



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 06:37 pm BST

PDB ID : 1SO2  
Title : CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 3B In COMPLEX WITH A DIHYDROPYRIDAZINE INHIBITOR  
Authors : Scapin, G.; Patel, S.B.; Chung, C.; Varnerin, J.P.; Edmondson, S.D.; Mastracchio, A.; Parmee, E.R.; Becker, J.W.; Singh, S.B.; Van Der Ploeg, L.H.; Tota, M.R.  
Deposited on : 2004-03-12  
Resolution : 2.40 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](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

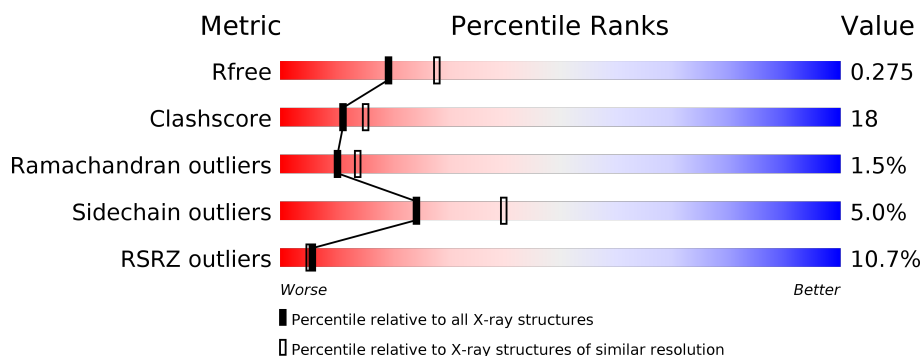
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	420	<div> <div>9%</div> <div> <div>61%</div> <div>23%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	420	<div> <div>8%</div> <div> <div>60%</div> <div>24%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	420	<div> <div>9%</div> <div> <div>63%</div> <div>24%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	420	<div> <div>12%</div> <div> <div>50%</div> <div>33%</div> <div>5%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12292 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.

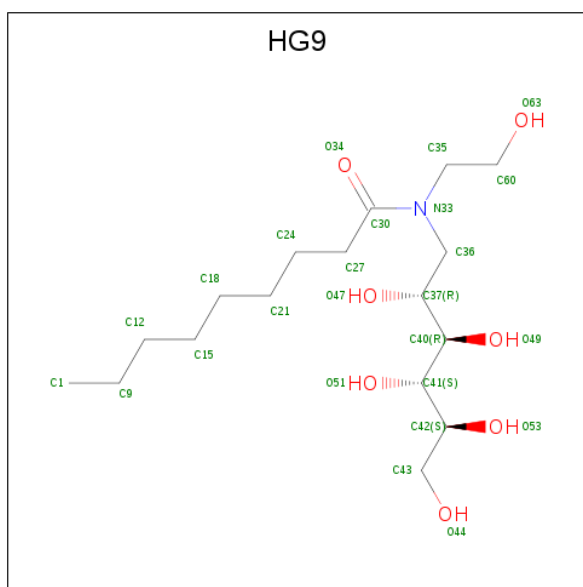
- Molecule 1 is a protein called cGMP-inhibited 3',5'-cyclic phosphodiesterase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2916	1868	501	533	14			
1	B	363	Total	C	N	O	S	0	0	0
			2909	1863	500	532	14			
1	C	372	Total	C	N	O	S	0	0	0
			2964	1897	508	545	14			
1	D	365	Total	C	N	O	S	0	0	0
			2916	1867	500	535	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

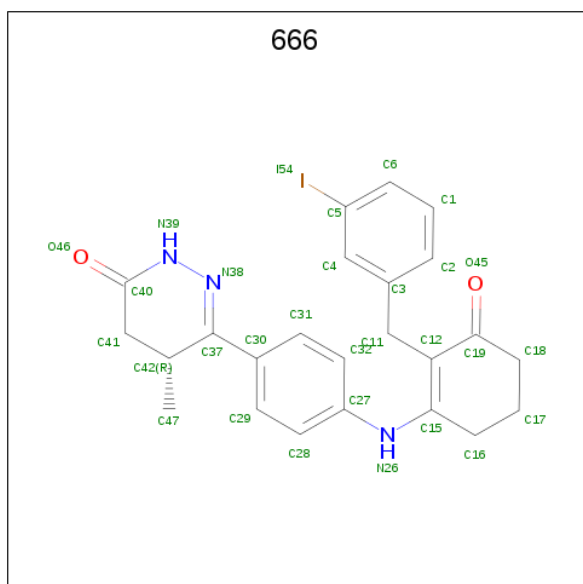
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	3	Total	Mg	0	0
			3	3		
2	D	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 1-DEOXY-1-[(2-HYDROXYETHYL)(NONANOYL)AMINO]HEXITOL (three-letter code: HG9) (formula: C<sub>17</sub>H<sub>35</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	16	1	7		
3	A	1	Total	C	N	O	0	0
			24	16	1	7		
3	B	1	Total	C	N	O	0	0
			24	16	1	7		
3	B	1	Total	C	N	O	0	0
			24	16	1	7		

- Molecule 4 is 6-(4-{[2-(3-iodobenzyl)-3-oxocyclohex-1-en-1-yl]amino}phenyl)-5-methyl-4,5-dihydropyridazin-3(2H)-one (three-letter code: 666) (formula:  $C_{24}H_{24}IN_3O_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	I	N	O	0	0
			30	24	1	3	2		
4	B	1	Total	C	I	N	O	0	0
			30	24	1	3	2		
4	C	1	Total	C	I	N	O	0	0
			30	24	1	3	2		
4	D	1	Total	C	I	N	O	0	0
			30	24	1	3	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	115	Total	O	0	0
			115	115		
5	C	70	Total	O	0	0
			70	70		
5	D	58	Total	O	0	0
			58	58		

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 ( $\text{RSRZ} > 2$ ). 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.

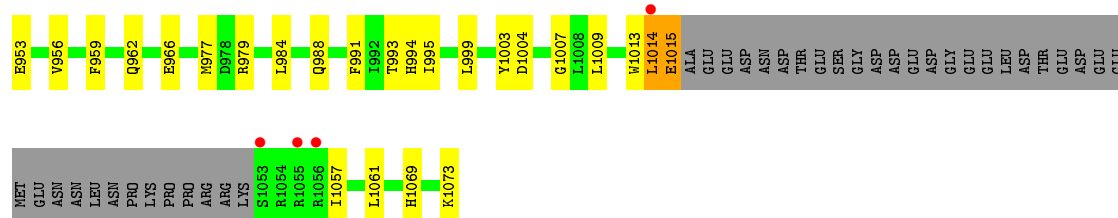
[illegible]

Chain B:

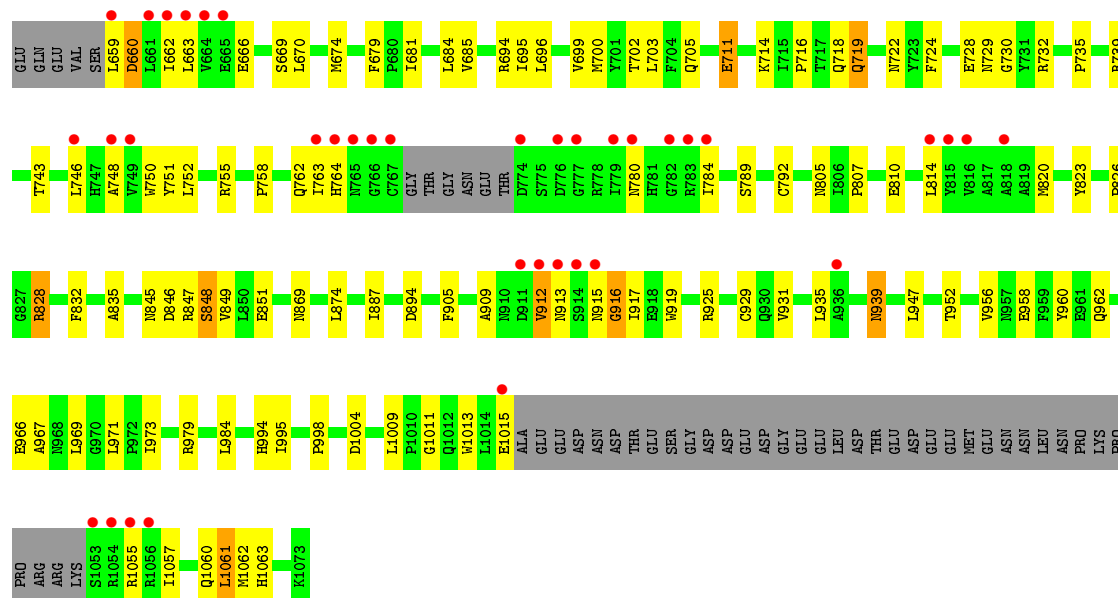
8% 60% 24% 14%

GLU GLN GLU VAL SER L569 D660 L661 L662 L663 V664 E665 E666 D668 S669 L670 L671 E672 K673 M674 S675 M676 I681 V685 G689 E690 K691 R694 I695 L696 S697 Q698 V699 M700 Q705 K714 Q719 E728 N729 G730 R739 I740 H741 A742 V745 L746 H747 A748 V749

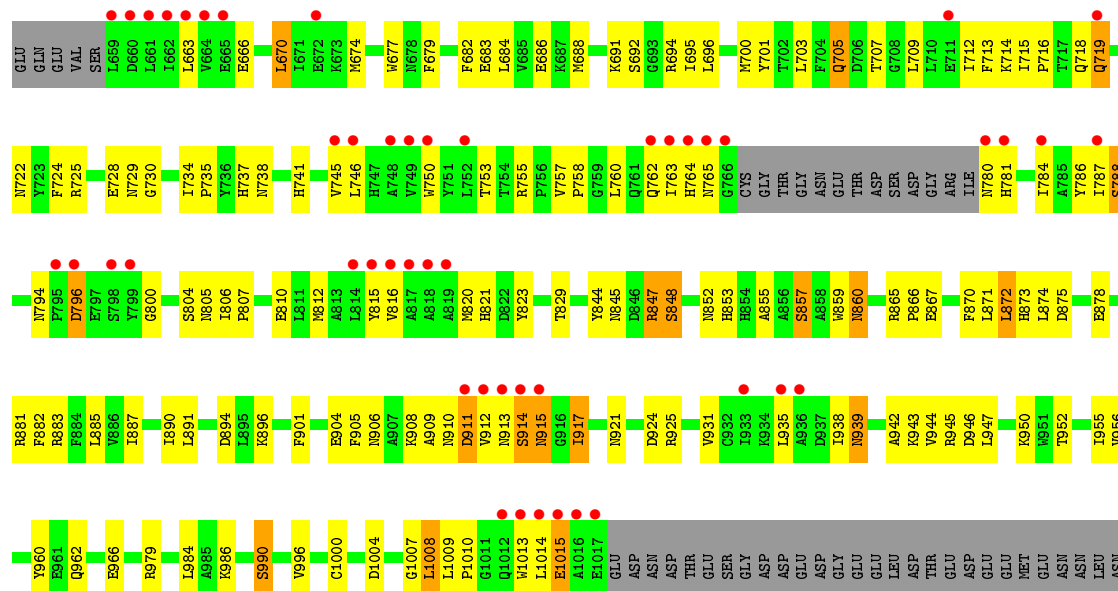
W750 Y751 R755 P758 G759 L760 Q761 Q762 L763 H764 V765 V766 Q767 G768 G769 L770 T771 A772 S773 L774 E775 L776 L777 L778 L779 L780 L781 L782 L783 L784 L785 L786 L787 L788 L789 L790 L791 L792 L793 L794 L795 L796 L797 L798 L799 L800 L801 L802 L803 L804 L805 L806 L807 L808 L809 L810 L811 L812 L813 L814 L815 L816 L817 L818 L819 L820 L821 L822 L823 L824 L825 L826 L827 L828 L829 L830 L831 L832 L833 L834 L835 L836 L837 L838 L839 L840 L841 L842 L843 L844 L845 L846 L847 L848 L849 L850 L851 L852 L853 L854 L855 L856 L857 L858 L859 L860 L861 L862 L863 L864 L865 L866 L867 L868 L869 L870 L871 L872 L873 L874 L875 L876 L877 L878 L879 L880 L881 L882 L883 L884 L885 L886 L887 L888 L889 L890 L891 L892 L893 L894 L895 L896 L897 L898 L899 L900 L901 L902 L903 L904 L905 L906 L907 L908 L909 L910 L911 L912 L913 L914 L915 L916 L917 L918 L919 L920 L921 L922 L923 L924 L925 L926 L927 L928 L929 L930 L931 L932 L933 L934 L935 L936 L937 L938 L939 L940 L941 L942 L943 L944 L945 L946 L947 L948 L949 L950 L951 L952 L953 L954 L955 L956 L957 L958 L959 L960 L961 L962 L963 L964 L965 L966 L967 L968 L969 L970 L971 L972 L973 L974 L975 L976 L977 L978 L979 L980 L981 L982 L983 L984 L985 L986 L987 L988 L989 L990 L991 L992 L993 L994 L995 L996 L997 L998 L999 L1000

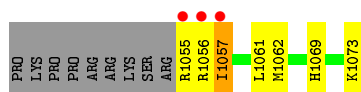


• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.48 Å   121.77 Å   126.67 Å 90.00°   100.74°   90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.40) 99.8 (29.82-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.39 Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.232   ,   0.277 0.228   ,   0.275	Depositor DCC
$R_{free}$ test set	4345 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.881	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 666, MG, HG9

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	0.59	0/2992	0.67	1/4063 (0.0%)
1	B	0.58	0/2985	0.70	1/4054 (0.0%)
1	C	0.55	0/3040	0.66	0/4129
1	D	0.58	0/2992	0.64	0/4065
All	All	0.57	0/12009	0.67	2/16311 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	828	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	821	HIS	N-CA-C	5.22	125.09	111.00

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	2916	0	2803	83	0
1	B	2909	0	2788	107	0
1	C	2964	0	2834	87	0
1	D	2916	0	2788	148	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	48	0	60	2	0
3	B	48	0	60	2	0
4	A	30	0	24	2	0
4	B	30	0	24	2	0
4	C	30	0	24	1	0
4	D	30	0	24	3	0
5	A	119	0	0	2	0
5	B	115	0	0	6	0
5	C	70	0	0	3	0
5	D	58	0	0	4	0
All	All	12292	0	11429	419	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 18.

