

wwPDB X-ray Structure Validation Summary Report (i)

Oct 19, 2023 – 09:37 AM EDT

PDB ID : 2IOD

Title: Binding of two substrate analogue molecules to dihydroflavonol-4-reductase

alters the functional geometry of the catalytic site

Authors : Petit, P.; Langlois d'Estaintot, B.; Granier, T.; Gallois, B.

Deposited on : 2006-10-10

Resolution : 2.06 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

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

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

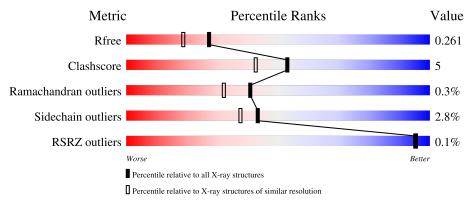
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.06 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	337	76%	18%	• 5%
1	В	337	82%	14%	
1	С	337	87%	9%	.
1	D	337	86%	9%	5%



2 Entry composition (i)

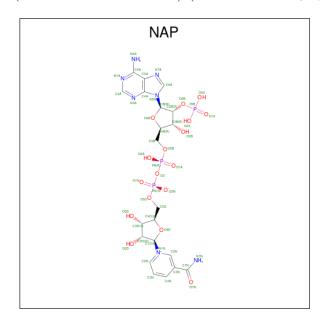
There are 4 unique types of molecules in this entry. The entry contains 11125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	Λ	320	Total	С	N	О	S	0	2	0
1	A	320	2477	1588	412	457	20	U	2	
1	В	326	Total	С	N	О	S	0	2	0
1	Ъ	320	2511	1608	415	466	22	0		0
1	С	325	Total	С	N	О	S	0	1	0
1		329	2509	1606	413	469	21	0	1	
1	1 D	D 321	Total	С	N	О	S	0	1	0
	D		2484	1590	410	463	21	U		U

• Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	Λ	1	Total	С	N	О	Р	0	0	
2	A	1	48	21	7	17	3	U		
2	D	1	Total	С	N	О	Р	0	0	
2	Б	$B \mid I \mid$		21	7	17	3	U		

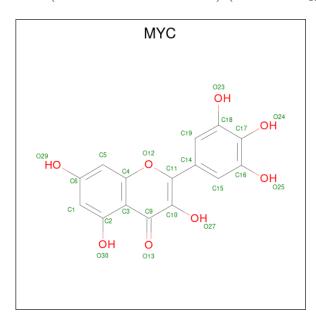
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	Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
	9	C	1	Total	С	N	О	Р	0	0	
		C	1	48	21	7	17	3	U		
ĺ	2	D	1	Total C N O P	0	0					
	2 D		1	48	21	7	17	3	U		

• Molecule 3 is 3,5,7-TRIHYDROXY-2-(3,4,5-TRIHYDROXYPHENYL)-4H-CHROMEN-4-ONE (three-letter code: MYC) (formula: $C_{15}H_{10}O_8$).



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

• Molecule 4 is water.



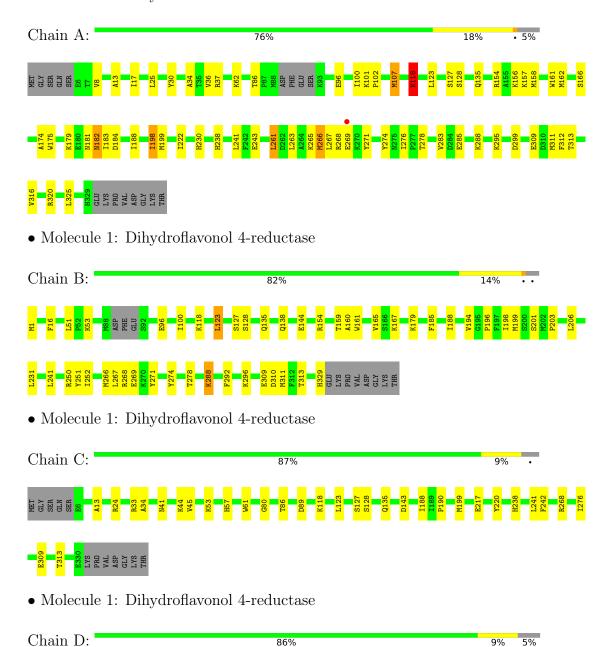
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	151	Total O 151 151	0	0
4	В	174	Total O 174 174	0	0
4	С	201	Total O 201 201	0	0
4	D	242	Total O 242 242	0	0



