



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:26 am BST

PDB ID : 3R5W  
Title : Structure of Ddn, the Deazaflavin-dependent nitroreductase from *Mycobacterium tuberculosis* involved in bioreductive activation of PA-824, with co-factor F420  
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Deposited on : 2011-03-20  
Resolution : 1.79 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](mailto: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.

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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	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

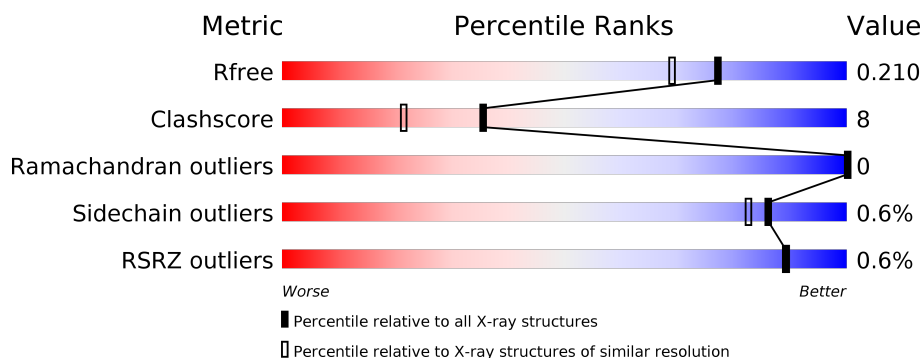
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	112	<div> <div></div> <div>87%11% .</div> </div>
1	B	112	<div> <div></div> <div>85%9% . .</div> </div>
1	C	112	<div> <div>%</div> <div>89%8% .</div> </div>
1	D	112	<div> <div></div> <div>90%7% .</div> </div>
1	E	112	<div> <div>%</div> <div>89%7% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	112	<div><div></div><div>82%13%</div><div></div></div>
1	L	112	<div><div></div><div>87%11%</div><div></div></div>
1	M	112	<div><div>%</div><div></div><div>88%10%</div><div></div></div>
1	N	112	<div><div>2%</div><div></div><div>82%15%</div><div></div></div>
1	O	112	<div><div>%</div><div></div><div>88%9%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10600 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 Deazaflavin-dependent nitroreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	1	0
			879	564	151	161	3			
1	B	109	Total	C	N	O	S	0	2	0
			885	568	151	163	3			
1	C	109	Total	C	N	O	S	0	1	0
			879	564	151	161	3			
1	D	109	Total	C	N	O	S	0	1	0
			879	564	151	161	3			
1	E	109	Total	C	N	O	S	0	0	0
			874	559	151	161	3			
1	K	109	Total	C	N	O	S	0	1	0
			879	564	151	161	3			
1	L	109	Total	C	N	O	S	0	1	0
			879	564	151	161	3			
1	M	109	Total	C	N	O	S	0	0	0
			874	559	151	161	3			
1	N	109	Total	C	N	O	S	0	1	0
			879	564	151	161	3			
1	O	109	Total	C	N	O	S	0	2	0
			883	568	151	161	3			

There are 10 discrepancies between the modelled and reference sequences:

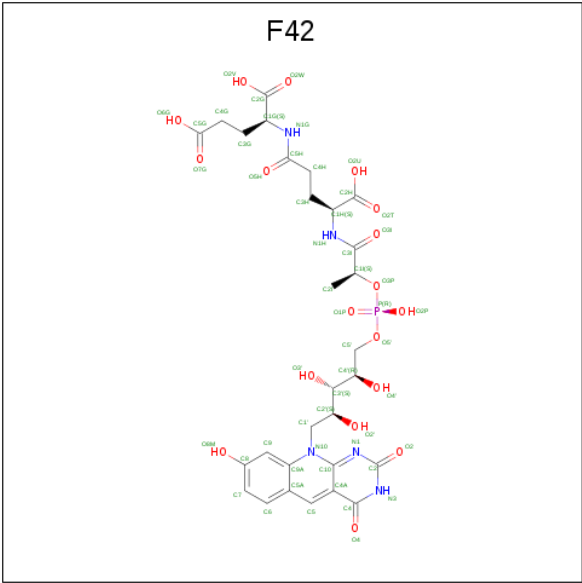
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLY	-	EXPRESSION TAG	UNP P71854
B	40	GLY	-	EXPRESSION TAG	UNP P71854
C	40	GLY	-	EXPRESSION TAG	UNP P71854
D	40	GLY	-	EXPRESSION TAG	UNP P71854
E	40	GLY	-	EXPRESSION TAG	UNP P71854
K	40	GLY	-	EXPRESSION TAG	UNP P71854
L	40	GLY	-	EXPRESSION TAG	UNP P71854
M	40	GLY	-	EXPRESSION TAG	UNP P71854
N	40	GLY	-	EXPRESSION TAG	UNP P71854

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Chain	Residue	Modelled	Actual	Comment	Reference
O	40	GLY	-	EXPRESSION TAG	UNP P71854

- Molecule 2 is COENZYME F420 (three-letter code: F42) (formula: C<sub>29</sub>H<sub>36</sub>N<sub>5</sub>O<sub>18</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	29	5	18	1	0	0
2	B	1	53	29	5	18	1	0	0
2	C	1	53	29	5	18	1	0	0
2	D	1	53	29	5	18	1	0	0
2	E	1	53	29	5	18	1	0	0
2	K	1	53	29	5	18	1	0	0
2	L	1	53	29	5	18	1	0	0
2	M	1	53	29	5	18	1	0	0
2	N	1	53	29	5	18	1	0	0
2	O	1	53	29	5	18	1	0	0


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total 137	O 137	0	0
3	B	142	Total 142	O 142	0	0
3	C	127	Total 127	O 127	0	0
3	D	123	Total 123	O 123	0	0
3	E	109	Total 109	O 109	0	0
3	K	138	Total 138	O 138	0	0
3	L	124	Total 124	O 124	0	0
3	M	148	Total 148	O 148	0	0
3	N	116	Total 116	O 116	0	0
3	O	116	Total 116	O 116	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Deazaflavin-dependent nitroreductase

Chain A:  87% 11% .




- Molecule 1: Deazaflavin-dependent nitroreductase

Chain B:  85% 9% . .



- Molecule 1: Deazaflavin-dependent nitroreductase

Chain C:  89% 8% .



- Molecule 1: Deazaflavin-dependent nitroreductase

Chain D:  90% 7% .




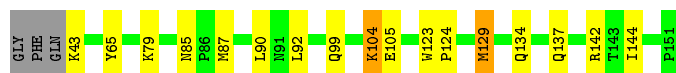
- Molecule 1: Deazaflavin-dependent nitroreductase

Chain E:  89% 7% . .




- Molecule 1: Deazaflavin-dependent nitroreductase

Chain K:  82% 13% . .




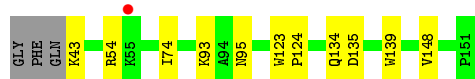
- Molecule 1: Deazaflavin-dependent nitroreductase

Chain L:  87% 11% .




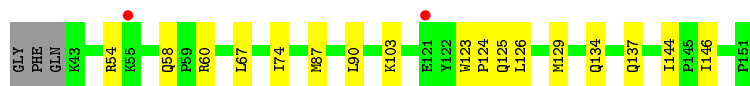
- Molecule 1: Deazaflavin-dependent nitroreductase

Chain M:  88% 10% .




- Molecule 1: Deazaflavin-dependent nitroreductase

Chain N:  82% 15% .



- Molecule 1: Deazaflavin-dependent nitroreductase

Chain O:  88% 9% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.34Å 89.42Å 127.68Å 90.00° 96.29° 90.00°	Depositor
Resolution (Å)	42.17 – 1.79 42.17 – 1.79	Depositor EDS
% Data completeness (in resolution range)	88.1 (42.17-1.79) 96.2 (42.17-1.79)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.173 , 0.206 0.178 , 0.210	Depositor DCC
$R_{free}$ test set	8674 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: F42

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	0.62	0/903	0.74	0/1231
1	B	0.62	0/912	0.81	2/1243 (0.2%)
1	C	0.63	0/903	0.72	0/1231
1	D	0.59	0/903	0.75	0/1231
1	E	0.56	0/895	0.74	0/1220
1	K	0.63	0/903	0.77	0/1231
1	L	0.60	0/903	0.72	0/1231
1	M	0.58	0/895	0.71	0/1220
1	N	0.58	0/903	0.70	0/1231
1	O	0.56	0/910	0.70	0/1241
All	All	0.60	0/9030	0.74	2/12310 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	67	LEU	CA-CB-CG	5.20	127.25	115.30

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	879	0	896	18	0
1	B	885	0	902	15	0
1	C	879	0	896	10	0
1	D	879	0	896	7	0
1	E	874	0	885	10	0
1	K	879	0	896	27	0
1	L	879	0	896	13	0
1	M	874	0	885	16	0
1	N	879	0	896	22	0
1	O	883	0	905	9	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
2	C	53	0	32	1	0
2	D	53	0	31	1	0
2	E	53	0	31	2	0
2	K	53	0	31	3	0
2	L	53	0	32	5	0
2	M	53	0	31	3	0
2	N	53	0	31	3	0
2	O	53	0	31	2	0
3	A	137	0	0	5	0
3	B	142	0	0	1	0
3	C	127	0	0	2	0
3	D	123	0	0	3	0
3	E	109	0	0	0	0
3	K	138	0	0	5	0
3	L	124	0	0	4	0
3	M	148	0	0	3	0
3	N	116	0	0	4	0
3	O	116	0	0	2	0
All	All	10600	0	9265	150	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 8.