The worst 5 of 419 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:A:700:MET:HE3	1:A:746:LEU:HD21	1.38	1.00
1:C:828:ARG:HG2	1:C:832:PHE:CD2	1.96	0.99
1:C:967:ALA:HB2	1:C:973:ILE:HD11	1.45	0.96
1:B:828:ARG:HG2	1:B:832:PHE:CD2	2.04	0.93
1:B:719:GLN:H	1:B:719:GLN:HE21	0.99	0.92

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	357/420 (85%)	337 (94%)	18 (5%)	2 (1%)	25	36
1	B	357/420 (85%)	325 (91%)	26 (7%)	6 (2%)	9	11
1	C	366/420 (87%)	336 (92%)	25 (7%)	5 (1%)	11	15
1	D	359/420 (86%)	319 (89%)	31 (9%)	9 (2%)	5	6
All	All	1439/1680 (86%)	1317 (92%)	100 (7%)	22 (2%)	10	14

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	912	VAL
1	B	913	ASN
1	C	660	ASP
1	D	914	SER
1	D	1015	GLU

### 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	310/370 (84%)	293 (94%)	17 (6%)	21	35
1	B	308/370 (83%)	295 (96%)	13 (4%)	30	47
1	C	313/370 (85%)	301 (96%)	12 (4%)	33	51
1	D	308/370 (83%)	288 (94%)	20 (6%)	17	27
All	All	1239/1480 (84%)	1177 (95%)	62 (5%)	24	40

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1014	LEU
1	C	780	ASN
1	D	939	ASN
1	C	705	GLN
1	C	820	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1060	GLN
1	C	719	GLN
1	D	913	ASN
1	C	705	GLN
1	C	722	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

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	HG9	B	451	-	23,23,24	1.86	5 (21%)	27,28,29	1.15	2 (7%)
4	666	A	461	-	33,33,33	3.89	25 (75%)	43,46,46	2.66	12 (27%)
3	HG9	B	452	-	23,23,24	1.47	3 (13%)	27,28,29	1.29	5 (18%)
4	666	B	462	-	33,33,33	3.81	22 (66%)	43,46,46	2.66	9 (20%)
3	HG9	A	453	-	23,23,24	1.51	3 (13%)	27,28,29	1.27	3 (11%)
4	666	C	463	-	33,33,33	3.83	24 (72%)	43,46,46	2.73	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	666	D	464	-	33,33,33	3.88	25 (75%)	43,46,46	2.74	13 (30%)
3	HG9	A	454	-	23,23,24	1.71	6 (26%)	27,28,29	1.48	4 (14%)

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	HG9	B	451	-	-	4/32/32/33	-
4	666	A	461	-	-	1/12/39/39	0/4/4/4
3	HG9	B	452	-	-	5/32/32/33	-
4	666	B	462	-	-	1/12/39/39	0/4/4/4
3	HG9	A	453	-	-	4/32/32/33	-
4	666	C	463	-	-	1/12/39/39	0/4/4/4
4	666	D	464	-	-	1/12/39/39	0/4/4/4
3	HG9	A	454	-	-	6/32/32/33	-

The worst 5 of 113 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	464	666	C15-N26	10.29	1.49	1.35
4	A	461	666	C15-N26	10.13	1.49	1.35
4	B	462	666	C37-N38	9.81	1.39	1.29
4	B	462	666	C15-N26	9.80	1.49	1.35
4	A	461	666	C37-N38	9.52	1.38	1.29

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	462	666	C11-C12-C19	-9.79	102.99	118.50
4	D	464	666	C11-C12-C19	-9.57	103.33	118.50
4	A	461	666	C11-C12-C19	-8.99	104.26	118.50
4	C	463	666	C11-C12-C19	-8.21	105.49	118.50
4	C	463	666	C19-C12-C15	-8.16	113.59	120.37

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	451	HG9	N33-C36-C37-C40
3	B	451	HG9	N33-C36-C37-O47
4	A	461	666	C3-C11-C12-C19
4	B	462	666	C3-C11-C12-C19
3	A	453	HG9	N33-C36-C37-C40

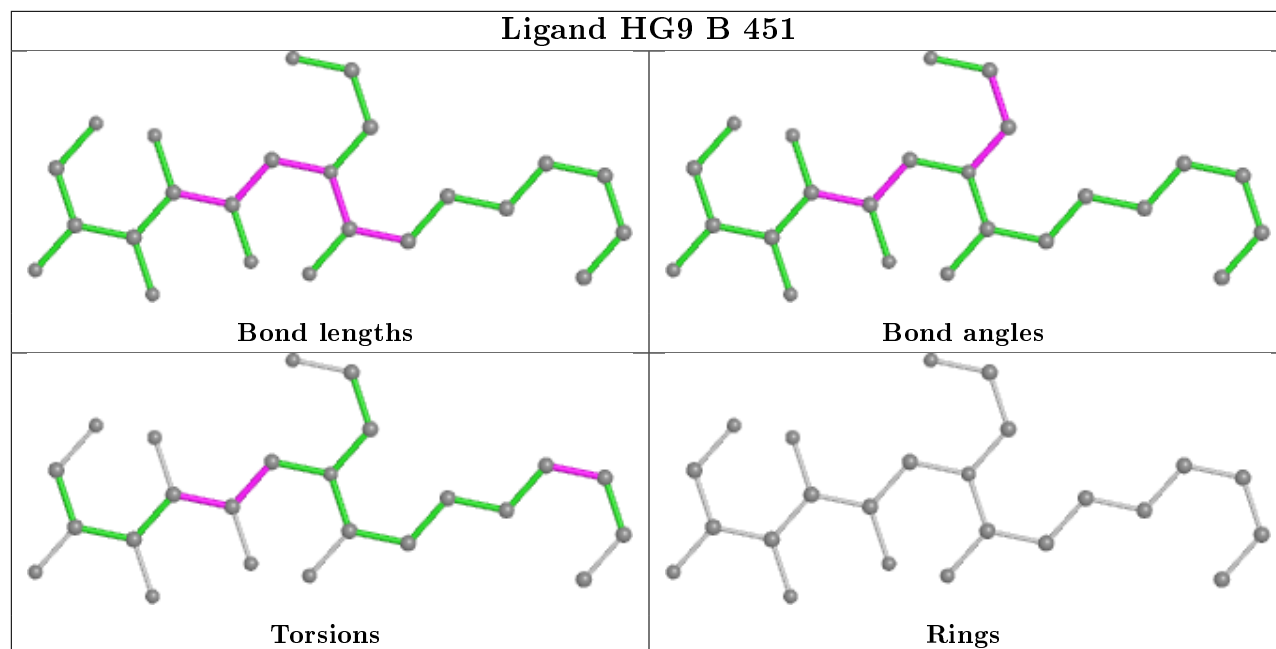
There are no ring outliers.

