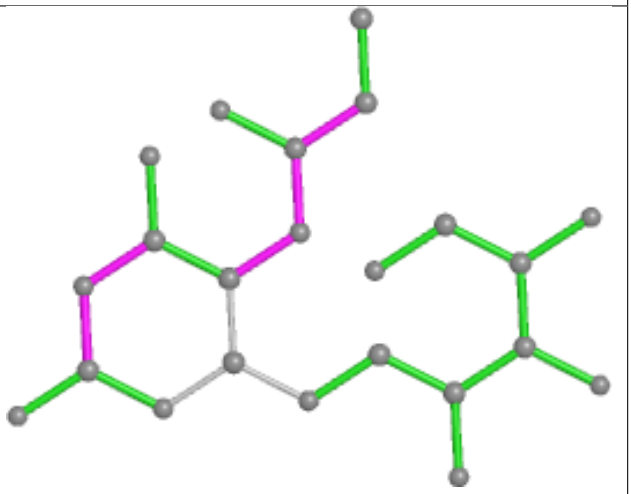
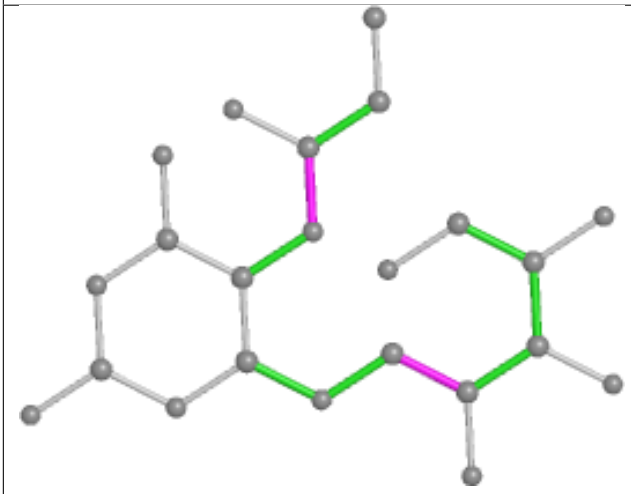
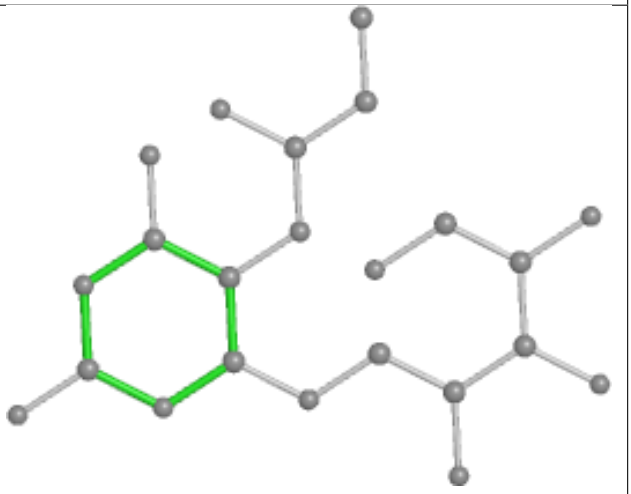


Bond angles

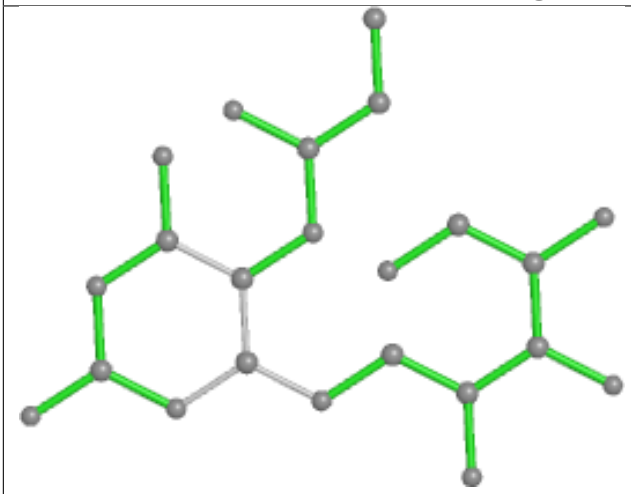


Torsions

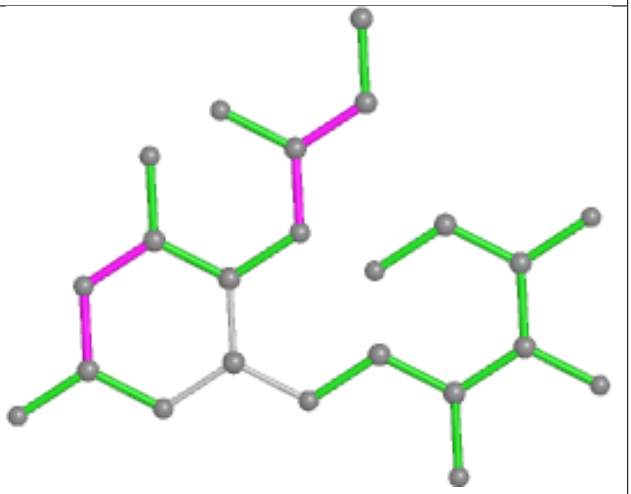


Rings

Ligand Y19 B 201



Bond lengths



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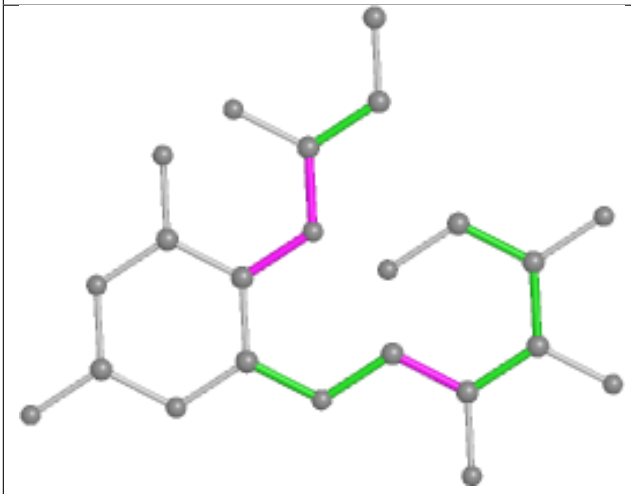

