



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 04:33 am BST

PDB ID : 3C1T  
Title : Binding of two substrate analogue molecules to dihydroflavonol 4-reductase alters the functional geometry of the catalytic site  
Authors : Trabelsi, N.; Petit, P.; Granier, T.; Langlois d'Estaintot, B.; Delrot, S.; Gallois, B.  
Deposited on : 2008-01-24  
Resolution : 2.25 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

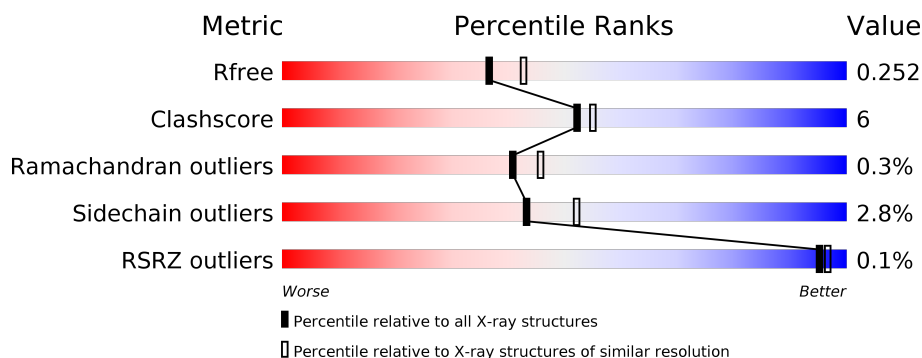
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	337	 76% 18% • 5%
1	B	337	 82% 14% • •
1	C	337	 87% 9% •
1	D	337	 86% 9% 5%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11125 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 dihydroflavonol 4-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	2	0
			2477	1588	412	457	20			
1	B	326	Total	C	N	O	S	0	2	0
			2511	1608	415	466	22			
1	C	325	Total	C	N	O	S	0	1	0
			2509	1606	413	469	21			
1	D	321	Total	C	N	O	S	0	1	0
			2484	1590	410	463	21			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



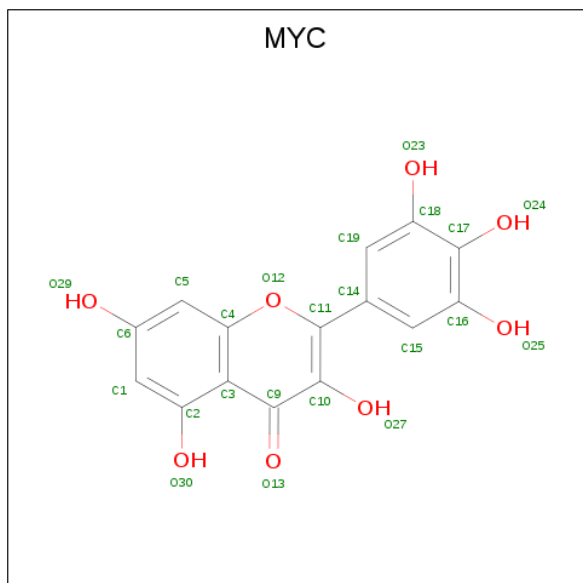
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O P	0	0
			48	21	7	17 3		
2	B	1	Total	C	N	O P	0	0
			48	21	7	17 3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 3,5,7-TRIHYDROXY-2-(3,4,5-TRIHYDROXYPHENYL)-4H-CHROMEN-4-ONE (three-letter code: MYC) (formula: C<sub>15</sub>H<sub>10</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	15	8		
3	A	1	Total	C	O	0	0
			23	15	8		
3	B	1	Total	C	O	0	0
			23	15	8		
3	B	1	Total	C	O	0	0
			23	15	8		
3	C	1	Total	C	O	0	0
			23	15	8		
3	C	1	Total	C	O	0	0
			23	15	8		
3	D	1	Total	C	O	0	0
			23	15	8		
3	D	1	Total	C	O	0	0
			23	15	8		

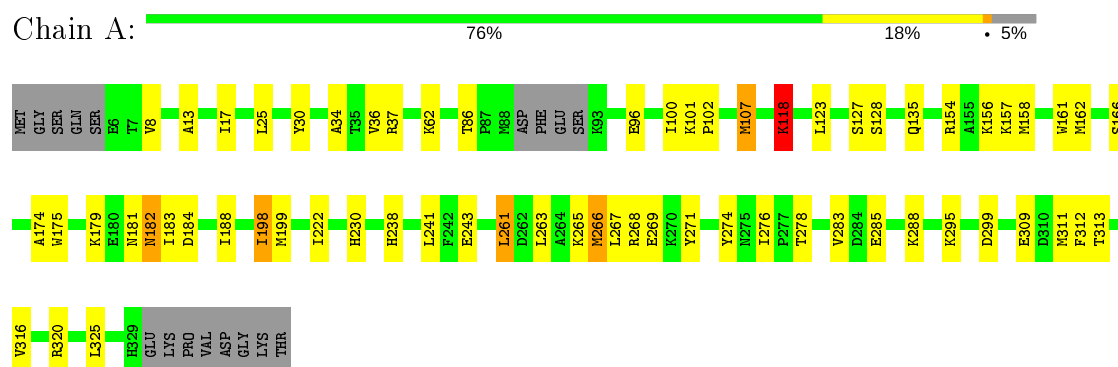
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total 151	O 151	0	0
4	B	174	Total 174	O 174	0	0
4	C	201	Total 201	O 201	0	0
4	D	242	Total 242	O 242	0	0

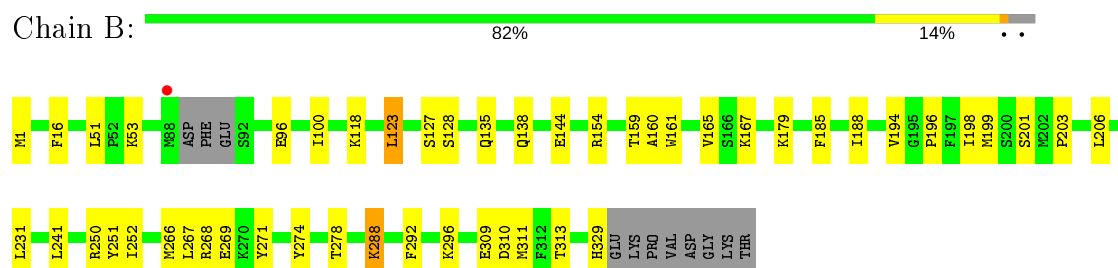
### 3 Residue-property plots [i](#)

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.

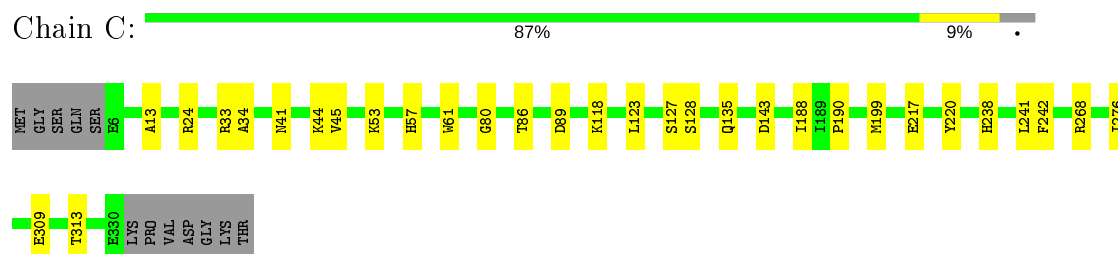
- Molecule 1: dihydroflavonol 4-reductase



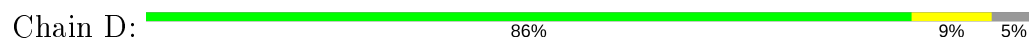
- Molecule 1: dihydroflavonol 4-reductase

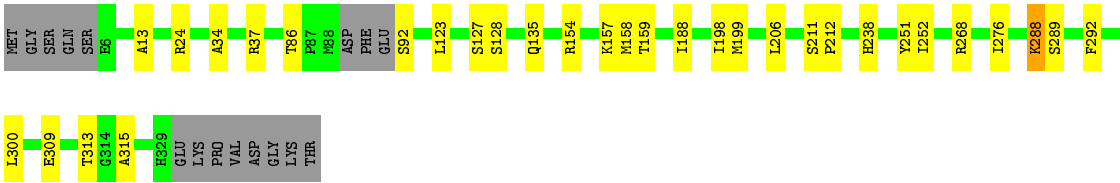


- Molecule 1: dihydroflavonol 4-reductase



- Molecule 1: dihydroflavonol 4-reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.23 Å 177.96 Å 92.60 Å 90.00° 104.77° 90.00°	Depositor
Resolution (Å)	89.09 – 2.25 88.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (89.09-2.25) 99.7 (88.98-2.25)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.25 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.186 , 0.255 0.185 , 0.252	Depositor DCC
$R_{free}$ test set	3486 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.169 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: NAP, MYC

