Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 03:46 AM EDT

PDB ID	:	6DL7
Title	:	Human mitochondrial ClpP in complex with ONC201 (TIC10)
Authors	:	Halgas, O.; Zarabi, S.F.; Schimmer, A.; Pai, E.F.
Deposited on	:	2018-05-31
Resolution	:	2.00 Å(reported)

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

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

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

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

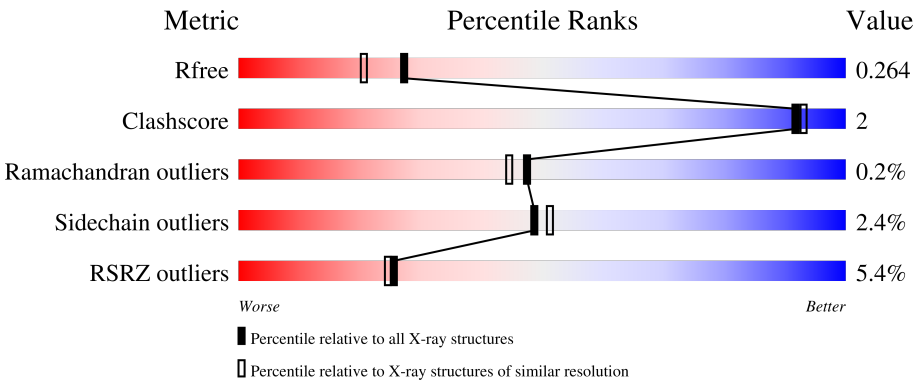
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	221	4% 76% • 21%
1	B	221	2% 74% • 21%
1	C	221	4% 77% • 19%
1	D	221	4% 72% 7% • 20%
1	E	221	6% 77% • • 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	221	5% 76% 19%
1	G	221	5% 79% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10643 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.

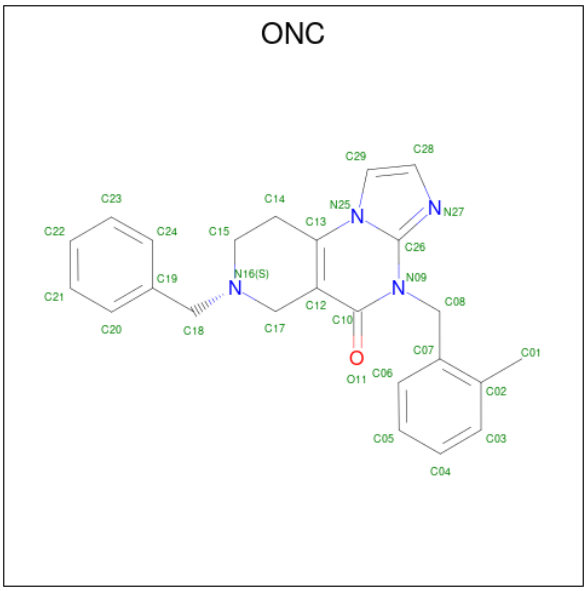
- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	175	1370	873	232	251	14	0	2	0
1	B	174	1354	866	230	245	13	0	1	0
1	C	178	1383	882	235	253	13	0	1	0
1	D	177	1394	889	237	254	14	0	3	0
1	E	180	1387	884	236	254	13	0	0	0
1	F	179	1389	885	236	255	13	0	1	0
1	G	181	1410	899	239	259	13	0	1	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	-	expression tag	UNP Q16740
B	57	SER	-	expression tag	UNP Q16740
C	57	SER	-	expression tag	UNP Q16740
D	57	SER	-	expression tag	UNP Q16740
E	57	SER	-	expression tag	UNP Q16740
F	57	SER	-	expression tag	UNP Q16740
G	57	SER	-	expression tag	UNP Q16740

- Molecule 2 is 7-benzyl-4-[(2-methylphenyl)methyl]-6,7,8,9-tetrahydroimidazo[1,2-a]pyrido[3,4-e]pyrimidin-5(4H)-one (three-letter code: ONC) (formula: $C_{24}H_{24}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	29	24	4	1	0	0
2	B	1	29	24	4	1	0	0
2	C	1	29	24	4	1	0	0
2	D	1	29	24	4	1	0	0
2	E	1	29	24	4	1	0	0
2	F	1	29	24	4	1	0	0
2	G	1	29	24	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	108	108	108	0	0
3	B	118	118	118	0	0
3	C	98	98	98	0	0
3	D	109	109	109	0	0
3	E	107	107	107	0	0

Continued on next page...

Continued from previous page...

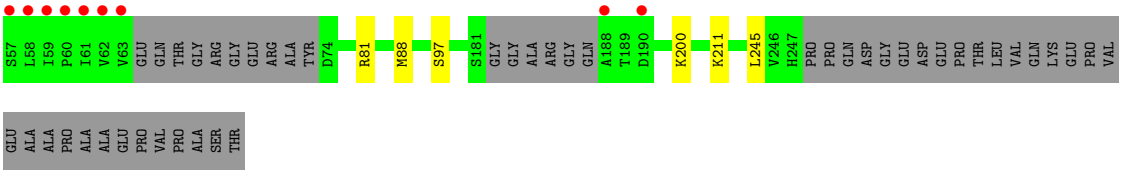
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	F	115	115	115	0	0
			Total	O		
3	G	98	98	98	0	0

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.

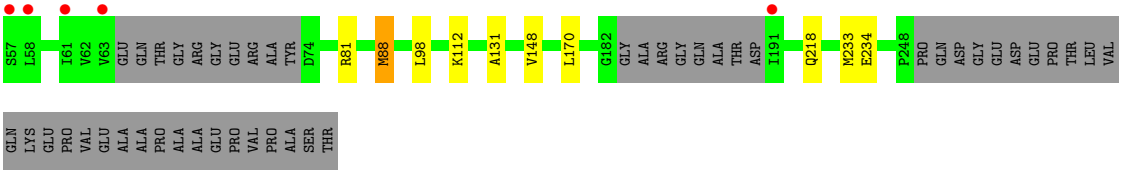
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain A:



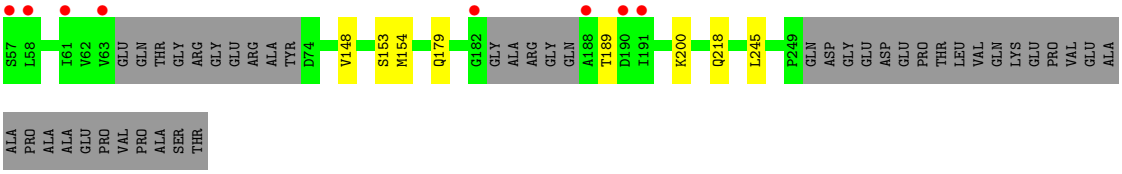
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain B:



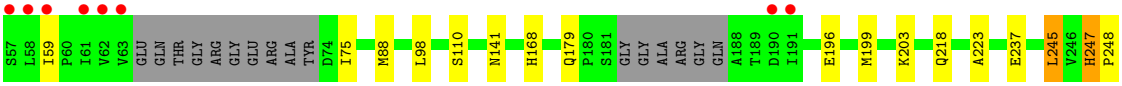
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

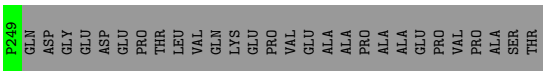
Chain C:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

