



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:55 PM UTC

PDB ID : 9ET3 / pdb\_00009et3  
Title : CDK2-cyclin A in complex with FragLite 10  
Authors : Hope, I.; Martin, M.P.; Waring, M.J.; Noble, M.E.M.; Endicott, J.A.; Tatum, N.J.  
Deposited on : 2024-03-26  
Resolution : 2.34 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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

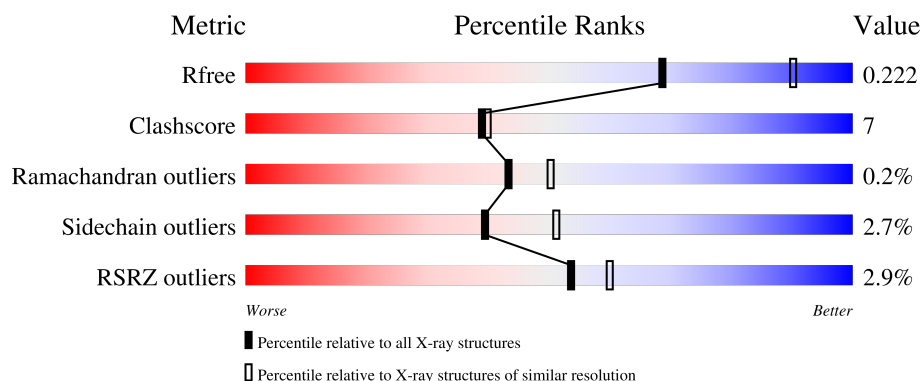
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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  $\geq 3$ , 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	B	268	
1	D	268	
2	A	302	
2	C	302	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1P8	A	604	-	-	X	-
3	1P8	B	501	-	-	X	-
3	1P8	D	503	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9203 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 Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	261	Total	C	N	O	S	0	0	0
			2103	1361	343	389	10			
1	B	261	Total	C	N	O	S	0	0	0
			2103	1361	343	389	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	171	GLY	-	expression tag	UNP P30274
D	433	HIS	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274
D	435	HIS	-	expression tag	UNP P30274
D	436	HIS	-	expression tag	UNP P30274
D	437	HIS	-	expression tag	UNP P30274
D	438	HIS	-	expression tag	UNP P30274
B	171	GLY	-	expression tag	UNP P30274
B	433	HIS	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
B	435	HIS	-	expression tag	UNP P30274
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274

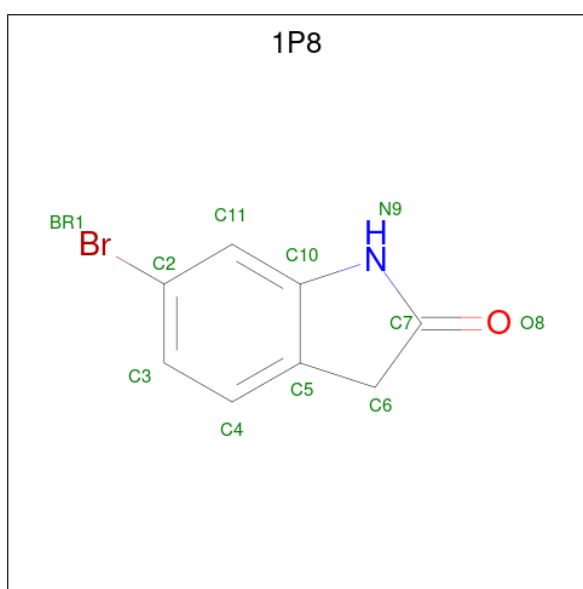
- Molecule 2 is a protein called Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	295	Total	C	N	O	P S	0	1	0
			2379	1543	406	421	1 8			
2	C	266	Total	C	N	O	P S	0	1	0
			2144	1389	367	380	1 7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 3 is 6-bromo-1,3-dihydro-2H-indol-2-one (CCD ID: 1P8) (formula: C<sub>8</sub>H<sub>6</sub>BrNO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	Br	C	N	O	0	0
			11	1	8	1	1		
3	D	1	Total	Br	C	N	O	0	0
			11	1	8	1	1		
3	D	1	Total	Br	C	N	O	0	0
			11	1	8	1	1		
3	A	1	Total	Br	C	N	O	0	0
			11	1	8	1	1		
3	A	1	Total	Br	C	N	O	0	0
			11	1	8	1	1		
3	A	1	Total	Br	C	N	O	0	1
			22	2	16	2	2		
3	A	1	Total	Br	C	N	O	0	0
			11	1	8	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 11	Br 1	C 8	N 1	O 1	0	0
3	B	1	Total 11	Br 1	C 8	N 1	O 1	0	0
3	B	1	Total 11	Br 1	C 8	N 1	O 1	0	0
3	B	1	Total 11	Br 1	C 8	N 1	O 1	0	0
3	C	1	Total 11	Br 1	C 8	N 1	O 1	0	0
3	C	1	Total 11	Br 1	C 8	N 1	O 1	0	0
3	C	1	Total 22	Br 2	C 16	N 2	O 2	0	1

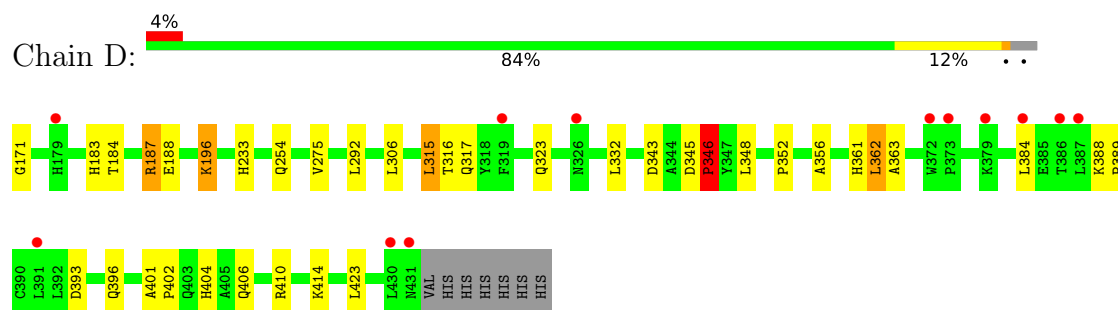
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	43	Total 43	O 43	0	0
4	A	111	Total 111	O 111	0	0
4	B	95	Total 95	O 95	0	0
4	C	49	Total 49	O 49	0	0

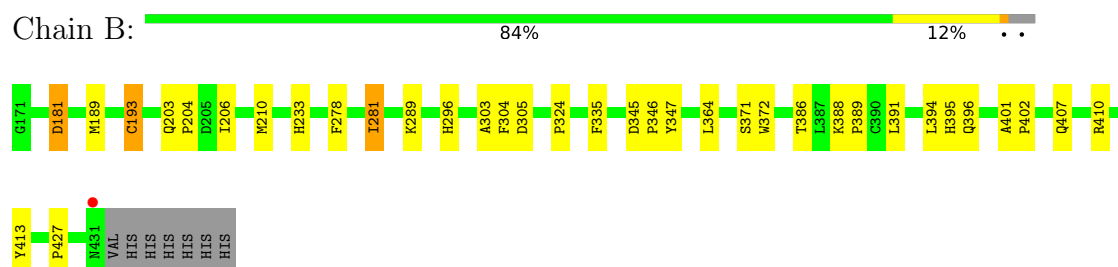
### 3 Residue-property plots [i](#)

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.

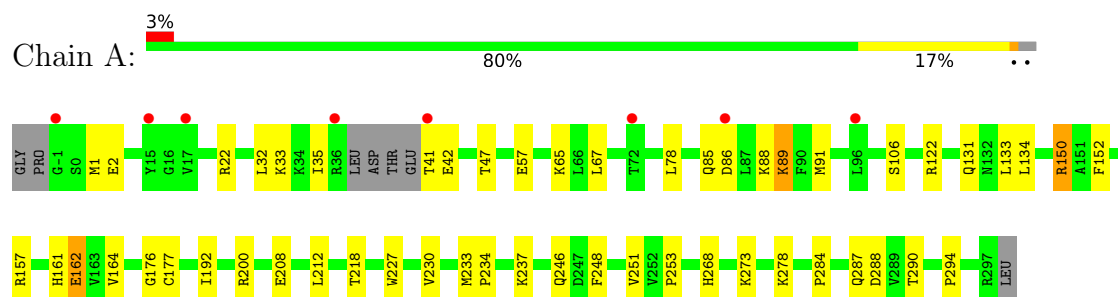
#### • Molecule 1: Cyclin-A2



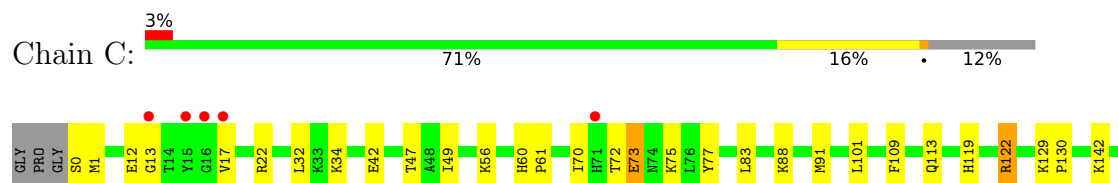
#### • Molecule 1: Cyclin-A2

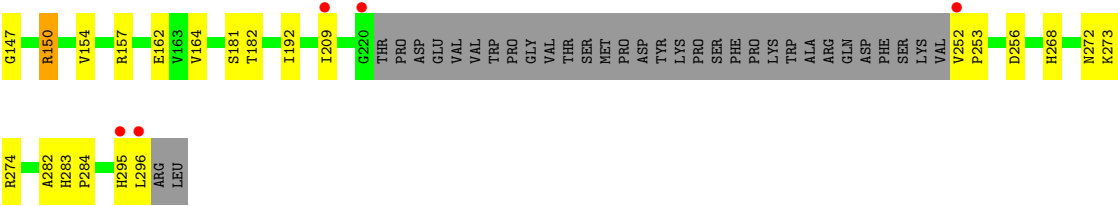


#### • Molecule 2: Cyclin-dependent kinase 2



#### • Molecule 2: Cyclin-dependent kinase 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.12Å 133.85Å 148.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.48 – 2.34 99.28 – 2.34	Depositor EDS
% Data completeness (in resolution range)	94.4 (99.48-2.34) 94.3 (99.28-2.34)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.183 , 0.221 0.183 , 0.222	Depositor DCC
$R_{free}$ test set	3102 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: 1P8, TPO

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	B	0.56	0/2153	1.18	3/2927 (0.1%)
1	D	0.55	0/2153	1.18	2/2927 (0.1%)
2	A	0.61	0/2428	1.23	6/3291 (0.2%)
2	C	0.57	0/2182	1.18	3/2954 (0.1%)
All	All	0.57	0/8916	1.19	14/12099 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	A	0	1
2	C	0	4
All	All	0	6

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	253	PRO	N-CA-C	8.29	120.81	110.70
2	C	253	PRO	N-CA-C	8.22	120.72	110.70
2	C	42	GLU	CB-CG-CD	6.29	123.28	112.60
2	A	161	HIS	CA-CB-CG	-6.23	107.57	113.80
1	B	364	LEU	N-CA-CB	-6.03	101.25	110.12
1	B	181	ASP	CA-CB-CG	5.99	118.58	112.60
2	A	162	GLU	CB-CG-CD	5.77	122.41	112.60
1	D	346	PRO	N-CA-CB	-5.67	96.36	102.60
2	A	294	PRO	N-CA-C	-5.47	102.85	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	89	LYS	CB-CG-CD	5.23	123.34	111.30
2	C	256	ASP	CA-CB-CG	5.14	117.74	112.60
1	D	196	LYS	CB-CA-C	-5.10	101.73	109.89
1	B	391	LEU	N-CA-CB	-5.09	102.62	110.16
2	A	47	THR	CA-CB-OG1	-5.04	102.04	109.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	150	ARG	Sidechain
2	C	122	ARG	Sidechain
2	C	150	ARG	Sidechain
2	C	157	ARG	Sidechain
2	C	274	ARG	Sidechain
1	D	187	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2103	0	2119	24	0
1	D	2103	0	2119	29	0
2	A	2379	0	2420	40	0
2	C	2144	0	2193	33	0
3	A	66	0	36	12	0
3	B	33	0	18	5	0
3	C	44	0	24	4	0
3	D	33	0	18	6	0
4	A	111	0	0	4	0
4	B	95	0	0	3	0
4	C	49	0	0	1	0
4	D	43	0	0	2	0
All	All	9203	0	8947	121	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 7.