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	0.66	0/2539	0.88	1/3450 (0.0%)
1	B	0.64	0/2573	0.87	0/3494
1	C	0.65	0/2568	0.85	2/3490 (0.1%)
1	D	0.69	0/2542	0.89	0/3453
All	All	0.66	0/10222	0.88	3/13887 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	107	MET	CG-SD-CE	5.36	108.78	100.20
1	C	24	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	2477	0	2431	44	0
1	B	2511	0	2457	31	0
1	C	2509	0	2447	19	0
1	D	2484	0	2432	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	25	4	0
2	B	48	0	25	1	0
2	C	48	0	25	4	0
2	D	48	0	25	2	0
3	A	46	0	11	2	0
3	B	46	0	11	4	0
3	C	46	0	15	2	0
3	D	46	0	10	1	0
4	A	151	0	0	3	0
4	B	174	0	0	1	0
4	C	201	0	0	3	0
4	D	242	0	0	1	0
All	All	11125	0	9914	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:GLU:O	1:D:313[B]:THR:HG22	1.65	0.95
1:A:312:PHE:O	1:A:316:VAL:HG23	1.81	0.80
1:D:199:MET:HE3	4:D:522:HOH:O	1.92	0.69
1:A:37:ARG:HD3	2:A:340:NAP:C6A	2.25	0.65
1:A:17:ILE:HD12	2:A:340:NAP:H51N	1.82	0.61
1:A:263:LEU:HD12	1:A:266:MET:HE2	1.82	0.61
1:D:309:GLU:O	1:D:313[A]:THR:HG23	2.01	0.60
1:B:16:PHE:CE1	1:B:231:LEU:HD22	2.37	0.60
1:A:175:TRP:O	1:A:179:LYS:HD3	2.02	0.59
1:B:309:GLU:O	1:B:313[A]:THR:HG23	2.04	0.58
1:A:8:VAL:HG21	1:A:25:LEU:HD13	1.86	0.58
1:A:182:ASN:HD21	1:D:159:THR:H	1.52	0.57
1:B:161:TRP:O	1:B:165:VAL:HG23	2.05	0.56
1:C:199:MET:HE1	4:C:439:HOH:O	2.07	0.55
1:A:128:SER:HG	3:A:342:MYC:HO3	1.54	0.55
1:B:96:GLU:OE2	1:B:154:ARG:NH1	2.39	0.55
1:B:128:SER:HG	3:B:342:MYC:HO3	1.55	0.54
1:B:196:PRO:O	1:B:231:LEU:HD23	2.08	0.54
1:A:285:GLU:CB	4:A:477:HOH:O	2.54	0.54
1:A:96:GLU:OE2	1:A:154:ARG:NH1	2.41	0.53
1:A:265:LYS:O	1:A:269:GLU:OE1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:SER:OG	3:A:342:MYC:O23	2.26	0.53
1:C:199:MET:HE3	4:C:390:HOH:O	2.09	0.53
1:A:271:TYR:CE2	1:A:316:VAL:HG21	2.44	0.52
1:A:316:VAL:HG13	1:A:325:LEU:CD1	2.40	0.52
1:D:37:ARG:NE	2:D:340:NAP:O3X	2.40	0.52
1:C:128:SER:OG	3:C:342:MYC:O23	2.28	0.51
1:D:188:ILE:CD1	1:D:238:HIS:HA	2.39	0.51
1:D:268:ARG:HG2	1:D:276:ILE:HB	1.93	0.51
1:A:188:ILE:CD1	1:A:241:LEU:HD12	2.41	0.51
1:A:157:LYS:HE3	1:A:161:TRP:CZ2	2.46	0.51
1:C:190:PRO:HG2	2:C:340:NAP:C6N	2.40	0.51
1:A:261:LEU:HD13	1:A:283:VAL:HG11	1.94	0.50
1:B:96:GLU:HA	1:B:100:ILE:HD12	1.94	0.50
1:B:267:LEU:O	1:B:271:TYR:N	2.39	0.50
1:D:13:ALA:CB	1:D:34:ALA:HB1	2.42	0.49
1:C:309:GLU:O	1:C:313[B]:THR:HG22	2.12	0.49
1:A:309:GLU:O	1:A:313[A]:THR:HG23	2.13	0.49
1:A:8:VAL:CG2	1:A:25:LEU:HD13	2.42	0.49
1:B:138:GLN:O	1:B:288:LYS:NZ	2.43	0.49
1:A:127:SER:O	2:A:340:NAP:H6N	2.12	0.49
1:A:13:ALA:CB	1:A:34:ALA:HB1	2.43	0.49
1:B:144:GLU:HG2	1:B:250:ARG:O	2.13	0.48
1:C:53:LYS:HE2	1:C:57:HIS:CD2	2.48	0.48
1:B:53:LYS:HD2	4:B:493:HOH:O	2.12	0.48
1:A:188:ILE:CD1	1:A:238:HIS:HA	2.44	0.48
1:A:184:ASP:OD1	1:A:184:ASP:C	2.50	0.47
1:C:309:GLU:O	1:C:313[B]:THR:CG2	2.61	0.47
1:A:268:ARG:HA	1:A:276:ILE:HD12	1.97	0.47
1:A:316:VAL:HG13	1:A:325:LEU:HD12	1.95	0.47
3:C:342:MYC:O23	4:C:519:HOH:O	2.21	0.47
1:A:30:TYR:OH	1:A:243:GLU:OE2	2.21	0.46
1:C:190:PRO:HG2	2:C:340:NAP:C5N	2.46	0.46
1:C:188:ILE:HD13	1:C:241:LEU:HD12	1.97	0.46
1:B:123:LEU:HD13	1:B:185:PHE:CD1	2.50	0.46
1:C:217:GLU:HG2	1:C:220:TYR:CE2	2.50	0.46
1:B:188:ILE:HG12	1:B:241:LEU:HD12	1.97	0.46
1:A:188:ILE:HD11	1:A:241:LEU:HD12	1.96	0.46
1:C:44:LYS:NZ	2:C:340:NAP:O1X	2.37	0.46
1:B:266:MET:CE	1:B:267:LEU:HD23	2.46	0.46
1:C:13:ALA:CB	1:C:34:ALA:HB1	2.46	0.46
1:D:251:TYR:OH	1:D:300:LEU:HD11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ASN:O	1:C:45:VAL:HG22	2.16	0.45
1:A:266:MET:HE3	1:A:267:LEU:HG	1.98	0.45
1:A:107:MET:HG2	1:A:174:ALA:HB2	1.98	0.45
1:A:230:HIS:HD2	1:A:311:MET:HA	1.82	0.45
1:A:157:LYS:HE3	1:A:161:TRP:CE2	2.52	0.45
1:B:199:MET:HE2	1:B:201:SER:O	2.17	0.45
1:B:251:TYR:CZ	1:B:296:LYS:HE2	2.52	0.45
1:A:37:ARG:HD3	2:A:340:NAP:N1A	2.32	0.45
1:C:188:ILE:CD1	1:C:241:LEU:HD12	2.46	0.45
1:B:252:ILE:HG21	1:B:292:PHE:HB3	1.99	0.44
1:D:252:ILE:HG21	1:D:292:PHE:HB3	1.99	0.44
1:B:199:MET:CE	1:B:201:SER:O	2.65	0.44
1:D:154:ARG:O	1:D:157:LYS:HE3	2.16	0.44
1:A:162:MET:O	1:A:166:SER:HB3	2.17	0.44
1:B:199:MET:HE1	1:B:203:PRO:HA	2.00	0.44
1:B:167:LYS:HG3	3:B:342:MYC:O24	2.18	0.43
1:B:268:ARG:CZ	1:B:278:THR:HA	2.49	0.43
1:A:36:VAL:O	1:A:62:LYS:HA	2.19	0.43
1:B:266:MET:HE1	1:B:267:LEU:HD23	2.01	0.43
1:B:271:TYR:OH	1:B:313[A]:THR:HA	2.19	0.43
1:C:268:ARG:HG2	1:C:276:ILE:HB	2.00	0.43
1:A:295:LYS:NZ	1:A:299:ASP:OD2	2.51	0.43
1:B:194:VAL:HG13	1:B:206:LEU:CD2	2.48	0.42
1:B:51:LEU:HD21	1:B:198:ILE:CD1	2.48	0.42
1:C:188:ILE:CD1	1:C:238:HIS:HA	2.49	0.42
1:D:288:LYS:HG2	1:D:289:SER:O	2.19	0.42
1:B:271:TYR:OH	1:B:313[B]:THR:HA	2.19	0.42
1:B:310:ASP:O	1:B:311:MET:C	2.57	0.42
1:B:274:TYR:HD1	1:B:329:HIS:ND1	2.16	0.42
1:A:118:LYS:NZ	4:A:358:HOH:O	2.53	0.42
1:A:101:LYS:HB3	1:A:102:PRO:HD3	2.02	0.42
1:A:230:HIS:CD2	1:A:311:MET:HA	2.55	0.41
1:B:159:THR:O	1:B:160:ALA:HB3	2.20	0.41
1:D:206:LEU:HD13	1:D:315:ALA:HB1	2.00	0.41
1:A:179:LYS:HE2	4:A:493:HOH:O	2.20	0.41
1:A:181:ASN:O	1:A:183:ILE:N	2.54	0.41
3:B:342:MYC:H15	3:B:342:MYC:O27	2.21	0.41
1:D:127:SER:O	2:D:340:NAP:H6N	2.21	0.41
1:B:127:SER:O	2:B:340:NAP:H6N	2.20	0.41
1:A:96:GLU:HA	1:A:100:ILE:HD12	2.03	0.41
1:A:274:TYR:OH	1:A:320:ARG:NE	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ALA:HB2	3:B:342:MYC:C4	2.50	0.41
1:D:211:SER:N	1:D:212:PRO:CD	2.84	0.41
1:A:198:ILE:HG21	1:A:198:ILE:HD13	1.82	0.40
1:C:80:GLY:HA3	1:C:242:PHE:CE1	2.56	0.40
1:A:268:ARG:HG2	1:A:276:ILE:HB	2.02	0.40
1:D:128:SER:OG	3:D:342:MYC:O25	2.36	0.40
1:D:24:ARG:HA	1:D:24:ARG:HD3	1.89	0.40
1:C:127:SER:O	2:C:340:NAP:H6N	2.20	0.40
1:C:33:ARG:HD3	1:C:61:TRP:CZ2	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	318/337 (94%)	302 (95%)	14 (4%)	2 (1%)	25	25
1	B	324/337 (96%)	308 (95%)	15 (5%)	1 (0%)	41	46
1	C	324/337 (96%)	316 (98%)	7 (2%)	1 (0%)	41	46
1	D	318/337 (94%)	307 (96%)	11 (4%)	0	100	100
All	All	1284/1348 (95%)	1233 (96%)	47 (4%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	118	LYS
1	B	118	LYS
1	C	118	LYS

### 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	267/293 (91%)	254 (95%)	13 (5%)	25	27
1	B	269/293 (92%)	263 (98%)	6 (2%)	52	61
1	C	269/293 (92%)	265 (98%)	4 (2%)	65	75
1	D	268/293 (92%)	261 (97%)	7 (3%)	46	55
All	All	1073/1172 (92%)	1043 (97%)	30 (3%)	43	52

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	THR
1	A	118	LYS
1	A	123	LEU
1	A	135	GLN
1	A	156	LYS
1	A	158	MET
1	A	198	ILE
1	A	199	MET
1	A	222	ILE
1	A	261	LEU
1	A	266	MET
1	A	278	THR
1	A	288	LYS
1	B	1	MET
1	B	123	LEU
1	B	135	GLN
1	B	179	LYS
1	B	269	GLU
1	B	288	LYS
1	C	86	THR
1	C	89	ASP
1	C	123	LEU
1	C	135	GLN
1	D	86	THR

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Mol	Chain	Res	Type
1	D	92	SER
1	D	123	LEU
1	D	135	GLN
1	D	158	MET
1	D	198	ILE
1	D	288	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	133	ASN
1	A	182	ASN
1	A	230	HIS
1	A	236	ASN
1	A	275	ASN
1	B	57	HIS
1	B	236	ASN
1	C	57	HIS
1	C	236	ASN
1	C	275	ASN
1	D	133	ASN
1	D	138	GLN
1	D	181	ASN
1	D	236	ASN
1	D	275	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MYC	C	341	-	22,25,25	1.14	2 (9%)	30,38,38	1.67	7 (23%)
2	NAP	D	340	-	45,52,52	1.64	5 (11%)	56,80,80	1.88	10 (17%)
3	MYC	D	341	-	22,25,25	1.07	0	30,38,38	1.33	6 (20%)
3	MYC	B	341	-	22,25,25	1.03	1 (4%)	30,38,38	1.45	5 (16%)
2	NAP	B	340	-	45,52,52	1.66	4 (8%)	56,80,80	2.03	14 (25%)
3	MYC	B	342	-	22,25,25	0.99	2 (9%)	30,38,38	1.45	5 (16%)
3	MYC	A	342	-	22,25,25	1.16	2 (9%)	30,38,38	1.47	5 (16%)
3	MYC	D	342	-	22,25,25	1.24	5 (22%)	30,38,38	1.69	8 (26%)
3	MYC	C	342	-	22,25,25	1.14	2 (9%)	30,38,38	2.03	9 (30%)
3	MYC	A	341	-	22,25,25	0.83	0	30,38,38	1.20	3 (10%)
2	NAP	C	340	-	45,52,52	1.64	2 (4%)	56,80,80	1.56	7 (12%)
2	NAP	A	340	-	45,52,52	1.68	5 (11%)	56,80,80	1.51	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MYC	C	341	-	-	2/4/4/4	0/3/3/3
2	NAP	D	340	-	-	8/31/67/67	0/5/5/5
3	MYC	D	341	-	-	2/4/4/4	0/3/3/3
3	MYC	B	341	-	-	2/4/4/4	0/3/3/3
2	NAP	B	340	-	-	6/31/67/67	0/5/5/5
3	MYC	B	342	-	-	2/4/4/4	0/3/3/3
3	MYC	A	342	-	-	2/4/4/4	0/3/3/3
3	MYC	D	342	-	-	2/4/4/4	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MYC	C	342	-	-	2/4/4/4	0/3/3/3
3	MYC	A	341	-	-	2/4/4/4	0/3/3/3
2	NAP	C	340	-	-	5/31/67/67	0/5/5/5
2	NAP	A	340	-	-	6/31/67/67	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	340	NAP	O7N-C7N	8.55	1.40	1.24
2	A	340	NAP	O7N-C7N	8.30	1.40	1.24
2	B	340	NAP	O7N-C7N	8.12	1.39	1.24
2	D	340	NAP	O7N-C7N	7.32	1.38	1.24
2	B	340	NAP	C2A-N3A	3.86	1.38	1.32
3	C	342	MYC	C18-C17	-3.67	1.35	1.40
2	D	340	NAP	C2N-N1N	3.46	1.39	1.35
2	A	340	NAP	C2A-N3A	3.41	1.37	1.32
2	D	340	NAP	C2A-N3A	3.39	1.37	1.32
2	A	340	NAP	O4D-C4D	-3.06	1.38	1.45
2	C	340	NAP	C2A-N3A	2.90	1.36	1.32
3	D	342	MYC	C16-C17	-2.66	1.36	1.40
2	A	340	NAP	C2N-N1N	2.53	1.38	1.35
3	D	342	MYC	C18-C17	-2.52	1.36	1.40
2	D	340	NAP	C3N-C7N	-2.45	1.46	1.50
3	C	341	MYC	O13-C9	2.43	1.27	1.23
3	A	342	MYC	C18-C17	-2.42	1.37	1.40
3	A	342	MYC	C14-C11	2.35	1.50	1.46
2	A	340	NAP	C2A-N1A	2.32	1.38	1.33
3	B	342	MYC	C18-C17	-2.27	1.37	1.40
3	D	342	MYC	C14-C11	2.26	1.50	1.46
3	C	341	MYC	C2-C3	-2.20	1.39	1.43
3	D	342	MYC	C3-C4	-2.16	1.38	1.41
3	D	342	MYC	C2-C3	-2.10	1.39	1.43
2	D	340	NAP	C2A-N1A	2.09	1.37	1.33
2	B	340	NAP	PN-O2N	-2.07	1.45	1.55
3	B	342	MYC	C14-C11	2.07	1.49	1.46
3	C	342	MYC	C14-C11	2.05	1.49	1.46
3	B	341	MYC	O13-C9	2.02	1.26	1.23
2	B	340	NAP	O4D-C4D	-2.00	1.40	1.45