6 monomers are involved in 12 short contacts:

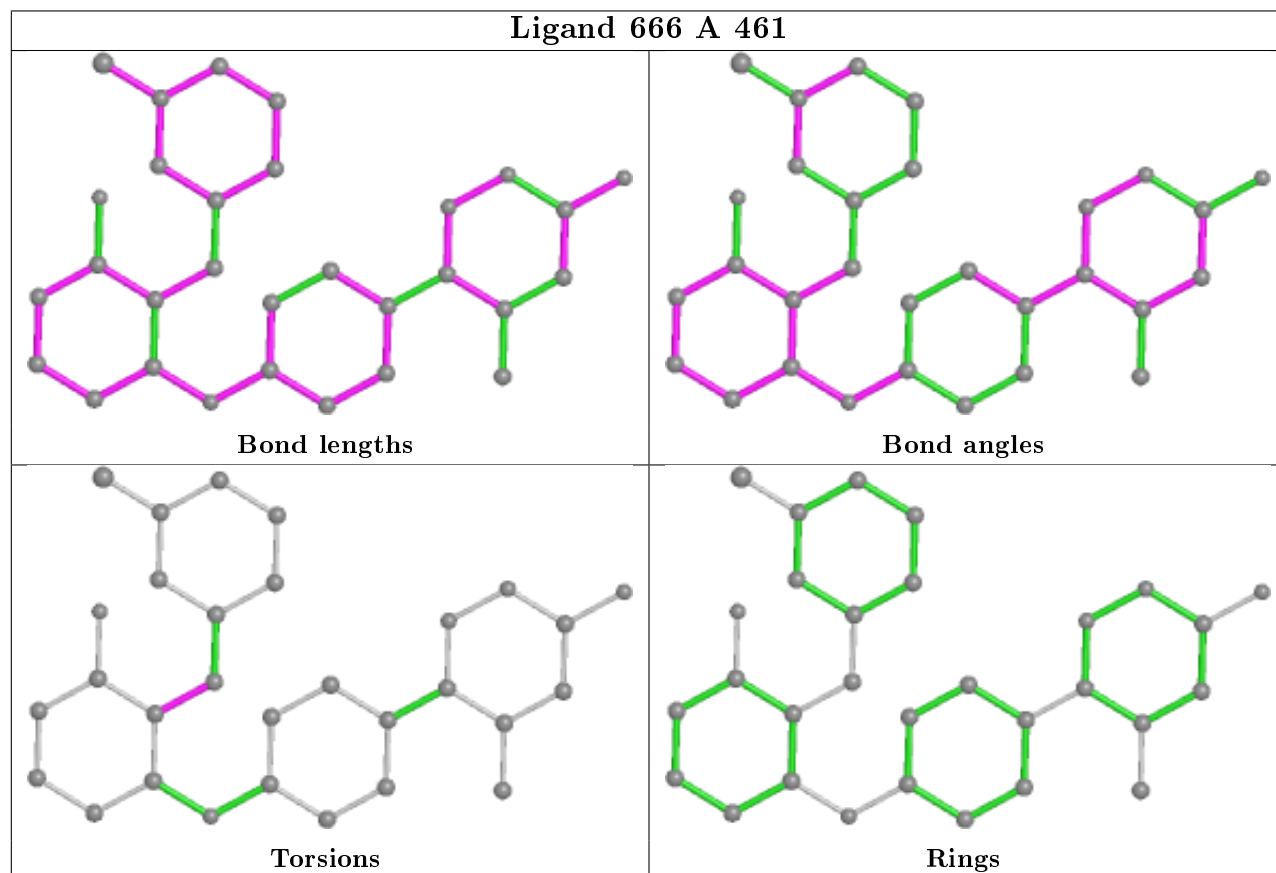
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	451	HG9	2	0
4	A	461	666	2	0
4	B	462	666	2	0
3	A	453	HG9	2	0
4	C	463	666	1	0
4	D	464	666	3	0