All (121) 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)
2:C:56:LYS:O	3:C:303[B]:1P8:H6	1.49	1.12
2:C:12:GLU:HG2	2:C:13:GLY:H	1.01	1.08
2:C:12:GLU:HG2	2:C:13:GLY:N	1.80	0.95
2:A:230:VAL:HA	2:A:233:MET:HE3	1.51	0.92
2:C:12:GLU:CG	2:C:13:GLY:H	1.82	0.92
1:D:404:HIS:HD2	1:D:406:GLN:H	1.17	0.88
1:D:348:LEU:HA	3:D:503:1P8:H6	1.58	0.86
1:B:193:CYS:CB	3:B:501:1P8:O8	2.27	0.83
2:A:227:TRP:CE2	2:A:233:MET:HE1	2.20	0.76
1:B:193:CYS:HB2	3:B:501:1P8:O8	1.85	0.75
4:A:712:HOH:O	1:B:189:MET:HE2	1.87	0.75
2:A:88:LYS:HG2	2:A:131:GLN:HE21	1.54	0.72
1:B:193:CYS:HB3	3:B:501:1P8:O8	1.89	0.71
2:A:227:TRP:CZ2	2:A:233:MET:HE1	2.28	0.69
2:A:246:GLN:HE21	2:A:251:VAL:HG22	1.62	0.65
2:C:56:LYS:O	3:C:303[B]:1P8:C3	2.36	0.65
3:A:601:1P8:H2	1:B:303:ALA:HB1	1.79	0.64
1:D:404:HIS:CD2	1:D:406:GLN:H	2.09	0.63
2:A:278:LYS:NZ	1:B:181:ASP:OD2	2.31	0.63
2:A:237:LYS:NZ	3:A:604:1P8:O8	2.32	0.62
2:A:88:LYS:HG2	2:A:131:GLN:NE2	2.14	0.62
1:D:233:HIS:HD2	4:D:604:HOH:O	1.84	0.61
2:C:295[A]:HIS:CG	2:C:295[A]:HIS:O	2.55	0.60
2:A:85:GLN:HG2	2:A:86:ASP:N	2.17	0.59
2:A:88:LYS:HA	2:A:91:MET:HE2	1.84	0.59
2:A:212:LEU:HD12	3:A:604:1P8:BR1	2.58	0.59
2:A:85:GLN:HG2	2:A:86:ASP:H	1.66	0.58
1:B:305:ASP:HB3	3:B:501:1P8:C10	2.33	0.58
1:D:306:LEU:HD12	2:C:49:ILE:HG23	1.86	0.56
2:C:60:HIS:CG	2:C:61:PRO:HD2	2.40	0.56
2:C:88:LYS:HA	2:C:91:MET:HE2	1.86	0.56
2:A:212:LEU:CD1	3:A:604:1P8:BR1	3.09	0.56
2:A:65:LYS:HG3	2:A:67:LEU:HD23	1.89	0.55
2:A:284:PRO:HA	3:A:603[A]:1P8:H2	1.89	0.55
2:A:106:SER:HB2	2:A:290:THR:O	2.07	0.54
2:C:47:THR:HG23	2:C:147:GLY:O	2.07	0.54
1:D:316:THR:HG23	2:C:154:VAL:O	2.07	0.54
2:A:268:HIS:NE2	2:A:273:LYS:HD2	2.22	0.54
4:A:712:HOH:O	1:B:189:MET:CE	2.50	0.54
1:D:348:LEU:CA	3:D:503:1P8:H6	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:GLN:HE21	2:A:89:LYS:CB	2.21	0.53
2:C:1:MET:HE1	2:C:32:LEU:HD13	1.90	0.53
2:A:230:VAL:CA	2:A:233:MET:HE3	2.34	0.53
2:A:177:CYS:SG	2:A:233:MET:SD	3.07	0.52
2:C:56:LYS:HD2	3:C:302:1P8:H6	1.93	0.51
1:B:278:PHE:O	1:B:281:ILE:HG13	2.10	0.51
2:A:287:GLN:HA	3:A:603[A]:1P8:C10	2.40	0.51
1:D:275:VAL:HG21	1:D:292:LEU:HD21	1.93	0.50
2:A:22:ARG:HD2	4:A:771:HOH:O	2.12	0.50
2:A:33:LYS:CE	3:A:602:1P8:H1	2.42	0.49
2:C:34:LYS:HG3	2:C:77:TYR:CE1	2.47	0.49
1:D:332:LEU:HD23	1:D:363:ALA:HA	1.95	0.49
1:D:315:LEU:HD13	1:D:356:ALA:HB1	1.94	0.49
2:C:268:HIS:CE1	2:C:273:LYS:HD2	2.48	0.49
1:D:401:ALA:HB1	1:D:410:ARG:HD2	1.94	0.49
1:B:206:ILE:HA	1:B:210:MET:SD	2.52	0.49
2:A:88:LYS:HE3	2:A:131:GLN:NE2	2.28	0.49
1:D:388:LYS:HB3	1:D:389:PRO:HD3	1.95	0.48
2:C:83:LEU:HD11	2:C:142:LYS:HD2	1.94	0.48
2:A:85:GLN:HE21	2:A:89:LYS:HB2	1.78	0.48
2:A:33:LYS:HE3	3:A:602:1P8:H1	1.95	0.48
2:A:57:GLU:HB3	3:B:501:1P8:BR1	2.69	0.48
1:D:315:LEU:CD1	1:D:356:ALA:HB1	2.44	0.47
2:A:218:THR:O	2:A:246:GLN:HG2	2.14	0.47
2:C:181:SER:OG	2:C:182:THR:N	2.48	0.47
2:C:70:ILE:HB	2:C:77:TYR:HB2	1.97	0.47
1:D:348:LEU:HD23	3:D:503:1P8:H6	1.97	0.46
1:D:348:LEU:HD23	3:D:503:1P8:C3	2.46	0.46
2:A:41:THR:HG23	2:A:42:GLU:H	1.80	0.46
1:D:171:GLY:HA3	2:C:272:ASN:OD1	2.16	0.46
1:B:345:ASP:HA	1:B:346:PRO:HA	1.76	0.45
2:C:56:LYS:C	3:C:303[B]:1P8:H6	2.34	0.45
2:A:122:ARG:HD3	4:A:744:HOH:O	2.17	0.45
2:C:101:LEU:HD13	2:C:101:LEU:O	2.16	0.45
2:C:72:THR:HG1	2:C:75:LYS:H	1.63	0.45
1:B:395:HIS:HE1	1:B:427:PRO:O	2.00	0.45
2:A:208:GLU:HB3	3:A:604:1P8:BR1	2.72	0.45
2:A:85:GLN:CG	2:A:86:ASP:H	2.30	0.45
1:D:401:ALA:N	1:D:402:PRO:CD	2.80	0.44
1:B:386:THR:HB	4:B:635:HOH:O	2.17	0.44
1:B:407:GLN:OE1	1:B:410:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:LYS:HD3	1:D:423:LEU:HD21	2.00	0.44
2:A:86:ASP:HA	2:A:134:LEU:HA	1.98	0.44
1:D:345:ASP:HA	1:D:346:PRO:HA	1.83	0.43
2:C:12:GLU:CG	2:C:13:GLY:N	2.52	0.43
1:D:184:THR:O	1:D:188:GLU:HG3	2.19	0.43
1:D:323:GLN:HA	1:D:323:GLN:OE1	2.19	0.43
1:D:183:HIS:HB2	1:D:317:GLN:HE22	1.84	0.43
2:A:122:ARG:HA	2:A:152:PHE:CE1	2.54	0.43
1:B:347:TYR:OH	1:B:394:LEU:HA	2.19	0.43
2:C:88:LYS:HB2	2:C:130:PRO:HB2	2.01	0.43
2:C:282:ALA:O	2:C:283:HIS:C	2.62	0.43
2:C:109:PHE:O	2:C:113:GLN:HG3	2.19	0.42
2:C:283:HIS:CG	2:C:284:PRO:HD2	2.54	0.42
1:D:343:ASP:OD1	1:D:404:HIS:HE1	2.03	0.42
2:A:2:GLU:OE1	2:C:73:GLU:HG2	2.19	0.42
1:B:233:HIS:HE1	4:B:645:HOH:O	2.02	0.42
3:A:601:1P8:H2	1:B:303:ALA:CB	2.47	0.42
1:B:388:LYS:HB3	1:B:389:PRO:HD3	2.01	0.42
2:C:88:LYS:HE2	2:C:91:MET:CE	2.49	0.42
2:A:176:GLY:O	2:A:234:PRO:HG2	2.19	0.42
2:A:1:MET:HE1	2:A:32:LEU:HD13	2.01	0.42
1:B:335:PHE:HB2	1:B:413:TYR:CD2	2.54	0.42
1:B:233:HIS:HD2	4:B:679:HOH:O	2.02	0.42
1:D:352:PRO:HG3	3:D:503:1P8:C6	2.50	0.41
2:A:133:LEU:HD11	2:A:192:ILE:HD13	2.02	0.41
2:A:288:ASP:OD1	2:A:288:ASP:N	2.51	0.41
1:B:371:SER:O	1:B:372:TRP:C	2.62	0.41
2:C:252:VAL:HG23	2:C:252:VAL:O	2.19	0.41
2:C:129:LYS:HA	2:C:192:ILE:HD11	2.01	0.41
2:A:287:GLN:HA	3:A:603[B]:1P8:C7	2.50	0.41
2:C:119:HIS:CE1	2:C:182:THR:HB	2.55	0.41
1:D:393:ASP:O	1:D:396:GLN:HB2	2.19	0.41
1:D:254:GLN:HG3	3:D:501:1P8:BR1	2.76	0.41
1:D:361:HIS:O	1:D:362:LEU:C	2.63	0.41
1:B:401:ALA:N	1:B:402:PRO:CD	2.84	0.41
2:C:22:ARG:NH1	4:C:404:HOH:O	2.49	0.41
1:D:233:HIS:CD2	4:D:604:HOH:O	2.65	0.41
3:A:605:1P8:BR1	1:B:304:PHE:HE2	2.59	0.40
1:B:203:GLN:HA	1:B:204:PRO:HD3	1.97	0.40
1:D:187:ARG:HA	1:D:187:ARG:HD2	1.92	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	B	259/268 (97%)	257 (99%)	2 (1%)	0	100	100
1	D	259/268 (97%)	251 (97%)	8 (3%)	0	100	100
2	A	291/302 (96%)	283 (97%)	7 (2%)	1 (0%)	36	41
2	C	262/302 (87%)	251 (96%)	10 (4%)	1 (0%)	30	32
All	All	1071/1140 (94%)	1042 (97%)	27 (2%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	164	VAL
2	C	164	VAL

### 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	B	233/240 (97%)	227 (97%)	6 (3%)	40	53
1	D	233/240 (97%)	228 (98%)	5 (2%)	47	60
2	A	259/264 (98%)	252 (97%)	7 (3%)	39	51
2	C	233/264 (88%)	225 (97%)	8 (3%)	32	42
All	All	958/1008 (95%)	932 (97%)	26 (3%)	39	51

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	196	LYS
1	D	315	LEU
1	D	346	PRO
1	D	362	LEU
1	D	384	LEU
2	A	35	ILE
2	A	78	LEU
2	A	150	ARG
2	A	157	ARG
2	A	162	GLU
2	A	200	ARG
2	A	248	PHE
1	B	193	CYS
1	B	281	ILE
1	B	289	LYS
1	B	296	HIS
1	B	324	PRO
1	B	396	GLN
2	C	0	SER
2	C	17	VAL
2	C	73	GLU
2	C	122	ARG
2	C	150	ARG
2	C	162	GLU
2	C	209	ILE
2	C	296	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	179	HIS
1	D	183	HIS
1	D	228	GLN
1	D	254	GLN
1	D	317	GLN
1	D	321	HIS
1	D	370	GLN
1	D	378	GLN
1	D	396	GLN
1	D	404	HIS
1	D	406	GLN
2	A	85	GLN
2	A	246	GLN

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Mol	Chain	Res	Type
1	B	179	HIS
1	B	254	GLN
1	B	312	ASN
1	B	317	GLN
1	B	322	GLN
1	B	378	GLN
1	B	395	HIS
1	B	403	GLN
1	B	425	ASN
2	C	161	HIS
2	C	287	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	TPO	C	160	2	8,10,11	0.56	0	10,14,16	0.91	0
2	TPO	A	160	2	8,10,11	0.76	0	10,14,16	0.78	0

