



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2022 – 01:25 pm GMT

PDB ID : 7ZH8  
Title : DYRK1a in Complex with a Bromo-Triazolo-Pyridine  
Authors : Dammann, M.; Stahlecker, J.; Stehle, T.; Boeckler, F.M.  
Deposited on : 2022-04-05  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

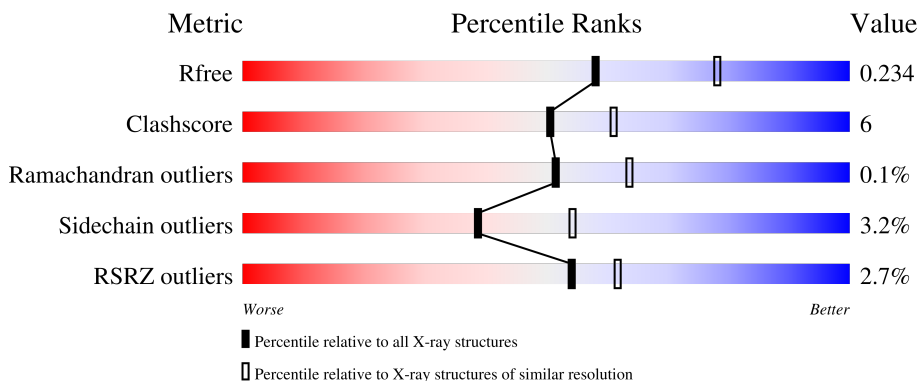
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


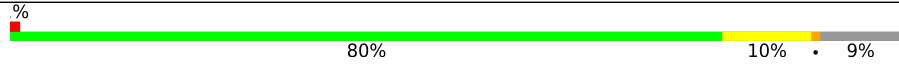
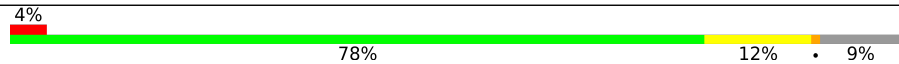

The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	382	 80% • 10% • 9%
1	B	382	 80% • 10% • 9%
1	C	382	 78% • 12% • 9%
1	D	382	 78% • 12% • 9%

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

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

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
10	CL	C	513	-	-	X	-

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 12103 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 Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	348	Total 2838	C 1822	N 488	O 510	P 1	S 17	0	1	0
1	B	347	Total 2810	C 1806	N 483	O 503	P 1	S 17	0	0	0
1	C	346	Total 2764	C 1780	N 465	O 501	P 1	S 17	0	1	0
1	D	346	Total 2785	C 1792	N 475	O 500	P 1	S 17	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	initiating methionine	UNP Q13627
A	105	HIS	-	expression tag	UNP Q13627
A	106	HIS	-	expression tag	UNP Q13627
A	107	HIS	-	expression tag	UNP Q13627
A	108	HIS	-	expression tag	UNP Q13627
A	109	HIS	-	expression tag	UNP Q13627
A	110	HIS	-	expression tag	UNP Q13627
A	111	SER	-	expression tag	UNP Q13627
A	112	SER	-	expression tag	UNP Q13627
A	113	GLY	-	expression tag	UNP Q13627
A	114	VAL	-	expression tag	UNP Q13627
A	115	ASP	-	expression tag	UNP Q13627
A	116	LEU	-	expression tag	UNP Q13627
A	117	GLY	-	expression tag	UNP Q13627
A	118	THR	-	expression tag	UNP Q13627
A	119	GLU	-	expression tag	UNP Q13627
A	120	ASN	-	expression tag	UNP Q13627
A	121	LEU	-	expression tag	UNP Q13627
A	122	TYR	-	expression tag	UNP Q13627
A	123	PHE	-	expression tag	UNP Q13627
A	124	GLN	-	expression tag	UNP Q13627

