



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:51 AM UTC

PDB ID : 3C1T / pdb_00003c1t
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

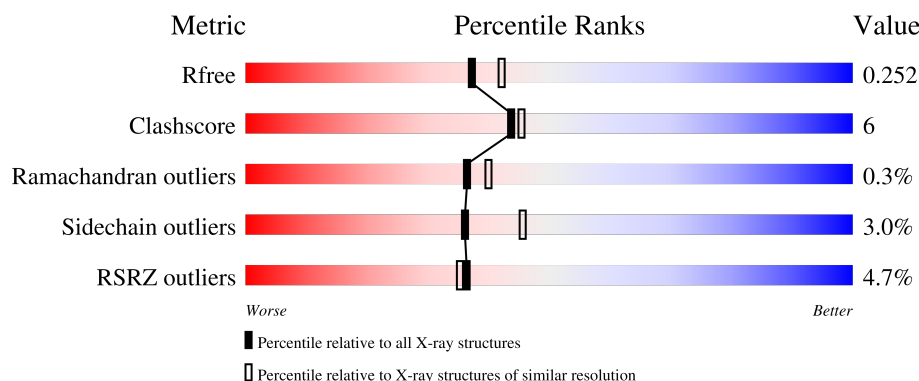
1 Overall quality at a glance

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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 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 $\leq 5\%$. 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.

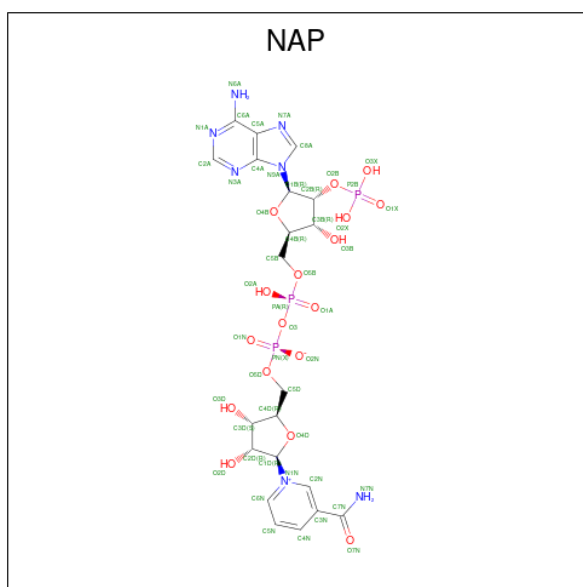
Mol	Chain	Length	Quality of chain
1	A	337	 7% 74% 20% • 5%
1	B	337	 7% 81% 15% • •
1	C	337	 3% 85% 12% •
1	D	337	 % 83% 11% • 5%

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 2477	C 1588	N 412	O 457	S 20	0	2	0
1	B	326	Total 2511	C 1608	N 415	O 466	S 22	0	2	0
1	C	325	Total 2509	C 1606	N 413	O 469	S 21	0	1	0
1	D	321	Total 2484	C 1590	N 410	O 463	S 21	0	1	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



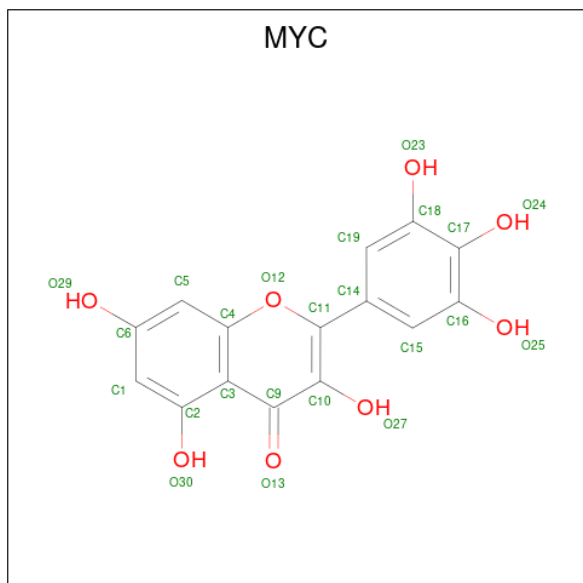
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

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-TRIHIDROXYPHENYL)-4H-CHROMEN-4-ONE (CCD ID: MYC) (formula: C₁₅H₁₀O₈).



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		

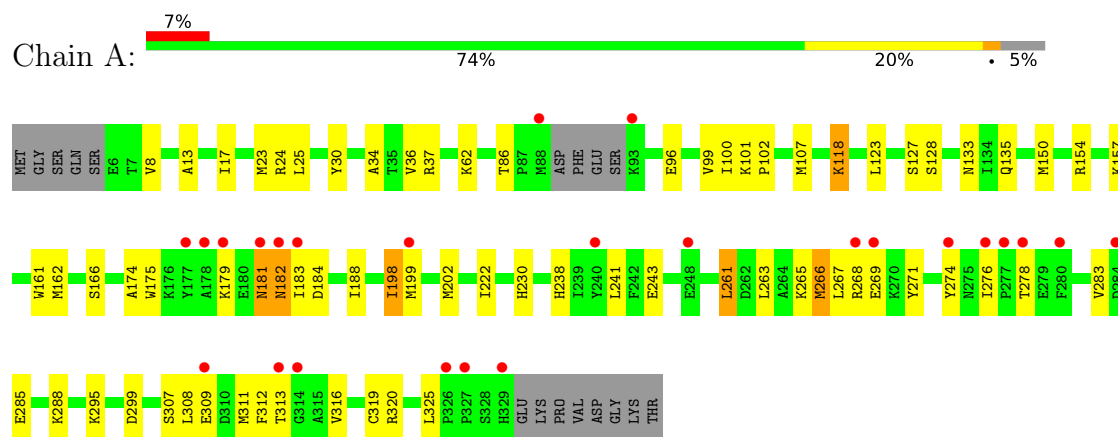
- Molecule 4 is water.

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

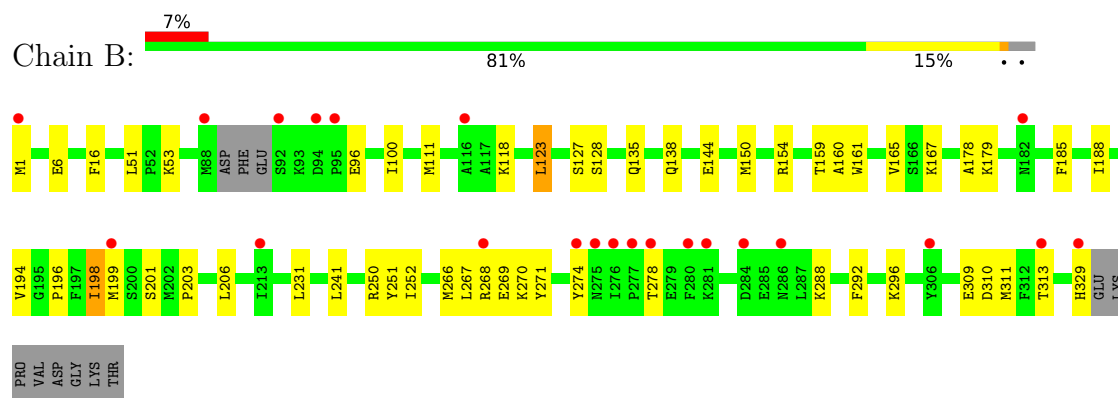
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

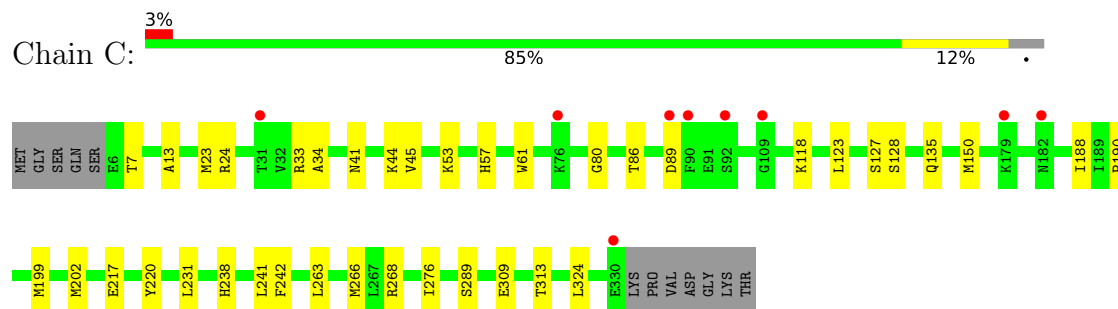
- Molecule 1: dihydroflavonol 4-reductase



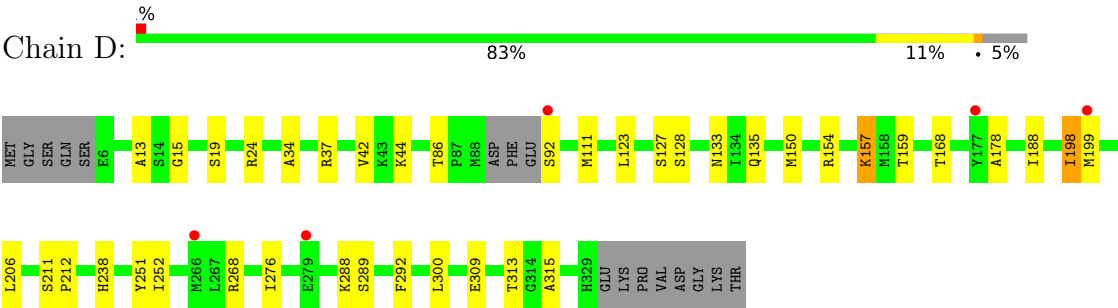
- Molecule 1: dihydroflavonol 4-reductase



- 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, α , β , γ	47.23Å 177.96Å 92.60Å 90.00° 104.77° 90.00°	Depositor
Resolution (Å)	89.09 – 2.25 89.09 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (89.09-2.25) 99.7 (89.09-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.25Å)	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 (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.85	0/2539	1.12	4/3450 (0.1%)
1	B	0.77	0/2573	1.09	0/3494
1	C	0.83	0/2568	1.10	3/3490 (0.1%)
1	D	0.86	0/2542	1.10	3/3453 (0.1%)
All	All	0.83	0/10222	1.10	10/13887 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	MET	CA-C-N	-6.97	113.20	120.38
1	A	202	MET	C-N-CA	-6.97	113.20	120.38
1	D	133	ASN	CA-C-N	-5.87	115.47	122.22
1	D	133	ASN	C-N-CA	-5.87	115.47	122.22
1	C	289	SER	N-CA-C	-5.48	102.37	110.48
1	C	231	LEU	N-CA-C	5.45	117.65	111.11
1	A	133	ASN	N-CA-C	5.33	119.38	111.87
1	C	7	THR	N-CA-C	5.28	117.33	108.73
1	D	15	GLY	N-CA-C	5.23	121.13	112.66
1	A	319	CYS	N-CA-C	5.07	116.80	111.28