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	TPO	C	160	2	-	0/9/11/13	-
2	TPO	A	160	2	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	1P8	D	501	-	12,12,12	0.52	0	17,17,17	0.80	0
3	1P8	A	601	-	12,12,12	0.66	0	17,17,17	1.90	5 (29%)
3	1P8	C	303[A]	-	12,12,12	0.51	0	17,17,17	0.77	0
3	1P8	C	302	-	12,12,12	0.54	0	17,17,17	1.02	1 (5%)
3	1P8	A	603[B]	-	12,12,12	0.55	0	17,17,17	0.77	0
3	1P8	C	301	-	12,12,12	0.59	0	17,17,17	2.39	4 (23%)
3	1P8	C	303[B]	-	12,12,12	0.54	0	17,17,17	1.54	3 (17%)
3	1P8	B	501	-	12,12,12	0.60	0	17,17,17	2.32	3 (17%)
3	1P8	D	503	-	12,12,12	0.54	0	17,17,17	1.27	2 (11%)
3	1P8	A	604	-	12,12,12	0.50	0	17,17,17	2.43	3 (17%)
3	1P8	B	502	-	12,12,12	0.54	0	17,17,17	0.98	0
3	1P8	A	602	-	12,12,12	0.61	0	17,17,17	1.58	3 (17%)
3	1P8	D	502	-	12,12,12	0.55	0	17,17,17	1.65	2 (11%)
3	1P8	B	503	-	12,12,12	0.56	0	17,17,17	0.69	0
3	1P8	A	603[A]	-	12,12,12	0.51	0	17,17,17	1.18	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1P8	A	605	-	12,12,12	0.53	0	17,17,17	1.09	1 (5%)

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	1P8	D	501	-	-	-	0/2/2/2
3	1P8	A	601	-	-	-	0/2/2/2
3	1P8	C	303[A]	-	-	-	0/2/2/2
3	1P8	C	302	-	-	-	0/2/2/2
3	1P8	A	603[B]	-	-	-	0/2/2/2
3	1P8	C	301	-	-	-	0/2/2/2
3	1P8	C	303[B]	-	-	-	0/2/2/2
3	1P8	B	501	-	-	-	0/2/2/2
3	1P8	D	503	-	-	-	0/2/2/2
3	1P8	A	604	-	-	-	0/2/2/2
3	1P8	B	502	-	-	-	0/2/2/2
3	1P8	A	602	-	-	-	0/2/2/2
3	1P8	D	502	-	-	-	0/2/2/2
3	1P8	B	503	-	-	-	0/2/2/2
3	1P8	A	603[A]	-	-	-	0/2/2/2
3	1P8	A	605	-	-	-	0/2/2/2

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	1P8	C10-N9-C7	-7.09	108.70	111.70
3	A	604	1P8	C10-N9-C7	-6.94	108.76	111.70
3	C	301	1P8	C10-N9-C7	-6.63	108.89	111.70
3	D	502	1P8	C10-N9-C7	-5.09	109.54	111.70
3	A	601	1P8	C10-N9-C7	-4.86	109.64	111.70
3	C	301	1P8	C5-C6-C7	-4.76	100.83	103.13
3	B	501	1P8	C5-C6-C7	-4.31	101.05	103.13
3	A	604	1P8	C5-C6-C7	-4.27	101.07	103.13
3	A	604	1P8	C6-C7-N9	-3.66	106.12	107.83
3	C	303[B]	1P8	C10-N9-C7	-3.41	110.25	111.70
3	C	303[B]	1P8	C6-C7-N9	-3.31	106.29	107.83
3	C	301	1P8	C6-C7-N9	-2.94	106.46	107.83
3	A	602	1P8	BR1-C2-C11	-2.80	115.27	119.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	1P8	O8-C7-C6	2.72	128.36	126.97
3	C	303[B]	1P8	C5-C6-C7	-2.72	101.82	103.13
3	A	601	1P8	C6-C7-N9	-2.70	106.57	107.83
3	C	302	1P8	C10-N9-C7	-2.58	110.60	111.70
3	D	503	1P8	C3-C4-C5	-2.54	118.08	121.39
3	A	601	1P8	C3-C4-C5	-2.53	118.08	121.39
3	A	601	1P8	C5-C6-C7	-2.43	101.96	103.13
3	C	301	1P8	O8-C7-C6	2.38	128.19	126.97
3	D	502	1P8	C5-C6-C7	-2.35	101.99	103.13
3	A	603[A]	1P8	C10-N9-C7	-2.35	110.70	111.70
3	A	605	1P8	C10-N9-C7	-2.32	110.71	111.70
3	D	503	1P8	C10-N9-C7	-2.23	110.75	111.70
3	A	602	1P8	C10-N9-C7	-2.20	110.77	111.70
3	B	501	1P8	C4-C5-C10	2.12	120.73	119.67
3	A	601	1P8	C3-C2-C11	2.05	124.49	121.53
3	A	603[A]	1P8	C6-C7-N9	-2.04	106.88	107.83

There are no chirality outliers.

There are no torsion outliers.

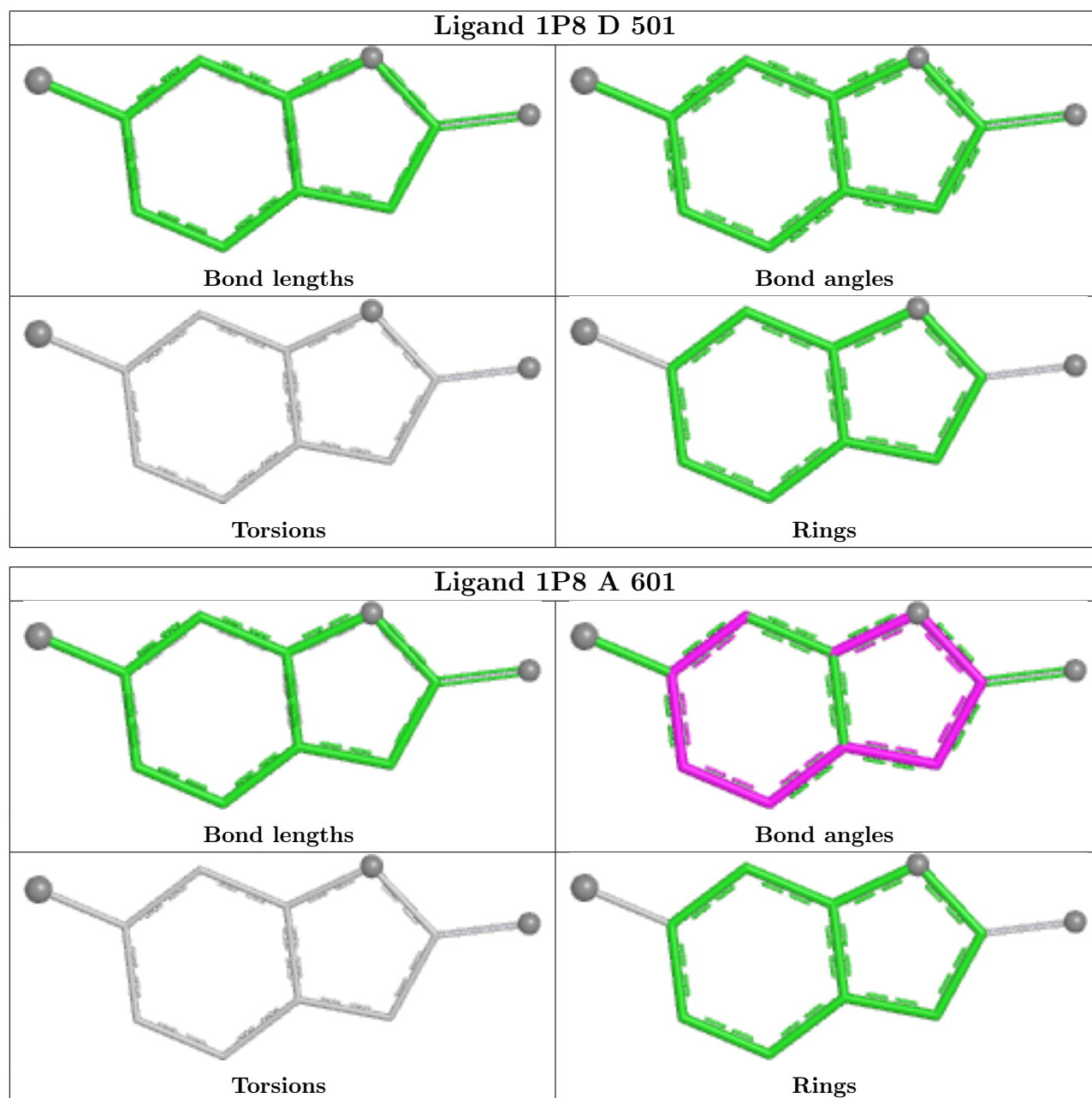
There are no ring outliers.

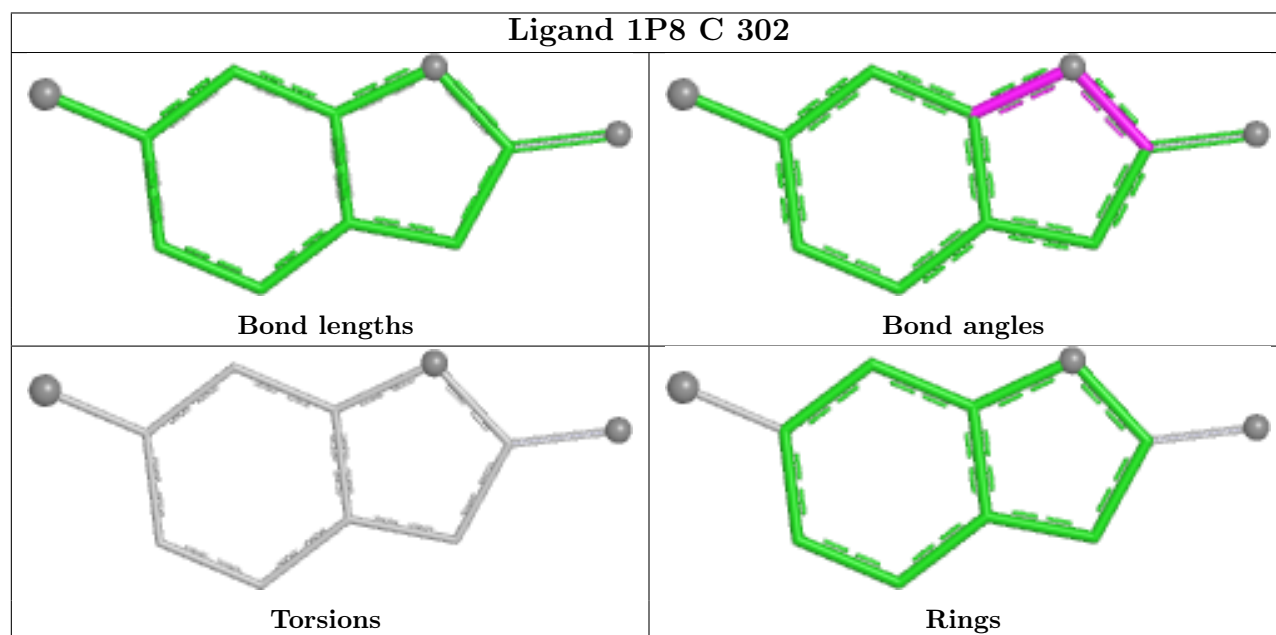
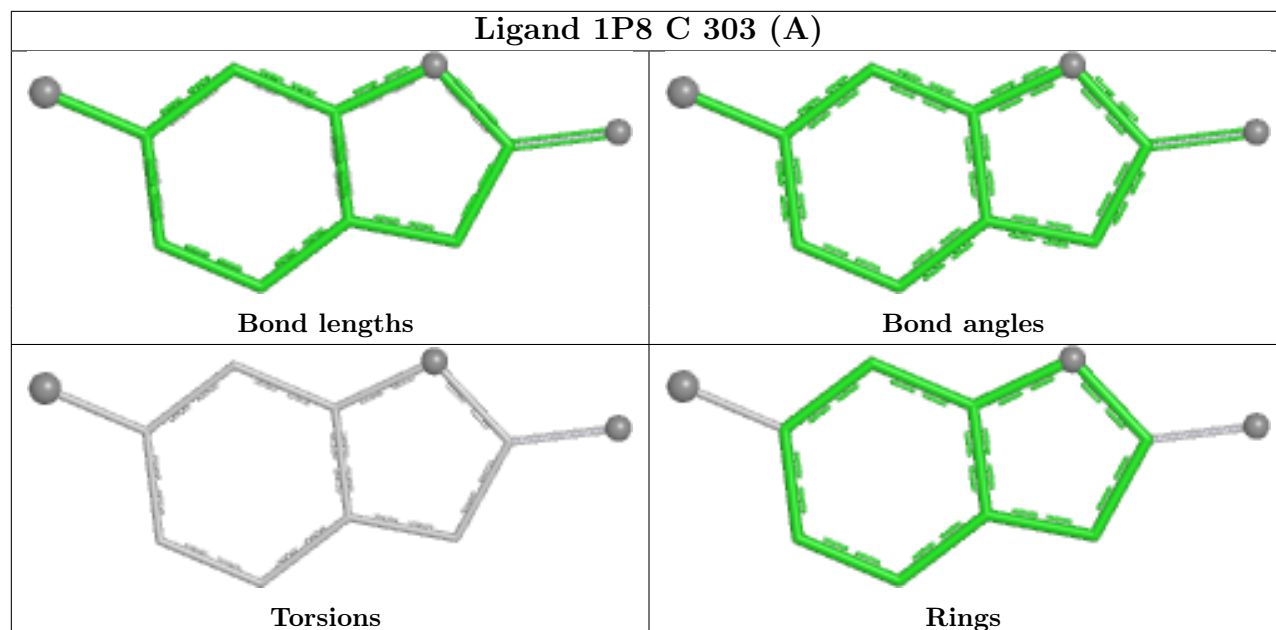
11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	1P8	1	0
3	A	601	1P8	2	0
3	C	302	1P8	1	0
3	A	603[B]	1P8	1	0
3	C	303[B]	1P8	3	0
3	B	501	1P8	5	0
3	D	503	1P8	5	0
3	A	604	1P8	4	0
3	A	602	1P8	2	0
3	A	603[A]	1P8	2	0
3	A	605	1P8	1	0