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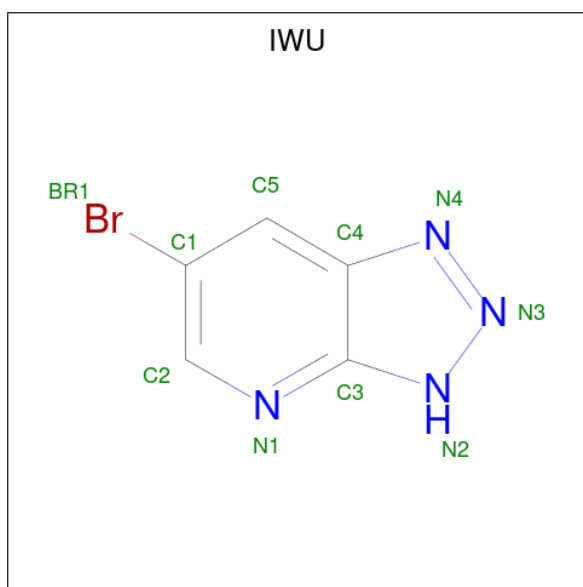
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	104	MET	-	initiating methionine	UNP Q13627
B	105	HIS	-	expression tag	UNP Q13627
B	106	HIS	-	expression tag	UNP Q13627
B	107	HIS	-	expression tag	UNP Q13627
B	108	HIS	-	expression tag	UNP Q13627
B	109	HIS	-	expression tag	UNP Q13627
B	110	HIS	-	expression tag	UNP Q13627
B	111	SER	-	expression tag	UNP Q13627
B	112	SER	-	expression tag	UNP Q13627
B	113	GLY	-	expression tag	UNP Q13627
B	114	VAL	-	expression tag	UNP Q13627
B	115	ASP	-	expression tag	UNP Q13627
B	116	LEU	-	expression tag	UNP Q13627
B	117	GLY	-	expression tag	UNP Q13627
B	118	THR	-	expression tag	UNP Q13627
B	119	GLU	-	expression tag	UNP Q13627
B	120	ASN	-	expression tag	UNP Q13627
B	121	LEU	-	expression tag	UNP Q13627
B	122	TYR	-	expression tag	UNP Q13627
B	123	PHE	-	expression tag	UNP Q13627
B	124	GLN	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	104	MET	-	initiating methionine	UNP Q13627
C	105	HIS	-	expression tag	UNP Q13627
C	106	HIS	-	expression tag	UNP Q13627
C	107	HIS	-	expression tag	UNP Q13627
C	108	HIS	-	expression tag	UNP Q13627
C	109	HIS	-	expression tag	UNP Q13627
C	110	HIS	-	expression tag	UNP Q13627
C	111	SER	-	expression tag	UNP Q13627
C	112	SER	-	expression tag	UNP Q13627
C	113	GLY	-	expression tag	UNP Q13627
C	114	VAL	-	expression tag	UNP Q13627
C	115	ASP	-	expression tag	UNP Q13627
C	116	LEU	-	expression tag	UNP Q13627
C	117	GLY	-	expression tag	UNP Q13627
C	118	THR	-	expression tag	UNP Q13627
C	119	GLU	-	expression tag	UNP Q13627
C	120	ASN	-	expression tag	UNP Q13627

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Chain	Residue	Modelled	Actual	Comment	Reference
C	121	LEU	-	expression tag	UNP Q13627
C	122	TYR	-	expression tag	UNP Q13627
C	123	PHE	-	expression tag	UNP Q13627
C	124	GLN	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627
D	104	MET	-	initiating methionine	UNP Q13627
D	105	HIS	-	expression tag	UNP Q13627
D	106	HIS	-	expression tag	UNP Q13627
D	107	HIS	-	expression tag	UNP Q13627
D	108	HIS	-	expression tag	UNP Q13627
D	109	HIS	-	expression tag	UNP Q13627
D	110	HIS	-	expression tag	UNP Q13627
D	111	SER	-	expression tag	UNP Q13627
D	112	SER	-	expression tag	UNP Q13627
D	113	GLY	-	expression tag	UNP Q13627
D	114	VAL	-	expression tag	UNP Q13627
D	115	ASP	-	expression tag	UNP Q13627
D	116	LEU	-	expression tag	UNP Q13627
D	117	GLY	-	expression tag	UNP Q13627
D	118	THR	-	expression tag	UNP Q13627
D	119	GLU	-	expression tag	UNP Q13627
D	120	ASN	-	expression tag	UNP Q13627
D	121	LEU	-	expression tag	UNP Q13627
D	122	TYR	-	expression tag	UNP Q13627
D	123	PHE	-	expression tag	UNP Q13627
D	124	GLN	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627
D	126	MET	-	expression tag	UNP Q13627

- Molecule 2 is 6-bromanyl-3H-[1,2,3]triazolo[4,5-b]pyridine (three-letter code: IWU) (formula:  $C_5H_3BrN_4$ ) (labeled as "Ligand of Interest" by depositor).



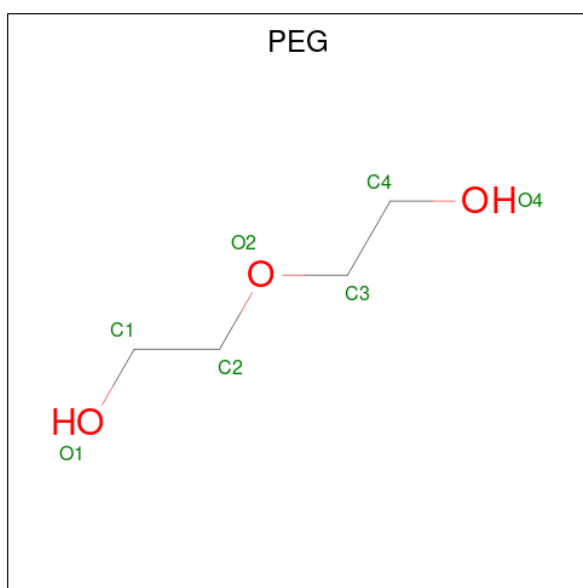
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	N		
2	A	1	10	1	5	4	0	0
2	A	1	10	1	5	4	0	0
2	B	1	10	1	5	4	0	0
2	B	1	10	1	5	4	0	0
2	C	1	10	1	5	4	0	0
2	C	1	10	1	5	4	0	0
2	D	1	10	1	5	4	0	0
2	D	1	10	1	5	4	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