All (150) 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:K:104:LYS:H	1:K:104:LYS:HE3	1.35	0.90
1:L:62:ASN:OD1	2:L:201:F42:H2I3	1.74	0.87
1:N:87:MET:HE3	3:N:338:HOH:O	1.78	0.83
1:K:65:TYR:HB3	1:K:129:MET:CE	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:67:LEU:HD12	1:N:129:MET:HE1	1.65	0.78
1:E:67:LEU:HD23	1:E:129:MET:HE1	1.65	0.76
1:K:87:MET:HE2	2:K:201:F42:H4G2	1.68	0.76
1:K:137:GLN:HE22	1:K:144:ILE:H	1.31	0.75
1:K:87:MET:HE3	1:K:87:MET:HA	1.70	0.74
1:M:123:TRP:HE1	1:M:134:GLN:HE22	1.34	0.73
1:L:137:GLN:HE22	1:L:144:ILE:H	1.36	0.72
1:A:87:MET:HG3	3:A:434:HOH:O	1.90	0.71
1:N:137:GLN:HE22	1:N:144:ILE:H	1.39	0.70
1:A:137:GLN:HE22	1:A:144:ILE:H	1.39	0.69
1:K:137:GLN:NE2	3:K:392:HOH:O	2.21	0.67
1:L:85:ASN:ND2	1:L:142:ARG:HH11	1.93	0.67
1:A:43:LYS:NZ	1:M:43:LYS:NZ	2.43	0.67
1:L:62:ASN:OD1	2:L:201:F42:C2I	2.44	0.65
1:B:103:LYS:HB2	1:B:104:LYS:HE3	1.77	0.64
1:K:104:LYS:HD2	1:K:105:GLU:N	2.13	0.63
1:K:87:MET:CE	1:K:90:LEU:HD12	2.28	0.63
1:C:123:TRP:HE1	1:C:134:GLN:HE22	1.45	0.62
1:D:137:GLN:HE22	1:D:144:ILE:H	1.48	0.62
1:B:103:LYS:CB	1:B:104:LYS:HE3	2.29	0.61
1:O:74[B]:ILE:HD12	1:O:148:VAL:HG22	1.84	0.59
1:A:137:GLN:NE2	3:A:309:HOH:O	2.18	0.59
1:B:85:ASN:ND2	1:B:142:ARG:HH11	2.00	0.59
1:M:93:LYS:HE2	3:M:414:HOH:O	2.03	0.59
1:C:54:ARG:NE	2:C:201:F42:O7G	2.32	0.59
1:K:87:MET:HE3	1:K:90:LEU:HD12	1.85	0.59
1:E:85:ASN:ND2	1:E:142:ARG:HH11	2.00	0.59
1:L:70:GLY:HA2	3:N:396:HOH:O	2.03	0.58
2:M:201:F42:O1P	2:M:201:F42:C2I	2.50	0.58
1:L:72:ARG:HD3	3:L:364:HOH:O	2.04	0.58
1:A:43:LYS:HZ2	1:M:43:LYS:NZ	1.98	0.58
1:N:103:LYS:HD2	3:N:362:HOH:O	2.03	0.58
1:L:65:TYR:HB3	1:L:129:MET:CE	2.34	0.57
1:B:104:LYS:HD2	1:B:105:GLU:N	2.19	0.57
1:B:67:LEU:HD13	1:B:126:LEU:HD23	1.87	0.57
1:K:104:LYS:HE3	1:K:104:LYS:N	2.14	0.57
1:K:79:LYS:HE2	3:K:394:HOH:O	2.05	0.56
1:K:65:TYR:HB3	1:K:129:MET:HE1	1.87	0.56
1:N:137:GLN:NE2	3:N:323:HOH:O	2.20	0.56
1:M:123:TRP:HE1	1:M:134:GLN:NE2	2.01	0.56
1:B:104:LYS:H	1:B:104:LYS:HE3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:43:LYS:NZ	3:K:387:HOH:O	2.39	0.55
1:M:95:ASN:HB2	3:M:403:HOH:O	2.06	0.55
1:B:104:LYS:CD	1:B:104:LYS:H	2.18	0.55
1:K:43:LYS:HD3	3:K:432:HOH:O	2.07	0.55
1:N:123:TRP:HE1	1:N:134:GLN:HE22	1.55	0.55
2:E:201:F42:O1P	2:E:201:F42:C2I	2.55	0.54
1:E:67:LEU:CD2	1:E:129:MET:HE1	2.36	0.54
1:L:85:ASN:HD22	1:L:142:ARG:NH1	2.06	0.53
1:A:123:TRP:HB3	1:A:124:PRO:HD3	1.90	0.53
1:A:85:ASN:ND2	1:A:142:ARG:HH11	2.07	0.53
1:C:123:TRP:HB3	1:C:124:PRO:HD3	1.92	0.52
2:D:201:F42:H2I2	3:D:416:HOH:O	2.07	0.52
1:K:87:MET:HE2	2:K:201:F42:C4G	2.38	0.52
1:L:85:ASN:ND2	1:L:142:ARG:NH1	2.58	0.51
1:A:43:LYS:NZ	1:M:43:LYS:HZ2	2.08	0.51
1:D:137:GLN:NE2	3:D:313:HOH:O	2.31	0.51
1:N:67:LEU:HD12	1:N:129:MET:CE	2.39	0.50
1:N:87:MET:HE2	1:N:87:MET:HA	1.93	0.50
1:C:123:TRP:HE1	1:C:134:GLN:NE2	2.08	0.50
1:L:137:GLN:NE2	3:L:330:HOH:O	2.29	0.50
1:M:54:ARG:NE	2:M:201:F42:O7G	2.40	0.50
1:M:134:GLN:NE2	3:M:416:HOH:O	2.43	0.50
1:C:43:LYS:NZ	3:C:398:HOH:O	2.46	0.49
1:K:99:GLN:NE2	3:K:416:HOH:O	2.40	0.49
1:A:123:TRP:HE1	1:A:134:GLN:HE22	1.60	0.49
1:N:67:LEU:HD21	1:N:125:GLN:HB2	1.95	0.48
1:N:123:TRP:HB3	1:N:124:PRO:HD3	1.95	0.48
1:O:85:ASN:ND2	1:O:142:ARG:HH11	2.12	0.48
1:B:65:TYR:HB3	1:B:129:MET:CE	2.43	0.48
1:K:85:ASN:ND2	1:K:142:ARG:HH11	2.11	0.48
1:K:87:MET:HA	1:K:87:MET:CE	2.41	0.47
1:K:123:TRP:HE1	1:K:134:GLN:HE22	1.62	0.47
1:B:85:ASN:HD22	1:B:142:ARG:NH1	2.12	0.47
1:A:43:LYS:HZ1	1:M:43:LYS:NZ	2.12	0.47
1:E:85:ASN:HD22	1:E:142:ARG:NH1	2.13	0.47
1:O:87:MET:HE2	3:O:338:HOH:O	2.15	0.47
1:C:74[A]:ILE:HD12	1:C:148:VAL:HG22	1.97	0.46
1:O:54:ARG:NE	2:O:201:F42:O7G	2.43	0.46
1:K:85:ASN:ND2	1:K:142:ARG:HD2	2.30	0.46
1:L:87:MET:HG3	2:L:201:F42:O2T	2.15	0.46
2:E:201:F42:O1P	2:E:201:F42:H2I3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:104:LYS:C	1:K:104:LYS:HD2	2.36	0.46
1:B:104:LYS:CE	1:B:104:LYS:H	2.28	0.45
1:A:103:LYS:HE2	3:A:345:HOH:O	2.17	0.45
1:B:77:ALA:HA	1:B:88:TRP:CZ2	2.52	0.45
1:E:61:VAL:HG12	3:O:336:HOH:O	2.17	0.45
1:K:123:TRP:HE1	1:K:134:GLN:NE2	2.14	0.45
1:L:87:MET:HG3	2:L:201:F42:H4H1	1.98	0.45
1:A:43:LYS:NZ	1:M:43:LYS:HZ1	2.12	0.45
1:M:43:LYS:HE3	1:M:43:LYS:HB2	1.72	0.45
1:C:123:TRP:CE3	1:C:146:ILE:HD11	2.53	0.44
1:O:85:ASN:ND2	1:O:142:ARG:HD2	2.32	0.44
1:N:60:ARG:HD2	2:N:201:F42:H4H2	1.99	0.44
1:N:123:TRP:HE3	1:N:146:ILE:HD11	1.82	0.44
1:N:60:ARG:HD2	2:N:201:F42:C4H	2.47	0.44
1:C:105:GLU:HG2	3:C:372:HOH:O	2.18	0.44
1:B:67:LEU:HD13	1:B:126:LEU:CD2	2.48	0.44
1:D:74[B]:ILE:HD12	1:D:148:VAL:HG22	2.00	0.44
1:C:123:TRP:HE3	1:C:146:ILE:HD11	1.82	0.43
1:B:103:LYS:HB3	1:B:104:LYS:HE3	2.00	0.43
1:M:74:ILE:HD12	1:M:148:VAL:HG22	1.99	0.43
1:M:123:TRP:HB3	1:M:124:PRO:HD3	2.00	0.43
1:M:135:ASP:HB3	1:M:139:TRP:CH2	2.53	0.43
1:A:123:TRP:HE1	1:A:134:GLN:NE2	2.16	0.43
1:E:67:LEU:CD2	1:E:129:MET:CE	2.97	0.43
1:K:123:TRP:HB3	1:K:124:PRO:HD3	2.01	0.43
2:A:201:F42:N1	2:A:201:F42:H2'	2.34	0.42
1:E:129:MET:HB2	1:E:129:MET:HE2	1.40	0.42
1:N:67:LEU:HD13	1:N:126:LEU:HD23	2.01	0.42
1:O:92:LEU:HD12	1:O:92:LEU:C	2.40	0.42
1:A:85:ASN:HD22	1:A:142:ARG:NH1	2.17	0.42
1:E:85:ASN:HD22	1:E:142:ARG:HH11	1.66	0.42
1:O:85:ASN:HD22	1:O:142:ARG:NH1	2.17	0.42
2:M:201:F42:O1P	2:M:201:F42:H2I3	2.19	0.42
1:N:123:TRP:HE1	1:N:134:GLN:NE2	2.15	0.42
2:A:201:F42:H9	2:A:201:F42:H1'1	1.80	0.42
2:B:201:F42:H1'1	2:B:201:F42:H9	1.78	0.42
1:K:87:MET:CE	2:K:201:F42:C5G	2.98	0.42
1:N:54:ARG:NE	2:N:201:F42:O7G	2.53	0.42
1:A:134:GLN:NE2	3:A:407:HOH:O	2.49	0.42
1:E:77:ALA:HA	1:E:88:TRP:CZ2	2.55	0.42
1:D:61:VAL:HG12	3:L:328:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ARG:O	3:D:303:HOH:O	2.21	0.41
1:L:123:TRP:CE3	1:L:146:ILE:HD11	2.55	0.41
1:K:104:LYS:H	1:K:104:LYS:CE	2.18	0.41
1:E:135:ASP:HB3	1:E:139:TRP:CH2	2.55	0.41
2:L:201:F42:H2I2	3:L:403:HOH:O	2.20	0.41
1:N:67:LEU:HD13	1:N:126:LEU:CD2	2.51	0.41
1:A:134:GLN:HG2	3:A:415:HOH:O	2.21	0.41
1:A:43:LYS:HZ1	1:M:43:LYS:HZ1	1.69	0.41
1:B:103:LYS:HE3	3:B:435:HOH:O	2.19	0.41
1:N:87:MET:CE	1:N:90:LEU:HD12	2.51	0.41
1:B:150:GLU:HA	1:B:151:PRO:HD3	1.86	0.41
1:K:87:MET:HE1	1:K:90:LEU:HD12	2.02	0.41
1:D:135:ASP:HB3	1:D:139:TRP:CH2	2.56	0.41
1:A:68:ARG:HD2	1:A:102:ILE:HD13	2.03	0.40
1:N:129:MET:HE2	1:N:129:MET:HB2	1.86	0.40
1:O:60:ARG:HE	2:O:201:F42:C5H	2.34	0.40
1:N:58:GLN:HA	1:N:58:GLN:NE2	2.35	0.40
1:O:77:ALA:HB3	1:O:145:PRO:HD2	2.04	0.40
1:K:92:LEU:HD12	1:K:92:LEU:C	2.42	0.40
1:N:123:TRP:CE3	1:N:146:ILE:HD11	2.56	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	108/112 (96%)	107 (99%)	1 (1%)	0	100	100
1	B	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
1	C	108/112 (96%)	107 (99%)	1 (1%)	0	100	100
1	D	108/112 (96%)	107 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	107/112 (96%)	106 (99%)	1 (1%)	0	100	100
1	K	108/112 (96%)	107 (99%)	1 (1%)	0	100	100
1	L	108/112 (96%)	107 (99%)	1 (1%)	0	100	100
1	M	107/112 (96%)	106 (99%)	1 (1%)	0	100	100
1	N	108/112 (96%)	107 (99%)	1 (1%)	0	100	100
1	O	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
All	All	1080/1120 (96%)	1070 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	96/97 (99%)	96 (100%)	0	100	100
1	B	97/97 (100%)	94 (97%)	3 (3%)	40	22
1	C	96/97 (99%)	96 (100%)	0	100	100
1	D	96/97 (99%)	96 (100%)	0	100	100
1	E	95/97 (98%)	94 (99%)	1 (1%)	73	65
1	K	96/97 (99%)	94 (98%)	2 (2%)	53	38
1	L	96/97 (99%)	96 (100%)	0	100	100
1	M	95/97 (98%)	95 (100%)	0	100	100
1	N	96/97 (99%)	96 (100%)	0	100	100
1	O	97/97 (100%)	97 (100%)	0	100	100
All	All	960/970 (99%)	954 (99%)	6 (1%)	86	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	ARG

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Mol	Chain	Res	Type
1	B	104	LYS
1	B	129	MET
1	E	129	MET
1	K	104	LYS
1	K	129	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	134	GLN
1	A	137	GLN
1	B	85	ASN
1	C	134	GLN
1	D	134	GLN
1	D	137	GLN
1	E	85	ASN
1	K	62	ASN
1	K	85	ASN
1	K	99	GLN
1	K	134	GLN
1	K	137	GLN
1	L	85	ASN
1	L	99	GLN
1	L	137	GLN
1	M	134	GLN
1	N	58	GLN
1	N	134	GLN
1	N	137	GLN
1	O	62	ASN
1	O	85	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	F42	K	201	-	42,55,55	3.37	14 (33%)	51,79,79	3.22	19 (37%)
2	F42	D	201	-	42,55,55	3.21	12 (28%)	51,79,79	3.06	15 (29%)
2	F42	M	201	-	42,55,55	3.24	12 (28%)	51,79,79	3.09	16 (31%)
2	F42	N	201	-	42,55,55	3.18	12 (28%)	51,79,79	3.12	17 (33%)
2	F42	O	201	-	42,55,55	3.21	12 (28%)	51,79,79	3.12	15 (29%)
2	F42	L	201	-	42,55,55	3.19	12 (28%)	51,79,79	3.06	20 (39%)
2	F42	A	201	-	42,55,55	3.30	14 (33%)	51,79,79	3.11	14 (27%)
2	F42	B	201	-	42,55,55	3.30	12 (28%)	51,79,79	3.06	16 (31%)
2	F42	C	201	-	42,55,55	3.27	12 (28%)	51,79,79	3.16	18 (35%)
2	F42	E	201	-	42,55,55	3.51	12 (28%)	51,79,79	3.08	17 (33%)

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	F42	K	201	-	-	8/43/53/53	0/3/3/3
2	F42	D	201	-	-	3/43/53/53	0/3/3/3
2	F42	M	201	-	-	8/43/53/53	0/3/3/3
2	F42	N	201	-	-	12/43/53/53	0/3/3/3
2	F42	O	201	-	-	8/43/53/53	0/3/3/3
2	F42	L	201	-	-	9/43/53/53	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	F42	A	201	-	-	3/43/53/53	0/3/3/3
2	F42	B	201	-	-	7/43/53/53	0/3/3/3
2	F42	C	201	-	-	7/43/53/53	0/3/3/3
2	F42	E	201	-	-	11/43/53/53	0/3/3/3