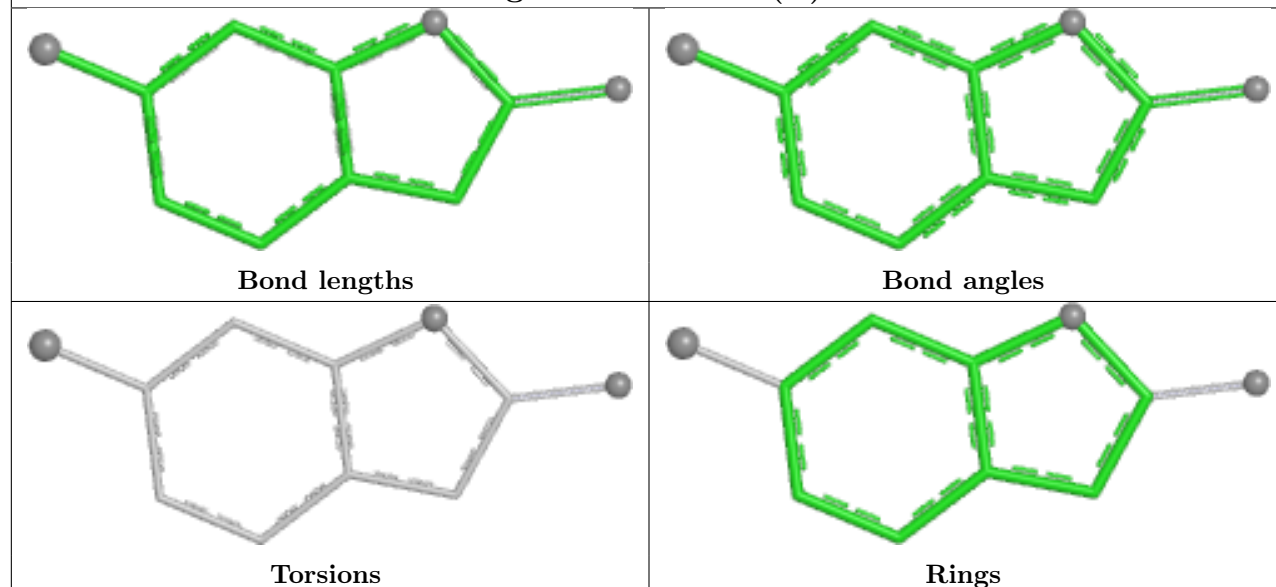
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

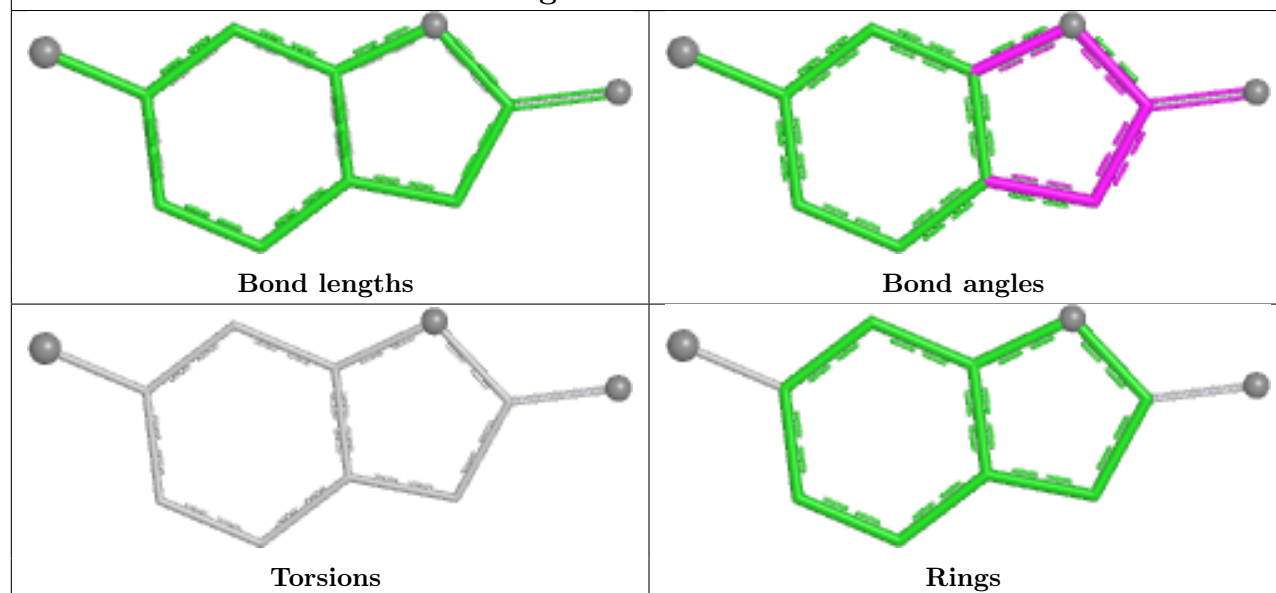




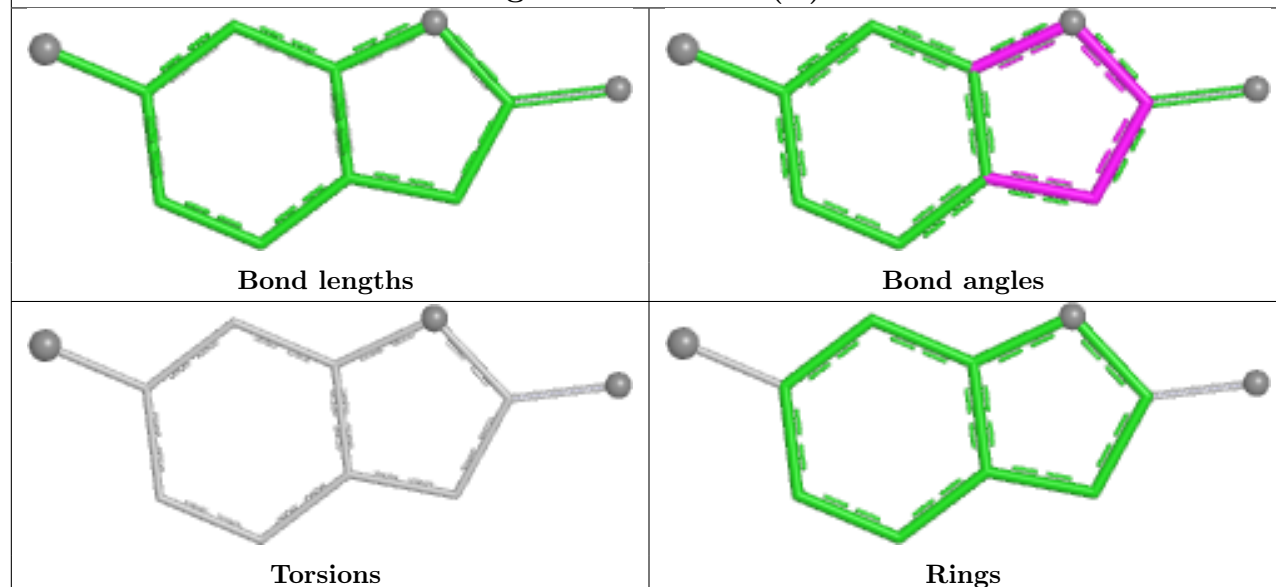
## Ligand 1P8 A 603 (B)