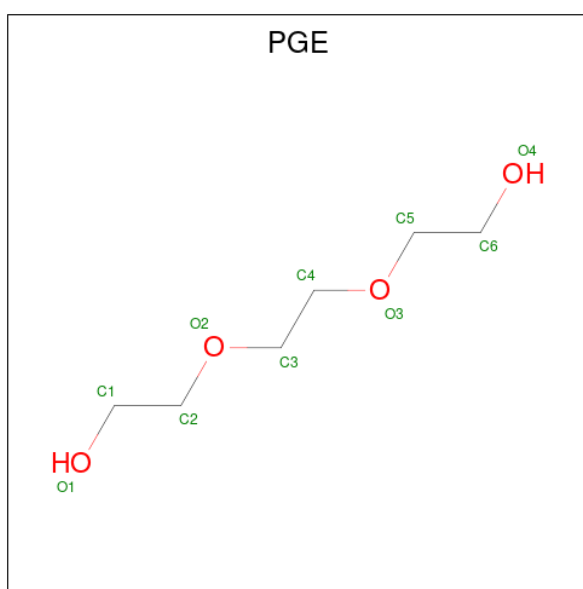
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



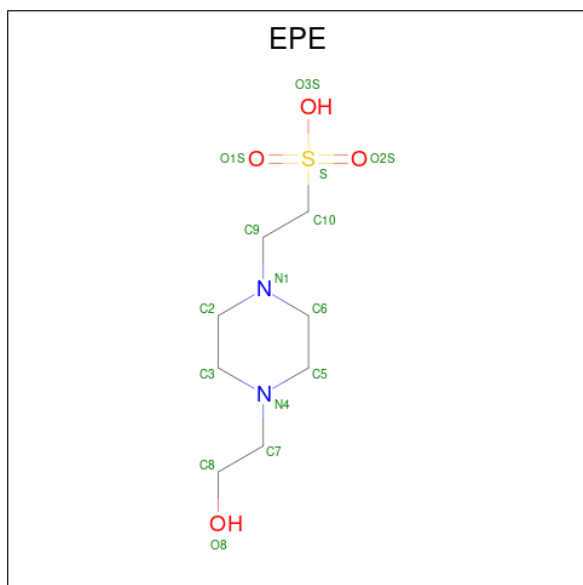
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	D	1	Total C O 10 6 4	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



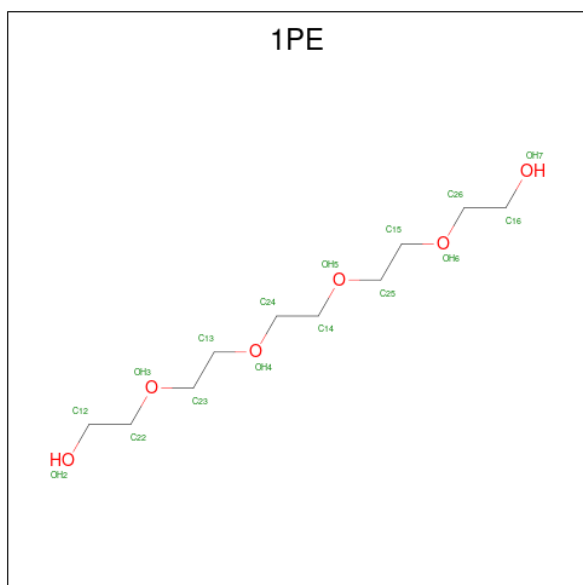
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	A	1	13	7	2	3	1	0	0
7	B	1	12	6	2	3	1	0	0
7	C	1	12	6	2	3	1	0	0
7	D	1	12	6	2	3	1	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			16	10	6		
8	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total Cl 3 3	0	0
10	B	1	Total Cl 1 1	0	0
10	C	1	Total Cl 1 1	0	0