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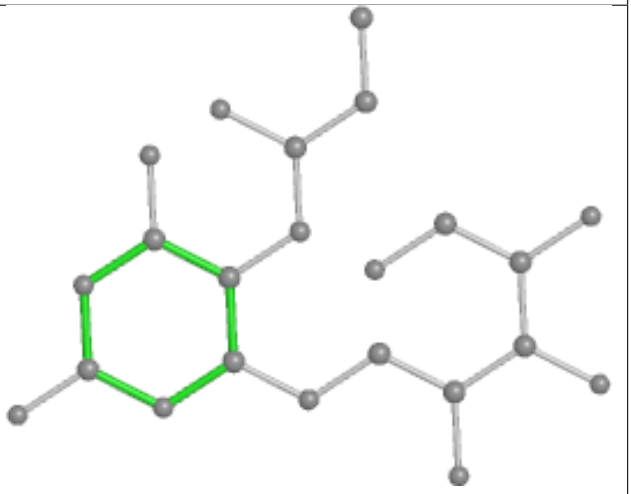
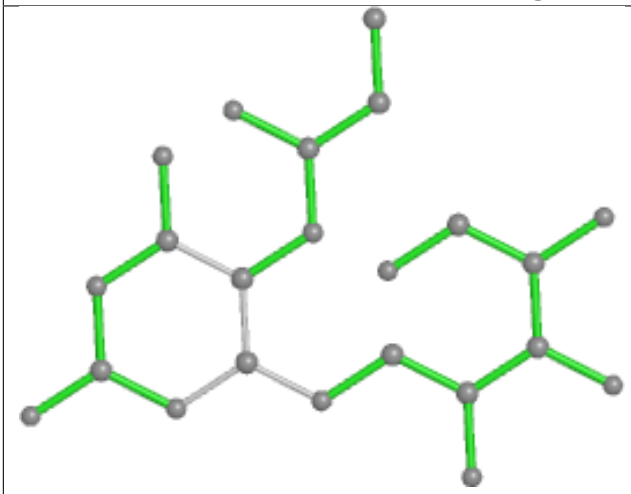
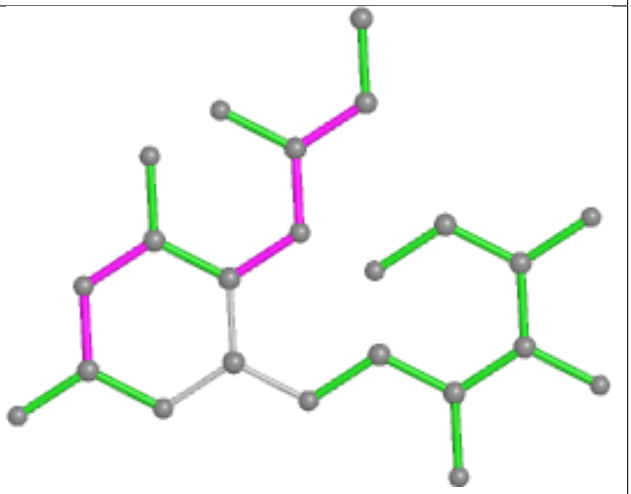


Rings

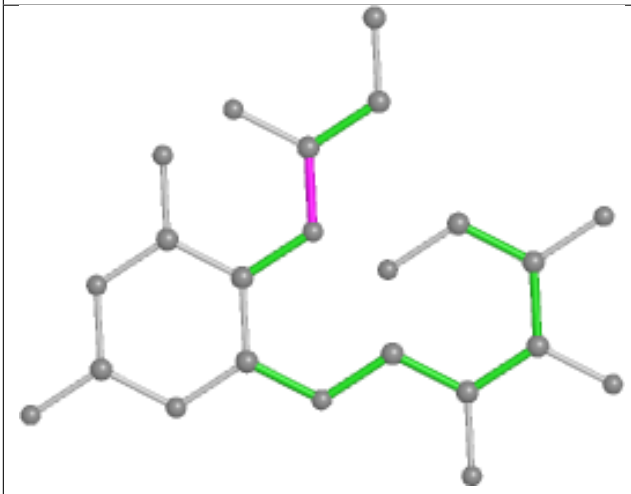
Ligand Y19 D 201



Bond lengths



Bond angles



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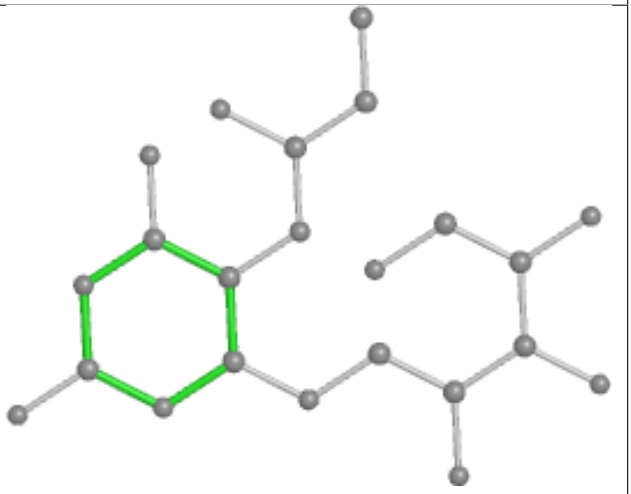
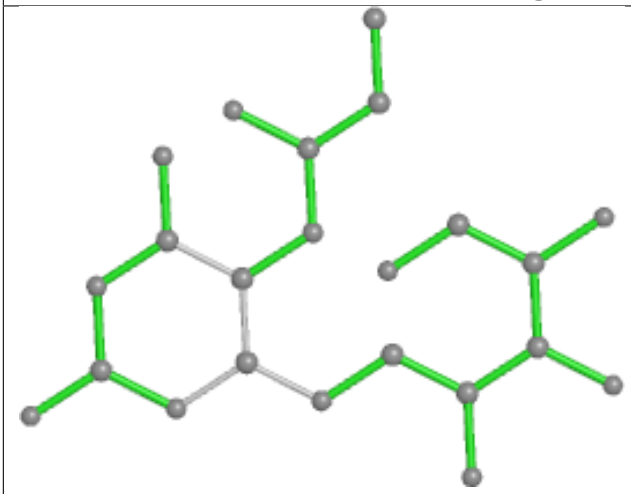


Rings

Ligand Y19 C 201



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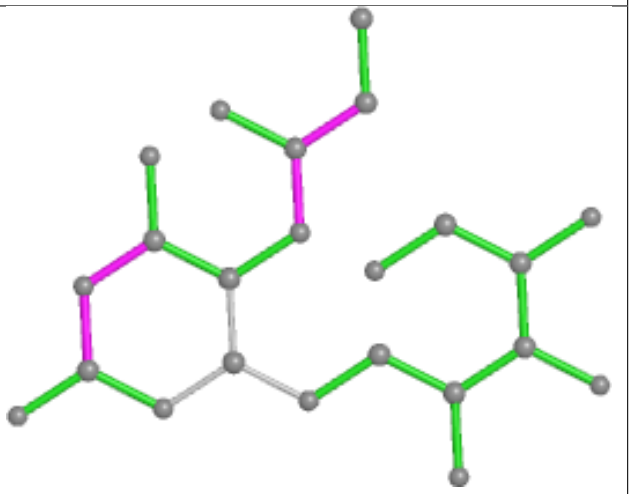
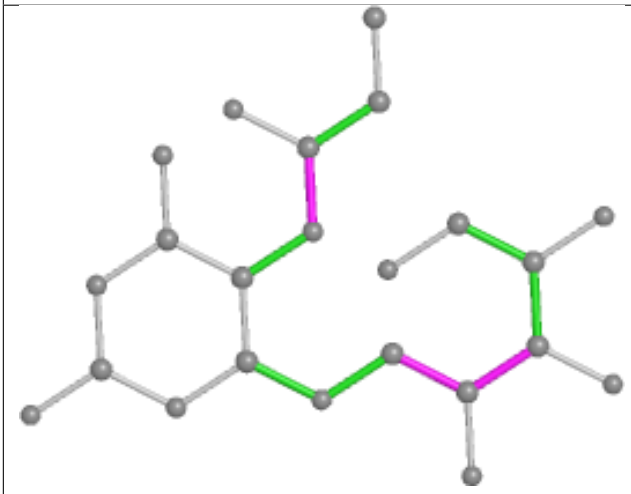
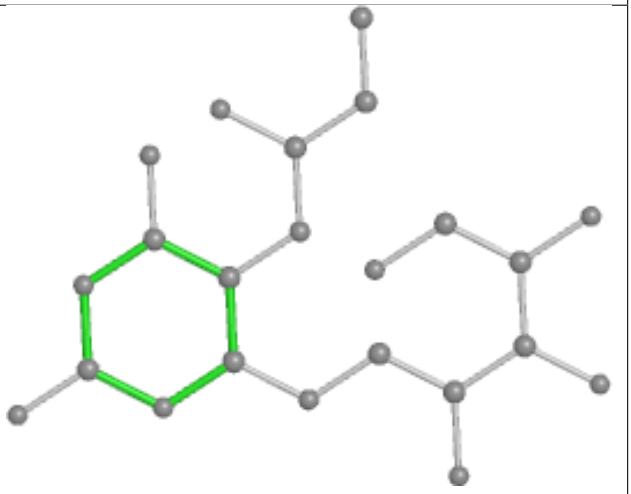


