



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2020 – 10:14 AM JST

PDB ID : 6LD8  
Title : Crystal structure of cystathionine gamma synthase from *Xanthomonas oryzae* pv. *oryzae* in complex with aminoacrylate and cysteine  
Authors : Ngo, H.P.T.; Nguyen, T.D.Q.; Kang, L.W.  
Deposited on : 2019-11-20  
Resolution : 2.31 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 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 : 2.14.6  
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) : 2.14.6

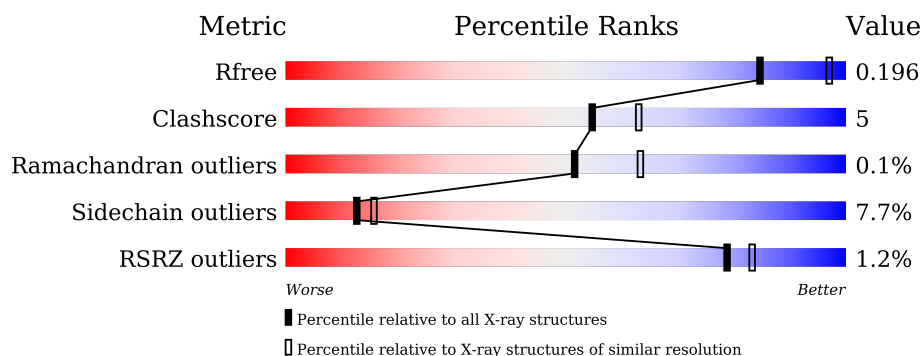
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	408	
1	B	408	
1	C	408	
1	D	408	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12208 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.

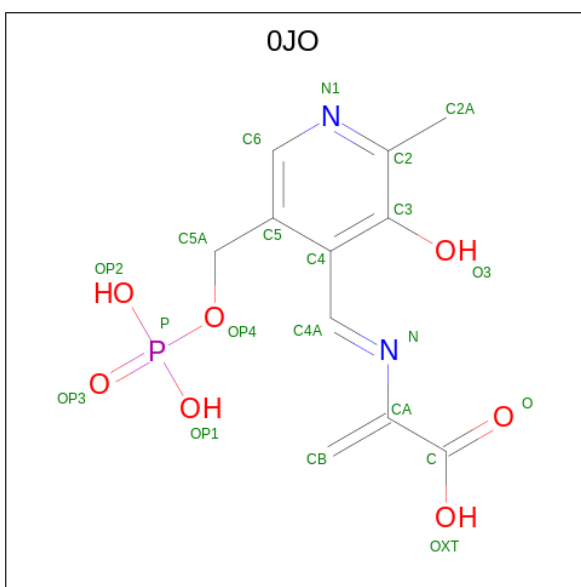
- Molecule 1 is a protein called Cystathionine gamma-synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	1	0
			2883	1823	508	545	7			
1	B	387	Total	C	N	O	S	0	0	0
			2870	1814	506	543	7			
1	C	387	Total	C	N	O	S	0	0	0
			2870	1814	506	543	7			
1	D	387	Total	C	N	O	S	0	1	0
			2876	1819	507	543	7			

There are 16 discrepancies between the modelled and reference sequences:

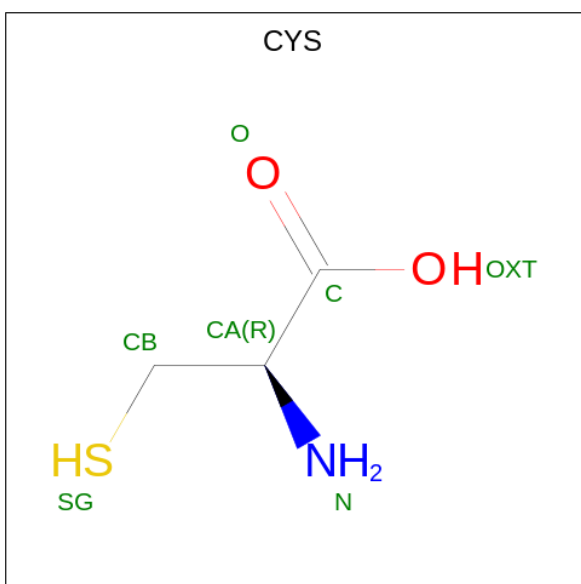
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q5H1U9
A	-1	SER	-	expression tag	UNP Q5H1U9
A	0	HIS	-	expression tag	UNP Q5H1U9
A	134	VAL	ASP	engineered mutation	UNP Q5H1U9
B	-2	GLY	-	expression tag	UNP Q5H1U9
B	-1	SER	-	expression tag	UNP Q5H1U9
B	0	HIS	-	expression tag	UNP Q5H1U9
B	134	VAL	ASP	engineered mutation	UNP Q5H1U9
C	-2	GLY	-	expression tag	UNP Q5H1U9
C	-1	SER	-	expression tag	UNP Q5H1U9
C	0	HIS	-	expression tag	UNP Q5H1U9
C	134	VAL	ASP	engineered mutation	UNP Q5H1U9
D	-2	GLY	-	expression tag	UNP Q5H1U9
D	-1	SER	-	expression tag	UNP Q5H1U9
D	0	HIS	-	expression tag	UNP Q5H1U9
D	134	VAL	ASP	engineered mutation	UNP Q5H1U9

- Molecule 2 is 2-[[[(E)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene]amino}prop-2-enoic acid (three-letter code: OJO) (formula: C<sub>11</sub>H<sub>13</sub>N<sub>2</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 3 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	D	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

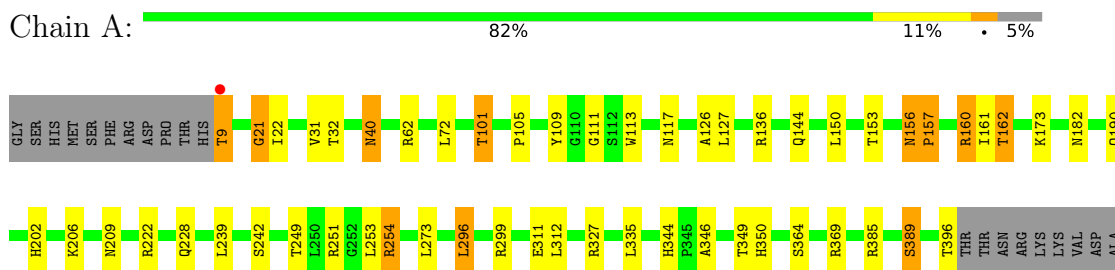
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total	O	0	0
			147	147		
4	B	149	Total	O	0	0
			149	149		
4	C	149	Total	O	0	0
			149	149		
4	D	152	Total	O	0	0
			152	152		

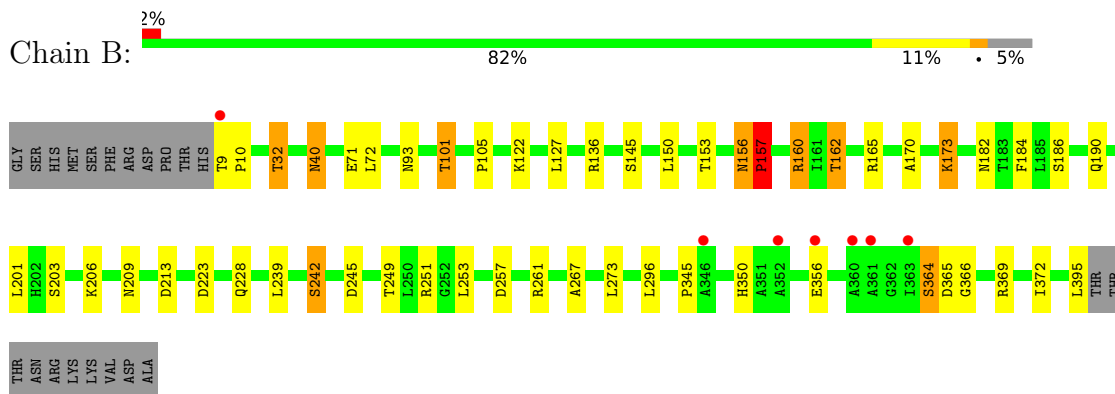
### 3 Residue-property plots [i](#)

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.

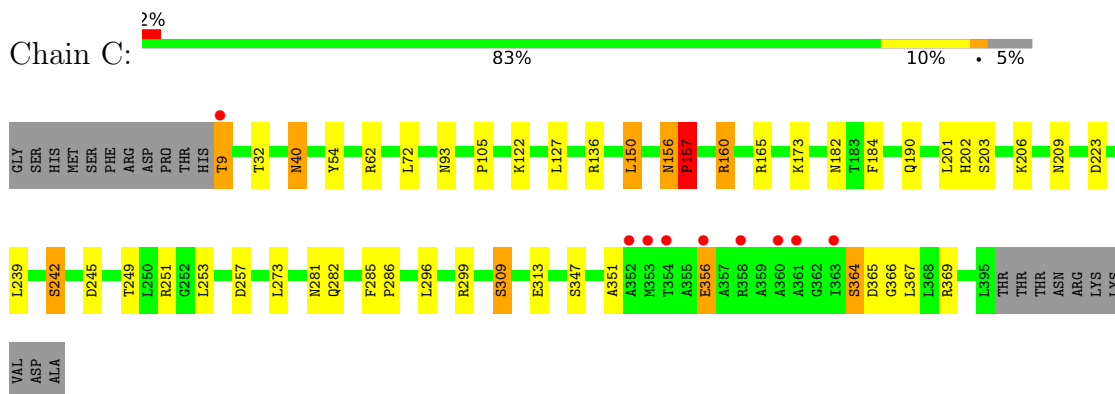
- Molecule 1: Cystathionine gamma-synthase



- Molecule 1: Cystathionine gamma-synthase



- Molecule 1: Cystathionine gamma-synthase



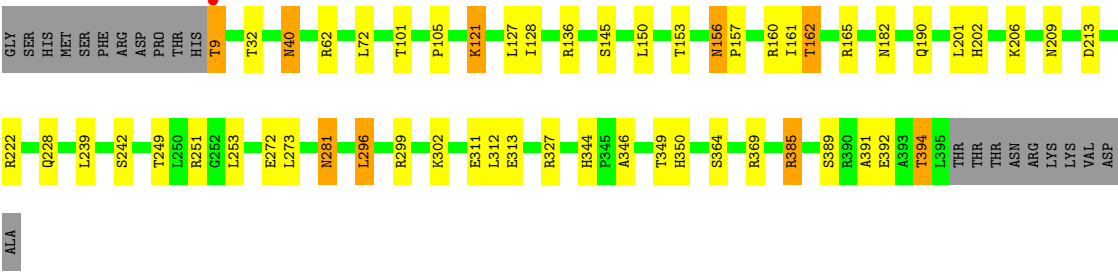
- Molecule 1: Cystathionine gamma-synthase