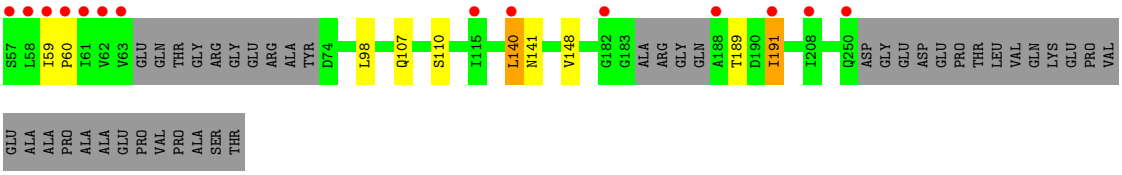
Chain D:





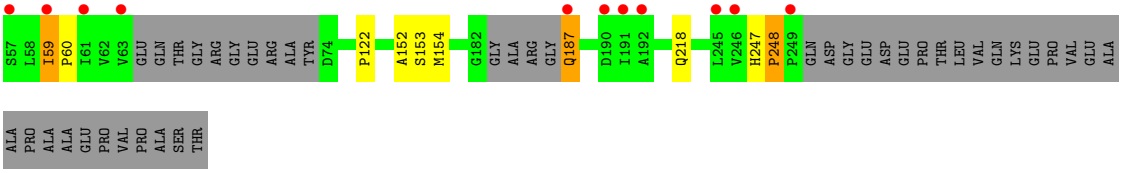
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain E:



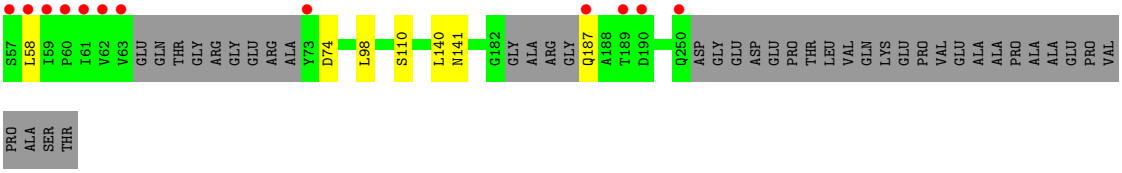
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain F:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.39Å 153.44Å 104.79Å 90.00° 117.58° 90.00°	Depositor
Resolution (Å)	49.33 – 2.00 49.33 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.33-2.00) 99.9 (49.33-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.226 , 0.262 0.231 , 0.264	Depositor DCC
R_{free} test set	7234 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10643	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.84% 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 (i)

5.1 Standard geometry (i)

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

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	0.24	0/1392	0.43	0/1881
1	B	0.24	0/1377	0.43	0/1862
1	C	0.24	0/1407	0.42	0/1904
1	D	0.24	0/1419	0.42	0/1921
1	E	0.24	0/1411	0.41	0/1909
1	F	0.24	0/1413	0.44	0/1912
1	G	0.24	0/1435	0.44	0/1942
All	All	0.24	0/9854	0.43	0/13331

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	1370	0	1413	3	0
1	B	1354	0	1403	4	0
1	C	1383	0	1425	4	0
1	D	1394	0	1434	10	0
1	E	1387	0	1429	5	0
1	F	1389	0	1430	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1410	0	1447	2	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
2	D	29	0	0	0	0
2	E	29	0	0	0	0
2	F	29	0	0	0	0
2	G	29	0	0	0	0
3	A	108	0	0	2	0
3	B	118	0	0	1	0
3	C	98	0	0	2	2
3	D	109	0	0	3	1
3	E	107	0	0	0	0
3	F	115	0	0	2	0
3	G	98	0	0	0	1
All	All	10643	0	9981	31	2

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 2.

All (31) 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:B:148[A]:VAL:HG23	1:B:170:LEU:HD12	1.67	0.77
1:C:179:GLN:OE1	3:C:401:HOH:O	2.06	0.74
1:B:218:GLN:N	3:B:401:HOH:O	2.23	0.71
1:A:211:LYS:NZ	3:A:402:HOH:O	2.25	0.69
1:D:237:GLU:OE1	3:D:401:HOH:O	2.10	0.68
1:E:189:THR:OG1	1:E:191:ILE:O	2.19	0.61
1:D:110:SER:O	1:D:141:ASN:ND2	2.34	0.56
1:C:153:SER:OG	1:C:154:MET:N	2.39	0.56
1:E:110:SER:O	1:E:141:ASN:ND2	2.40	0.55
1:C:200:LYS:NZ	3:C:404:HOH:O	2.38	0.55
1:F:187:GLN:N	3:F:407:HOH:O	2.41	0.54
1:F:187:GLN:N	3:F:404:HOH:O	2.40	0.53
1:D:168:HIS:HB3	1:D:245:LEU:CD2	2.43	0.49
1:F:247:HIS:HB2	1:F:248:PRO:HD2	1.95	0.48
1:A:200:LYS:NZ	3:A:404:HOH:O	2.30	0.47
1:B:131:ALA:HB1	1:C:148:VAL:HG22	1.97	0.47
1:E:98:LEU:HD11	1:F:60:PRO:HD2	1.97	0.45
1:D:196:GLU:OE1	1:D:196:GLU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:GLN:OE1	1:E:140:LEU:HD22	2.18	0.44
1:F:59:ILE:HD12	1:G:58:LEU:HB2	2.00	0.43
1:D:223:ALA:O	3:D:402:HOH:O	2.21	0.42
1:D:98:LEU:HD11	1:E:60:PRO:CD	2.50	0.41
1:D:247[B]:HIS:HB2	1:D:248:PRO:CD	2.50	0.41
1:F:247:HIS:HB2	1:F:248:PRO:CD	2.50	0.41
1:A:97:SER:HB3	1:B:88:MET:HG2	2.02	0.41
1:D:59:ILE:HD12	1:D:59:ILE:N	2.35	0.41
1:F:153[A]:SER:OG	1:F:154:MET:N	2.52	0.41
1:D:199:MET:HG3	1:D:203:LYS:HE2	2.01	0.40
1:D:179:GLN:NE2	3:D:407:HOH:O	2.34	0.40
1:F:122:PRO:HA	1:F:152:ALA:HB3	2.04	0.40
1:G:110:SER:O	1:G:141:ASN:ND2	2.45	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:490:HOH:O	3:D:432:HOH:O[2_554]	2.08	0.12
3:C:486:HOH:O	3:G:491:HOH:O[4_544]	2.18	0.02

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	171/221 (77%)	163 (95%)	8 (5%)	0	100	100
1	B	169/221 (76%)	162 (96%)	7 (4%)	0	100	100
1	C	173/221 (78%)	169 (98%)	4 (2%)	0	100	100
1	D	174/221 (79%)	168 (97%)	6 (3%)	0	100	100
1	E	174/221 (79%)	167 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	174/221 (79%)	165 (95%)	7 (4%)	2 (1%)	14	8
1	G	176/221 (80%)	168 (96%)	7 (4%)	1 (1%)	25	19
All	All	1211/1547 (78%)	1162 (96%)	46 (4%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	74	ASP
1	F	59	ILE
1	F	248	PRO