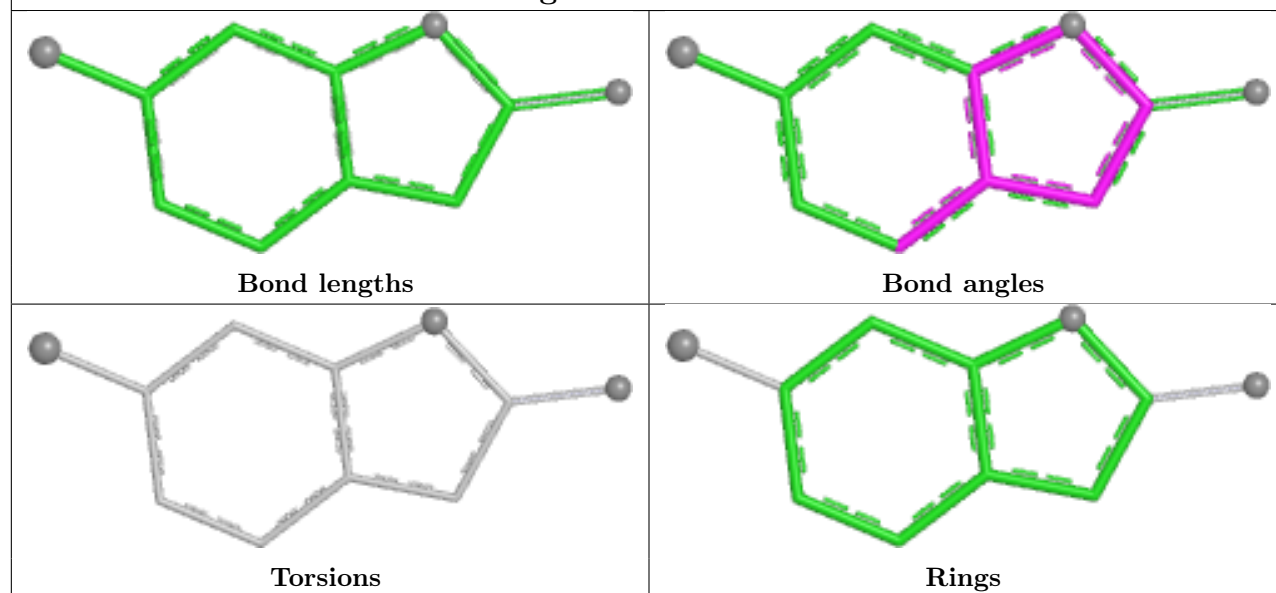
## Ligand 1P8 C 301



## Ligand 1P8 C 303 (B)

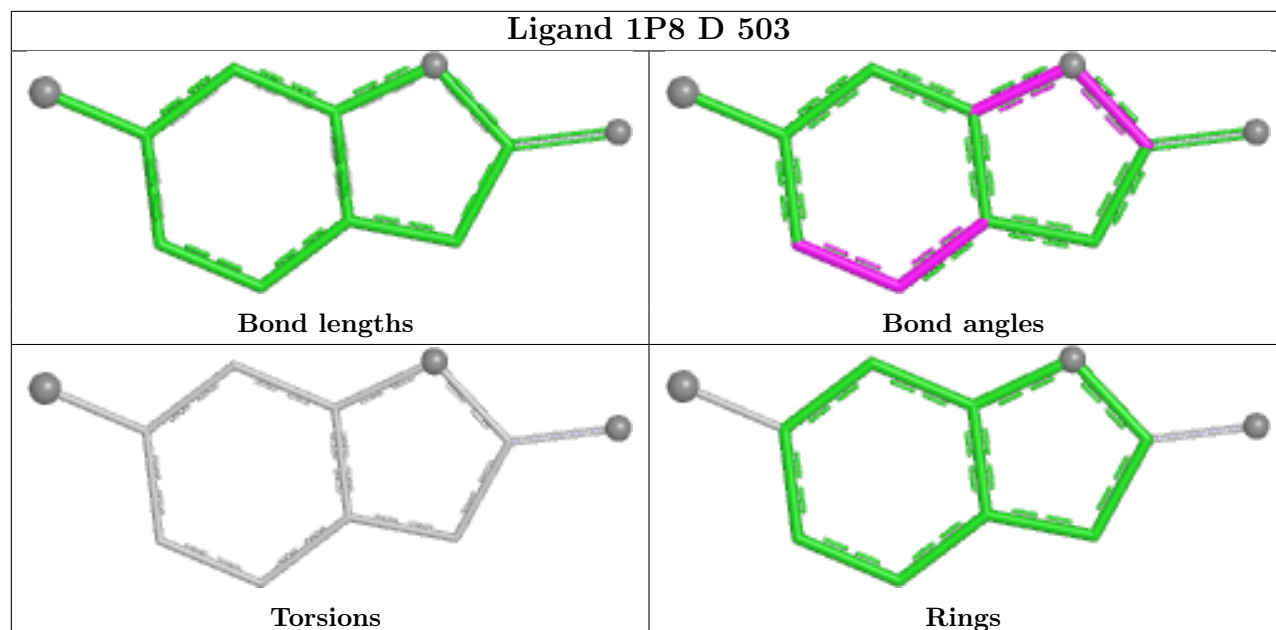


## Ligand 1P8 B 501

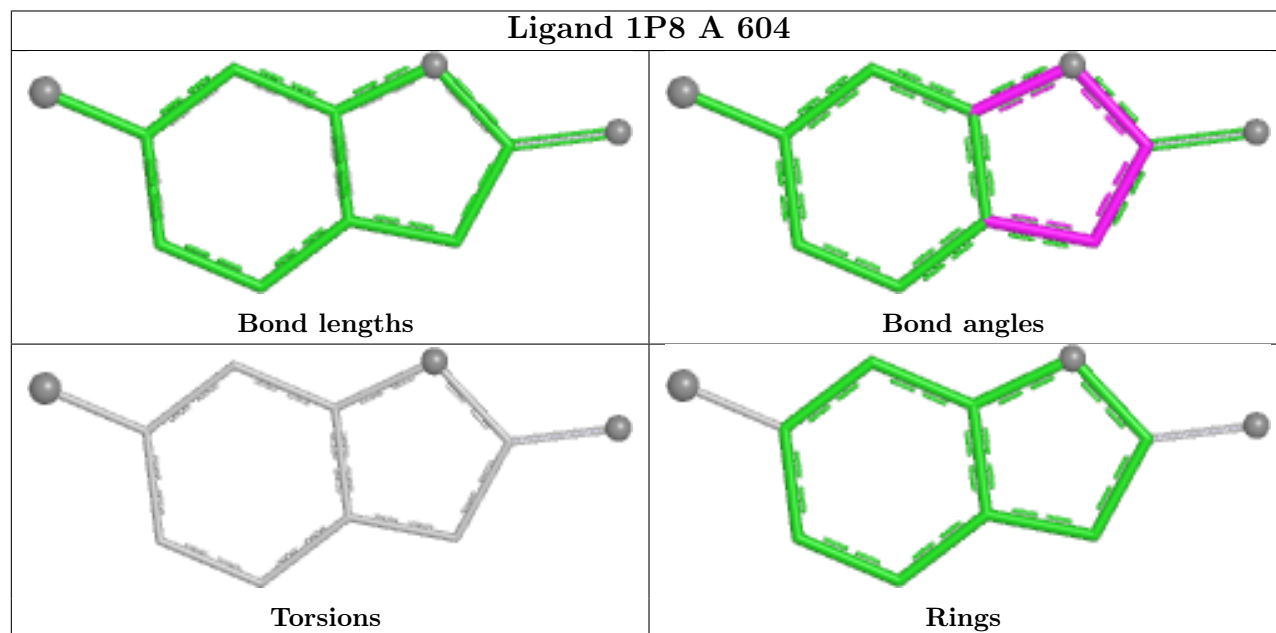




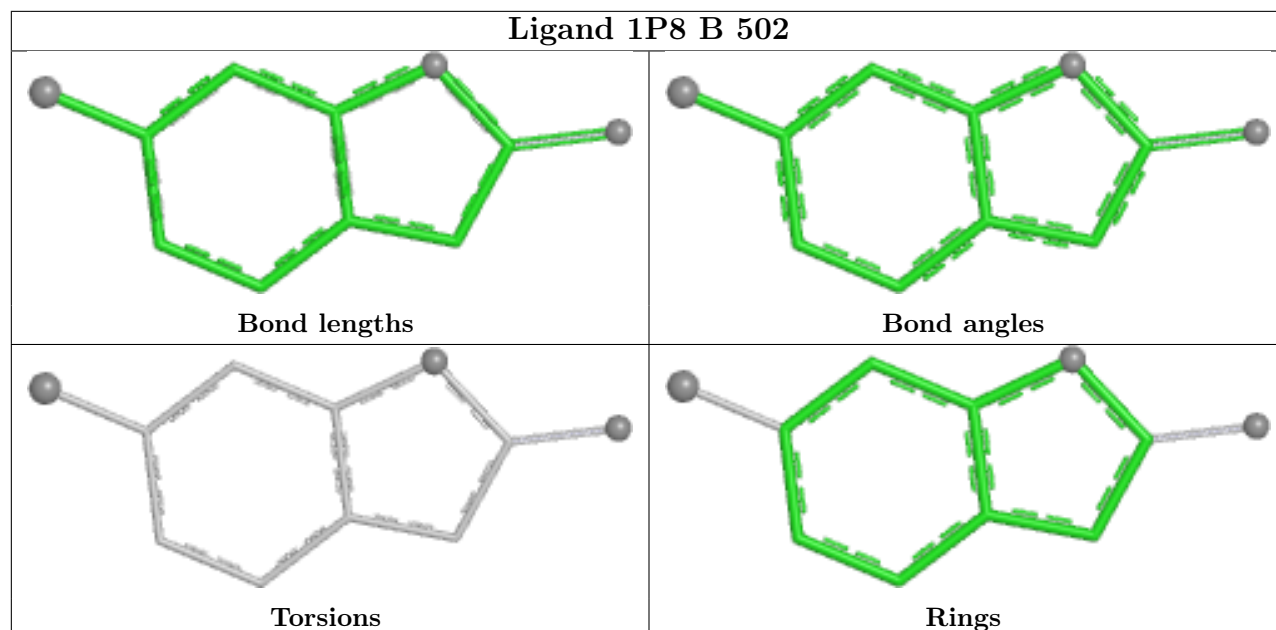
## Ligand 1P8 D 503



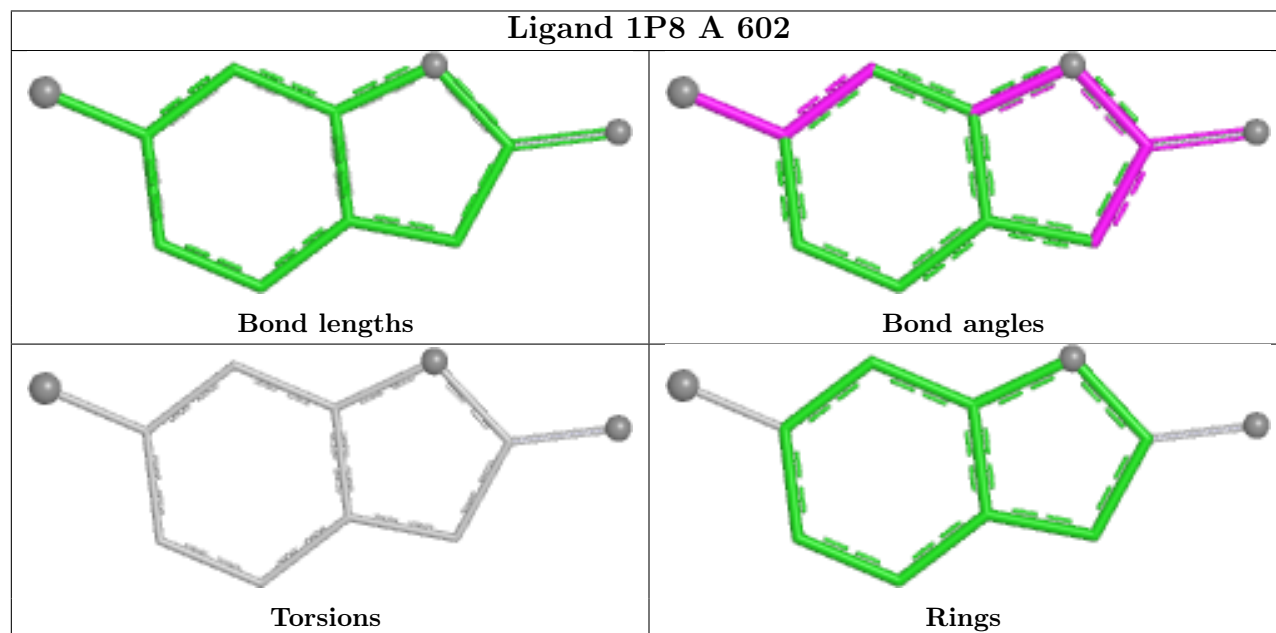
## Ligand 1P8 A 604



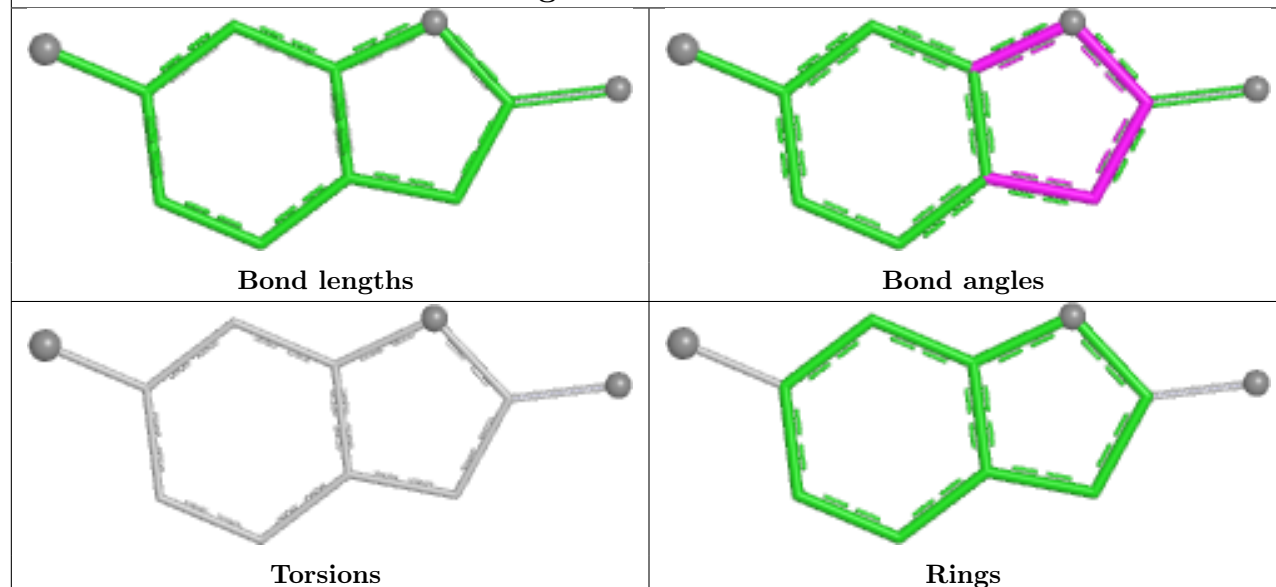
## Ligand 1P8 B 502



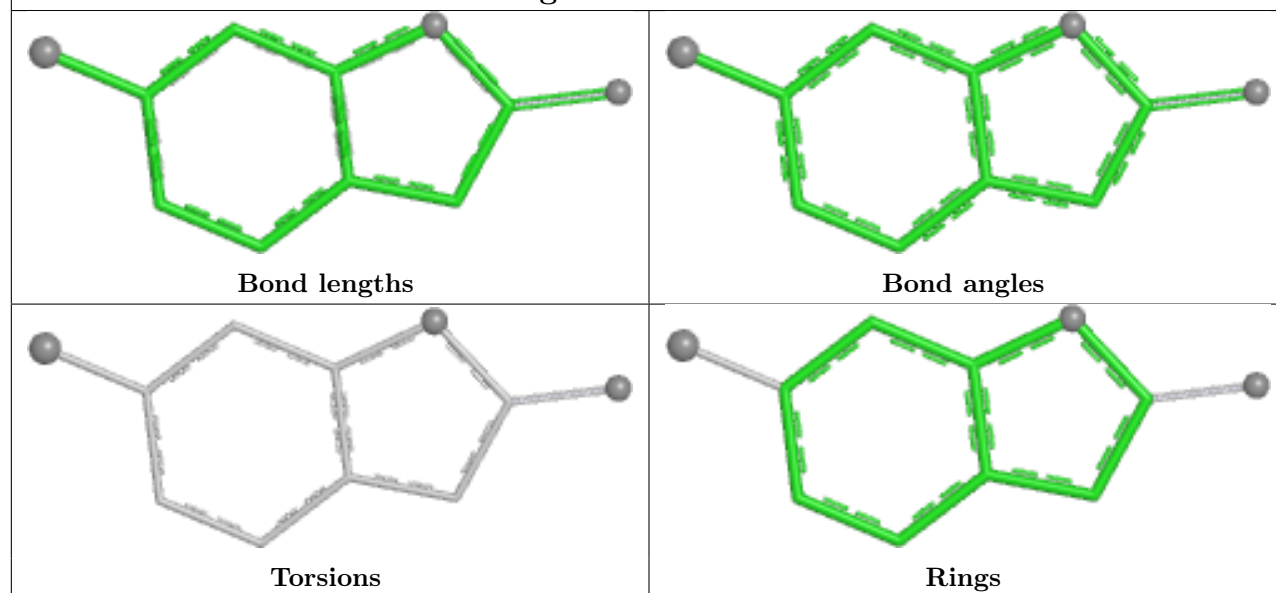
## Ligand 1P8 A 602

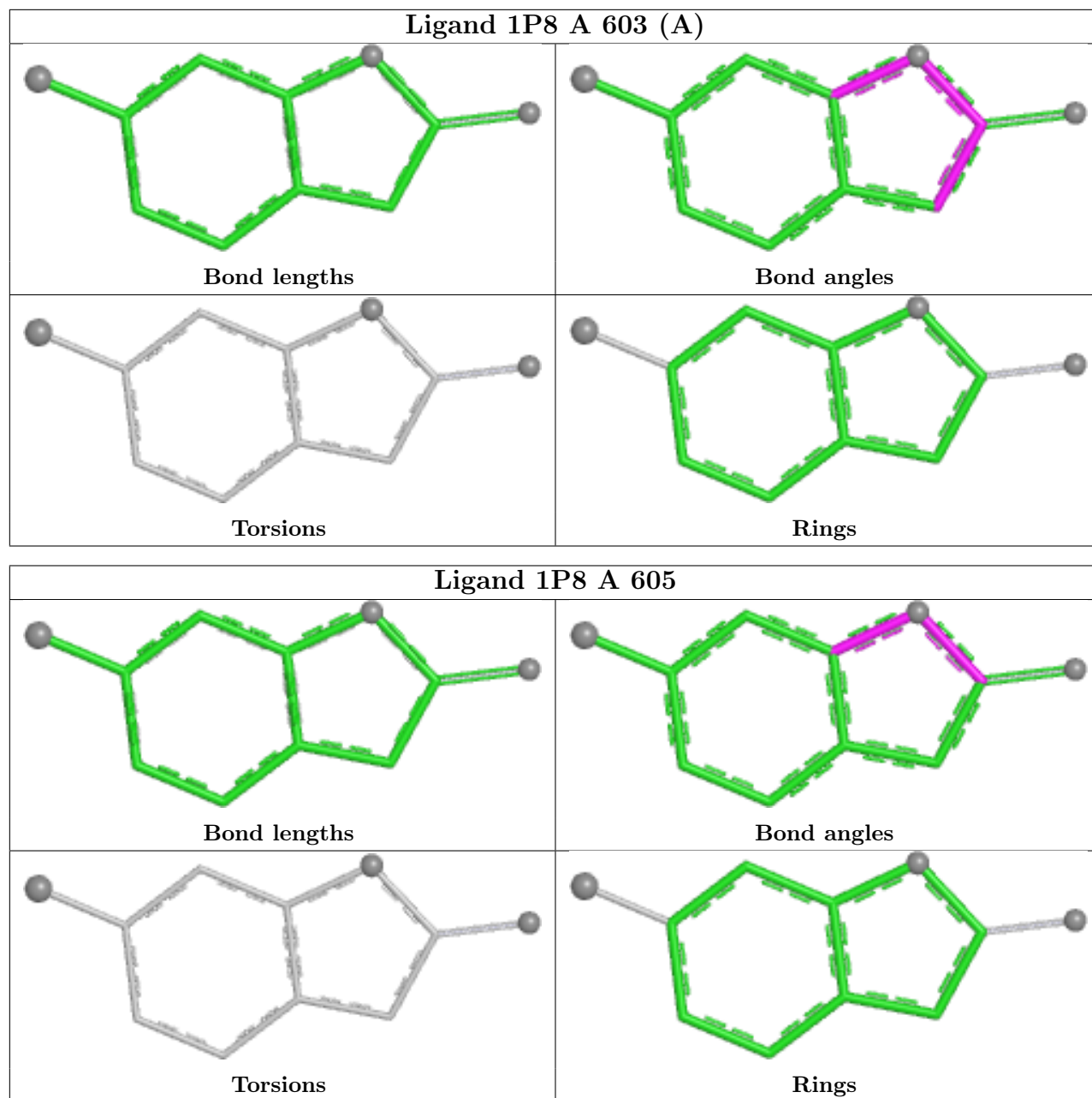


## Ligand 1P8 D 502



## Ligand 1P8 B 503





## 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, 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	B	261/268 (97%)	-0.33	1 (0%) 88 90	31, 46, 71, 113	0
1	D	261/268 (97%)	0.24	12 (4%) 37 43	35, 64, 102, 141	0
2	A	294/302 (97%)	-0.24	8 (2%) 56 62	24, 42, 90, 130	1 (0%)
2	C	265/302 (87%)	0.16	10 (3%) 44 50	9, 56, 94, 181	2 (0%)
All	All	1081/1140 (94%)	-0.05	31 (2%) 53 60	9, 52, 97, 181	3 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	71	HIS	19.3
2	C	295[A]	HIS	8.3
1	D	391	LEU	4.9
2	C	15	TYR	4.9
2	A	15	TYR	3.9
2	A	41	THR	3.9
2	A	86	ASP	3.2
2	A	96	LEU	2.8
1	D	372	TRP	2.6
2	C	252	VAL	2.6
1	D	386	THR	2.5
2	C	209	ILE	2.5
2	A	-1	GLY	2.5
1	D	431	ASN	2.4
1	D	326	ASN	2.4
1	B	431	ASN	2.4
2	C	17	VAL	2.3
2	A	36	ARG	2.3
1	D	379	LYS	2.3
1	D	319	PHE	2.2
2	A	17	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	220	GLY	2.2
2	C	13	GLY	2.2
1	D	387	LEU	2.2
1	D	179	HIS	2.1
1	D	384	LEU	2.1
1	D	373	PRO	2.1
2	C	16	GLY	2.1
2	A	72	THR	2.0
1	D	430	LEU	2.0