Chain D: 

81%

11%

5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.99Å 161.99Å 245.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.61 – 2.31 40.61 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.61-2.31) 99.9 (40.61-2.31)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.15 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.166 , 0.195 0.171 , 0.196	Depositor DCC
$R_{free}$ test set	6941 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 12.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: 0JO

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	0.84	0/2940	1.03	9/4001 (0.2%)
1	B	0.82	3/2924 (0.1%)	1.00	6/3980 (0.2%)
1	C	0.84	3/2924 (0.1%)	1.00	5/3980 (0.1%)
1	D	0.84	0/2933	1.02	7/3991 (0.2%)
All	All	0.83	6/11721 (0.1%)	1.01	27/15952 (0.2%)

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	A	0	3
1	C	0	3
1	D	0	2
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	366	GLY	C-O	7.62	1.35	1.23
1	C	257	ASP	CG-OD2	6.84	1.41	1.25
1	B	366	GLY	C-O	6.35	1.33	1.23
1	B	203	SER	CA-CB	-6.01	1.44	1.52
1	C	203	SER	CA-CB	-5.39	1.44	1.52
1	B	257	ASP	CG-OD2	5.24	1.37	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	ARG	NE-CZ-NH2	-11.03	114.79	120.30
1	A	160	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	D	160	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	D	62	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	B	32	THR	CA-CB-OG1	-7.79	92.64	109.00
1	A	62	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	160	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	157	PRO	N-CA-CB	-6.93	94.97	102.60
1	C	32	THR	CA-CB-OG1	-6.56	95.22	109.00
1	D	62	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	D	385	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	385	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	160	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	62	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	389	SER	N-CA-CB	5.99	119.48	110.50
1	C	157	PRO	N-CA-CB	-5.79	96.23	102.60
1	D	160	ARG	CG-CD-NE	-5.77	99.68	111.80
1	D	385	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	C	160	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	385	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	261	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	254	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	62	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	395	LEU	CA-C-O	5.31	131.25	120.10
1	B	160	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	157	PRO	N-CA-CB	-5.17	96.92	102.60
1	C	299	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	HIS	Peptide
1	A	21	GLY	Peptide
1	A	9	THR	Peptide
1	C	202	HIS	Peptide
1	C	356	GLU	Peptide
1	C	9	THR	Peptide
1	D	202	HIS	Peptide
1	D	9	THR	Peptide

## 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	2883	0	2893	31	0
1	B	2870	0	2873	35	0
1	C	2870	0	2873	32	0
1	D	2876	0	2886	37	0
2	A	21	0	9	3	0
2	B	21	0	9	4	0
2	C	21	0	9	3	0
2	D	21	0	9	3	0
3	A	7	0	4	0	0
3	B	7	0	4	0	0
3	C	7	0	4	0	0
3	D	7	0	4	0	0
4	A	147	0	0	7	0
4	B	149	0	0	5	0
4	C	149	0	0	1	0
4	D	152	0	0	9	0
All	All	12208	0	11577	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (120) 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:B:101:THR:HG22	4:B:627:HOH:O	1.80	0.81
1:C:206:LYS:NZ	2:C:501:OJO:C4A	2.44	0.80
1:D:228:GLN:HG2	4:D:749:HOH:O	1.83	0.77
1:A:21:GLY:H	1:A:254:ARG:HH12	1.34	0.74
1:B:251:ARG:HH22	1:D:209:ASN:HD21	1.36	0.74
1:B:206:LYS:NZ	2:B:501:OJO:C4A	2.50	0.74
1:B:209:ASN:HD21	1:D:251:ARG:HH22	1.36	0.74
1:C:206:LYS:HZ3	2:C:501:OJO:C4A	2.01	0.72
1:B:122:LYS:NZ	1:C:93:ASN:O	2.23	0.70
1:D:281:ASN:OD1	1:D:313:GLU:OE1	2.09	0.70
1:D:228:GLN:CG	4:D:749:HOH:O	2.39	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:HD21	1:C:251:ARG:HH22	1.38	0.69
1:A:209:ASN:HD22	1:A:249:THR:HA	1.58	0.68
1:A:251:ARG:HH22	1:C:209:ASN:HD21	1.42	0.68
1:B:156:ASN:HD21	1:B:369:ARG:HH11	1.43	0.66
1:B:40:ASN:H	1:B:40:ASN:HD22	1.44	0.66
1:A:101:THR:HG22	4:A:620:HOH:O	1.97	0.65
1:B:101:THR:CG2	4:B:627:HOH:O	2.42	0.64
1:A:113:TRP:CZ2	1:A:117:ASN:ND2	2.66	0.63
1:D:161:ILE:HG22	1:D:296:LEU:HD13	1.79	0.63
1:A:344:HIS:CE1	1:A:346:ALA:HB3	2.33	0.63
1:B:209:ASN:HD21	1:D:251:ARG:NH2	1.95	0.63
1:B:206:LYS:HZ3	2:B:501:OJO:C4A	2.11	0.62
1:D:209:ASN:HD22	1:D:249:THR:HA	1.65	0.62
1:B:206:LYS:HZ1	2:B:501:OJO:C4A	2.11	0.61
1:B:201:LEU:HD12	1:B:201:LEU:C	2.21	0.61
1:C:40:ASN:HD22	1:C:40:ASN:H	1.47	0.61
1:C:206:LYS:HZ1	2:C:501:OJO:C4A	2.13	0.60
1:D:391:ALA:O	1:D:394:THR:HB	2.02	0.60
1:A:311:GLU:HG2	4:A:650:HOH:O	2.01	0.60
1:C:156:ASN:HD21	1:C:369:ARG:HH11	1.50	0.59
1:A:156:ASN:HD21	1:A:369:ARG:HH11	1.50	0.59
1:B:9:THR:HG22	1:B:10:PRO:O	2.02	0.59
1:A:40:ASN:HD22	1:A:40:ASN:H	1.51	0.59
1:B:93:ASN:O	1:C:122:LYS:NZ	2.31	0.58
1:D:40:ASN:H	1:D:40:ASN:HD22	1.51	0.58
1:D:101:THR:HG21	1:D:128:ILE:HD12	1.86	0.57
1:A:105:PRO:HD3	1:A:150:LEU:O	2.04	0.57
1:B:251:ARG:NH2	1:D:209:ASN:HD21	2.02	0.57
1:D:311:GLU:HG2	4:D:657:HOH:O	2.03	0.57
1:D:153:THR:HB	1:D:162:THR:HG23	1.86	0.56
1:A:113:TRP:CE2	1:A:117:ASN:ND2	2.73	0.56
1:B:40:ASN:N	1:B:40:ASN:HD22	2.03	0.56
1:A:162:THR:CG2	4:A:666:HOH:O	2.53	0.55
1:A:251:ARG:NH2	1:C:209:ASN:HD21	2.03	0.55
1:D:344:HIS:CE1	1:D:346:ALA:HB3	2.41	0.55
1:C:209:ASN:HD22	1:C:249:THR:HA	1.72	0.54
1:D:206[A]:LYS:HZ3	2:D:501:OJO:C4A	2.21	0.54
1:B:105:PRO:HD3	1:B:150:LEU:O	2.08	0.54
1:C:157:PRO:O	1:C:309:SER:OG	2.26	0.54
1:A:206[A]:LYS:HZ3	2:A:501:OJO:C4A	2.20	0.54
1:D:156:ASN:HD21	1:D:369:ARG:HH11	1.56	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ASN:N	1:C:40:ASN:HD22	2.04	0.53
1:B:162:THR:CG2	4:B:690:HOH:O	2.57	0.53
1:C:105:PRO:HD3	1:C:150:LEU:O	2.09	0.52
1:A:162:THR:HG21	4:A:720:HOH:O	2.08	0.52
1:D:162:THR:HG21	4:D:724:HOH:O	2.08	0.52
1:B:170:ALA:HA	1:B:173:LYS:HD3	1.92	0.52
1:B:32:THR:HG21	1:D:213:ASP:HB3	1.92	0.52
1:A:209:ASN:HD21	1:C:251:ARG:NH2	2.06	0.50
1:B:162:THR:HG21	4:B:716:HOH:O	2.13	0.49
1:D:40:ASN:N	1:D:40:ASN:HD22	2.09	0.49
1:D:392:GLU:C	1:D:394:THR:H	2.16	0.49
1:B:162:THR:HG22	4:B:690:HOH:O	2.11	0.49
1:C:201:LEU:C	1:C:201:LEU:HD12	2.34	0.48
1:A:162:THR:HG22	4:A:666:HOH:O	2.11	0.48
1:B:209:ASN:HD22	1:B:249:THR:HA	1.79	0.48
1:A:153:THR:HB	1:A:162:THR:HG23	1.95	0.48
1:D:206[A]:LYS:NZ	2:D:501:OJO:C4A	2.77	0.47
1:A:101:THR:CG2	4:A:620:HOH:O	2.59	0.47
1:B:245:ASP:OD2	1:C:242:SER:HB2	2.13	0.47
1:C:364:SER:OG	1:C:365:ASP:N	2.47	0.47
1:A:161:ILE:HG22	1:A:296:LEU:HD13	1.96	0.47
1:C:105:PRO:CD	1:C:150:LEU:HD23	2.45	0.47
1:D:105:PRO:HD3	1:D:150:LEU:O	2.15	0.47
1:B:239:LEU:HD23	1:C:239:LEU:HD23	1.97	0.46
1:B:242:SER:HB2	1:C:245:ASP:OD2	2.15	0.46
1:A:239:LEU:HD23	1:D:239:LEU:HD23	1.97	0.46
1:D:162:THR:CG2	4:D:674:HOH:O	2.64	0.46
1:D:162:THR:HG22	4:D:674:HOH:O	2.15	0.46
1:C:105:PRO:HD2	1:C:150:LEU:HD23	1.98	0.45
1:B:364:SER:OG	1:B:365:ASP:N	2.48	0.45
1:A:206[A]:LYS:NZ	2:A:501:OJO:C4A	2.79	0.45
1:C:281:ASN:ND2	1:C:313:GLU:OE1	2.27	0.44
1:A:40:ASN:N	1:A:40:ASN:HD22	2.09	0.44
1:A:101:THR:HB	1:A:126:ALA:HB3	1.99	0.44
1:B:182:ASN:HD21	1:B:190:GLN:HB3	1.81	0.44
1:D:201:LEU:C	1:D:201:LEU:HD12	2.39	0.44
1:A:206[A]:LYS:HD2	1:A:335:LEU:O	2.18	0.43
1:D:101:THR:CG2	1:D:128:ILE:HD12	2.48	0.43
1:B:156:ASN:HA	1:B:157:PRO:HA	1.74	0.43
1:B:213:ASP:HB3	1:D:32:THR:HG21	2.01	0.43
1:D:121:LYS:HB3	1:D:121:LYS:HE2	1.71	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASN:HD22	1:C:157:PRO:CA	2.31	0.42
2:B:501:OJO:OP1	1:C:54:TYR:OH	2.30	0.42
1:C:156:ASN:HB2	1:C:184:PHE:CZ	2.54	0.42
1:C:182:ASN:HD21	1:C:190:GLN:HB3	1.84	0.42
1:B:153:THR:HB	1:B:162:THR:HG23	2.02	0.42
1:C:285:PHE:HA	1:C:286:PRO:HD3	1.89	0.42
1:D:228:GLN:HG3	4:D:749:HOH:O	2.16	0.42
1:A:349:THR:OG1	1:A:350:HIS:HD2	2.01	0.42
2:A:501:OJO:N	2:A:501:OJO:O3	2.53	0.42
1:D:394:THR:CG2	4:D:602:HOH:O	2.67	0.42
1:D:385:ARG:NH2	4:D:606:HOH:O	2.44	0.41
1:C:282:GLN:NE2	4:C:607:HOH:O	2.52	0.41
1:C:309:SER:HB2	1:C:367:LEU:HD11	2.02	0.41
1:B:209:ASN:ND2	1:D:251:ARG:HH22	2.12	0.41
1:D:349:THR:OG1	1:D:350:HIS:HD2	2.01	0.41
2:D:501:OJO:N	2:D:501:OJO:O3	2.53	0.41
1:B:267:ALA:HA	1:B:372:ILE:HD13	2.03	0.41
1:A:109:TYR:CE2	1:A:111:GLY:HA3	2.55	0.41
1:A:182:ASN:HD21	1:A:190:GLN:HB3	1.86	0.41
1:D:156:ASN:ND2	1:D:369:ARG:HH11	2.18	0.41
1:B:345:PRO:O	1:B:350:HIS:N	2.49	0.40
1:C:156:ASN:HA	1:C:157:PRO:HA	1.71	0.40
1:D:182:ASN:HD21	1:D:190:GLN:HB3	1.86	0.40
1:C:347:SER:O	1:C:351:ALA:HB2	2.20	0.40
1:A:222:ARG:HG2	4:A:618:HOH:O	2.22	0.40
1:A:22:ILE:HA	1:A:31:VAL:O	2.22	0.40
1:B:40:ASN:ND2	1:B:40:ASN:N	2.68	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	387/408 (95%)	375 (97%)	12 (3%)	0	100	100
1	B	385/408 (94%)	371 (96%)	14 (4%)	0	100	100
1	C	385/408 (94%)	374 (97%)	10 (3%)	1 (0%)	41	50
1	D	386/408 (95%)	373 (97%)	13 (3%)	0	100	100
All	All	1543/1632 (94%)	1493 (97%)	49 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	364	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/310 (94%)	269 (92%)	24 (8%)	11	14
1	B	291/310 (94%)	268 (92%)	23 (8%)	12	15
1	C	291/310 (94%)	273 (94%)	18 (6%)	18	24
1	D	292/310 (94%)	267 (91%)	25 (9%)	10	12
All	All	1167/1240 (94%)	1077 (92%)	90 (8%)	13	16