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	2477	0	2431	46	0
1	B	2511	0	2457	33	0
1	C	2509	0	2447	23	0
1	D	2484	0	2432	21	0
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	2	0
4	B	174	0	0	1	0
4	C	201	0	0	3	0
4	D	242	0	0	2	0
All	All	11125	0	9914	124	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 (124) 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:C:199:MET:HE1	4:C:439:HOH:O	1.86	0.73
1:A:150:MET:HA	1:A:150:MET:HE2	1.76	0.68
1:A:37:ARG:HD3	2:A:340:NAP:C6A	2.25	0.65
1:A:23:MET:HE3	1:A:24:ARG:NH1	2.11	0.65
1:A:17:ILE:HD12	2:A:340:NAP:H51N	1.82	0.61
1:C:202:MET:HE2	1:C:324:LEU:HB3	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:B:199:MET:HE3	1:B:201:SER:O	2.02	0.59
1:B:111:MET:HE1	1:B:178:ALA:HB2	1.83	0.59
1:A:175:TRP:O	1:A:179:LYS:HD3	2.02	0.59
1:A:128:SER:HG	3:A:342:MYC:HO3	1.52	0.58
1:B:309:GLU:O	1:B:313[A]:THR:HG23	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:150:MET:HE2	1:C:150:MET:HA	1.88	0.56
1:C:23:MET:HE3	1:C:24:ARG:NH1	2.21	0.56
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:263:LEU:HD12	1:A:266:MET:HE2	1.88	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
1:D:199:MET:HE3	4:D:522:HOH:O	2.09	0.53
1:A:271:TYR:CE2	1:A:316:VAL:HG21	2.44	0.52
1:A:184:ASP:C	1:A:184:ASP:OD1	2.50	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:C:263:LEU:HD12	1:C:266:MET:HE2	1.93	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:199:MET:HE2	1:B:203:PRO:HG3	1.92	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:8:VAL:CG2	1:A:25:LEU:HD13	2.42	0.49
1:A:309:GLU:O	1:A:313[A]:THR:HG23	2.13	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:C:309:GLU:O	1:C:313[B]:THR:CG2	2.61	0.47
1:B:310:ASP:O	1:B:311:MET:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:HE3	1:A:267:LEU:HG	1.96	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
1:B:266:MET:HE1	1:B:267:LEU:HD23	1.97	0.47
3:C:342:MYC:O23	4:C:519:HOH:O	2.21	0.47
1:B:150:MET:HA	1:B:150:MET:HE2	1.97	0.46
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:A:128:SER:OG	3:A:342:MYC:O23	2.26	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
1:C:41:ASN:O	1:C:45:VAL:HG22	2.16	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: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: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: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:D:44:LYS:NZ	4:D:480:HOH:O	2.50	0.43
1:A:36:VAL:O	1:A:62:LYS:HA	2.19	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:D:111:MET:HE1	1:D:178:ALA:HB2	2.00	0.43
1:A:295:LYS:NZ	1:A:299:ASP:OD2	2.51	0.43
1:B:51:LEU:HD21	1:B:198:ILE:CD1	2.48	0.42
1:B:194:VAL:HG13	1:B:206:LEU:CD2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:TYR:OH	1:B:313[B]:THR:HA	2.19	0.42
1:A:307:SER:O	1:A:308:LEU:C	2.63	0.42
1:B:199:MET:CE	1:B:201:SER:O	2.65	0.42
1:B:274:TYR:HD1	1:B:329:HIS:ND1	2.16	0.42
1:D:150:MET:HE3	1:D:168:THR:HG21	2.01	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:19:SER:C	1:D:198:ILE:HD11	2.46	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
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:HD13	1:A:198:ILE:HG21	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:C:199:MET:HE3	4:C:390:HOH:O	2.20	0.40
1:D:24:ARG:HD3	1:D:24:ARG:HA	1.89	0.40
1:C:33:ARG:HD3	1:C:61:TRP:CZ2	2.56	0.40
1:C:127:SER:O	2:C:340:NAP:H6N	2.20	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%)	21	21
1	B	324/337 (96%)	308 (95%)	15 (5%)	1 (0%)	36	40
1	C	324/337 (96%)	316 (98%)	7 (2%)	1 (0%)	36	40
1	D	318/337 (94%)	307 (96%)	11 (4%)	0	100	100
All	All	1284/1348 (95%)	1233 (96%)	47 (4%)	4 (0%)	36	40

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%)	22	24
1	B	269/293 (92%)	261 (97%)	8 (3%)	36	45
1	C	269/293 (92%)	265 (98%)	4 (2%)	57	68
1	D	268/293 (92%)	261 (97%)	7 (3%)	40	50
All	All	1073/1172 (92%)	1041 (97%)	32 (3%)	36	45

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	THR
1	A	99	VAL
1	A	118	LYS
1	A	123	LEU
1	A	135	GLN
1	A	181	ASN
1	A	198	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	6	GLU
1	B	123	LEU
1	B	135	GLN
1	B	179	LYS
1	B	198	ILE
1	B	269	GLU
1	B	270	LYS
1	C	86	THR
1	C	89	ASP
1	C	123	LEU
1	C	135	GLN
1	D	42	VAL
1	D	86	THR
1	D	92	SER
1	D	123	LEU
1	D	135	GLN
1	D	157	LYS
1	D	198	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
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	181	ASN
1	D	236	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	275	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	NAP	A	340	-	50,52,52	1.78	8 (16%)	71,80,80	1.84	17 (23%)
2	NAP	D	340	-	50,52,52	1.72	7 (14%)	71,80,80	2.12	21 (29%)
3	MYC	A	342	-	25,25,25	1.57	4 (16%)	38,38,38	1.80	9 (23%)
3	MYC	C	342	-	25,25,25	1.43	3 (12%)	38,38,38	2.08	12 (31%)
2	NAP	B	340	-	50,52,52	1.81	8 (16%)	71,80,80	2.04	20 (28%)
3	MYC	D	342	-	25,25,25	1.34	5 (20%)	38,38,38	1.85	11 (28%)
3	MYC	B	342	-	25,25,25	1.43	3 (12%)	38,38,38	1.77	9 (23%)
3	MYC	C	341	-	25,25,25	1.38	4 (16%)	38,38,38	1.87	11 (28%)
3	MYC	B	341	-	25,25,25	1.04	1 (4%)	38,38,38	1.56	8 (21%)
2	NAP	C	340	-	50,52,52	1.57	2 (4%)	71,80,80	1.67	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MYC	A	341	-	25,25,25	0.95	2 (8%)	38,38,38	1.39	6 (15%)
3	MYC	D	341	-	25,25,25	1.26	2 (8%)	38,38,38	1.79	8 (21%)

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	NAP	A	340	-	-	4/35/67/67	0/5/5/5
2	NAP	D	340	-	-	8/35/67/67	0/5/5/5
3	MYC	A	342	-	-	0/4/4/4	0/3/3/3
3	MYC	C	342	-	-	0/4/4/4	0/3/3/3
2	NAP	B	340	-	-	7/35/67/67	0/5/5/5
3	MYC	D	342	-	-	0/4/4/4	0/3/3/3
3	MYC	B	342	-	-	0/4/4/4	0/3/3/3
3	MYC	C	341	-	-	4/4/4/4	0/3/3/3
3	MYC	B	341	-	-	4/4/4/4	0/3/3/3
2	NAP	C	340	-	-	6/35/67/67	0/5/5/5
3	MYC	A	341	-	-	4/4/4/4	0/3/3/3
3	MYC	D	341	-	-	4/4/4/4	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	340	NAP	O7N-C7N	8.81	1.40	1.24
2	A	340	NAP	O7N-C7N	8.55	1.40	1.24
2	B	340	NAP	O7N-C7N	8.36	1.39	1.24
2	D	340	NAP	O7N-C7N	7.54	1.38	1.24
3	A	342	MYC	C10-C11	5.18	1.41	1.36
2	B	340	NAP	PA-O3	4.76	1.64	1.59
3	B	342	MYC	C10-C11	4.59	1.40	1.36
2	D	340	NAP	PA-O3	4.29	1.64	1.59
2	A	340	NAP	PA-O3	3.95	1.63	1.59
3	C	341	MYC	C10-C11	3.83	1.40	1.36
2	D	340	NAP	C2N-N1N	3.82	1.39	1.35
3	C	342	MYC	C18-C17	-3.82	1.35	1.40
2	B	340	NAP	PN-O3	3.79	1.63	1.59
3	C	342	MYC	C10-C11	3.64	1.40	1.36
3	D	341	MYC	C10-C11	3.61	1.40	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	340	NAP	PN-O3	3.30	1.63	1.59
3	B	342	MYC	C10-C9	-3.23	1.37	1.46
2	D	340	NAP	C8A-N7A	3.14	1.37	1.31
2	A	340	NAP	O4D-C4D	-3.08	1.38	1.45
2	A	340	NAP	C2N-N1N	2.79	1.38	1.35
3	D	342	MYC	C16-C17	-2.77	1.36	1.40
3	D	341	MYC	C10-C9	-2.72	1.39	1.46
2	A	340	NAP	C5A-N7A	-2.70	1.34	1.39
3	C	341	MYC	C10-C9	-2.68	1.39	1.46
3	A	342	MYC	C10-C9	-2.63	1.39	1.46
3	D	342	MYC	C18-C17	-2.62	1.36	1.40
3	A	342	MYC	C18-C17	-2.52	1.37	1.40
3	A	341	MYC	C10-C11	2.49	1.38	1.36
2	D	340	NAP	C3N-C7N	-2.48	1.46	1.50
2	B	340	NAP	C2A-N3A	2.46	1.38	1.33
2	A	340	NAP	C2A-N1A	2.41	1.38	1.33
3	D	342	MYC	C10-C11	2.38	1.38	1.36
3	B	342	MYC	C18-C17	-2.36	1.37	1.40
3	D	342	MYC	O12-C4	-2.33	1.35	1.38
3	C	342	MYC	C10-C9	-2.31	1.40	1.46
3	C	341	MYC	C19-C14	2.30	1.42	1.39
3	A	342	MYC	C19-C14	2.28	1.42	1.39
3	A	341	MYC	C10-C9	-2.23	1.40	1.46
3	D	342	MYC	C10-C9	-2.22	1.40	1.46
2	C	340	NAP	C5A-N7A	-2.22	1.35	1.39
2	D	340	NAP	C2A-N1A	2.17	1.37	1.33
2	B	340	NAP	C8A-N7A	2.14	1.35	1.31
2	B	340	NAP	PN-O2N	-2.10	1.45	1.55
3	C	341	MYC	O13-C9	2.07	1.27	1.23
2	A	340	NAP	C2A-N3A	2.06	1.37	1.33
2	D	340	NAP	C2A-N3A	2.04	1.37	1.33
3	B	341	MYC	C10-C9	-2.03	1.40	1.46
2	B	340	NAP	C5A-N7A	-2.02	1.35	1.39
2	B	340	NAP	O4D-C4D	-2.01	1.40	1.45