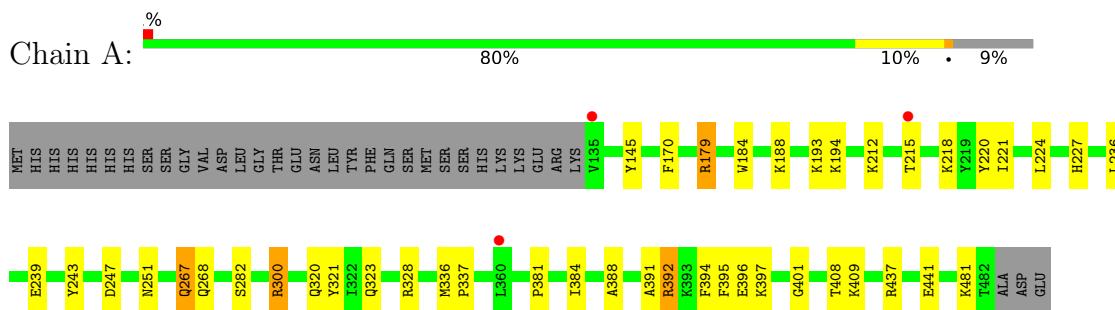
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	199	Total O 199 199	0	0
11	B	153	Total O 153 153	0	0
11	C	93	Total O 93 93	0	0
11	D	74	Total O 74 74	0	0

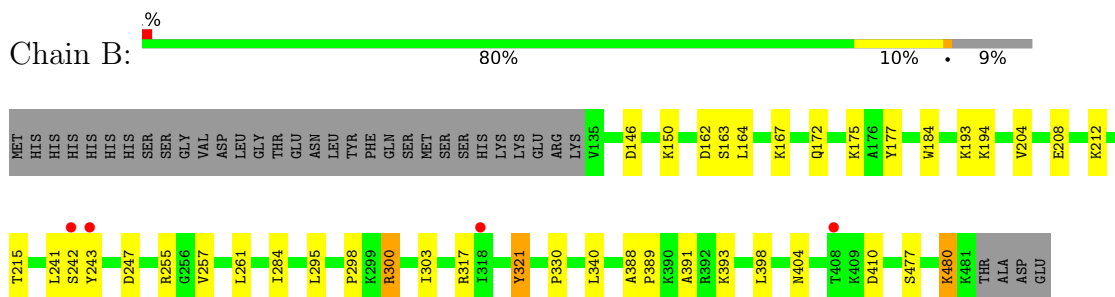
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

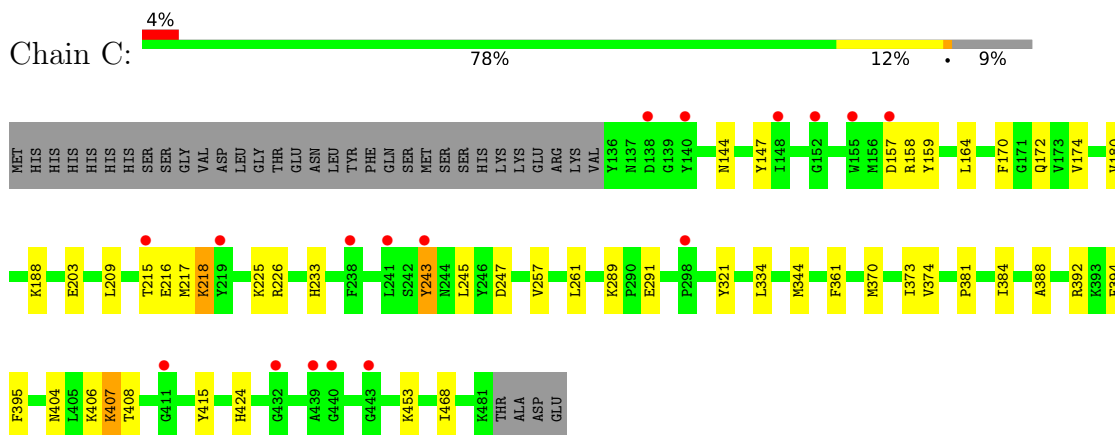
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	245.00Å 64.66Å 147.31Å 90.00° 115.58° 90.00°	Depositor
Resolution (Å)	48.60 – 2.30 48.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.60-2.30) 100.0 (48.60-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.199 , 0.235 0.197 , 0.234	Depositor DCC
$R_{free}$ test set	1487 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12103	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.09% 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: GOL, EPE, PG4, CL, PTR, PGE, 1PE, SO4, IWU, PEG

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	0.56	0/2887	0.71	0/3896
1	B	0.50	0/2859	0.68	0/3860
1	C	0.43	0/2813	0.63	0/3807
1	D	0.43	0/2834	0.62	0/3829
All	All	0.49	0/11393	0.66	0/15392

