Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2024 – 12:35 PM EDT

PDB ID	:	9BNJ
Title	:	Proteus vulgaris tryptophan indole-lyase aminoacrylate complex with benzimidazole
Authors	:	Phillips, R.S.
Deposited on	:	2024-05-02
Resolution	:	1.51 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

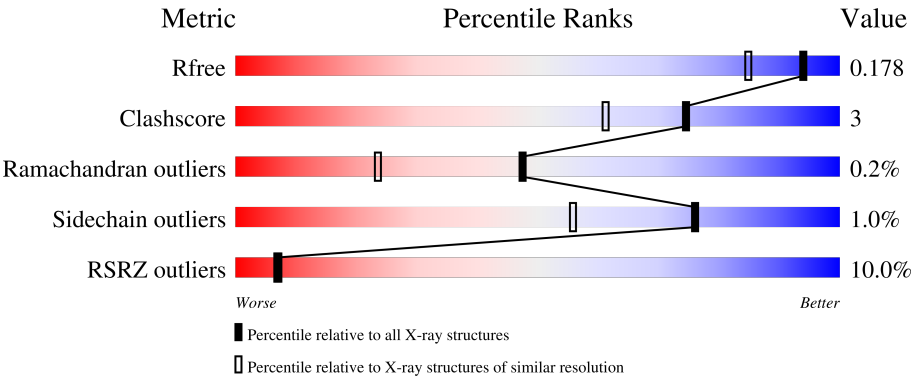
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	467	17% 85% 12%
1	B	467	2% 94% 5%
1	C	467	3% 95% 5%
1	D	467	17% 90% 10%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 36133 atoms, of which 17210 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.

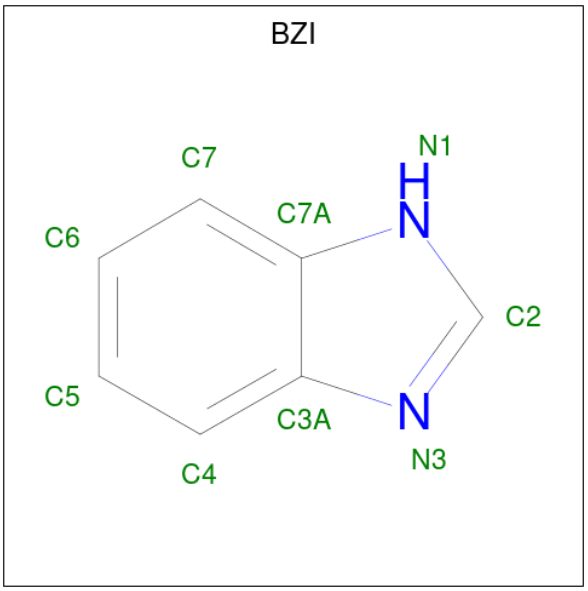
- Molecule 1 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	459	Total	C	H	N	O	S	0	138	0
			9437	3022	4739	800	853	23			
1	B	465	Total	C	H	N	O	S	0	15	0
			7570	2419	3796	645	689	21			
1	C	465	Total	C	H	N	O	S	0	17	0
			7585	2426	3803	642	693	21			
1	D	465	Total	C	H	N	O	S	0	139	0
			9522	3051	4778	806	864	23			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

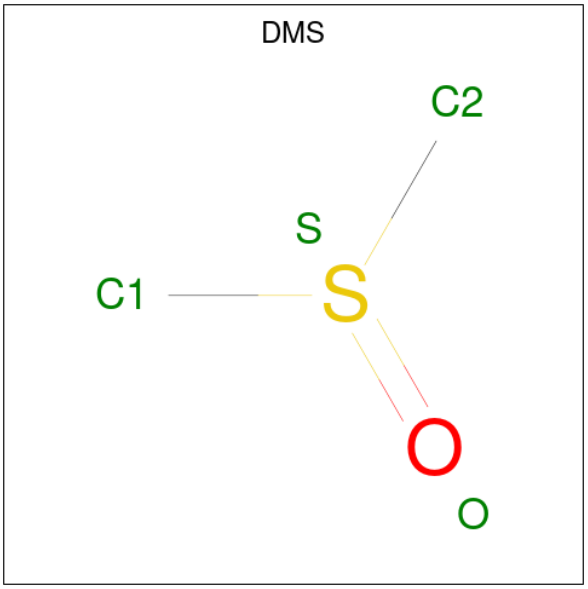
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		
2	C	2	Total	K	0	0
			2	2		

- Molecule 3 is BENZIMIDAZOLE (three-letter code: BZI) (formula: $C_7H_6N_2$) (labeled as "Ligand of Interest" by depositor).



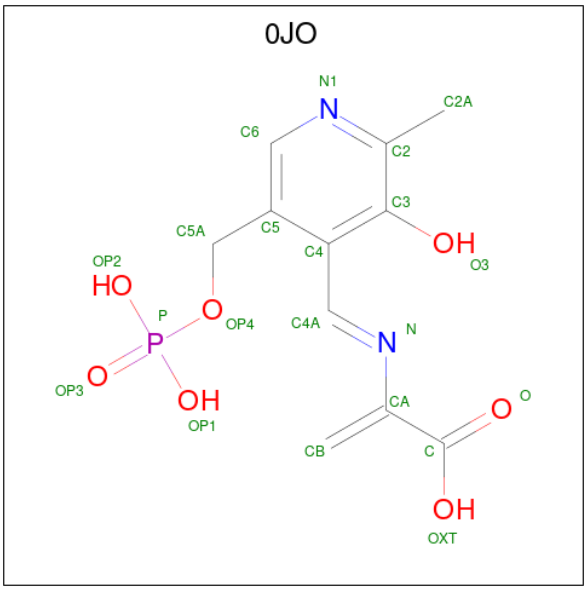
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N 30 14 12 4	0	1
3	A	1	Total C H N 15 7 6 2	0	0
3	B	1	Total C H N 15 7 6 2	0	0
3	C	1	Total C H N 30 14 12 4	0	1
3	D	1	Total C H N 30 14 12 4	0	1

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 5 is 2-{[(E)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene]amino}prop-2-enoic acid (three-letter code: 0JO) (formula: $C_{11}H_{13}N_2O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			31	11	10	2	7	1		
5	B	1	Total	C	H	N	O	P	0	0
			31	11	10	2	7	1		
5	C	1	Total	C	H	N	O	P	0	0
			31	11	10	2	7	1		
5	D	1	Total	C	H	N	O	P	0	0
			31	11	10	2	7	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

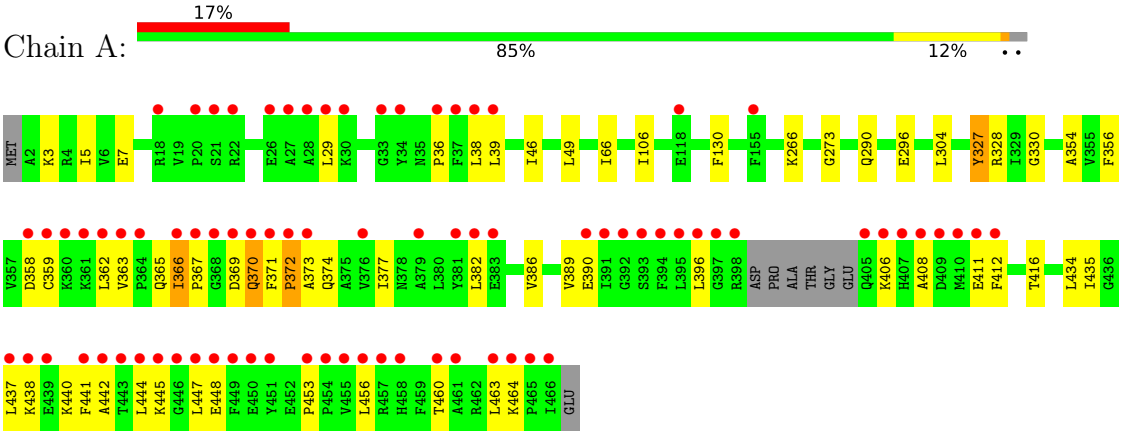
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	422	Total O 422 422	0	49
7	B	454	Total O 454 454	0	25
7	C	456	Total O 456 456	0	31
7	D	428	Total O 428 428	0	39

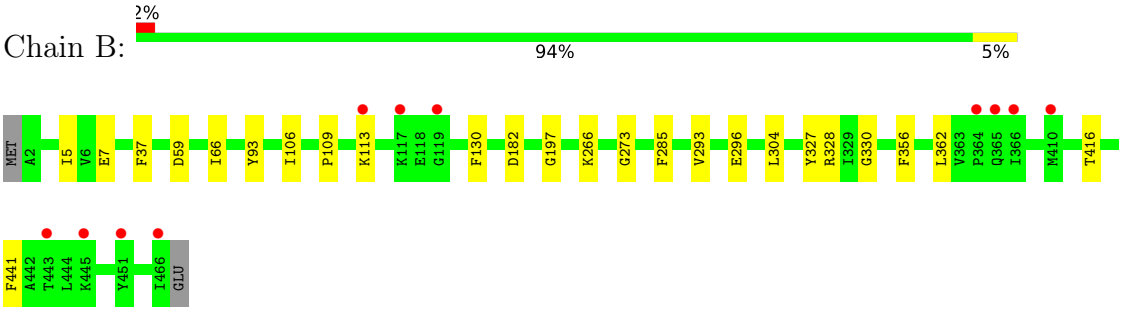
3 Residue-property plots (i)

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.

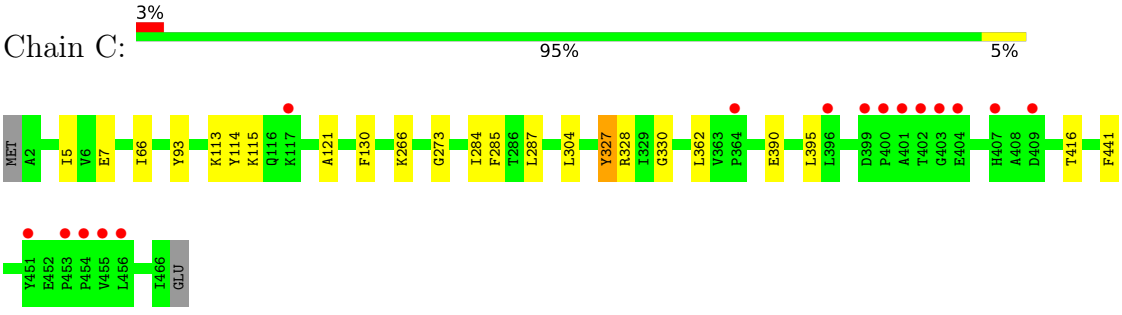
• Molecule 1: Tryptophanase



• Molecule 1: Tryptophanase

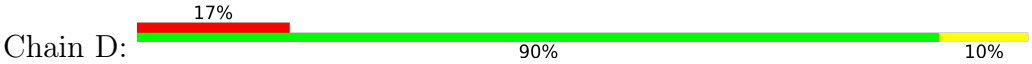


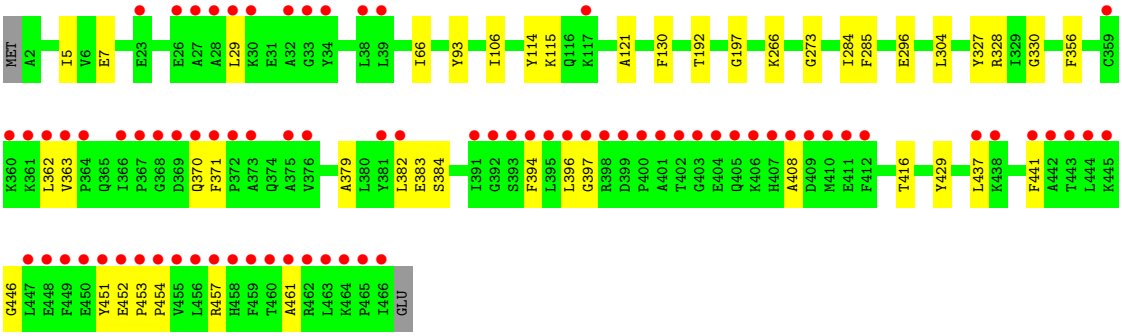
• Molecule 1: Tryptophanase



• Molecule 1: Tryptophanase

Chain D:


17%
90%
10%


MET A2 I5 V6 E7 E23 E26 A27 A28 L29 K30 E31 A32 G33 Y34 L38 L39 I66 Y93 I106 Y114 K115 Q116 K117 A121 F130 T192 G197 K266 G273 I284 F285 E296 L304 Y327 R328 I329 G330 F356 C359
K360 K361 L362 V363 P364 Q365 I366 P367 G368 D369 Q370 F371 P372 A373 Q374 A375 V376 A379 L380 Y381 L382 E383 S384 I391 G392 S393 F394 L395 L396 G397 R398 D399 P400 A401 T402 G403 E404 Q405 K406 H407 A408 D409 M410 E411 F412 T416 Y429 L437 K438 F441 A442 T443 L444 K445
G446 L447 E448 F449 E450 Y451 E452 P453 P454 V455 L456 R457 H458 F459 T460 A461 R462 L463 K464 P465 I466 GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.94Å 118.22Å 152.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.27 – 1.51 91.27 – 1.51	Depositor EDS
% Data completeness (in resolution range)	99.4 (91.27-1.51) 99.4 (91.27-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.51Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.158 , 0.180 0.155 , 0.178	Depositor DCC
R_{free} test set	15878 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	36133	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BZI, 0JO, CL, K, DMS