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	201	F42	C10-N1	-11.06	1.33	1.46
2	C	201	F42	C10-N1	-10.51	1.33	1.46
2	B	201	F42	C10-N1	-10.49	1.33	1.46
2	E	201	F42	C10-N1	-10.45	1.33	1.46
2	A	201	F42	C10-N1	-10.37	1.34	1.46
2	M	201	F42	C10-N1	-10.23	1.34	1.46
2	E	201	F42	C5-C4A	-10.06	1.38	1.53
2	D	201	F42	C10-N1	-9.40	1.35	1.46
2	C	201	F42	C5-C4A	-9.34	1.39	1.53
2	O	201	F42	C10-N1	-9.34	1.35	1.46
2	N	201	F42	C5-C4A	-9.34	1.39	1.53
2	D	201	F42	C5-C4A	-9.24	1.40	1.53
2	L	201	F42	C10-N1	-9.09	1.35	1.46
2	N	201	F42	C10-N1	-9.03	1.35	1.46
2	A	201	F42	C5-C4A	-8.49	1.41	1.53
2	O	201	F42	C5-C4A	-8.42	1.41	1.53
2	M	201	F42	C5-C4A	-8.41	1.41	1.53
2	L	201	F42	C5-C4A	-8.14	1.41	1.53
2	K	201	F42	C5-C4A	-7.75	1.42	1.53
2	B	201	F42	C5-C4A	-7.63	1.42	1.53
2	E	201	F42	C9-C9A	-7.51	1.37	1.53
2	A	201	F42	C5A-C9A	-7.32	1.39	1.53
2	K	201	F42	C5A-C9A	-7.22	1.39	1.53
2	B	201	F42	C5A-C9A	-7.07	1.39	1.53
2	L	201	F42	C5A-C9A	-6.98	1.39	1.53
2	O	201	F42	C9-C8	-6.97	1.39	1.51
2	D	201	F42	C5A-C9A	-6.91	1.39	1.53
2	E	201	F42	C9-C8	-6.86	1.39	1.51
2	M	201	F42	C9-C8	-6.67	1.39	1.51
2	N	201	F42	C5A-C9A	-6.61	1.40	1.53
2	B	201	F42	C9-C9A	-6.58	1.39	1.53
2	M	201	F42	C5A-C9A	-6.55	1.40	1.53
2	K	201	F42	C9-C8	-6.50	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	F42	C9-C8	-6.41	1.40	1.51
2	O	201	F42	C9-C9A	-6.32	1.40	1.53
2	E	201	F42	C5A-C9A	-6.30	1.41	1.53
2	C	201	F42	C5A-C9A	-6.23	1.41	1.53
2	O	201	F42	C5A-C9A	-6.22	1.41	1.53
2	C	201	F42	C9-C8	-6.21	1.40	1.51
2	D	201	F42	C9-C8	-6.17	1.40	1.51
2	L	201	F42	C9-C8	-6.06	1.40	1.51
2	E	201	F42	C7-C6	-6.04	1.37	1.52
2	D	201	F42	C9-C9A	-6.02	1.40	1.53
2	M	201	F42	C9-C9A	-5.93	1.40	1.53
2	N	201	F42	C9-C8	-5.93	1.41	1.51
2	C	201	F42	C9-C9A	-5.88	1.40	1.53
2	A	201	F42	C9-C8	-5.86	1.41	1.51
2	L	201	F42	C9-C9A	-5.83	1.41	1.53
2	K	201	F42	C9-C9A	-5.82	1.41	1.53
2	E	201	F42	C5-C5A	-5.72	1.40	1.53
2	A	201	F42	C9-C9A	-5.69	1.41	1.53
2	N	201	F42	C9-C9A	-5.68	1.41	1.53
2	A	201	F42	C7-C8	-5.59	1.38	1.51
2	O	201	F42	C6-C5A	-5.50	1.40	1.53
2	B	201	F42	C7-C8	-5.49	1.38	1.51
2	O	201	F42	C5-C5A	-5.46	1.40	1.53
2	L	201	F42	C7-C8	-5.38	1.38	1.51
2	A	201	F42	C6-C5A	-5.38	1.40	1.53
2	D	201	F42	C7-C8	-5.36	1.38	1.51
2	B	201	F42	C7-C6	-5.30	1.39	1.52
2	O	201	F42	C7-C6	-5.29	1.39	1.52
2	N	201	F42	C7-C8	-5.26	1.39	1.51
2	M	201	F42	C7-C8	-5.26	1.39	1.51
2	E	201	F42	C6-C5A	-5.20	1.40	1.53
2	E	201	F42	C7-C8	-5.20	1.39	1.51
2	L	201	F42	C7-C6	-5.19	1.39	1.52
2	C	201	F42	C7-C6	-5.19	1.40	1.52
2	K	201	F42	C6-C5A	-5.18	1.40	1.53
2	K	201	F42	C9A-N10	-5.17	1.39	1.48
2	M	201	F42	C7-C6	-5.17	1.40	1.52
2	N	201	F42	C6-C5A	-5.17	1.40	1.53
2	C	201	F42	C6-C5A	-5.12	1.40	1.53
2	N	201	F42	C7-C6	-5.12	1.40	1.52
2	A	201	F42	C7-C6	-5.12	1.40	1.52
2	K	201	F42	C7-C6	-5.11	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	F42	C5-C5A	-5.08	1.41	1.53
2	B	201	F42	C5-C5A	-5.06	1.41	1.53
2	D	201	F42	C6-C5A	-5.03	1.41	1.53
2	M	201	F42	C6-C5A	-5.03	1.41	1.53
2	N	201	F42	C5-C5A	-5.02	1.41	1.53
2	K	201	F42	C7-C8	-4.98	1.39	1.51
2	M	201	F42	C5-C5A	-4.95	1.41	1.53
2	D	201	F42	C7-C6	-4.89	1.40	1.52
2	K	201	F42	C5-C5A	-4.88	1.42	1.53
2	O	201	F42	C7-C8	-4.80	1.40	1.51
2	L	201	F42	C5-C5A	-4.78	1.42	1.53
2	B	201	F42	C6-C5A	-4.72	1.41	1.53
2	L	201	F42	C6-C5A	-4.68	1.42	1.53
2	C	201	F42	C7-C8	-4.63	1.40	1.51
2	A	201	F42	C9A-N10	-4.51	1.40	1.48
2	A	201	F42	C5-C5A	-4.49	1.42	1.53
2	D	201	F42	C5-C5A	-4.41	1.43	1.53
2	L	201	F42	C9A-N10	-4.27	1.40	1.48
2	C	201	F42	C9A-N10	-4.10	1.40	1.48
2	E	201	F42	C9A-N10	-4.02	1.41	1.48
2	L	201	F42	C4A-C4	-3.96	1.45	1.51
2	B	201	F42	C9A-N10	-3.93	1.41	1.48
2	N	201	F42	C9A-N10	-3.62	1.41	1.48
2	O	201	F42	C9A-N10	-3.50	1.42	1.48
2	D	201	F42	C9A-N10	-3.47	1.42	1.48
2	M	201	F42	C9A-N10	-3.41	1.42	1.48
2	K	201	F42	C4A-C4	-3.26	1.46	1.51
2	D	201	F42	C4A-C4	-2.91	1.47	1.51
2	B	201	F42	O8M-C8	-2.84	1.34	1.43
2	E	201	F42	C4A-C4	-2.70	1.47	1.51
2	N	201	F42	C4A-C4	-2.60	1.47	1.51
2	K	201	F42	O8M-C8	-2.59	1.35	1.43
2	B	201	F42	C4-N3	-2.59	1.32	1.37
2	M	201	F42	O8M-C8	-2.57	1.35	1.43
2	E	201	F42	O8M-C8	-2.55	1.35	1.43
2	O	201	F42	O8M-C8	-2.50	1.35	1.43
2	K	201	F42	C4-N3	-2.49	1.33	1.37
2	O	201	F42	C4A-C4	-2.40	1.47	1.51
2	M	201	F42	C1'-C2'	2.38	1.56	1.52
2	A	201	F42	O8M-C8	-2.30	1.36	1.43
2	D	201	F42	O8M-C8	-2.24	1.36	1.43
2	N	201	F42	O8M-C8	-2.24	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	F42	C2-N3	-2.18	1.33	1.37
2	A	201	F42	C4A-C4	-2.15	1.48	1.51
2	K	201	F42	C1'-C2'	2.15	1.55	1.52
2	A	201	F42	C4-N3	-2.12	1.33	1.37
2	C	201	F42	O8M-C8	-2.11	1.37	1.43
2	A	201	F42	C2-N3	-2.11	1.33	1.37
2	C	201	F42	C4A-C4	-2.03	1.48	1.51

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	F42	C5-C4A-C10	12.30	123.04	107.74
2	K	201	F42	C5-C4A-C10	11.57	122.13	107.74
2	O	201	F42	C5-C4A-C10	11.49	122.03	107.74
2	N	201	F42	C5-C4A-C10	11.46	121.99	107.74
2	C	201	F42	C5-C4A-C10	10.64	120.97	107.74
2	M	201	F42	C5-C4A-C10	10.33	120.58	107.74
2	D	201	F42	C5-C4A-C10	10.31	120.56	107.74
2	E	201	F42	C9-C8-C7	9.90	122.38	110.55
2	C	201	F42	C9-C8-C7	9.89	122.36	110.55
2	O	201	F42	C9-C8-C7	9.84	122.30	110.55
2	K	201	F42	C9-C8-C7	9.74	122.18	110.55
2	B	201	F42	C5-C4A-C10	9.68	119.77	107.74
2	L	201	F42	C5-C4A-C10	9.59	119.66	107.74
2	N	201	F42	C9-C8-C7	9.41	121.79	110.55
2	M	201	F42	C9-C8-C7	9.36	121.73	110.55
2	B	201	F42	C9-C8-C7	9.28	121.63	110.55
2	D	201	F42	C5-C5A-C9A	9.13	122.58	110.04
2	E	201	F42	C5-C4A-C10	8.95	118.86	107.74
2	A	201	F42	C9-C8-C7	8.82	121.08	110.55
2	M	201	F42	C5-C5A-C9A	8.34	121.49	110.04
2	L	201	F42	C5-C5A-C9A	8.26	121.38	110.04
2	A	201	F42	C5-C5A-C9A	8.23	121.34	110.04
2	L	201	F42	C9-C8-C7	8.06	120.18	110.55
2	E	201	F42	C5-C5A-C9A	8.01	121.04	110.04
2	C	201	F42	C5-C5A-C9A	7.89	120.87	110.04
2	O	201	F42	C5-C5A-C9A	7.52	120.37	110.04
2	D	201	F42	C9-C8-C7	7.50	119.51	110.55
2	N	201	F42	C5-C5A-C9A	7.39	120.18	110.04
2	K	201	F42	C5-C5A-C9A	7.16	119.87	110.04
2	L	201	F42	C5-C4A-C4	7.12	125.60	111.13
2	B	201	F42	C5-C5A-C9A	7.03	119.70	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	F42	N3-C2-N1	6.88	123.36	116.12
2	K	201	F42	N3-C2-N1	6.76	123.23	116.12
2	E	201	F42	C5-C4A-C4	6.70	124.74	111.13
2	B	201	F42	C5-C4A-C4	6.53	124.40	111.13
2	C	201	F42	C5-C4A-C4	6.33	123.99	111.13
2	M	201	F42	N3-C2-N1	6.31	122.76	116.12
2	D	201	F42	C5-C4A-C4	6.15	123.62	111.13
2	C	201	F42	N3-C2-N1	6.09	122.53	116.12
2	M	201	F42	C5-C4A-C4	5.99	123.30	111.13
2	L	201	F42	C6-C7-C8	5.91	121.70	111.61
2	N	201	F42	C5-C4A-C4	5.70	122.70	111.13
2	O	201	F42	C5-C4A-C4	5.68	122.67	111.13
2	A	201	F42	C5-C4A-C4	5.65	122.61	111.13
2	E	201	F42	N3-C2-N1	5.56	121.97	116.12
2	D	201	F42	O8M-C8-C9	5.50	120.80	109.85
2	K	201	F42	C5-C4A-C4	5.40	122.11	111.13
2	E	201	F42	C6-C7-C8	5.34	120.72	111.61
2	D	201	F42	N3-C2-N1	5.26	121.66	116.12
2	D	201	F42	C6-C7-C8	5.25	120.57	111.61
2	B	201	F42	C6-C7-C8	5.03	120.20	111.61
2	O	201	F42	N3-C2-N1	5.02	121.40	116.12
2	A	201	F42	O8M-C8-C9	4.92	119.65	109.85
2	A	201	F42	C6-C7-C8	4.89	119.96	111.61
2	N	201	F42	C6-C7-C8	4.87	119.93	111.61
2	N	201	F42	N3-C2-N1	4.87	121.24	116.12
2	O	201	F42	C6-C7-C8	4.79	119.79	111.61
2	N	201	F42	O8M-C8-C9	4.69	119.19	109.85
2	M	201	F42	C6-C7-C8	4.58	119.44	111.61
2	L	201	F42	O8M-C8-C7	4.43	121.44	110.16
2	K	201	F42	O8M-C8-C9	4.38	118.57	109.85
2	B	201	F42	C5-C5A-C6	4.32	120.56	112.66
2	L	201	F42	O8M-C8-C9	4.28	118.37	109.85
2	C	201	F42	C6-C7-C8	4.25	118.87	111.61
2	B	201	F42	O8M-C8-C9	4.22	118.25	109.85
2	L	201	F42	N3-C2-N1	4.19	120.53	116.12
2	C	201	F42	O8M-C8-C9	4.17	118.16	109.85
2	K	201	F42	C7-C6-C5A	4.13	121.54	112.24
2	M	201	F42	O8M-C8-C7	4.11	120.64	110.16
2	K	201	F42	O2-C2-N1	-4.08	114.79	122.92
2	E	201	F42	C6-C5A-C9A	4.01	120.67	109.73
2	E	201	F42	O8M-C8-C9	3.98	117.78	109.85
2	K	201	F42	C5-C5A-C6	3.98	119.92	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	201	F42	C6-C5A-C9A	3.97	120.57	109.73
2	O	201	F42	O8M-C8-C9	3.96	117.73	109.85
2	C	201	F42	C6-C5A-C9A	3.96	120.53	109.73
2	M	201	F42	O8M-C8-C9	3.90	117.61	109.85
2	B	201	F42	O8M-C8-C7	3.90	120.09	110.16
2	O	201	F42	C6-C5A-C9A	3.86	120.28	109.73
2	O	201	F42	O8M-C8-C7	3.85	119.97	110.16
2	K	201	F42	C6-C5A-C9A	3.83	120.19	109.73
2	E	201	F42	O8M-C8-C7	3.80	119.84	110.16
2	E	201	F42	C4-N3-C2	-3.78	121.19	126.25
2	D	201	F42	O8M-C8-C7	3.74	119.68	110.16
2	C	201	F42	O8M-C8-C7	3.66	119.48	110.16
2	O	201	F42	C5-C5A-C6	3.66	119.34	112.66
2	B	201	F42	C6-C5A-C9A	3.65	119.70	109.73
2	D	201	F42	C7-C6-C5A	3.63	120.42	112.24
2	A	201	F42	C6-C5A-C9A	3.63	119.64	109.73
2	E	201	F42	O2-C2-N1	-3.63	115.69	122.92
2	A	201	F42	N3-C2-N1	3.63	119.94	116.12
2	L	201	F42	C5-C5A-C6	3.62	119.27	112.66
2	N	201	F42	C5-C5A-C6	3.60	119.24	112.66
2	M	201	F42	C6-C5A-C9A	3.57	119.48	109.73
2	K	201	F42	O8M-C8-C7	3.56	119.23	110.16
2	A	201	F42	O8M-C8-C7	3.54	119.17	110.16
2	A	201	F42	C7-C6-C5A	3.51	120.14	112.24
2	L	201	F42	C6-C5A-C9A	3.51	119.31	109.73
2	M	201	F42	C7-C6-C5A	3.50	120.11	112.24
2	A	201	F42	C5-C5A-C6	3.48	119.02	112.66
2	N	201	F42	O8M-C8-C7	3.48	119.01	110.16
2	M	201	F42	C5-C5A-C6	3.47	119.01	112.66
2	C	201	F42	C7-C6-C5A	3.42	119.95	112.24
2	D	201	F42	C5-C5A-C6	3.38	118.83	112.66
2	K	201	F42	C6-C7-C8	3.36	117.35	111.61
2	N	201	F42	O3P-C1I-C3I	-3.36	100.03	108.99
2	A	201	F42	O4-C4-C4A	-3.34	116.31	122.04
2	C	201	F42	C4-N3-C2	-3.25	121.90	126.25
2	C	201	F42	C5-C5A-C6	3.25	118.59	112.66
2	D	201	F42	C6-C5A-C9A	3.25	118.59	109.73
2	B	201	F42	C4-N3-C2	-3.23	121.93	126.25
2	C	201	F42	O2-C2-N1	-3.22	116.50	122.92
2	N	201	F42	C7-C6-C5A	3.16	119.36	112.24
2	K	201	F42	O4-C4-C4A	-3.08	116.75	122.04
2	E	201	F42	C5-C5A-C6	3.08	118.29	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	201	F42	O2-C2-N1	-3.06	116.82	122.92
2	E	201	F42	C4A-C5-C5A	3.02	119.99	109.93
2	O	201	F42	C7-C6-C5A	3.00	119.00	112.24
2	B	201	F42	C7-C6-C5A	2.99	118.97	112.24
2	O	201	F42	O2-C2-N1	-2.99	116.97	122.92
2	N	201	F42	C4-N3-C2	-2.93	122.33	126.25
2	L	201	F42	C7-C6-C5A	2.90	118.78	112.24
2	K	201	F42	C4-N3-C2	-2.90	122.38	126.25
2	O	201	F42	O4-C4-C4A	-2.85	117.15	122.04
2	B	201	F42	C4A-C5-C5A	2.80	119.25	109.93
2	L	201	F42	C2I-C1I-C3I	-2.77	104.25	111.11
2	L	201	F42	C1H-N1H-C3I	-2.76	119.05	123.19
2	L	201	F42	C3H-C1H-N1H	2.74	114.19	110.19
2	D	201	F42	C9-C9A-N10	2.68	118.86	113.83
2	L	201	F42	C4A-C5-C5A	2.68	118.85	109.93
2	N	201	F42	O2-C2-N1	-2.68	117.58	122.92
2	N	201	F42	O4-C4-C4A	-2.68	117.44	122.04
2	K	201	F42	C4H-C3H-C1H	-2.67	106.81	113.41
2	D	201	F42	C4-N3-C2	-2.66	122.69	126.25
2	L	201	F42	C9-C9A-N10	2.66	118.81	113.83
2	D	201	F42	O2-C2-N1	-2.64	117.65	122.92
2	O	201	F42	C4-N3-C2	-2.64	122.72	126.25
2	B	201	F42	C3H-C4H-C5H	-2.63	107.17	113.04
2	L	201	F42	O4-C4-C4A	-2.53	117.70	122.04
2	C	201	F42	O4-C4-C4A	-2.47	117.80	122.04
2	K	201	F42	O4-C4-N3	2.46	125.39	121.01
2	E	201	F42	C7-C6-C5A	2.43	117.70	112.24
2	C	201	F42	O5H-C5H-C4H	-2.42	117.58	122.02
2	C	201	F42	C4A-C5-C5A	2.40	117.92	109.93
2	C	201	F42	C4G-C3G-C1G	-2.38	108.22	113.04
2	N	201	F42	C4A-C5-C5A	2.36	117.77	109.93
2	N	201	F42	O2P-P-O3P	2.35	116.06	106.78
2	A	201	F42	O4-C4-N3	2.34	125.18	121.01
2	A	201	F42	O2-C2-N1	-2.33	118.28	122.92
2	M	201	F42	C3H-C4H-C5H	-2.32	107.86	113.04
2	O	201	F42	C4A-C5-C5A	2.31	117.62	109.93
2	B	201	F42	O2-C2-N1	-2.31	118.31	122.92
2	K	201	F42	O5H-C5H-C4H	-2.31	117.80	122.02
2	C	201	F42	C9-C9A-N10	2.28	118.11	113.83
2	M	201	F42	C4A-C5-C5A	2.20	117.26	109.93
2	E	201	F42	O4-C4-C4A	-2.20	118.26	122.04
2	D	201	F42	C4A-C5-C5A	2.20	117.25	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	F42	C2I-C1I-C3I	-2.13	105.85	111.11
2	K	201	F42	C3G-C4G-C5G	-2.12	109.04	113.59
2	L	201	F42	O2-C2-N1	-2.09	118.75	122.92
2	E	201	F42	C9-C9A-N10	2.08	117.73	113.83
2	L	201	F42	C4-N3-C2	-2.06	123.50	126.25
2	B	201	F42	O5H-C5H-C4H	-2.03	118.30	122.02
2	M	201	F42	C4-N3-C2	-2.03	123.54	126.25
2	K	201	F42	C4A-C5-C5A	2.02	116.65	109.93
2	M	201	F42	C1H-N1H-C3I	-2.02	120.17	123.19
2	L	201	F42	O3P-C1I-C3I	2.00	114.34	108.99