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	340	NAP	N3A-C2A-N1A	-7.16	117.74	128.58
2	C	340	NAP	N3A-C2A-N1A	-6.68	118.47	128.58
3	D	341	MYC	O12-C11-C14	5.79	118.99	110.87
2	B	340	NAP	N3A-C2A-N1A	-5.64	120.04	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	342	MYC	O27-C10-C11	5.26	126.19	120.74
2	B	340	NAP	O3X-P2B-O2X	5.18	127.22	107.80
2	D	340	NAP	N9A-C8A-N7A	-5.17	106.60	113.94
2	B	340	NAP	N9A-C8A-N7A	-4.99	106.85	113.94
2	B	340	NAP	C3N-C7N-N7N	4.77	123.62	117.74
2	A	340	NAP	N3A-C2A-N1A	-4.70	121.47	128.58
3	B	342	MYC	O27-C10-C11	4.63	125.53	120.74
2	B	340	NAP	O7N-C7N-C3N	-4.61	113.97	119.60
3	D	341	MYC	C14-C11-C10	-4.55	121.28	128.44
3	C	342	MYC	O27-C10-C11	4.50	125.39	120.74
3	C	341	MYC	C14-C11-C10	-4.38	121.54	128.44
2	D	340	NAP	O7N-C7N-C3N	-4.25	114.40	119.60
3	C	342	MYC	C2-C3-C4	4.13	121.35	117.41
2	A	340	NAP	O7N-C7N-C3N	-4.12	114.55	119.60
2	D	340	NAP	O2X-P2B-O1X	4.11	126.84	110.83
2	A	340	NAP	C5A-C4A-N3A	-4.10	121.08	126.72
3	C	342	MYC	C18-C17-C16	4.08	122.06	119.53
2	D	340	NAP	C4A-N9A-C8A	3.89	109.82	105.74
3	D	342	MYC	C11-C10-C9	-3.80	118.80	121.52
2	B	340	NAP	C5A-N7A-C8A	3.77	109.37	103.45
3	D	342	MYC	O27-C10-C11	3.76	124.64	120.74
2	A	340	NAP	O3-PA-O1A	-3.74	99.44	110.70
3	C	342	MYC	O23-C18-C19	3.74	129.55	119.45
3	C	342	MYC	O24-C17-C18	-3.67	109.78	119.46
3	D	342	MYC	O12-C4-C5	3.62	120.96	115.83
2	D	340	NAP	C6N-N1N-C2N	-3.56	118.85	121.88
2	B	340	NAP	O3X-P2B-O1X	-3.53	97.07	110.83
3	A	342	MYC	C4-C3-C9	-3.52	115.78	120.03
3	B	342	MYC	O12-C11-C14	3.48	115.75	110.87
3	C	341	MYC	O12-C11-C14	3.45	115.70	110.87
2	D	340	NAP	C2A-N3A-C4A	3.42	120.19	111.83
2	A	340	NAP	N9A-C8A-N7A	-3.41	109.10	113.94
2	A	340	NAP	C3N-C7N-N7N	3.37	121.89	117.74
3	A	341	MYC	O12-C11-C14	3.33	115.54	110.87
3	C	341	MYC	O13-C9-C10	3.33	126.37	119.61
3	B	341	MYC	C15-C14-C11	-3.29	116.01	120.65
3	C	342	MYC	O24-C17-C16	3.29	128.12	119.46
2	D	340	NAP	C5A-N7A-C8A	3.23	108.53	103.45
3	B	342	MYC	C2-C3-C4	3.22	120.48	117.41
3	D	342	MYC	O25-C16-C15	3.22	128.14	119.45
3	C	342	MYC	C11-C10-C9	-3.20	119.23	121.52
3	C	342	MYC	O23-C18-C17	-3.19	109.69	117.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	340	NAP	O3-PA-O1A	-3.13	101.28	110.70
2	D	340	NAP	C2N-C3N-C4N	3.12	121.89	118.26
2	B	340	NAP	C4A-N9A-C1B	-3.12	119.34	126.63
2	B	340	NAP	C4A-C5A-N7A	-3.11	107.02	110.58
2	D	340	NAP	C5N-C4N-C3N	-3.11	117.31	120.36
3	C	341	MYC	O13-C9-C3	-3.11	116.44	122.06
2	C	340	NAP	N9A-C8A-N7A	-3.10	109.53	113.94
2	B	340	NAP	C2N-C3N-C4N	3.10	121.86	118.26
2	D	340	NAP	O3X-P2B-O2B	3.09	117.91	105.85
2	D	340	NAP	O2A-PA-O3	-3.09	98.92	107.27
2	C	340	NAP	C2B-C1B-N9A	-3.09	108.67	113.75
2	D	340	NAP	O3-PA-O1A	-3.08	101.43	110.70
2	A	340	NAP	O2X-P2B-O1X	3.04	122.68	110.83
3	D	341	MYC	C2-C3-C4	3.03	120.30	117.41
2	D	340	NAP	C5A-C4A-N3A	-3.02	122.56	126.72
2	A	340	NAP	O3-PN-O1N	-3.00	101.69	110.70
3	C	341	MYC	C2-C3-C4	3.00	120.27	117.41
2	A	340	NAP	N3A-C4A-N9A	2.97	132.22	127.17
3	D	342	MYC	C4-O12-C11	2.96	125.20	120.67
3	D	342	MYC	O25-C16-C17	-2.95	110.32	117.90
2	C	340	NAP	C2A-N1A-C6A	2.94	123.56	118.73
3	A	341	MYC	C2-C3-C4	2.94	120.21	117.41
3	A	342	MYC	O23-C18-C19	2.93	127.38	119.45
2	A	340	NAP	C6A-C5A-C4A	2.93	121.17	117.18
3	C	341	MYC	C15-C14-C11	-2.89	116.57	120.65
2	D	340	NAP	C4A-N9A-C1B	-2.89	119.88	126.63
3	C	341	MYC	O12-C4-C5	2.88	119.91	115.83
2	C	340	NAP	C2A-N3A-C4A	2.85	118.78	111.83
2	C	340	NAP	O2X-P2B-O1X	2.83	121.88	110.83
2	B	340	NAP	C4A-N9A-C8A	2.80	108.67	105.74
3	A	341	MYC	C14-C11-C10	-2.78	124.07	128.44
3	B	342	MYC	C18-C17-C16	2.77	121.25	119.53
3	B	341	MYC	O12-C11-C14	2.76	114.74	110.87
2	C	340	NAP	O3X-P2B-O2X	-2.76	97.46	107.80
2	B	340	NAP	C2A-N3A-C4A	2.75	118.55	111.83
3	D	342	MYC	O12-C4-C3	-2.75	118.50	121.19
3	C	341	MYC	C18-C17-C16	2.74	121.23	119.53
2	C	340	NAP	C5A-N7A-C8A	2.74	107.76	103.45
3	D	342	MYC	O24-C17-C18	2.73	126.66	119.46
3	A	342	MYC	C18-C17-C16	2.72	121.22	119.53
2	A	340	NAP	C5A-N7A-C8A	2.71	107.71	103.45
3	D	342	MYC	O13-C9-C3	-2.71	117.17	122.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	340	NAP	O2N-PN-O5D	2.70	119.81	107.57
2	C	340	NAP	C1B-N9A-C8A	2.70	133.09	127.09
3	C	342	MYC	C4-C3-C9	-2.70	116.77	120.03
3	C	341	MYC	O12-C11-C10	2.69	122.73	120.19
3	B	341	MYC	C19-C14-C11	2.69	124.45	120.65
3	B	341	MYC	C14-C11-C10	-2.67	124.23	128.44
2	A	340	NAP	C2A-N3A-C4A	2.67	118.36	111.83
2	C	340	NAP	C4A-N9A-C1B	-2.65	120.43	126.63
2	A	340	NAP	C4D-O4D-C1D	2.64	112.34	109.92
3	A	342	MYC	C19-C18-C17	-2.63	118.63	120.45
3	A	342	MYC	C2-C3-C4	2.58	119.87	117.41
3	D	342	MYC	C2-C3-C4	2.54	119.84	117.41
3	B	342	MYC	O12-C4-C5	2.54	119.43	115.83
2	A	340	NAP	O2A-PA-O1A	2.53	124.23	112.44
3	A	341	MYC	C1-C2-C3	-2.51	118.11	120.92
2	D	340	NAP	O5B-PA-O1A	2.49	118.81	108.94
2	A	340	NAP	O2N-PN-O1N	2.46	123.89	112.44
3	A	342	MYC	O12-C11-C10	-2.45	117.86	120.19
2	B	340	NAP	O2X-P2B-O2B	-2.45	96.32	105.85
3	A	341	MYC	O27-C10-C11	-2.44	118.22	120.74
2	D	340	NAP	N3A-C4A-N9A	2.43	131.30	127.17
3	D	342	MYC	O24-C17-C16	-2.43	113.06	119.46
2	B	340	NAP	C5A-C4A-N3A	-2.42	123.38	126.72
2	B	340	NAP	C2D-C3D-C4D	2.41	107.27	102.61
3	B	341	MYC	O27-C10-C9	2.40	121.31	116.89
3	C	342	MYC	C1-C2-C3	-2.33	118.31	120.92
3	D	341	MYC	O12-C4-C5	2.32	119.13	115.83
2	D	340	NAP	C3N-C7N-N7N	2.32	120.60	117.74
3	D	341	MYC	C15-C14-C11	-2.32	117.37	120.65
2	C	340	NAP	C5A-C4A-N3A	-2.32	123.53	126.72
2	D	340	NAP	C4B-O4B-C1B	-2.31	104.36	109.47
2	A	340	NAP	O4B-C1B-N9A	2.26	112.44	108.09
3	A	342	MYC	O27-C10-C9	-2.26	112.74	116.89
3	C	342	MYC	C3-C9-C10	2.25	120.07	116.88
3	B	341	MYC	O12-C4-C5	2.24	119.01	115.83
3	A	342	MYC	C3-C9-C10	2.24	120.05	116.88
3	A	341	MYC	O27-C10-C9	2.24	121.00	116.89
3	C	342	MYC	C14-C19-C18	-2.23	118.14	120.09
3	D	341	MYC	C19-C14-C11	2.23	123.80	120.65
3	D	341	MYC	C4-C3-C9	-2.23	117.34	120.03
3	B	342	MYC	C3-C9-C10	2.22	120.03	116.88
3	B	342	MYC	C4-C3-C9	-2.22	117.35	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	340	NAP	C4B-O4B-C1B	-2.21	104.60	109.47
3	B	341	MYC	C11-C10-C9	-2.18	119.96	121.52
2	B	340	NAP	O2X-P2B-O1X	2.17	119.28	110.83
2	C	340	NAP	C6N-N1N-C2N	-2.15	120.05	121.88
3	D	341	MYC	O29-C6-C5	-2.15	114.23	119.85
3	B	342	MYC	O23-C18-C19	2.11	125.15	119.45
2	C	340	NAP	C4B-O4B-C1B	-2.10	104.83	109.47
3	B	341	MYC	O30-C2-C3	-2.10	117.26	121.14
2	B	340	NAP	C1B-N9A-C8A	2.09	131.73	127.09
2	C	340	NAP	C4A-C5A-N7A	-2.07	108.21	110.58
3	C	341	MYC	O27-C10-C9	2.06	120.69	116.89
2	D	340	NAP	C2A-N1A-C6A	2.05	122.10	118.73
3	C	341	MYC	C19-C14-C11	2.04	123.53	120.65
2	C	340	NAP	C5A-C4A-N9A	2.03	108.02	105.81
2	B	340	NAP	C5B-C4B-C3B	-2.03	107.91	115.21
2	D	340	NAP	C2B-C3B-C4B	2.02	106.33	101.99
2	C	340	NAP	O2B-P2B-O1X	-2.01	102.17	109.33
3	B	342	MYC	C14-C11-C10	-2.01	125.28	128.44

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	340	NAP	C5D-O5D-PN-O3
2	A	340	NAP	C5D-O5D-PN-O1N
2	A	340	NAP	C5D-O5D-PN-O2N
2	B	340	NAP	C5B-O5B-PA-O1A
2	B	340	NAP	C5D-O5D-PN-O3
2	B	340	NAP	C5D-O5D-PN-O2N
2	C	340	NAP	C5D-O5D-PN-O3
2	C	340	NAP	C5D-O5D-PN-O2N
2	D	340	NAP	C5D-O5D-PN-O3
2	D	340	NAP	C5D-O5D-PN-O1N
2	D	340	NAP	C5D-O5D-PN-O2N
3	A	341	MYC	C10-C11-C14-C15
3	A	341	MYC	C10-C11-C14-C19
3	B	341	MYC	C10-C11-C14-C15
3	B	341	MYC	C10-C11-C14-C19
3	C	341	MYC	C10-C11-C14-C15
3	C	341	MYC	C10-C11-C14-C19
3	D	341	MYC	C10-C11-C14-C15
3	D	341	MYC	C10-C11-C14-C19

Continued on next page...

Continued from previous page...

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

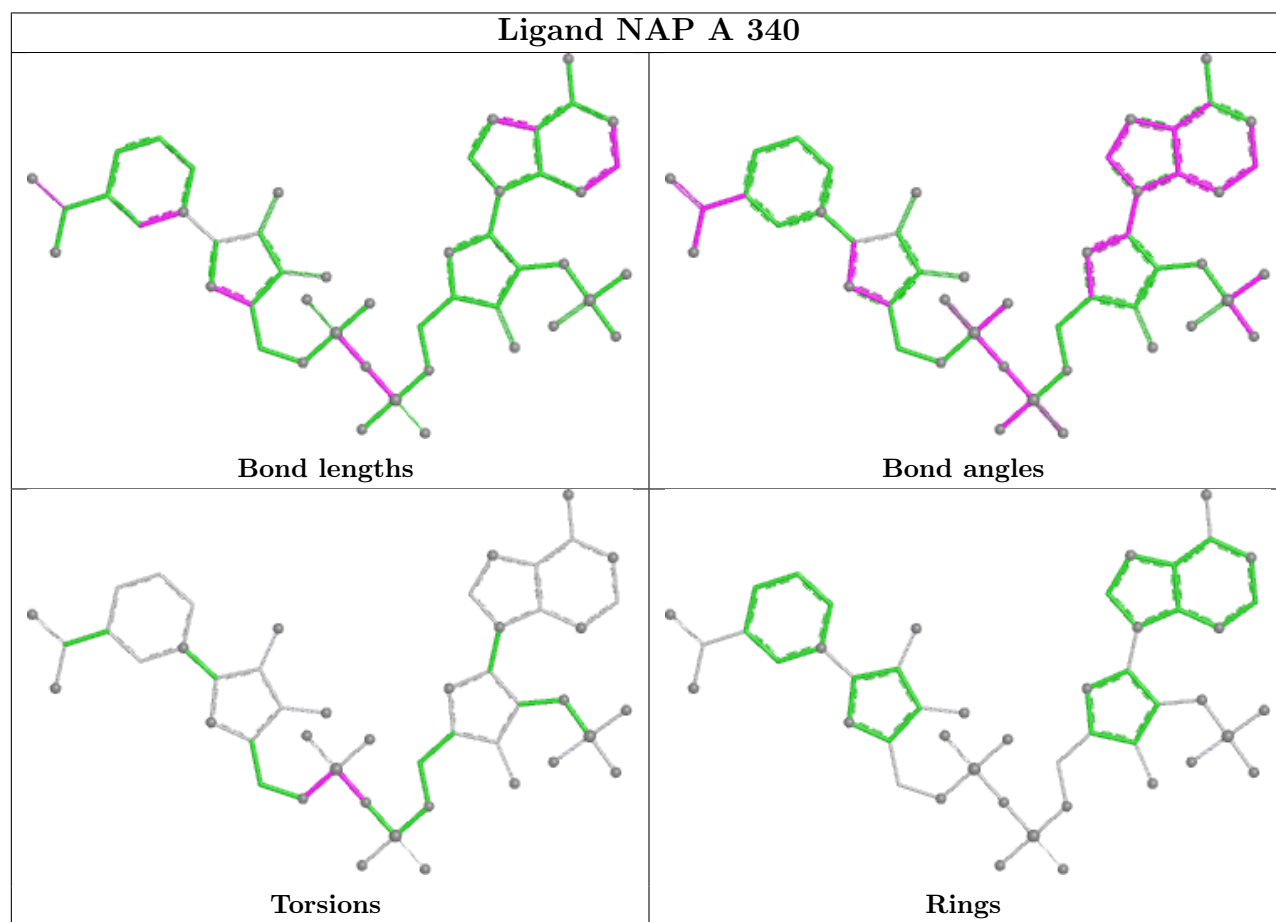
There are no ring outliers.