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2838	0	2810	34	0
1	B	2810	0	2779	33	0
1	C	2764	0	2676	30	0
1	D	2785	0	2734	27	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	3	0
2	D	20	0	0	2	0
3	A	13	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	13	0	18	0	0
4	A	7	0	10	3	0
4	B	7	0	10	1	0
4	C	21	0	30	0	0
4	D	7	0	10	0	0
5	A	20	0	28	1	0
5	C	10	0	14	1	0
5	D	10	0	14	0	0
6	A	6	0	8	1	0
6	B	30	0	39	6	0
6	C	12	0	16	0	0
7	A	13	0	13	2	0
7	B	12	0	13	5	0
7	C	12	0	12	4	0
7	D	12	0	13	5	0
8	A	16	0	22	1	0
8	B	16	0	22	4	0
9	A	25	0	0	1	0
9	B	15	0	0	0	0
9	C	10	0	0	0	0
9	D	15	0	0	1	0
10	A	3	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	2	0
11	A	199	0	0	9	0
11	B	153	0	0	2	0
11	C	93	0	0	1	0
11	D	74	0	0	2	0
All	All	12103	0	11309	130	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 6.

All (130) 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:366:GLU:HG3	7:D:505:EPE:H91	1.51	0.91
7:A:508:EPE:H61	9:A:511:SO4:O4	1.89	0.73
1:B:175:LYS:HZ3	8:B:509:1PE:H221	1.54	0.72
1:B:477:SER:HA	1:B:480:LYS:HD3	1.72	0.71
1:D:162:ASP:OD2	1:D:175:LYS:HE3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:NE2	11:A:601:HOH:O	2.26	0.69
1:B:150:LYS:NZ	11:B:601:HOH:O	2.27	0.67
1:B:194:LYS:HB3	6:B:503:GOL:H2	1.76	0.66
1:C:159:TYR:OH	1:C:226[A]:ARG:NH1	2.30	0.64
1:B:193:LYS:HD2	6:B:503:GOL:H31	1.80	0.63
1:C:321:PTR:HD2	7:C:510:EPE:H31	1.81	0.63
1:D:226:ARG:NH1	11:D:601:HOH:O	2.31	0.63
1:A:179:ARG:NH1	11:A:602:HOH:O	2.27	0.63
1:C:321:PTR:CD2	7:C:510:EPE:H31	2.29	0.63
1:D:437:ARG:NH2	9:D:507:SO4:O2	2.32	0.62
1:A:381:PRO:HD2	1:A:384:ILE:HD12	1.80	0.62
1:B:243:TYR:CE2	1:B:298:PRO:HB3	2.34	0.62
1:D:469:GLN:NE2	11:D:605:HOH:O	2.33	0.61
1:A:282:SER:HB2	6:A:507:GOL:H2	1.82	0.61
1:D:388:ALA:HB3	1:D:391:ALA:HB2	1.83	0.60
7:A:508:EPE:H102	7:A:508:EPE:H31	1.84	0.60
1:B:243:TYR:HA	11:B:608:HOH:O	2.03	0.59
1:C:188:LYS:NZ	1:C:203:GLU:OE2	2.28	0.58
1:D:365:ASN:HB2	7:D:505:EPE:H101	1.86	0.58
1:A:320:GLN:NE2	11:A:606:HOH:O	2.37	0.57
1:A:441:GLU:OE2	5:A:506:PGE:H6	2.04	0.57
1:A:184:TRP:CE2	8:A:509:1PE:H231	2.39	0.57
1:A:328:ARG:HG3	1:A:328:ARG:HH11	1.69	0.56
1:D:400:ASP:OD1	1:D:400:ASP:N	2.38	0.56
1:D:284:ILE:HG12	1:D:340:LEU:HG	1.87	0.56
1:A:239:GLU:HB3	4:A:504:PEG:H32	1.87	0.56
1:C:164:LEU:HA	1:C:174:VAL:HG12	1.88	0.56
1:A:392:ARG:NH1	11:A:605:HOH:O	2.37	0.56
1:B:184:TRP:CZ2	8:B:509:1PE:H252	2.42	0.55
1:B:321:PTR:HD1	7:B:510:EPE:H52	1.88	0.55
1:C:216:GLU:O	1:C:218:LYS:N	2.39	0.55
1:A:227:HIS:HE1	11:A:616:HOH:O	1.90	0.54
1:A:392:ARG:HH12	1:A:396:GLU:HG3	1.72	0.54
1:C:164:LEU:HD11	1:C:172:GLN:HB3	1.90	0.54
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.90	0.53
1:B:295:LEU:HD23	1:B:303:ILE:HG22	1.91	0.53
1:A:300:ARG:HD2	11:A:603:HOH:O	2.07	0.53
1:D:145:TYR:CE1	1:D:193:LYS:HD3	2.44	0.53
1:D:290:PRO:HD3	1:D:350:ILE:HG12	1.91	0.52
1:A:145:TYR:CZ	1:A:193:LYS:HE3	2.43	0.52
1:B:300:ARG:HB3	1:B:300:ARG:CZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:GLU:HG3	7:D:505:EPE:C9	2.34	0.52
1:A:323:GLN:HB2	1:A:328:ARG:HG3	1.91	0.51
1:B:164:LEU:HD11	1:B:172:GLN:HB3	1.91	0.51
1:C:407:LYS:HB3	5:C:509:PGE:H32	1.91	0.51
1:C:424:HIS:HB2	2:C:504:IWU:N3	2.25	0.50
1:B:175:LYS:NZ	8:B:509:1PE:H221	2.23	0.50
1:A:239:GLU:HB3	4:A:504:PEG:H22	1.94	0.50
1:D:215:THR:O	1:D:216:GLU:HB2	2.12	0.50
1:A:392:ARG:NH2	1:A:397:LYS:H	2.10	0.49
1:A:323:GLN:O	1:A:328:ARG:NH1	2.45	0.49
1:C:225:LYS:O	1:C:226[B]:ARG:HG3	2.13	0.49
1:D:398:LEU:HD11	1:D:404:ASN:ND2	2.27	0.49
1:D:366:GLU:CG	7:D:505:EPE:H91	2.33	0.48
1:B:389:PRO:HA	4:B:504:PEG:H32	1.94	0.48
1:A:243:TYR:HB2	1:A:247:ASP:OD2	2.14	0.48
1:B:242:SER:OG	1:B:298:PRO:HD3	2.13	0.48