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	201	F42	C2H-C1H-C3H-C4H
2	D	201	F42	C2H-C1H-C3H-C4H
2	M	201	F42	C2I-C1I-O3P-P
2	M	201	F42	C1I-C3I-N1H-C1H
2	M	201	F42	C2H-C1H-C3H-C4H
2	N	201	F42	C1I-O3P-P-O2P
2	N	201	F42	C2H-C1H-C3H-C4H
2	O	201	F42	C2H-C1H-C3H-C4H
2	L	201	F42	C2I-C1I-O3P-P
2	L	201	F42	C2H-C1H-N1H-C3I
2	L	201	F42	C3H-C1H-N1H-C3I
2	L	201	F42	C4H-C5H-N1G-C1G
2	B	201	F42	C2H-C1H-C3H-C4H
2	C	201	F42	C2H-C1H-C3H-C4H
2	E	201	F42	C2I-C1I-O3P-P
2	E	201	F42	C1I-C3I-N1H-C1H
2	E	201	F42	C2H-C1H-N1H-C3I
2	E	201	F42	C2H-C1H-C3H-C4H
2	E	201	F42	C4H-C5H-N1G-C1G
2	L	201	F42	O5H-C5H-N1G-C1G
2	M	201	F42	O3I-C3I-N1H-C1H
2	E	201	F42	O3I-C3I-N1H-C1H
2	E	201	F42	O5H-C5H-N1G-C1G
2	D	201	F42	N1H-C1H-C3H-C4H
2	N	201	F42	N1H-C1H-C3H-C4H
2	B	201	F42	N1H-C1H-C3H-C4H
2	K	201	F42	C1I-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
2	O	201	F42	C1I-O3P-P-O5'
2	B	201	F42	C1I-O3P-P-O5'
2	C	201	F42	C1I-O3P-P-O5'
2	K	201	F42	N1H-C1H-C3H-C4H
2	O	201	F42	N1H-C1H-C3H-C4H
2	C	201	F42	N1H-C1H-C3H-C4H
2	N	201	F42	O5H-C5H-N1G-C1G
2	N	201	F42	C4H-C5H-N1G-C1G
2	N	201	F42	C1I-O3P-P-O5'
2	M	201	F42	N1H-C1H-C3H-C4H
2	C	201	F42	C3H-C4H-C5H-O5H
2	N	201	F42	C3H-C4H-C5H-O5H
2	E	201	F42	C3H-C1H-N1H-C3I
2	M	201	F42	C2'-C1'-N10-C9A
2	O	201	F42	C2'-C1'-N10-C9A
2	M	201	F42	C1I-O3P-P-O5'
2	C	201	F42	C3H-C4H-C5H-N1G
2	K	201	F42	C1I-O3P-P-O1P
2	N	201	F42	C1I-O3P-P-O1P
2	O	201	F42	C1I-O3P-P-O1P
2	B	201	F42	C1I-O3P-P-O1P
2	C	201	F42	C1I-O3P-P-O1P
2	N	201	F42	C3H-C4H-C5H-N1G
2	E	201	F42	C1I-O3P-P-O5'
2	N	201	F42	N1G-C1G-C3G-C4G
2	O	201	F42	C3H-C4H-C5H-O5H
2	L	201	F42	C1I-O3P-P-O5'
2	N	201	F42	O3P-C1I-C3I-N1H
2	O	201	F42	C3H-C4H-C5H-N1G
2	K	201	F42	C3H-C4H-C5H-O5H
2	L	201	F42	C3H-C4H-C5H-O5H
2	K	201	F42	C2'-C1'-N10-C9A
2	D	201	F42	C2'-C1'-N10-C9A
2	N	201	F42	C2'-C1'-N10-C9A
2	L	201	F42	C2'-C1'-N10-C9A
2	A	201	F42	C2'-C1'-N10-C9A
2	B	201	F42	C2'-C1'-N10-C9A
2	C	201	F42	C2'-C1'-N10-C9A
2	E	201	F42	C2'-C1'-N10-C9A
2	A	201	F42	O5H-C5H-N1G-C1G
2	K	201	F42	C1I-O3P-P-O2P
2	O	201	F42	C1I-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	K	201	F42	C3H-C4H-C5H-N1G
2	B	201	F42	C3H-C4H-C5H-O5H
2	E	201	F42	N1H-C1H-C3H-C4H
2	L	201	F42	C3H-C4H-C5H-N1G
2	B	201	F42	C3H-C4H-C5H-N1G
2	A	201	F42	N1H-C1H-C3H-C4H
2	M	201	F42	C3H-C4H-C5H-O5H

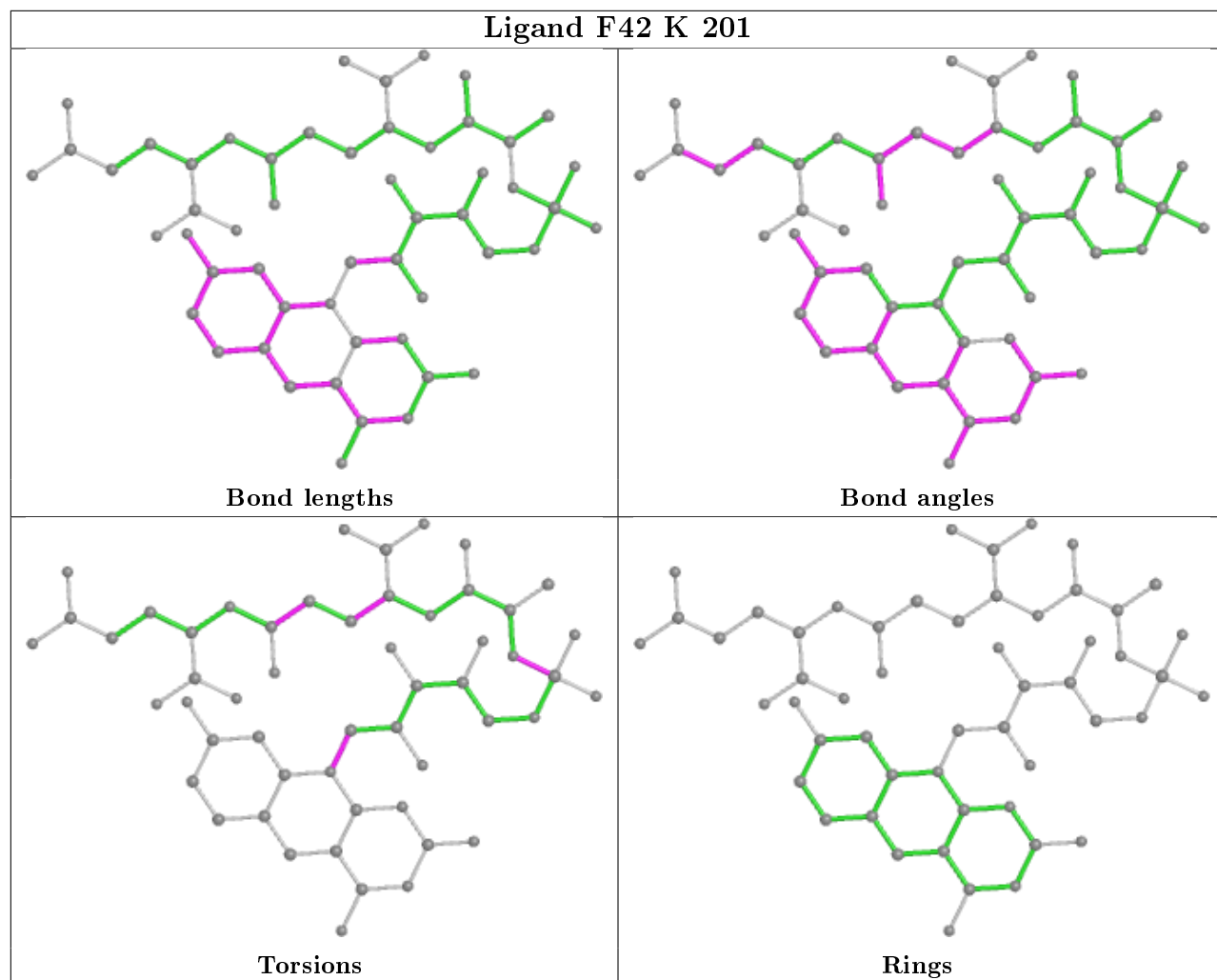
There are no ring outliers.