3 Residue-property plots (i)

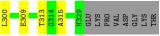
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	47.23Å 177.96Å 92.60Å	Donositon
a, b, c, α , β , γ	90.00° 104.77° 90.00°	Depositor
Resolution (Å)	89.44 - 2.06	Depositor
Resolution (A)	89.54 - 2.06	EDS
% Data completeness	98.9 (89.44-2.06)	Depositor
(in resolution range)	98.9 (89.54-2.06)	EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	2.17 (at 2.07Å)	Xtriage
Refinement program	REFMAC	Depositor
Ρ. Р.	0.189 , 0.257	Depositor
R, R_{free}	0.195 , 0.261	DCC
R_{free} test set	4501 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 55.9	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.170 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 4.25% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
Mol		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.66	0/2539	0.89	$2/3450 \ (0.1\%)$	
1	В	0.64	0/2573	0.87	0/3494	
1	С	0.65	0/2568	0.85	2/3490 (0.1%)	
1	D	0.69	0/2542	0.90	$1/3453 \ (0.0\%)$	
All	All	0.66	0/10222	0.88	5/13887 (0.0%)	

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	37	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	D	24	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	С	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	С	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 (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.

\mathbf{N}	Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
	1	A	2477	0	2431	42	0
	1	В	2511	0	2457	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	2509	0	2447	19	0
1	D	2484	0	2432	16	0
2	A	48	0	25	2	0
2	В	48	0	25	1	0
2	С	48	0	25	4	0
2	D	48	0	25	2	0
3	A	46	0	11	2	0
3	В	46	0	11	4	0
3	С	46	0	15	2	0
3	D	46	0	10	1	0
4	A	151	0	0	3	0
4	В	174	0	0	1	0
4	С	201	0	0	3	0
4	D	242	0	0	1	0
All	All	11125	0	9914	109	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 5.

The worst 5 of 109 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
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:4522:HOH:O	1.92	0.69
1:A:17:ILE:HD12	2:A:1340:NAP:H51N	1.82	0.61
1:A:263:LEU:HD12	1:A:266:MET:HE2	1.82	0.61

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	15	
1	В	324/337~(96%)	308 (95%)	15 (5%)	1 (0%)	41	32	
1	C	324/337~(96%)	316 (98%)	7 (2%)	1 (0%)	41	32	
1	D	318/337 (94%)	307 (96%)	11 (4%)	0	100	100	
All	All	1284/1348~(95%)	1233 (96%)	47 (4%)	4 (0%)	41	32	

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	118	LYS
1	В	118	LYS
1	С	118	LYS

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	267/293~(91%)	254 (95%)	13 (5%)	25	17	
1	В	269/293~(92%)	263 (98%)	6 (2%)	52	46	
1	С	269/293~(92%)	265 (98%)	4 (2%)	65	62	
1	D	268/293~(92%)	261 (97%)	7 (3%)	46	40	
All	All	$1073/1172\ (92\%)$	1043 (97%)	30 (3%)	43	37	

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	123	LEU
1	D	158	MET
1	В	269	GLU
1	D	288	LYS
1	D	92	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16



such sidechains are listed below:

Mol	Chain	Res	Type
1	D	236	ASN
1	D	181	ASN
1	С	57	HIS
1	D	138	GLN
1	В	236	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 monosaccharides 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	Mol Type Chain Res		Peg	Link	Во	ond leng	ths	В	ond ang	gles
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	В	2340	-	45,52,52	1.66	4 (8%)	56,80,80	2.03	14 (25%)
2	NAP	D	4340	-	45,52,52	1.64	5 (11%)	56,80,80	1.88	10 (17%)
3	MYC	A	1341	-	22,25,25	1.18	2 (9%)	27,38,38	1.31	4 (14%)
3	MYC	В	2342	-	22,25,25	1.14	3 (13%)	27,38,38	1.55	5 (18%)
3	MYC	С	3342	-	22,25,25	1.34	3 (13%)	27,38,38	2.21	10 (37%)
3	MYC	D	4341	-	22,25,25	1.29	2 (9%)	27,38,38	1.28	4 (14%)
3	MYC	A	1342	-	22,25,25	1.45	3 (13%)	27,38,38	1.62	6 (22%)