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	154/185 (83%)	151 (98%)	3 (2%)	57	61
1	B	152/185 (82%)	146 (96%)	6 (4%)	32	30
1	C	155/185 (84%)	151 (97%)	4 (3%)	46	48
1	D	157/185 (85%)	151 (96%)	6 (4%)	33	31
1	E	155/185 (84%)	151 (97%)	4 (3%)	46	48
1	F	156/185 (84%)	154 (99%)	2 (1%)	69	74
1	G	158/185 (85%)	155 (98%)	3 (2%)	57	61
All	All	1087/1295 (84%)	1059 (97%)	28 (3%)	49	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	88	MET
1	A	245	LEU
1	B	81	ARG
1	B	88	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	98	LEU
1	B	112	LYS
1	B	233	MET
1	B	234	GLU
1	C	189	THR
1	C	218[A]	GLN
1	C	218[B]	GLN
1	C	245	LEU
1	D	75	ILE
1	D	88	MET
1	D	218	GLN
1	D	245	LEU
1	D	247[A]	HIS
1	D	247[B]	HIS
1	E	59	ILE
1	E	140	LEU
1	E	148	VAL
1	E	191	ILE
1	F	187	GLN
1	F	218	GLN
1	G	98	LEU
1	G	140	LEU
1	G	187	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	ONC	B	301	-	30,33,33	1.75	8 (26%)	34,47,47	2.08	10 (29%)
2	ONC	G	301	-	30,33,33	2.12	9 (30%)	34,47,47	1.87	6 (17%)
2	ONC	F	301	-	30,33,33	2.39	9 (30%)	34,47,47	1.64	6 (17%)
2	ONC	E	301	-	30,33,33	2.33	9 (30%)	34,47,47	1.76	6 (17%)
2	ONC	A	301	-	30,33,33	2.35	11 (36%)	34,47,47	1.94	7 (20%)
2	ONC	D	301	-	30,33,33	2.42	13 (43%)	34,47,47	1.78	6 (17%)
2	ONC	C	301	-	30,33,33	1.92	10 (33%)	34,47,47	1.62	4 (11%)

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	ONC	B	301	-	-	1/8/17/17	0/4/5/5
2	ONC	G	301	-	-	2/8/17/17	0/4/5/5
2	ONC	F	301	-	-	0/8/17/17	0/4/5/5
2	ONC	E	301	-	-	0/8/17/17	0/4/5/5
2	ONC	A	301	-	-	1/8/17/17	0/4/5/5
2	ONC	D	301	-	-	0/8/17/17	0/4/5/5
2	ONC	C	301	-	-	2/8/17/17	0/4/5/5

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	ONC	C17-N16	-8.34	1.39	1.46
2	F	301	ONC	C17-N16	-7.72	1.39	1.46
2	D	301	ONC	C29-N25	6.02	1.44	1.38
2	A	301	ONC	C29-N25	5.85	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ONC	C17-N16	-5.32	1.41	1.46
2	G	301	ONC	C17-N16	-5.27	1.41	1.46
2	A	301	ONC	C17-N16	-5.17	1.42	1.46
2	E	301	ONC	C10-N09	4.67	1.46	1.38
2	D	301	ONC	C17-N16	-4.52	1.42	1.46
2	D	301	ONC	C08-C07	-4.51	1.43	1.51
2	G	301	ONC	C10-N09	4.31	1.45	1.38
2	F	301	ONC	C29-C28	4.19	1.52	1.36
2	F	301	ONC	C14-C13	-4.11	1.45	1.50
2	A	301	ONC	C14-C13	-4.11	1.45	1.50
2	F	301	ONC	C29-N25	3.86	1.42	1.38
2	G	301	ONC	C15-N16	-3.79	1.36	1.46
2	A	301	ONC	C29-C28	3.79	1.50	1.36
2	B	301	ONC	C29-C28	3.78	1.50	1.36
2	B	301	ONC	C29-N25	3.78	1.42	1.38
2	G	301	ONC	O11-C10	-3.76	1.15	1.23
2	G	301	ONC	C18-N16	-3.56	1.40	1.47
2	F	301	ONC	C17-C12	-3.50	1.46	1.51
2	D	301	ONC	C29-C28	3.50	1.49	1.36
2	B	301	ONC	C10-N09	3.48	1.44	1.38
2	F	301	ONC	C18-N16	-3.38	1.41	1.47
2	C	301	ONC	C29-C28	3.37	1.49	1.36
2	A	301	ONC	O11-C10	-3.35	1.16	1.23
2	D	301	ONC	C17-C12	-3.35	1.46	1.51
2	D	301	ONC	C10-N09	3.35	1.44	1.38
2	A	301	ONC	C10-N09	3.34	1.44	1.38
2	A	301	ONC	C15-N16	-3.33	1.37	1.46
2	E	301	ONC	C15-N16	-3.27	1.38	1.46
2	F	301	ONC	O11-C10	-3.25	1.16	1.23
2	C	301	ONC	C10-N09	3.24	1.43	1.38
2	B	301	ONC	C26-N27	3.23	1.40	1.35
2	G	301	ONC	C29-C28	3.23	1.48	1.36
2	B	301	ONC	C15-N16	-3.21	1.38	1.46
2	G	301	ONC	C17-C12	-3.20	1.46	1.51
2	C	301	ONC	C15-N16	-3.16	1.38	1.46
2	D	301	ONC	O11-C10	-3.13	1.16	1.23
2	E	301	ONC	C14-C13	-3.07	1.46	1.50
2	A	301	ONC	C18-N16	-3.03	1.41	1.47
2	D	301	ONC	C18-N16	-2.96	1.41	1.47
2	G	301	ONC	C29-N25	2.95	1.41	1.38
2	C	301	ONC	C08-N09	-2.93	1.42	1.46
2	E	301	ONC	C29-C28	2.93	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	ONC	C15-N16	-2.85	1.39	1.46
2	E	301	ONC	C17-C12	-2.83	1.46	1.51
2	E	301	ONC	O11-C10	-2.71	1.17	1.23
2	C	301	ONC	O11-C10	-2.71	1.17	1.23
2	D	301	ONC	C26-N27	2.67	1.40	1.35
2	D	301	ONC	C14-C13	-2.65	1.47	1.50
2	F	301	ONC	C26-N27	2.56	1.39	1.35
2	E	301	ONC	C29-N25	2.56	1.41	1.38
2	B	301	ONC	C17-N16	-2.50	1.44	1.46
2	B	301	ONC	O11-C10	-2.50	1.18	1.23
2	G	301	ONC	C26-N27	2.48	1.39	1.35
2	A	301	ONC	C17-C12	-2.46	1.47	1.51
2	A	301	ONC	C26-N27	2.46	1.39	1.35
2	C	301	ONC	C18-N16	-2.45	1.42	1.47
2	C	301	ONC	C26-N27	2.43	1.39	1.35
2	A	301	ONC	C08-C07	-2.40	1.47	1.51
2	C	301	ONC	C14-C13	-2.33	1.47	1.50
2	D	301	ONC	C06-C07	-2.25	1.36	1.39
2	F	301	ONC	C15-N16	-2.24	1.40	1.46
2	D	301	ONC	C05-C06	-2.23	1.35	1.38
2	C	301	ONC	C17-C12	-2.18	1.47	1.51
2	B	301	ONC	C24-C19	-2.03	1.34	1.38
2	E	301	ONC	C26-N27	2.00	1.38	1.35