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	0.30	0/4854	0.57	0/6545
1	B	0.31	0/3900	0.58	1/5260 (0.0%)
1	C	0.31	0/3918	0.58	0/5286
1	D	0.30	0/4907	0.57	0/6624
All	All	0.30	0/17579	0.57	1/23715 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	59	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4698	4739	4712	55	0
1	B	3774	3796	3794	12	0
1	C	3782	3803	3785	13	0
1	D	4744	4778	4749	30	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	18	18	0	0
3	B	9	6	6	0	0
3	C	18	12	12	0	0
3	D	18	12	12	0	0
4	A	4	6	6	2	0
5	A	21	10	10	2	0
5	B	21	10	10	1	0
5	C	21	10	10	2	0
5	D	21	10	10	2	0
6	B	1	0	0	0	0
7	A	422	0	0	6	0
7	B	454	0	0	1	0
7	C	456	0	0	2	0
7	D	428	0	0	0	0
All	All	18923	17210	17134	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 3.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396[B]:LEU:HD22	1:D:408[B]:ALA:HB2	1.51	0.90
1:A:373[B]:ALA:HB2	1:A:411[B]:GLU:OE2	1.87	0.73
1:A:396[B]:LEU:HD12	1:A:408[B]:ALA:HB2	1.71	0.73
1:A:38[B]:LEU:HD21	1:A:460[B]:THR:HA	1.79	0.64
1:A:354[B]:ALA:HB3	1:A:356[B]:PHE:CE1	2.37	0.60
1:A:371[B]:PHE:N	1:A:372[B]:PRO:HD2	2.17	0.60
1:A:362[B]:LEU:HD23	1:A:362[B]:LEU:O	2.01	0.60
1:A:444[A]:LEU:HD23	1:A:445[A]:LYS:N	2.18	0.59
1:C:114:TYR:CG	1:C:284[A]:ILE:HD11	2.38	0.58
1:A:266:LYS:HZ1	5:A:504:0JO:C4A	2.17	0.58
1:A:365[A]:GLN:HG2	1:A:445[A]:LYS:HD2	1.86	0.57
1:A:46:ILE:HB	1:A:386[B]:VAL:HG22	1.87	0.56
1:D:29[B]:LEU:HD22	1:D:382[B]:LEU:HD21	1.87	0.56
1:A:373[A]:ALA:HB3	1:A:390[A]:GLU:HG3	1.87	0.56
1:D:383[B]:GLU:HG3	1:D:437[B]:LEU:HD21	1.89	0.55
1:A:36[B]:PRO:HA	1:A:39[B]:LEU:HD12	1.90	0.54
4:A:503:DMS:H21	7:A:968:HOH:O	2.07	0.54
1:B:106:ILE:HD11	1:B:296:GLU:HG3	1.90	0.54
1:D:114:TYR:CG	1:D:284[A]:ILE:HD11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366[A]:ILE:HG22	1:A:367[A]:PRO:O	2.07	0.53
1:C:5:ILE:HD12	1:C:330:GLY:HA3	1.91	0.53
1:A:359[B]:CYS:O	1:A:363[B]:VAL:HG22	2.08	0.53
1:A:266:LYS:HZ1	5:A:504:0JO:H4	1.73	0.53
1:D:363[A]:VAL:HG23	1:D:363[A]:VAL:O	2.08	0.53
1:A:106:ILE:HD11	1:A:296:GLU:HG3	1.91	0.52
1:A:448[B]:GLU:O	1:A:464[B]:LYS:N	2.41	0.52
1:D:453[A]:PRO:N	1:D:454[A]:PRO:HD3	2.25	0.51
1:A:7:GLU:HG3	1:A:327[B]:TYR:CZ	2.46	0.51
1:A:447[A]:LEU:HD22	1:A:463[A]:LEU:HB3	1.93	0.51
1:D:362[B]:LEU:HD21	1:D:441[B]:PHE:CZ	2.44	0.51
1:C:273:GLY:HA2	1:C:304:LEU:HD21	1.93	0.51
1:A:362[B]:LEU:HD21	1:A:441[B]:PHE:CE2	2.46	0.50
1:D:396[B]:LEU:CD2	1:D:408[B]:ALA:HB2	2.34	0.50
1:A:273:GLY:HA2	1:A:304:LEU:HD21	1.93	0.49
1:A:365[A]:GLN:HG2	1:A:445[A]:LYS:CD	2.43	0.49
1:B:182:ASP:OD1	7:B:601:HOH:O	2.20	0.49
1:A:366[A]:ILE:HG13	1:A:445[A]:LYS:HD2	1.95	0.49
1:D:273:GLY:HA2	1:D:304:LEU:HD21	1.95	0.49
1:C:287:LEU:HD13	7:C:829:HOH:O	2.12	0.49
1:C:7:GLU:HG3	1:C:327[B]:TYR:CZ	2.49	0.48
1:D:29[B]:LEU:CD2	1:D:382[B]:LEU:HD21	2.44	0.48
1:D:266:LYS:HZ1	5:D:502:0JO:C4A	2.26	0.48
1:A:366[A]:ILE:HD11	1:A:445[A]:LYS:HG3	1.94	0.48
1:D:453[A]:PRO:N	1:D:454[A]:PRO:CD	2.77	0.48
1:A:456[B]:LEU:HD12	7:A:648:HOH:O	2.14	0.47
1:A:396[A]:LEU:HD13	1:A:408[A]:ALA:HB2	1.96	0.47
1:B:266[A]:LYS:HZ1	5:B:503:0JO:C4A	2.27	0.47
1:D:266:LYS:HZ1	5:D:502:0JO:H4	1.78	0.47
1:A:366[A]:ILE:HB	1:A:372[A]:PRO:HB3	1.97	0.47
1:B:273:GLY:HA2	1:B:304:LEU:HD21	1.97	0.47
1:B:7:GLU:HG3	1:B:327[A]:TYR:CZ	2.50	0.47
1:A:373[B]:ALA:HB3	1:A:390[B]:GLU:HG3	1.96	0.47
1:B:197:GLY:HA2	1:B:356:PHE:CE1	2.50	0.47
1:D:370[B]:GLN:HB3	1:D:446[B]:GLY:HA3	1.96	0.46
1:D:397[B]:GLY:O	1:D:457[B]:ARG:NH2	2.48	0.46
4:A:503:DMS:H23	7:A:965:HOH:O	2.15	0.46
1:D:371[B]:PHE:CE1	1:D:394[B]:PHE:HA	2.51	0.46
1:C:266:LYS:HZ1	5:C:503:0JO:C4A	2.28	0.46
1:D:7:GLU:HG3	1:D:327[A]:TYR:CZ	2.50	0.46
1:D:451[A]:TYR:O	1:D:452[A]:GLU:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359[B]:CYS:HB2	1:A:411[B]:GLU:OE1	2.16	0.45
1:C:362:LEU:HD22	1:C:441:PHE:CD2	2.51	0.45
1:A:396[B]:LEU:CD1	1:A:408[B]:ALA:HB2	2.45	0.45
1:A:362[A]:LEU:HD11	1:A:441[A]:PHE:CE2	2.51	0.45
1:A:358[B]:ASP:HA	1:A:412[B]:PHE:CD1	2.53	0.44
1:A:444[A]:LEU:O	1:A:445[A]:LYS:HB2	2.16	0.44
1:A:435[B]:ILE:O	1:A:438[B]:LYS:HG2	2.18	0.44
1:C:266:LYS:HZ1	5:C:503:0JO:H4	1.82	0.44
1:A:371[B]:PHE:O	1:A:372[B]:PRO:C	2.56	0.44
1:D:453[B]:PRO:HD2	1:D:461[B]:ALA:HB2	1.99	0.44
1:D:5:ILE:HD12	1:D:330:GLY:HA3	1.98	0.43
1:B:362:LEU:O	1:B:441:PHE:HB3	2.18	0.43
1:A:49:LEU:HD12	1:A:389[B]:VAL:HB	1.99	0.43
1:D:379[A]:ALA:O	1:D:383[A]:GLU:HG2	2.18	0.43
1:A:363[A]:VAL:HG13	1:A:365[A]:GLN:NE2	2.34	0.43
1:D:384[B]:SER:HB2	1:D:429:TYR:CE1	2.53	0.43
1:A:374[B]:GLN:HB2	1:A:390[B]:GLU:OE1	2.19	0.43
1:A:396[B]:LEU:CD2	1:A:406[B]:LYS:HB3	2.49	0.43
1:A:456[A]:LEU:HD13	1:B:293:VAL:HG12	2.00	0.43
1:A:362[B]:LEU:HD21	1:A:441[B]:PHE:CD2	2.54	0.43
1:A:38[B]:LEU:HD11	1:A:460[B]:THR:O	2.18	0.43
1:A:3:LYS:HE2	7:A:941:HOH:O	2.19	0.42
1:C:395:LEU:HD23	1:C:395:LEU:C	2.39	0.42
1:A:5:ILE:HD12	1:A:330:GLY:HA3	2.00	0.42
1:A:366[A]:ILE:HG12	1:A:445[A]:LYS:HG2	2.02	0.42
1:A:29[B]:LEU:CD2	1:A:382[B]:LEU:HD21	2.49	0.42
1:B:5:ILE:HD12	1:B:330:GLY:HA3	2.00	0.42
1:D:452[A]:GLU:HG3	1:D:454[A]:PRO:CD	2.50	0.42
1:C:93:TYR:HB3	1:C:285:PHE:CD1	2.55	0.42
1:A:453[B]:PRO:HG3	1:A:460[B]:THR:OG1	2.20	0.41
1:D:394[A]:PHE:HZ	1:D:461[A]:ALA:HB3	1.84	0.41
1:A:366[A]:ILE:HG21	1:A:372[A]:PRO:HA	2.02	0.41
1:C:113:LYS:HD3	7:C:913:HOH:O	2.20	0.41
1:B:93:TYR:HB3	1:B:285:PHE:CD1	2.56	0.41
1:A:440[B]:LYS:C	1:A:442[B]:ALA:N	2.74	0.41
1:D:197:GLY:HA2	1:D:356[A]:PHE:CE1	2.55	0.41
1:A:434[B]:LEU:HD12	1:A:437[B]:LEU:HD12	2.02	0.41
1:C:115:LYS:HG2	1:C:121:ALA:HB2	2.03	0.41
1:A:377[B]:ILE:HG23	7:A:604:HOH:O	2.21	0.41
1:B:109:PRO:O	1:B:113:LYS:HG2	2.21	0.41
1:D:29[B]:LEU:HD22	1:D:382[B]:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369[B]:ASP:O	1:A:370[B]:GLN:HB2	2.19	0.41
1:D:106:ILE:HD11	1:D:296:GLU:HG3	2.02	0.41
1:D:115:LYS:HG2	1:D:121:ALA:HB2	2.03	0.41
1:A:440[B]:LYS:O	1:A:444[B]:LEU:N	2.54	0.40
1:A:290:GLN:OE1	7:A:601:HOH:O	2.22	0.40
1:D:93:TYR:HB3	1:D:285:PHE:CD1	2.57	0.40
1:A:66:ILE:CD1	1:D:66[A]:ILE:HG13	2.51	0.40
1:B:66:ILE:CD1	1:C:66[A]:ILE:HG13	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	590/467 (126%)	551 (93%)	33 (6%)	6 (1%)	15 3
1	B	478/467 (102%)	464 (97%)	14 (3%)	0	100 100
1	C	480/467 (103%)	463 (96%)	17 (4%)	0	100 100
1	D	601/467 (129%)	578 (96%)	22 (4%)	1 (0%)	47 23
All	All	2149/1868 (115%)	2056 (96%)	86 (4%)	7 (0%)	47 18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372[A]	PRO
1	A	372[B]	PRO
1	A	366[A]	ILE
1	A	366[B]	ILE
1	A	370[A]	GLN
1	A	370[B]	GLN
1	D	192	THR

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	497/386 (129%)	491 (99%)	6 (1%)	71	47
1	B	398/386 (103%)	394 (99%)	4 (1%)	76	56
1	C	401/386 (104%)	395 (98%)	6 (2%)	65	38
1	D	502/386 (130%)	498 (99%)	4 (1%)	81	65
All	All	1798/1544 (116%)	1778 (99%)	20 (1%)	76	52

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	PHE
1	A	327[A]	TYR
1	A	327[B]	TYR
1	A	328	ARG
1	A	416[A]	THR
1	A	416[B]	THR
1	B	37	PHE
1	B	130	PHE
1	B	328	ARG
1	B	416	THR
1	C	130	PHE
1	C	327[A]	TYR
1	C	327[B]	TYR
1	C	328	ARG
1	C	390	GLU
1	C	416	THR
1	D	130	PHE
1	D	328	ARG
1	D	416[A]	THR
1	D	416[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	B	243	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)

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	BZI	D	501[A]	-	8,10,10	0.95	0	6,13,13	1.26	1 (16%)
3	BZI	C	502[A]	-	8,10,10	0.95	0	6,13,13	1.25	1 (16%)
3	BZI	B	502	-	8,10,10	0.95	0	6,13,13	1.27	1 (16%)
3	BZI	A	502[A]	-	8,10,10	0.94	0	6,13,13	1.24	1 (16%)
3	BZI	C	502[B]	-	8,10,10	0.94	0	6,13,13	1.26	1 (16%)
3	BZI	A	502[B]	-	8,10,10	0.95	0	6,13,13	1.25	1 (16%)
3	BZI	D	501[B]	-	8,10,10	0.93	0	6,13,13	1.26	1 (16%)
4	DMS	A	503	-	3,3,3	0.60	0	3,3,3	0.32	0
5	0JO	A	504	-	20,21,21	1.28	2 (10%)	23,30,30	0.82	1 (4%)
5	0JO	D	502	-	20,21,21	1.22	2 (10%)	23,30,30	0.69	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	0JO	C	503	-	20,21,21	1.21	2 (10%)	23,30,30	0.79	1 (4%)
3	BZI	A	505	-	8,10,10	0.93	0	6,13,13	1.24	1 (16%)
5	0JO	B	503	-	20,21,21	1.16	2 (10%)	23,30,30	0.84	1 (4%)

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	BZI	D	501[A]	-	-	-	0/2/2/2
3	BZI	C	502[A]	-	-	-	0/2/2/2
3	BZI	B	502	-	-	-	0/2/2/2
3	BZI	A	502[A]	-	-	-	0/2/2/2
3	BZI	C	502[B]	-	-	-	0/2/2/2
3	BZI	A	502[B]	-	-	-	0/2/2/2
3	BZI	D	501[B]	-	-	-	0/2/2/2
5	0JO	A	504	-	-	0/10/15/15	0/1/1/1
5	0JO	D	502	-	-	0/10/15/15	0/1/1/1
5	0JO	C	503	-	-	0/10/15/15	0/1/1/1
3	BZI	A	505	-	-	-	0/2/2/2
5	0JO	B	503	-	-	0/10/15/15	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	0JO	CA-C	-4.65	1.40	1.50
5	C	503	0JO	CA-C	-4.30	1.41	1.50
5	D	502	0JO	CA-C	-4.27	1.41	1.50
5	B	503	0JO	CA-C	-3.89	1.42	1.50
5	B	503	0JO	OXT-C	-2.87	1.22	1.30
5	D	502	0JO	OXT-C	-2.79	1.22	1.30
5	C	503	0JO	OXT-C	-2.75	1.22	1.30
5	A	504	0JO	OXT-C	-2.67	1.22	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	503	0JO	CB-CA-C	-2.81	114.27	121.06
5	A	504	0JO	CB-CA-C	-2.43	115.19	121.06
3	B	502	BZI	C6-C7-C7A	-2.42	116.60	120.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502[B]	BZI	C6-C7-C7A	-2.38	116.65	120.08
3	D	501[B]	BZI	C6-C7-C7A	-2.37	116.67	120.08
3	C	502[B]	BZI	C6-C7-C7A	-2.37	116.67	120.08
3	A	505	BZI	C6-C7-C7A	-2.36	116.69	120.08
3	C	502[A]	BZI	C6-C7-C7A	-2.36	116.69	120.08
3	A	502[A]	BZI	C6-C7-C7A	-2.35	116.69	120.08
3	D	501[A]	BZI	C6-C7-C7A	-2.35	116.70	120.08
5	C	503	0JO	CB-CA-C	-2.32	115.47	121.06
5	D	502	0JO	CB-CA-C	-2.08	116.03	121.06

There are no chirality outliers.

There are no torsion outliers.

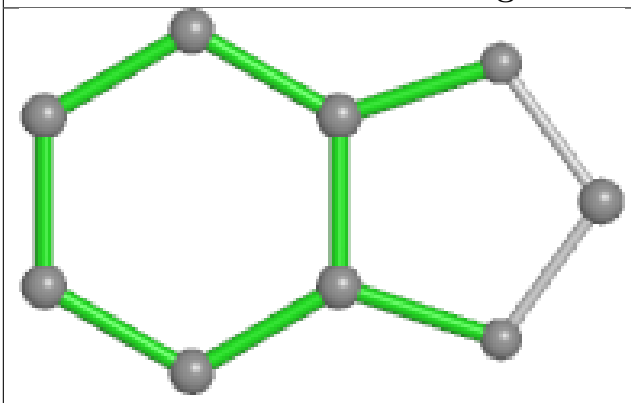
There are no ring outliers.

5 monomers are involved in 9 short contacts:

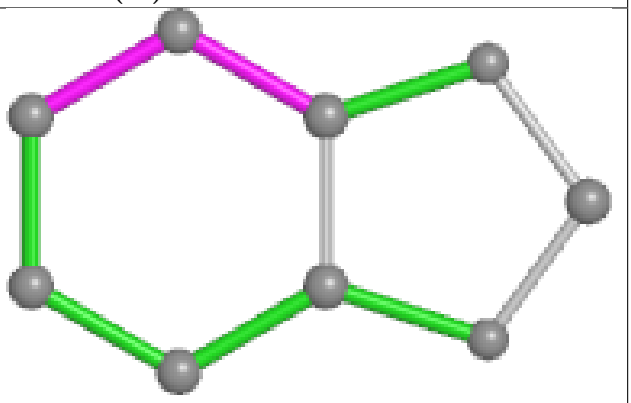
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	DMS	2	0
5	A	504	0JO	2	0
5	D	502	0JO	2	0
5	C	503	0JO	2	0
5	B	503	0JO	1	0

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.