Mol	Mol Type		Res	Link	Во	ond leng	ths	Bond angles		
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MYC	С	3341	-	22,25,25	1.27	3 (13%)	27,38,38	1.59	6 (22%)
2	NAP	С	3340	-	45,52,52	1.64	2 (4%)	56,80,80	1.56	7 (12%)
2	NAP	A	1340	-	45,52,52	1.68	5 (11%)	56,80,80	1.51	6 (10%)
3	MYC	В	2341	-	22,25,25	1.46	3 (13%)	27,38,38	1.31	3 (11%)
3	MYC	D	4342	-	22,25,25	1.36	6 (27%)	27,38,38	1.83	9 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	В	2340	-	-	6/31/67/67	0/5/5/5
2	NAP	D	4340	-	-	8/31/67/67	0/5/5/5
3	MYC	A	1341	-	-	0/0/4/4	0/3/3/3
3	MYC	В	2342	-	-	0/0/4/4	0/3/3/3
3	MYC	С	3342	-	-	0/0/4/4	0/3/3/3
3	MYC	D	4341	-	-	0/0/4/4	0/3/3/3
3	MYC	A	1342	-	-	0/0/4/4	0/3/3/3
3	MYC	С	3341	-	-	0/0/4/4	0/3/3/3
2	NAP	С	3340	-	-	5/31/67/67	0/5/5/5
2	NAP	A	1340	-	-	6/31/67/67	0/5/5/5
3	MYC	В	2341	-	-	0/0/4/4	0/3/3/3
3	MYC	D	4342	-	-	0/0/4/4	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
2	С	3340	NAP	O7N-C7N	8.55	1.40	1.24
2	A	1340	NAP	O7N-C7N	8.30	1.40	1.24
2	В	2340	NAP	O7N-C7N	8.12	1.39	1.24
2	D	4340	NAP	O7N-C7N	7.32	1.38	1.24
3	В	2341	MYC	C15-C16	4.27	1.41	1.37

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	D	4340	NAP	N3A-C2A-N1A	-6.99	117.75	128.68
2	С	3340	NAP	N3A-C2A-N1A	-6.53	118.47	128.68
2	В	2340	NAP	N3A-C2A-N1A	-5.53	120.04	128.68

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	В	2340	NAP	O3X-P2B-O2X	5.12	127.22	107.64
2	В	2340	NAP	C3N-C7N-N7N	4.89	123.62	117.75

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1340	NAP	C5D-O5D-PN-O1N
2	A	1340	NAP	C5D-O5D-PN-O2N
2	В	2340	NAP	C5B-O5B-PA-O1A
2	В	2340	NAP	C5D-O5D-PN-O2N
2	С	3340	NAP	C5D-O5D-PN-O2N

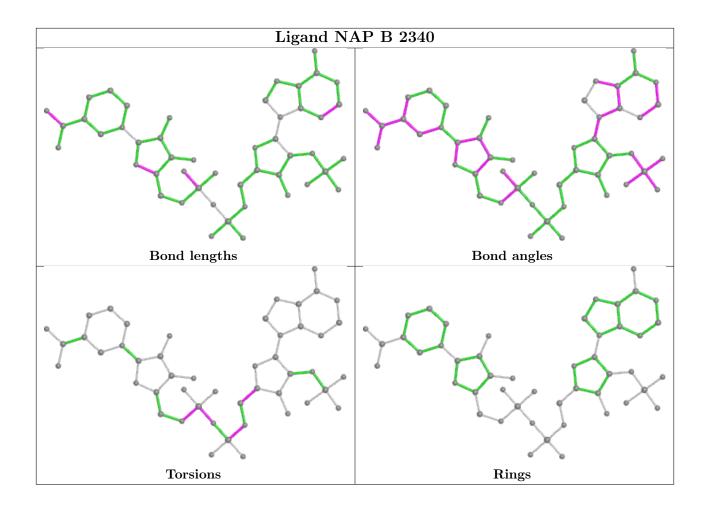
There are no ring outliers.