2	C	296	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	TPO	C	160	11/12	0.98	0.05	46,49,52,54	0
2	TPO	A	160	11/12	0.99	0.04	37,42,46,49	0

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	1P8	D	503	11/11	0.70	0.50	73,78,85,101	11
3	1P8	B	503	11/11	0.74	0.18	139,183,190,191	0
3	1P8	C	302	11/11	0.74	0.34	58,64,70,79	11
3	1P8	D	501	11/11	0.77	0.18	98,112,134,140	0
3	1P8	D	502	11/11	0.78	0.20	158,171,178,179	0
3	1P8	B	501	11/11	0.79	0.21	57,131,145,145	0

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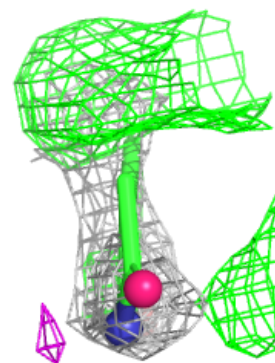
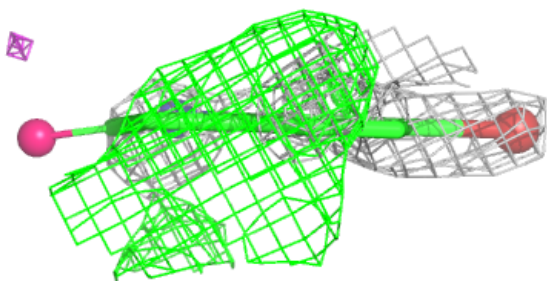
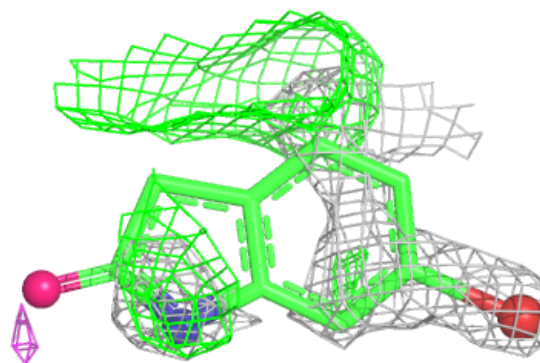
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1P8	C	303[A]	11/11	0.79	0.32	90,120,140,178	11
3	1P8	C	303[B]	11/11	0.79	0.32	94,114,133,168	11
3	1P8	C	301	11/11	0.80	0.22	69,97,109,113	0
3	1P8	A	602	11/11	0.80	0.22	78,86,105,107	0
3	1P8	B	502	11/11	0.82	0.21	125,131,137,145	0
3	1P8	A	604	11/11	0.82	0.39	59,72,80,80	11
3	1P8	A	603[A]	11/11	0.88	0.27	95,108,129,129	11
3	1P8	A	603[B]	11/11	0.88	0.27	66,79,116,125	11
3	1P8	A	605	11/11	0.92	0.15	49,51,59,65	11
3	1P8	A	601	11/11	0.92	0.18	40,46,57,58	11

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 1P8 D 503:

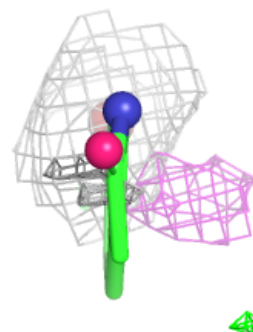
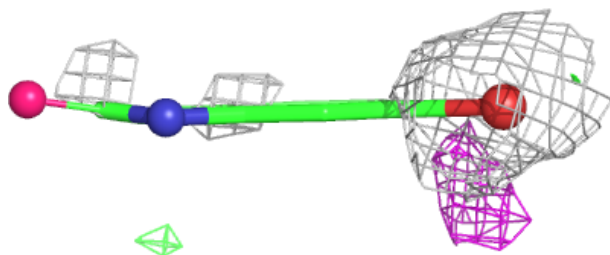
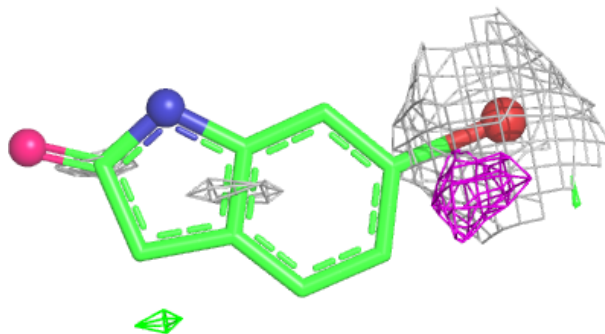
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



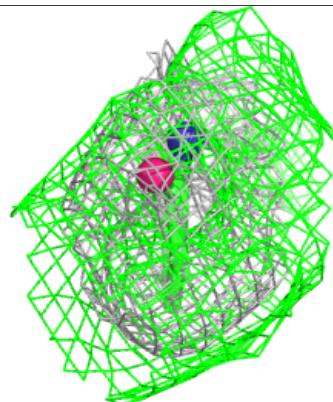
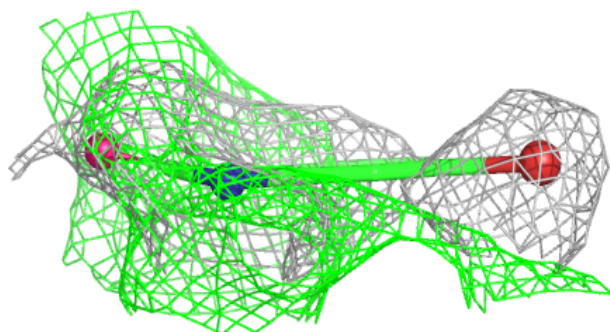
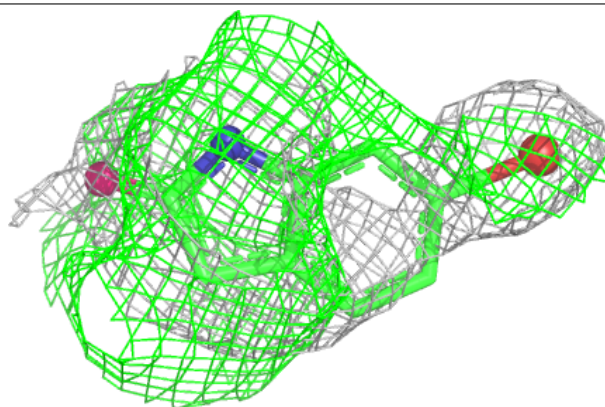