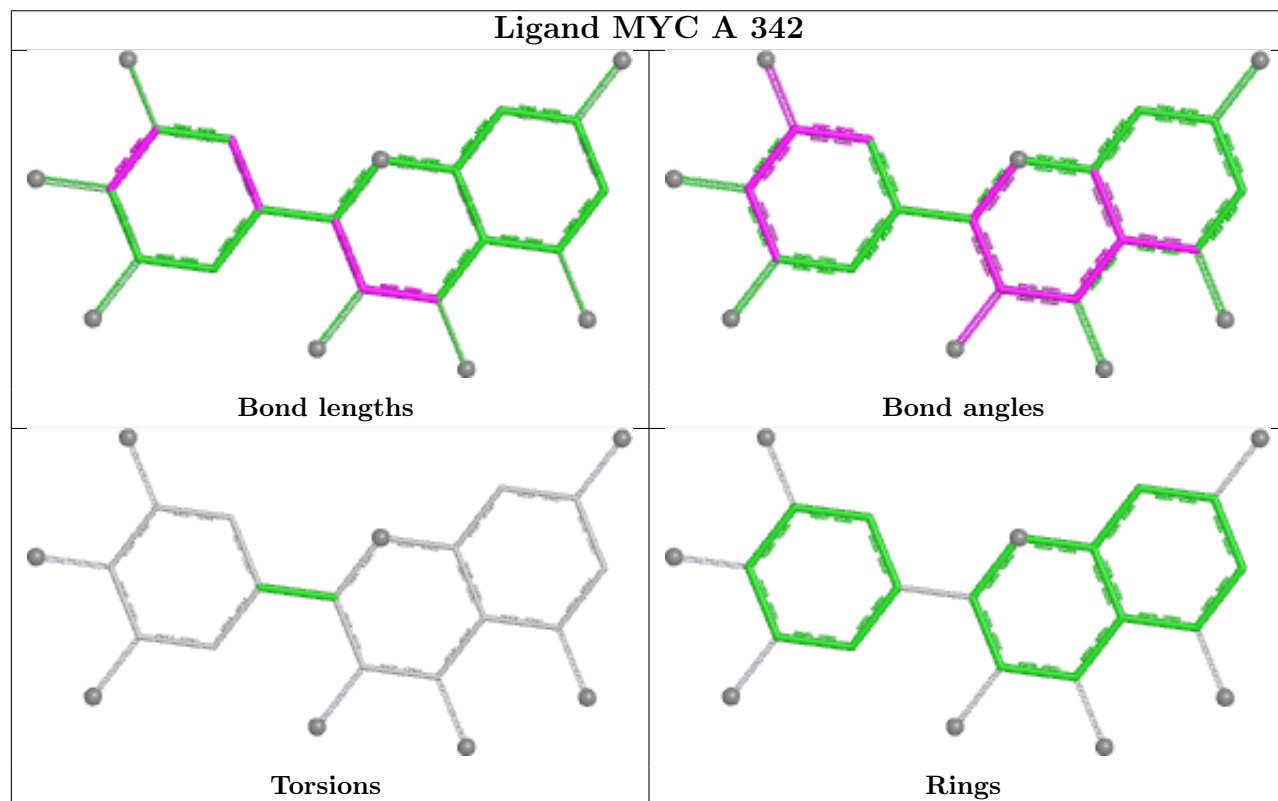
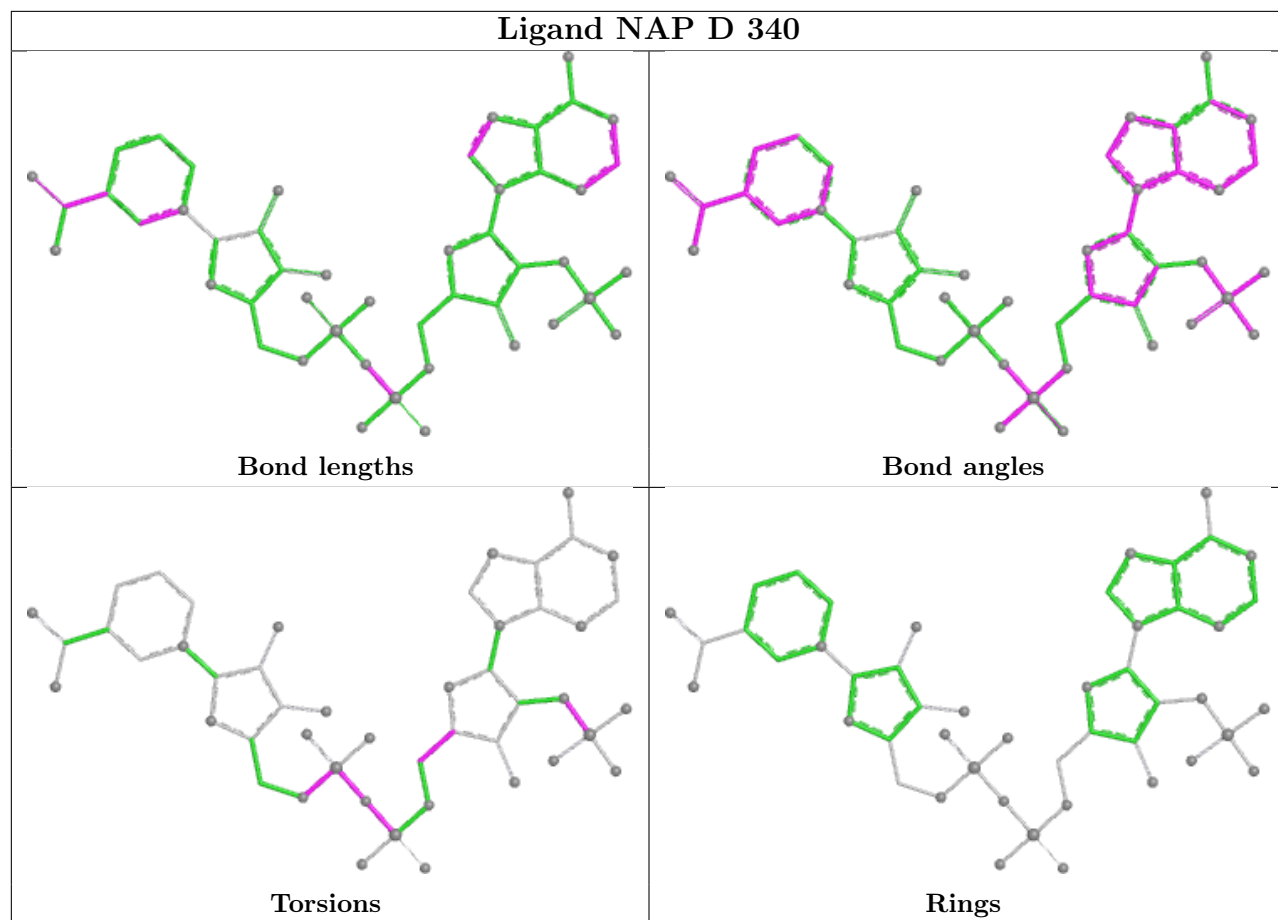
8 monomers are involved in 20 short contacts:

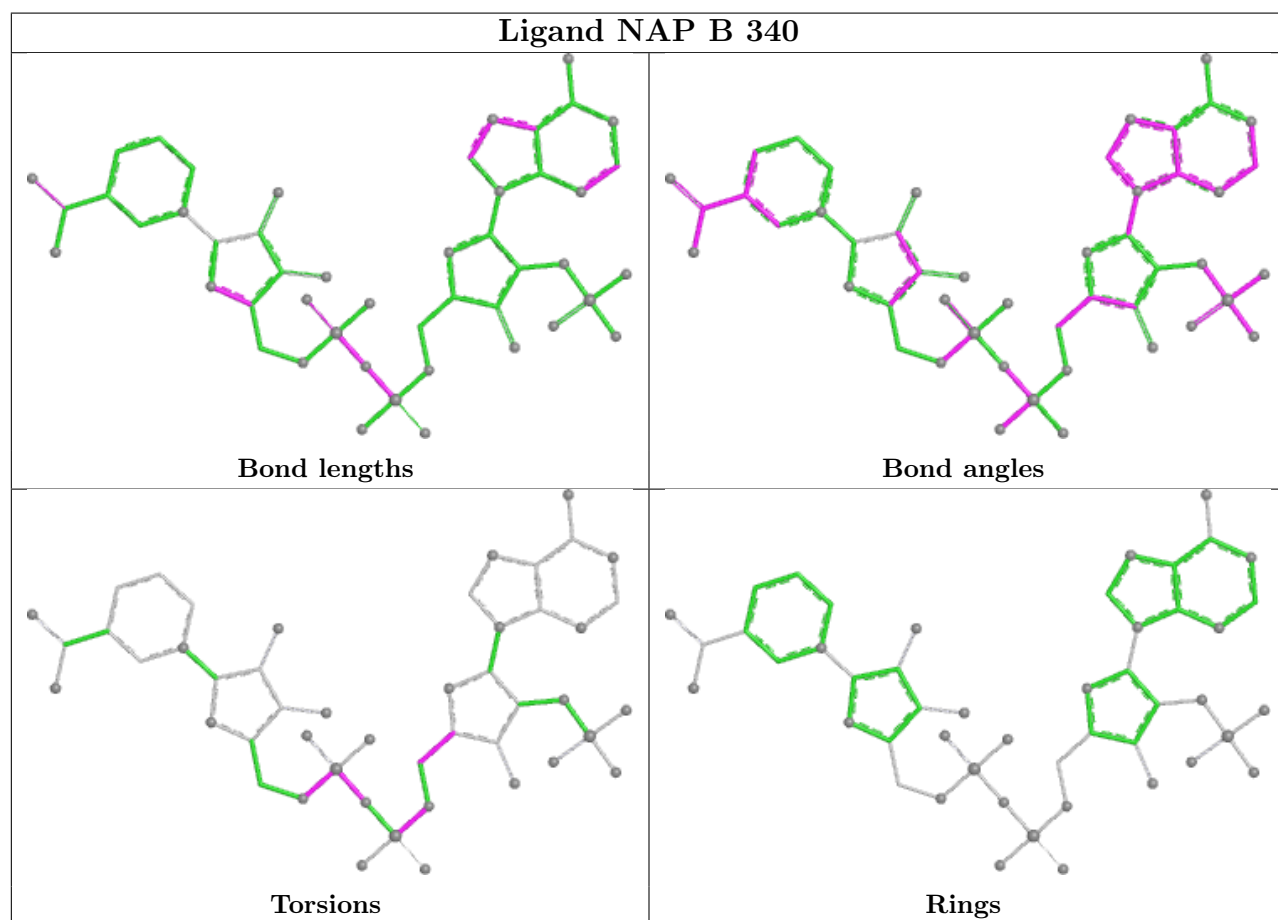
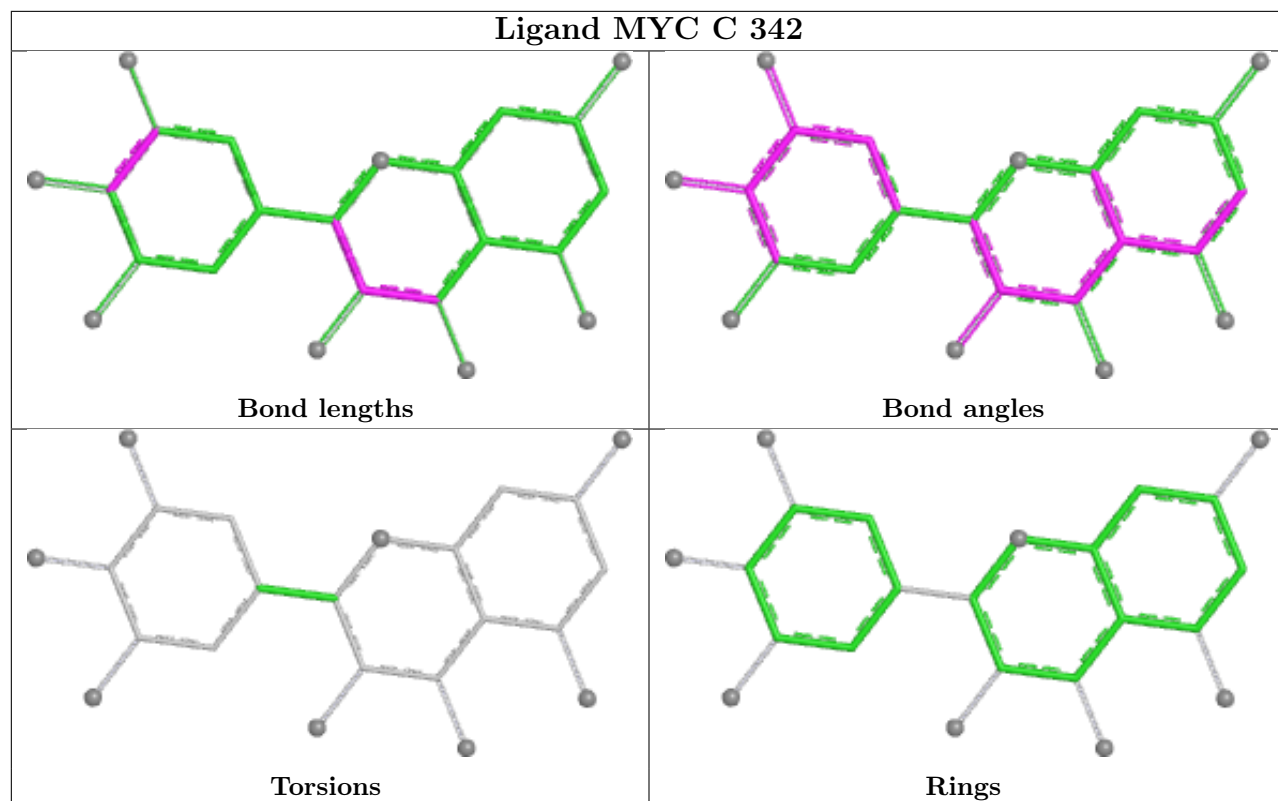
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	340	NAP	4	0
2	D	340	NAP	2	0
3	A	342	MYC	2	0
3	C	342	MYC	2	0
2	B	340	NAP	1	0
3	D	342	MYC	1	0
3	B	342	MYC	4	0
2	C	340	NAP	4	0