8 monomers are involved in 18 short contacts:

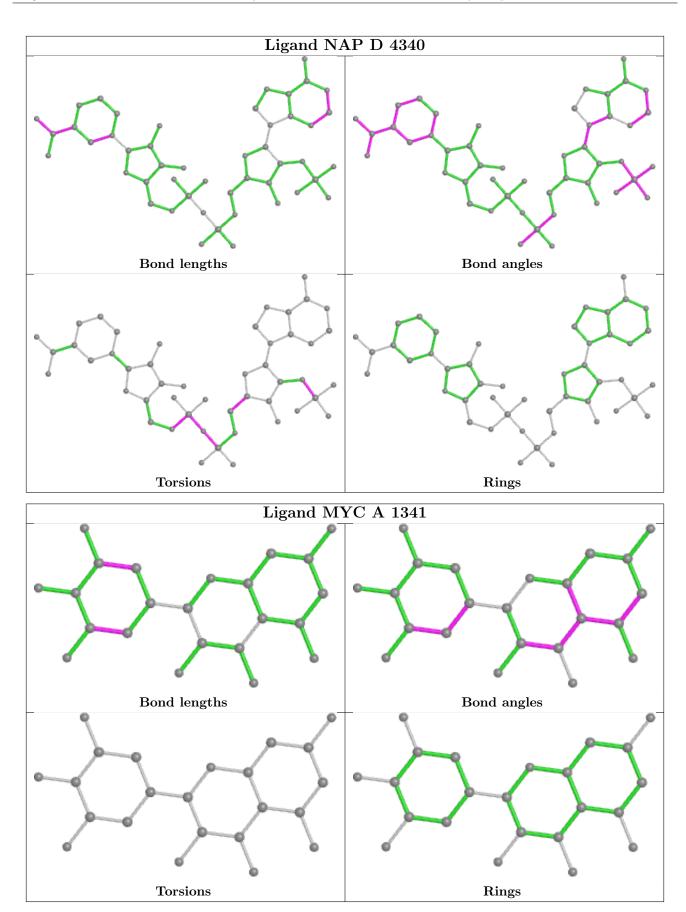
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	2340	NAP	1	0
2	D	4340	NAP	2	0
3	В	2342	MYC	4	0
3	С	3342	MYC	2	0
3	A	1342	MYC	2	0
2	С	3340	NAP	4	0
2	A	1340	NAP	2	0
3	D	4342	MYC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