**Electron density around 1P8 B 503:**

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

**Electron density around 1P8 C 302:**

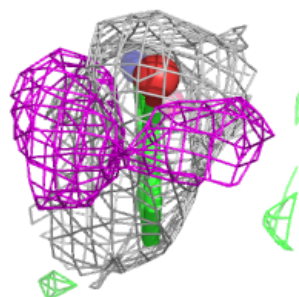
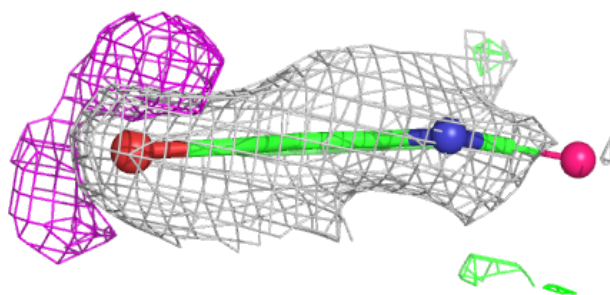
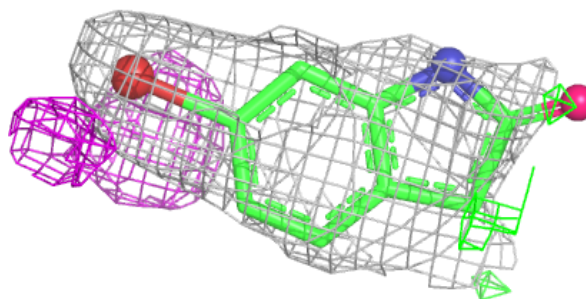
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



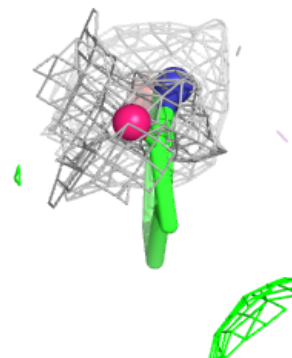
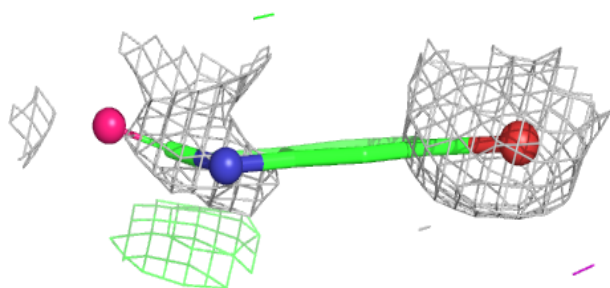
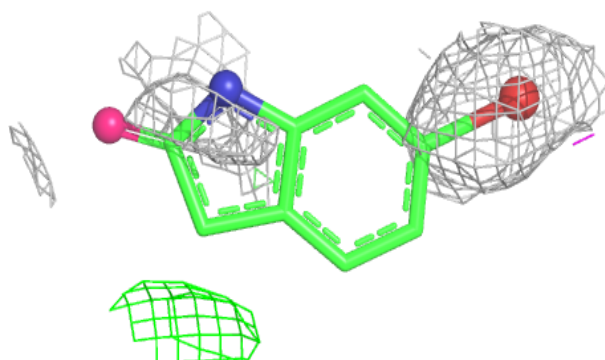


**Electron density around 1P8 D 501:**

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

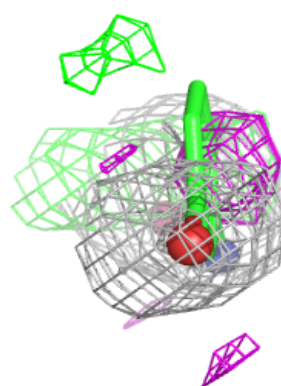
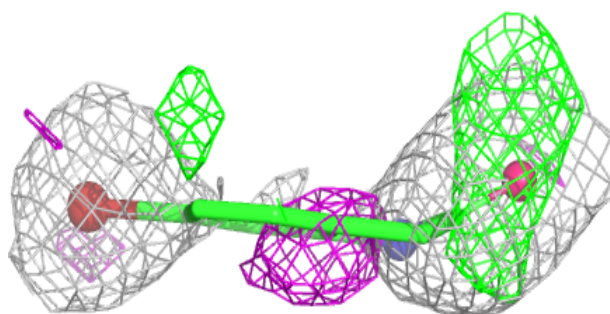
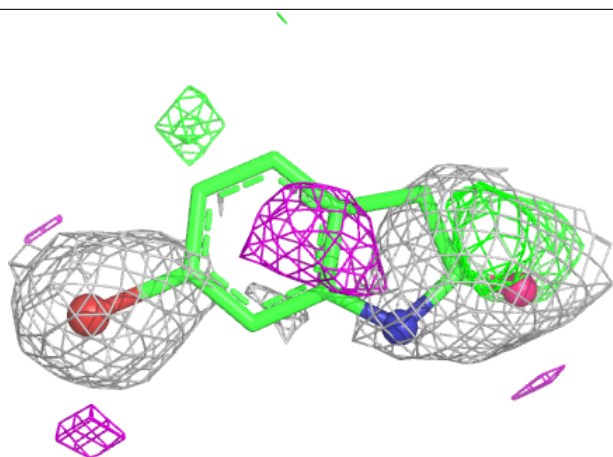
**Electron density around 1P8 D 502:**

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



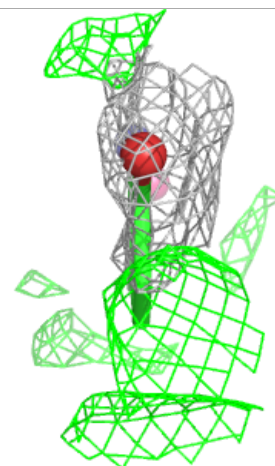
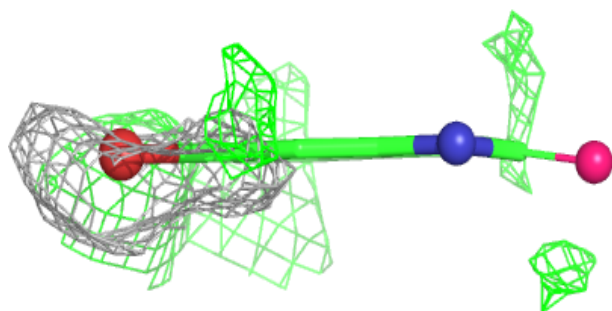
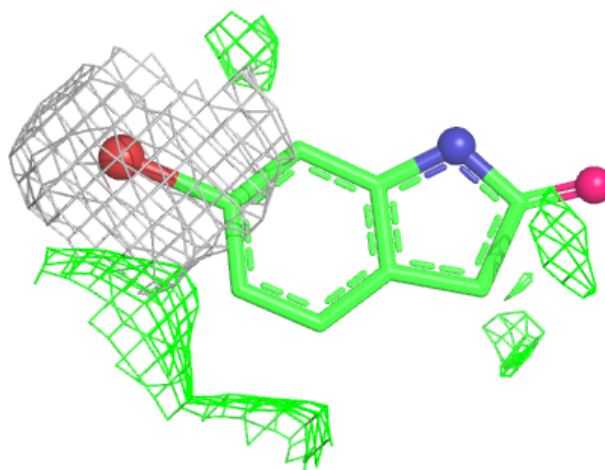
**Electron density around 1P8 B 501:**

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



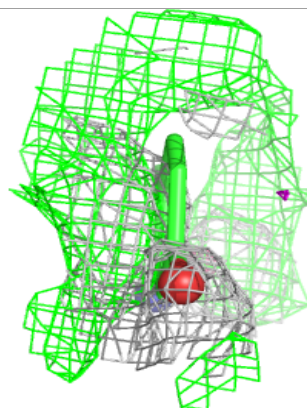
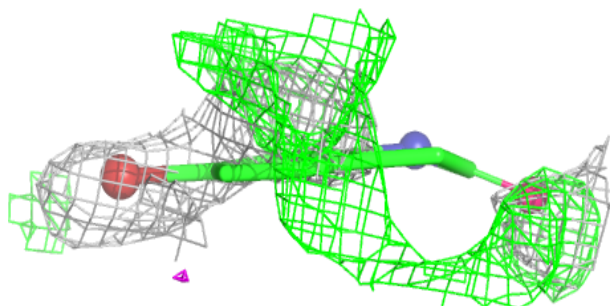
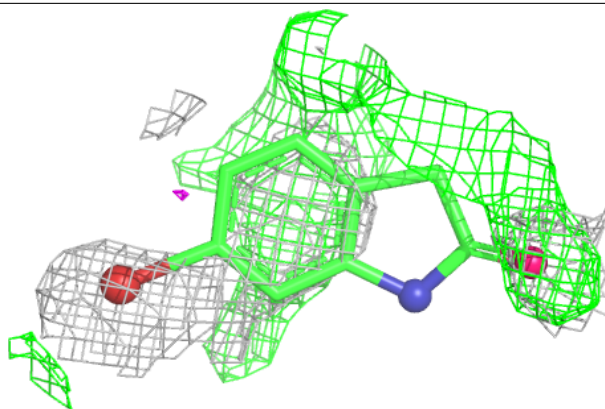
**Electron density around 1P8 C 303 (A):**

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and green (positive)

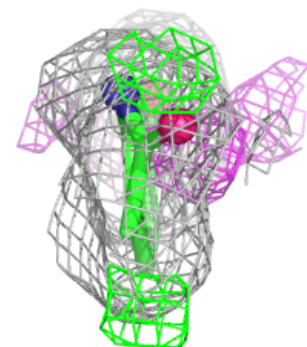
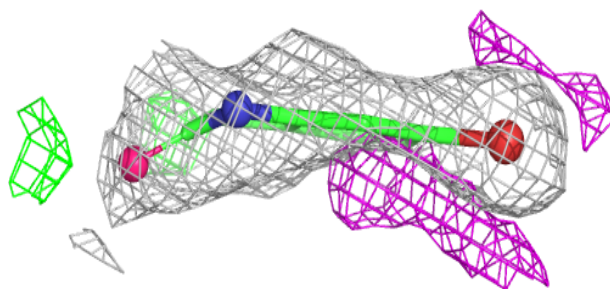
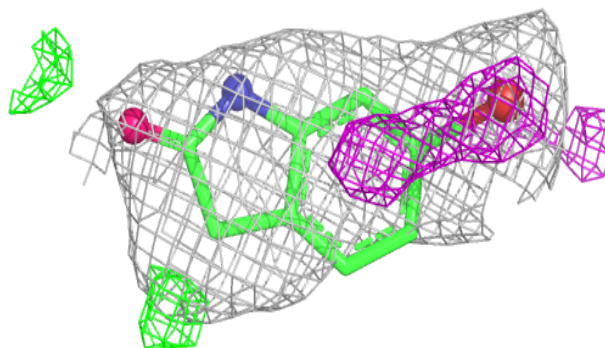


**Electron density around 1P8 C 303 (B):**

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

**Electron density around 1P8 C 301:**

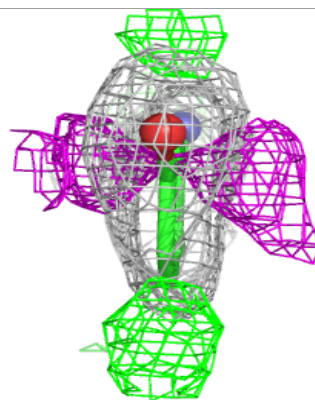
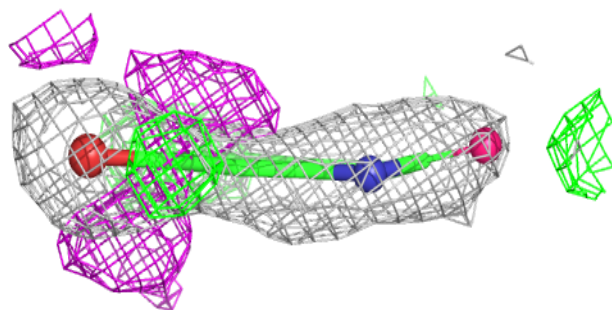
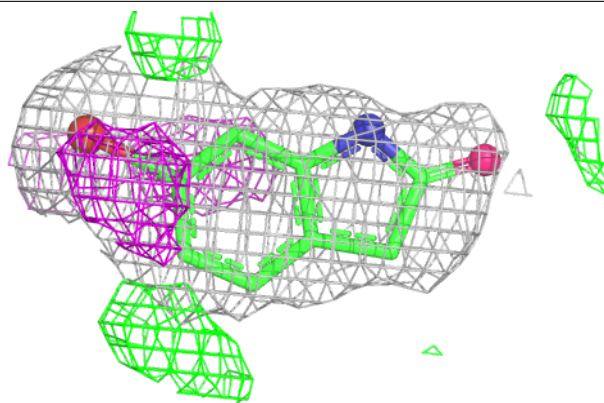
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