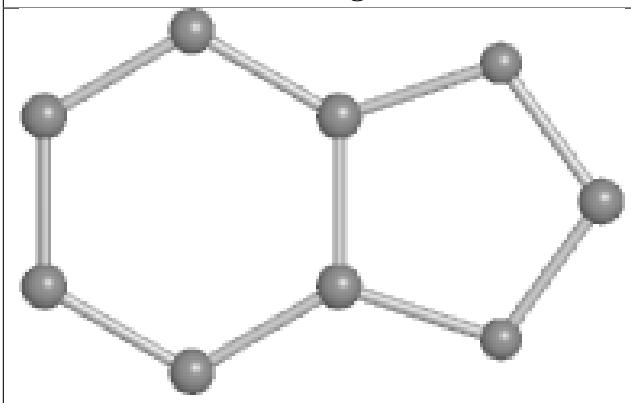
Ligand BZI D 501 (A)



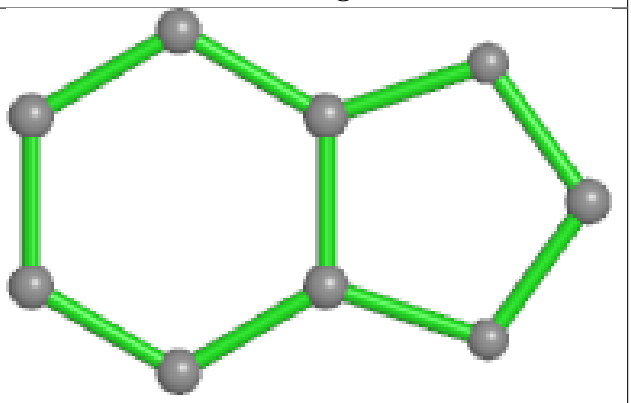
Bond lengths



Bond angles

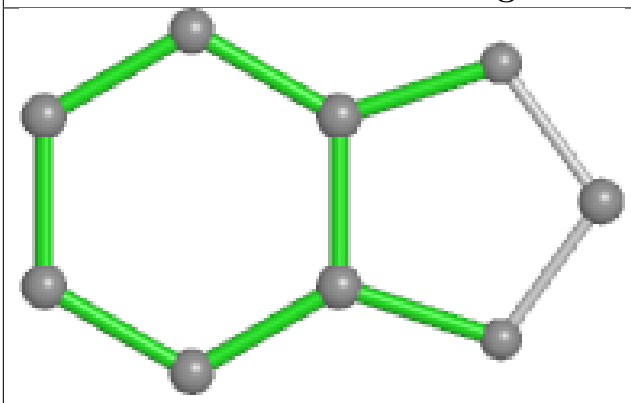


Torsions



Rings

Ligand BZI C 502 (A)



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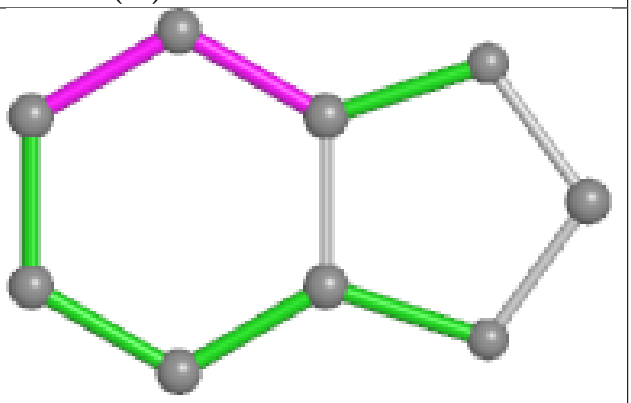

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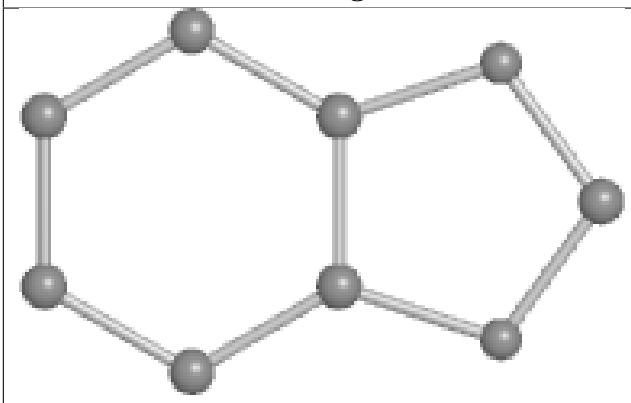

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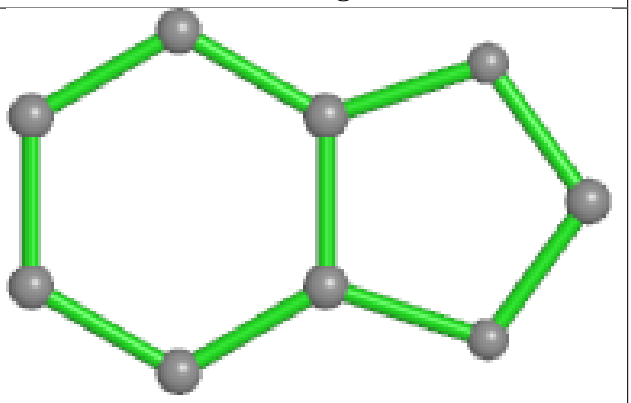
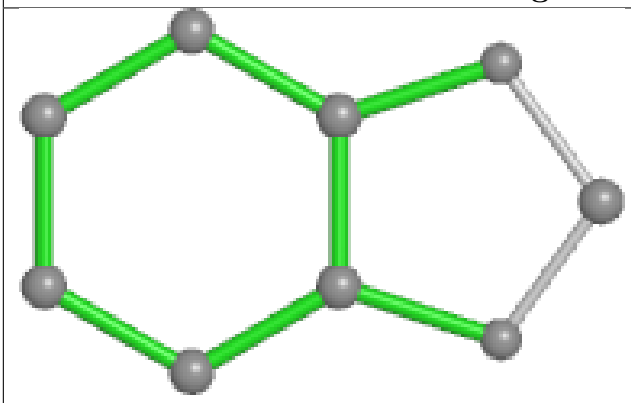


Rings

Ligand BZI B 502



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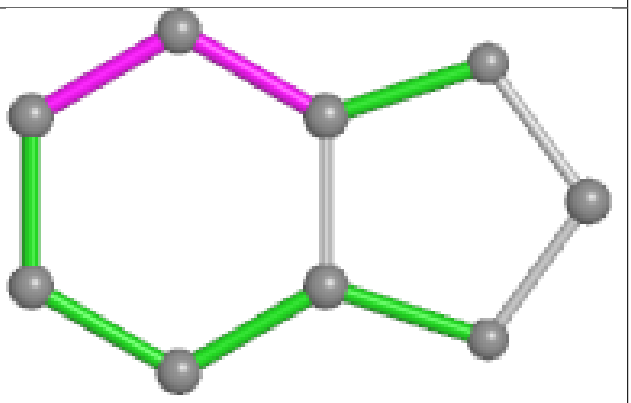
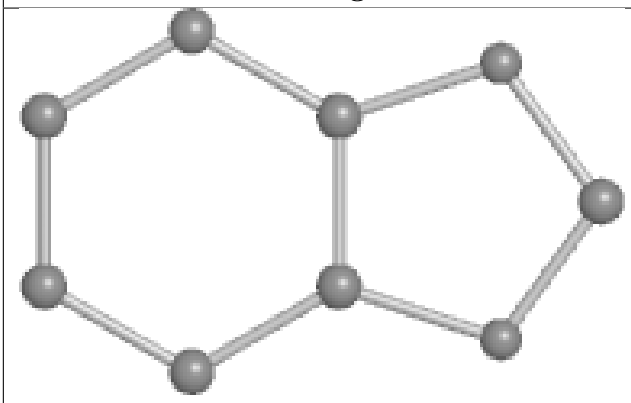


Bond angles



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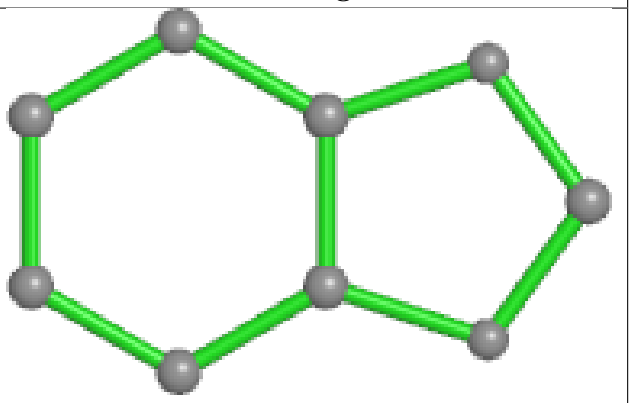
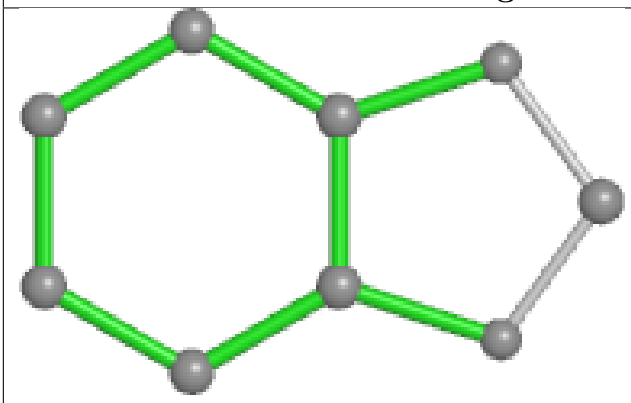


Rings

Ligand BZI A 502 (A)



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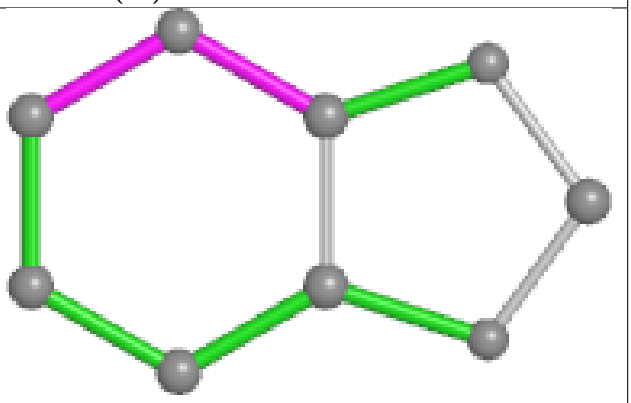

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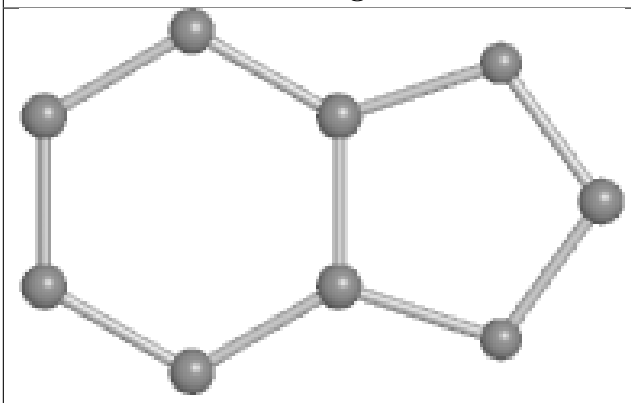

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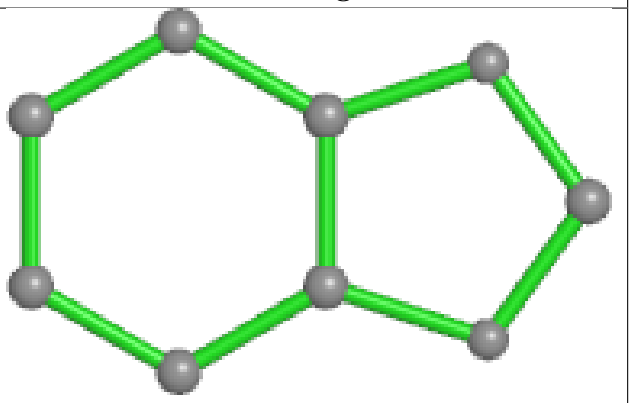
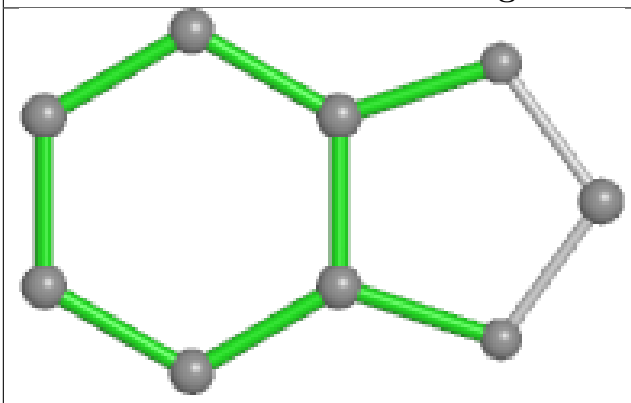
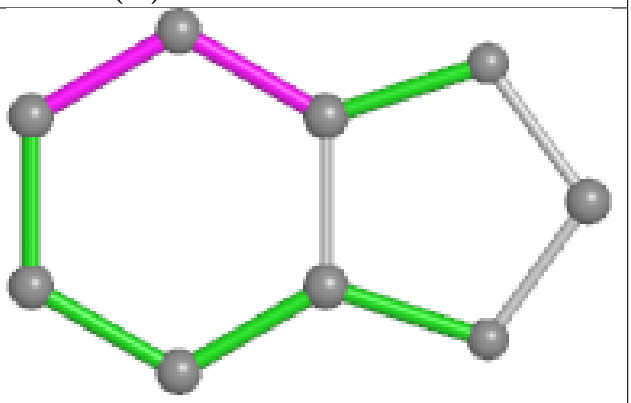


Rings

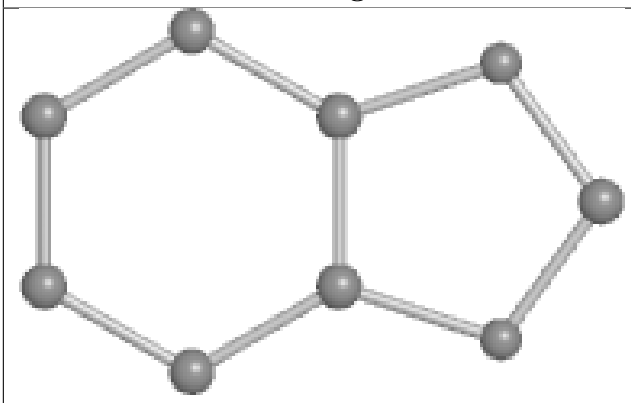
Ligand BZI C 502 (B)



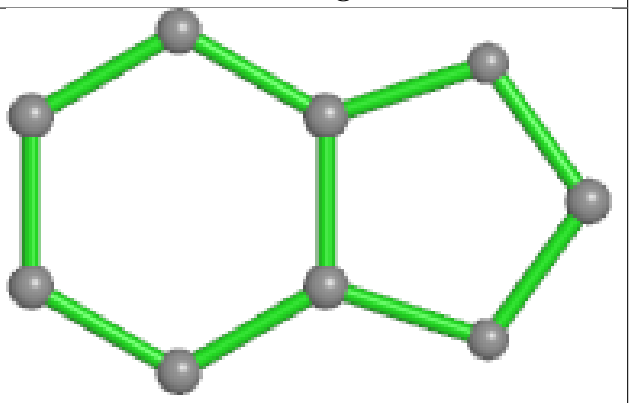
Bond lengths



Bond angles



Torsions



Rings

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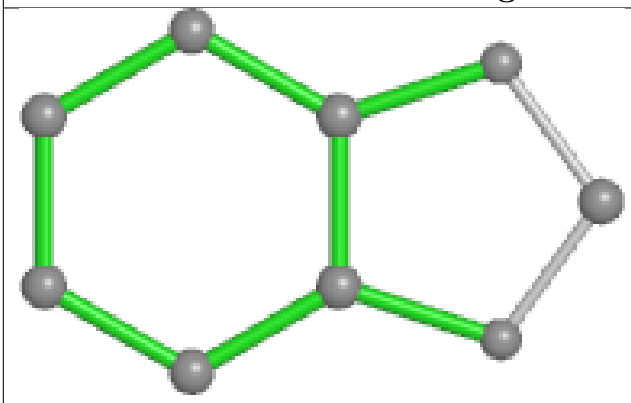
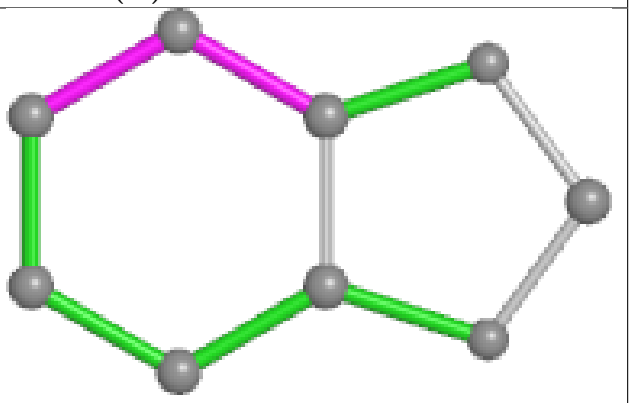
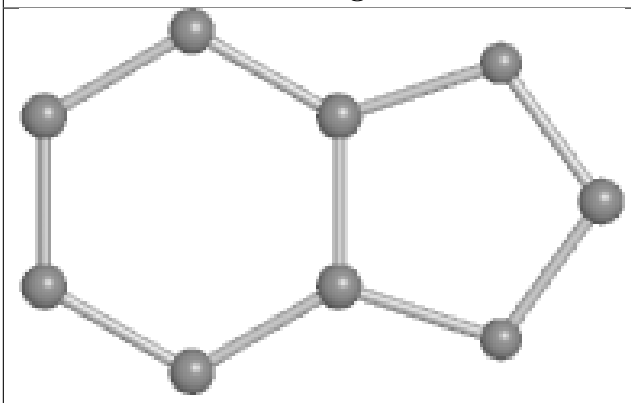