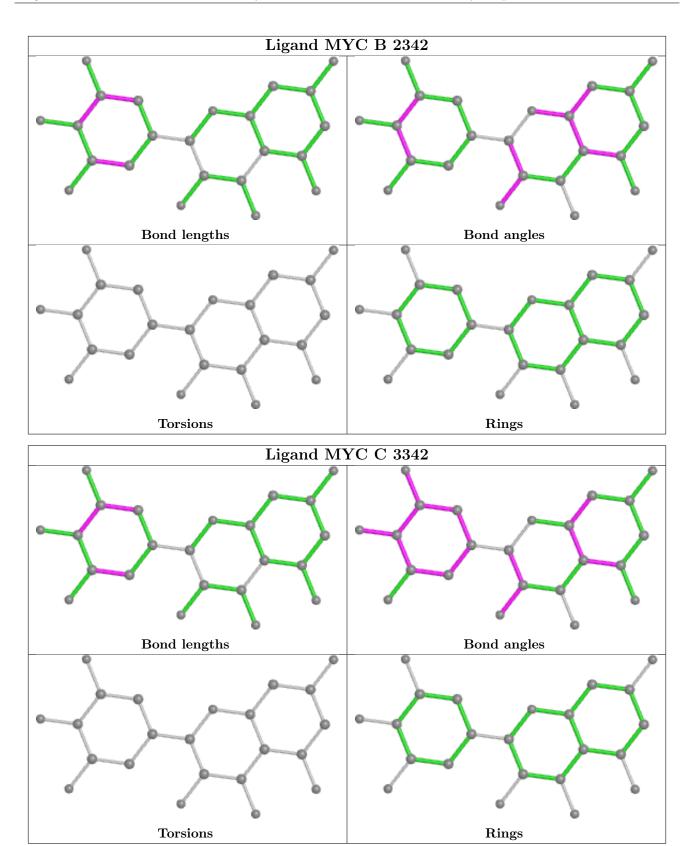




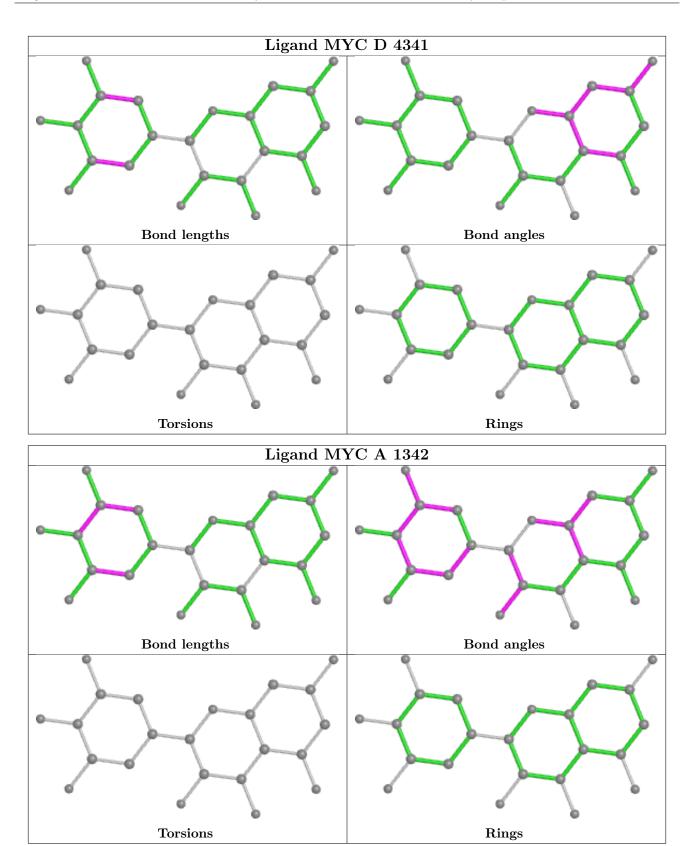




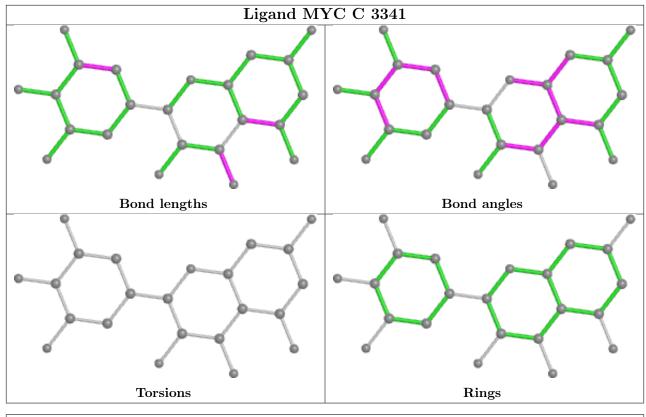


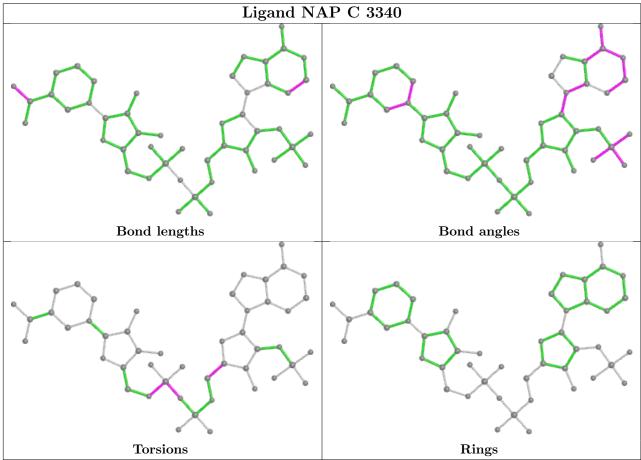




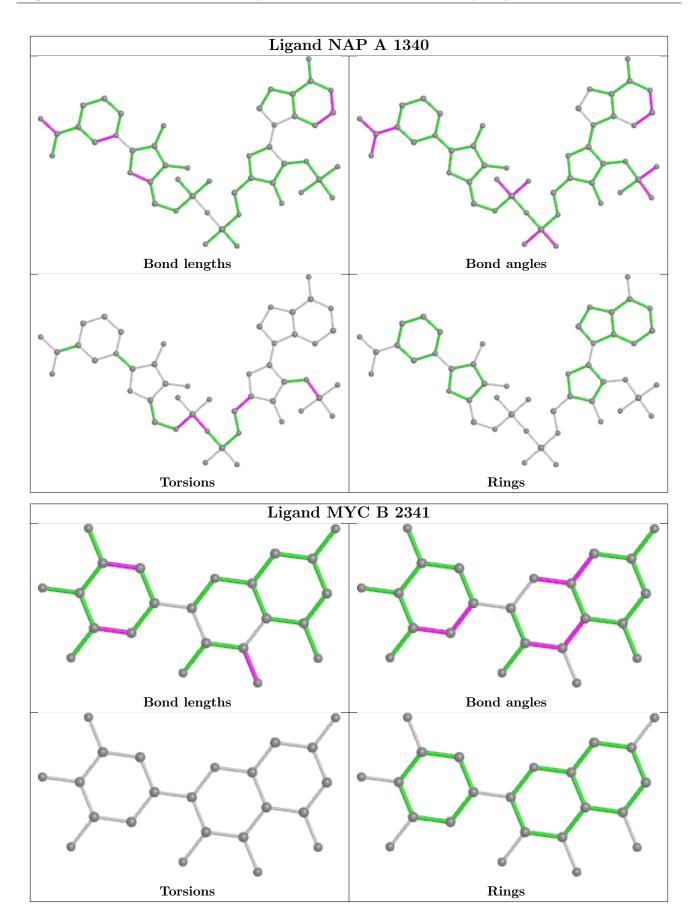




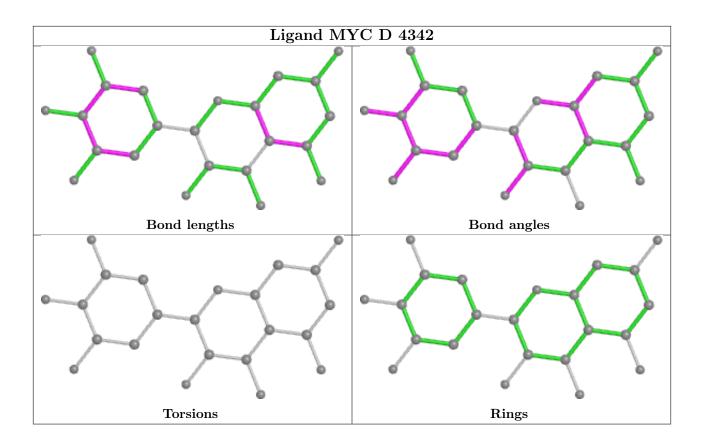












5.7 Other polymers (i)

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	# RSRZ > 2	$OWAB(\AA^2)$	Q < 0.9
1	A	320/337 (94%)	-0.21	1 (0%) 94 94	29, 45, 64, 79	0
1	В	326/337~(96%)	-0.29	0 100 100	29, 44, 65, 88	0
1	С	325/337~(96%)	-0.37	0 100 100	27, 42, 62, 80	0
1	D	321/337 (95%)	-0.38	0 100 100	27, 41, 60, 80	0