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	ONC	C18-N16-C17	7.57	120.11	110.51
2	A	301	ONC	C07-C08-N09	4.97	121.93	113.27
2	C	301	ONC	C15-C14-C13	4.93	118.14	108.56
2	A	301	ONC	C08-N09-C10	4.93	121.97	116.72
2	D	301	ONC	C15-C14-C13	4.93	118.14	108.56
2	A	301	ONC	C15-C14-C13	4.82	117.93	108.56
2	G	301	ONC	C08-N09-C10	4.81	121.84	116.72
2	G	301	ONC	C07-C08-N09	4.69	121.45	113.27
2	E	301	ONC	C08-N09-C10	4.55	121.56	116.72
2	D	301	ONC	C18-N16-C17	4.54	116.26	110.51
2	G	301	ONC	C15-C14-C13	4.44	117.19	108.56
2	F	301	ONC	C07-C08-N09	4.36	120.87	113.27
2	C	301	ONC	C08-N09-C10	4.00	120.98	116.72
2	F	301	ONC	C15-C14-C13	3.93	116.20	108.56
2	D	301	ONC	C18-N16-C15	-3.92	102.64	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	ONC	C15-C14-C13	3.90	116.14	108.56
2	E	301	ONC	C15-C14-C13	3.82	115.98	108.56
2	B	301	ONC	C08-N09-C10	3.73	120.69	116.72
2	E	301	ONC	C07-C08-N09	3.67	119.66	113.27
2	A	301	ONC	C18-N16-C17	3.62	115.11	110.51
2	A	301	ONC	C18-N16-C15	-3.58	103.37	111.07
2	B	301	ONC	C07-C08-N09	3.46	119.31	113.27
2	E	301	ONC	C18-N16-C17	3.42	114.84	110.51
2	G	301	ONC	C18-N16-C17	3.32	114.72	110.51
2	F	301	ONC	C18-N16-C15	-3.29	103.98	111.07
2	F	301	ONC	C18-N16-C17	3.27	114.65	110.51
2	C	301	ONC	C18-N16-C15	-3.26	104.04	111.07
2	G	301	ONC	C18-N16-C15	-3.20	104.17	111.07
2	D	301	ONC	C07-C08-N09	3.09	118.67	113.27
2	F	301	ONC	C08-N09-C10	3.02	119.94	116.72
2	E	301	ONC	C14-C15-N16	-3.01	108.49	111.19
2	D	301	ONC	C08-N09-C10	2.96	119.88	116.72
2	C	301	ONC	C18-N16-C17	2.83	114.09	110.51
2	E	301	ONC	C18-N16-C15	-2.66	105.35	111.07
2	B	301	ONC	C14-C15-N16	-2.55	108.90	111.19
2	D	301	ONC	C12-C10-N09	2.22	119.43	115.17
2	B	301	ONC	C19-C18-N16	2.21	117.66	113.15
2	A	301	ONC	O11-C10-C12	-2.19	120.89	125.06
2	B	301	ONC	C12-C10-N09	2.17	119.33	115.17
2	B	301	ONC	O11-C10-C12	-2.14	120.99	125.06
2	B	301	ONC	C17-N16-C15	2.14	113.17	110.10
2	B	301	ONC	C18-N16-C15	-2.11	106.53	111.07
2	A	301	ONC	C12-C10-N09	2.10	119.21	115.17
2	F	301	ONC	C12-C10-N09	2.09	119.19	115.17
2	G	301	ONC	C14-C15-N16	-2.02	109.38	111.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

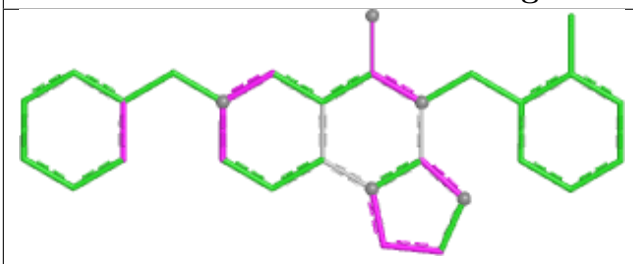
Mol	Chain	Res	Type	Atoms
2	C	301	ONC	C19-C18-N16-C17
2	B	301	ONC	C19-C18-N16-C17
2	G	301	ONC	C19-C18-N16-C17
2	C	301	ONC	C19-C18-N16-C15
2	G	301	ONC	C19-C18-N16-C15
2	A	301	ONC	C19-C18-N16-C17

There are no ring outliers.

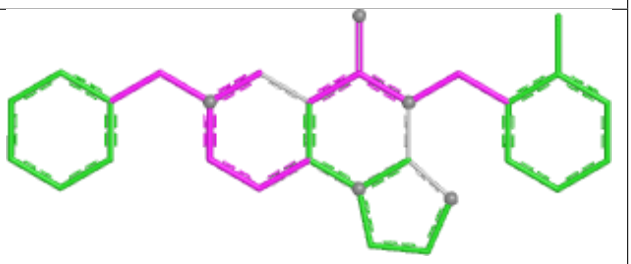
No monomer is involved in short contacts.

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.