Bond angles

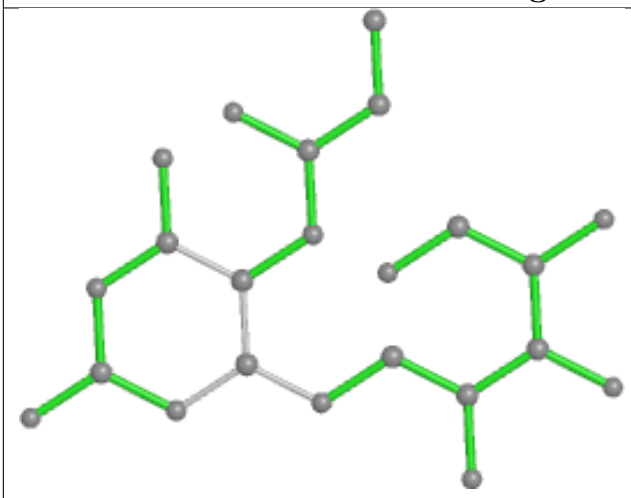


Torsions

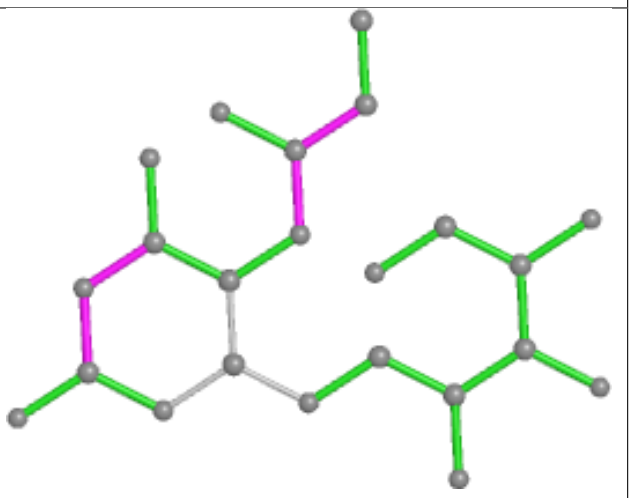


Rings

Ligand Y19 A 201



Bond lengths



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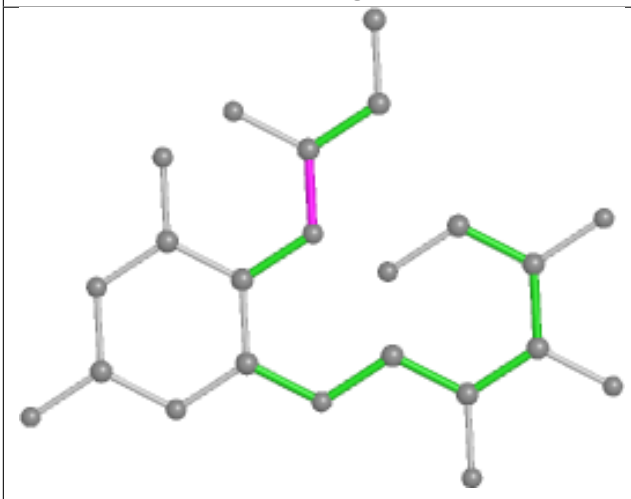
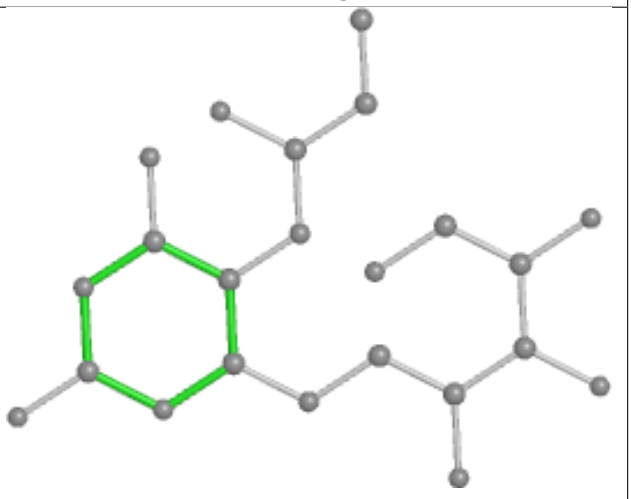


Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	150/160 (93%)	1.12	22 (14%)	2	3	36, 39, 43, 54	0
1	B	147/160 (91%)	1.18	25 (17%)	1	2	36, 39, 42, 48	0
1	C	146/160 (91%)	1.41	33 (22%)	0	1	36, 39, 42, 46	0
1	D	148/160 (92%)	1.15	23 (15%)	2	3	36, 39, 43, 49	0
1	E	151/160 (94%)	1.21	25 (16%)	1	2	36, 39, 44, 54	0
1	F	147/160 (91%)	1.26	30 (20%)	1	1	36, 39, 42, 48	0
1	G	147/160 (91%)	1.37	30 (20%)	1	1	36, 39, 42, 47	0
1	H	148/160 (92%)	1.16	23 (15%)	2	3	36, 39, 42, 49	0
1	I	150/160 (93%)	1.27	32 (21%)	0	1	36, 39, 43, 52	0
1	J	146/160 (91%)	1.19	21 (14%)	2	3	36, 39, 42, 46	0
All	All	1480/1600 (92%)	1.23	264 (17%)	1	1	36, 39, 43, 54	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	12	SER	9.4
1	A	12	SER	8.8
1	H	158	ALA	8.7
1	G	160	SER	8.5
1	H	133	THR	7.5
1	E	10	LEU	7.1
1	D	159	HIS	7.1
1	J	160	SER	6.7
1	I	135	ALA	6.6
1	G	18	VAL	6.2
1	C	154	ARG	6.0
1	G	125	ALA	5.9
1	I	159	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	125	ALA	5.7
1	H	89	HIS	5.6
1	E	158	ALA	5.5
1	D	160	SER	5.4
1	F	132	PRO	5.3
1	B	14	ASP	5.2
1	E	133	THR	5.0
1	C	81	VAL	4.9
1	B	155	GLU	4.9
1	I	158	ALA	4.9
1	G	48	LEU	4.9
1	A	11	PRO	4.8
1	I	134	SER	4.7
1	C	135	ALA	4.7
1	C	160	SER	4.7
1	I	133	THR	4.7
1	A	158	ALA	4.7
1	A	132	PRO	4.7
1	F	88	PRO	4.6
1	B	160	SER	4.6
1	C	131	LEU	4.6
1	E	160	SER	4.6
1	I	119	THR	4.4
1	H	160	SER	4.4
1	E	15	ALA	4.4
1	A	13	LEU	4.3
1	G	89	HIS	4.3
1	I	11	PRO	4.2
1	D	57	LEU	4.1
1	J	27	TRP	4.0
1	H	131	LEU	4.0
1	E	12	SER	3.9
1	D	125	ALA	3.9
1	H	121	THR	3.9
1	G	126	LEU	3.9
1	C	117	LEU	3.8
1	C	155	GLU	3.8
1	A	159	HIS	3.7
1	G	158	ALA	3.7
1	B	62	ILE	3.7
1	I	57	LEU	3.6
1	F	86	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	11	PRO	3.6
1	F	156	LEU	3.6
1	F	159	HIS	3.6
1	D	158	ALA	3.6
1	D	123	GLU	3.6
1	F	160	SER	3.6
1	D	14	ASP	3.6
1	B	27	TRP	3.5
1	E	159	HIS	3.5
1	E	90	PHE	3.5
1	F	85	GLY	3.5
1	I	87	THR	3.5
1	C	132	PRO	3.5
1	I	121	THR	3.5
1	H	125	ALA	3.5
1	C	159	HIS	3.4
1	G	23	VAL	3.4
1	D	13	LEU	3.4
1	F	126	LEU	3.4
1	C	79	LEU	3.4
1	E	91	ASP	3.4
1	A	155	GLU	3.4
1	C	125	ALA	3.4
1	E	18	VAL	3.3
1	D	88	PRO	3.3
1	D	97	VAL	3.3
1	B	89	HIS	3.3
1	G	120	ASN	3.3
1	B	57	LEU	3.3
1	G	27	TRP	3.3
1	B	30	LYS	3.2
1	B	81	VAL	3.2
1	F	18	VAL	3.2
1	F	28	HIS	3.2
1	H	155	GLU	3.2
1	F	15	ALA	3.2
1	D	48	LEU	3.2
1	J	155	GLU	3.1
1	D	135	ALA	3.1
1	F	14	ASP	3.1
1	A	27	TRP	3.1
1	F	117	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	16	SER	3.1
1	F	99	GLN	3.1
1	F	57	LEU	3.1
1	C	138	LYS	3.1
1	J	16	SER	3.1
1	J	18	VAL	3.0
1	D	89	HIS	3.0
1	G	140	ALA	3.0
1	G	37	ASP	3.0
1	I	127	ASP	3.0
1	I	126	LEU	3.0
1	I	44	ALA	2.9
1	C	49	ASP	2.9
1	B	70	ALA	2.9
1	C	15	ALA	2.9
1	I	132	PRO	2.9
1	C	122	GLU	2.9
1	E	14	ASP	2.9
1	B	118	THR	2.8
1	J	57	LEU	2.8
1	A	85	GLY	2.8
1	H	50	ASP	2.8
1	C	116	VAL	2.8
1	C	59	ALA	2.8
1	D	28	HIS	2.8
1	H	134	SER	2.8
1	I	120	ASN	2.8
1	I	125	ALA	2.8
1	B	154	ARG	2.8
1	G	135	ALA	2.7
1	A	133	THR	2.7
1	G	133	THR	2.7
1	E	125	ALA	2.7
1	I	81	VAL	2.7
1	J	126	LEU	2.7
1	G	128	ARG	2.7
1	B	49	ASP	2.7
1	H	13	LEU	2.7
1	F	87	THR	2.7
1	G	121	THR	2.7
1	H	81	VAL	2.7
1	D	144	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	49	ASP	2.6
1	C	53	VAL	2.6
1	I	160	SER	2.6
1	J	145	ALA	2.6
1	B	18	VAL	2.6
1	H	126	LEU	2.6
1	D	124	GLN	2.6
1	B	109	SER	2.6
1	J	42	VAL	2.6
1	H	154	ARG	2.6
1	C	86	GLN	2.6
1	E	121	THR	2.6
1	F	59	ALA	2.6
1	B	124	GLN	2.5
1	J	49	ASP	2.5
1	A	89	HIS	2.5
1	G	90	PHE	2.5
1	A	160	SER	2.5
1	G	155	GLU	2.5
1	H	91	ASP	2.5
1	E	83	ILE	2.5
1	E	86	GLN	2.5
1	A	14	ASP	2.5
1	G	87	THR	2.5
1	J	132	PRO	2.5
1	I	89	HIS	2.5
1	C	147	LEU	2.5
1	F	154	ARG	2.5
1	J	84	ARG	2.5
1	C	123	GLU	2.5
1	A	83	ILE	2.5
1	B	100	GLY	2.5
1	C	83	ILE	2.5
1	A	88	PRO	2.4
1	C	119	THR	2.4
1	F	51	PRO	2.4
1	F	49	ASP	2.4
1	G	59	ALA	2.4
1	D	27	TRP	2.4
1	G	49	ASP	2.4
1	G	154	ARG	2.4
1	H	159	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	83	ILE	2.4
1	J	30	LYS	2.4
1	C	27	TRP	2.4
1	C	38	GLY	2.4
1	C	126	LEU	2.4
1	G	156	LEU	2.4
1	F	125	ALA	2.4
1	A	144	VAL	2.4
1	J	90	PHE	2.4
1	A	59	ALA	2.3
1	G	33	ASP	2.3
1	B	92	TYR	2.3
1	G	131	LEU	2.3
1	I	13	LEU	2.3
1	F	89	HIS	2.3
1	G	88	PRO	2.3
1	C	140	ALA	2.3
1	E	84	ARG	2.3
1	E	157	ARG	2.3
1	H	135	ALA	2.3
1	E	27	TRP	2.3
1	C	22	ILE	2.3
1	C	24	ALA	2.3
1	J	149	THR	2.3
1	E	92	TYR	2.3
1	J	81	VAL	2.3
1	A	50	ASP	2.3
1	J	44	ALA	2.3
1	D	92	TYR	2.2
1	A	121	THR	2.2
1	C	139	GLY	2.2
1	E	32	CYS	2.2
1	A	70	ALA	2.2
1	E	85	GLY	2.2
1	F	145	ALA	2.2
1	F	152	THR	2.2
1	B	129	ALA	2.2
1	E	135	ALA	2.2
1	E	23	VAL	2.2
1	D	90	PHE	2.2
1	G	35	LEU	2.2
1	H	57	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	128	ARG	2.2
1	F	123	GLU	2.2
1	F	44	ALA	2.2
1	F	98	THR	2.2
1	G	129	ALA	2.1
1	E	37	ASP	2.1
1	A	128	ARG	2.1
1	H	66	ALA	2.1
1	D	45	GLY	2.1
1	H	130	GLY	2.1
1	D	15	ALA	2.1
1	D	18	VAL	2.1
1	H	90	PHE	2.1
1	H	129	ALA	2.1
1	I	70	ALA	2.1
1	F	35	LEU	2.1
1	B	50	ASP	2.1
1	B	87	THR	2.1
1	C	152	THR	2.1
1	I	93	VAL	2.1
1	B	88	PRO	2.1
1	J	38	GLY	2.1
1	A	118	THR	2.1
1	B	135	ALA	2.1
1	I	145	ALA	2.1
1	I	86	GLN	2.1
1	I	117	LEU	2.1
1	I	151	LEU	2.1
1	J	154	ARG	2.1
1	B	82	VAL	2.1
1	F	92	TYR	2.1
1	H	84	ARG	2.0
1	D	133	THR	2.0
1	F	134	SER	2.0
1	I	16	SER	2.0
1	J	89	HIS	2.0
1	J	139	GLY	2.0
1	C	129	ALA	2.0
1	G	34	ALA	2.0
1	G	159	HIS	2.0
1	I	55	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	Y19	G	201	23/23	0.76	0.24	45,45,46,46	0
2	Y19	I	201	23/23	0.79	0.23	37,38,38,38	0
2	Y19	J	201	23/23	0.79	0.23	43,47,49,49	0
2	Y19	F	201	23/23	0.80	0.22	44,45,46,46	0
2	Y19	E	201	23/23	0.81	0.20	40,41,42,42	0
2	Y19	C	201	23/23	0.82	0.19	39,40,40,40	0
2	Y19	A	201	23/23	0.82	0.22	38,43,46,46	0
2	Y19	D	201	23/23	0.83	0.20	36,37,38,38	0
2	Y19	H	201	23/23	0.84	0.23	38,40,41,41	0
3	K	C	603	1/1	0.85	0.10	46,46,46,46	0
3	K	E	603	1/1	0.85	0.21	63,63,63,63	0
2	Y19	B	201	23/23	0.86	0.19	41,42,43,43	0
3	K	D	603	1/1	0.89	0.11	52,52,52,52	0
4	PO4	B	702	5/5	0.91	0.27	54,54,54,54	0
4	PO4	E	702	5/5	0.91	0.13	36,36,36,36	0
4	PO4	G	702	5/5	0.91	0.14	31,31,31,31	0
4	PO4	A	702	5/5	0.92	0.12	37,37,37,38	0
3	K	A	603	1/1	0.92	0.07	43,43,43,43	0
4	PO4	C	702	5/5	0.93	0.15	28,28,29,29	0
3	K	C	601	1/1	0.93	0.11	32,32,32,32	0
4	PO4	F	702	5/5	0.93	0.22	58,58,58,58	0
3	K	B	601	1/1	0.93	0.09	31,31,31,31	0
4	PO4	H	702	5/5	0.93	0.15	38,38,38,38	0
4	PO4	I	702	5/5	0.93	0.15	25,26,26,26	0
4	PO4	J	702	5/5	0.94	0.11	36,36,36,36	0
3	K	G	601	1/1	0.95	0.12	38,38,38,38	0
3	K	B	603	1/1	0.97	0.06	39,39,39,39	0