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	340	NAP	N3A-C2A-N1A	-7.00	117.74	128.68
2	C	340	NAP	N3A-C2A-N1A	-6.53	118.47	128.68
2	B	340	NAP	N3A-C2A-N1A	-5.53	120.04	128.68
2	B	340	NAP	O3X-P2B-O2X	5.12	127.22	107.64
2	B	340	NAP	C3N-C7N-N7N	4.89	123.62	117.75
2	B	340	NAP	O7N-C7N-C3N	-4.74	113.97	119.63
2	A	340	NAP	N3A-C2A-N1A	-4.61	121.47	128.68
2	D	340	NAP	O7N-C7N-C3N	-4.37	114.40	119.63
2	A	340	NAP	O7N-C7N-C3N	-4.24	114.55	119.63
2	B	340	NAP	C1B-N9A-C4A	-4.15	119.34	126.64
3	D	342	MYC	O12-C4-C5	4.14	120.96	116.11
2	D	340	NAP	O2X-P2B-O1X	4.13	126.84	110.68
3	C	342	MYC	C18-C17-C16	4.00	122.06	119.51
2	D	340	NAP	C1B-N9A-C4A	-3.85	119.88	126.64
3	C	341	MYC	C5-C4-C3	-3.78	118.86	123.05
3	C	342	MYC	O23-C18-C19	3.77	129.55	119.46
3	C	342	MYC	O24-C17-C18	-3.65	109.78	119.50
2	B	340	NAP	C3N-C2N-N1N	-3.56	116.95	120.43
2	C	340	NAP	C1B-N9A-C4A	-3.54	120.43	126.64
2	B	340	NAP	O3X-P2B-O1X	-3.48	97.07	110.68
2	A	340	NAP	C3N-C7N-N7N	3.45	121.89	117.75
2	D	340	NAP	C6N-N1N-C2N	-3.43	118.85	121.97
3	C	342	MYC	C5-C4-C3	-3.26	119.44	123.05
3	C	341	MYC	O12-C4-C5	3.25	119.91	116.11
3	D	342	MYC	O25-C16-C15	3.24	128.14	119.46
3	C	342	MYC	O24-C17-C16	3.24	128.12	119.50
2	D	340	NAP	C2N-C3N-C4N	3.21	121.89	118.26
3	C	342	MYC	C14-C19-C18	-3.19	118.14	120.68
2	B	340	NAP	C2N-C3N-C4N	3.18	121.86	118.26
3	C	342	MYC	O23-C18-C17	-3.18	109.69	117.90
2	A	340	NAP	O2X-P2B-O1X	3.07	122.68	110.68
3	B	341	MYC	C15-C14-C11	-3.07	116.01	120.29
3	C	342	MYC	C2-C3-C4	3.05	121.35	117.82
3	C	341	MYC	C10-C9-C3	-3.05	117.12	121.38
3	B	341	MYC	C19-C14-C11	2.98	124.45	120.29
3	A	342	MYC	O23-C18-C19	2.95	127.38	119.46
3	D	342	MYC	O25-C16-C17	-2.93	110.32	117.90
2	C	340	NAP	O2X-P2B-O1X	2.86	121.88	110.68
3	A	342	MYC	C5-C4-C3	-2.85	119.90	123.05
3	B	342	MYC	O12-C4-C5	2.83	119.43	116.11
2	C	340	NAP	C2A-N1A-C6A	2.81	123.56	118.75
3	B	342	MYC	C18-C17-C16	2.73	121.25	119.51
3	C	341	MYC	C18-C17-C16	2.70	121.23	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	342	MYC	O24-C17-C18	2.69	126.66	119.50
3	A	342	MYC	C18-C17-C16	2.68	121.22	119.51
3	A	342	MYC	C19-C18-C17	-2.68	118.63	120.47
3	C	341	MYC	C15-C14-C11	-2.67	116.57	120.29
2	C	340	NAP	O3X-P2B-O2X	-2.66	97.46	107.64
2	D	340	NAP	O3X-P2B-O2B	2.66	117.91	105.99
3	B	342	MYC	C5-C4-C3	-2.65	120.11	123.05
2	B	340	NAP	O2N-PN-O5D	2.60	119.81	107.75
3	D	341	MYC	O12-C4-C5	2.58	119.13	116.11
3	D	342	MYC	O12-C4-C3	-2.58	118.50	121.03
3	D	342	MYC	C14-C15-C16	-2.56	118.64	120.68
2	D	340	NAP	C5N-C4N-C3N	-2.56	117.31	120.34
3	D	341	MYC	C5-C4-C3	-2.55	120.23	123.05
3	D	341	MYC	C19-C14-C11	2.51	123.80	120.29
2	D	340	NAP	O5B-PA-O1A	2.49	118.81	109.07
3	B	341	MYC	O12-C4-C5	2.48	119.01	116.11
2	A	340	NAP	O2A-PA-O1A	2.43	124.23	112.24
3	D	342	MYC	O24-C17-C16	-2.42	113.06	119.50
3	B	341	MYC	C14-C15-C16	-2.41	118.76	120.68
2	B	340	NAP	C2D-C3D-C4D	2.38	107.27	102.64
2	D	340	NAP	C3N-C7N-N7N	2.38	120.60	117.75
2	A	340	NAP	O2N-PN-O1N	2.36	123.89	112.24
3	D	341	MYC	O29-C6-C5	-2.35	114.23	120.98
3	C	341	MYC	C19-C14-C11	2.33	123.53	120.29
3	B	342	MYC	C2-C3-C4	2.30	120.48	117.82
3	B	341	MYC	C10-C9-C3	-2.29	118.17	121.38
3	A	341	MYC	C10-C9-C3	-2.29	118.17	121.38
2	B	340	NAP	C4A-C5A-N7A	-2.28	107.02	109.40
3	D	342	MYC	C5-C4-C3	-2.26	120.54	123.05
2	B	340	NAP	O2X-P2B-O1X	2.20	119.28	110.68
2	B	340	NAP	O2X-P2B-O2B	-2.16	96.32	105.99
3	A	341	MYC	C1-C2-C3	-2.16	118.11	120.61
3	D	341	MYC	C2-C3-C4	2.14	120.30	117.82
3	B	342	MYC	O23-C18-C19	2.12	125.15	119.46
2	C	340	NAP	C6N-N1N-C2N	-2.12	120.05	121.97
3	C	341	MYC	C2-C3-C4	2.11	120.27	117.82
2	B	340	NAP	O4D-C1D-C2D	2.10	110.00	106.93
3	A	342	MYC	O12-C4-C5	2.10	118.56	116.11
3	D	341	MYC	C15-C14-C11	-2.09	117.37	120.29
3	A	341	MYC	C2-C3-C4	2.06	120.21	117.82
2	C	340	NAP	C5A-C6A-N6A	2.02	123.42	120.35
3	C	342	MYC	C14-C15-C16	-2.01	119.08	120.68

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	340	NAP	C5D-O5D-PN-O1N
2	D	340	NAP	C5D-O5D-PN-O2N
2	B	340	NAP	C5B-O5B-PA-O1A
2	B	340	NAP	C5D-O5D-PN-O2N
3	B	342	MYC	C10-C11-C14-C15
3	B	342	MYC	C10-C11-C14-C19
3	A	342	MYC	C10-C11-C14-C15
3	A	342	MYC	C10-C11-C14-C19
3	D	342	MYC	C10-C11-C14-C15
3	D	342	MYC	C10-C11-C14-C19
3	C	342	MYC	C10-C11-C14-C15
3	C	342	MYC	C10-C11-C14-C19
2	C	340	NAP	C5D-O5D-PN-O2N
2	A	340	NAP	C5D-O5D-PN-O1N
2	A	340	NAP	C5D-O5D-PN-O2N
3	C	341	MYC	O12-C11-C14-C15
3	C	341	MYC	O12-C11-C14-C19
3	D	341	MYC	O12-C11-C14-C15
3	D	341	MYC	O12-C11-C14-C19
3	B	341	MYC	O12-C11-C14-C15
3	B	341	MYC	O12-C11-C14-C19
3	A	341	MYC	O12-C11-C14-C15
3	A	341	MYC	O12-C11-C14-C19
2	D	340	NAP	PN-O3-PA-O5B
2	D	340	NAP	C2B-O2B-P2B-O3X
2	C	340	NAP	C5D-O5D-PN-O3
2	D	340	NAP	PA-O3-PN-O2N
2	B	340	NAP	C5D-O5D-PN-O1N
2	C	340	NAP	C5D-O5D-PN-O1N
2	B	340	NAP	PA-O3-PN-O2N
2	D	340	NAP	O4B-C4B-C5B-O5B
2	C	340	NAP	O4B-C4B-C5B-O5B
2	C	340	NAP	PA-O3-PN-O2N
2	A	340	NAP	C2B-O2B-P2B-O1X
2	B	340	NAP	O4B-C4B-C5B-O5B
2	D	340	NAP	C5D-O5D-PN-O3
2	B	340	NAP	C5D-O5D-PN-O3
2	A	340	NAP	C5D-O5D-PN-O3
2	A	340	NAP	O4B-C4B-C5B-O5B
2	D	340	NAP	PA-O3-PN-O1N