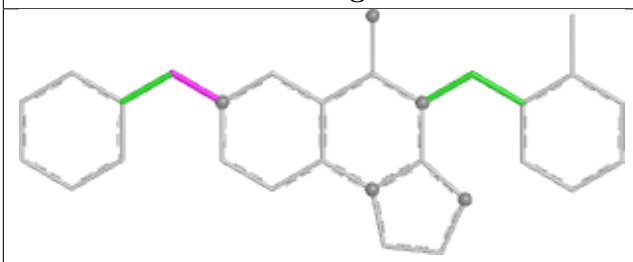
Ligand ONC B 301



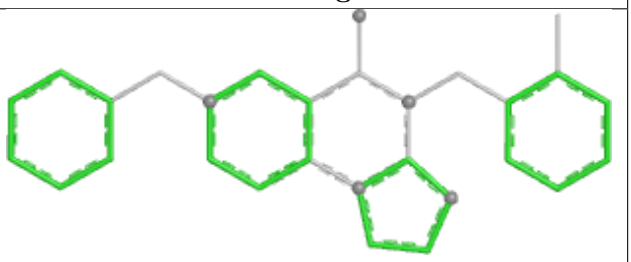
Bond lengths



Bond angles

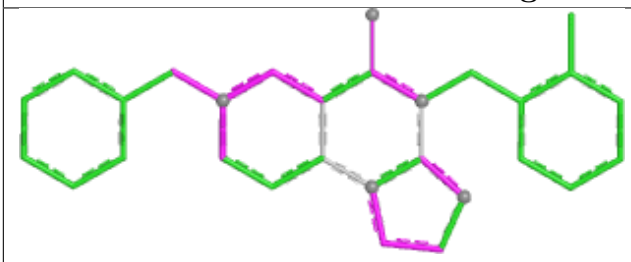


Torsions

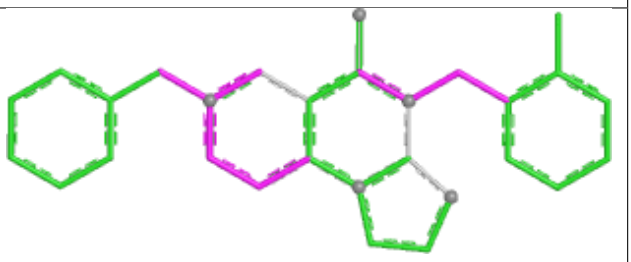


Rings

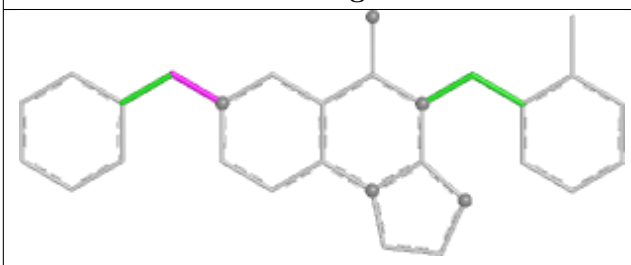
Ligand ONC G 301



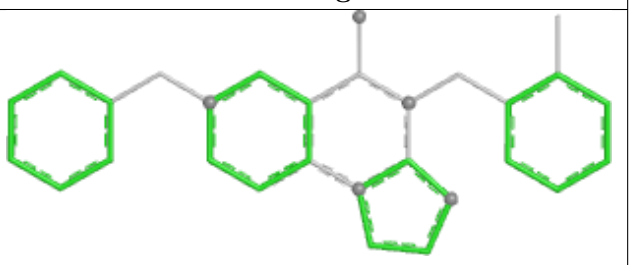
Bond lengths



Bond angles

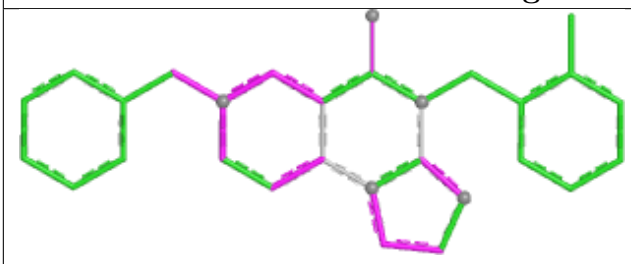


Torsions

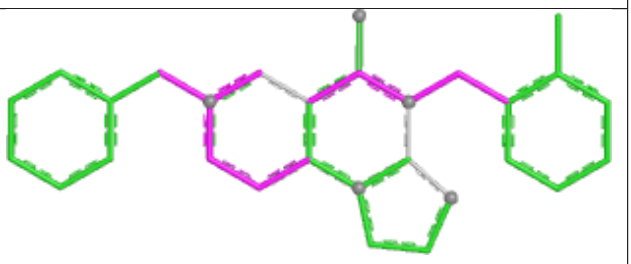


Rings

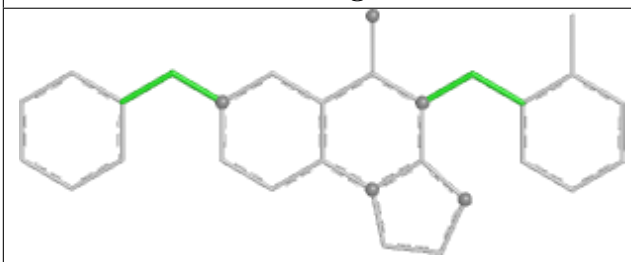
Ligand ONC F 301



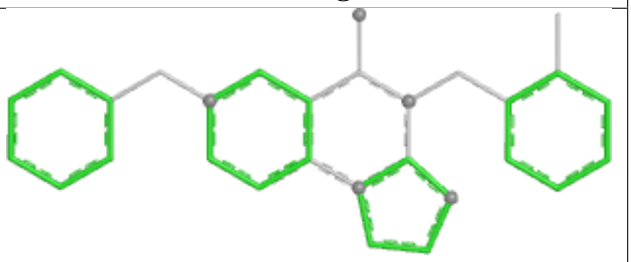
Bond lengths



Bond angles

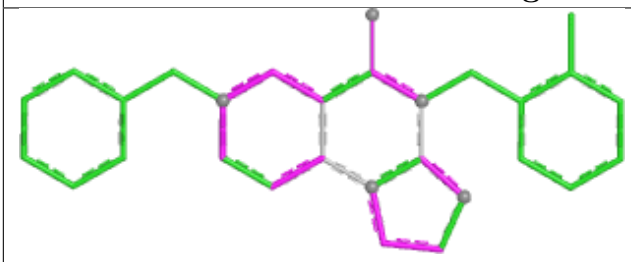


Torsions

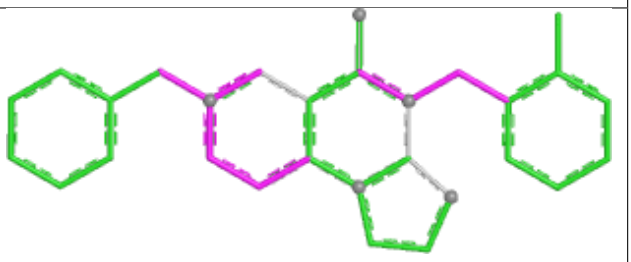


Rings

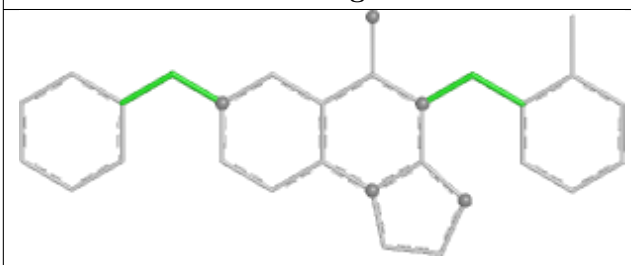
Ligand ONC E 301



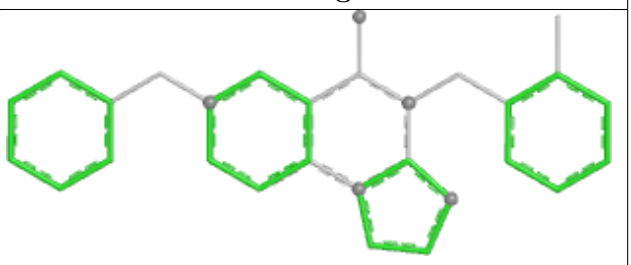
Bond lengths



Bond angles

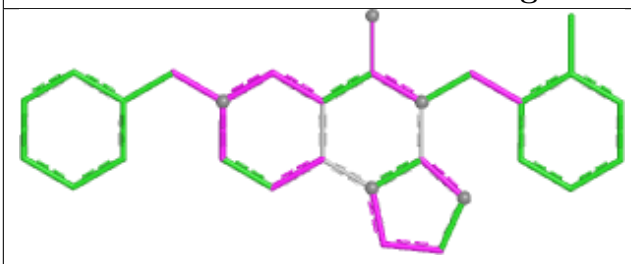


Torsions

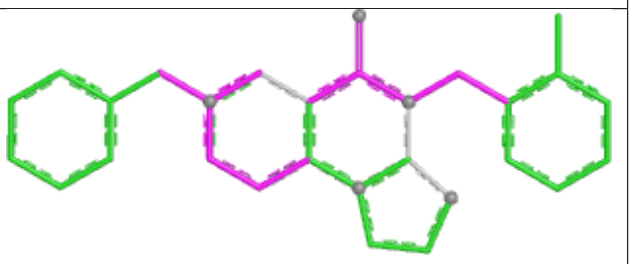


Rings

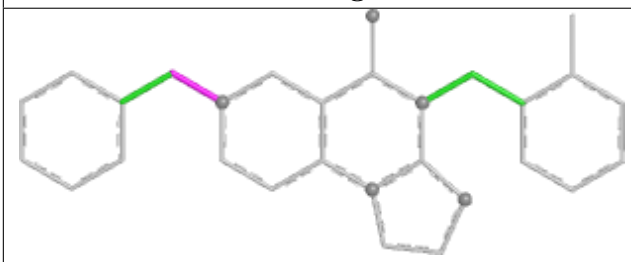
Ligand ONC A 301



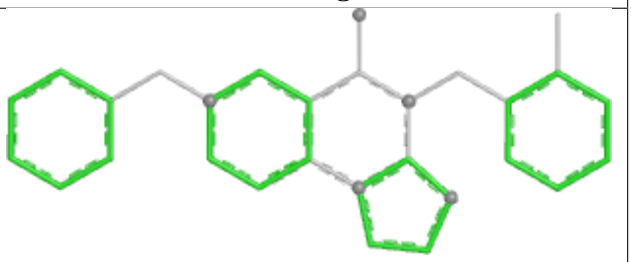
Bond lengths



Bond angles

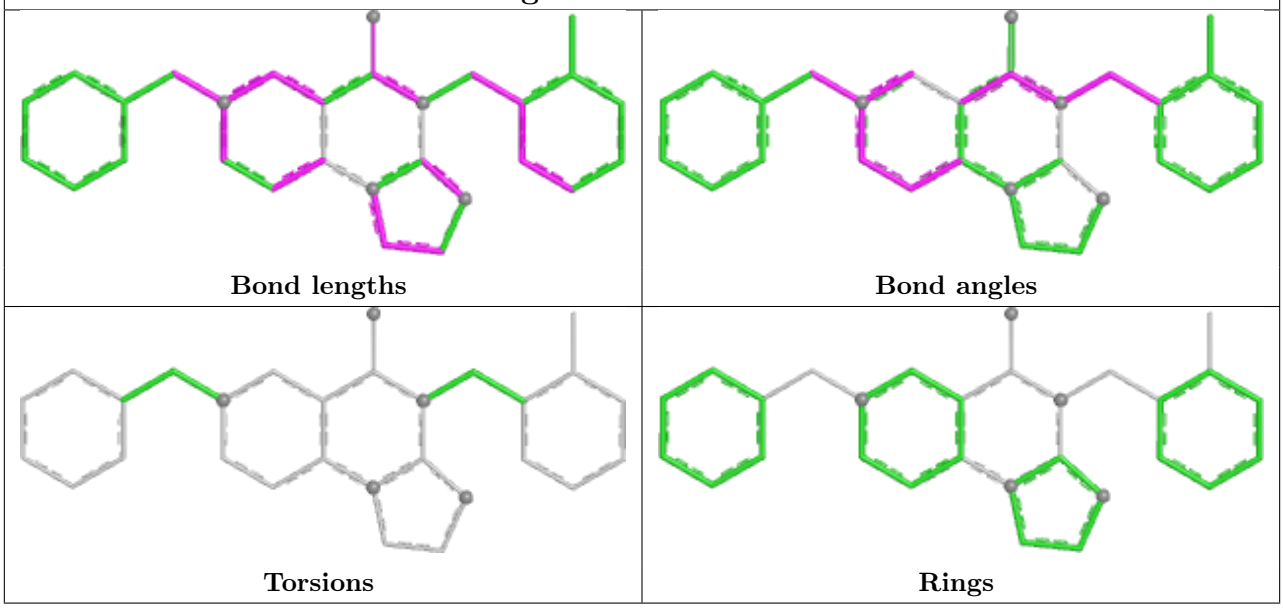


Torsions

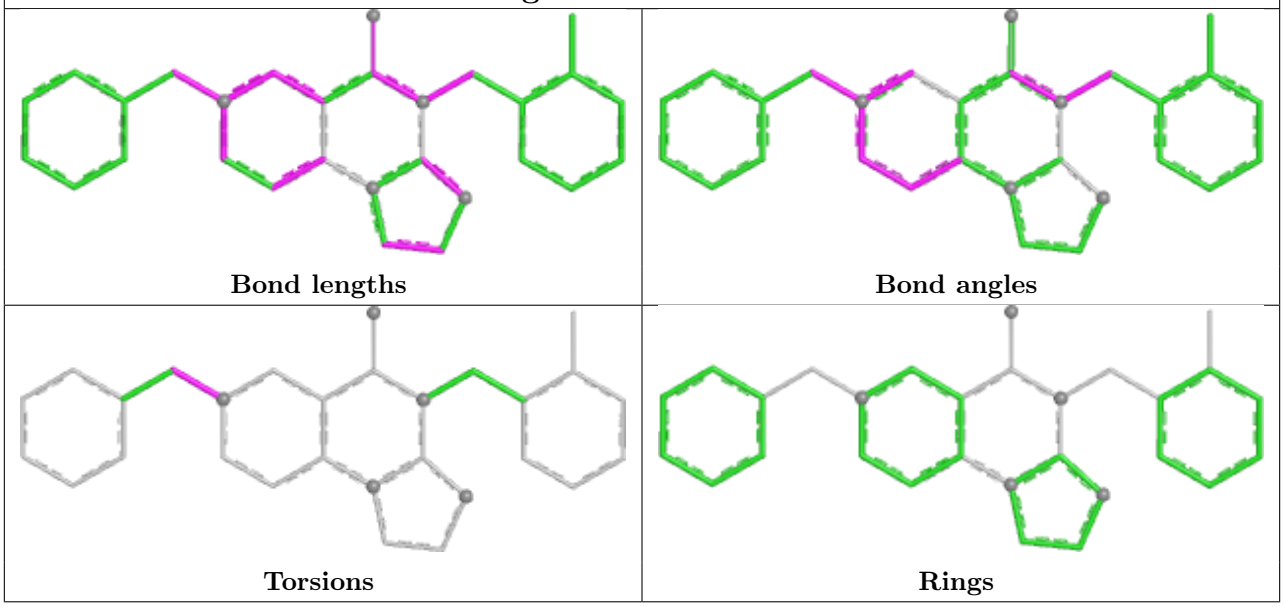


Rings

Ligand ONC D 301



Ligand ONC C 301



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	175/221 (79%)	-0.08	9 (5%)	28	27	32, 44, 97, 153	0
1	B	174/221 (78%)	-0.11	5 (2%)	51	50	30, 42, 99, 160	0
1	C	178/221 (80%)	-0.07	8 (4%)	33	32	30, 41, 94, 123	0
1	D	177/221 (80%)	-0.12	8 (4%)	33	32	30, 42, 106, 145	0