All	All	1292/1348 (95%)	-0.31	1 (0%) 95 95	27, 43, 63, 88	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	MYC	В	2342	23/23	0.92	0.17	44,55,56,57	0

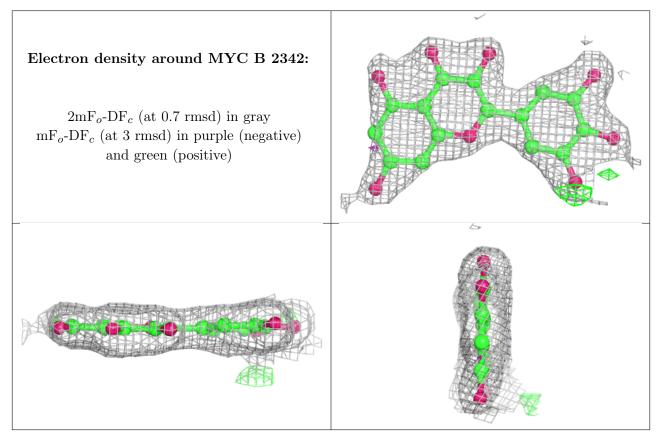
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	MYC	A	1342	23/23	0.94	0.13	34,50,52,53	0
3	MYC	В	2341	23/23	0.95	0.09	36,41,42,43	0
3	MYC	A	1341	23/23	0.96	0.10	36,40,41,42	0
3	MYC	С	3341	23/23	0.97	0.08	29,31,32,34	0
3	MYC	С	3342	23/23	0.97	0.09	26,30,33,33	0
3	MYC	D	4342	23/23	0.97	0.09	28,31,33,34	0
2	NAP	D	4340	48/48	0.98	0.09	22,31,48,53	0
2	NAP	A	1340	48/48	0.98	0.09	30,35,53,59	0
2	NAP	В	2340	48/48	0.98	0.10	29,35,51,55	0
3	MYC	D	4341	23/23	0.98	0.08	28,31,32,33	0
2	NAP	С	3340	48/48	0.98	0.10	24,32,46,51	0