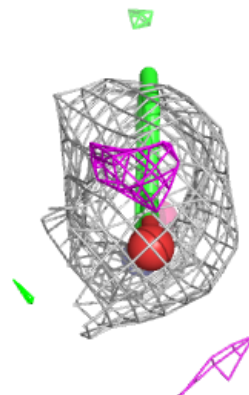
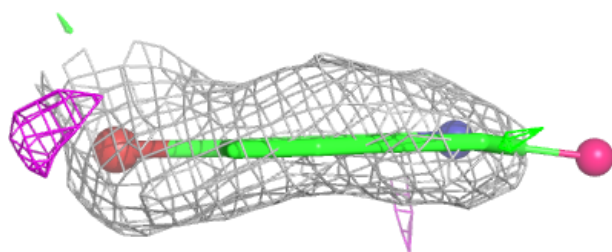
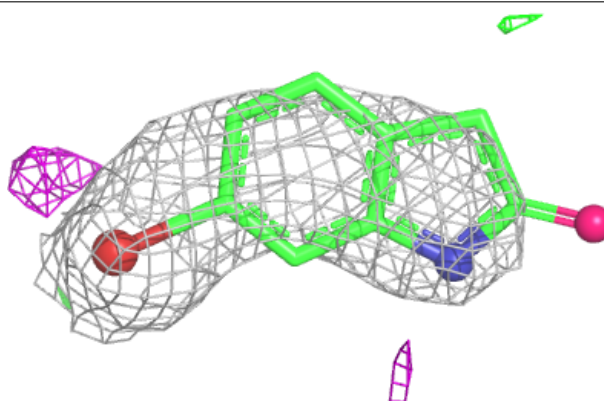


**Electron density around 1P8 A 602:**

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

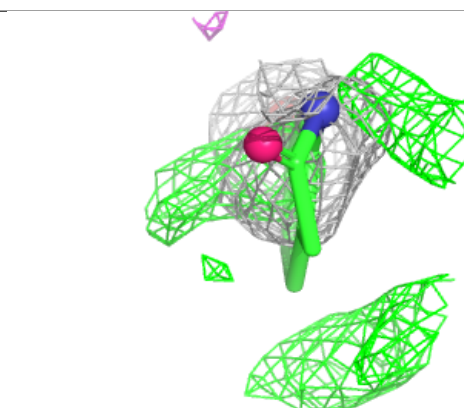
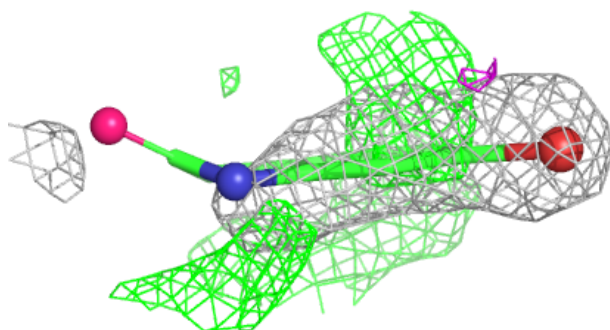
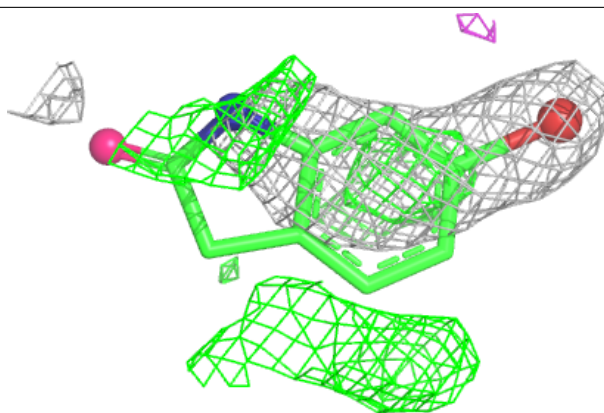
**Electron density around 1P8 B 502:**

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

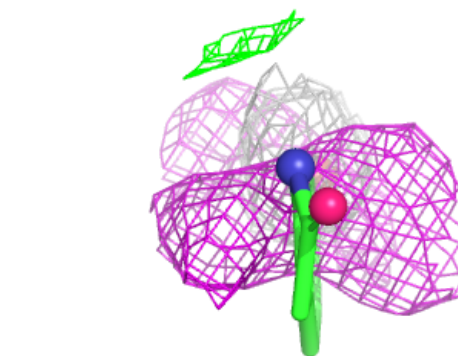
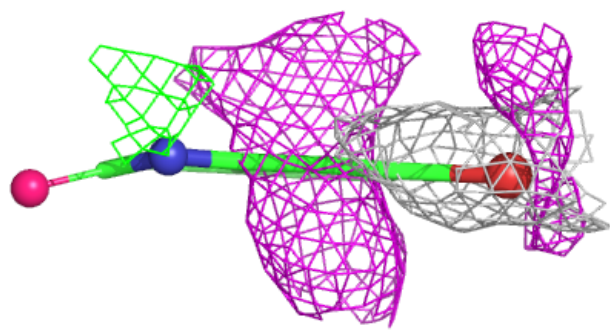
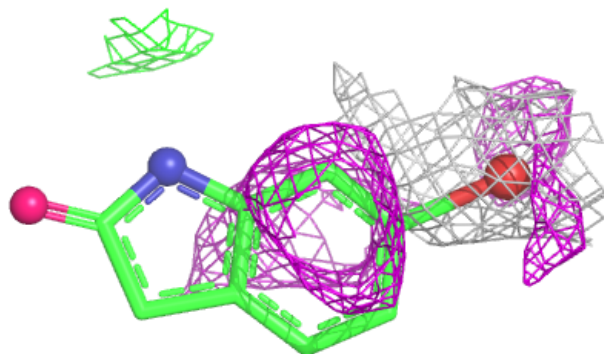


**Electron density around 1P8 A 604:**

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

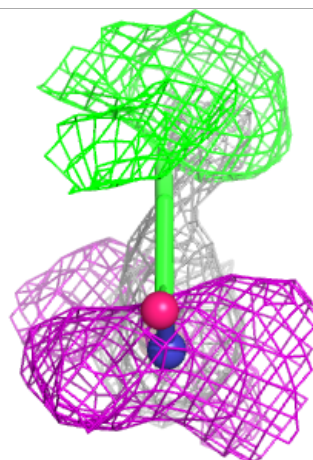
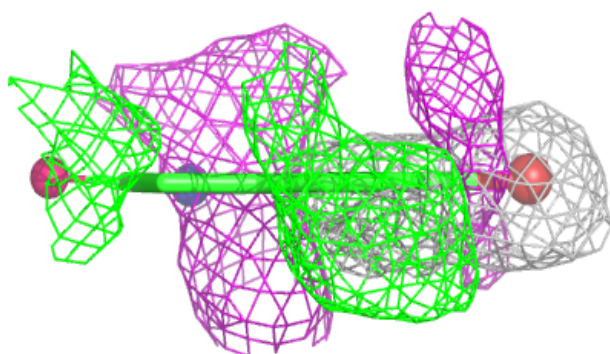
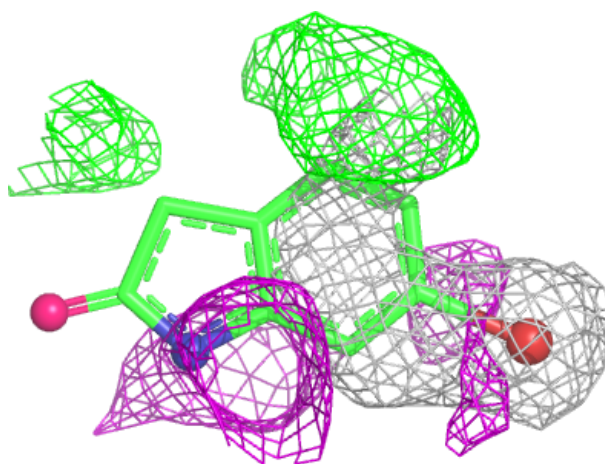
**Electron density around 1P8 A 603 (A):**

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



**Electron density around 1P8 A 603 (B):**

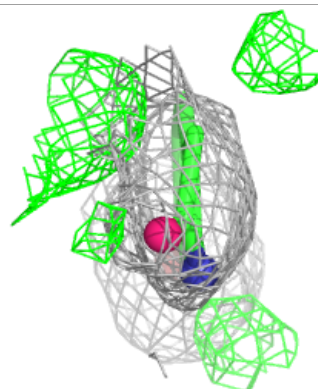
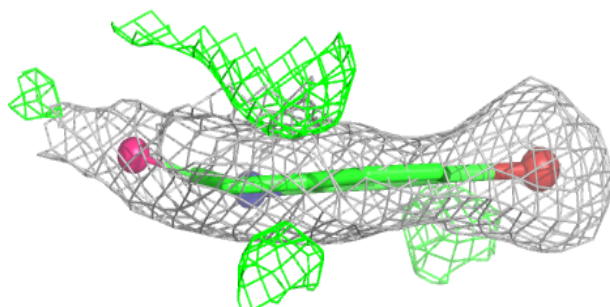
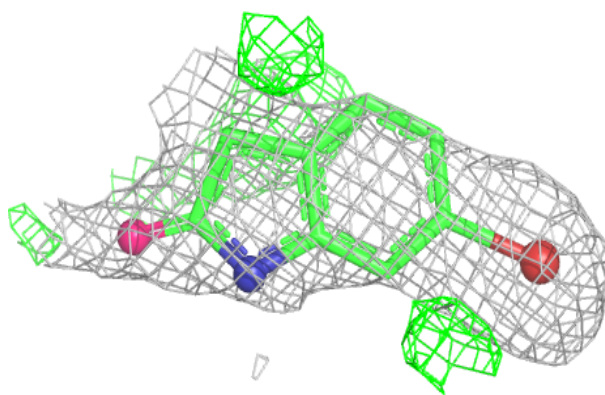
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



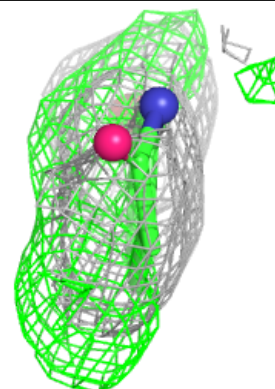
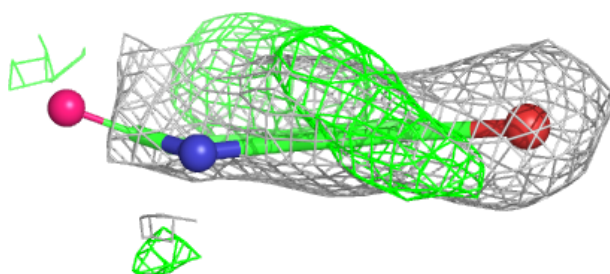
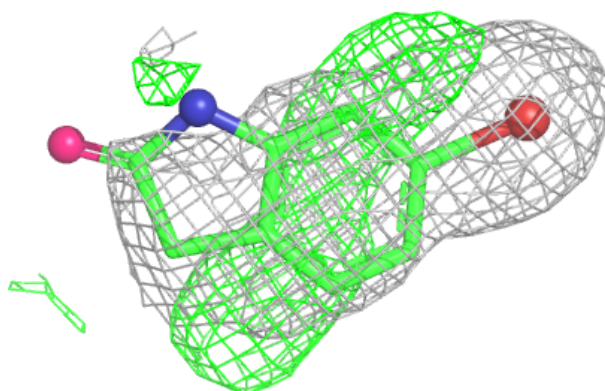


**Electron density around 1P8 A 605:**

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

**Electron density around 1P8 A 601:**

$2mF_o-DF_c$  (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.