1	E	180/221 (81%)	0.39	14 (7%)	13	12	29, 40, 101, 140	0
1	F	179/221 (80%)	-0.07	11 (6%)	21	20	30, 42, 97, 160	0
1	G	181/221 (81%)	0.07	12 (6%)	18	17	30, 39, 105, 156	0
All	All	1244/1547 (80%)	0.00	67 (5%)	25	24	29, 42, 100, 160	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	SER	9.5
1	E	57	SER	7.6
1	E	58	LEU	7.3
1	D	58	LEU	6.5
1	C	57	SER	6.5
1	A	63	VAL	6.2
1	B	57	SER	6.2
1	G	58	LEU	5.9
1	A	58	LEU	5.6
1	F	61	ILE	5.6
1	G	57	SER	5.6
1	G	250	GLN	5.5
1	G	73	TYR	5.3
1	A	61	ILE	5.2
1	F	249	PRO	5.2
1	G	63	VAL	5.1
1	D	57	SER	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	188	ALA	5.0
1	C	58	LEU	4.9
1	G	59	ILE	4.9
1	E	250	GLN	4.7
1	G	61	ILE	4.7
1	D	190	ASP	4.6
1	E	61	ILE	4.6
1	F	59	ILE	4.6
1	B	61	ILE	4.5
1	F	187	GLN	4.2
1	D	63	VAL	4.2
1	C	191	ILE	4.0
1	B	63	VAL	3.8
1	D	62	VAL	3.5
1	D	61	ILE	3.5
1	D	191	ILE	3.3
1	F	57	SER	3.3
1	A	59	ILE	3.1
1	C	63	VAL	3.1
1	G	60	PRO	3.1
1	F	63	VAL	3.1
1	A	190	ASP	3.0
1	C	190	ASP	3.0
1	G	190	ASP	3.0
1	F	191	ILE	3.0
1	B	191	ILE	3.0
1	E	62	VAL	2.9
1	F	246	VAL	2.9
1	A	60	PRO	2.8
1	E	59	ILE	2.8
1	C	182	GLY	2.8
1	F	190	ASP	2.8
1	D	59	ILE	2.7
1	G	62	VAL	2.6
1	G	187	GLN	2.5
1	F	245	LEU	2.4
1	E	188	ALA	2.4
1	B	58	LEU	2.4
1	E	182	GLY	2.4
1	E	191	ILE	2.4
1	C	61	ILE	2.3
1	A	62	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	189	THR	2.3
1	E	60	PRO	2.3
1	E	140	LEU	2.3
1	A	188	ALA	2.2
1	E	63	VAL	2.2
1	E	208	ILE	2.1
1	E	115	ILE	2.0
1	F	192	ALA	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)