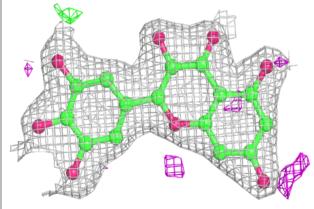
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

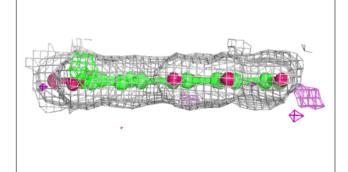


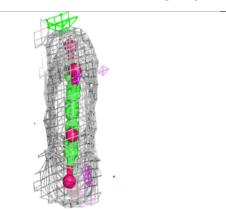


Electron density around MYC A 1342:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

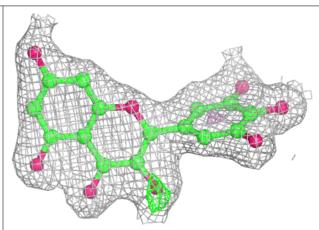


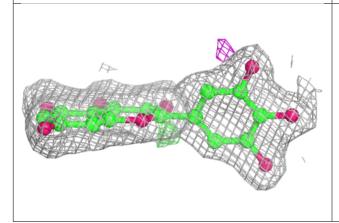


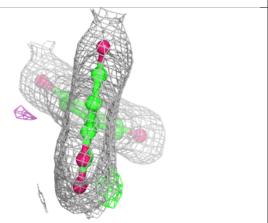


Electron density around MYC B 2341:

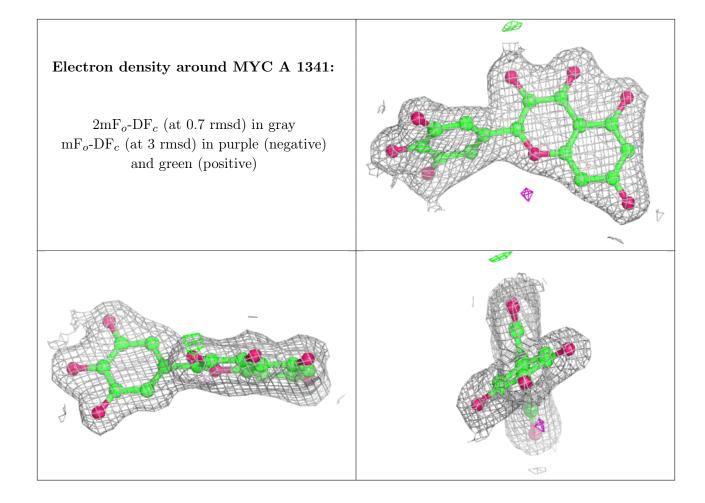
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



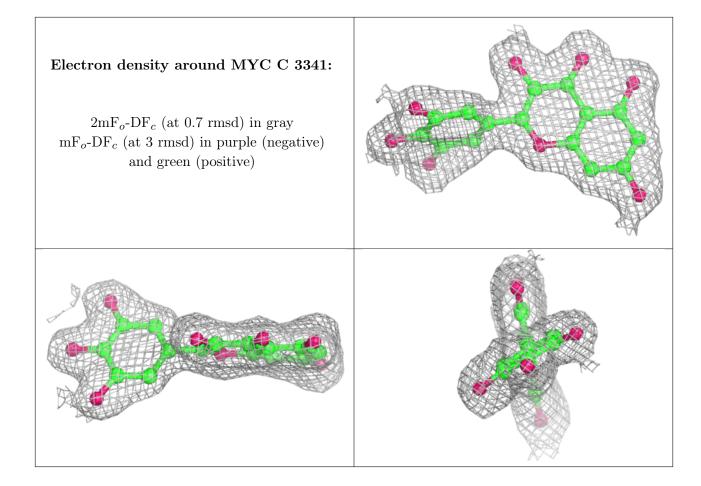












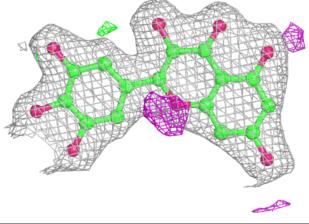


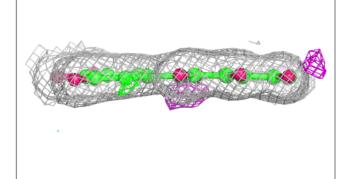
Electron density around MYC C 3342: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