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	32	THR
1	A	40	ASN
1	A	72	LEU
1	A	101	THR
1	A	127	LEU
1	A	136	ARG
1	A	144	GLN
1	A	156	ASN
1	A	157	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	160	ARG
1	A	162	THR
1	A	173	LYS
1	A	228	GLN
1	A	242	SER
1	A	253	LEU
1	A	273	LEU
1	A	296	LEU
1	A	299	ARG
1	A	312	LEU
1	A	327	ARG
1	A	364	SER
1	A	389	SER
1	A	396	THR
1	B	40	ASN
1	B	71	GLU
1	B	72	LEU
1	B	101	THR
1	B	127	LEU
1	B	136	ARG
1	B	145	SER
1	B	156	ASN
1	B	157	PRO
1	B	160	ARG
1	B	162	THR
1	B	165	ARG
1	B	173	LYS
1	B	184	PHE
1	B	186	SER
1	B	223	ASP
1	B	228	GLN
1	B	242	SER
1	B	253	LEU
1	B	273	LEU
1	B	296	LEU
1	B	356	GLU
1	B	364	SER
1	C	9	THR
1	C	40	ASN
1	C	72	LEU
1	C	127	LEU
1	C	136	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	150	LEU
1	C	156	ASN
1	C	157	PRO
1	C	160	ARG
1	C	165	ARG
1	C	173	LYS
1	C	223	ASP
1	C	242	SER
1	C	253	LEU
1	C	273	LEU
1	C	296	LEU
1	C	309	SER
1	C	356	GLU
1	D	9	THR
1	D	40	ASN
1	D	72	LEU
1	D	121	LYS
1	D	127	LEU
1	D	136	ARG
1	D	145	SER
1	D	156	ASN
1	D	157	PRO
1	D	162	THR
1	D	165	ARG
1	D	222	ARG
1	D	242	SER
1	D	253	LEU
1	D	272	GLU
1	D	273	LEU
1	D	281	ASN
1	D	296	LEU
1	D	299	ARG
1	D	302	LYS
1	D	312	LEU
1	D	327	ARG
1	D	364	SER
1	D	389	SER
1	D	394	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	97	GLN
1	A	156	ASN
1	A	182	ASN
1	A	190	GLN
1	A	209	ASN
1	A	350	HIS
1	B	40	ASN
1	B	48	ASN
1	B	51	GLN
1	B	97	GLN
1	B	156	ASN
1	B	182	ASN
1	B	190	GLN
1	B	209	ASN
1	B	282	GLN
1	C	40	ASN
1	C	48	ASN
1	C	51	GLN
1	C	97	GLN
1	C	156	ASN
1	C	182	ASN
1	C	190	GLN
1	C	209	ASN
1	D	40	ASN
1	D	48	ASN
1	D	156	ASN
1	D	182	ASN
1	D	190	GLN
1	D	209	ASN
1	D	350	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	OJO	A	501	-	18,21,21	1.24	1 (5%)	21,30,30	1.11	3 (14%)
2	OJO	D	501	-	18,21,21	1.12	1 (5%)	21,30,30	1.20	2 (9%)
2	OJO	B	501	-	18,21,21	1.41	3 (16%)	21,30,30	1.16	3 (14%)
3	CYS	B	502	-	3,6,6	1.42	1 (33%)	1,7,7	1.71	0
3	CYS	C	502	-	3,6,6	1.38	1 (33%)	1,7,7	0.84	0
3	CYS	A	502	-	3,6,6	1.09	0	1,7,7	1.53	0
3	CYS	D	502	-	3,6,6	0.83	0	1,7,7	1.40	0
2	OJO	C	501	-	18,21,21	1.56	3 (16%)	21,30,30	1.25	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OJO	A	501	-	-	0/9/15/15	0/1/1/1
2	OJO	D	501	-	-	0/9/15/15	0/1/1/1
2	OJO	B	501	-	-	1/9/15/15	0/1/1/1
3	CYS	B	502	-	-	2/2/6/6	-
3	CYS	C	502	-	-	2/2/6/6	-
3	CYS	A	502	-	-	0/2/6/6	-
3	CYS	D	502	-	-	0/2/6/6	-
2	OJO	C	501	-	-	0/9/15/15	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	OJO	C-CA	-4.55	1.45	1.52
2	A	501	OJO	C-CA	-4.13	1.45	1.52
2	B	501	OJO	C-CA	-4.01	1.46	1.52
2	D	501	OJO	C-CA	-3.78	1.46	1.52
2	B	501	OJO	CA-N	2.44	1.46	1.36
2	C	501	OJO	C4A-N	2.37	1.31	1.28
2	C	501	OJO	CA-N	2.34	1.46	1.36
3	C	502	CYS	CA-N	2.21	1.52	1.47
2	B	501	OJO	C4A-N	2.21	1.31	1.28
3	B	502	CYS	CA-N	2.14	1.51	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	OJO	OP4-C5A-C5	2.76	114.61	109.35
2	B	501	OJO	OP2-P-OP4	-2.66	99.67	106.73
2	D	501	OJO	OP1-P-OP4	-2.57	99.88	106.73
2	B	501	OJO	OP2-P-OP1	2.56	117.42	107.64
2	C	501	OJO	OP2-P-OP1	2.50	117.18	107.64
2	C	501	OJO	OP2-P-OP4	-2.37	100.42	106.73
2	C	501	OJO	C3-C4-C5	-2.36	116.45	118.26
2	A	501	OJO	OP4-P-OP3	-2.21	100.27	106.47
2	A	501	OJO	OP2-P-OP1	2.13	115.78	107.64
2	B	501	OJO	C3-C4-C5	-2.10	116.65	118.26
2	D	501	OJO	OP4-C5A-C5	2.09	113.34	109.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	CYS	C-CA-CB-SG
3	C	502	CYS	C-CA-CB-SG
3	B	502	CYS	N-CA-CB-SG
3	C	502	CYS	N-CA-CB-SG
2	B	501	OJO	C4-C4A-N-CA