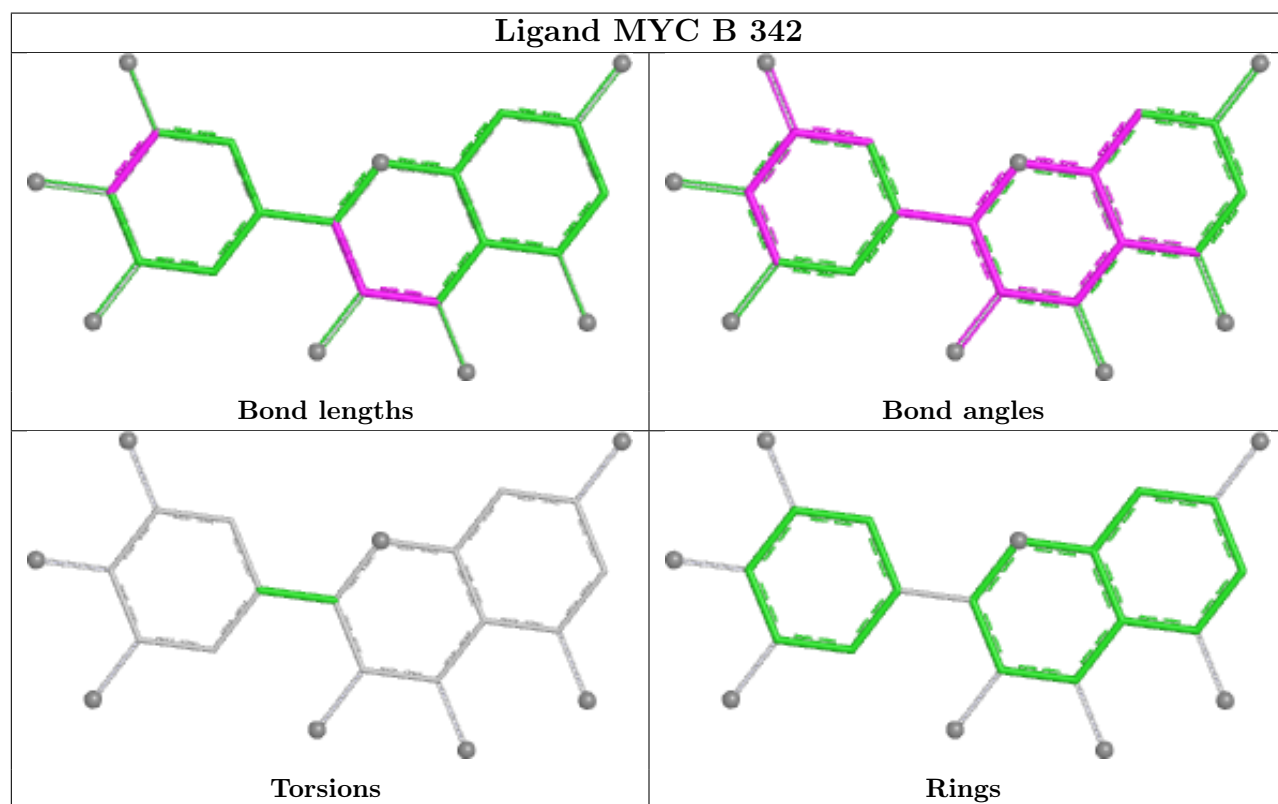
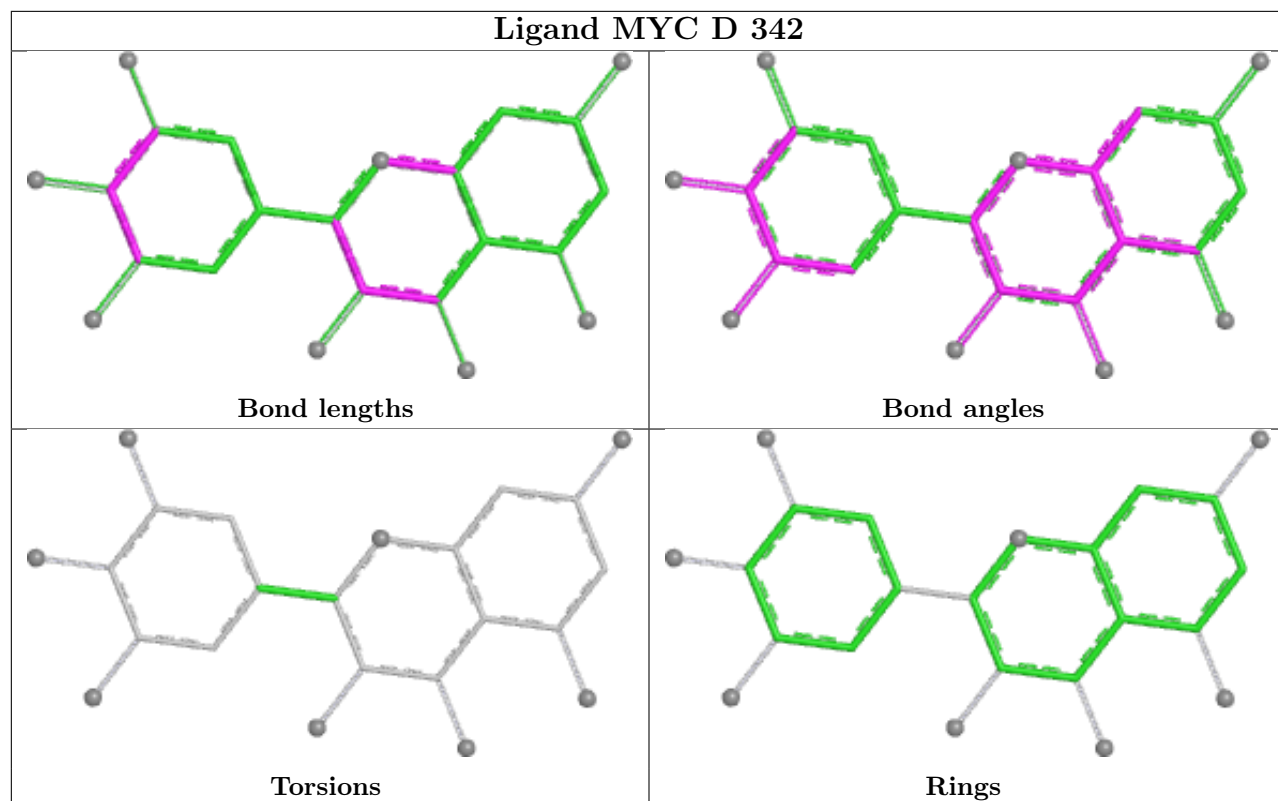
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