1:D:241:LEU:HD12	2:D:501:IWU:BR1	2.69	0.48
1:B:146:ASP:HB3	1:B:172:GLN:NE2	2.28	0.48
1:A:397:LYS:HE2	1:A:401:GLY:HA2	1.96	0.48
1:C:257:VAL:HB	1:C:261:LEU:HD23	1.96	0.48
1:C:289:LYS:HE2	1:C:291:GLU:OE2	2.13	0.48
1:C:392:ARG:O	1:C:406:LYS:NZ	2.41	0.47
1:B:321:PTR:CD1	7:B:510:EPE:H32	2.44	0.47
1:C:404:ASN:HB3	11:C:627:HOH:O	2.14	0.47
1:B:243:TYR:HB2	1:B:247:ASP:OD2	2.14	0.47
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.96	0.47
1:C:424:HIS:HB2	2:C:504:IWU:N2	2.30	0.46
1:B:393:LYS:HZ1	7:B:510:EPE:H101	1.79	0.46
1:B:204:VAL:O	1:B:208:GLU:HG3	2.16	0.46
1:A:239:GLU:CB	4:A:504:PEG:H22	2.44	0.46
1:A:220:TYR:CE1	1:A:268:GLN:HG2	2.51	0.46
1:C:147:TYR:HB2	1:C:233:HIS:CD2	2.51	0.46
1:A:394:PHE:HB2	1:A:395:PHE:CD2	2.51	0.45
1:C:334:LEU:HB3	1:C:388:ALA:HB1	1.97	0.45
1:C:344:MET:HG2	1:C:468:ILE:O	2.16	0.45
1:B:162:ASP:OD1	8:B:509:1PE:H162	2.16	0.45
1:B:257:VAL:HB	1:B:261:LEU:HD23	1.98	0.45
1:C:408:THR:HG21	1:C:415:TYR:HE2	1.81	0.45
1:D:330:PRO:HD3	1:D:345:TRP:CE2	2.51	0.45
1:D:471:TYR:O	1:D:475:GLN:HG3	2.17	0.45
1:A:300:ARG:HD3	1:B:177:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ILE:HG12	1:B:340:LEU:HD12	1.98	0.45
1:C:370:MET:O	1:C:374:VAL:HG23	2.17	0.45
1:A:170:PHE:CD1	1:A:188:LYS:HE3	2.52	0.45
1:D:453:LYS:NZ	2:D:502:IWU:N3	2.64	0.44
1:B:317:ARG:CZ	6:B:505:GOL:H31	2.48	0.44
1:B:317:ARG:O	6:B:505:GOL:O3	2.35	0.44
1:D:447:ALA:O	1:D:451:LYS:HG3	2.18	0.44
1:C:209:LEU:HD12	1:C:209:LEU:HA	1.81	0.44
1:C:243:TYR:CD2	1:C:247:ASP:HB3	2.52	0.44
1:A:392:ARG:NH2	11:A:619:HOH:O	2.51	0.43
1:B:398:LEU:HD11	1:B:404:ASN:ND2	2.32	0.43
1:D:210:MET:HG2	1:D:281:LEU:HD13	2.00	0.43
1:A:392:ARG:NH1	1:A:396:GLU:HA	2.32	0.43
1:A:194:LYS:NZ	11:A:611:HOH:O	2.39	0.43
6:B:506:GOL:H11	7:B:510:EPE:H62	2.00	0.43
1:C:164:LEU:CD1	1:C:172:GLN:HB3	2.48	0.43
1:C:394:PHE:HB2	1:C:395:PHE:CD2	2.53	0.43
1:C:170:PHE:CD2	1:C:188:LYS:HE3	2.52	0.43
1:B:162:ASP:OD1	1:B:163:SER:OG	2.33	0.43
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.83	0.43
7:D:505:EPE:S	7:D:505:EPE:H21	2.58	0.42
1:A:437[A]:ARG:NH1	11:A:620:HOH:O	2.52	0.42
1:C:361:PHE:CE1	1:C:373:ILE:HA	2.54	0.42
1:C:453:LYS:NZ	2:C:504:IWU:N3	2.67	0.42
7:C:510:EPE:H51	10:C:513:CL:CL	2.56	0.42
1:B:321:PTR:CG	7:B:510:EPE:H32	2.49	0.42
1:D:392:ARG:O	1:D:406:LYS:HD2	2.20	0.42
1:A:336:MET:HB3	1:A:337:PRO:HD2	2.02	0.42
1:B:317:ARG:H	1:B:317:ARG:HG3	1.66	0.42
1:A:392:ARG:HD2	1:A:392:ARG:HA	1.76	0.42
1:C:158:ARG:HG3	1:C:180:VAL:HG23	2.01	0.42
7:C:510:EPE:C5	10:C:513:CL:CL	3.05	0.41
1:D:434:PRO:O	1:D:437:ARG:HG3	2.20	0.41
1:A:224:LEU:HD11	1:A:236:LEU:HB3	2.03	0.41
1:A:408:THR:HG22	1:A:409:LYS:N	2.35	0.41
1:B:242:SER:HB2	1:B:295:LEU:O	2.21	0.41
1:C:245:LEU:HD23	1:C:245:LEU:HA	1.82	0.41
1:C:381:PRO:HG2	1:C:384:ILE:HD12	2.03	0.41
1:D:303:ILE:O	1:D:304:LYS:HD2	2.22	0.40
6:B:507:GOL:O1	6:B:507:GOL:O3	2.29	0.40
1:D:164:LEU:HD21	1:D:172:GLN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:PHE:CE2	1:D:231:ARG:HD2	2.55	0.40
1:D:469:GLN:H	1:D:469:GLN:HG2	1.36	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	346/382 (91%)	330 (95%)	15 (4%)	1 (0%)	41	50
1	B	344/382 (90%)	329 (96%)	15 (4%)	0	100	100
1	C	344/382 (90%)	324 (94%)	20 (6%)	0	100	100
1	D	343/382 (90%)	323 (94%)	20 (6%)	0	100	100
All	All	1377/1528 (90%)	1306 (95%)	70 (5%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	LYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/339 (89%)	293 (97%)	9 (3%)	41	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	298/339 (88%)	290 (97%)	8 (3%)	44	61
1	C	286/339 (84%)	279 (98%)	7 (2%)	49	66
1	D	292/339 (86%)	278 (95%)	14 (5%)	25	36
All	All	1178/1356 (87%)	1140 (97%)	38 (3%)	39	54