Bond lengths



Bond angles



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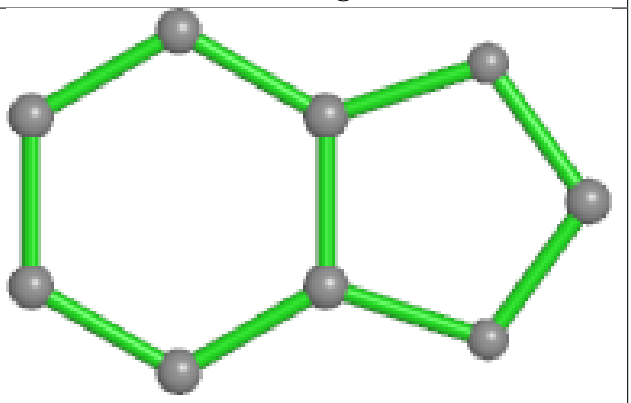
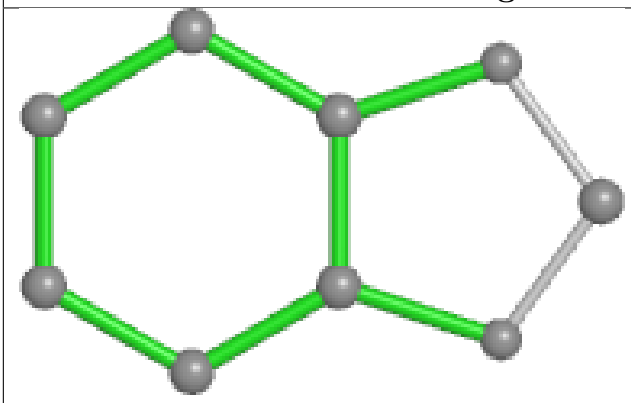
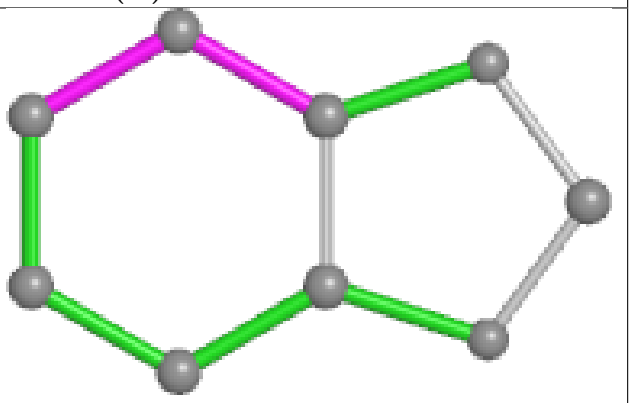


Rings

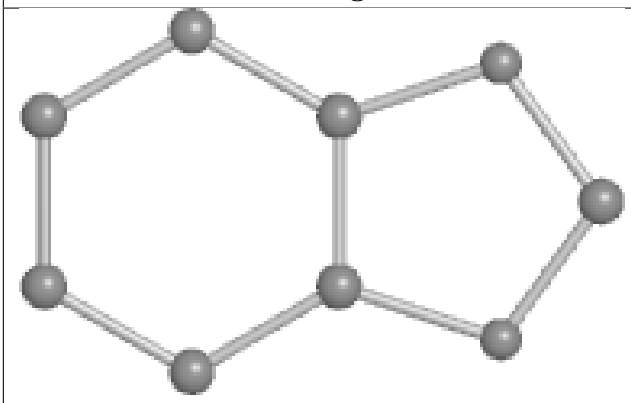
Ligand BZI D 501 (B)