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

## Ligand HG9 B 451

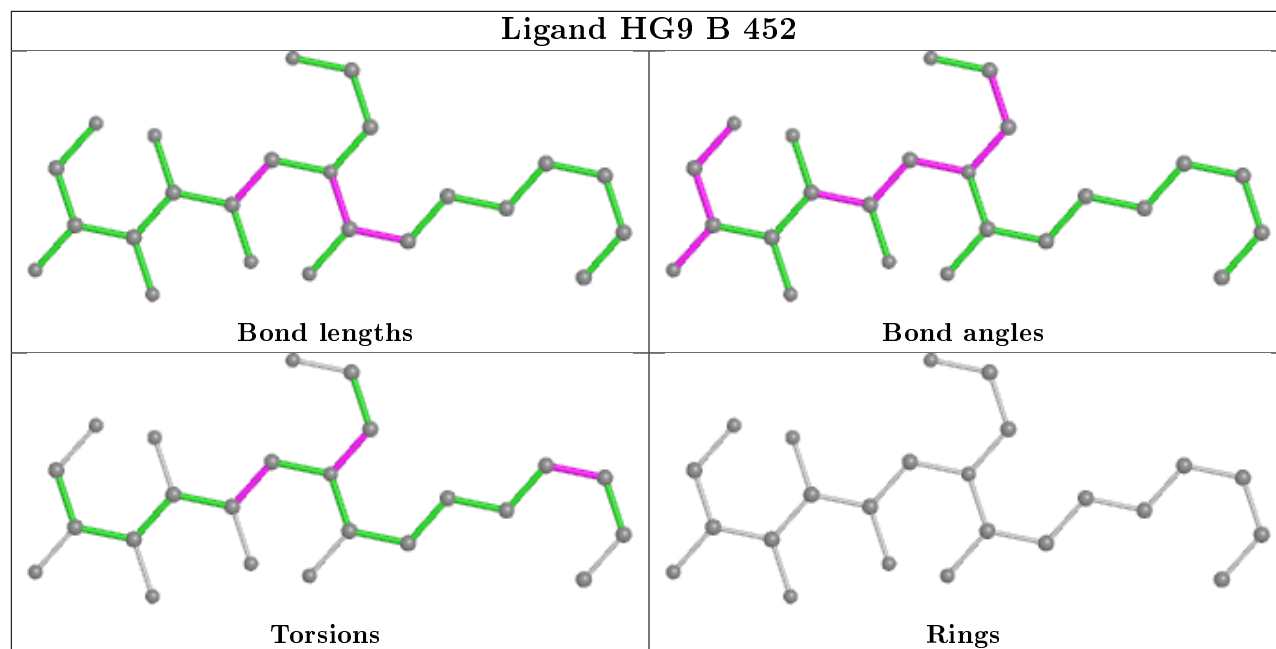


## Ligand 666 A 461

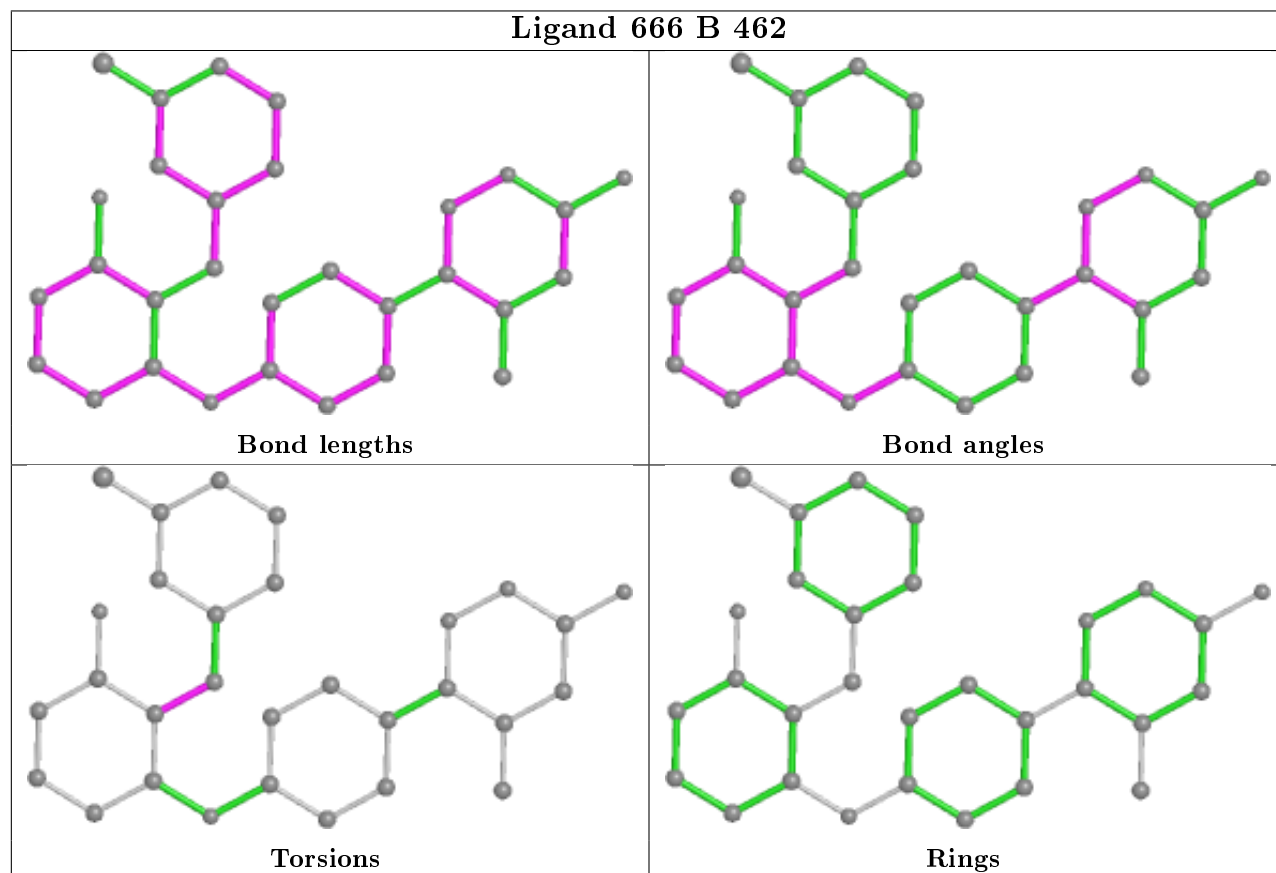


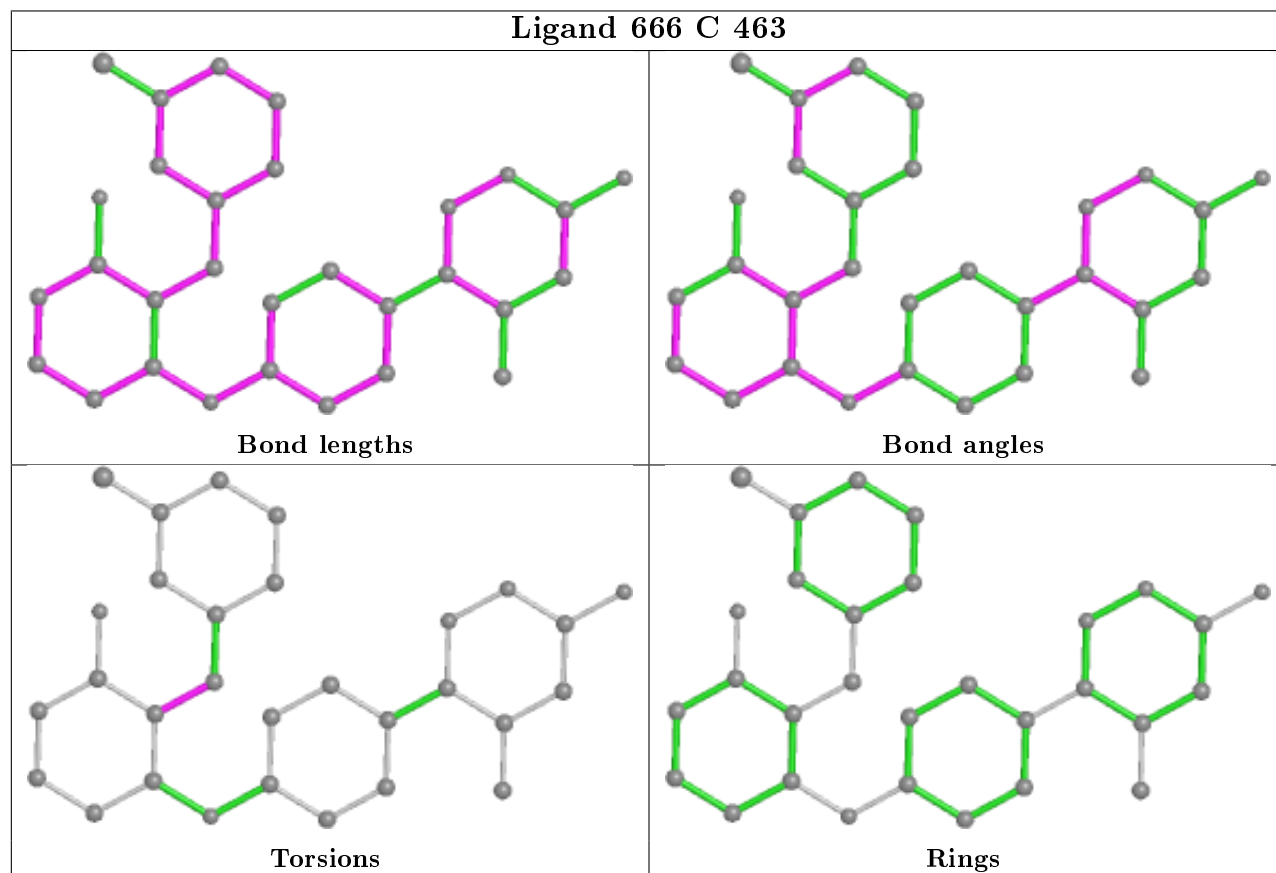
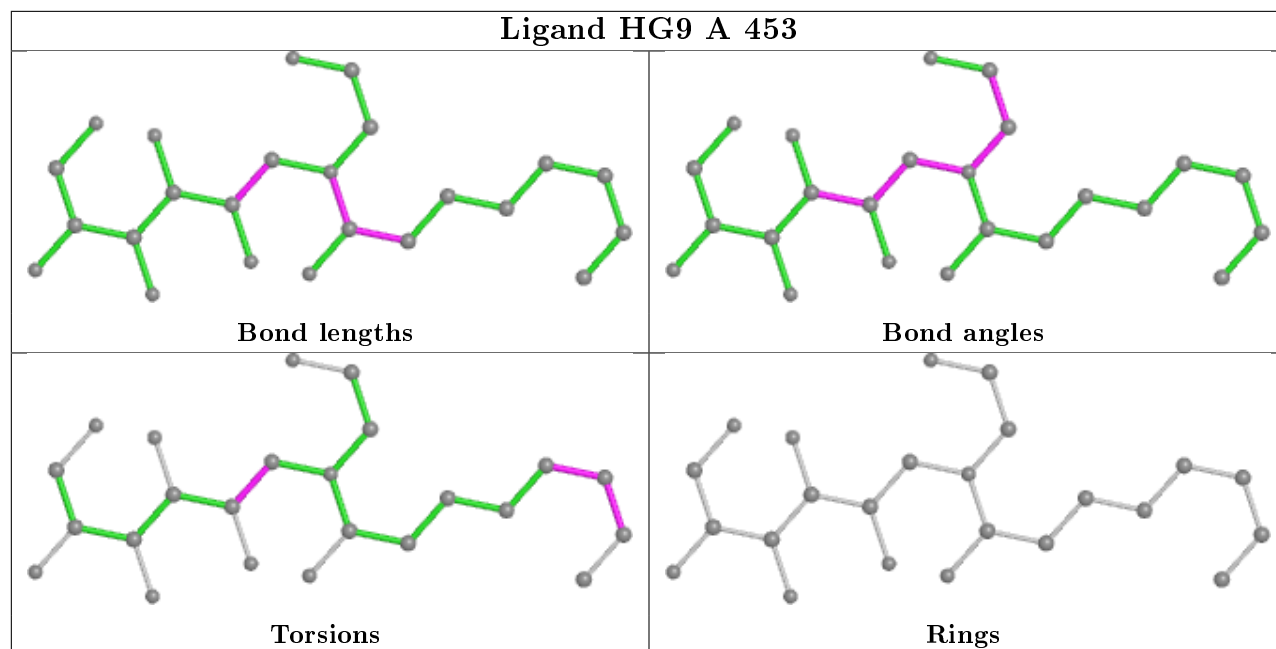