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	ARG
1	A	212	LYS
1	A	215	THR
1	A	218	LYS
1	A	221	ILE
1	A	251	ASN
1	A	267	GLN
1	A	300	ARG
1	A	392	ARG
1	B	167	LYS
1	B	212	LYS
1	B	215	THR
1	B	255	ARG
1	B	300	ARG
1	B	330	PRO
1	B	410	ASP
1	B	480	LYS
1	C	144	ASN
1	C	157	ASP
1	C	215	THR
1	C	217	MET
1	C	218	LYS
1	C	243	TYR
1	C	407	LYS
1	D	182	GLN
1	D	194	LYS
1	D	217	MET
1	D	226	ARG
1	D	232	ASN
1	D	240	MET
1	D	245	LEU
1	D	251	ASN
1	D	304	LYS

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Mol	Chain	Res	Type
1	D	318	ILE
1	D	324	SER
1	D	400	ASP
1	D	465	LYS
1	D	469	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	383	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PTR	A	321	1	15,16,17	0.77	0	19,22,24	1.15	1 (5%)
1	PTR	D	321	1	15,16,17	0.86	0	19,22,24	1.07	0
1	PTR	B	321	1	15,16,17	0.84	0	19,22,24	1.53	4 (21%)
1	PTR	C	321	1	15,16,17	0.80	0	19,22,24	0.92	0