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	OJO	3	0
2	D	501	OJO	3	0

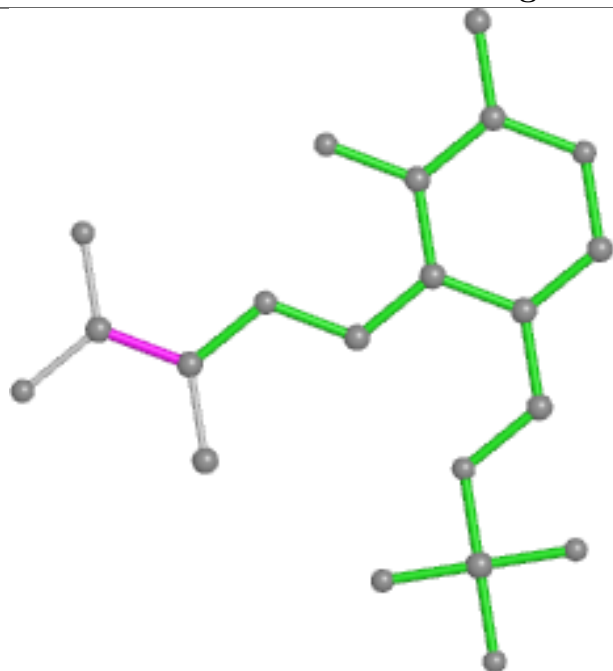
*Continued on next page...*

*Continued from previous page...*

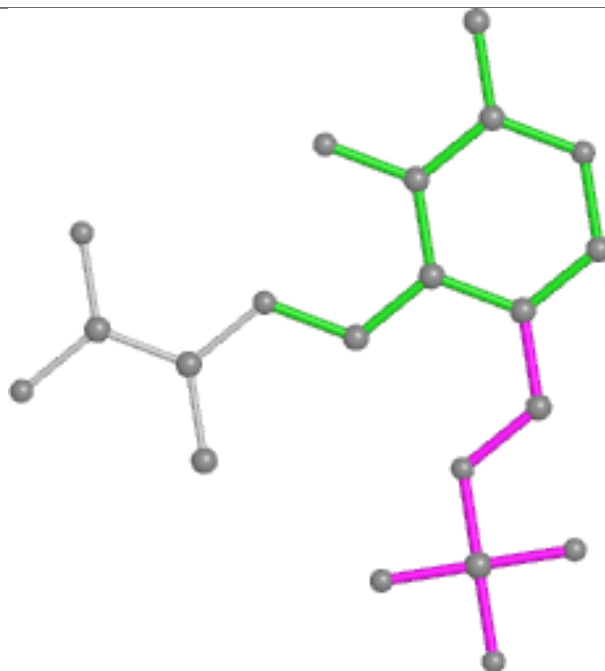
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	OJO	4	0
2	C	501	OJO	3	0