10 monomers are involved in 23 short contacts:

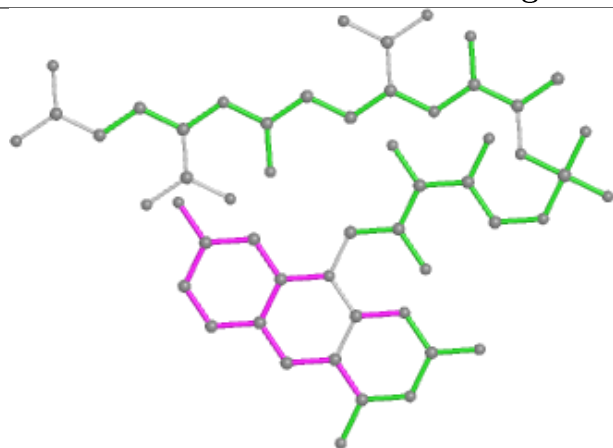
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	201	F42	3	0
2	D	201	F42	1	0
2	M	201	F42	3	0
2	N	201	F42	3	0
2	O	201	F42	2	0
2	L	201	F42	5	0
2	A	201	F42	2	0
2	B	201	F42	1	0
2	C	201	F42	1	0
2	E	201	F42	2	0

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 than 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.

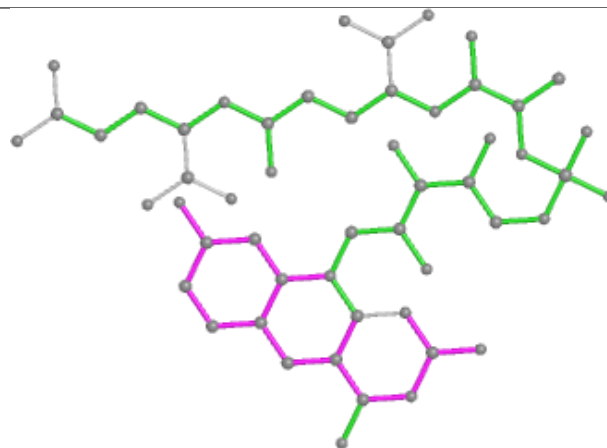
## Ligand F42 K 201



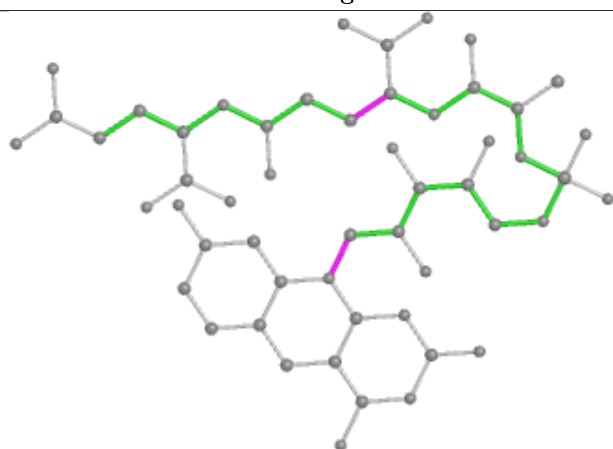
## Ligand F42 D 201



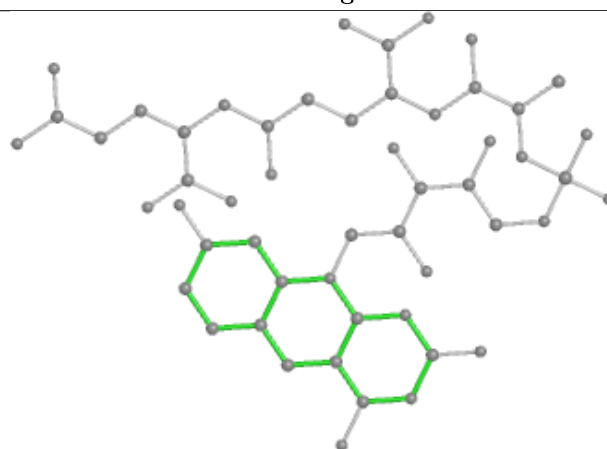
Bond lengths



Bond angles

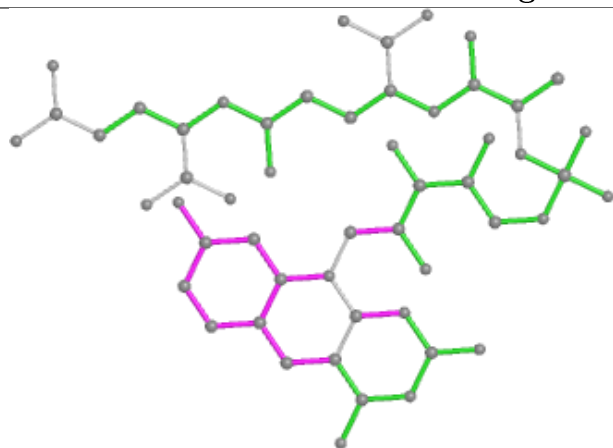


Torsions

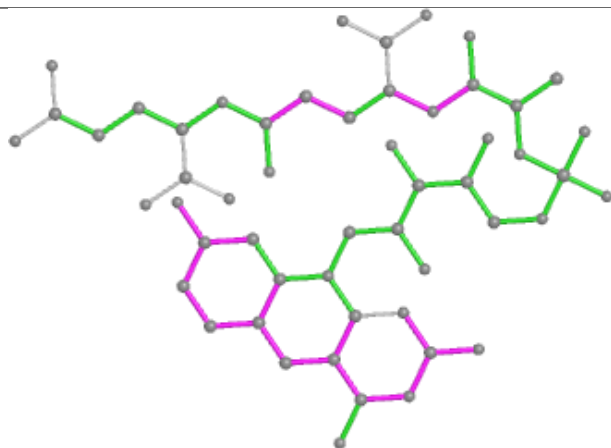


Rings

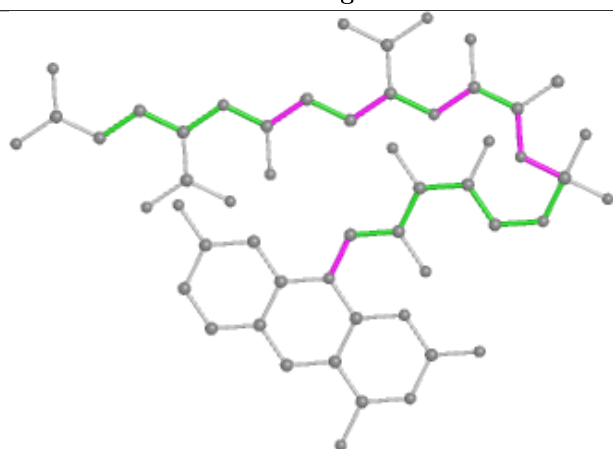
## Ligand F42 M 201



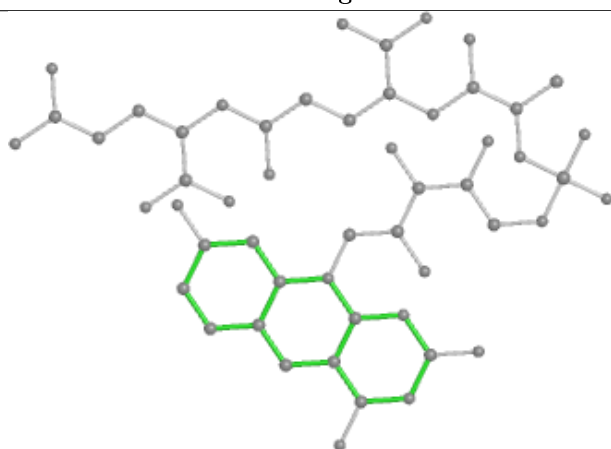
Bond lengths



Bond angles

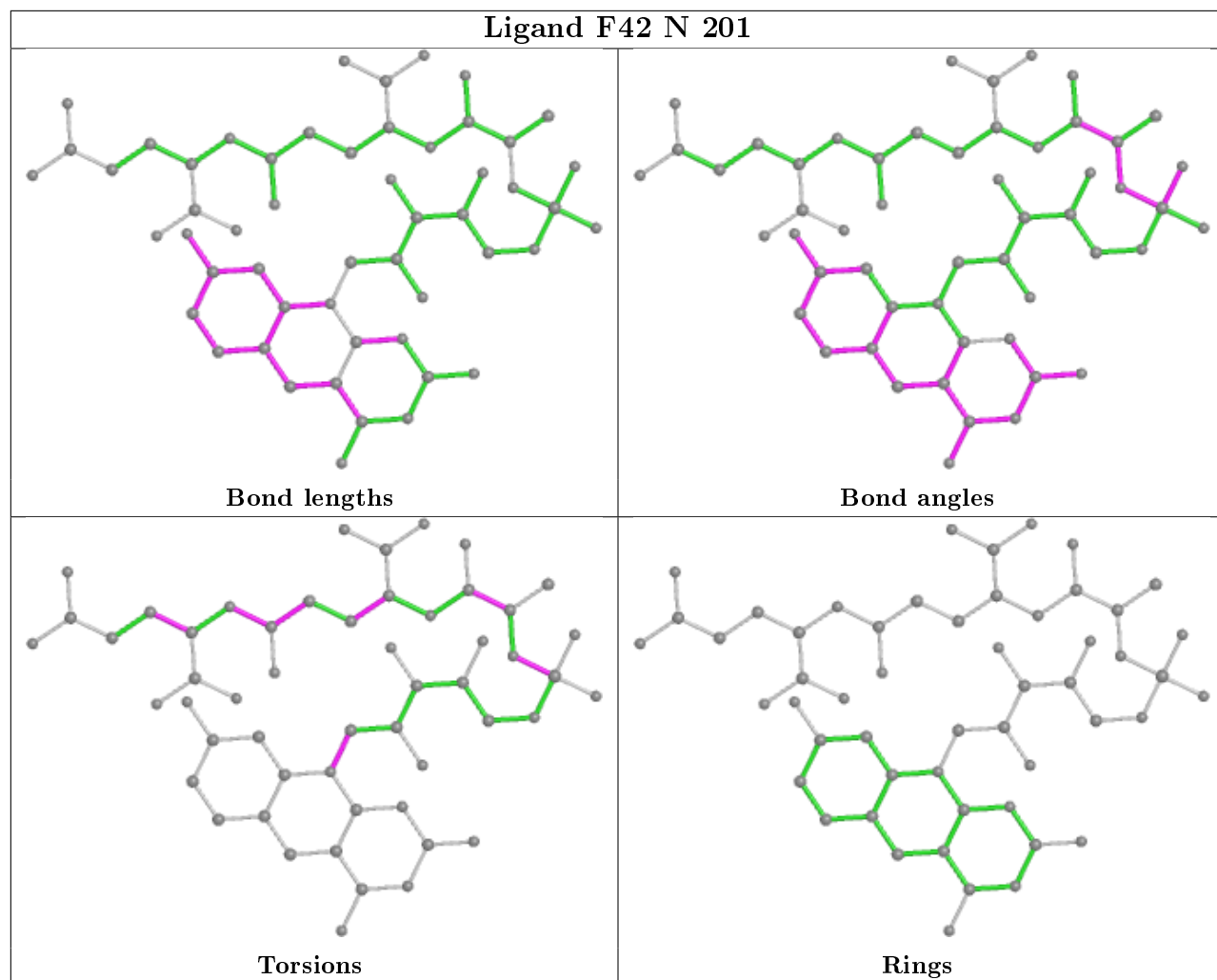


Torsions



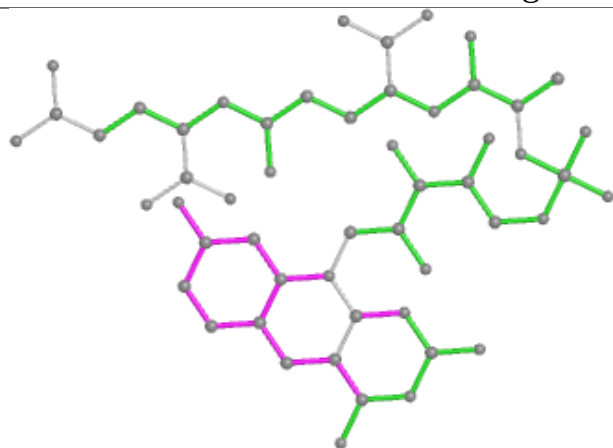
Rings

## Ligand F42 N 201

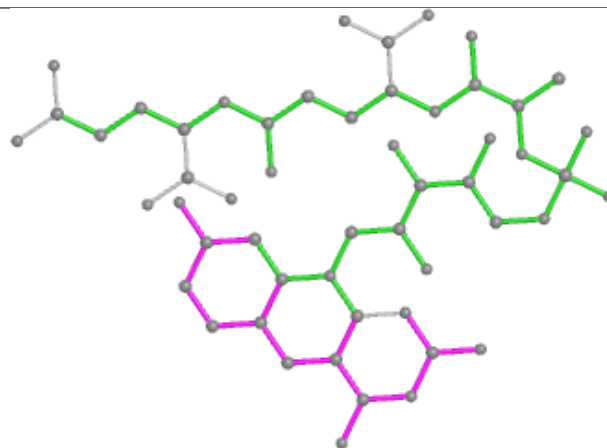




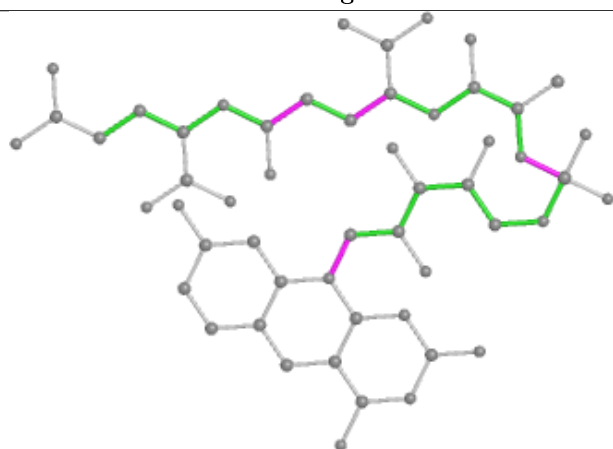
## Ligand F42 O 201



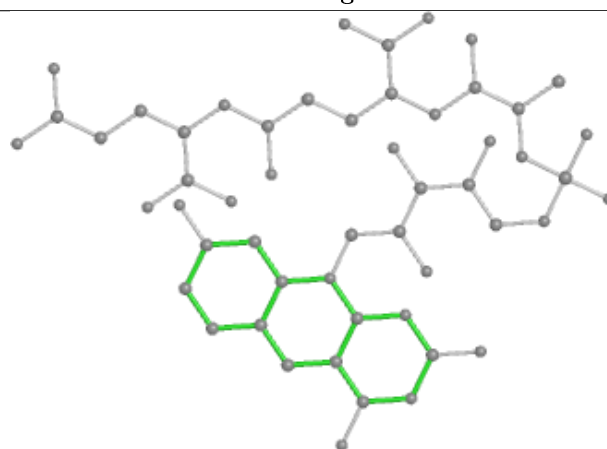
Bond lengths



Bond angles

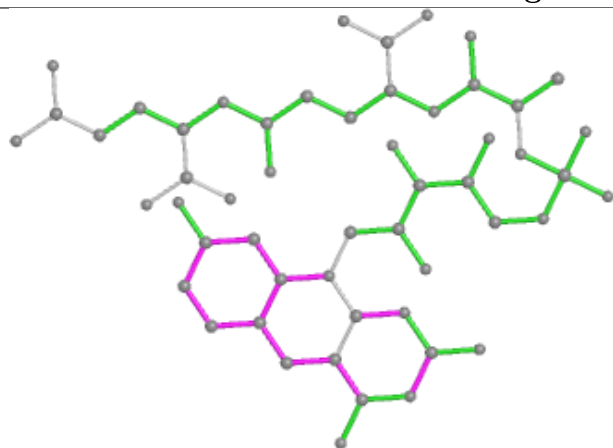


Torsions

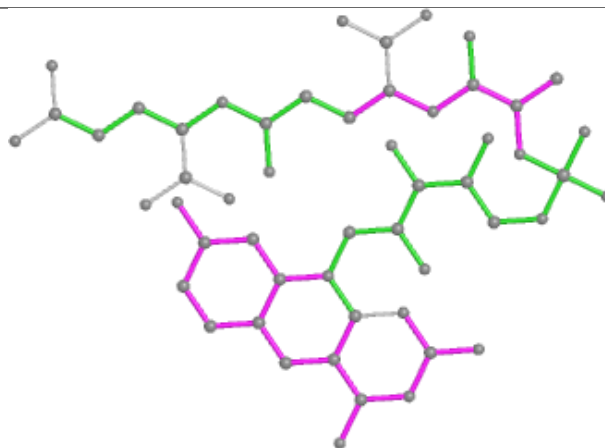


Rings

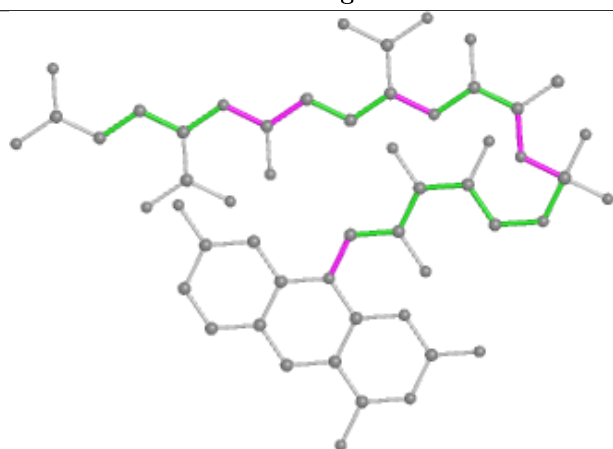
## Ligand F42 L 201



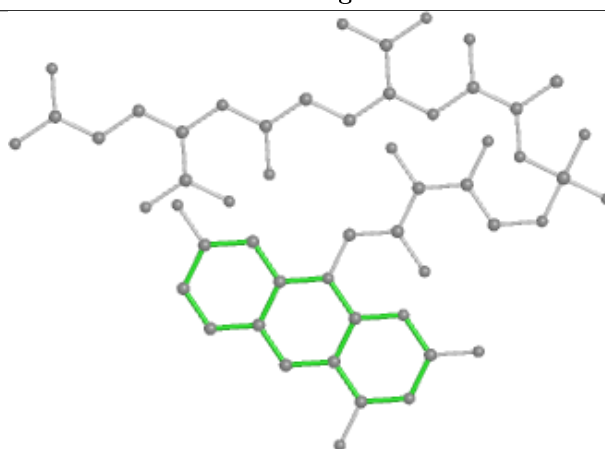
Bond lengths