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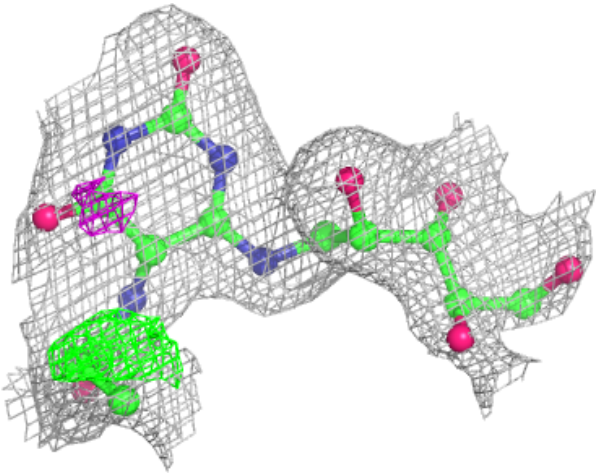
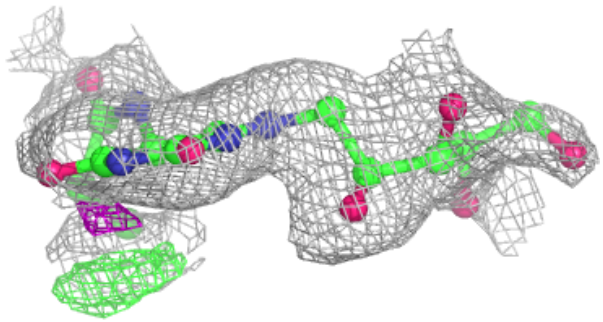
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	A	601	1/1	0.97	0.10	26,26,26,26	0
3	K	H	601	1/1	0.97	0.07	22,22,22,22	0
4	PO4	D	702	5/5	0.97	0.13	34,34,34,34	0
3	K	J	601	1/1	0.97	0.08	25,25,25,25	0
3	K	I	601	1/1	0.98	0.05	24,24,24,24	0
3	K	D	601	1/1	0.98	0.04	27,27,27,27	0
3	K	E	601	1/1	0.99	0.04	27,27,27,27	0
3	K	F	601	1/1	0.99	0.14	32,32,32,32	0

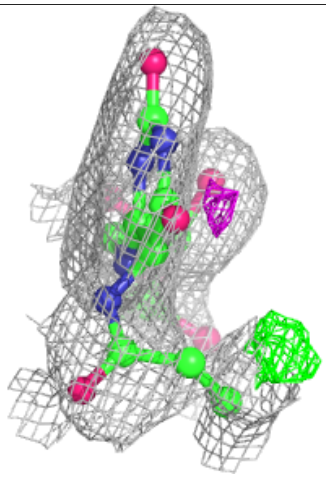
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Y19 G 201:

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

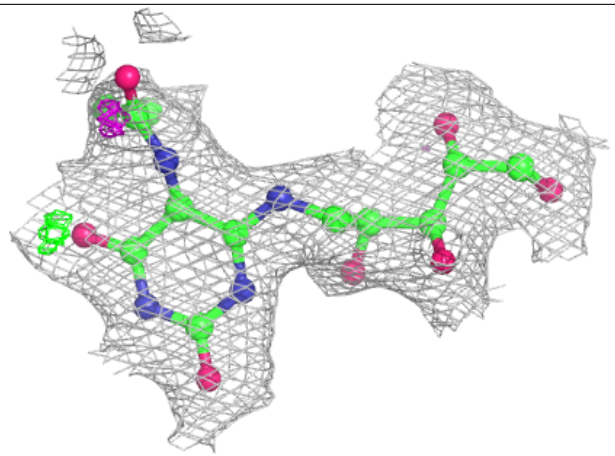


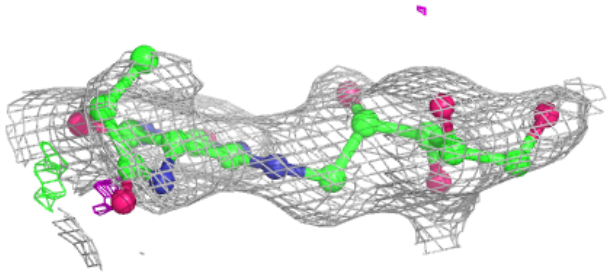


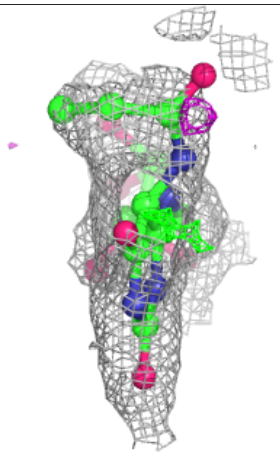


Electron density around Y19 I 201:

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

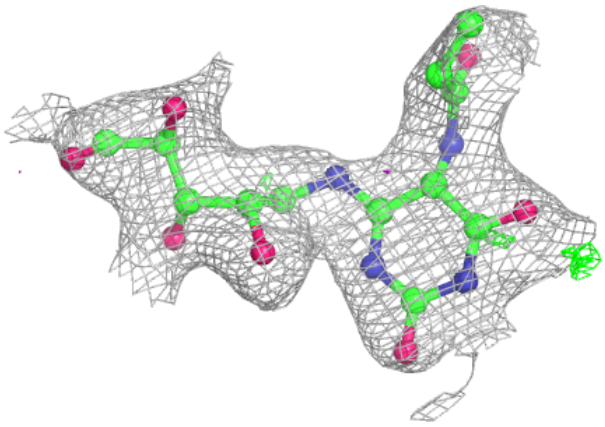


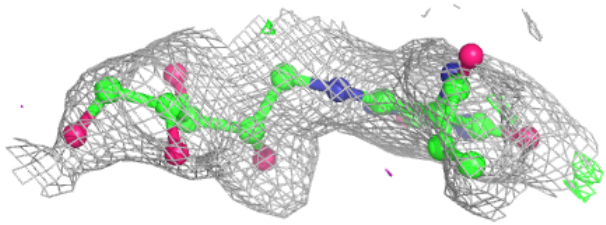


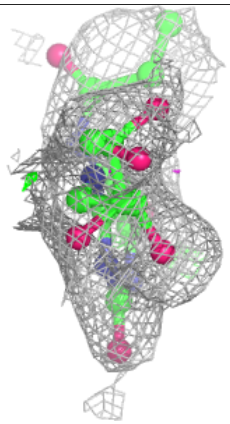


Electron density around Y19 J 201:

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

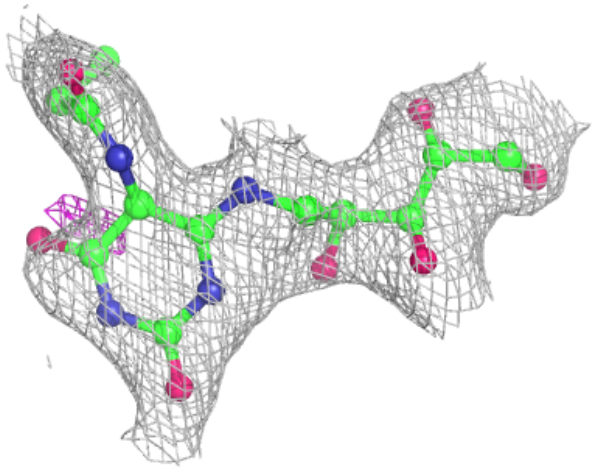


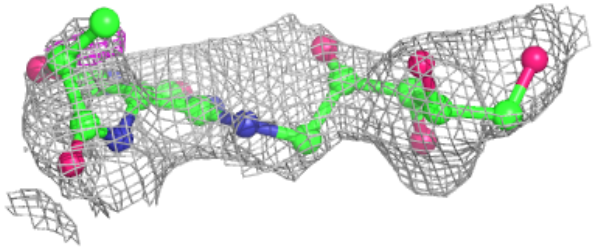


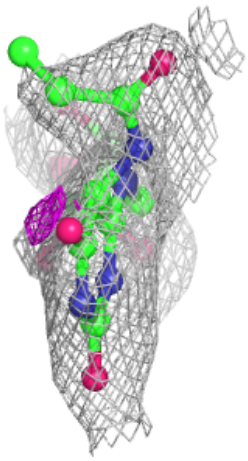


Electron density around Y19 F 201:

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

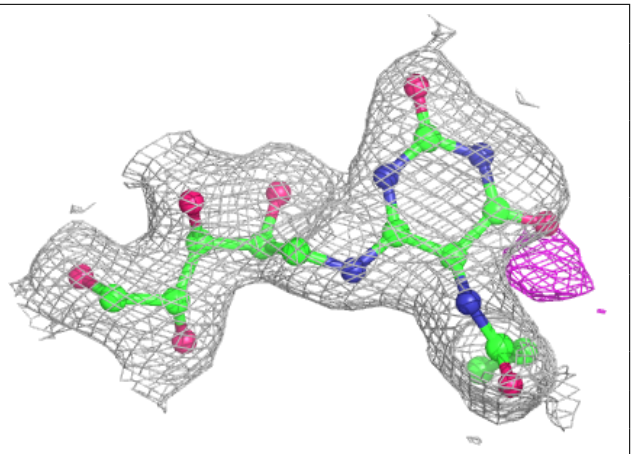


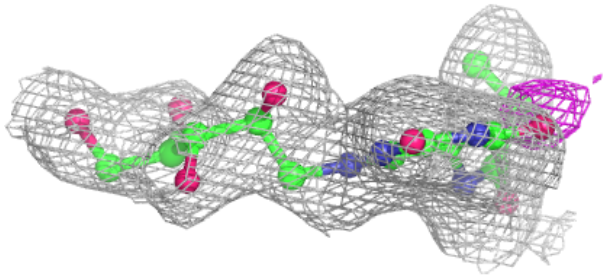


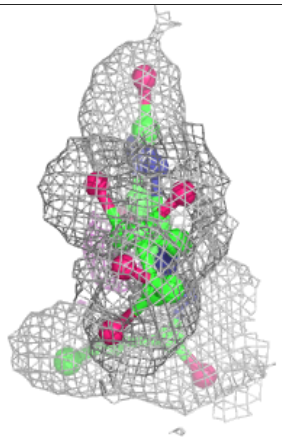


Electron density around Y19 E 201:

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

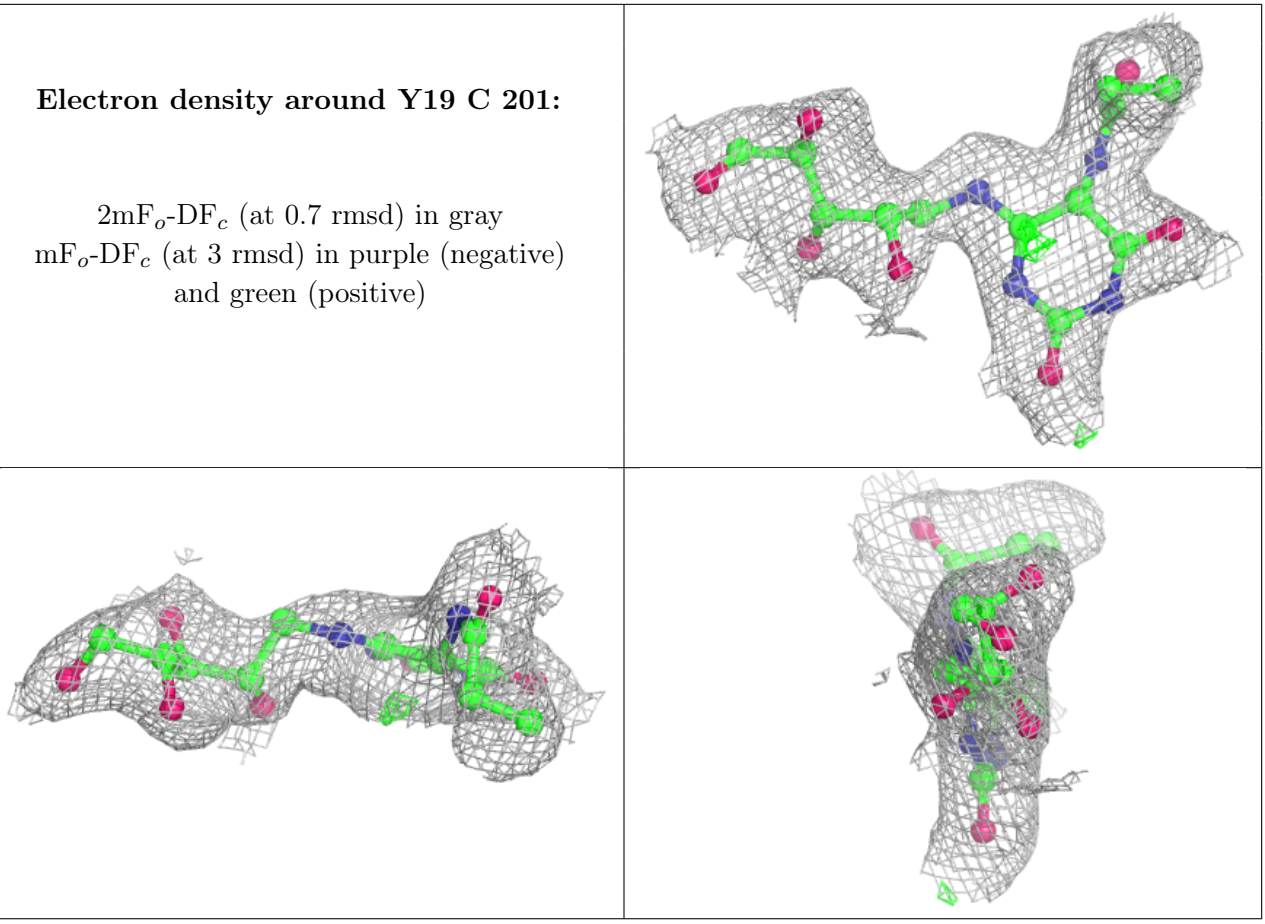






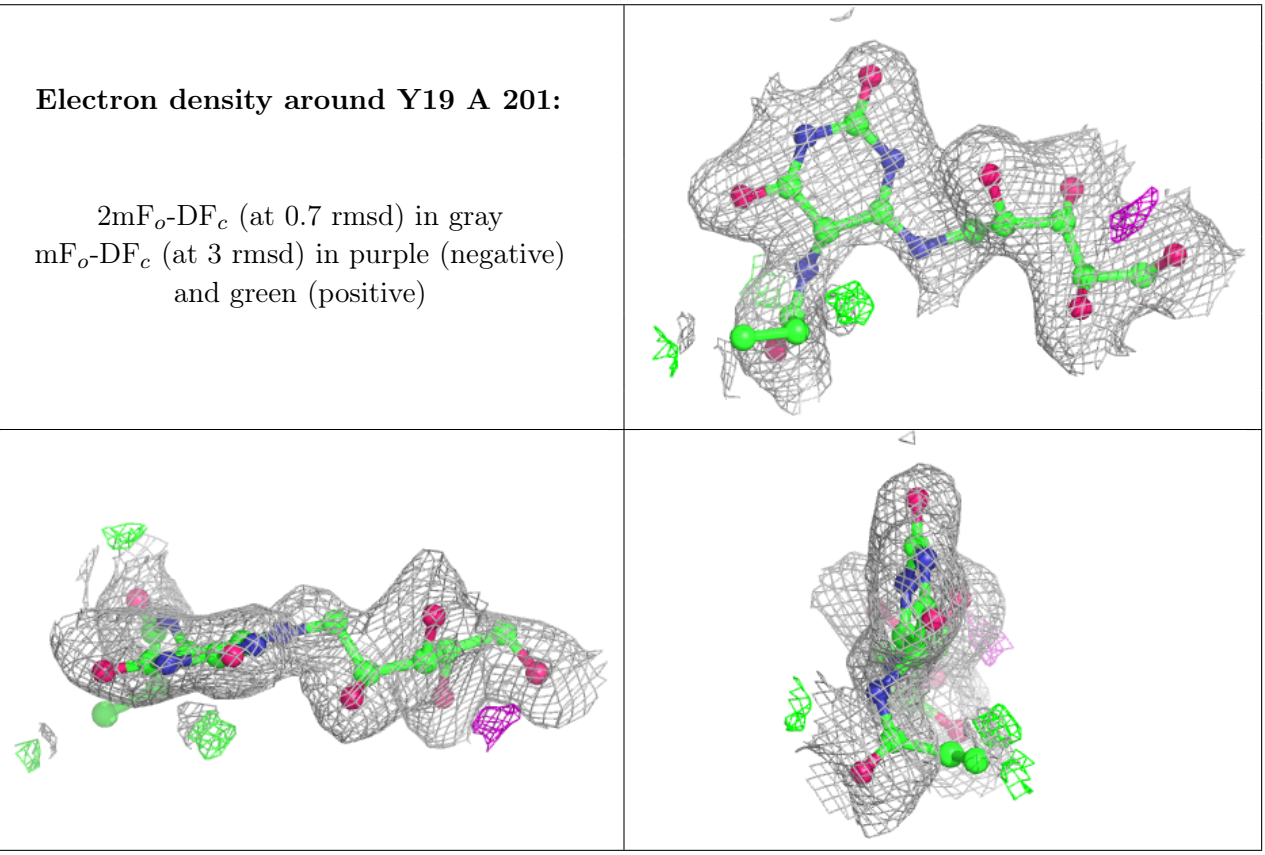
Electron density around Y19 C 201:

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



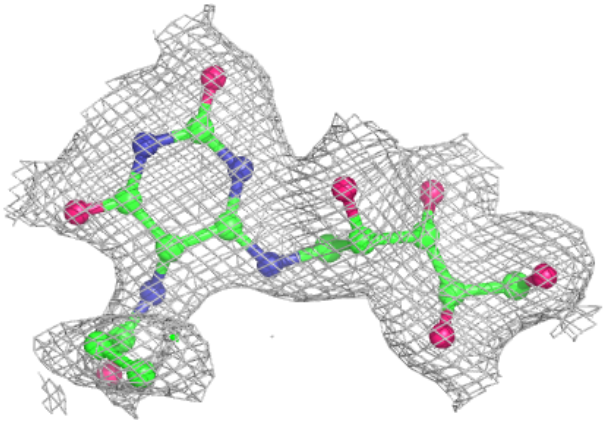
Electron density around Y19 A 201:

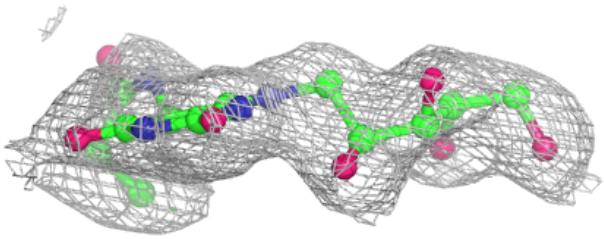
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

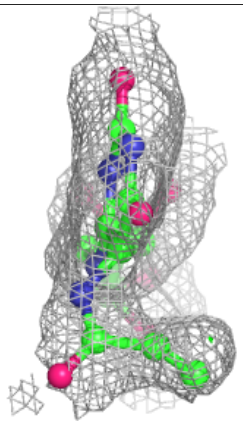


Electron density around Y19 D 201:

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

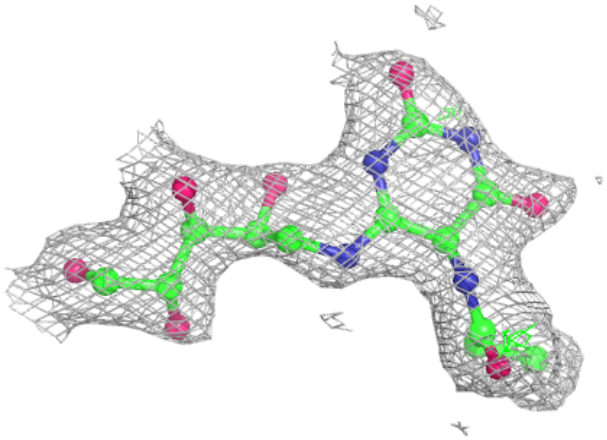


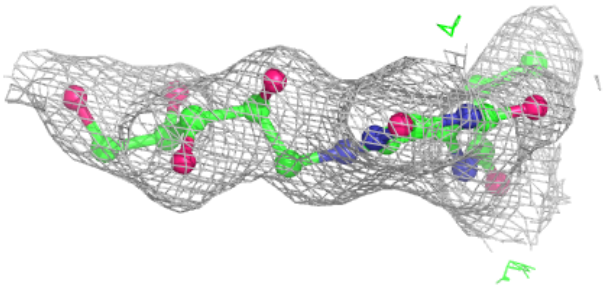




Electron density around Y19 H 201:

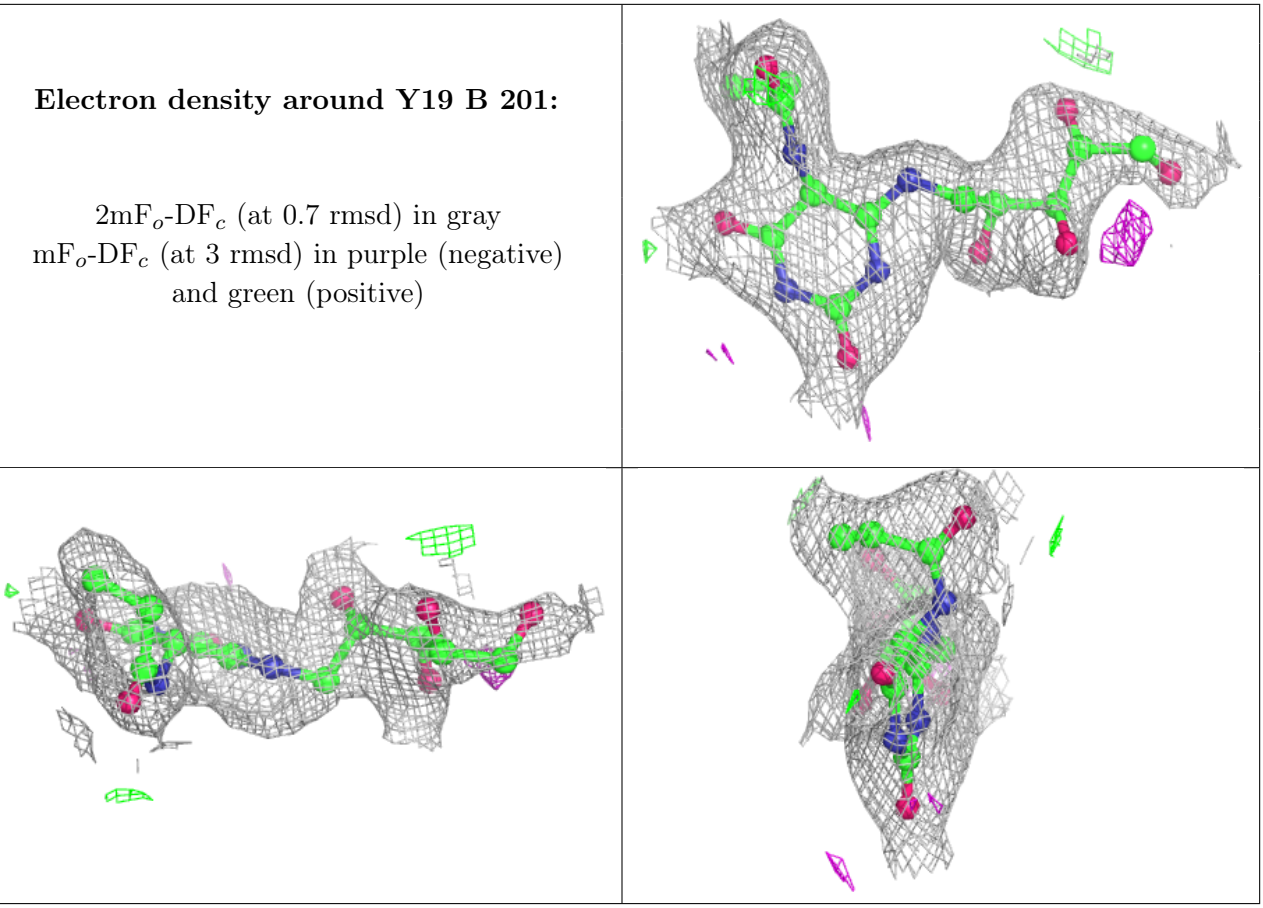
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around Y19 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)



6.5 Other polymers

There are no such residues in this entry.