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

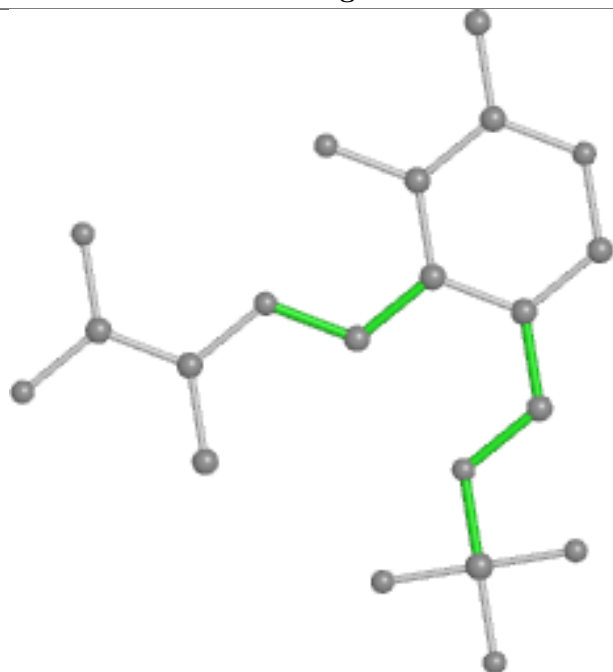
## Ligand 0JO A 501



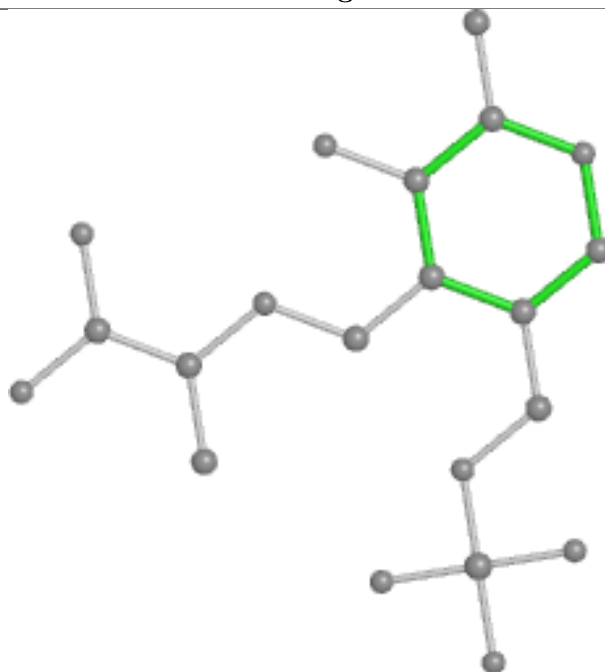
Bond lengths



Bond angles

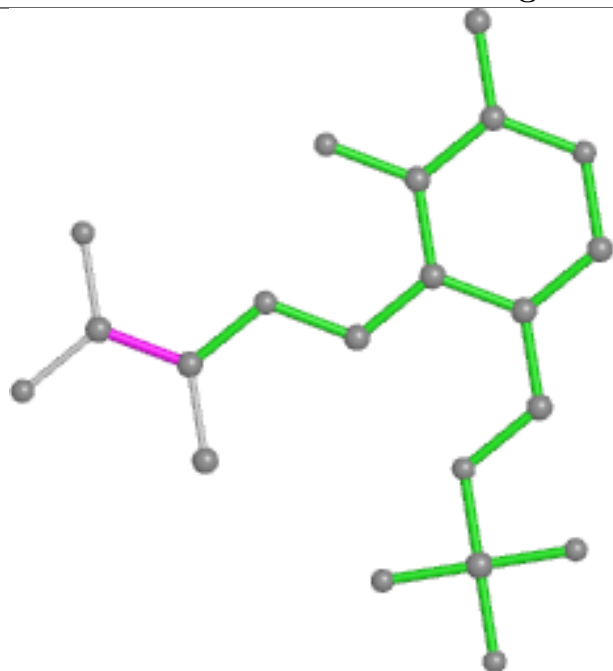


Torsions

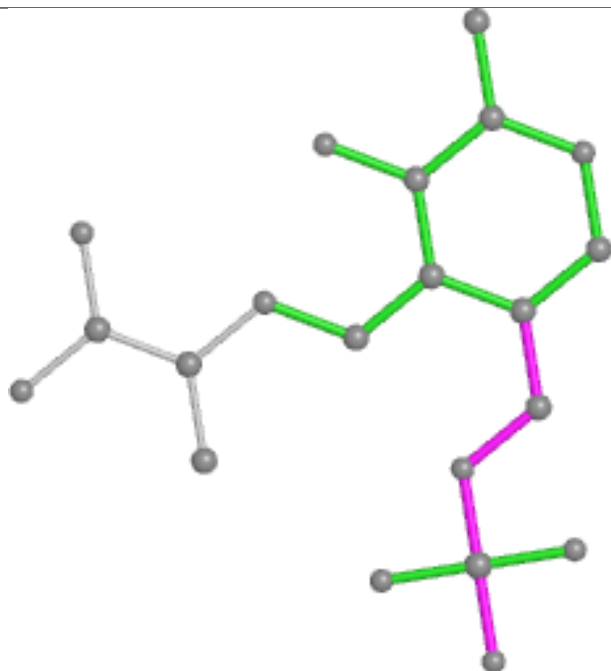


Rings

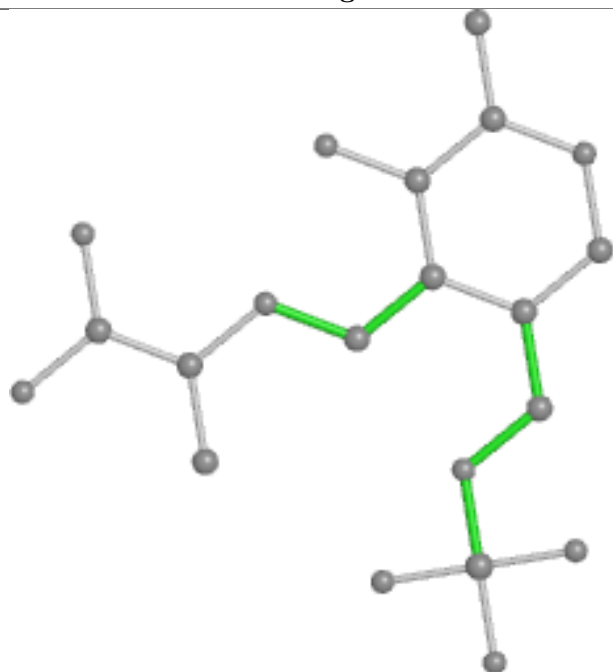
## Ligand 0JO D 501



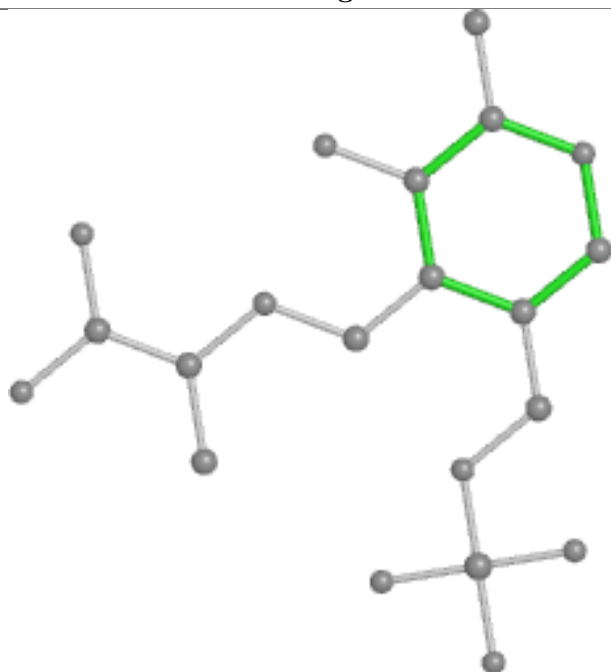
Bond lengths



Bond angles

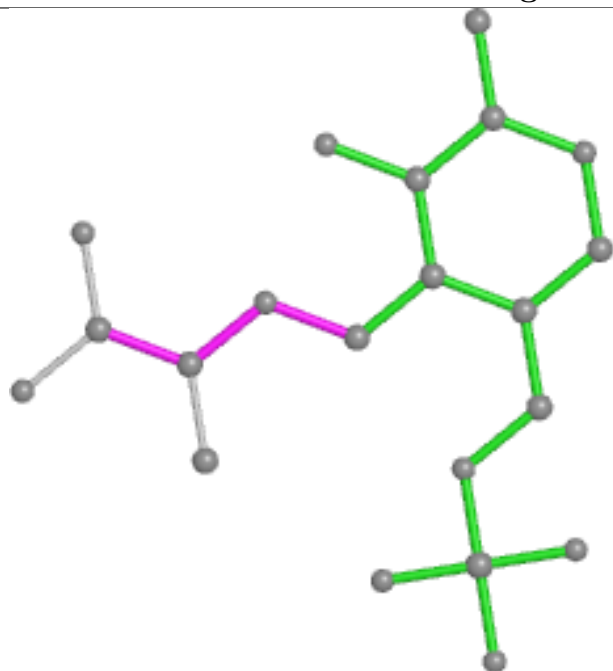


Torsions

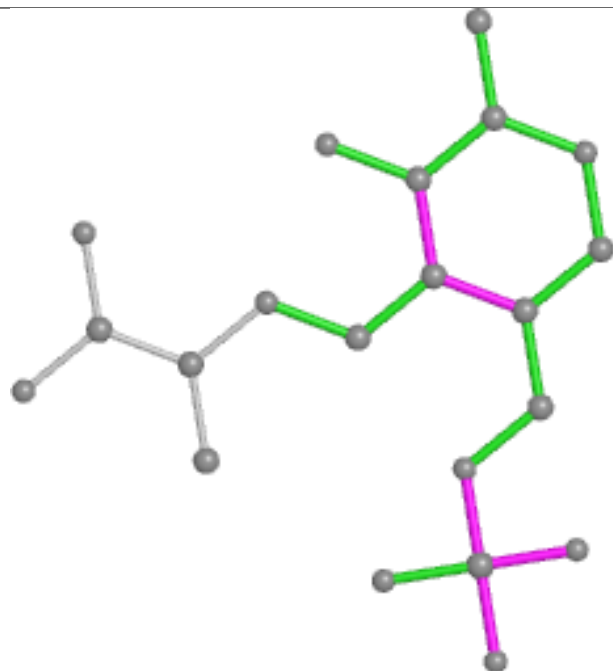


Rings

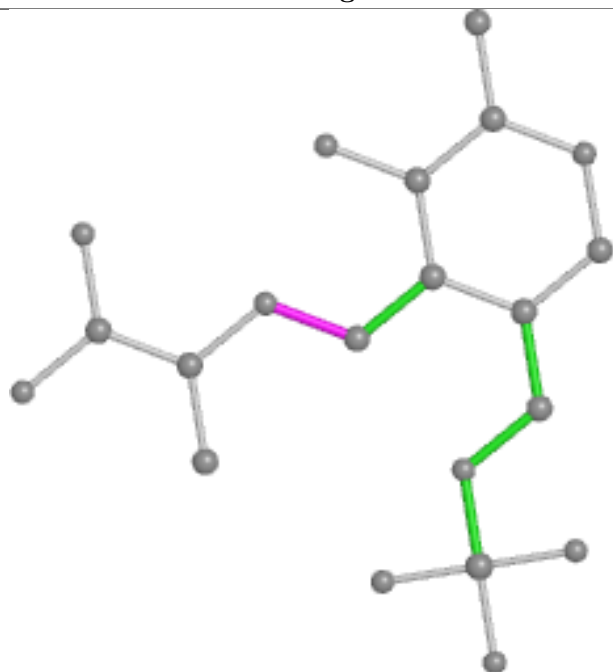
## Ligand 0JO B 501



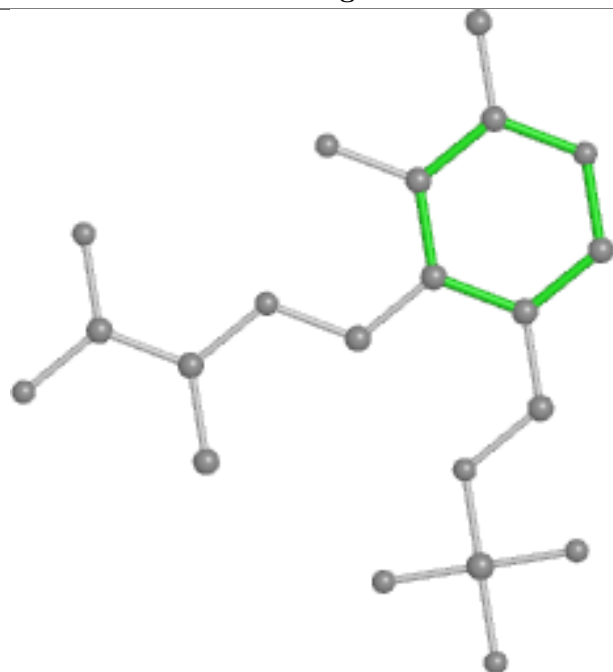
Bond lengths



Bond angles

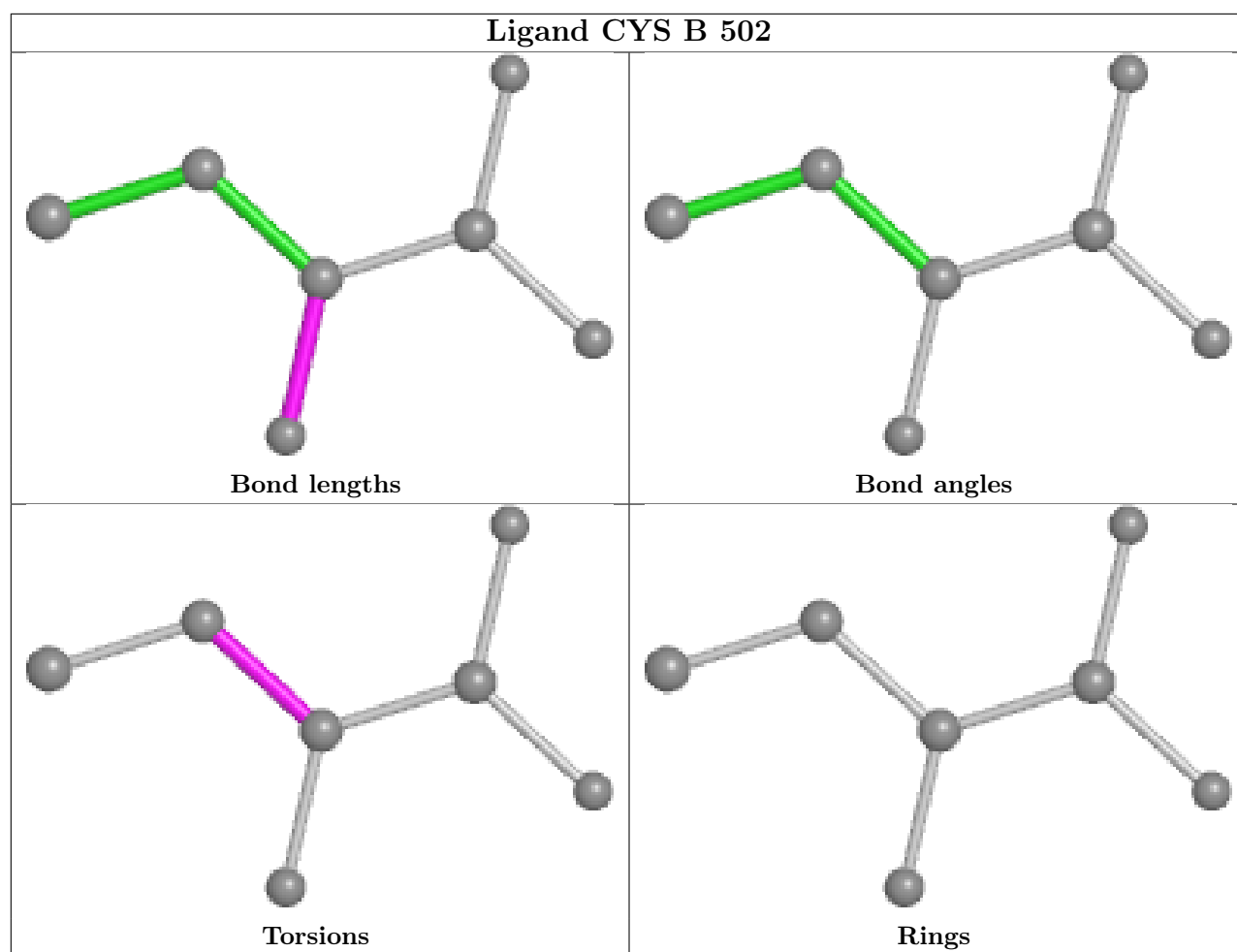


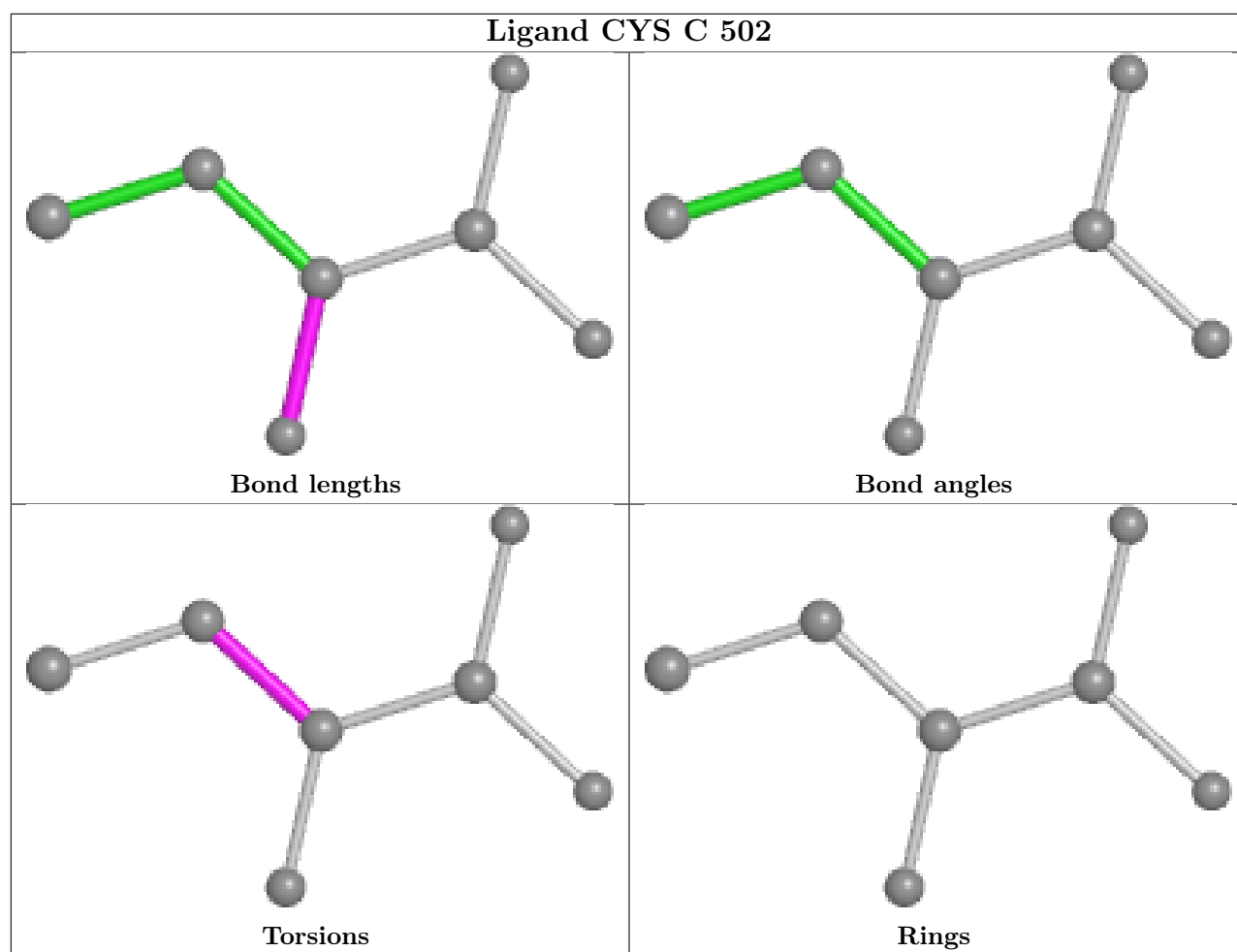
Torsions

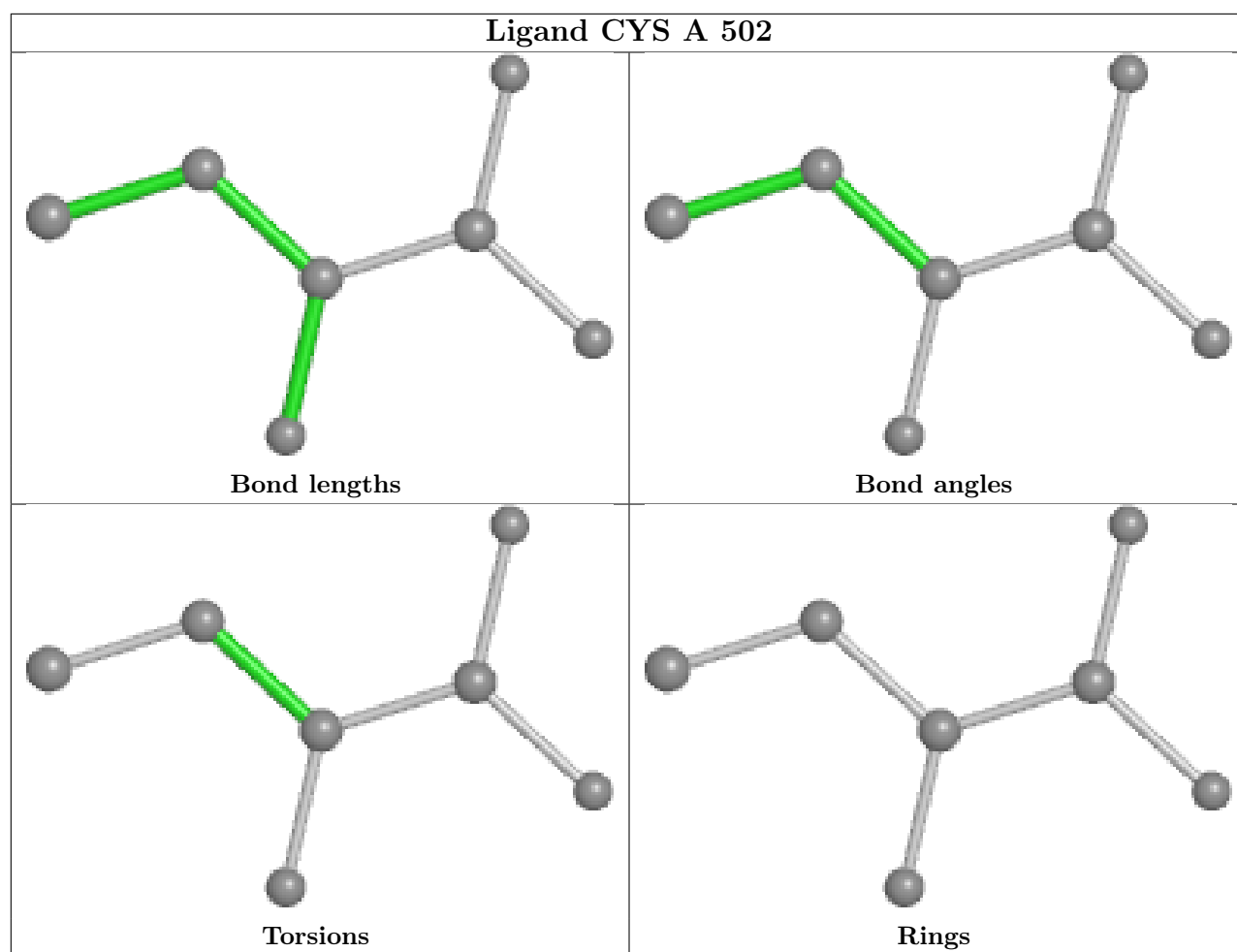


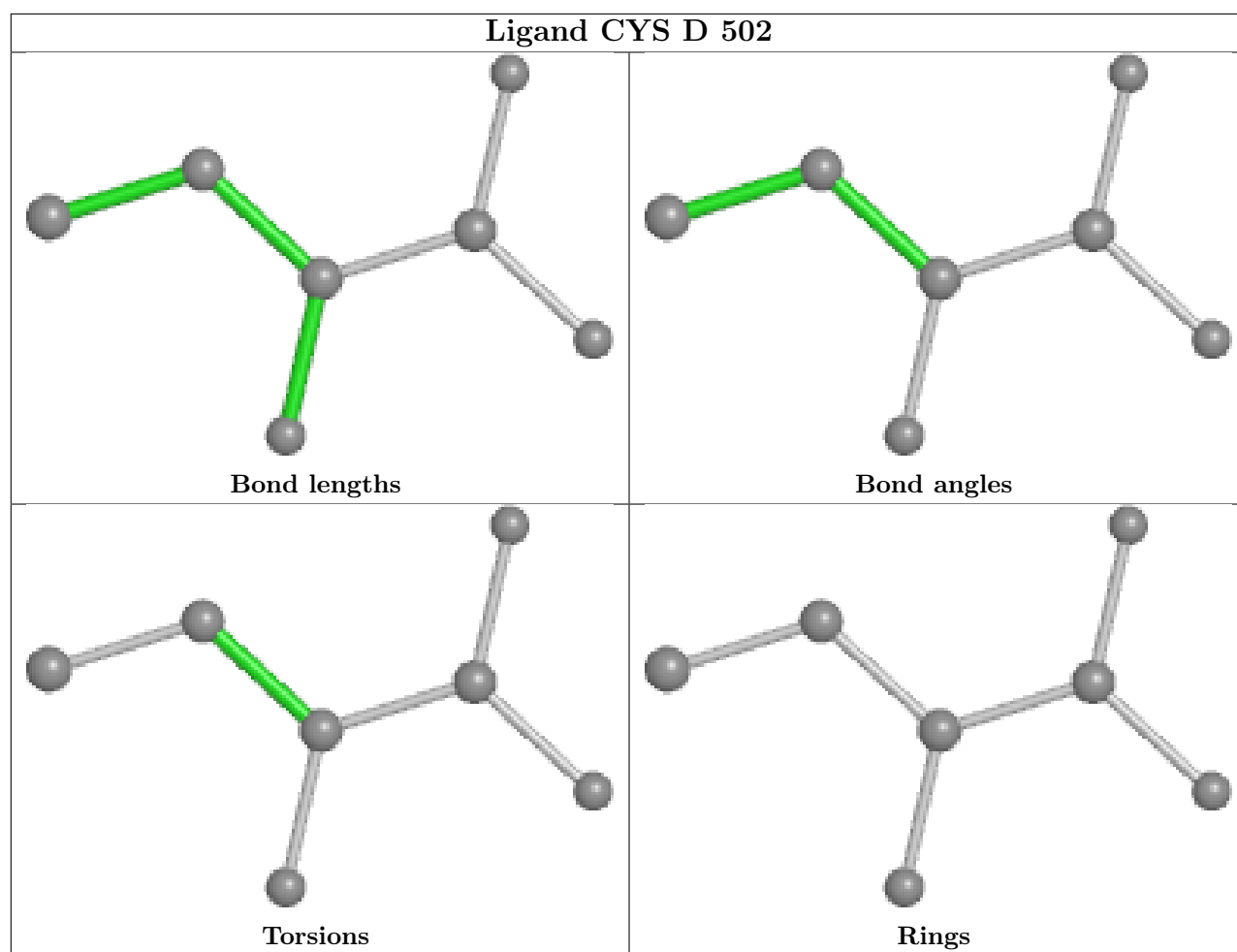
Rings