Bond angles

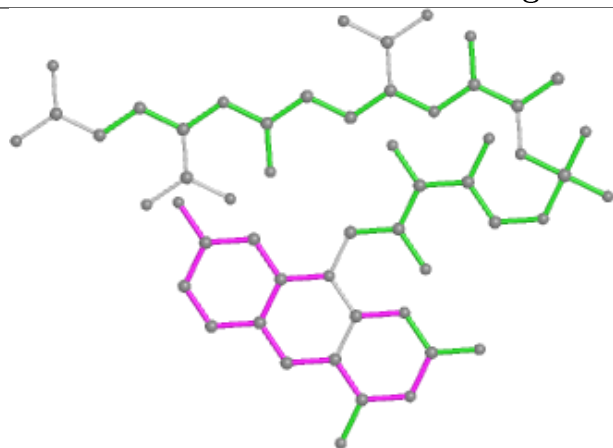


Torsions

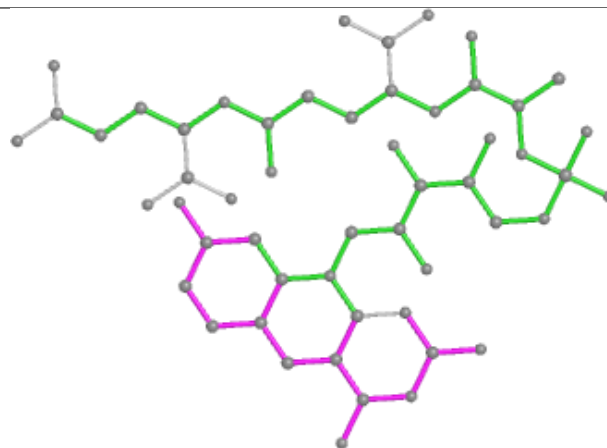


Rings

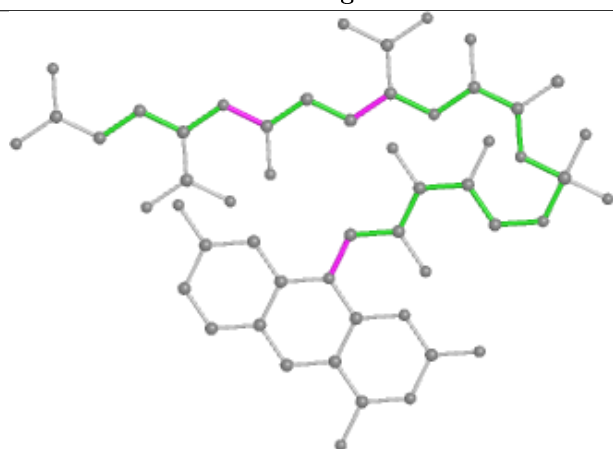
## Ligand F42 A 201



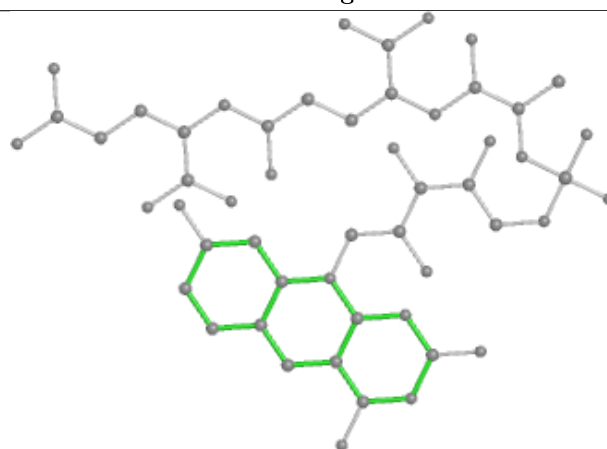
Bond lengths



Bond angles

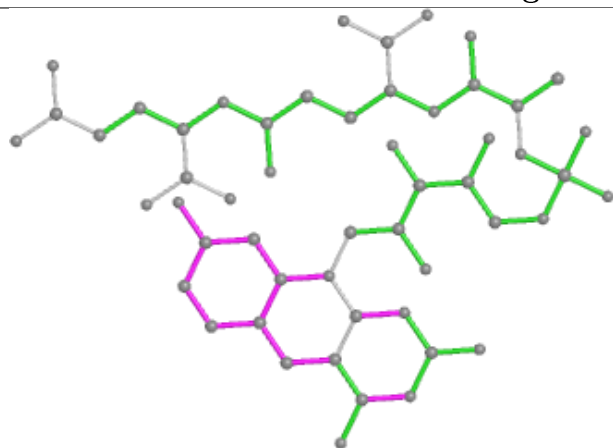


Torsions

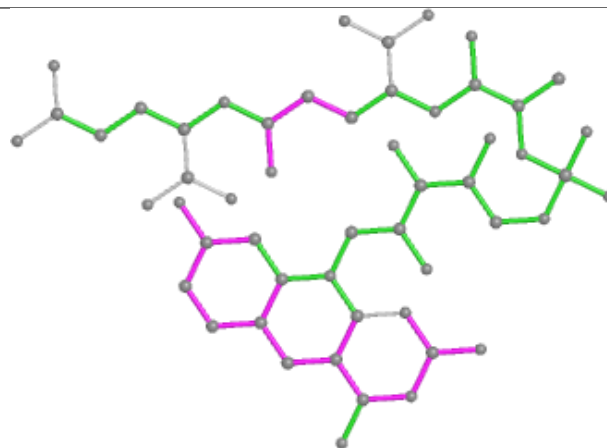


Rings

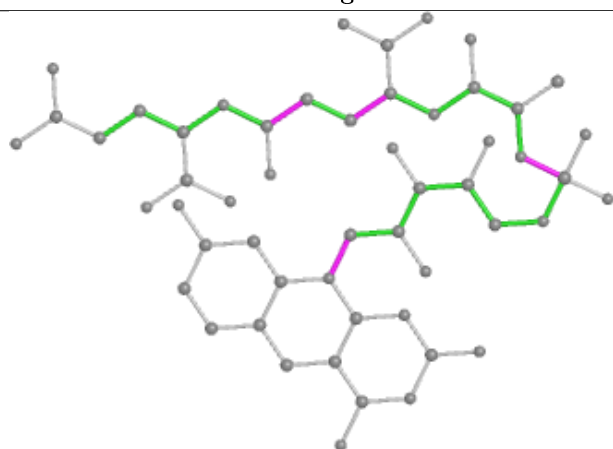
## Ligand F42 B 201



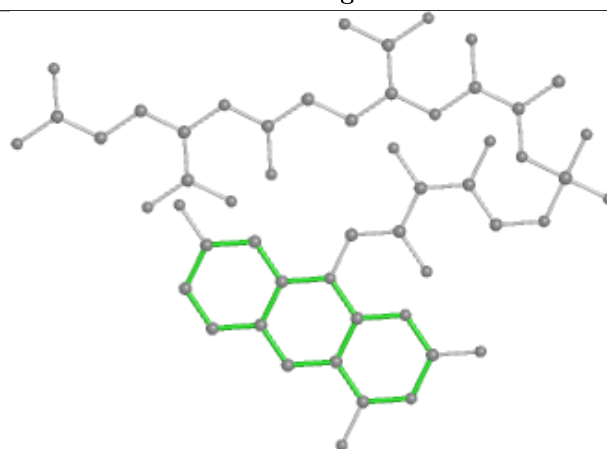
Bond lengths



Bond angles

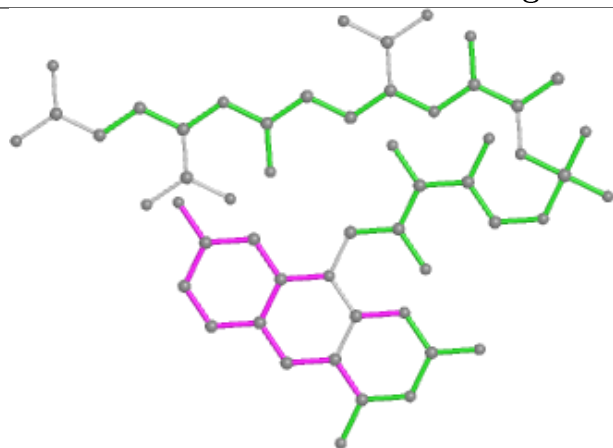


Torsions

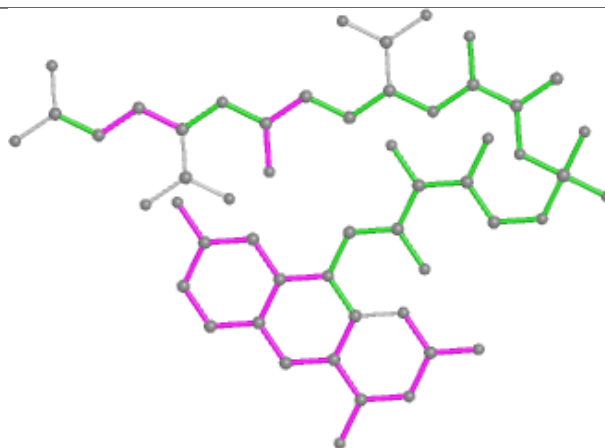


Rings

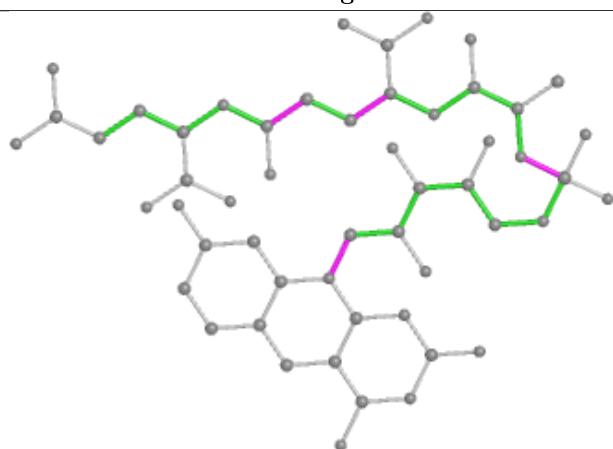
## Ligand F42 C 201



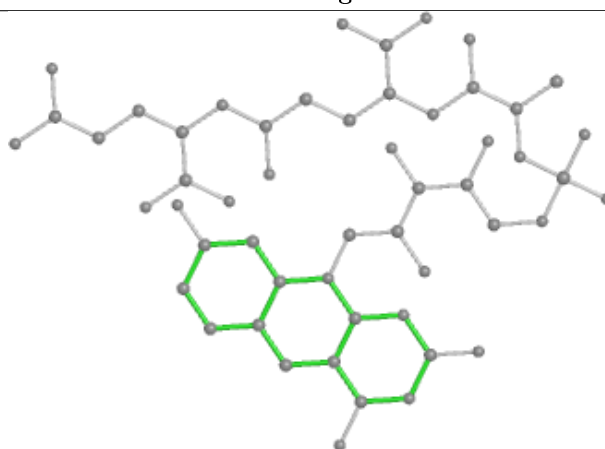
Bond lengths



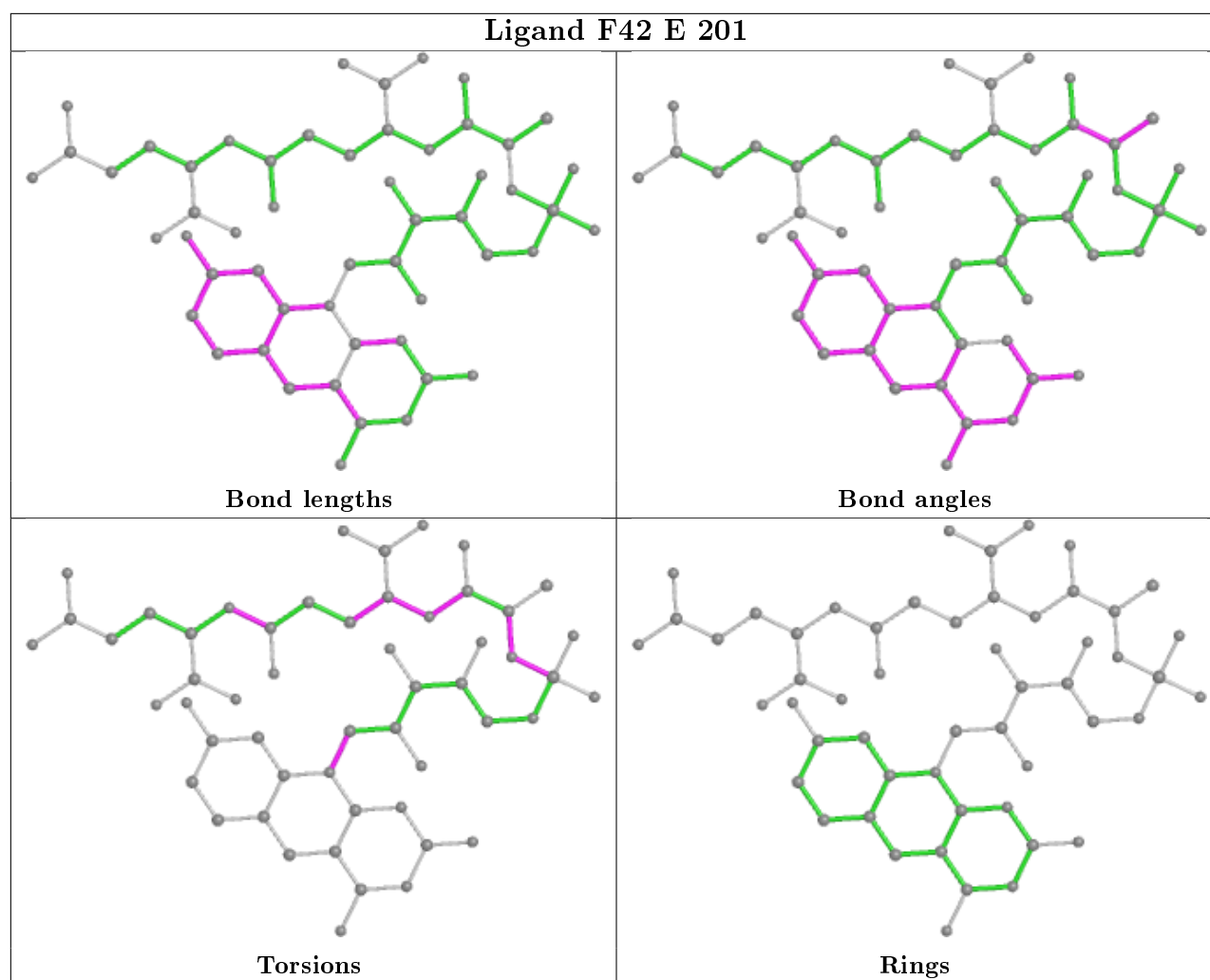
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	109/112 (97%)	-0.19	0 100 100	13, 24, 45, 57	0
1	B	109/112 (97%)	-0.27	0 100 100	14, 24, 45, 58	0
1	C	109/112 (97%)	-0.16	1 (0%) 84 84	12, 24, 43, 58	0
1	D	109/112 (97%)	-0.16	0 100 100	16, 28, 49, 63	0
1	E	109/112 (97%)	-0.23	1 (0%) 84 84	17, 28, 48, 61	0
1	K	109/112 (97%)	-0.21	0 100 100	13, 24, 44, 57	0
1	L	109/112 (97%)	-0.22	0 100 100	16, 25, 48, 62	0
1	M	109/112 (97%)	-0.15	1 (0%) 84 84	14, 24, 44, 56	0
1	N	109/112 (97%)	-0.15	2 (1%) 68 68	16, 28, 51, 62	0
1	O	109/112 (97%)	-0.19	1 (0%) 84 84	16, 29, 50, 67	0