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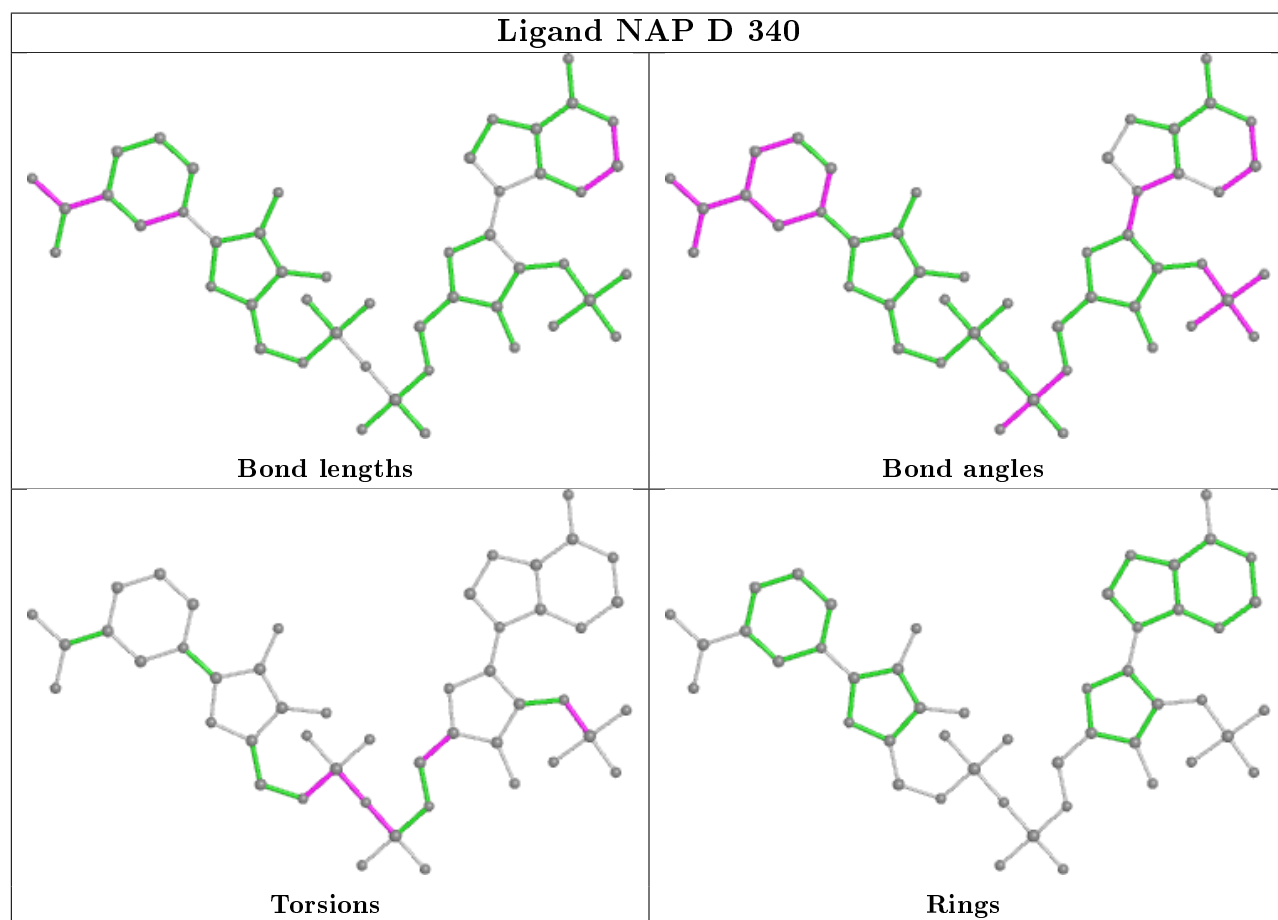
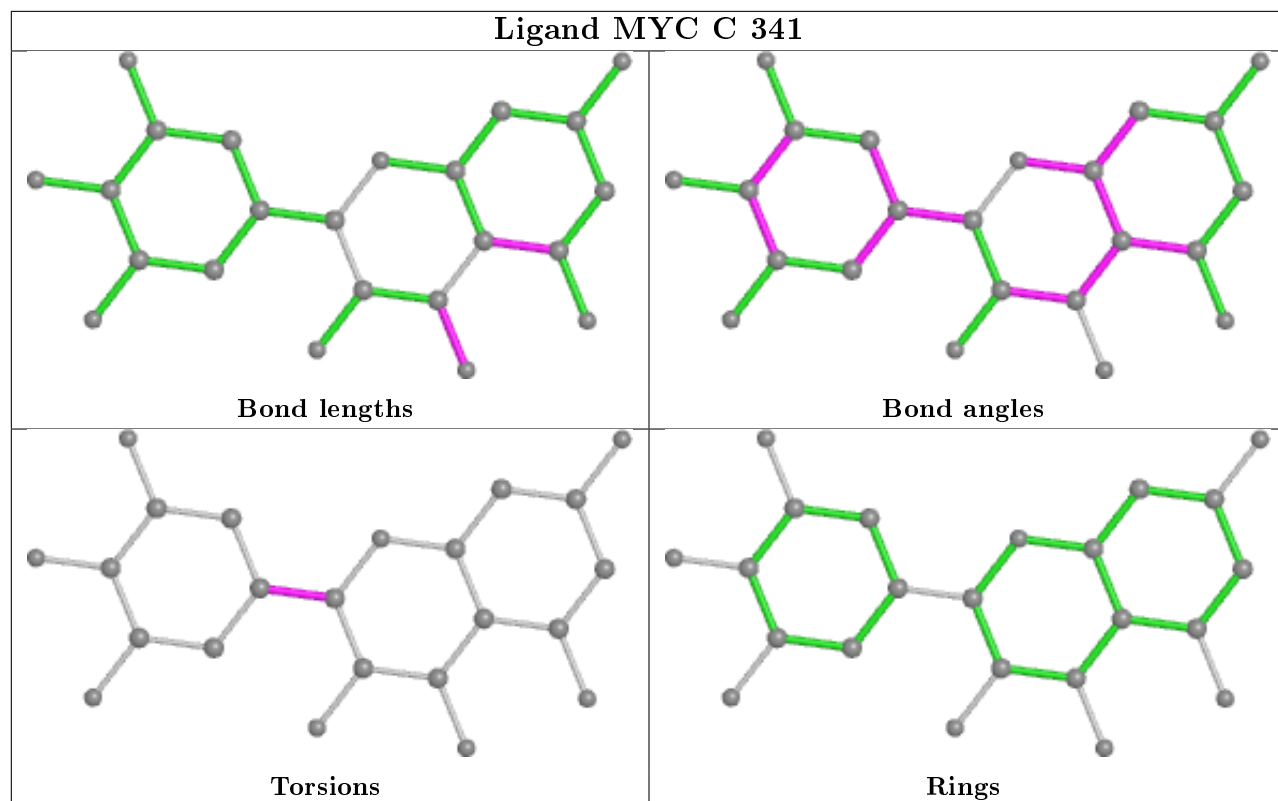
Mol	Chain	Res	Type	Atoms
2	A	340	NAP	PA-O3-PN-O1N

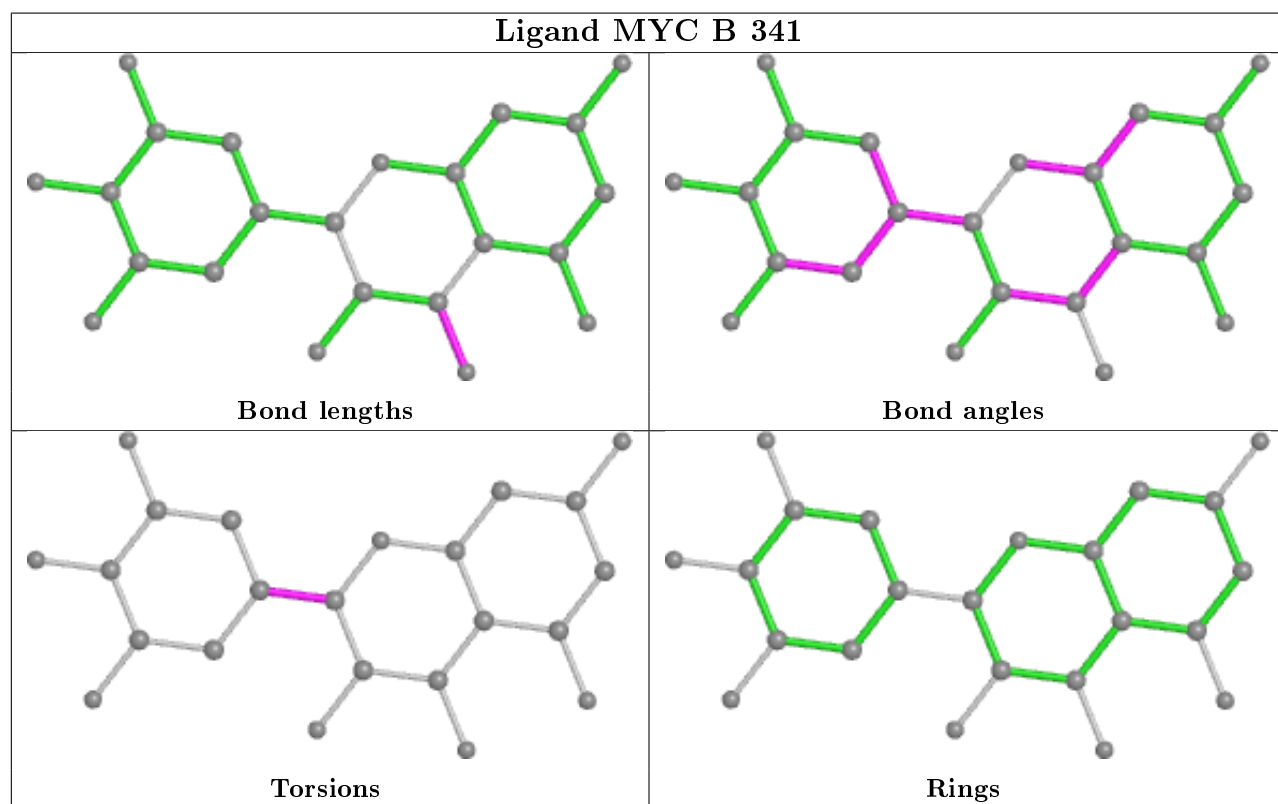
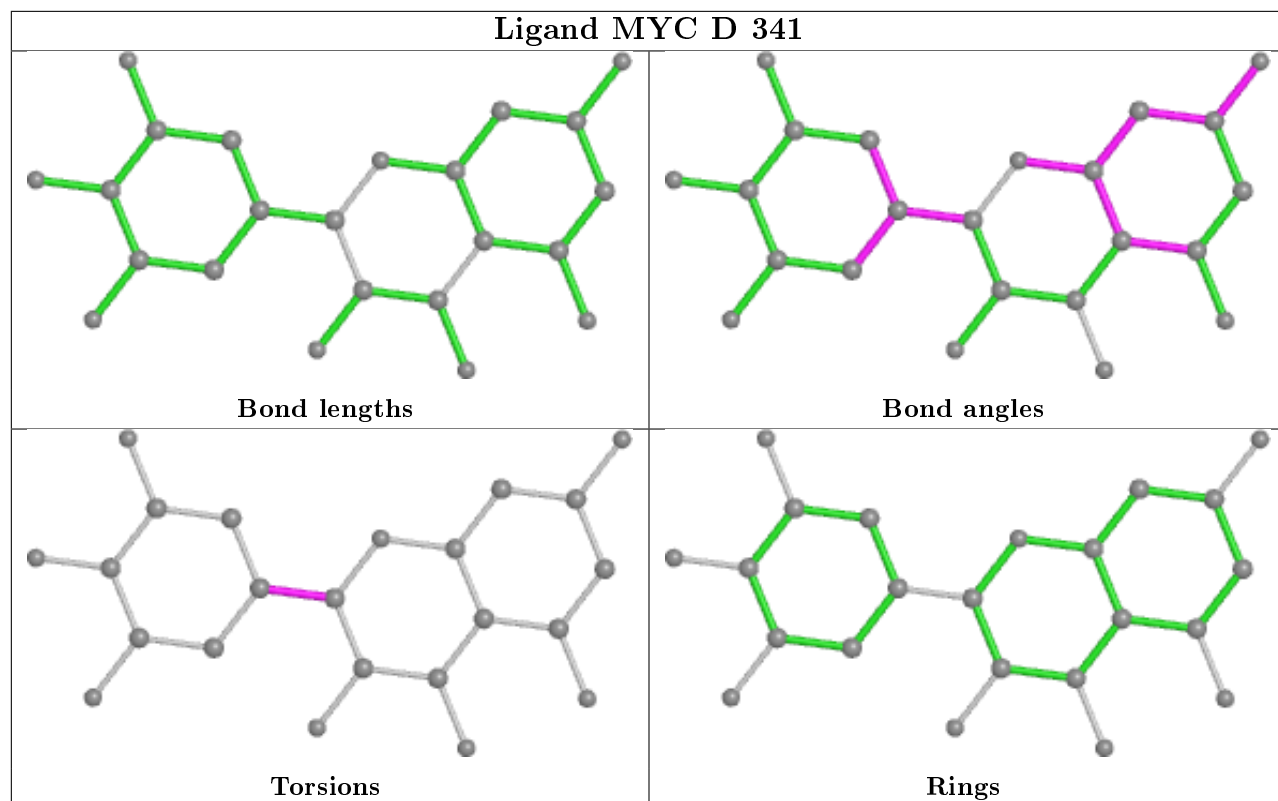
There are no ring outliers.