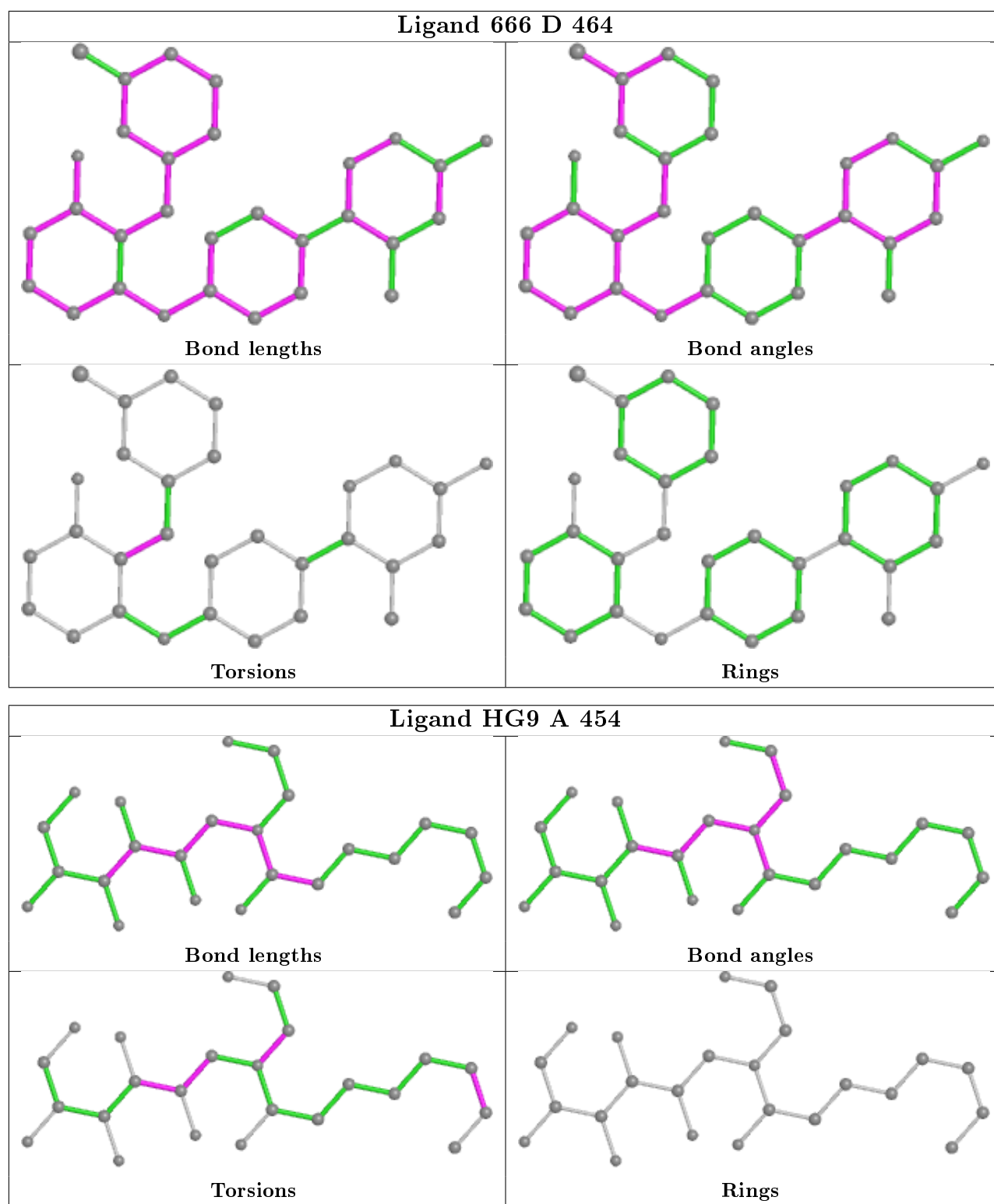
## Ligand HG9 B 452



## Ligand 666 B 462







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	363/420 (86%)	0.28	36 (9%) 7 6	26, 42, 69, 77	0
1	B	363/420 (86%)	0.29	32 (8%) 10 9	23, 43, 70, 79	0
1	C	372/420 (88%)	0.39	37 (9%) 7 6	34, 49, 72, 78	0
1	D	365/420 (86%)	0.73	52 (14%) 2 2	33, 55, 74, 79	0
All	All	1463/1680 (87%)	0.42	157 (10%) 6 5	23, 48, 72, 79	0

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1016	ALA	9.5
1	A	662	ILE	8.1
1	C	661	LEU	8.0
1	A	1053	SER	7.4
1	A	659	LEU	7.1