All	All	1090/1120 (97%)	-0.19	6 (0%) 89 89	12, 26, 49, 67	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	151	PRO	2.6
1	N	121	GLU	2.3
1	N	55	LYS	2.2
1	O	151	PRO	2.1
1	C	117	GLU	2.1
1	M	55	LYS	2.1

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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<sup>th</sup> 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.

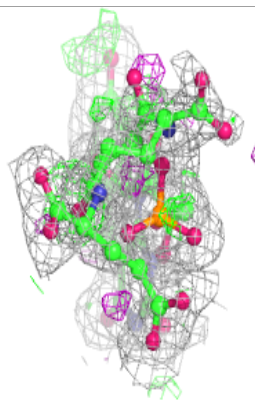
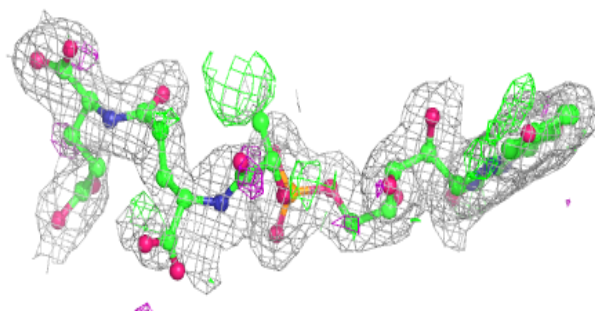
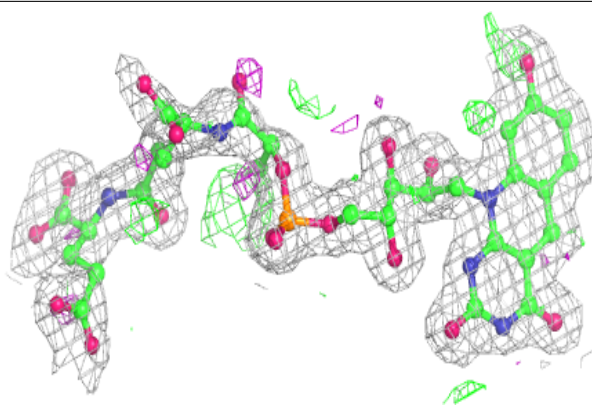
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	F42	M	201	53/53	0.95	0.15	13,21,89,92	0
2	F42	A	201	53/53	0.95	0.14	11,20,81,96	0
2	F42	C	201	53/53	0.95	0.15	10,19,84,86	0
2	F42	O	201	53/53	0.96	0.10	14,23,83,97	0
2	F42	L	201	53/53	0.96	0.13	13,22,87,98	0
2	F42	K	201	53/53	0.96	0.12	9,20,80,82	0
2	F42	B	201	53/53	0.96	0.12	10,19,73,89	0
2	F42	N	201	53/53	0.96	0.13	13,21,96,107	0
2	F42	E	201	53/53	0.96	0.14	13,22,82,91	0
2	F42	D	201	53/53	0.97	0.12	12,21,97,103	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.

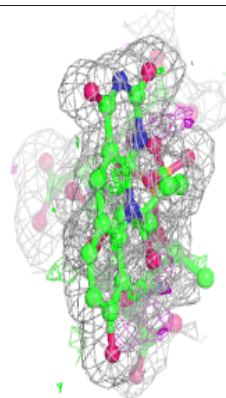
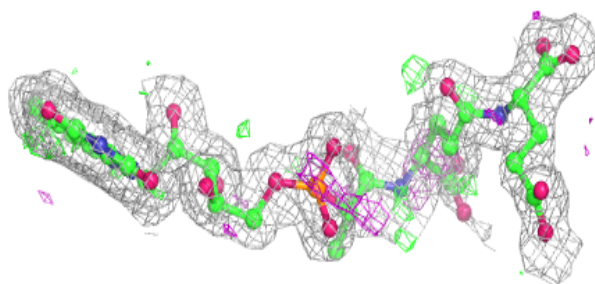
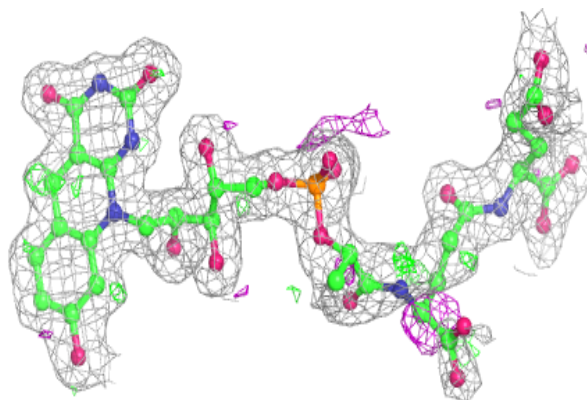


**Electron density around F42 M 201:**

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

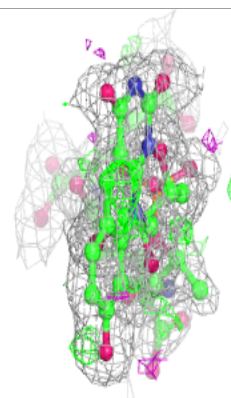
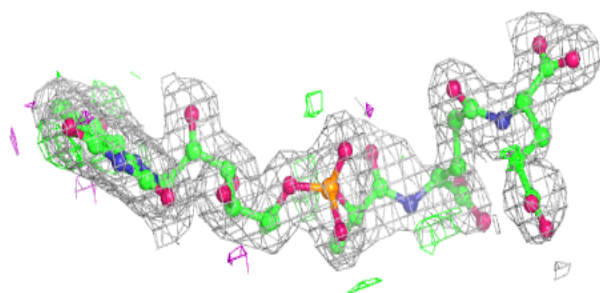
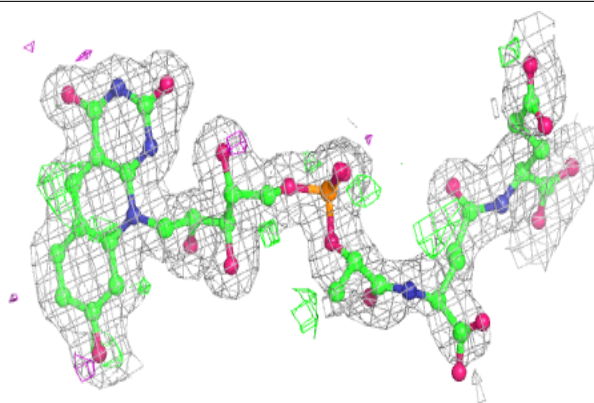
**Electron density around F42 A 201:**