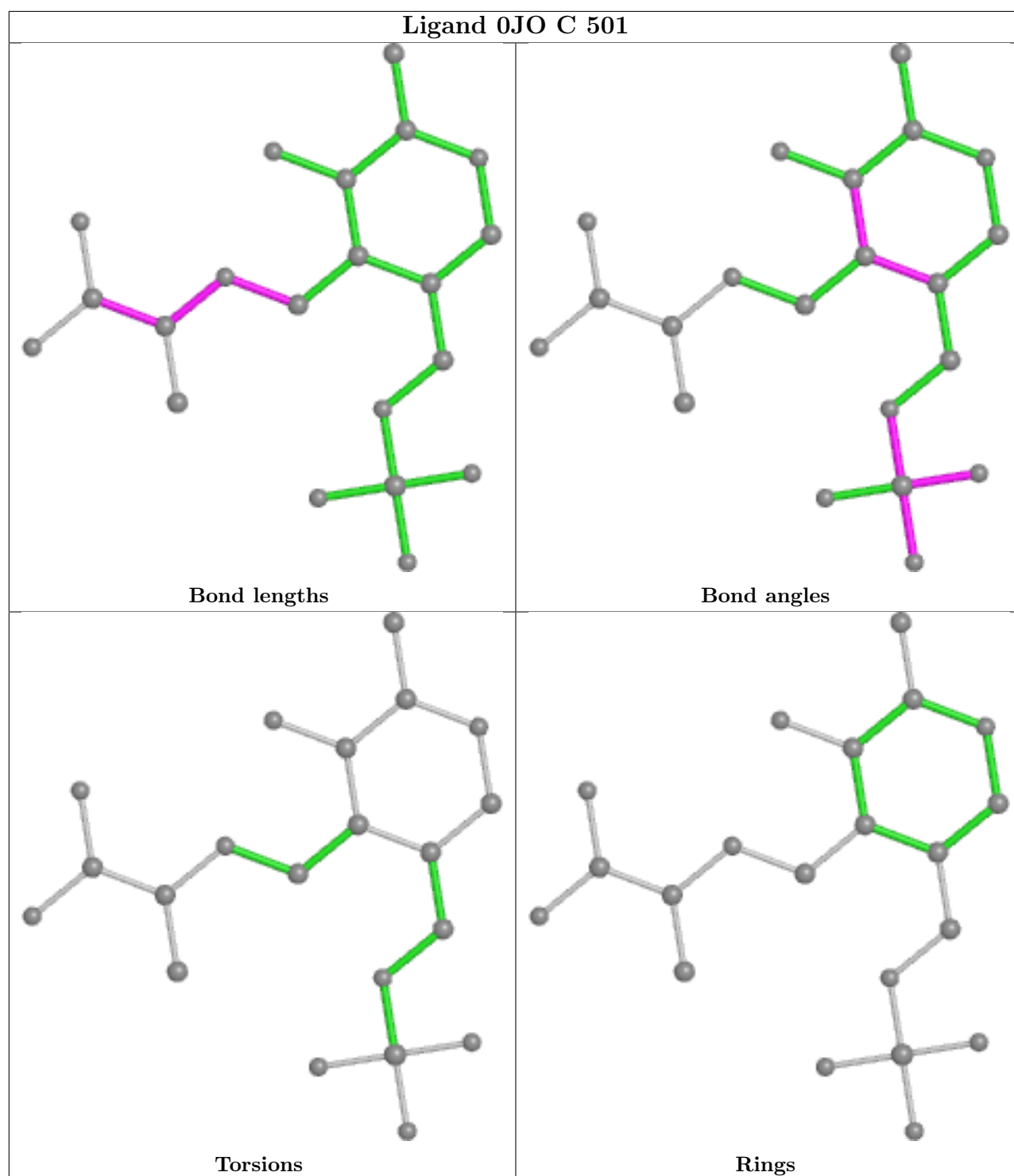












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	A	388/408 (95%)	-0.13	1 (0%) 94 96	18, 31, 55, 101	0
1	B	387/408 (94%)	-0.06	7 (1%) 68 75	17, 31, 67, 98	0
1	C	387/408 (94%)	-0.05	9 (2%) 60 67	18, 30, 67, 93	0
1	D	387/408 (94%)	-0.10	1 (0%) 94 96	18, 31, 56, 102	0
All	All	1549/1632 (94%)	-0.08	18 (1%) 79 83	17, 31, 62, 102	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	9	THR	4.3
1	C	363	ILE	4.1
1	C	352	ALA	3.7
1	C	354	THR	3.2
1	A	9	THR	2.9
1	C	9	THR	2.7
1	B	361	ALA	2.6
1	B	363	ILE	2.5
1	C	356	GLU	2.5
1	C	361	ALA	2.5
1	B	346	ALA	2.4
1	B	9	THR	2.4
1	B	356	GLU	2.3
1	B	352	ALA	2.3
1	C	353	MET	2.1
1	C	358	ARG	2.1
1	C	360	ALA	2.1
1	B	360	ALA	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

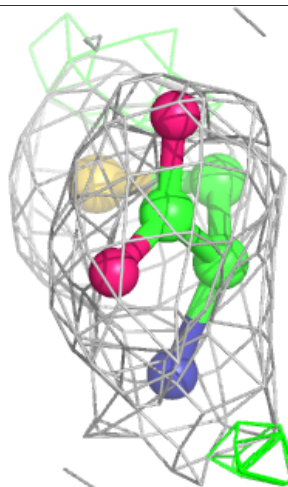
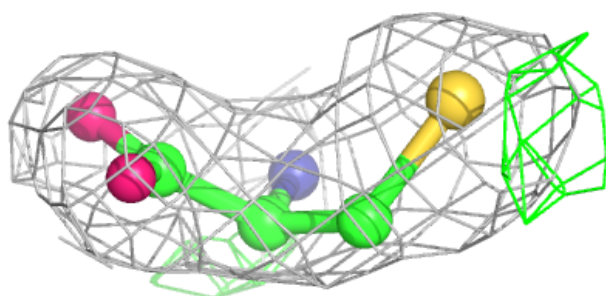