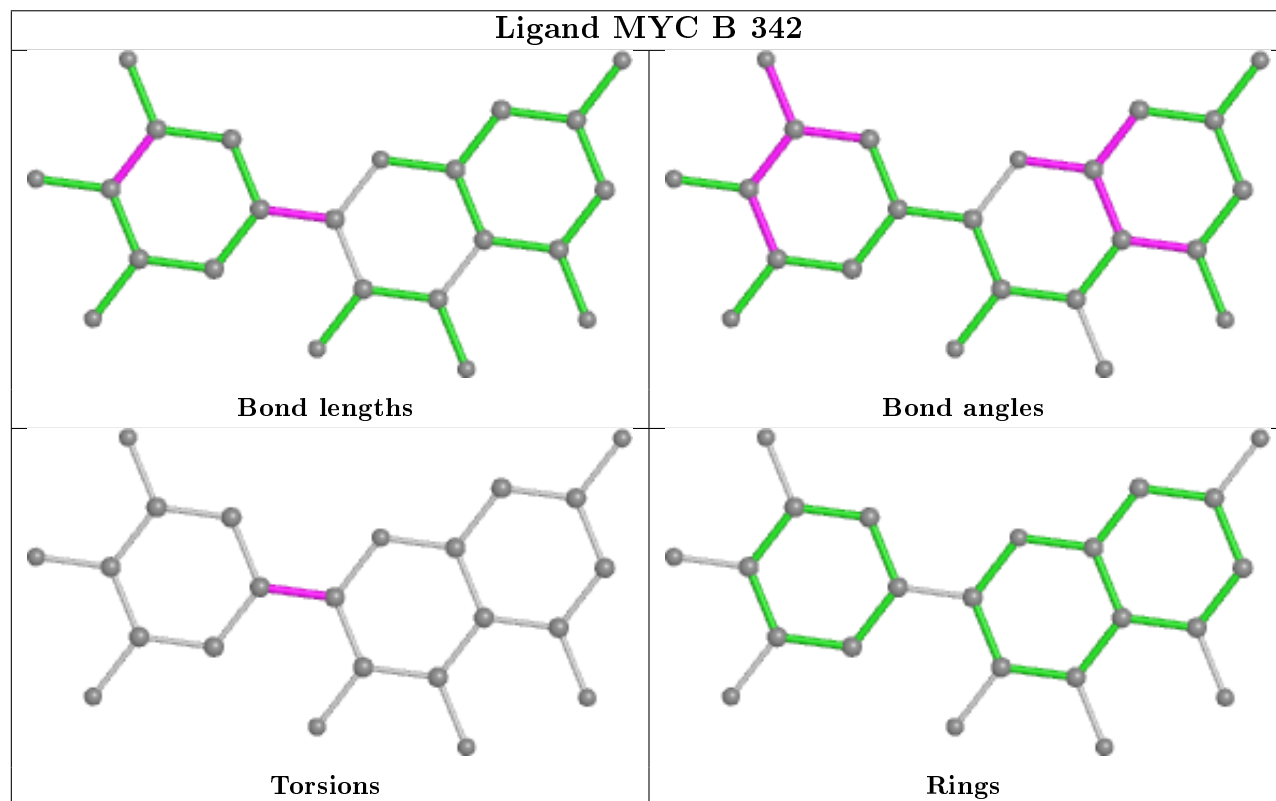
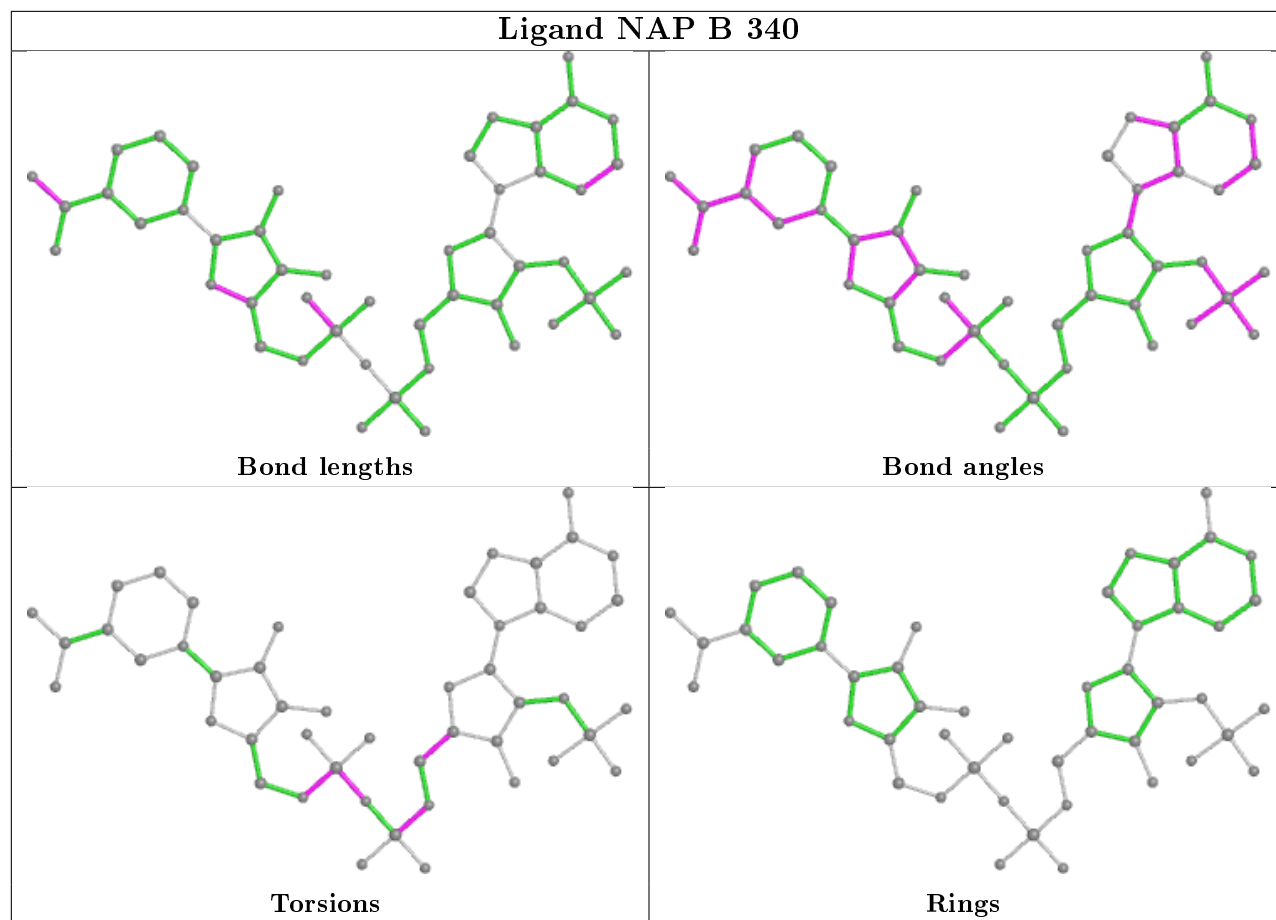
8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	340	NAP	2	0
2	B	340	NAP	1	0
3	B	342	MYC	4	0
3	A	342	MYC	2	0
3	D	342	MYC	1	0
3	C	342	MYC	2	0
2	C	340	NAP	4	0
2	A	340	NAP	4	0

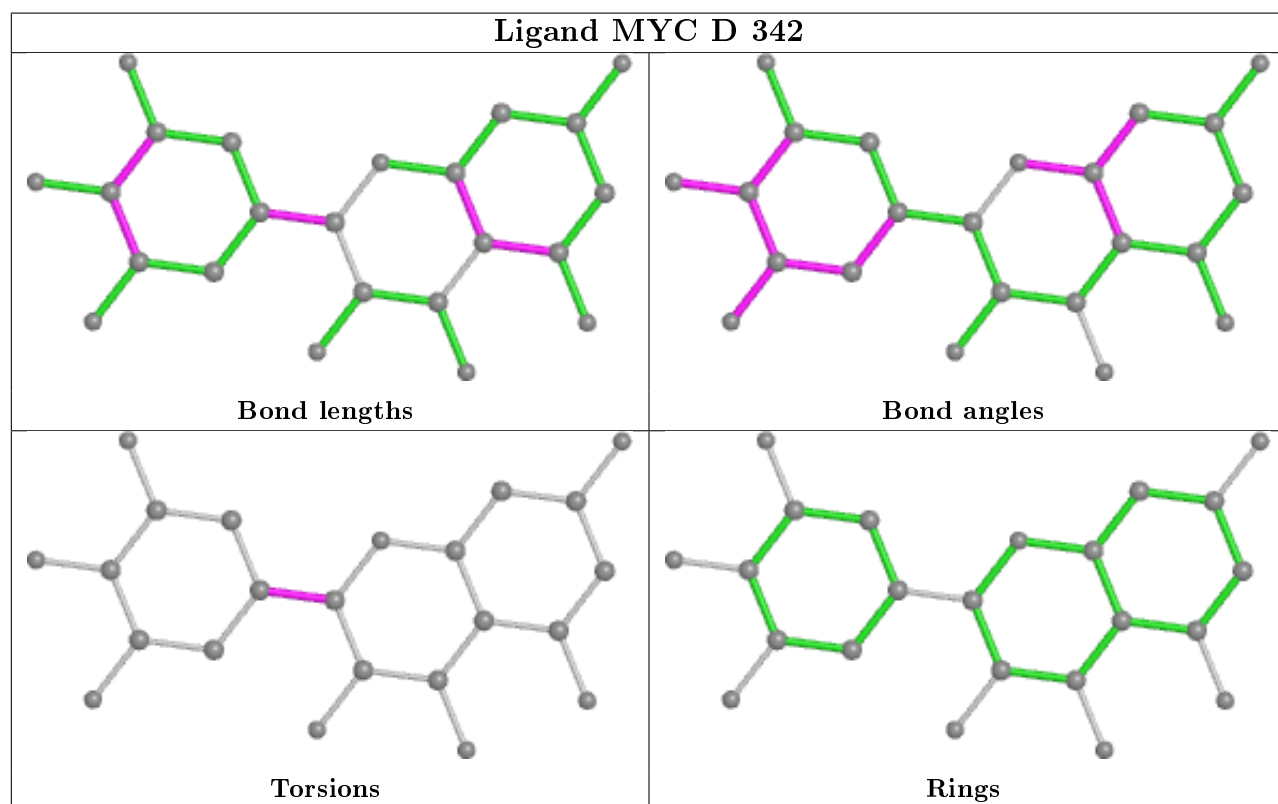
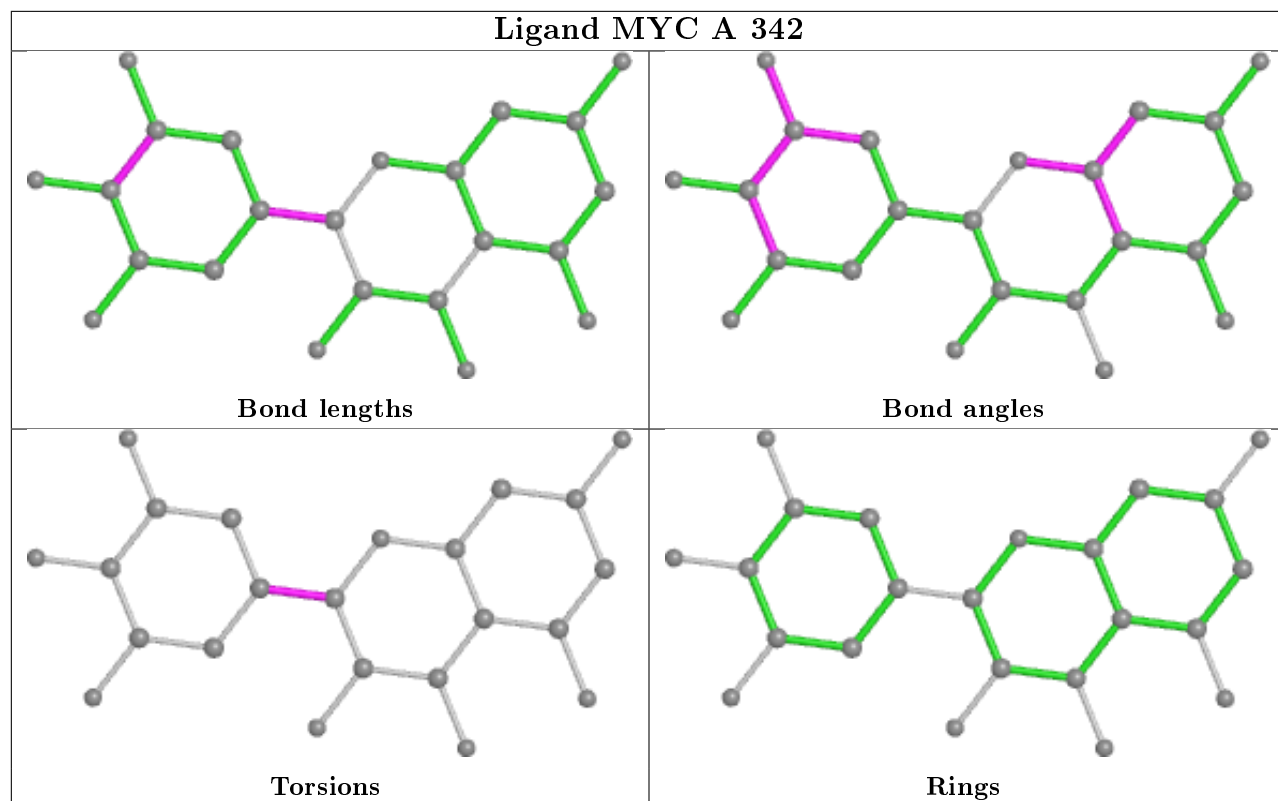
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