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

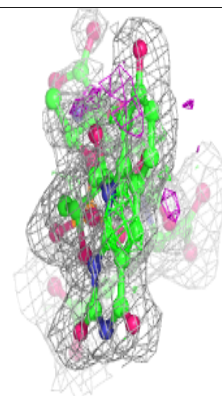
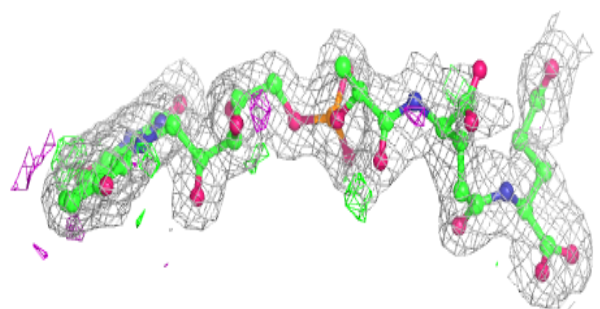
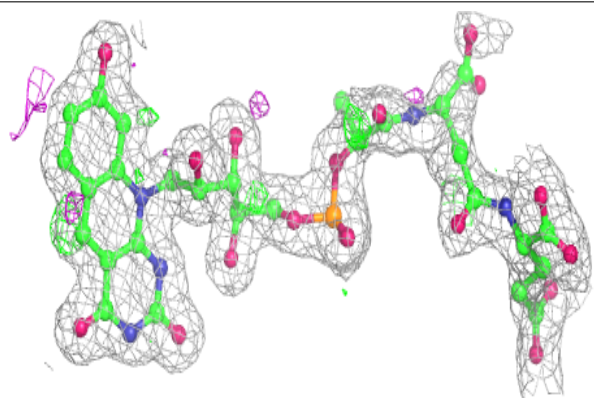


**Electron density around F42 C 201:**

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

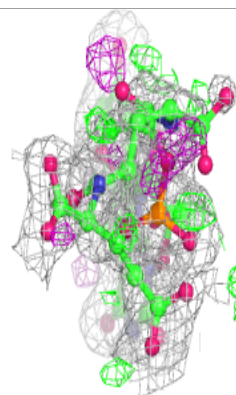
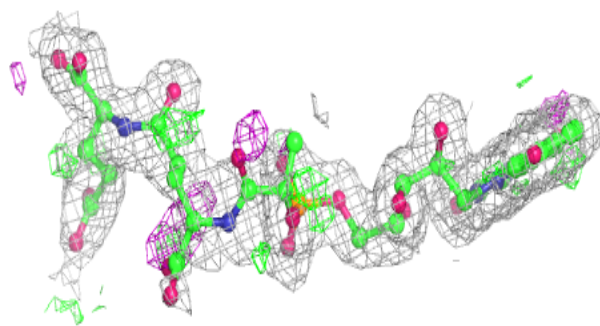
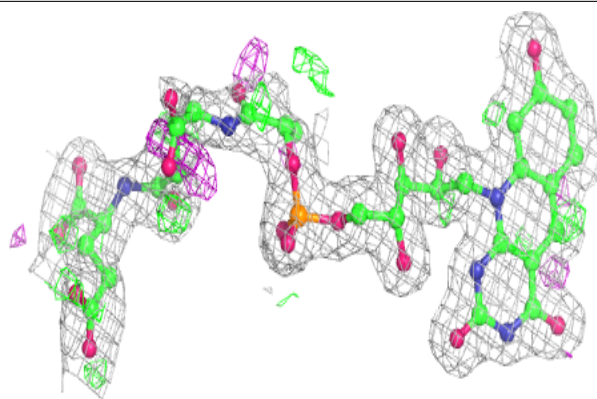
**Electron density around F42 O 201:**

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

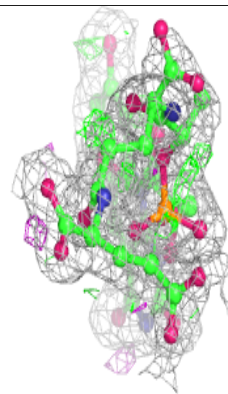
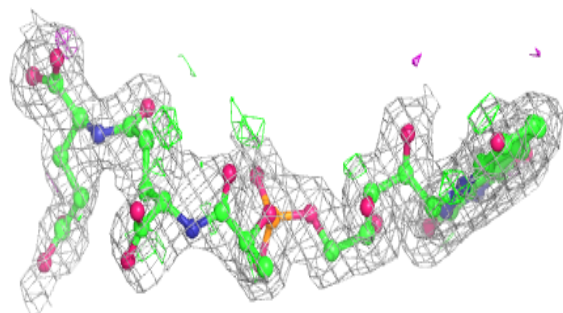
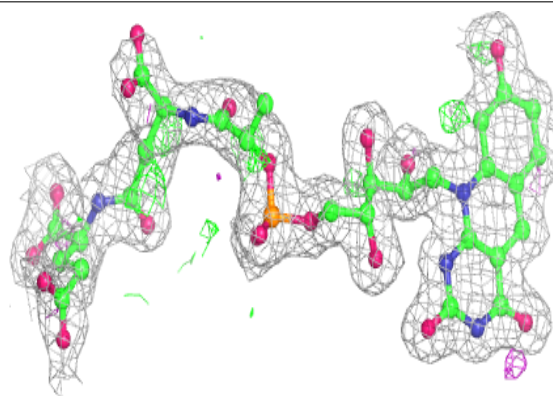


**Electron density around F42 L 201:**

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

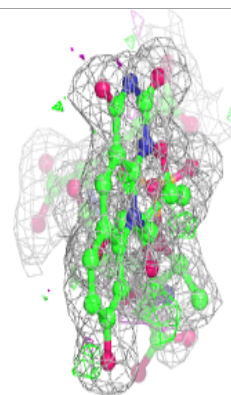
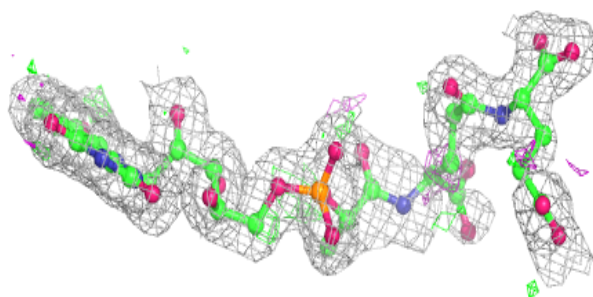
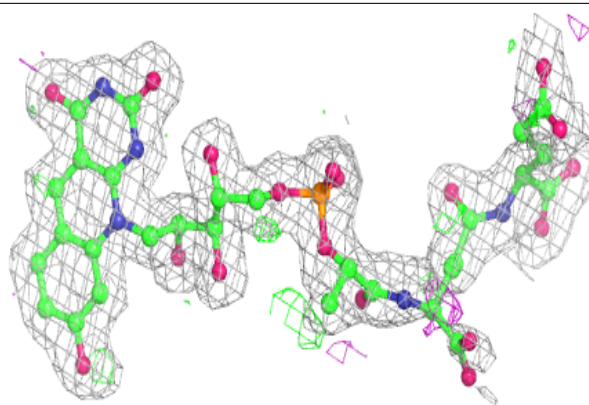
**Electron density around F42 K 201:**

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

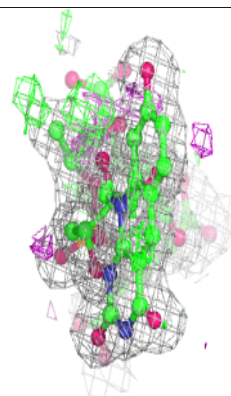
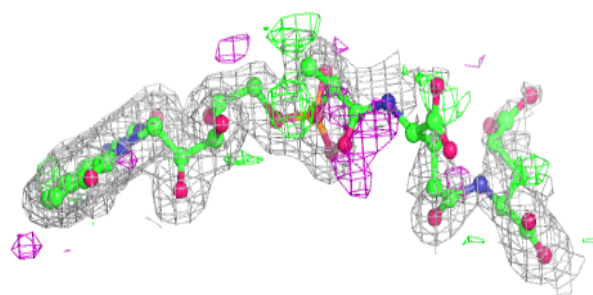
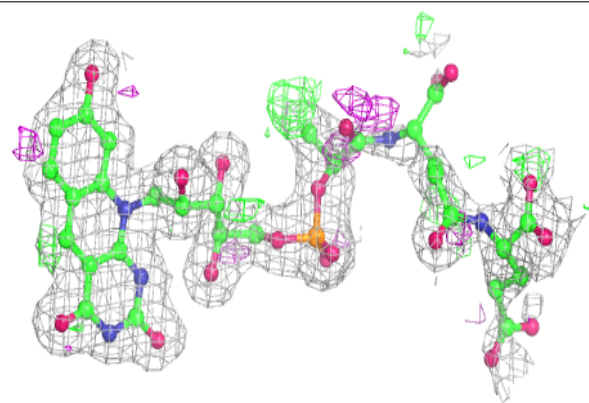


**Electron density around F42 B 201:**

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

**Electron density around F42 N 201:**

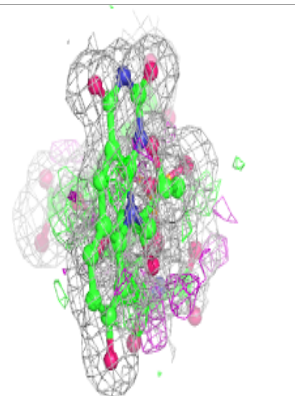
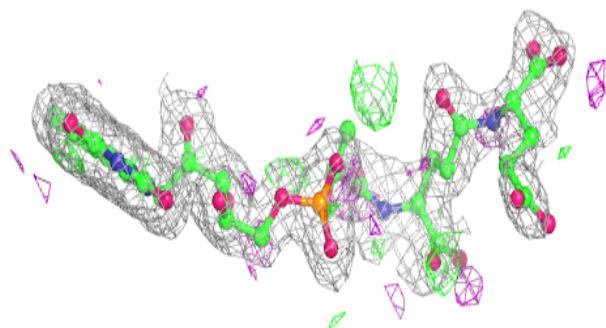
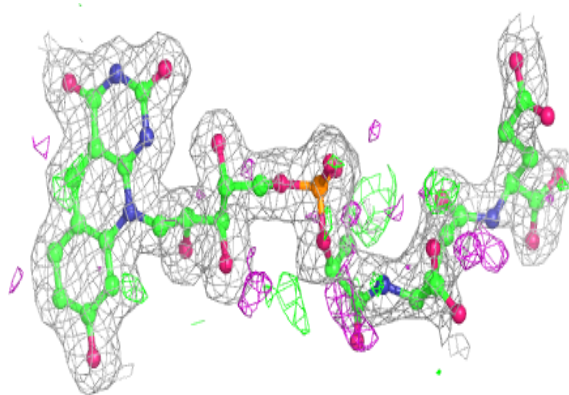
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



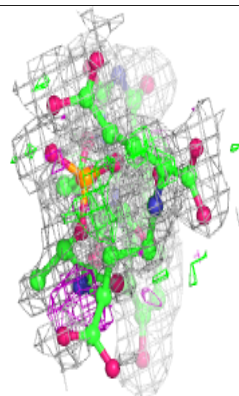
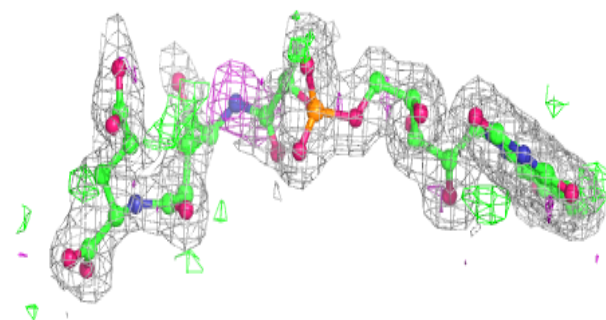
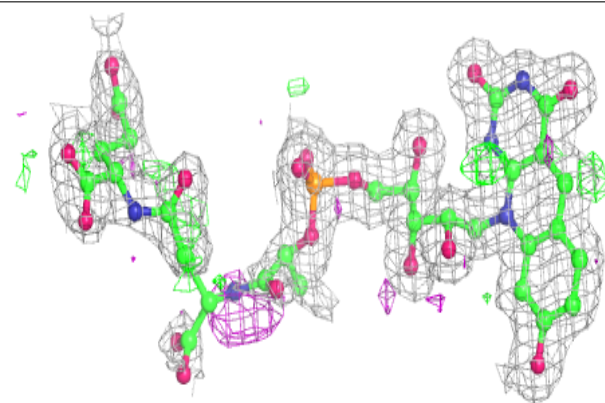


**Electron density around F42 E 201:**

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

**Electron density around F42 D 201:**

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



## 6.5 Other polymers

There are no such residues in this entry.