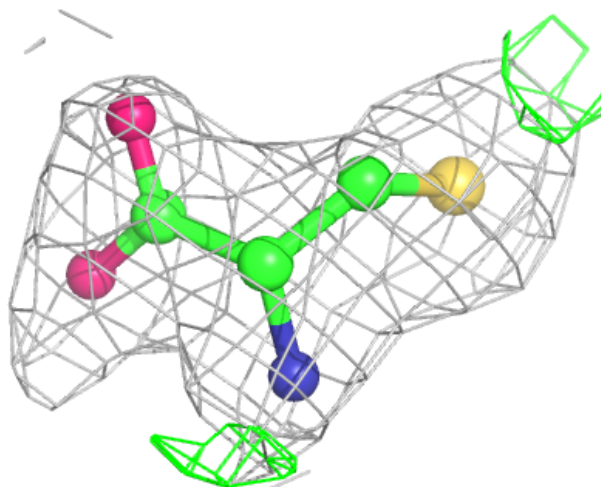
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CYS	B	502	7/7	0.89	0.16	55,61,70,76	0
3	CYS	C	502	7/7	0.91	0.16	59,67,71,77	0
3	CYS	D	502	7/7	0.93	0.14	42,51,61,67	0
3	CYS	A	502	7/7	0.96	0.16	43,49,63,66	0
2	OJO	A	501	21/21	0.98	0.12	17,25,37,38	0
2	OJO	B	501	21/21	0.98	0.13	20,33,46,48	0
2	OJO	C	501	21/21	0.98	0.12	19,30,44,46	0
2	OJO	D	501	21/21	0.99	0.10	16,25,35,38	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.



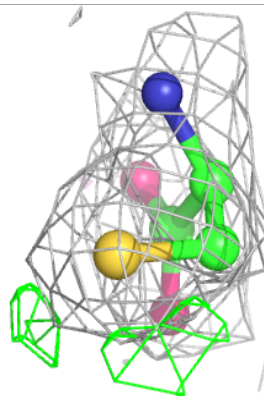
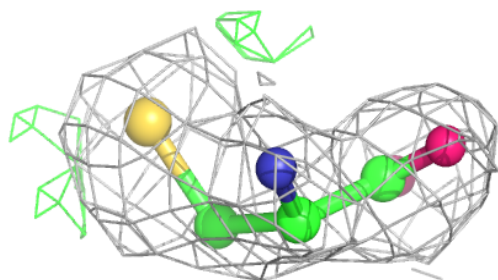
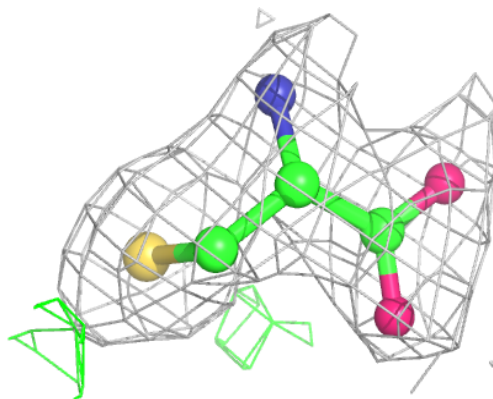
**Electron density around CYS B 502:**

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



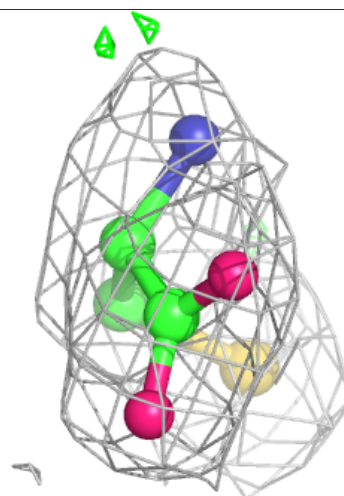
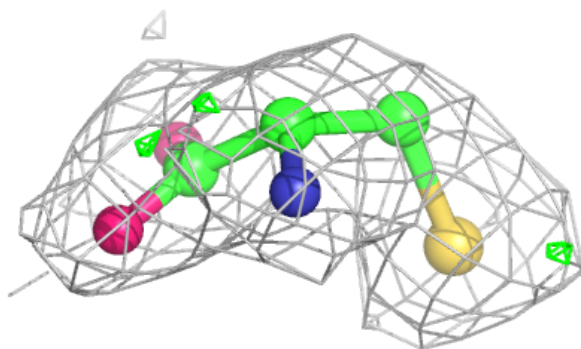
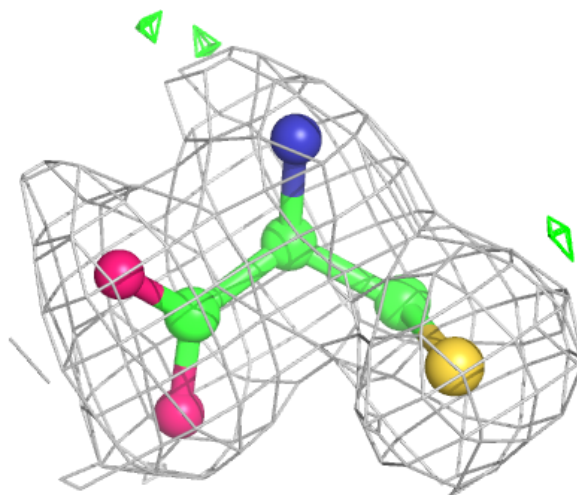
**Electron density around CYS C 502:**