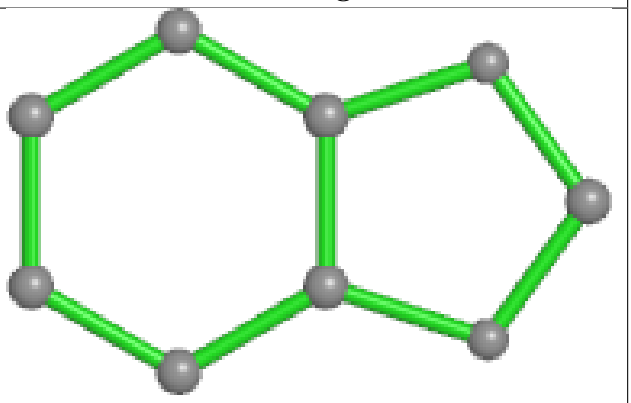
Bond lengths



Bond angles

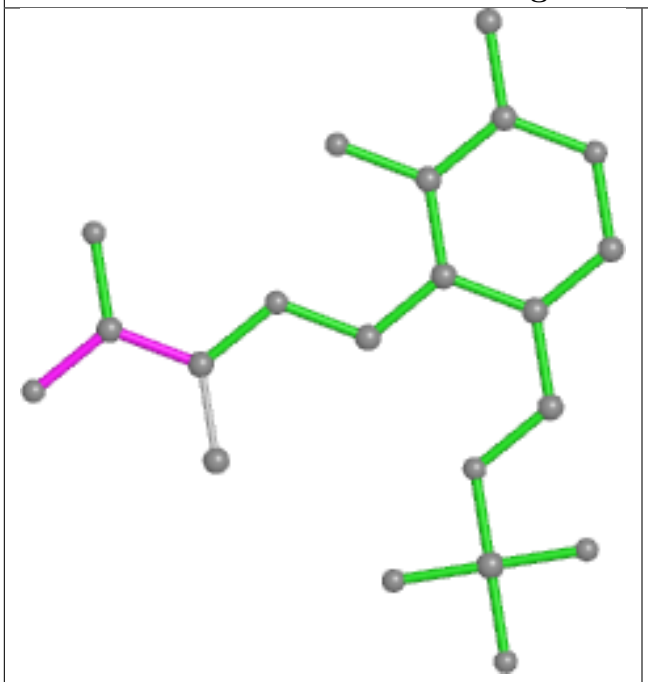


Torsions

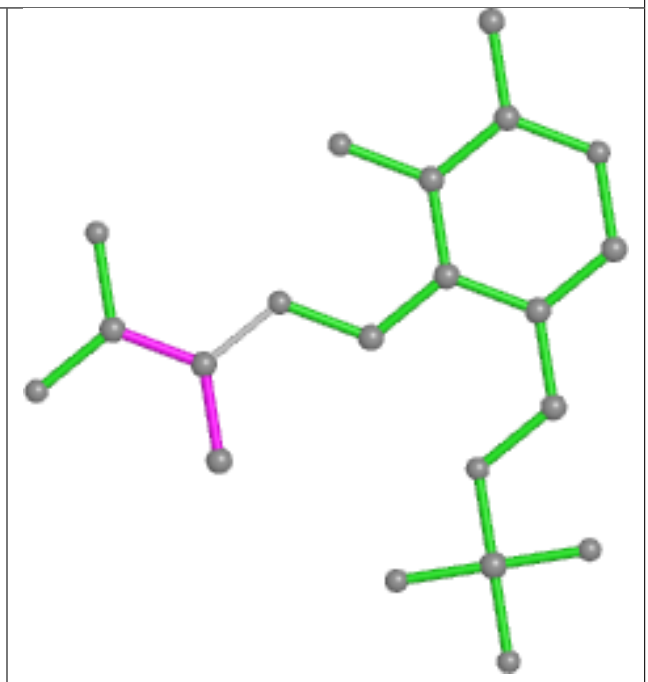


Rings

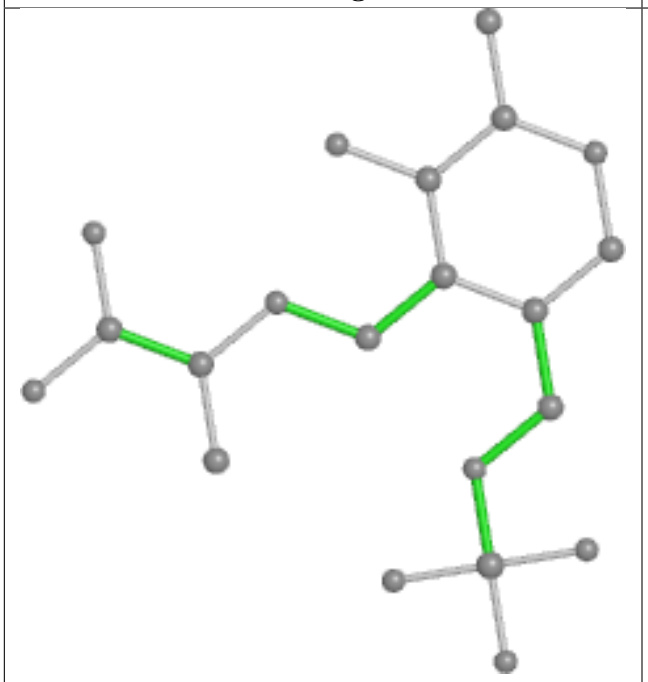
Ligand 0JO A 504



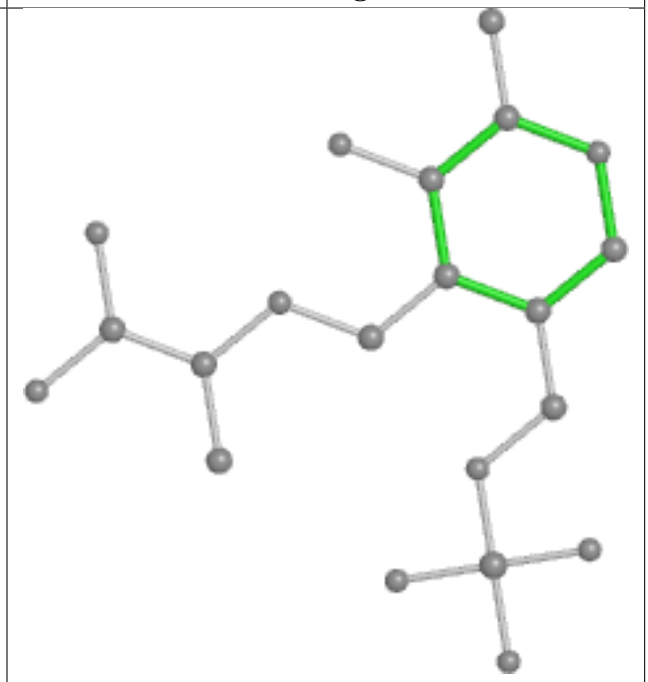
Bond lengths



Bond angles

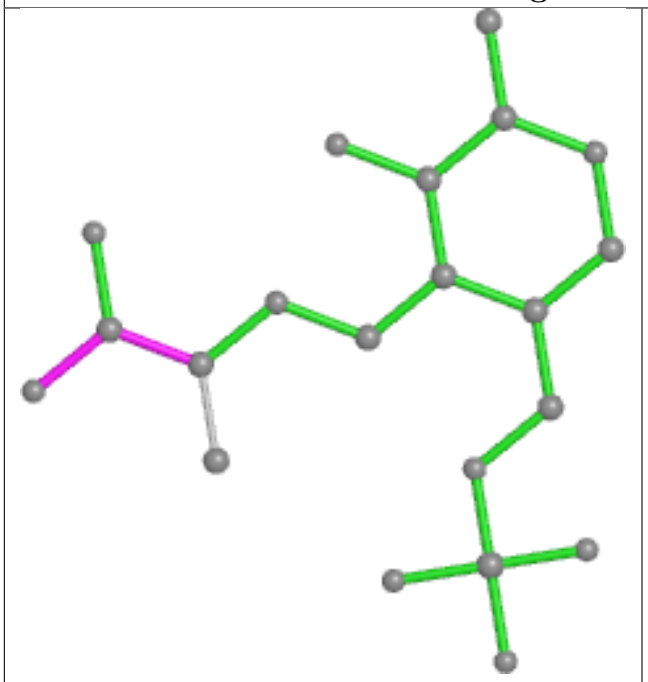


Torsions

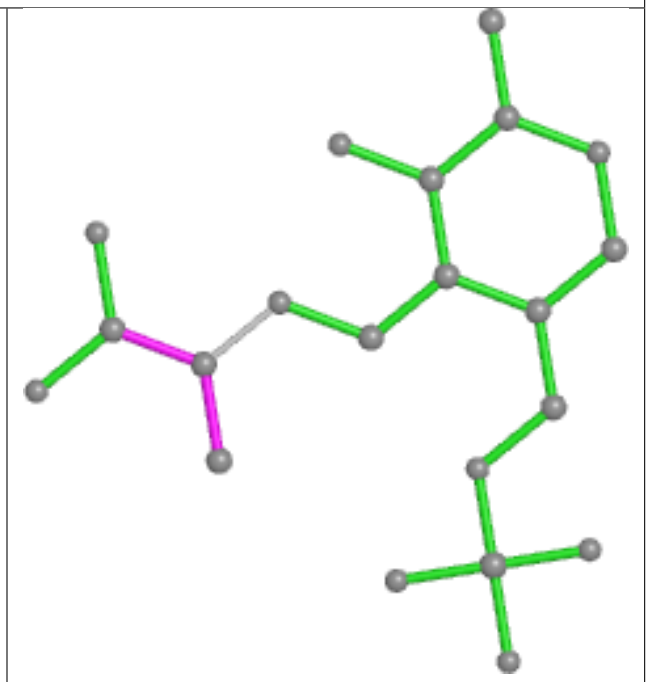


Rings

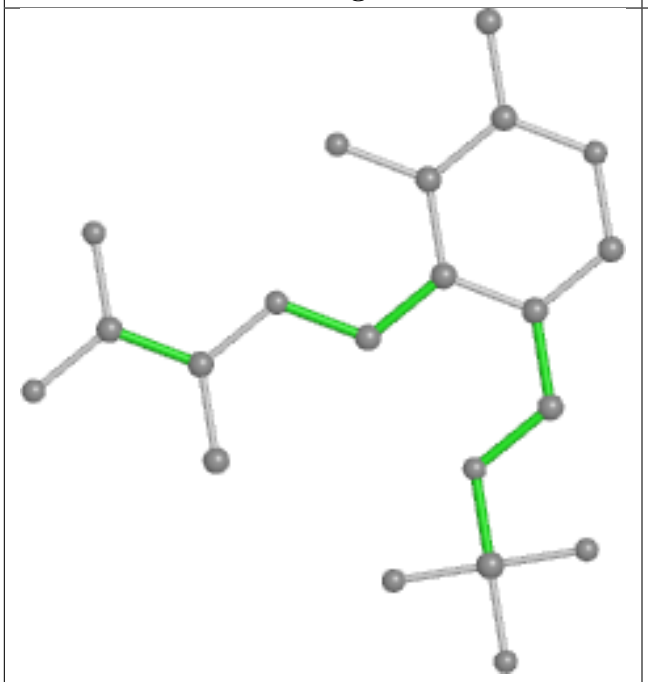
Ligand 0JO D 502



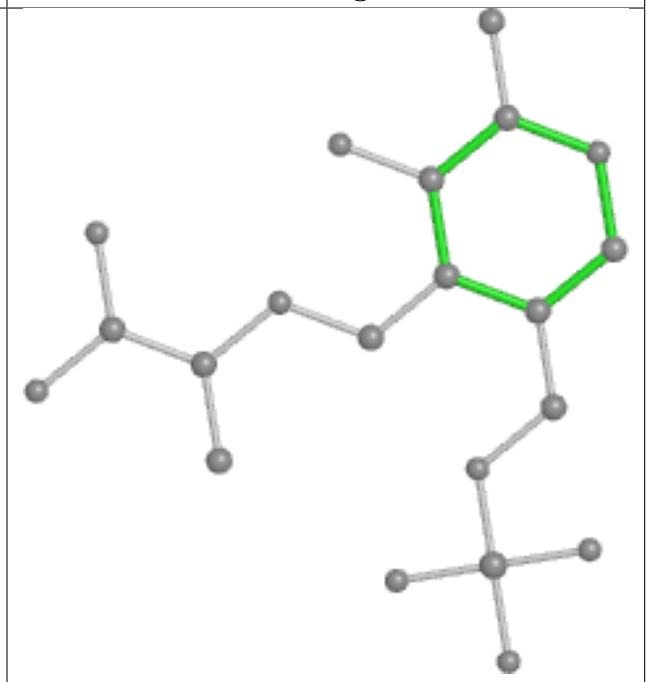
Bond lengths



Bond angles

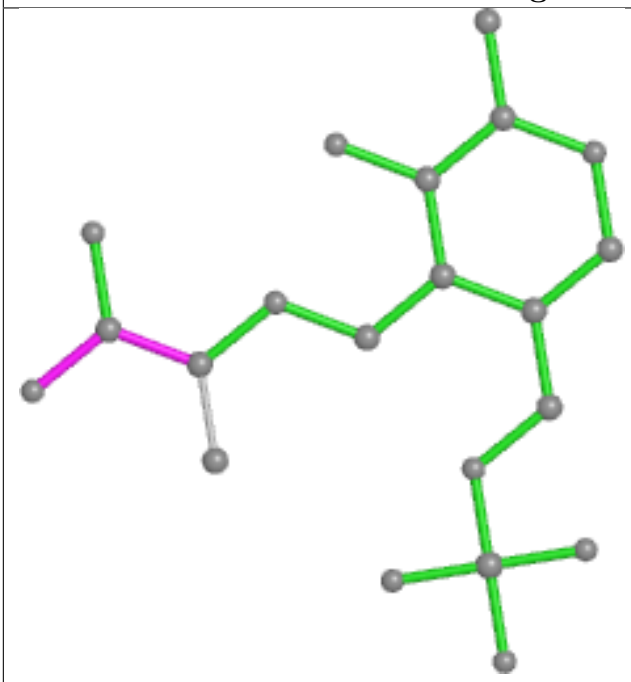


Torsions

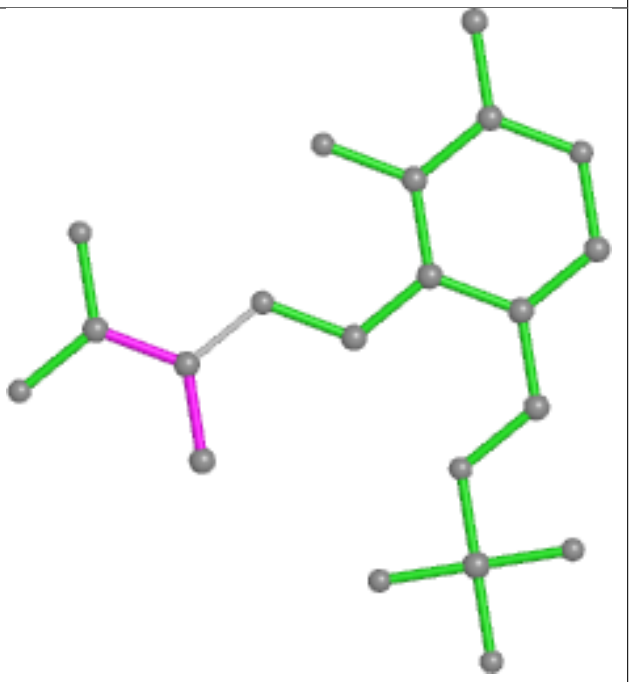


Rings

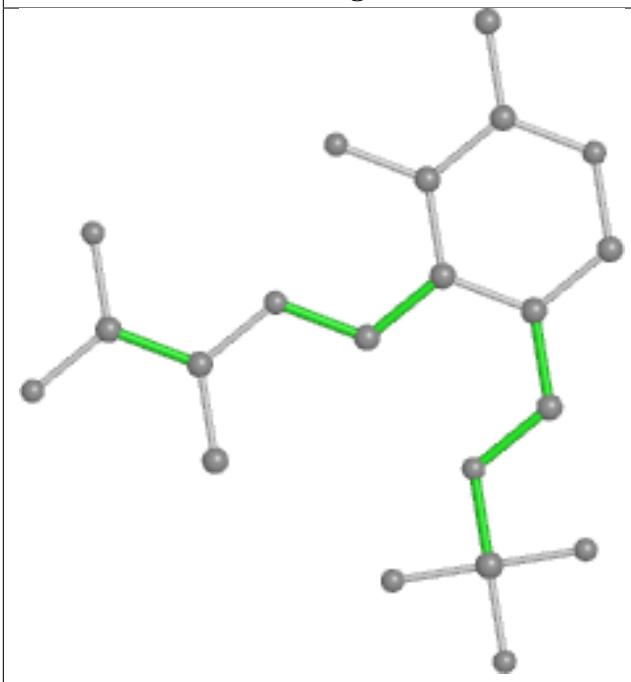
Ligand 0JO C 503



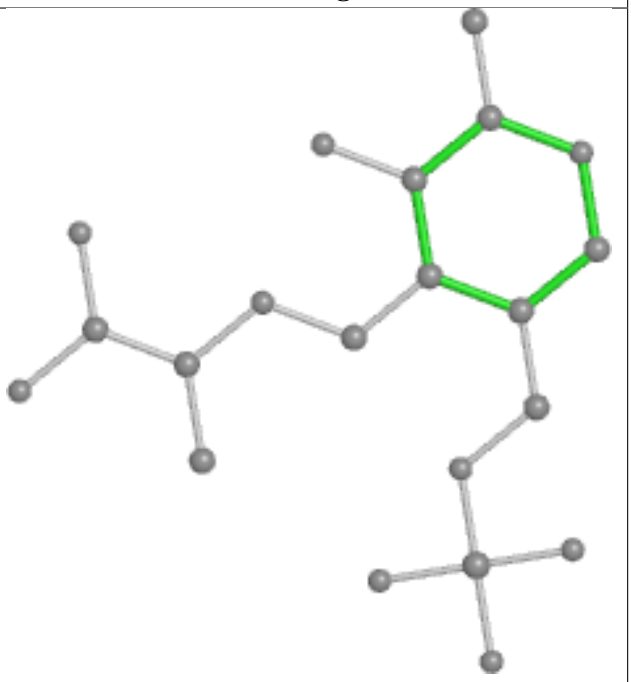
Bond lengths



Bond angles

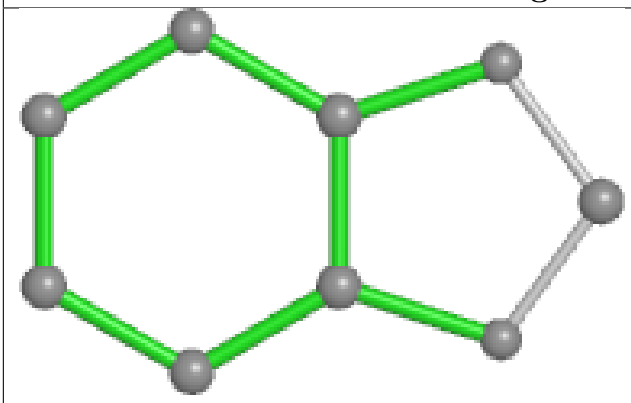


Torsions

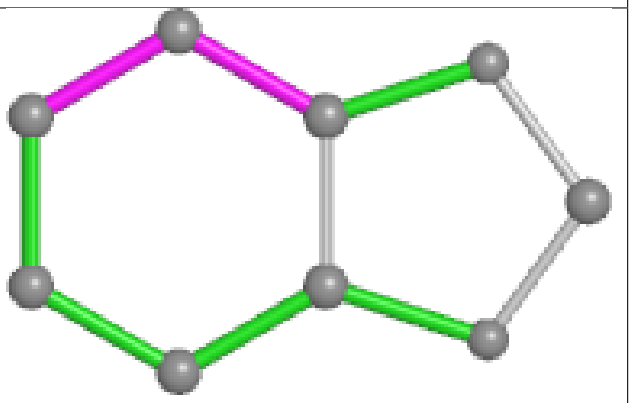


Rings

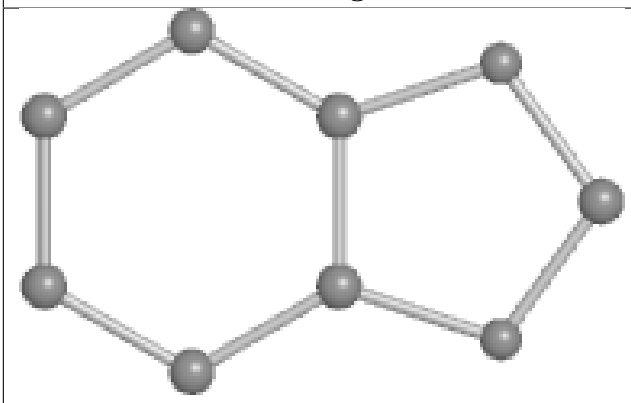
Ligand BZI A 505



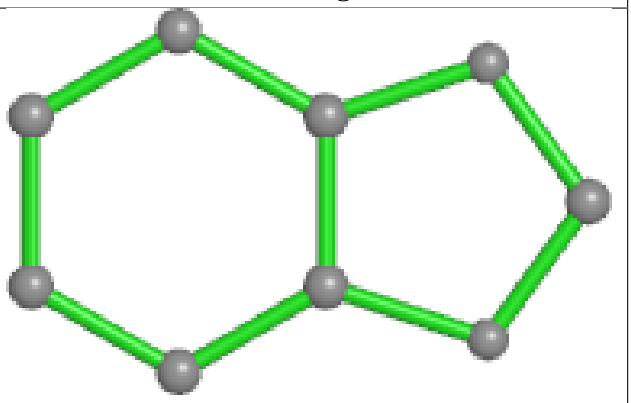
Bond lengths



Bond angles

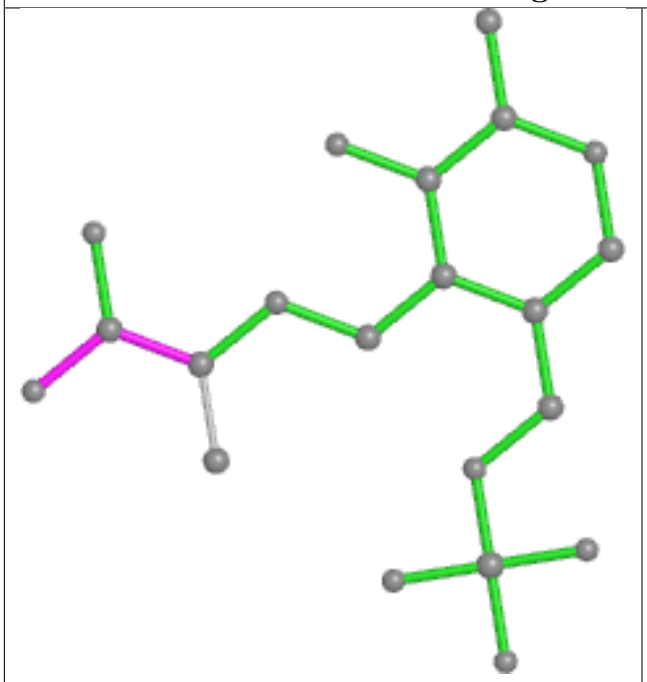


Torsions

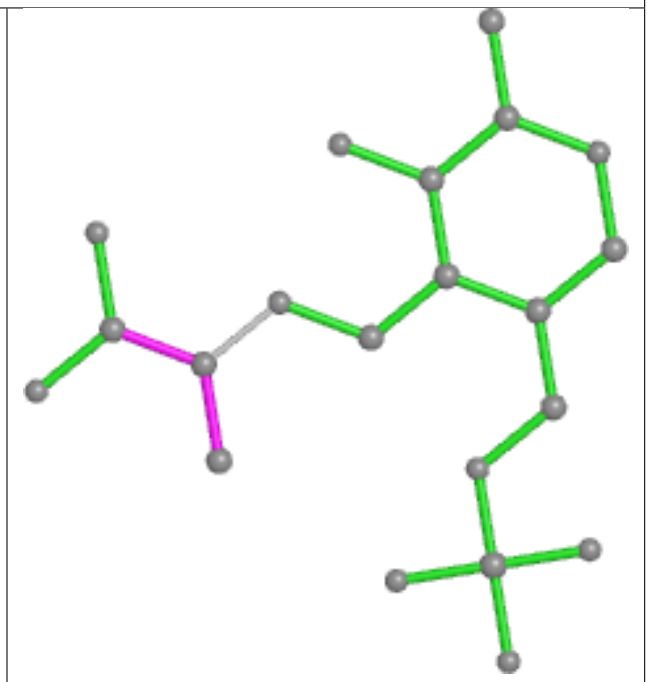


Rings

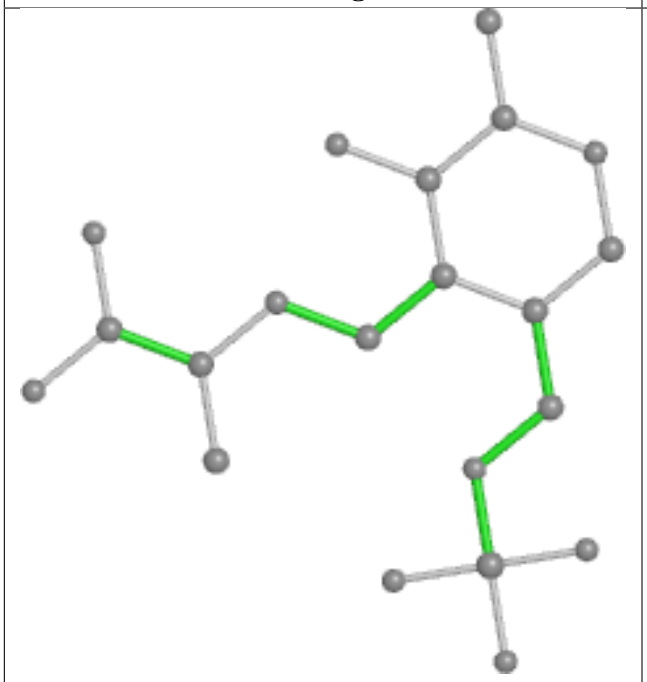
Ligand 0JO B 503



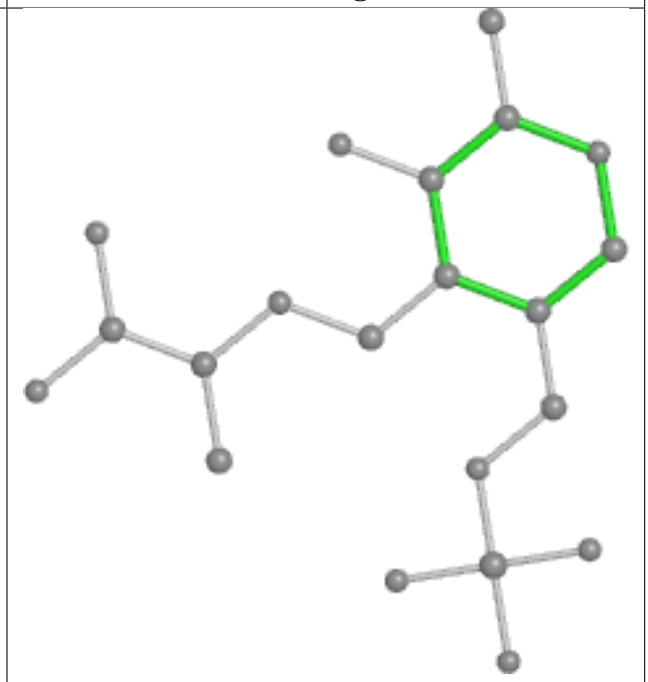
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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^{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(Å^2)	Q<0.9
1	A	459/467 (98%)	0.85	80 (17%) 1 1	15, 26, 65, 100	0
1	B	465/467 (99%)	0.04	11 (2%) 59 63	15, 25, 53, 76	0
1	C	465/467 (99%)	0.04	16 (3%) 45 50	16, 25, 60, 95	0
1	D	465/467 (99%)	0.98	79 (16%) 1 1	15, 23, 73, 122	0
All	All	1854/1868 (99%)	0.48	186 (10%) 7 7	15, 25, 65, 122	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	451[A]	TYR	14.3
1	D	396[A]	LEU	13.2
1	D	455[A]	VAL	12.3
1	A	407[A]	HIS	11.1
1	D	371[A]	PHE	10.8
1	D	456[A]	LEU	10.7
1	A	371[A]	PHE	10.6
1	D	407[A]	HIS	10.5
1	D	447[A]	LEU	10.1
1	A	405[A]	GLN	9.3
1	D	393[A]	SER	9.3
1	A	366[A]	ILE	9.3
1	D	402	THR	9.1
1	A	362[A]	LEU	9.1
1	D	408[A]	ALA	9.0
1	A	447[A]	LEU	8.7
1	A	466[A]	ILE	8.3
1	D	397[A]	GLY	8.2
1	A	441[A]	PHE	8.1
1	D	466[A]	ILE	8.1
1	D	445[A]	LYS	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	359[A]	CYS	8.0
1	D	449[A]	PHE	8.0
1	D	463[A]	LEU	8.0
1	A	412[A]	PHE	7.9
1	D	363[A]	VAL	7.6
1	A	456[A]	LEU	7.5
1	A	368[A]	GLY	7.4
1	C	455	VAL	7.4
1	D	394[A]	PHE	7.4
1	A	444[A]	LEU	7.3
1	A	442[A]	ALA	7.1
1	A	34[A]	TYR	7.1
1	D	444[A]	LEU	7.0
1	A	367[A]	PRO	6.9
1	A	408[A]	ALA	6.8
1	D	366[A]	ILE	6.8
1	D	454[A]	PRO	6.8
1	D	448[A]	GLU	6.7
1	A	360	LYS	6.7
1	A	443[A]	THR	6.6
1	A	369[A]	ASP	6.6
1	D	360[A]	LYS	6.6
1	D	441[A]	PHE	6.4
1	D	34[A]	TYR	6.2
1	A	361[A]	LYS	6.2
1	A	449[A]	PHE	6.2
1	D	369[A]	ASP	6.1
1	D	406[A]	LYS	6.0
1	A	364[A]	PRO	5.8
1	A	396[A]	LEU	5.8
1	D	464[A]	LYS	5.8
1	A	394[A]	PHE	5.8
1	A	464[A]	LYS	5.6
1	D	450[A]	GLU	5.5
1	A	455[A]	VAL	5.4
1	A	29[A]	LEU	5.4
1	A	463[A]	LEU	5.4
1	D	382[A]	LEU	5.4
1	A	381[A]	TYR	5.3
1	D	401	ALA	5.2
1	A	363[A]	VAL	5.2
1	D	395[A]	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	439[A]	GLU	5.0
1	A	406[A]	LYS	5.0
1	D	398[A]	ARG	4.8
1	B	410	MET	4.7
1	D	442[A]	ALA	4.7
1	D	359[A]	CYS	4.7
1	D	33[A]	GLY	4.7
1	A	410[A]	MET	4.6
1	D	364[A]	PRO	4.6
1	D	29[A]	LEU	4.6
1	A	372[A]	PRO	4.6
1	D	453[A]	PRO	4.6
1	D	362[A]	LEU	4.6
1	A	411[A]	GLU	4.5
1	A	451[A]	TYR	4.5
1	A	437[A]	LEU	4.5