### 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](#)

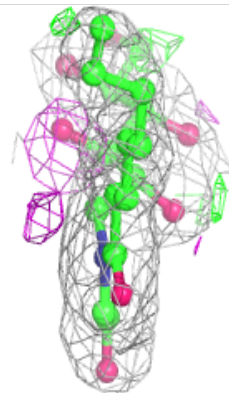
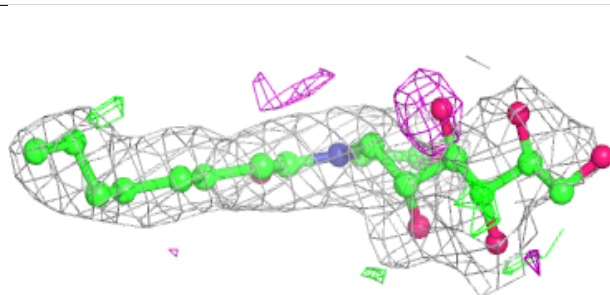
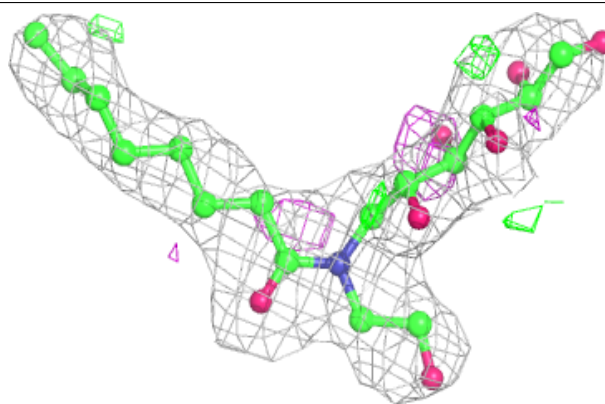
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HG9	B	452	24/25	0.76	0.26	48,54,68,70	0
3	HG9	B	451	24/25	0.78	0.28	37,49,69,70	0
3	HG9	A	453	24/25	0.80	0.27	42,53,65,67	0
3	HG9	A	454	24/25	0.83	0.22	46,61,71,74	0
4	666	C	463	30/30	0.93	0.20	39,53,72,85	0
4	666	A	461	30/30	0.94	0.17	32,43,59,73	0
4	666	B	462	30/30	0.95	0.20	36,43,60,68	0
4	666	D	464	30/30	0.95	0.18	46,50,65,82	0
2	MG	B	474	1/1	0.97	0.14	33,33,33,33	0
2	MG	A	479	1/1	0.97	0.06	39,39,39,39	0
2	MG	C	476	1/1	0.97	0.18	37,37,37,37	0
2	MG	A	472	1/1	0.97	0.19	32,32,32,32	0
2	MG	D	477	1/1	0.99	0.18	34,34,34,34	0
2	MG	B	473	1/1	0.99	0.29	23,23,23,23	0
2	MG	A	471	1/1	0.99	0.27	34,34,34,34	0
2	MG	D	478	1/1	0.99	0.13	31,31,31,31	0
2	MG	C	475	1/1	0.99	0.16	28,28,28,28	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.

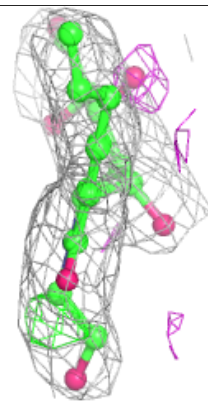
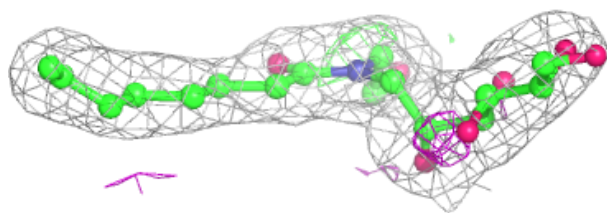
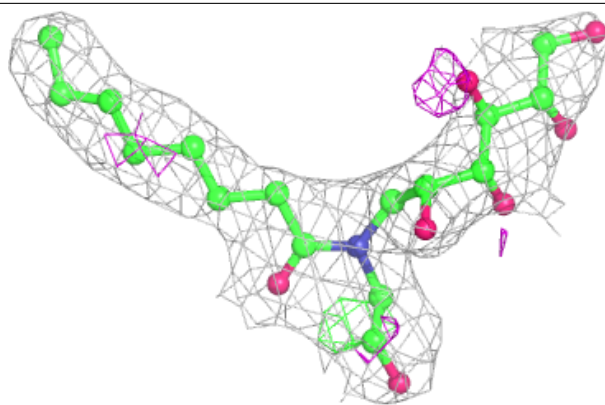
#### Electron density around HG9 B 452:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

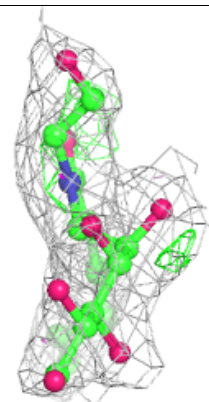
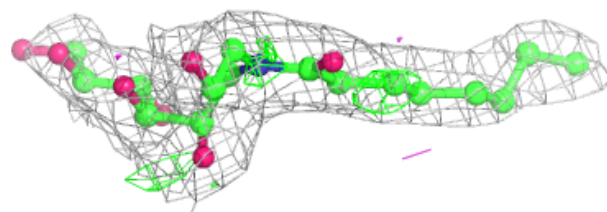
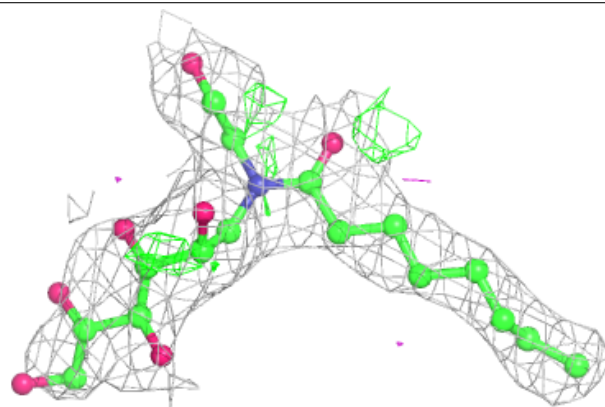


**Electron density around HG9 B 451:**

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

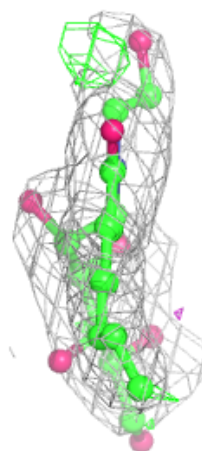
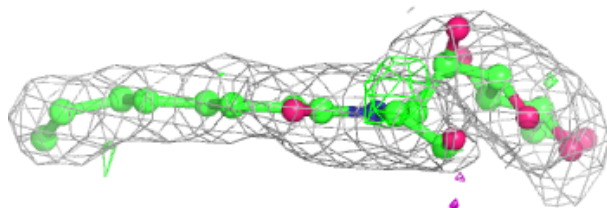
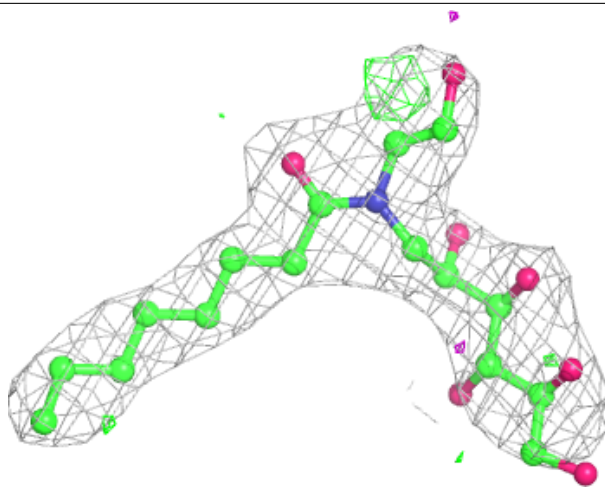
**Electron density around HG9 A 453:**