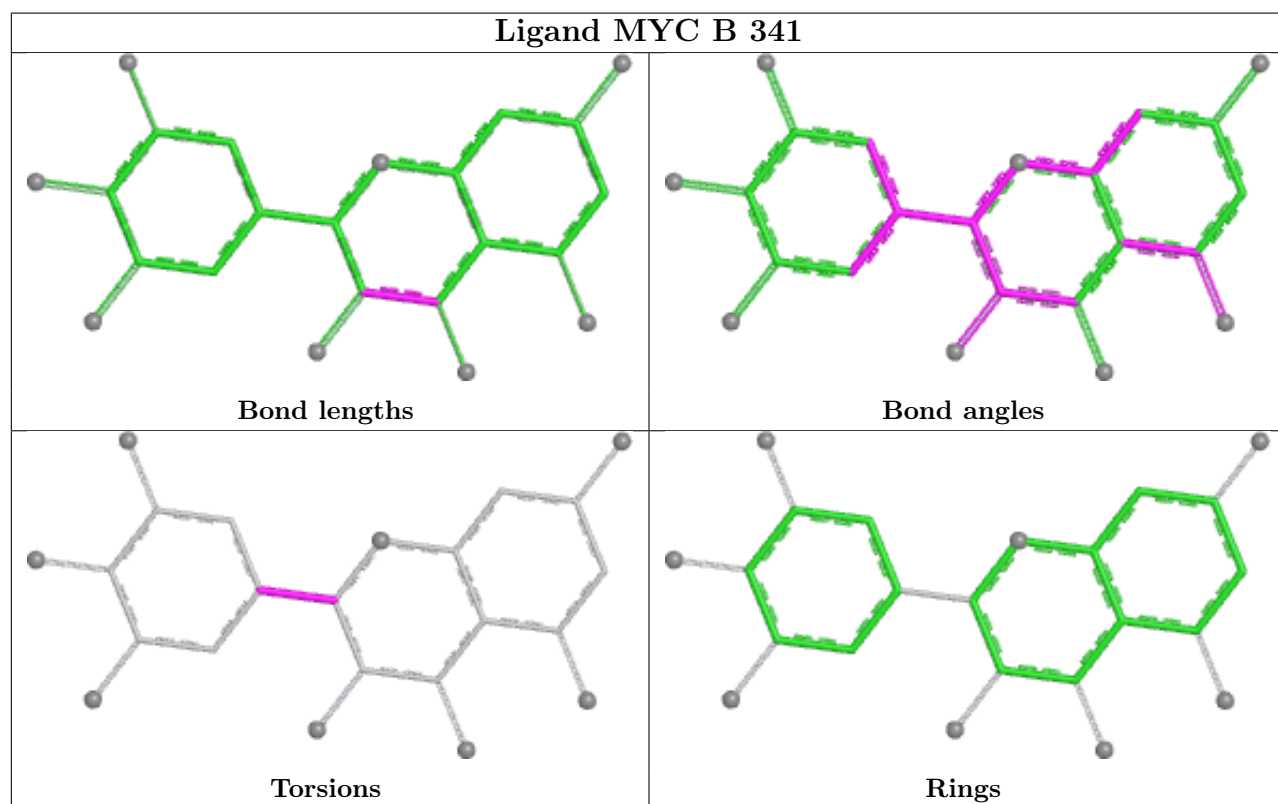
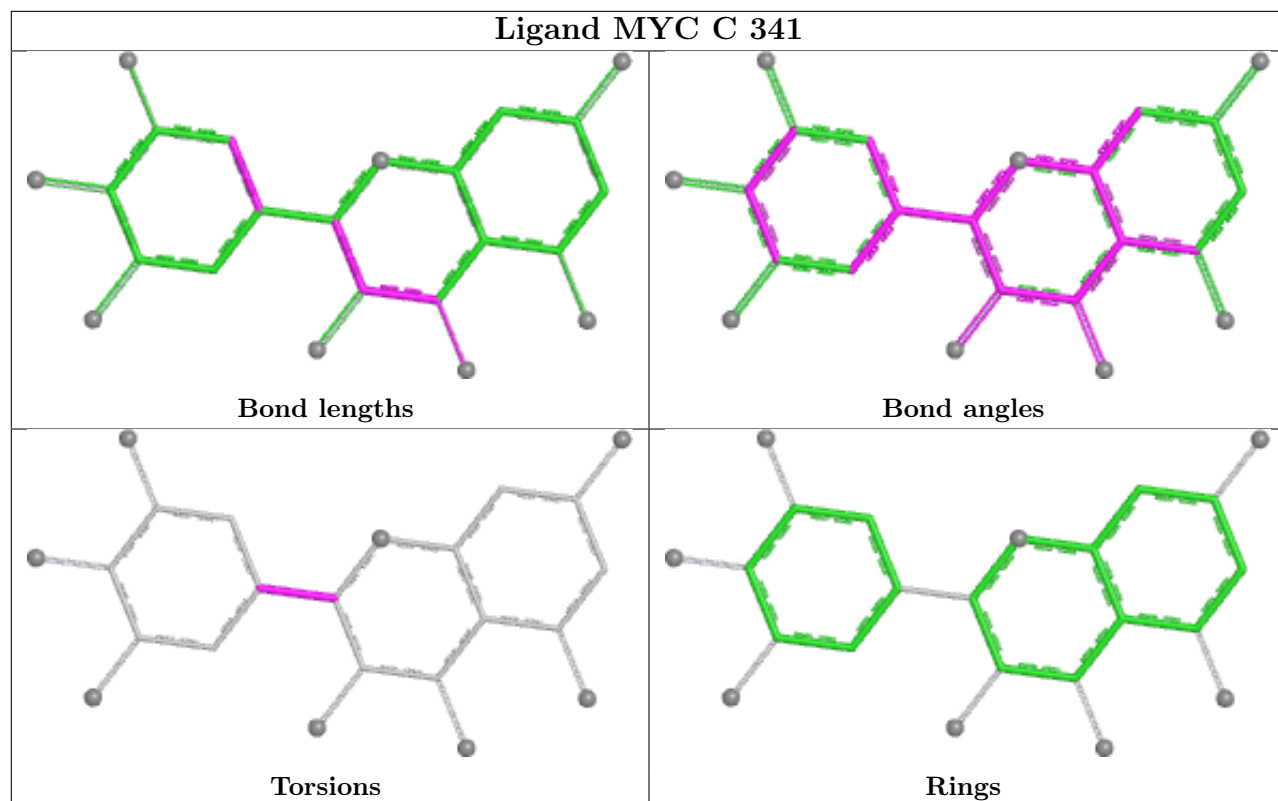
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

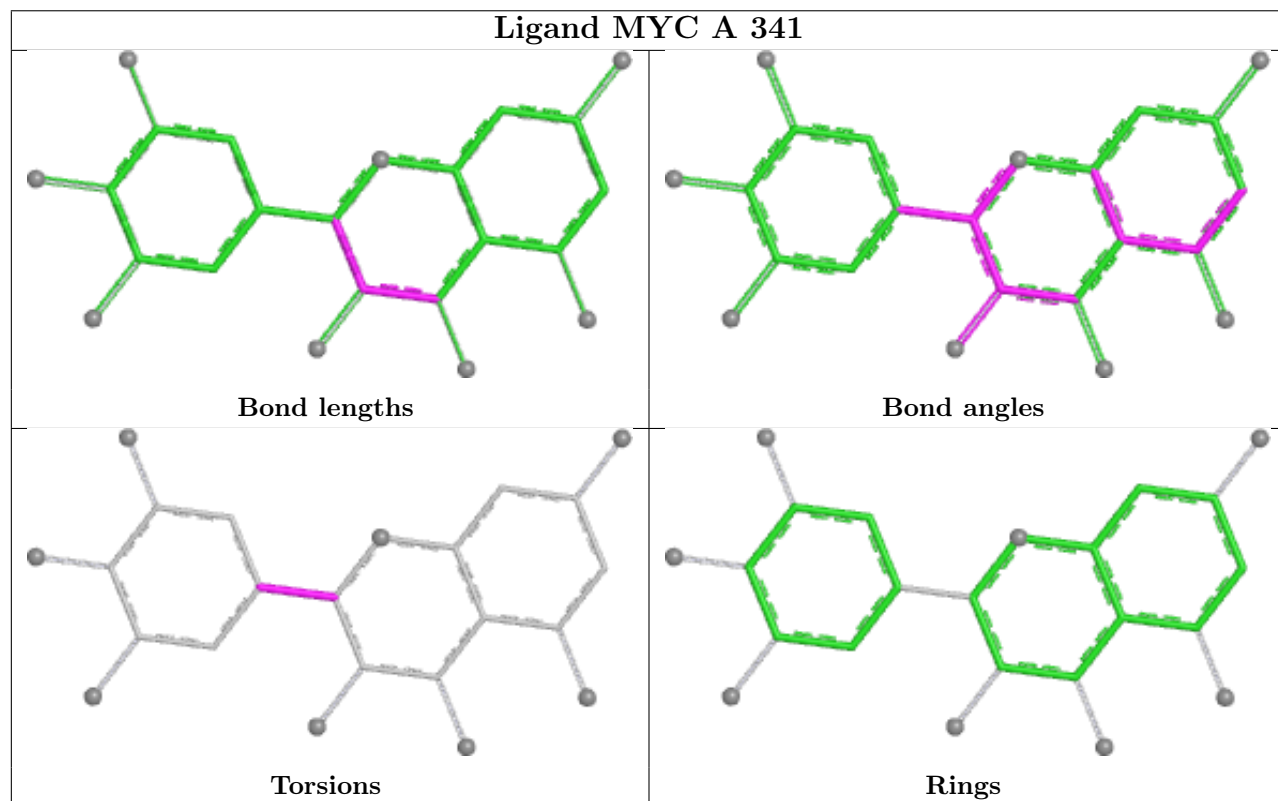
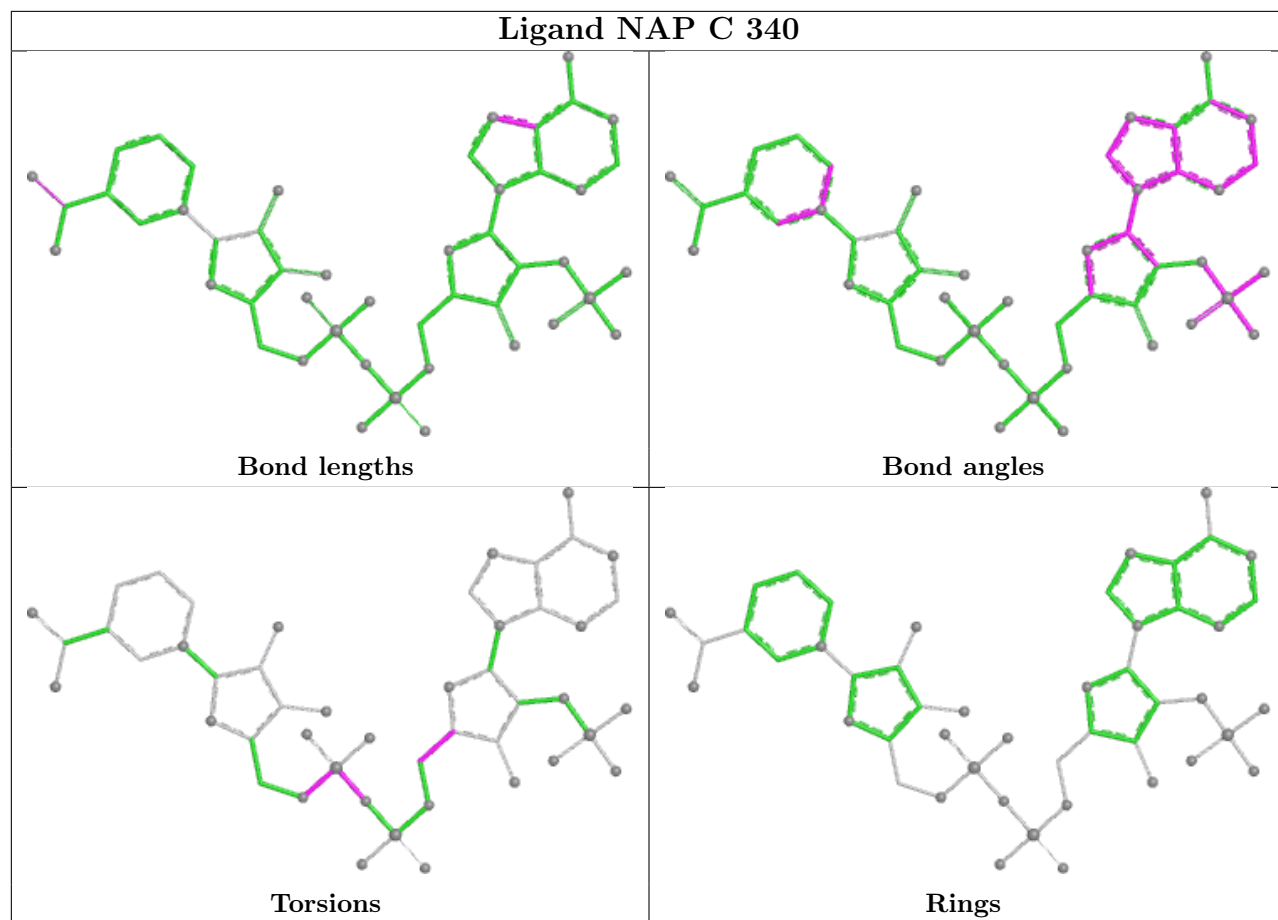