1	D	460[A]	THR	4.5
1	D	32[A]	ALA	4.5
1	D	462[A]	ARG	4.4
1	D	409[A]	ASP	4.4
1	C	396	LEU	4.4
1	D	452[A]	GLU	4.4
1	D	30[A]	LYS	4.4
1	D	443[A]	THR	4.3
1	A	30[A]	LYS	4.3
1	A	370[A]	GLN	4.3
1	D	400	PRO	4.3
1	D	372[A]	PRO	4.2
1	A	395[A]	LEU	4.2
1	A	409[A]	ASP	4.2
1	B	451	TYR	4.1
1	C	451	TYR	4.0
1	D	38[A]	LEU	4.0
1	A	448[A]	GLU	4.0
1	C	402	THR	4.0
1	A	382[A]	LEU	3.9
1	C	404	GLU	3.9
1	A	36[A]	PRO	3.8
1	D	412[A]	PHE	3.8
1	A	465[A]	PRO	3.7
1	A	393[A]	SER	3.7
1	A	445[A]	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	404	GLU	3.7
1	D	458[A]	HIS	3.6
1	A	460[A]	THR	3.6
1	D	410[A]	MET	3.6
1	C	400	PRO	3.5
1	D	117	LYS	3.5
1	D	403	GLY	3.5
1	C	456	LEU	3.5
1	D	399	ASP	3.5
1	D	26[A]	GLU	3.4
1	D	367[A]	PRO	3.4
1	A	22[A]	ARG	3.4
1	A	390[A]	GLU	3.3
1	A	438[A]	LYS	3.2
1	A	28[A]	ALA	3.2
1	D	461[A]	ALA	3.2
1	A	446[A]	GLY	3.2
1	A	458[A]	HIS	3.2
1	A	373[A]	ALA	3.2
1	C	453	PRO	3.2
1	D	411[A]	GLU	3.1
1	A	358[A]	ASP	3.1
1	D	361[A]	LYS	3.1
1	D	39[A]	LEU	3.1
1	A	391[A]	ILE	3.1
1	D	370[A]	GLN	3.0
1	A	397[A]	GLY	3.0
1	C	401	ALA	3.0
1	A	454[A]	PRO	3.0
1	A	118	GLU	2.9
1	A	398[A]	ARG	2.9
1	D	28[A]	ALA	2.9
1	B	443	THR	2.9
1	D	391[A]	ILE	2.9
1	D	392[A]	GLY	2.8
1	C	364	PRO	2.8
1	A	155	PHE	2.8
1	C	403	GLY	2.8
1	A	453[A]	PRO	2.8
1	B	364	PRO	2.8
1	D	405[A]	GLN	2.8
1	A	461[A]	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	438[A]	LYS	2.7
1	B	366	ILE	2.6
1	A	39[A]	LEU	2.6
1	D	457[A]	ARG	2.6
1	A	379[A]	ALA	2.6
1	D	381[A]	TYR	2.6
1	D	465[A]	PRO	2.6
1	A	392[A]	GLY	2.5
1	D	376[A]	VAL	2.5
1	C	454	PRO	2.5
1	A	450[A]	GLU	2.5
1	C	399	ASP	2.5
1	D	23[A]	GLU	2.4
1	A	27[A]	ALA	2.3
1	A	457[A]	ARG	2.3
1	A	33[A]	GLY	2.3
1	A	21[A]	SER	2.3
1	D	373[A]	ALA	2.3
1	A	26[A]	GLU	2.3
1	D	459[A]	PHE	2.3
1	A	38[A]	LEU	2.3
1	C	409	ASP	2.3
1	A	20[A]	PRO	2.2
1	A	37[A]	PHE	2.2
1	A	376[A]	VAL	2.2
1	D	437[A]	LEU	2.2
1	A	383[A]	GLU	2.2
1	B	466	ILE	2.2
1	B	445	LYS	2.1
1	D	368[A]	GLY	2.1
1	C	407	HIS	2.1
1	D	27[A]	ALA	2.1
1	D	375[A]	ALA	2.1
1	A	18[A]	ARG	2.1
1	B	365	GLN	2.0
1	B	119	GLY	2.0
1	C	117[A]	LYS	2.0
1	B	117	LYS	2.0
1	B	113	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

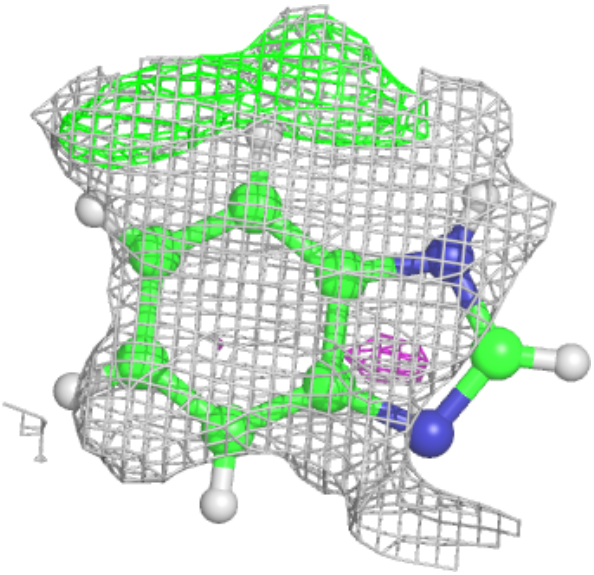
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

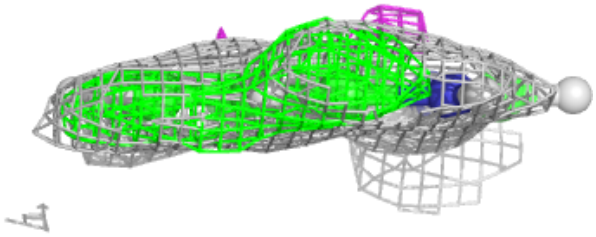
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BZI	A	505	9/9	0.45	0.26	67,83,99,103	0
4	DMS	A	503	4/4	0.61	0.19	51,65,66,104	0
3	BZI	B	502	9/9	0.71	0.12	35,44,54,63	0
3	BZI	D	501[B]	9/9	0.80	0.19	26,35,43,44	15
3	BZI	D	501[A]	9/9	0.80	0.19	27,33,41,44	15
3	BZI	A	502[B]	9/9	0.84	0.23	32,37,44,47	15
3	BZI	A	502[A]	9/9	0.84	0.23	29,34,40,41	15
3	BZI	C	502[B]	9/9	0.87	0.14	27,34,41,41	15
3	BZI	C	502[A]	9/9	0.87	0.14	28,33,41,42	15
5	0JO	B	503	21/21	0.95	0.11	15,24,32,37	0
6	CL	B	501	1/1	0.95	0.10	56,56,56,56	0
5	0JO	C	503	21/21	0.97	0.09	15,21,28,30	0
5	0JO	D	502	21/21	0.97	0.10	14,20,26,36	0
5	0JO	A	504	21/21	0.97	0.08	16,22,34,40	0
2	K	C	501	1/1	1.00	0.09	20,20,20,20	0
2	K	C	504	1/1	1.00	0.09	19,19,19,19	0
2	K	A	501	1/1	1.00	0.09	21,21,21,21	0
2	K	A	506	1/1	1.00	0.10	19,19,19,19	0

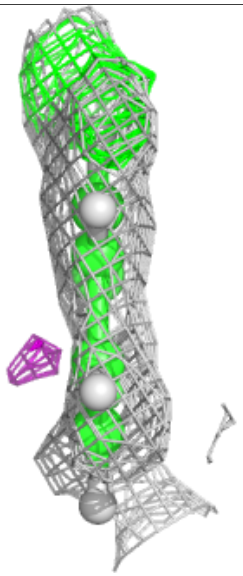
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BZI A 505:

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

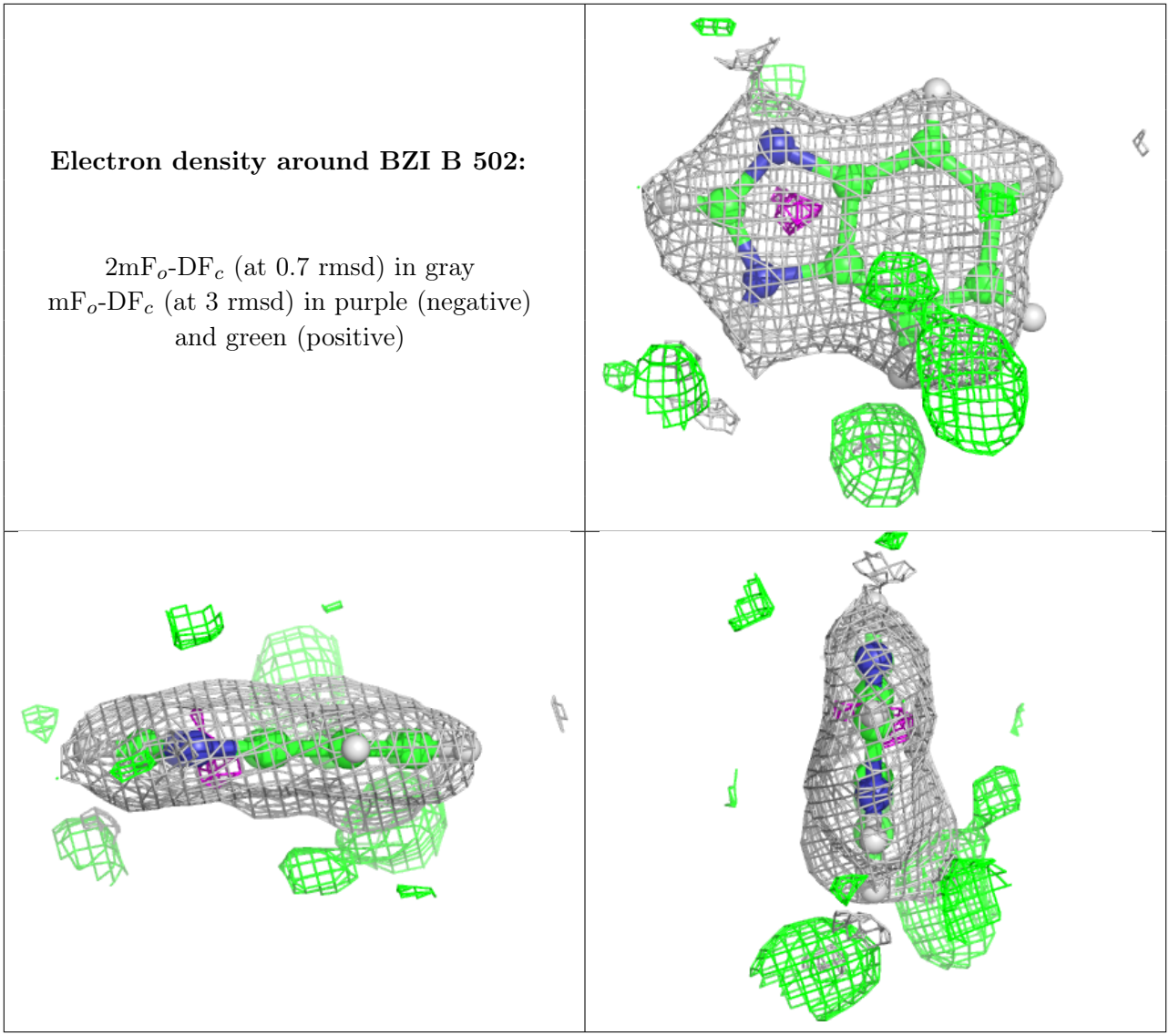






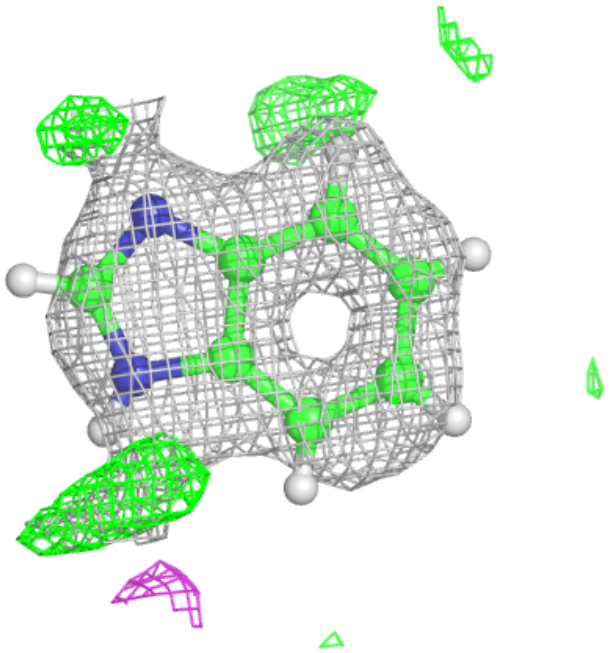
Electron density around BZI B 502:

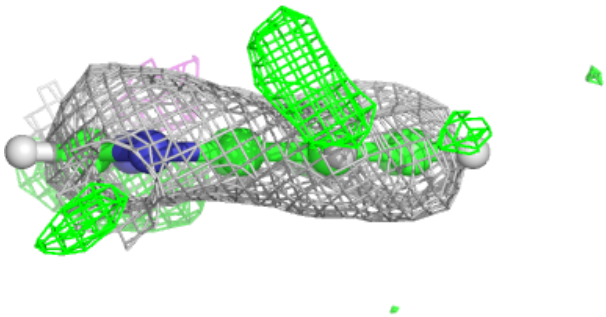
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

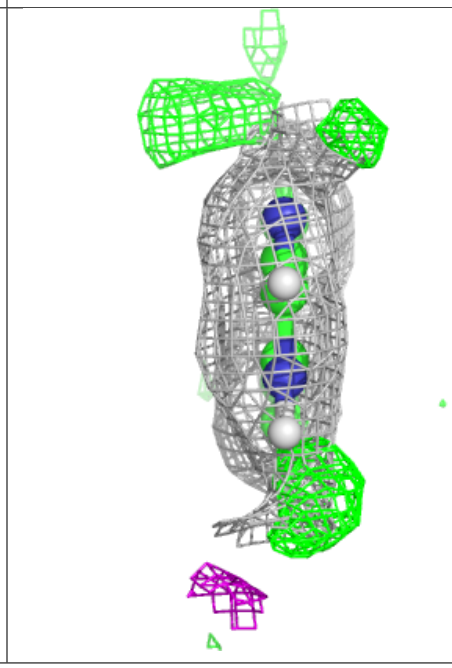


Electron density around BZI D 501 (B):

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

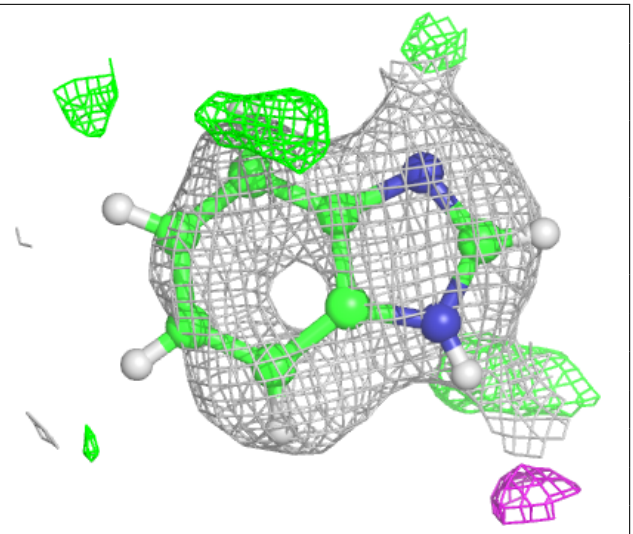


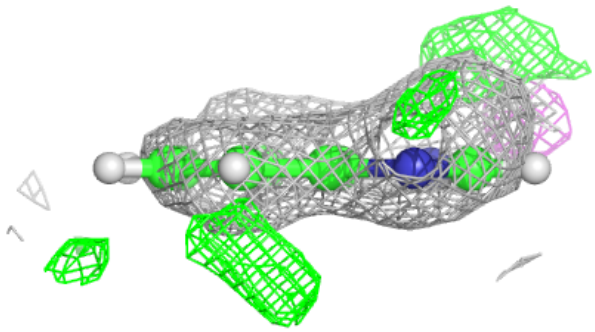


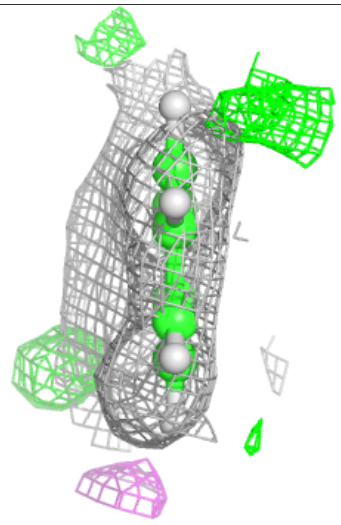


Electron density around BZI D 501 (A):

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

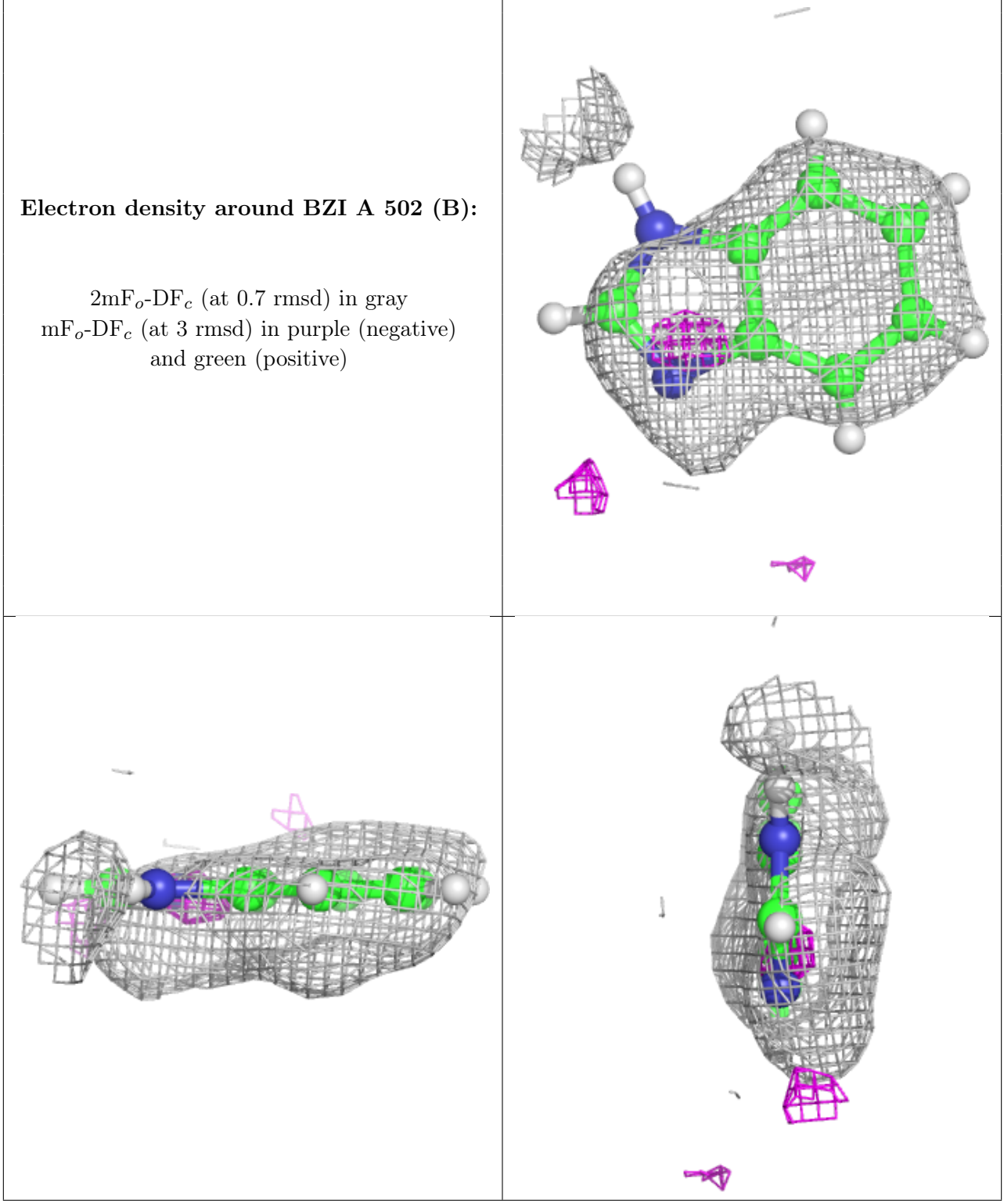






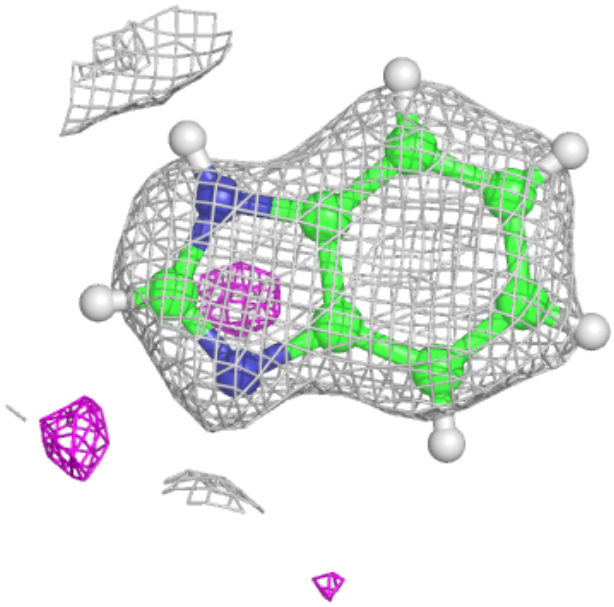
Electron density around BZI A 502 (B):

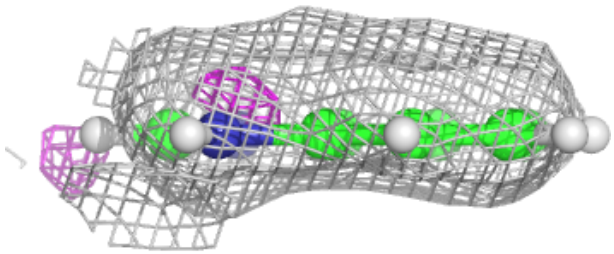
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

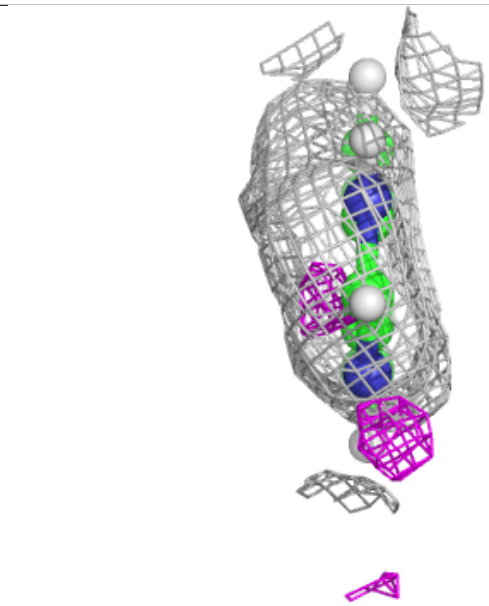


Electron density around BZI A 502 (A):

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

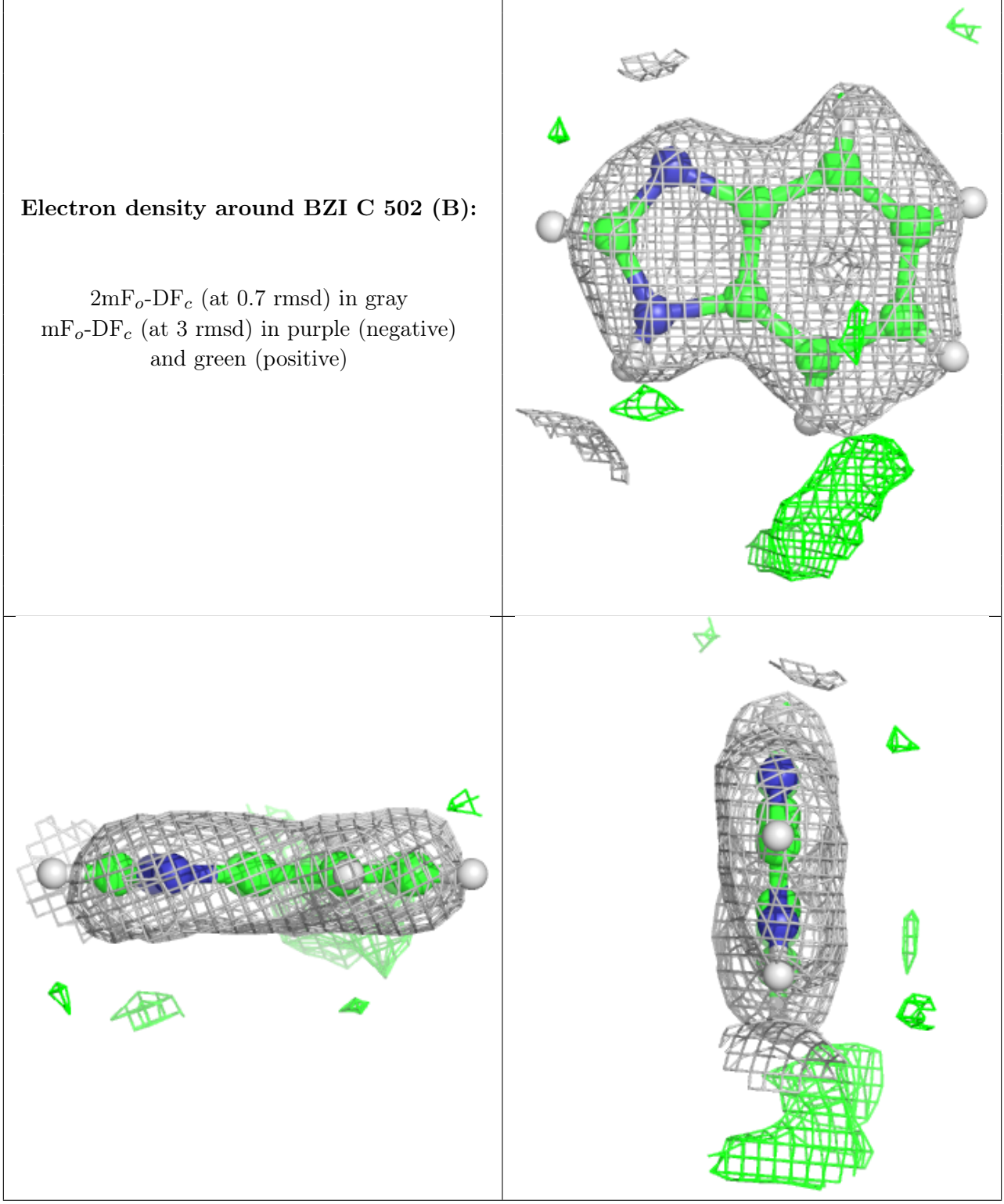






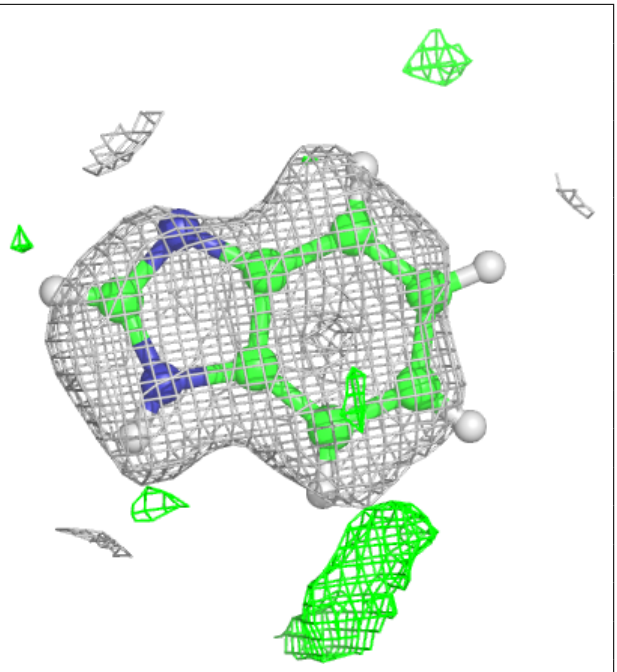
Electron density around BZI C 502 (B):