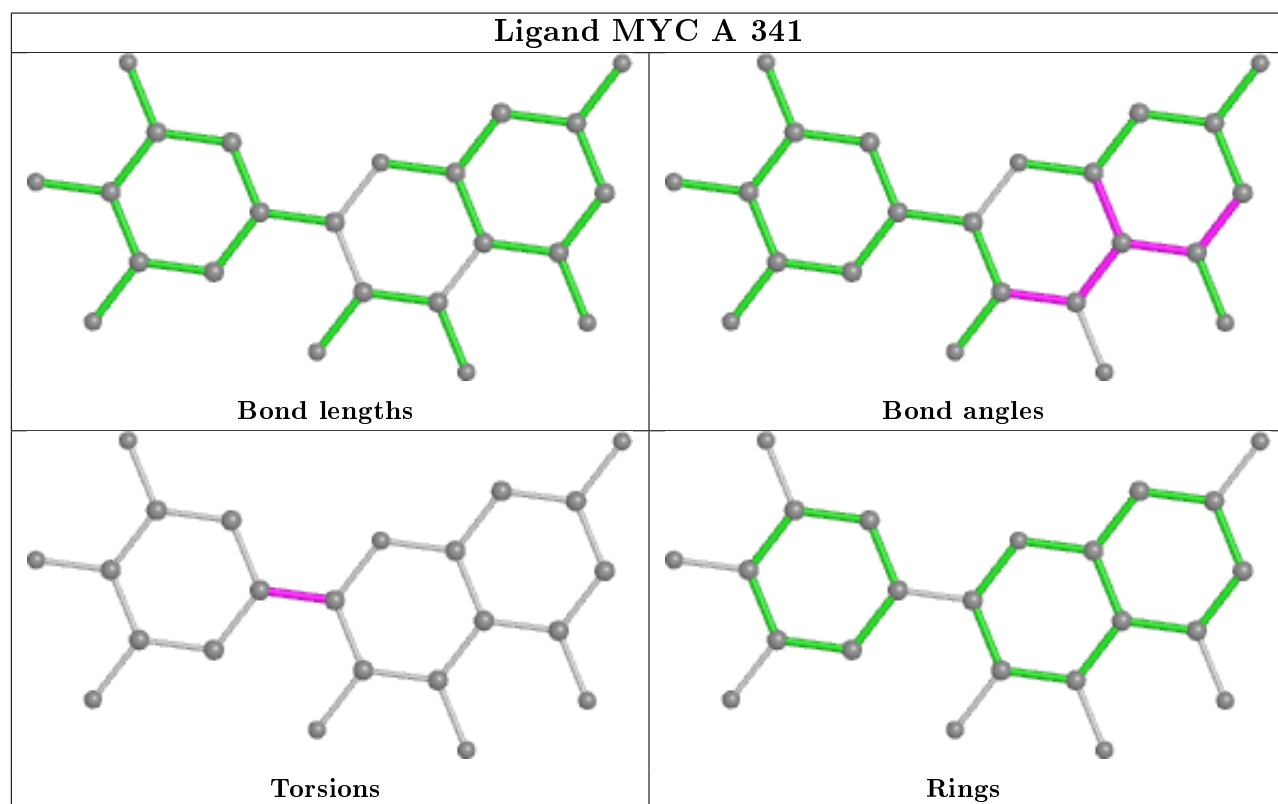
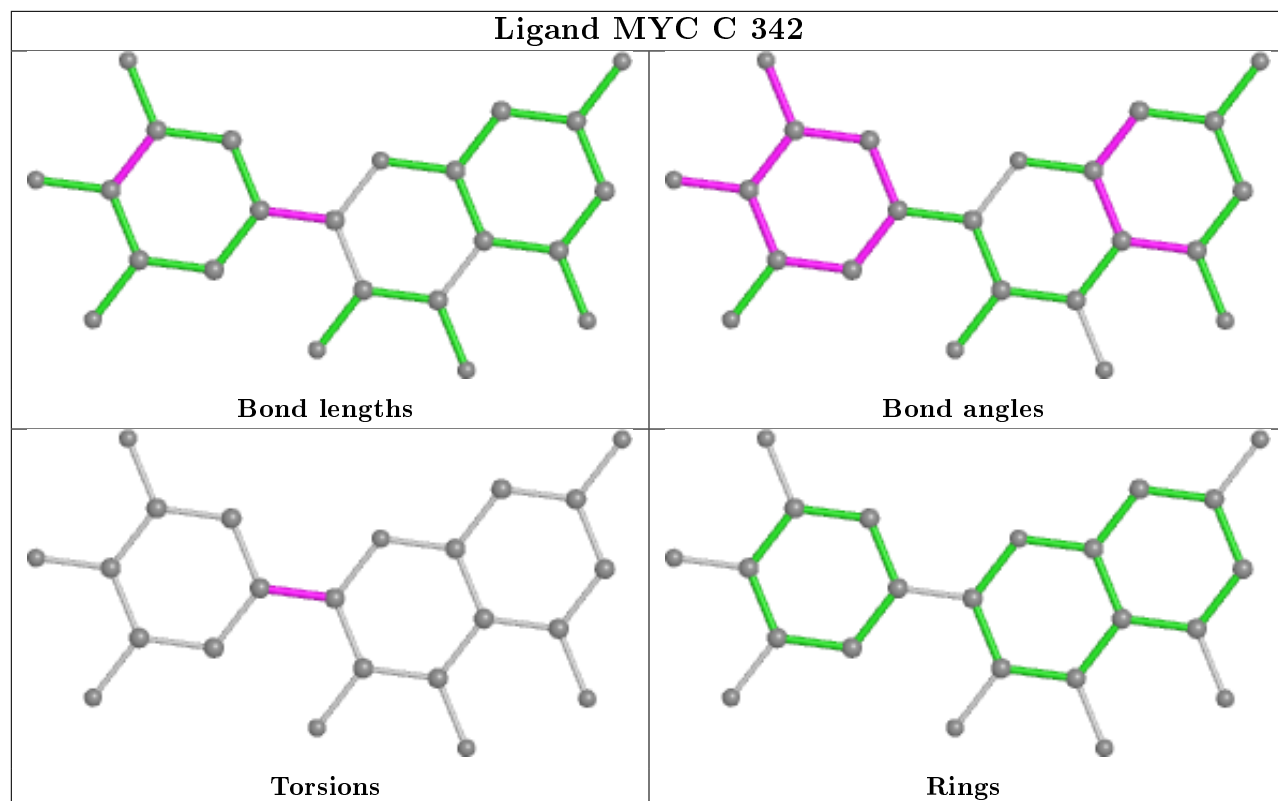