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



**Electron density around HG9 A 454:**

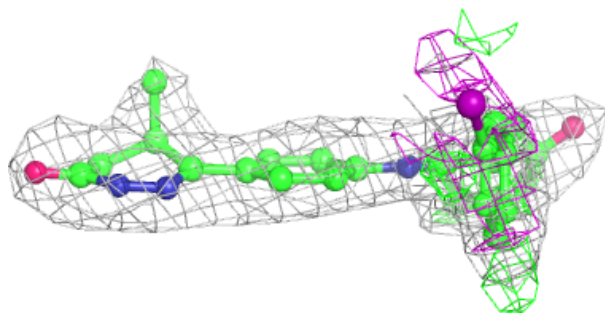
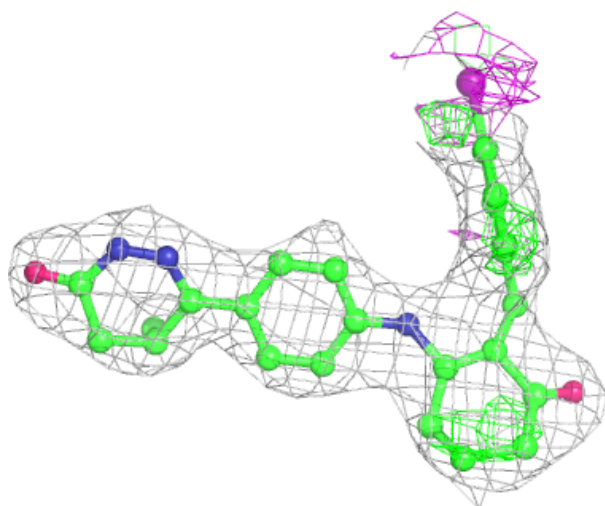
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





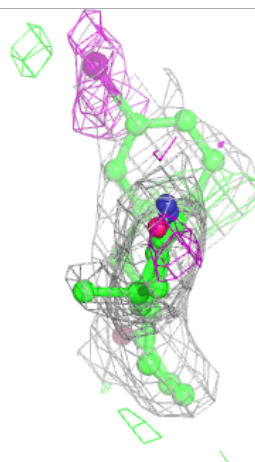
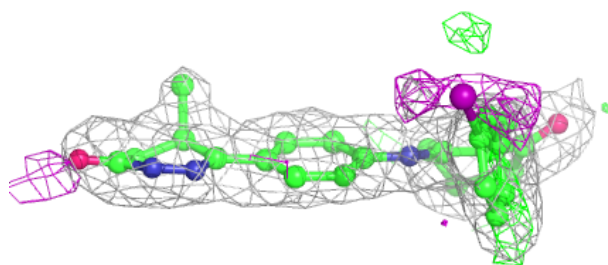
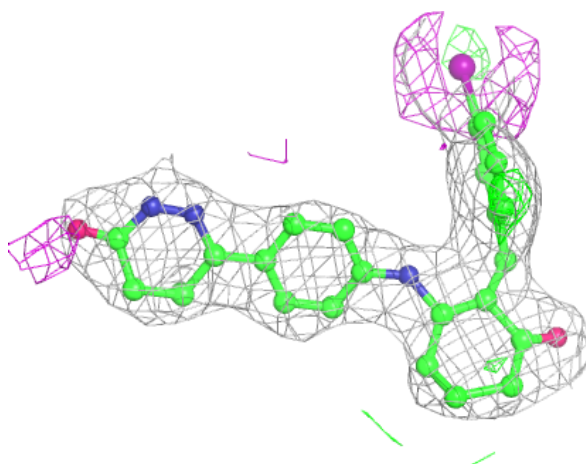
**Electron density around 666 C 463:**

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



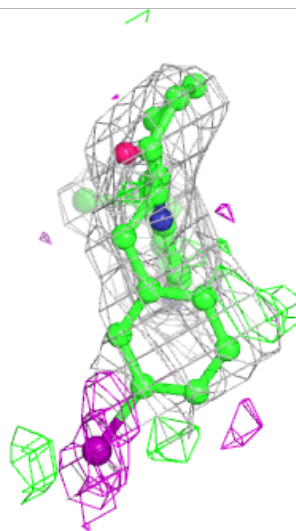
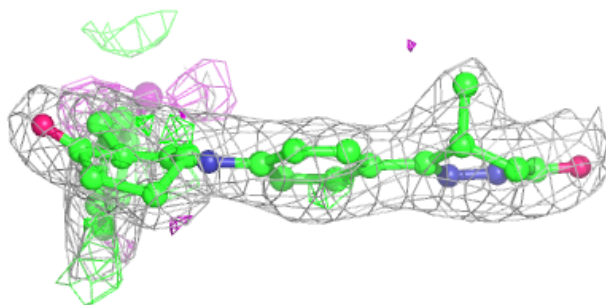
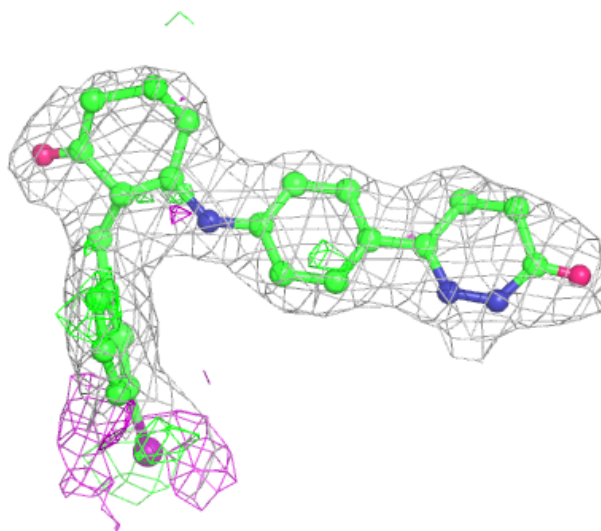
**Electron density around 666 A 461:**

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



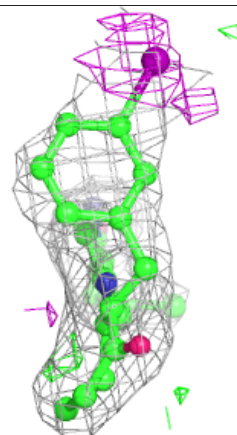
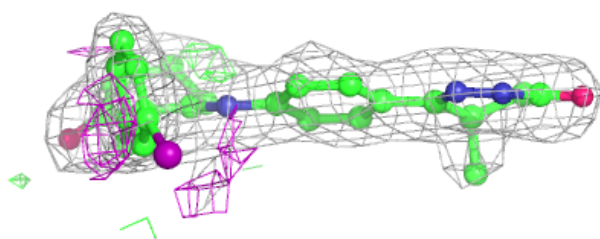
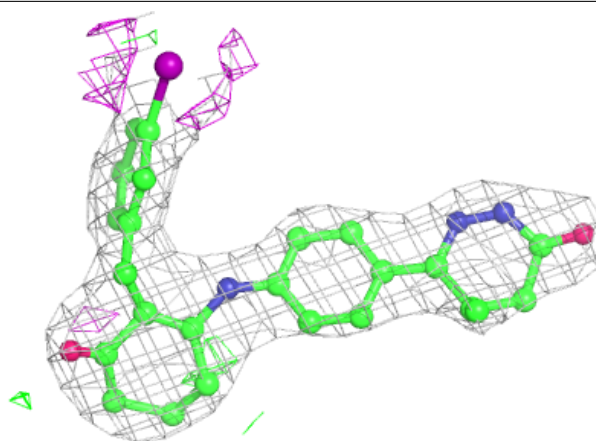
**Electron density around 666 B 462:**

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



**Electron density around 666 D 464:**

$2mF_o-DF_c$  (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.