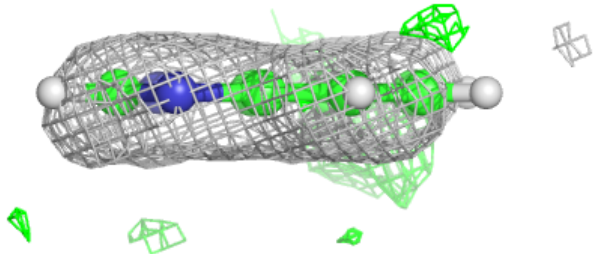
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

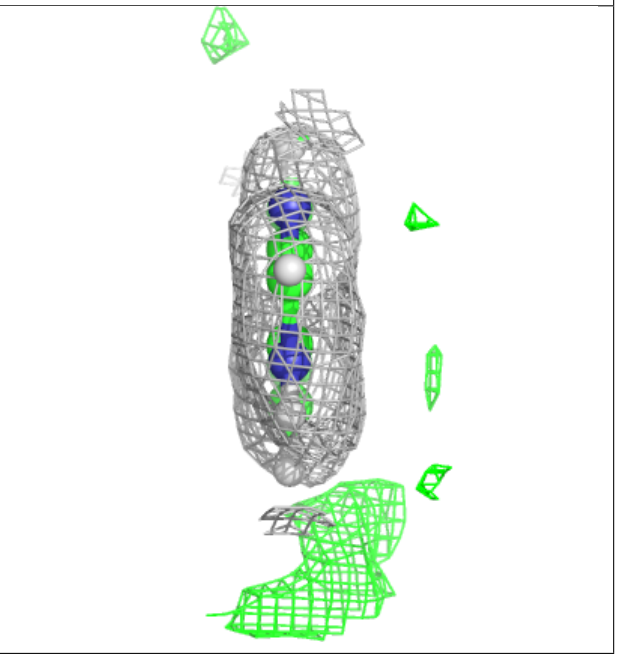


Electron density around BZI C 502 (A):

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

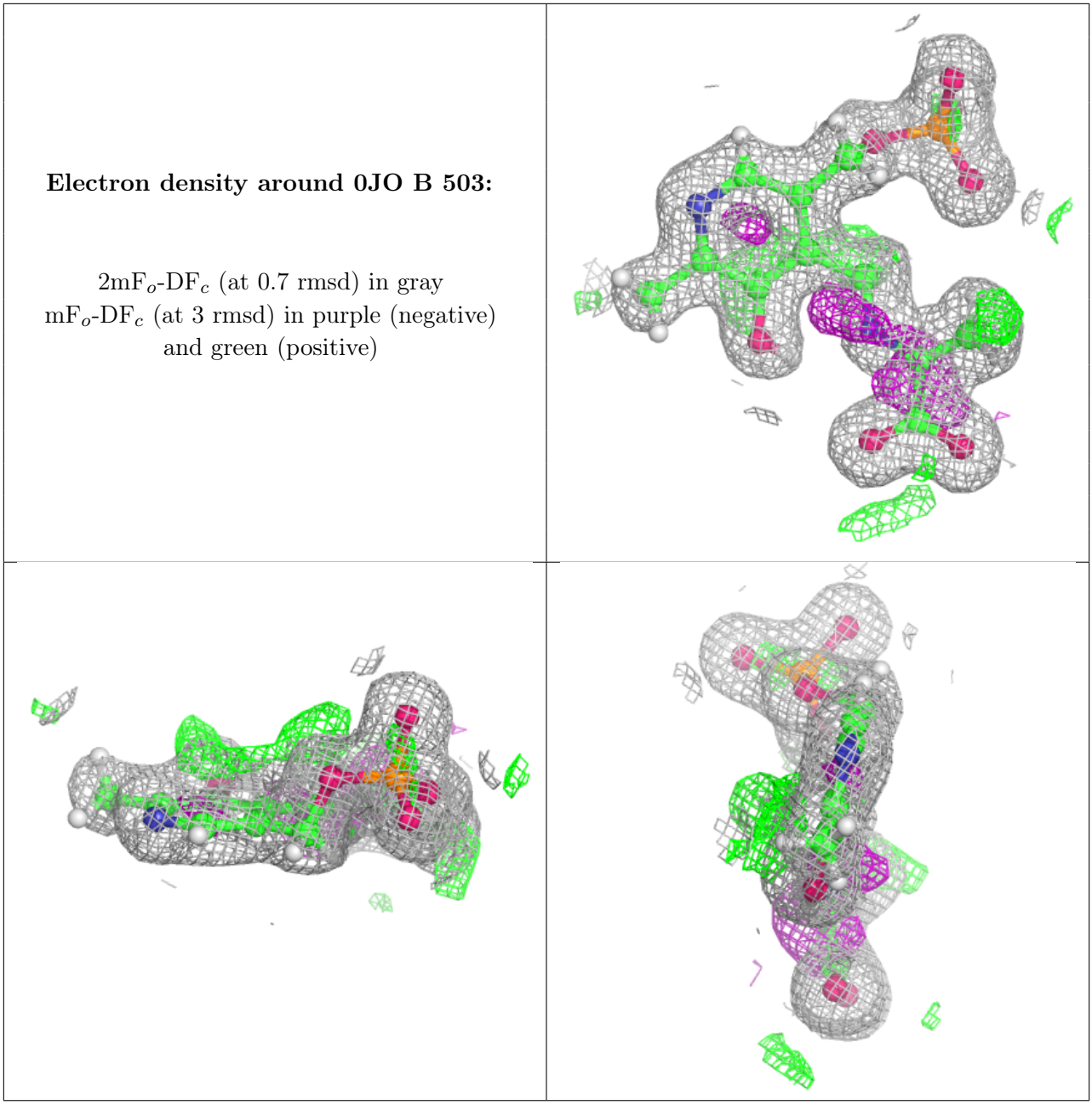






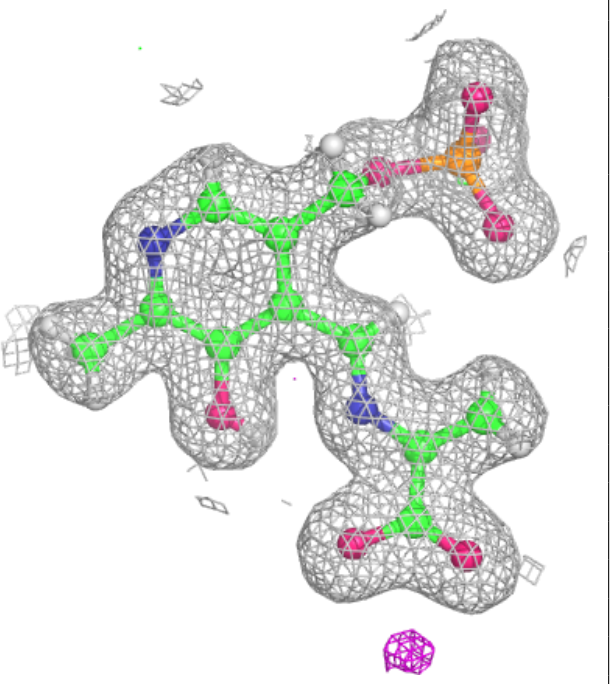
Electron density around 0JO B 503:

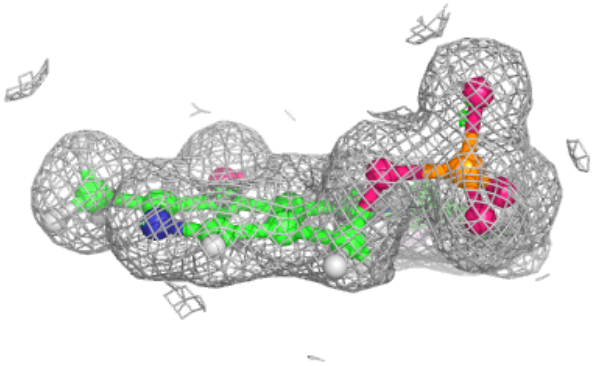
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

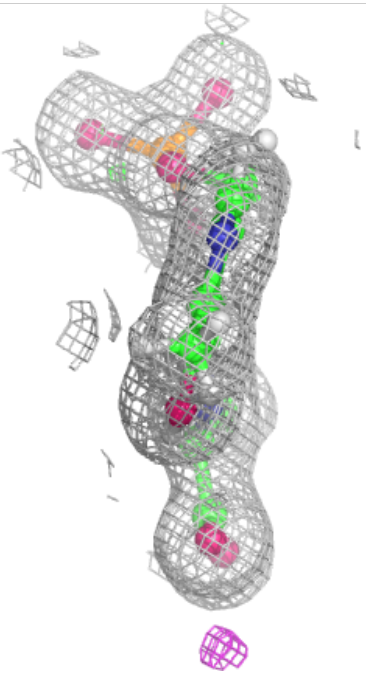


Electron density around 0JO C 503:

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

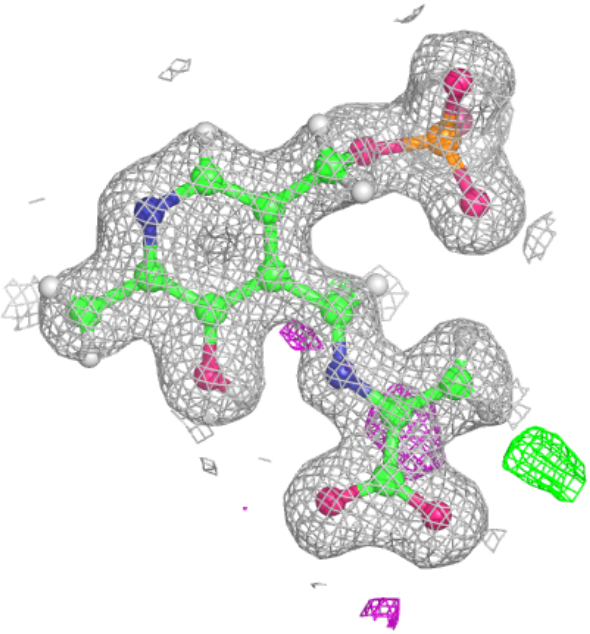


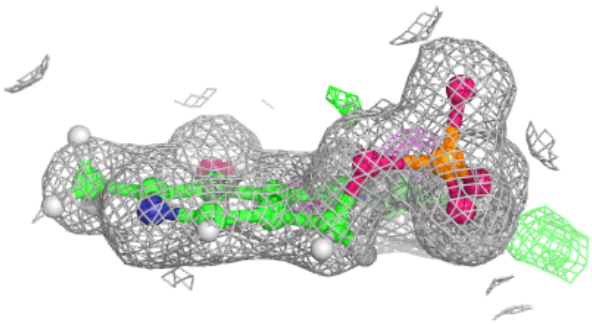


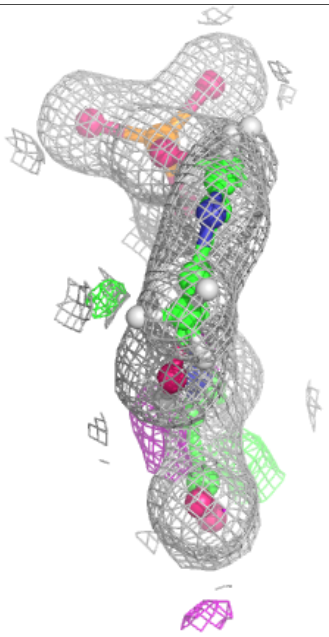


Electron density around 0JO D 502:

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

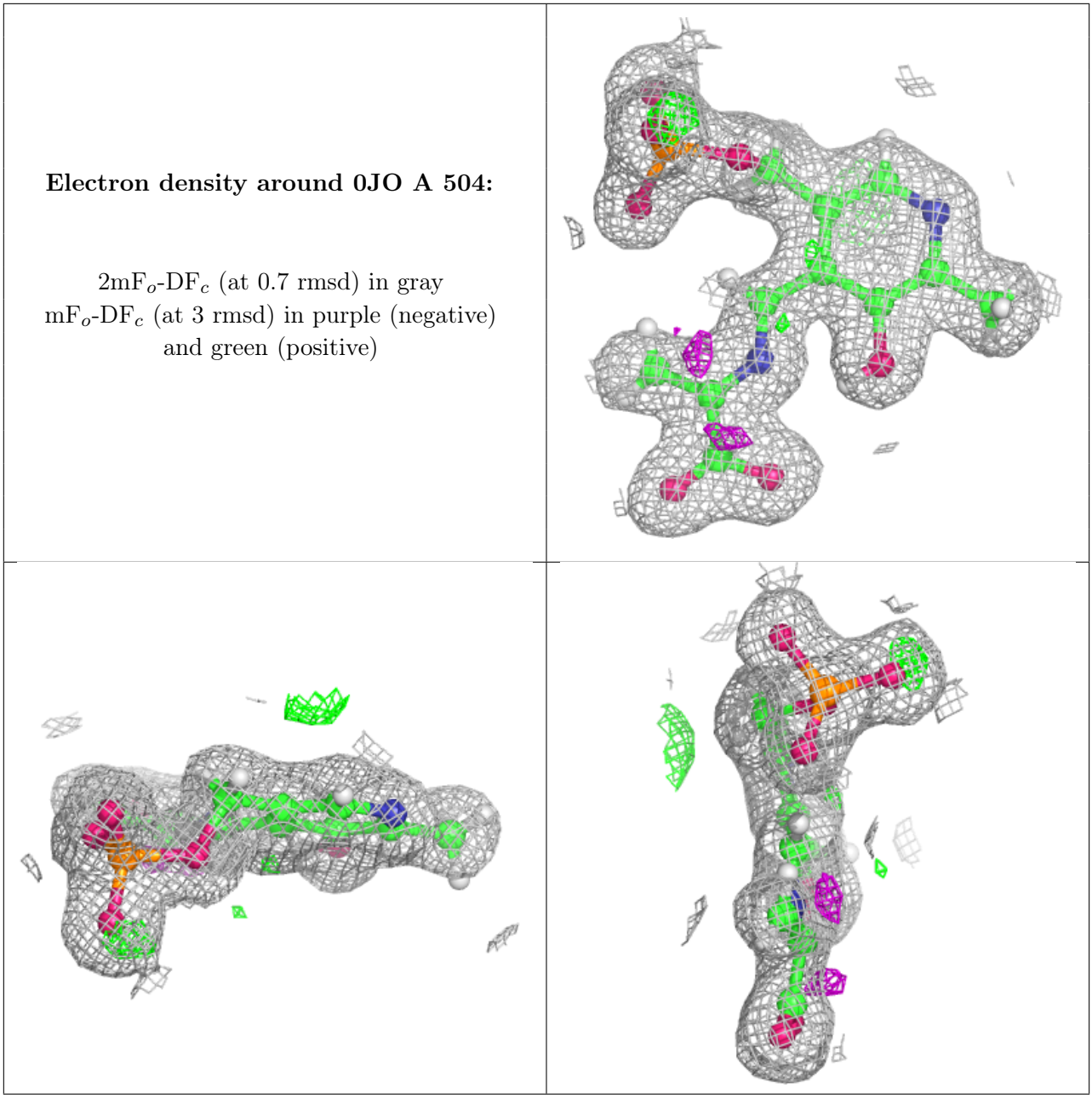






Electron density around 0JO A 504:

$2mF_o$-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.