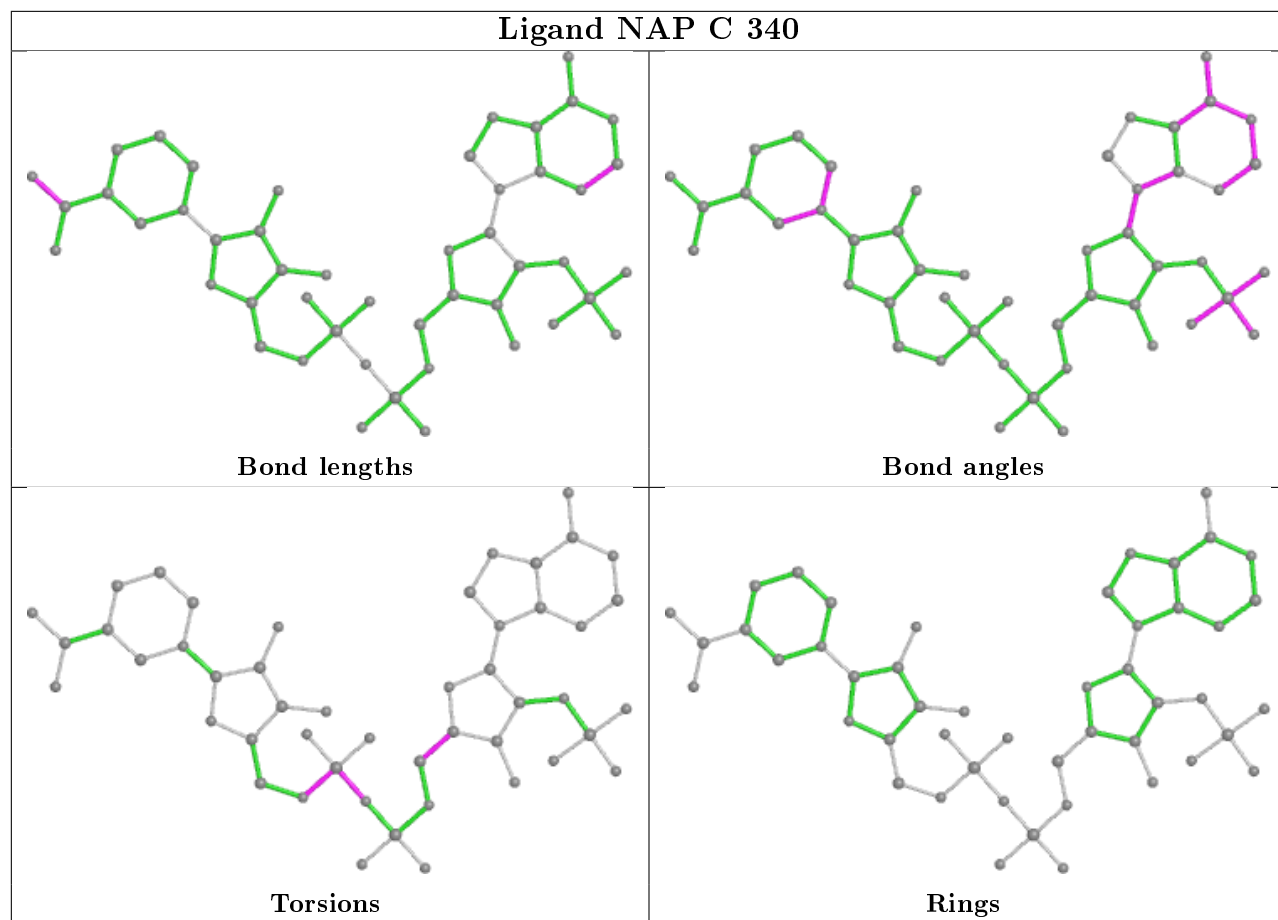


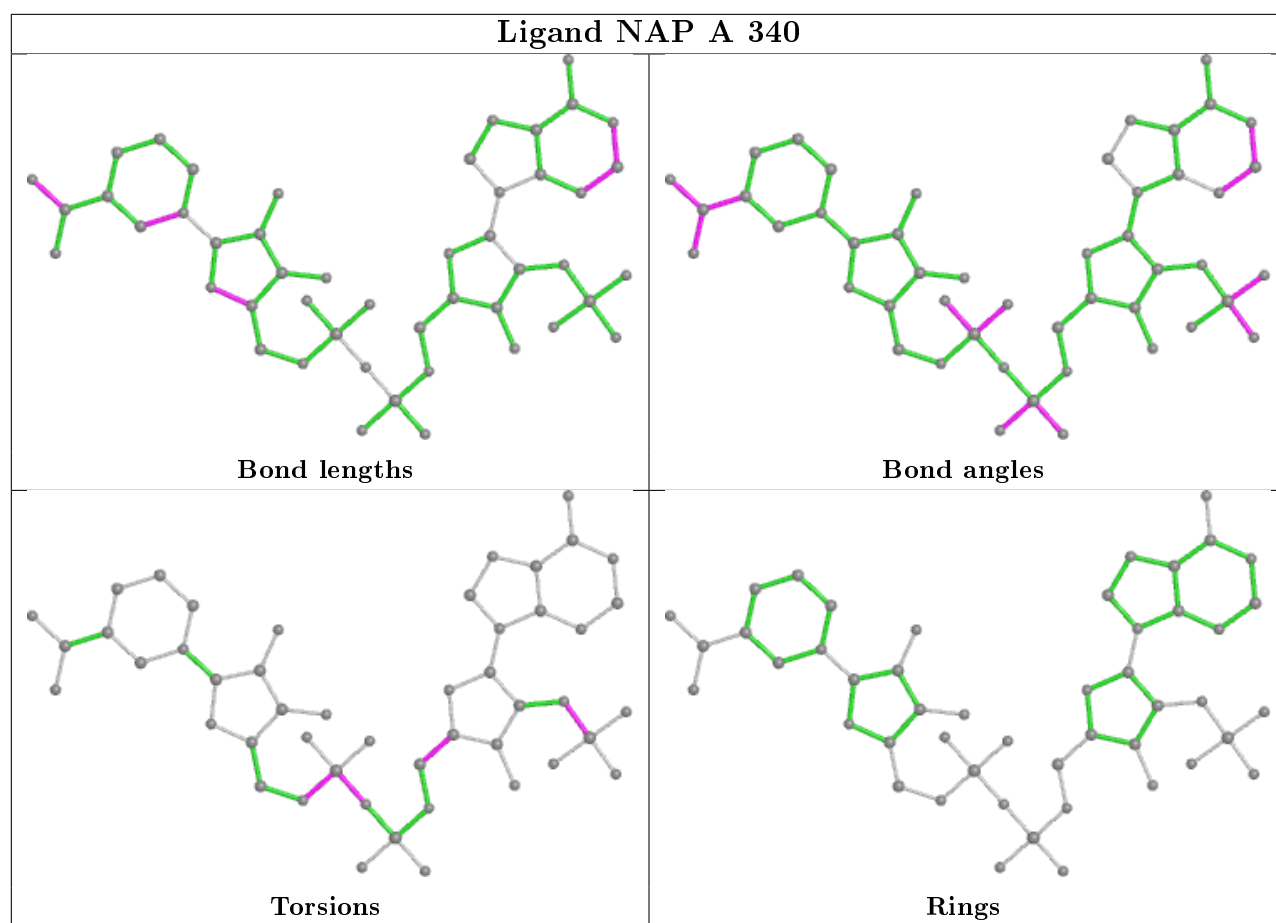












## 5.7 Other polymers [i](#)

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, 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	320/337 (94%)	-0.16	0 <b>100</b> <b>100</b>	29, 45, 64, 79	0
1	B	326/337 (96%)	-0.20	1 (0%) <b>94</b> <b>94</b>	29, 44, 65, 88	0
1	C	325/337 (96%)	-0.32	0 <b>100</b> <b>100</b>	27, 42, 62, 80	0
1	D	321/337 (95%)	-0.30	0 <b>100</b> <b>100</b>	27, 41, 60, 80	0
All	All	1292/1348 (95%)	-0.25	1 (0%) <b>95</b> <b>96</b>	27, 43, 63, 88	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	MET	2.1

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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.

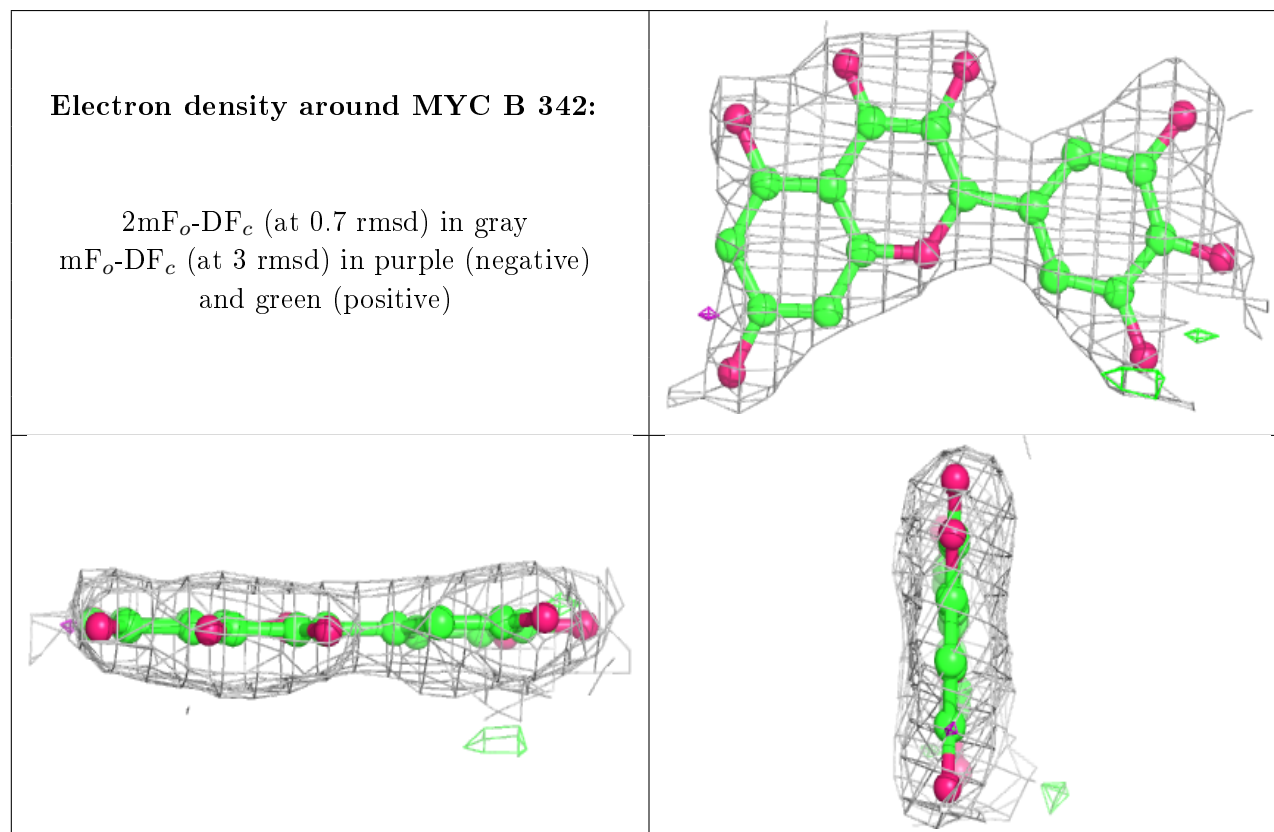
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MYC	B	342	23/23	0.94	0.18	44,55,56,57	0

*Continued on next page...*

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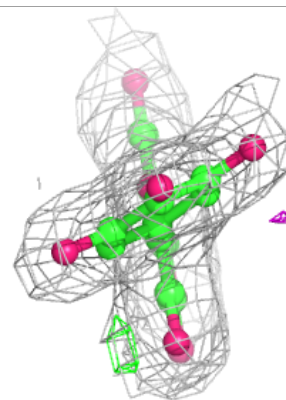
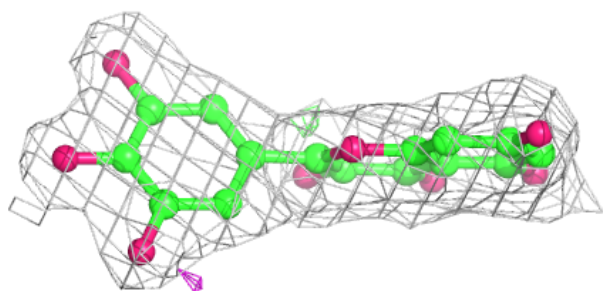
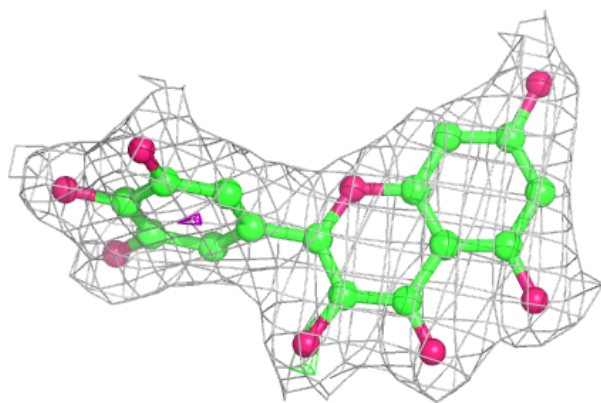
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MYC	B	341	23/23	0.95	0.10	36,41,42,43	0
3	MYC	A	342	23/23	0.95	0.15	34,50,52,53	0
3	MYC	D	342	23/23	0.96	0.11	28,31,33,34	0
3	MYC	A	341	23/23	0.97	0.12	36,40,41,42	0
2	NAP	D	340	48/48	0.98	0.11	22,31,48,53	0
3	MYC	D	341	23/23	0.98	0.10	28,31,32,33	0
3	MYC	C	341	23/23	0.98	0.10	29,31,32,34	0
3	MYC	C	342	23/23	0.98	0.11	26,30,33,33	0
2	NAP	B	340	48/48	0.98	0.11	29,35,51,55	0
2	NAP	C	340	48/48	0.98	0.11	24,32,46,51	0
2	NAP	A	340	48/48	0.98	0.11	30,35,53,59	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.

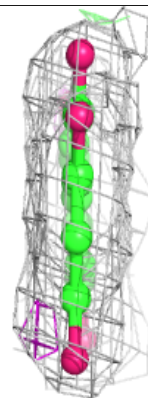
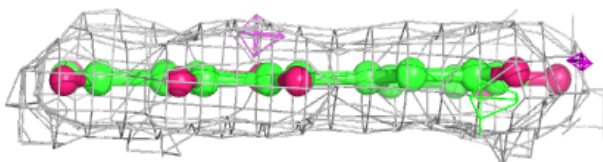
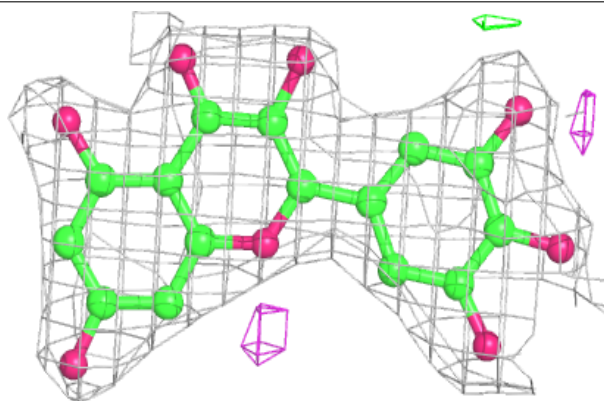


**Electron density around MYC B 341:**

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

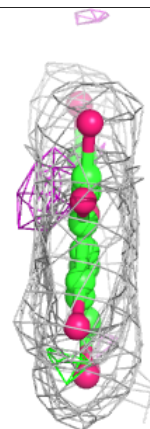
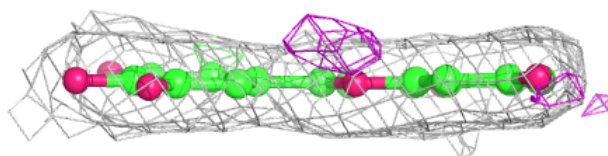
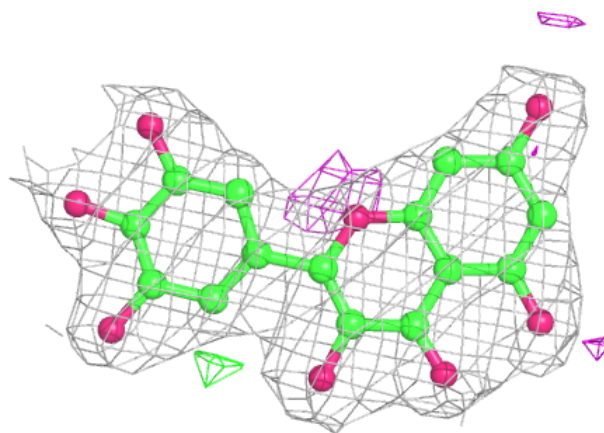
**Electron density around MYC A 342:**