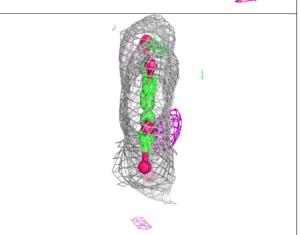


Electron density around MYC D 4342:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

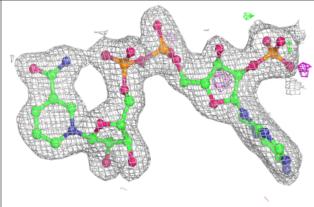


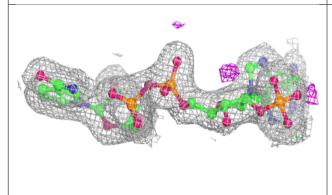


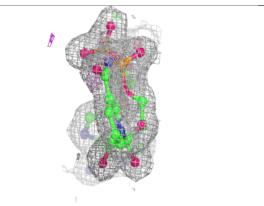


Electron density around NAP D 4340:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



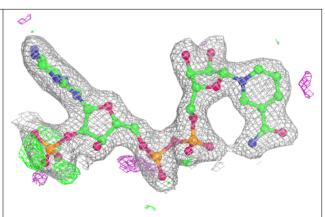


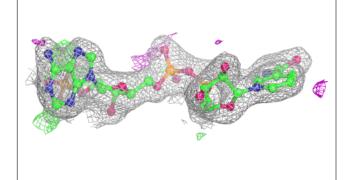


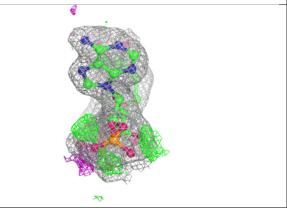


Electron density around NAP A 1340:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

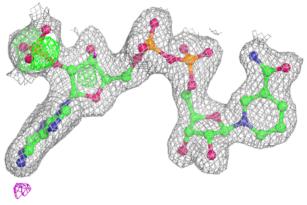


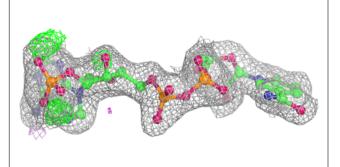


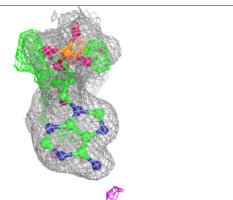


Electron density around NAP B 2340:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



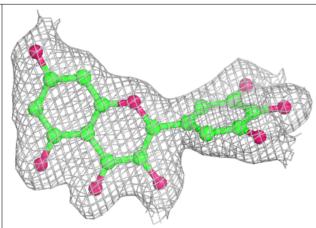


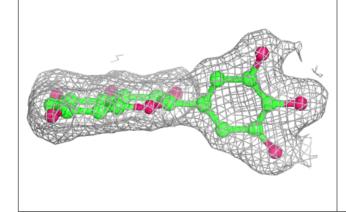


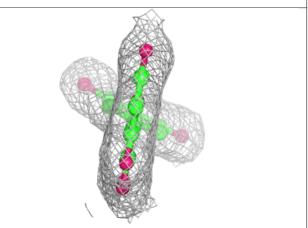


Electron density around MYC D 4341:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

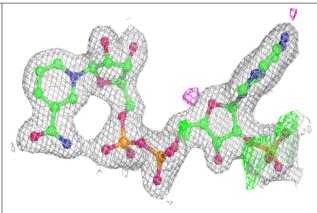


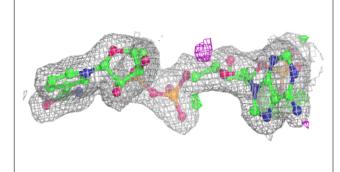


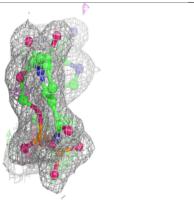


Electron density around NAP C 3340:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