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



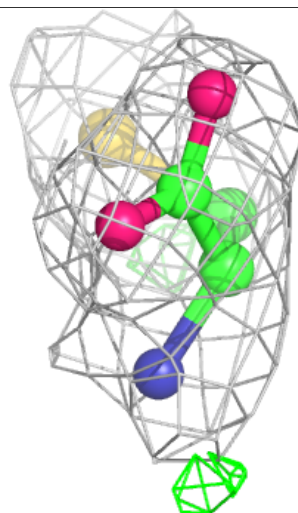
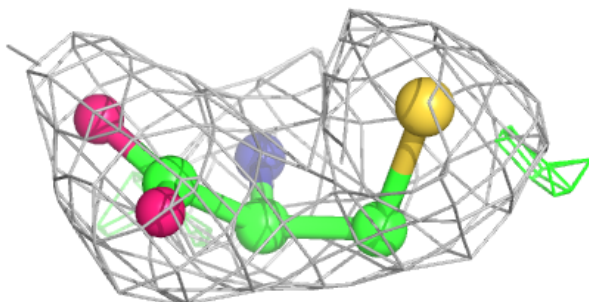
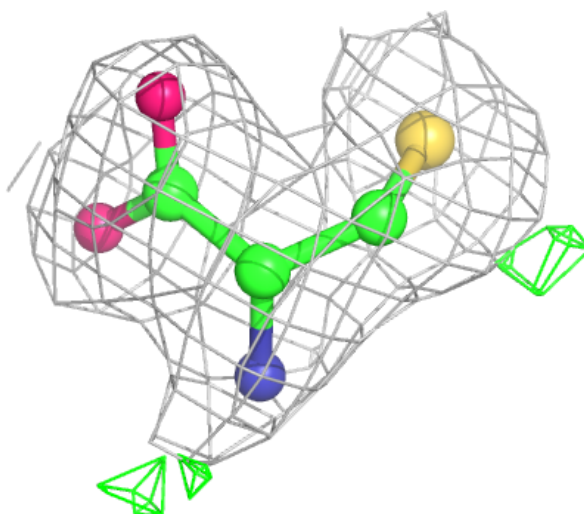
**Electron density around CYS D 502:**

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



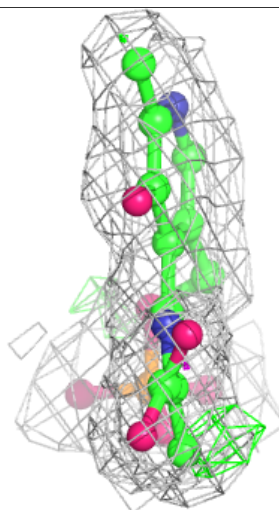
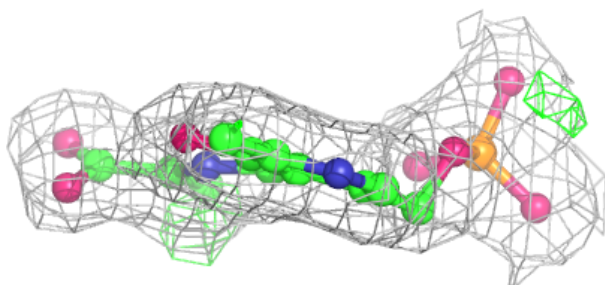
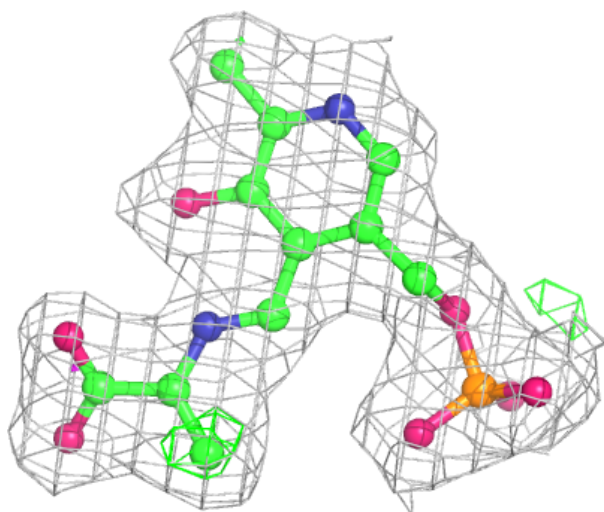
**Electron density around CYS A 502:**

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



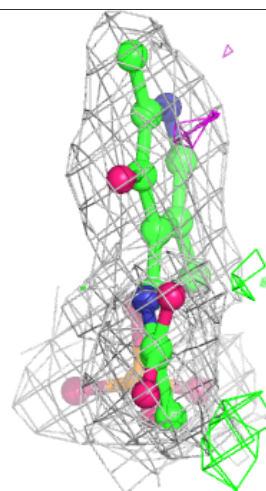
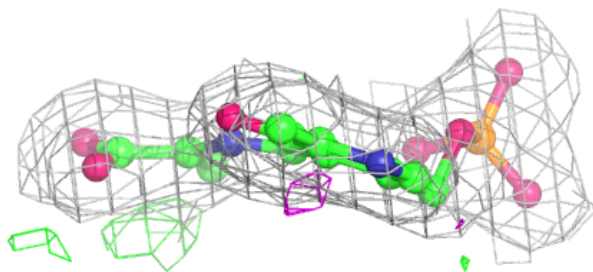
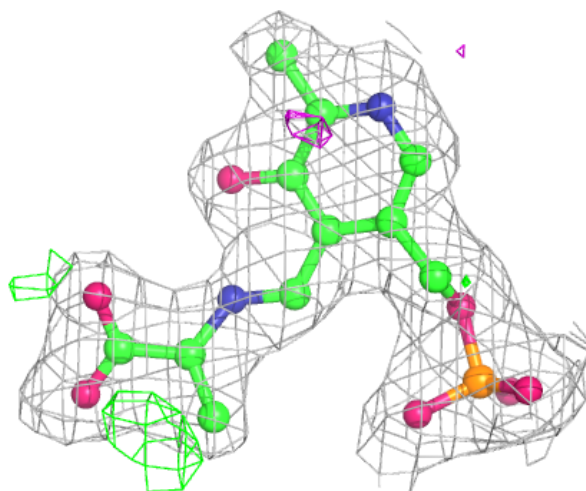
**Electron density around 0JO A 501:**

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



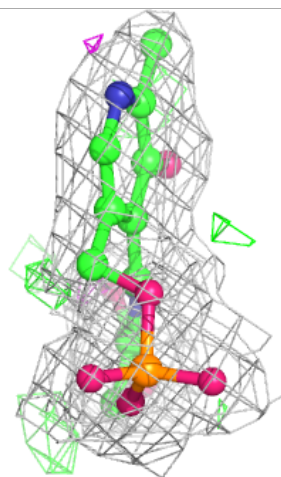
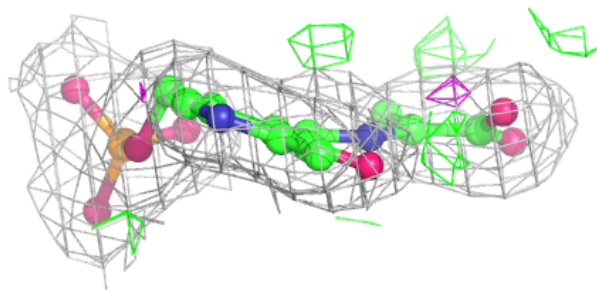
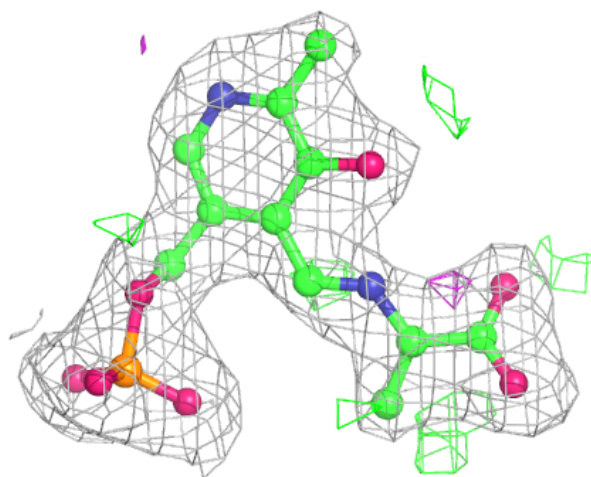
**Electron density around 0JO B 501:**

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



**Electron density around 0JO C 501:**

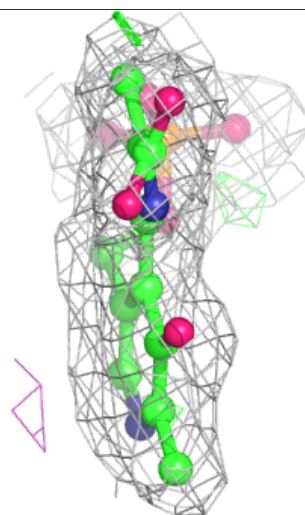
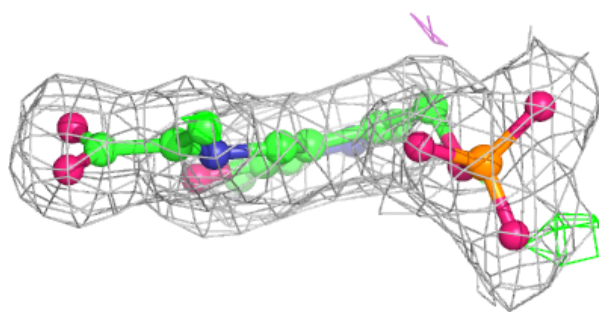
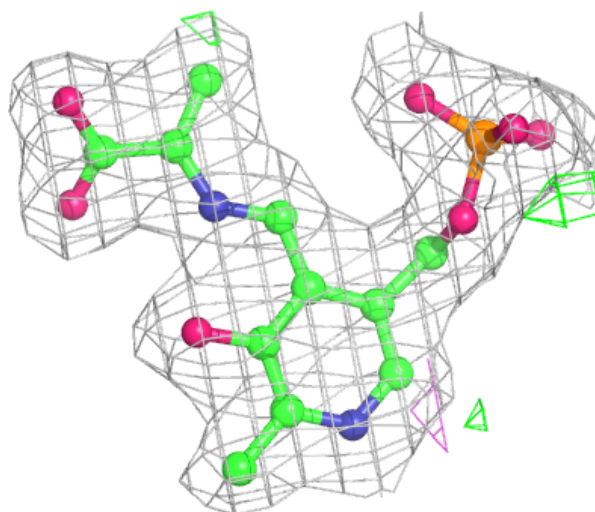
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 0JO D 501:**

$2mF_o-DF_c$  (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.