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



**Electron density around MYC D 342:**

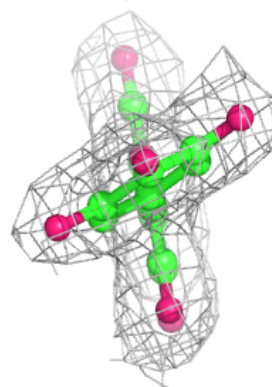
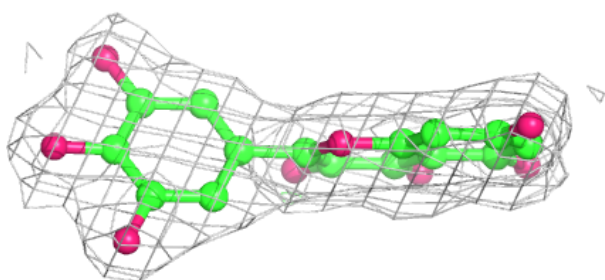
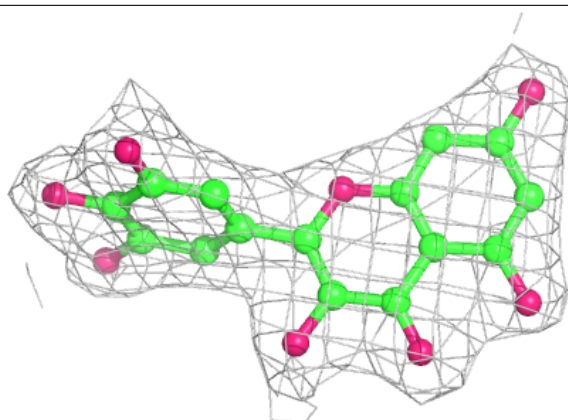
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



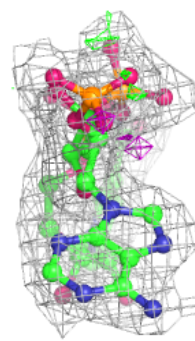
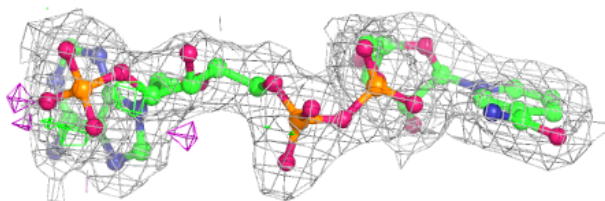
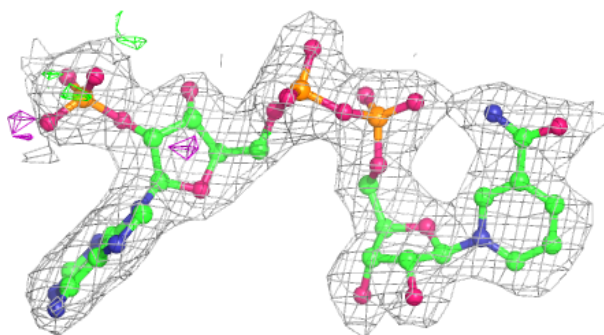


**Electron density around MYC A 341:**

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

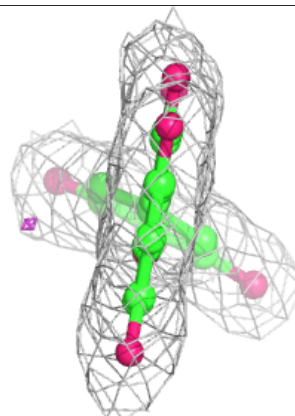
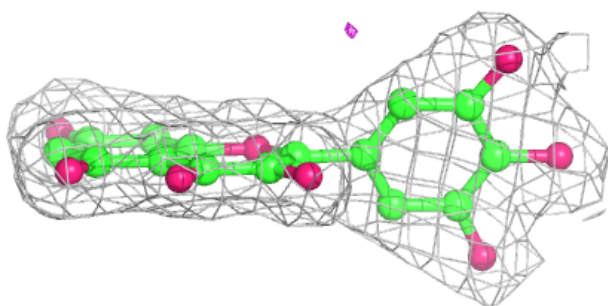
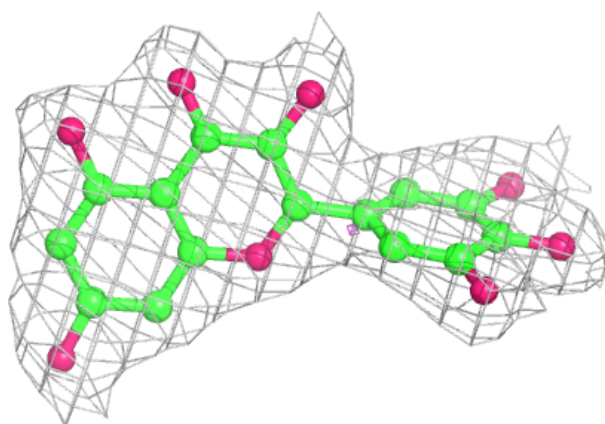
**Electron density around NAP D 340:**

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and green (positive)

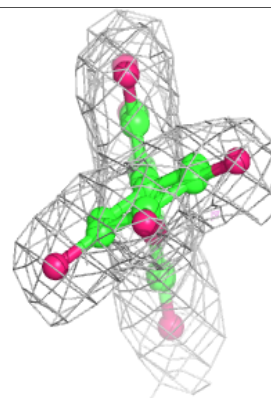
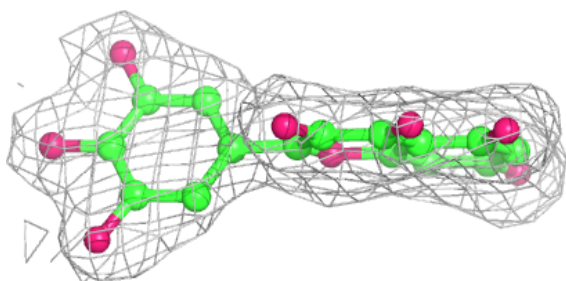
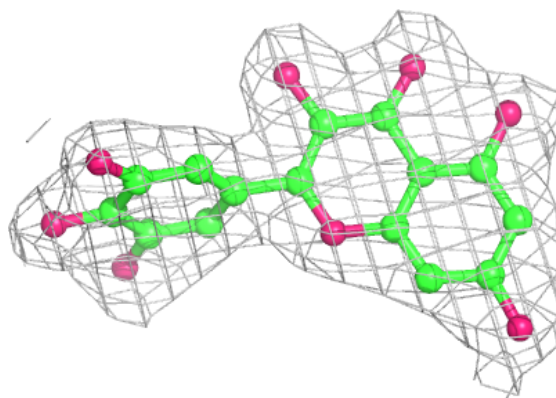


**Electron density around MYC D 341:**

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and green (positive)

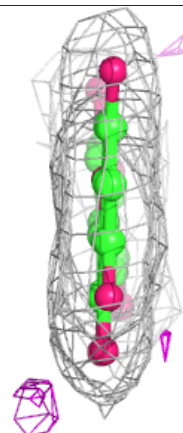
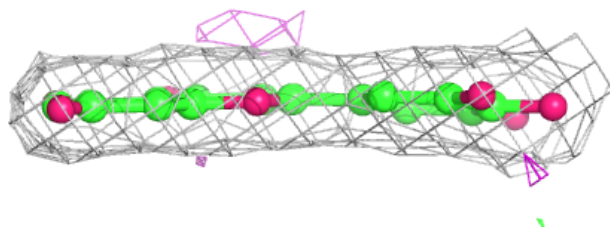
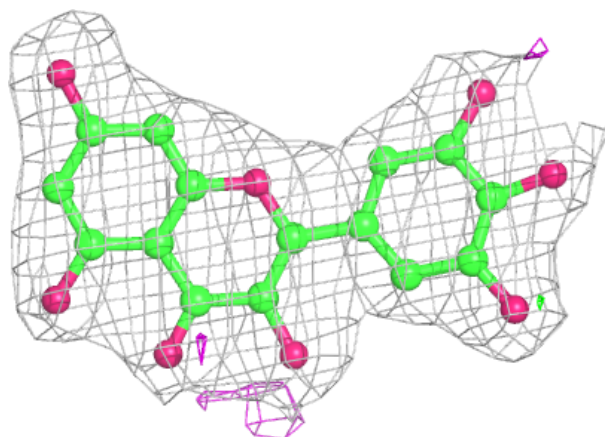
**Electron density around MYC C 341:**

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and green (positive)

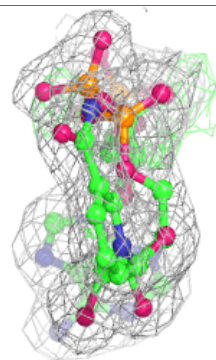
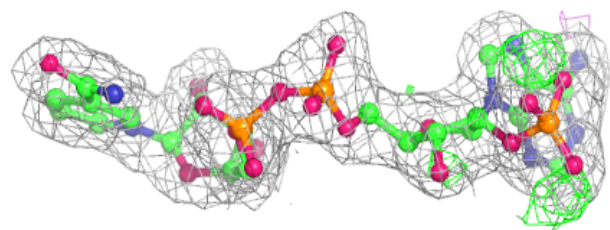
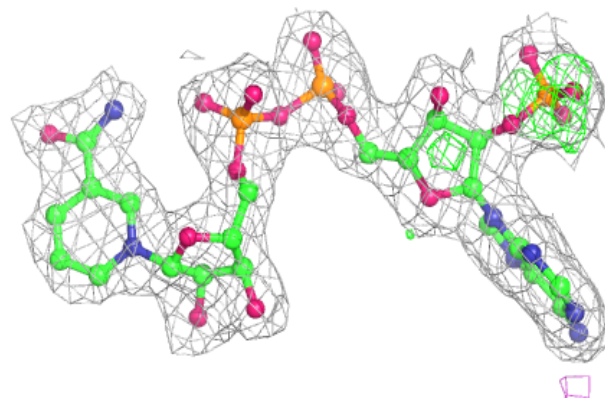


**Electron density around MYC C 342:**

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

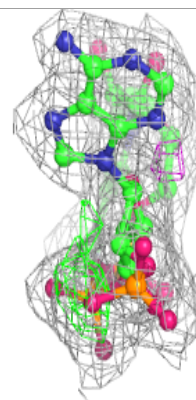
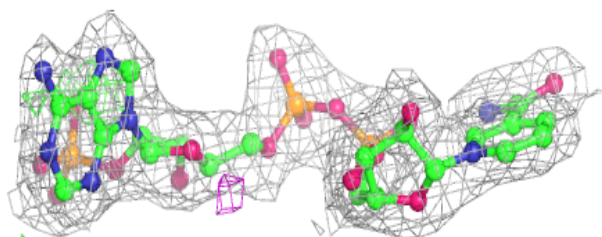
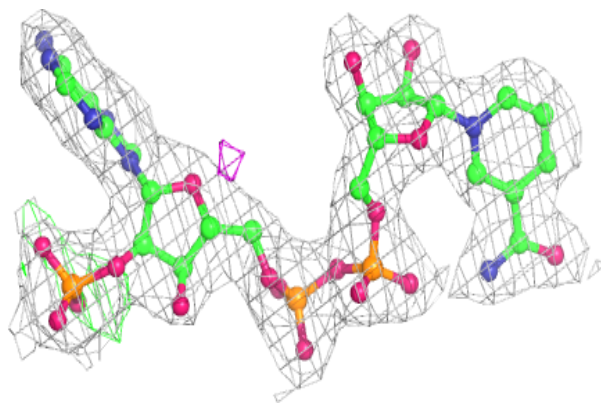
**Electron density around NAP B 340:**

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

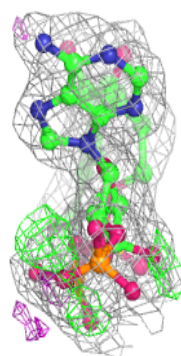
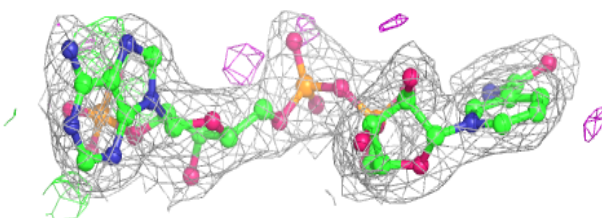
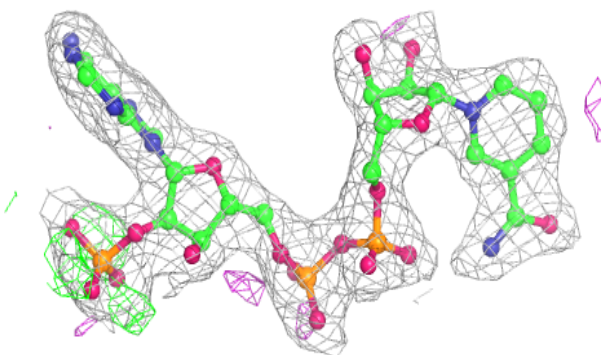


**Electron density around NAP C 340:**

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

**Electron density around NAP A 340:**

$2mF_o-DF_c$  (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.