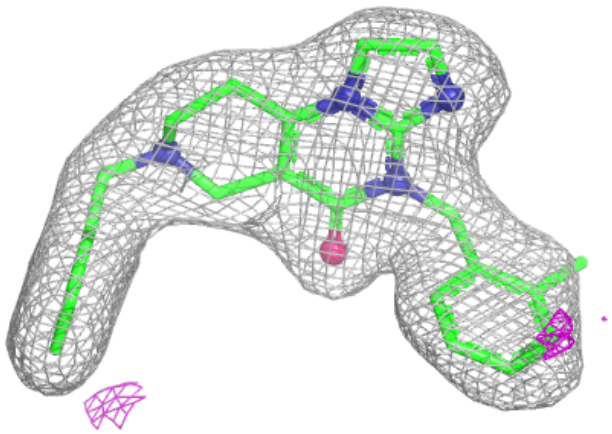
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

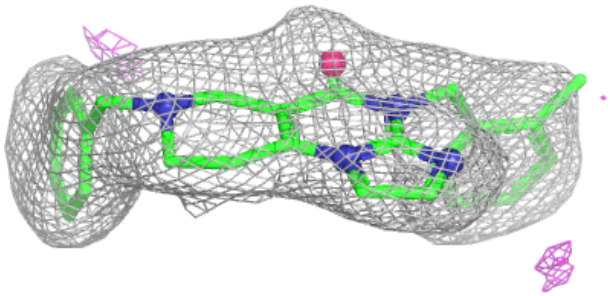
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ONC	B	301	29/29	0.94	0.10	31,52,72,75	0
2	ONC	E	301	29/29	0.95	0.10	36,42,49,50	0
2	ONC	G	301	29/29	0.95	0.09	35,45,54,56	0
2	ONC	D	301	29/29	0.96	0.09	35,44,59,62	0
2	ONC	A	301	29/29	0.96	0.10	34,42,58,65	0
2	ONC	F	301	29/29	0.96	0.09	34,41,54,60	0
2	ONC	C	301	29/29	0.96	0.09	31,44,66,68	0

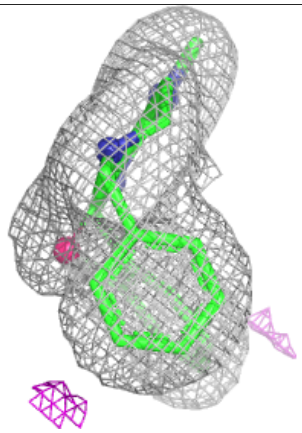
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ONC B 301:

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

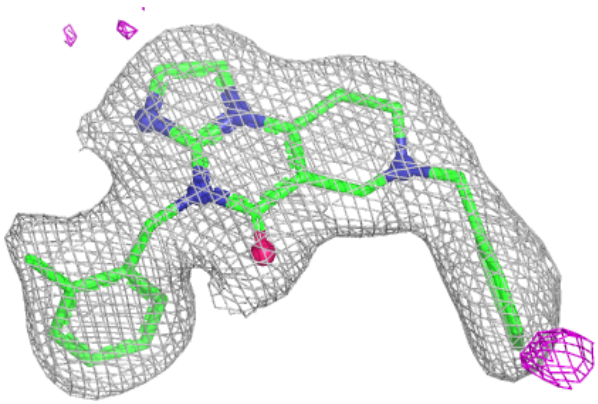


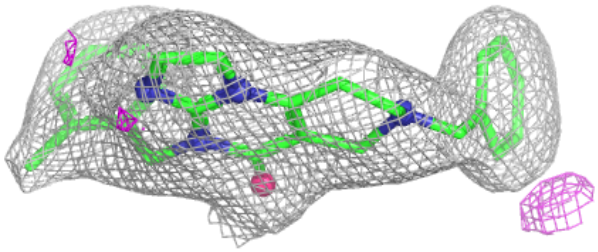


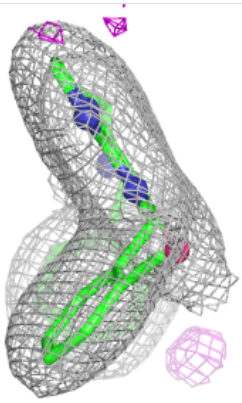


Electron density around ONC E 301:

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

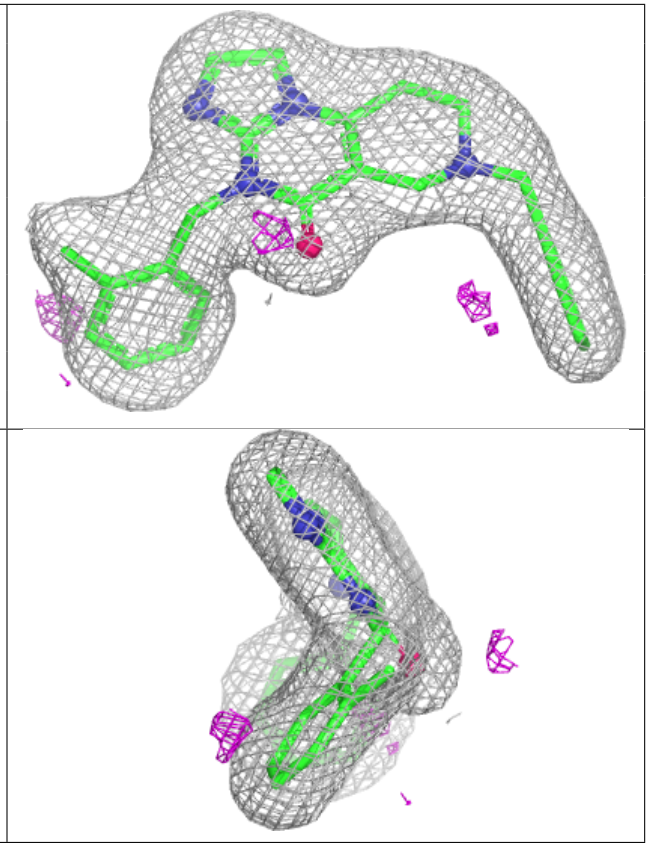






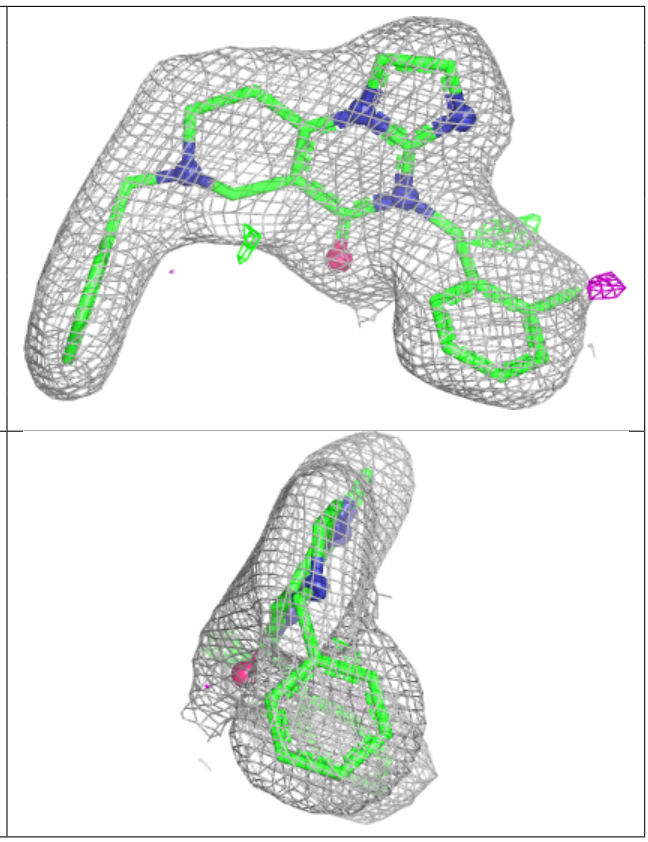
Electron density around ONC G 301:

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



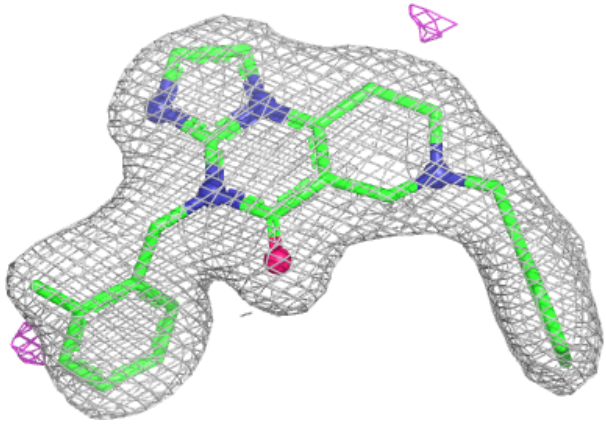
Electron density around ONC D 301:

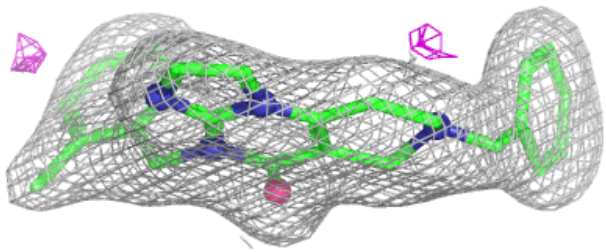
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

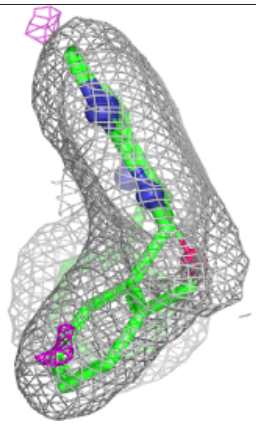


Electron density around ONC A 301:

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

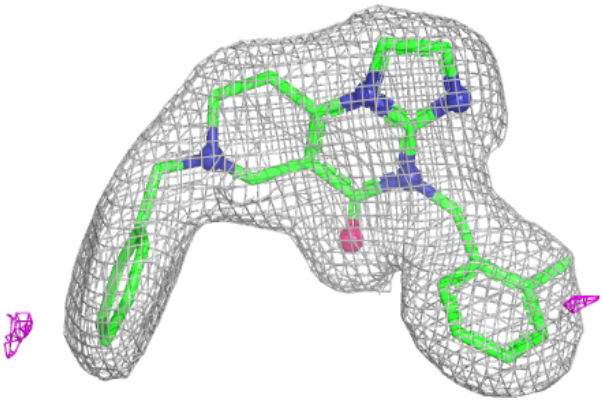


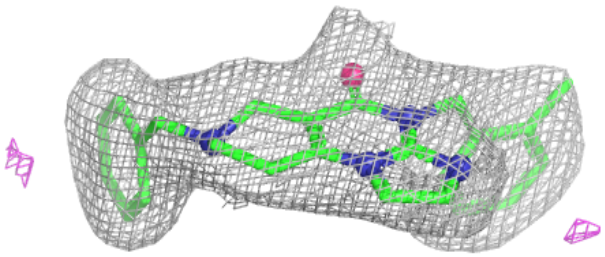


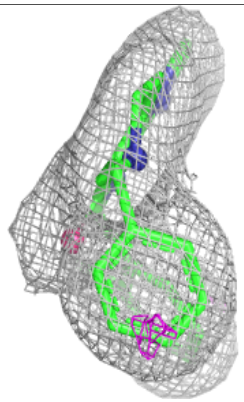


Electron density around ONC F 301:

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

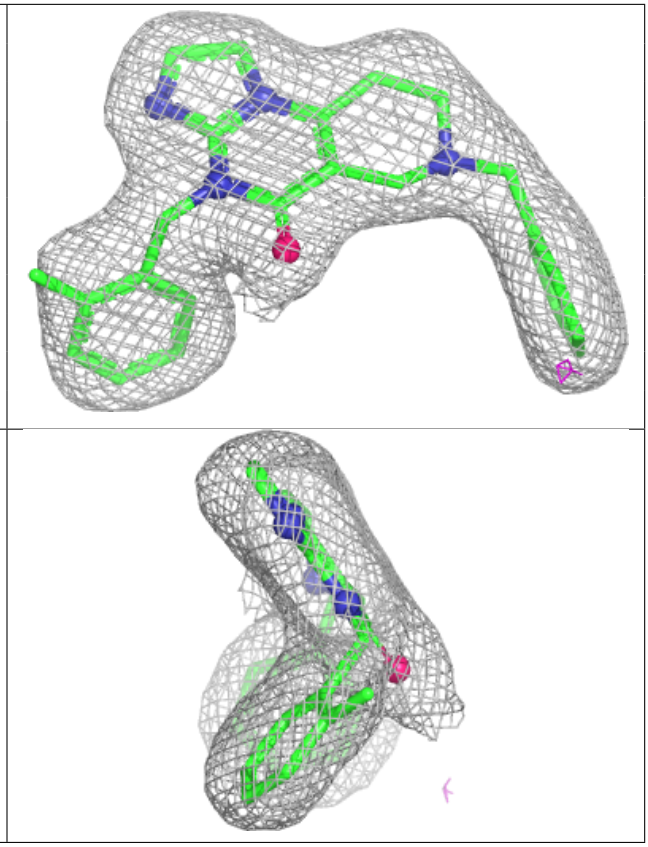






Electron density around ONC C 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.