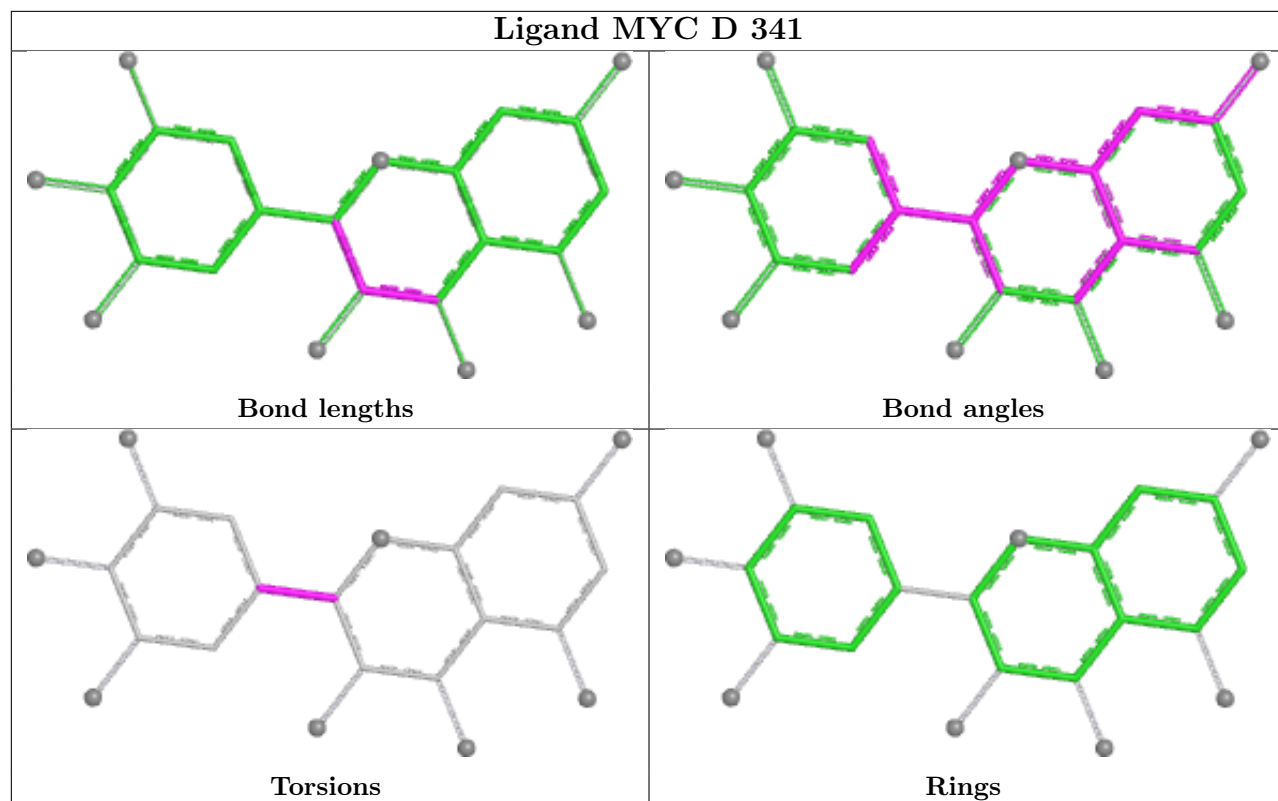












5.7 Other polymers [i](#)

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 ⓘ

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, 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	320/337 (94%)	0.70	25 (7%)	19 17	24, 45, 64, 79	2 (0%)
1	B	326/337 (96%)	0.52	22 (6%)	24 22	23, 44, 65, 88	2 (0%)
1	C	325/337 (96%)	0.29	9 (2%)	55 55	21, 42, 62, 80	1 (0%)
1	D	321/337 (95%)	0.29	5 (1%)	70 71	20, 41, 60, 80	1 (0%)
All	All	1292/1348 (95%)	0.45	61 (4%)	36 35	20, 43, 63, 88	6 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ASN	4.3
1	A	277	PRO	4.2
1	A	178	ALA	3.3
1	B	88	MET	3.1
1	B	329	HIS	2.9
1	A	177	TYR	2.8
1	A	248	GLU	2.8
1	C	90	PHE	2.8
1	C	89	ASP	2.8
1	B	274	TYR	2.8
1	A	314	GLY	2.7
1	D	199	MET	2.7
1	A	309	GLU	2.7
1	A	274	TYR	2.6
1	A	329	HIS	2.6
1	B	278	THR	2.6
1	A	278	THR	2.5
1	A	327	PRO	2.5
1	B	313[A]	THR	2.5
1	B	280	PHE	2.4
1	A	181	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	182	ASN	2.4
1	A	326	PRO	2.4
1	C	330	GLU	2.4
1	B	92	SER	2.4
1	D	279	GLU	2.3
1	B	182	ASN	2.3
1	B	306	TYR	2.3
1	D	177	TYR	2.3
1	A	268	ARG	2.3
1	C	109	GLY	2.3
1	A	269	GLU	2.3
1	A	183	ILE	2.3
1	B	94	ASP	2.2
1	B	277	PRO	2.2
1	A	313[A]	THR	2.2
1	A	276	ILE	2.2
1	B	275	ASN	2.2
1	D	92	SER	2.2
1	A	284	ASP	2.2
1	B	286	ASN	2.2
1	B	1	MET	2.2
1	B	116	ALA	2.2
1	A	240	TYR	2.1
1	B	268	ARG	2.1
1	A	88	MET	2.1
1	A	199	MET	2.1
1	B	284	ASP	2.1
1	A	280	PHE	2.1
1	C	92	SER	2.1
1	A	93	LYS	2.1
1	B	276	ILE	2.1
1	C	76	LYS	2.1
1	C	179	LYS	2.1
1	B	281	LYS	2.0
1	D	266	MET	2.0
1	B	199	MET	2.0
1	C	31	THR	2.0
1	B	95	PRO	2.0
1	B	213	ILE	2.0
1	A	179	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

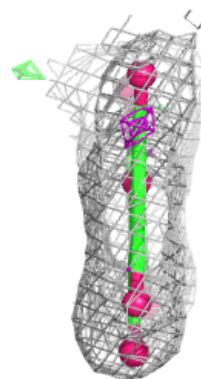
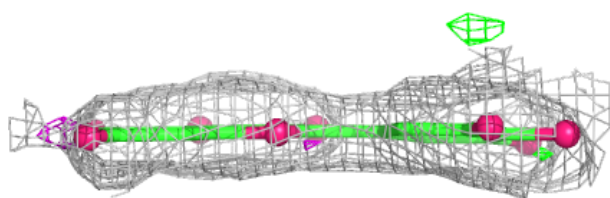
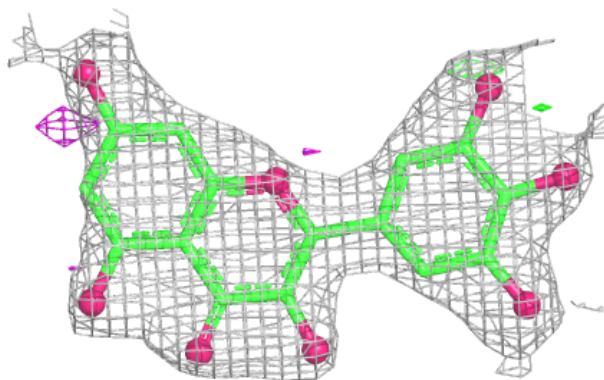
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MYC	B	342	23/23	0.91	0.11	44,55,56,57	0
3	MYC	A	342	23/23	0.92	0.09	34,50,52,53	0
3	MYC	B	341	23/23	0.95	0.08	36,41,42,43	0
3	MYC	A	341	23/23	0.95	0.08	36,40,41,42	0
3	MYC	D	342	23/23	0.95	0.07	28,31,33,34	0
2	NAP	B	340	48/48	0.96	0.07	29,35,51,55	0
3	MYC	C	342	23/23	0.96	0.06	26,30,33,33	0
2	NAP	A	340	48/48	0.96	0.07	30,35,53,59	0
3	MYC	C	341	23/23	0.97	0.06	29,31,32,34	0
2	NAP	C	340	48/48	0.97	0.07	24,32,46,51	0
3	MYC	D	341	23/23	0.97	0.06	28,31,32,33	0
2	NAP	D	340	48/48	0.97	0.06	22,31,48,53	0

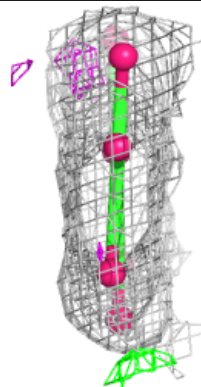
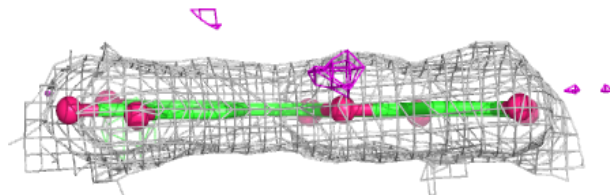
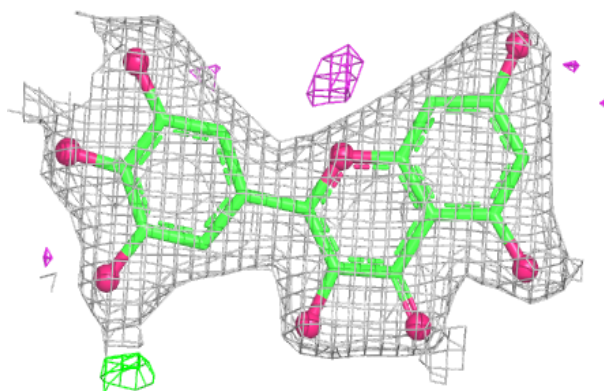
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MYC B 342:

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

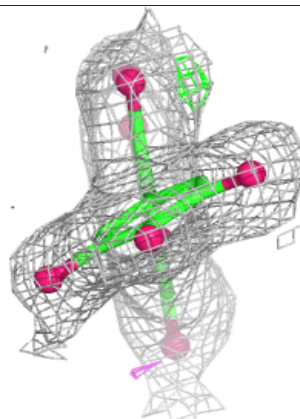
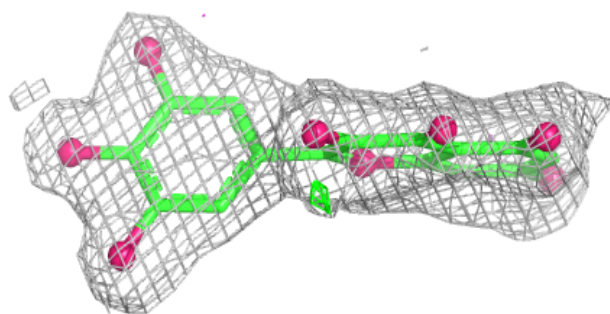
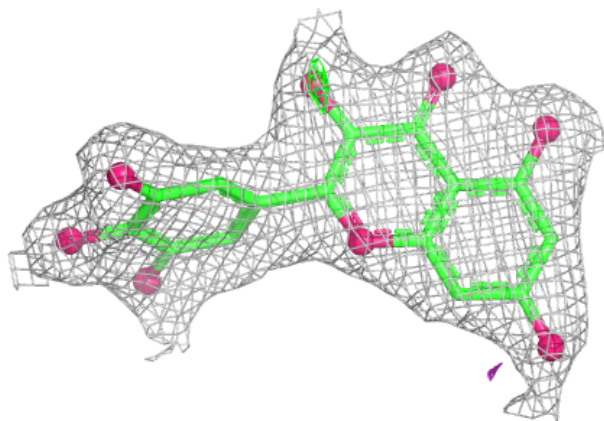
**Electron density around MYC A 342:**

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



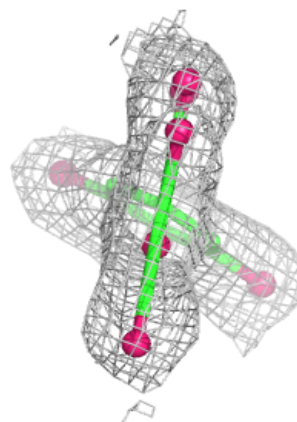
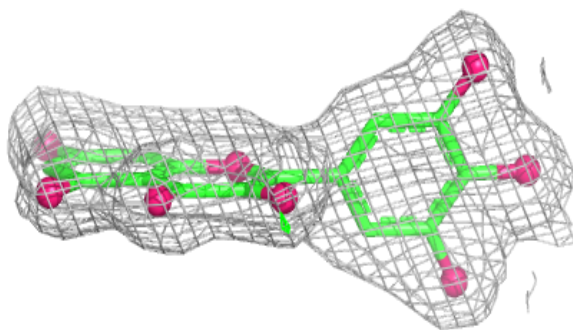
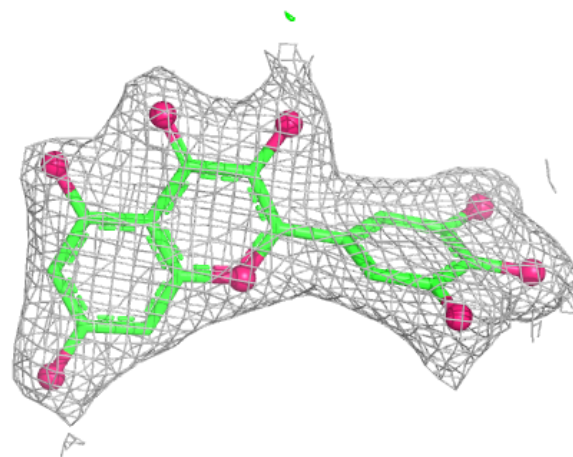
Electron density around MYC B 341:

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



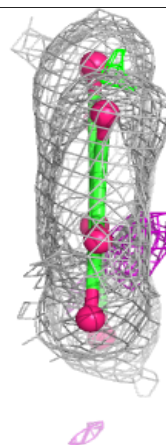
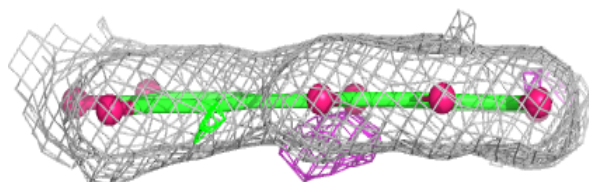
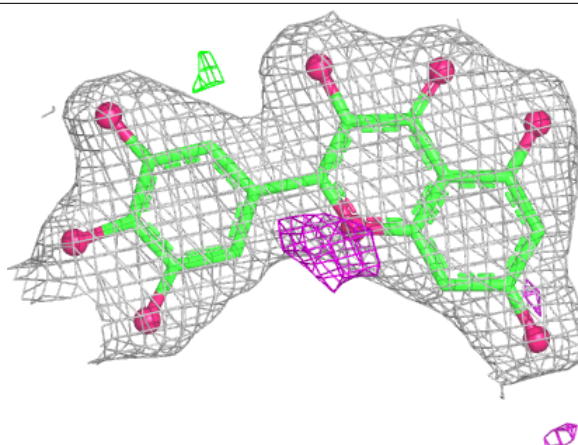
Electron density around MYC A 341:

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

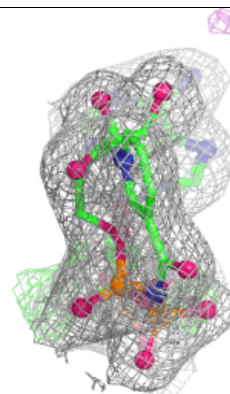
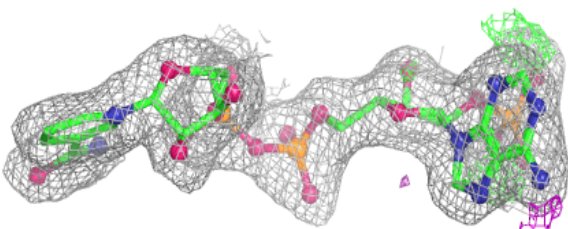
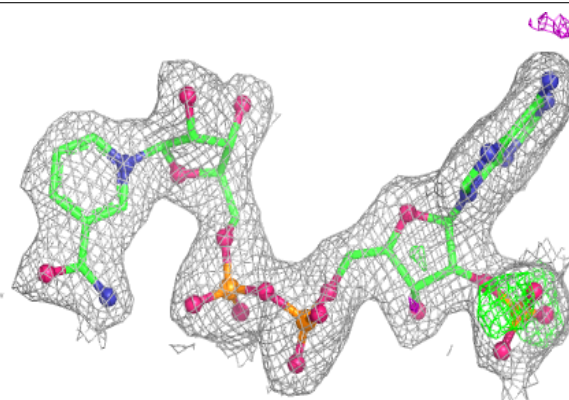


Electron density around MYC D 342:

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

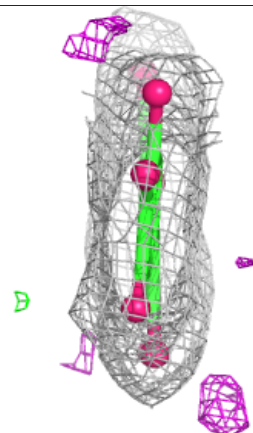
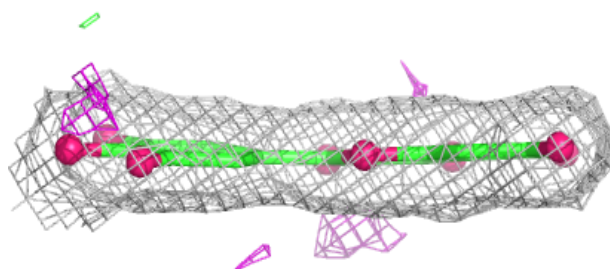
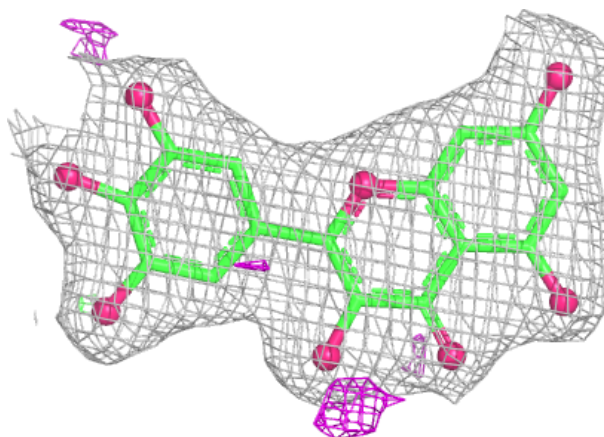
**Electron density around NAP B 340:**

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

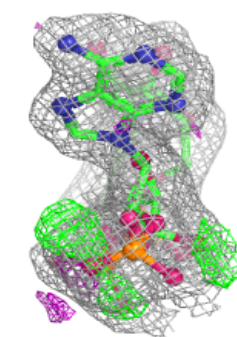
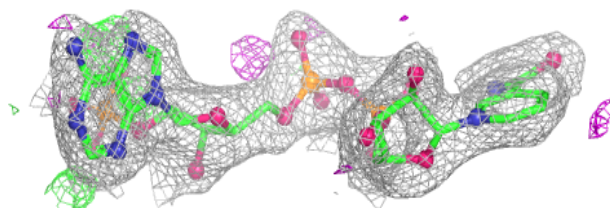
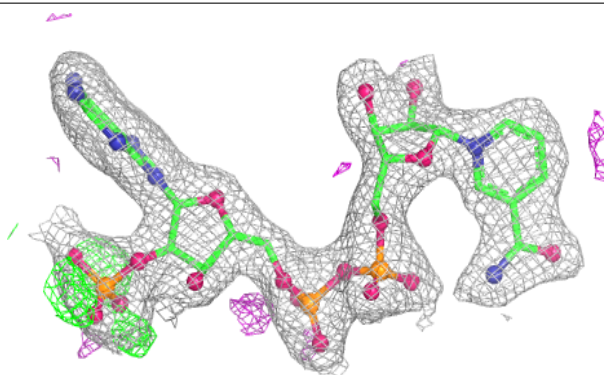


Electron density around MYC C 342:

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

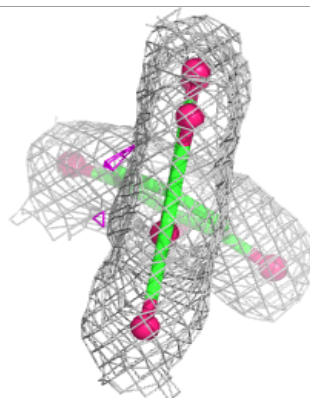
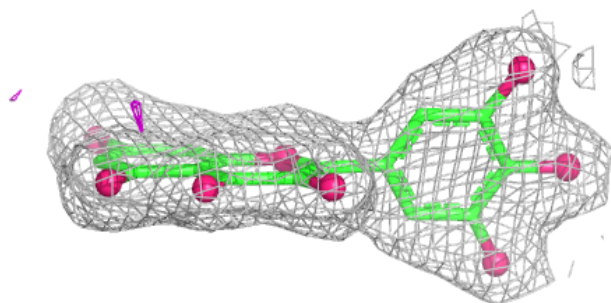
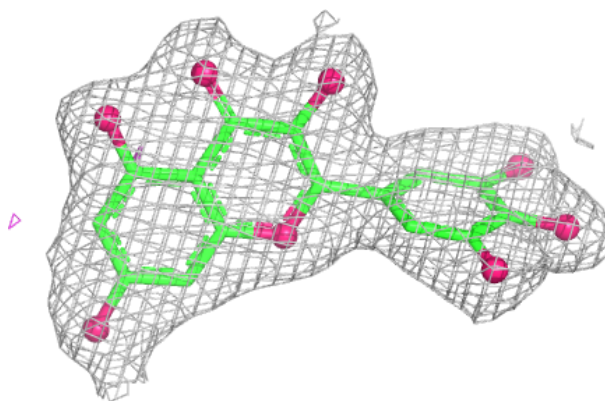
**Electron density around NAP A 340:**

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

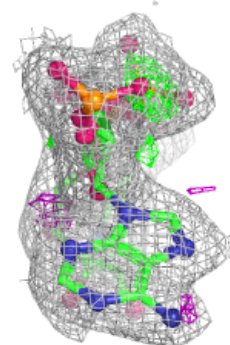
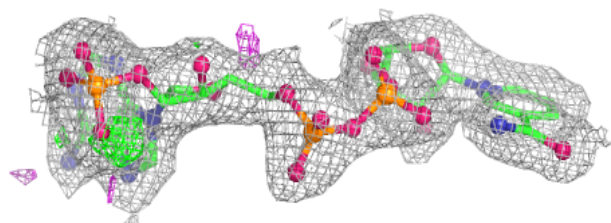
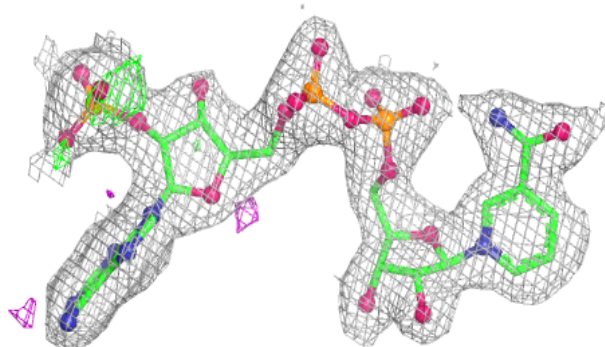


Electron density around MYC C 341:

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

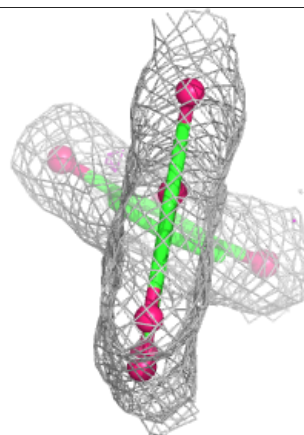
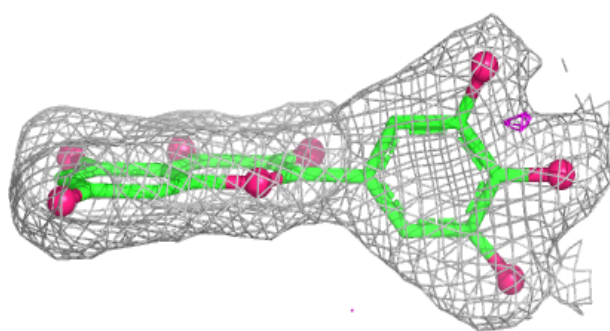
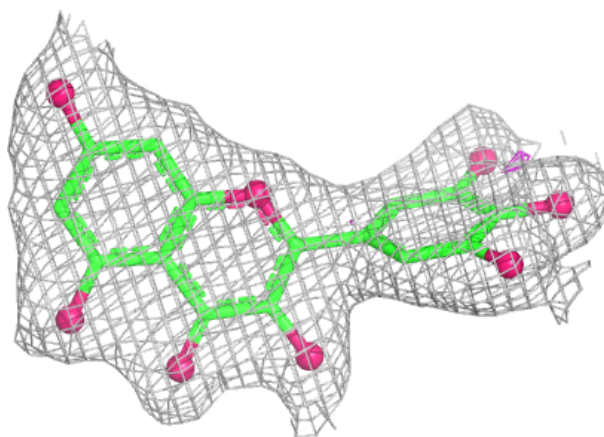
**Electron density around NAP C 340:**

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

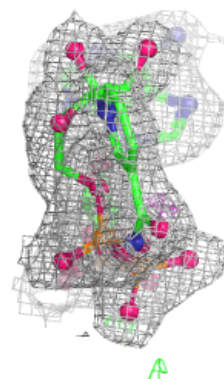
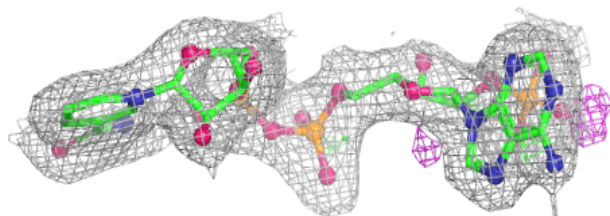
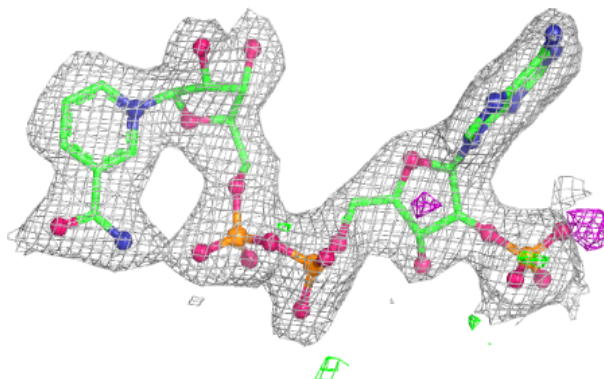


Electron density around MYC D 341:

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

**Electron density around NAP D 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.