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1
1	PTR	D	321	1	-	1/10/11/13	0/1/1/1
1	PTR	B	321	1	-	1/10/11/13	0/1/1/1
1	PTR	C	321	1	-	1/10/11/13	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	PTR	CG-CB-CA	3.10	120.38	114.10
1	B	321	PTR	CB-CG-CD2	-2.95	115.06	120.91
1	A	321	PTR	P-OH-CZ	2.44	131.58	123.75
1	B	321	PTR	CB-CG-CD1	2.05	124.98	120.91
1	B	321	PTR	O3P-P-O1P	2.04	118.68	110.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	321	PTR	O-C-CA-CB
1	B	321	PTR	O-C-CA-CB
1	C	321	PTR	O-C-CA-CB
1	D	321	PTR	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	321	PTR	3	0
1	C	321	PTR	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 5 are monoatomic - leaving 47 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
7	EPE	D	505	-	12,12,15	0.88	1 (8%)	14,16,20	0.82	0
2	IWU	D	502	-	8,11,11	1.26	0	7,15,15	1.69	3 (42%)
6	GOL	B	506	-	5,5,5	0.84	0	5,5,5	0.86	0
4	PEG	C	506	-	6,6,6	0.14	0	5,5,5	0.15	0
9	SO4	A	514	-	4,4,4	0.22	0	6,6,6	0.19	0
6	GOL	A	507	-	5,5,5	0.98	0	5,5,5	1.09	0
9	SO4	B	512	-	4,4,4	0.21	0	6,6,6	0.19	0
6	GOL	B	508	-	5,5,5	0.88	0	5,5,5	0.94	0
5	PGE	D	504	-	9,9,9	0.40	0	8,8,8	0.31	0
7	EPE	C	510	-	12,12,15	1.18	1 (8%)	14,16,20	1.56	2 (14%)
9	SO4	C	511	-	4,4,4	0.10	0	6,6,6	0.39	0
3	PG4	A	502	-	12,12,12	0.20	0	11,11,11	0.50	0
9	SO4	A	510	-	4,4,4	0.18	0	6,6,6	0.20	0
4	PEG	D	503	-	6,6,6	0.22	0	5,5,5	0.08	0
8	IPE	B	509	-	15,15,15	0.24	0	14,14,14	0.22	0
9	SO4	D	507	-	4,4,4	0.20	0	6,6,6	0.19	0
9	SO4	B	511	-	4,4,4	0.15	0	6,6,6	0.43	0
4	PEG	B	504	-	6,6,6	0.31	0	5,5,5	0.13	0
4	PEG	C	501	-	6,6,6	0.33	0	5,5,5	0.20	0
2	IWU	C	502	-	8,11,11	1.29	2 (25%)	7,15,15	1.65	3 (42%)
6	GOL	B	503	-	5,5,5	0.97	0	5,5,5	0.78	0
2	IWU	A	501	-	8,11,11	1.22	1 (12%)	7,15,15	1.89	3 (42%)
6	GOL	B	507	-	5,5,5	1.25	0	5,5,5	1.78	2 (40%)
9	SO4	A	511	-	4,4,4	0.63	0	6,6,6	0.87	0
5	PGE	A	505	-	9,9,9	0.48	0	8,8,8	0.40	0
2	IWU	B	501	-	8,11,11	1.28	1 (12%)	7,15,15	1.72	3 (42%)
9	SO4	A	512	-	4,4,4	0.31	0	6,6,6	0.48	0
9	SO4	A	513	-	4,4,4	0.31	0	6,6,6	0.71	0
9	SO4	B	513	-	4,4,4	0.20	0	6,6,6	0.28	0
5	PGE	A	506	-	9,9,9	0.44	0	8,8,8	0.70	0
5	PGE	C	509	-	9,9,9	0.37	0	8,8,8	0.53	0
6	GOL	C	507	-	5,5,5	0.76	0	5,5,5	0.96	0
6	GOL	C	508	-	5,5,5	0.94	0	5,5,5	0.98	0
9	SO4	C	512	-	4,4,4	0.15	0	6,6,6	0.36	0
3	PG4	C	503	-	12,12,12	0.25	0	11,11,11	0.42	0
4	PEG	C	505	-	6,6,6	0.30	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EPE	B	510	-	12,12,15	0.77	1 (8%)	14,16,20	0.90	1 (7%)
2	IWU	A	503	-	8,11,11	1.30	0	7,15,15	1.58	2 (28%)
8	1PE	A	509	-	15,15,15	0.27	0	14,14,14	0.28	0
4	PEG	A	504	-	6,6,6	0.16	0	5,5,5	0.15	0
6	GOL	B	505	-	5,5,5	1.06	1 (20%)	5,5,5	1.08	0
2	IWU	B	502	-	8,11,11	1.29	0	7,15,15	1.70	1 (14%)
9	SO4	D	506	-	4,4,4	0.15	0	6,6,6	0.36	0
9	SO4	D	508	-	4,4,4	0.14	0	6,6,6	0.28	0
2	IWU	D	501	-	8,11,11	1.29	1 (12%)	7,15,15	1.76	3 (42%)
7	EPE	A	508	-	13,13,15	0.82	1 (7%)	16,18,20	1.03	1 (6%)
2	IWU	C	504	-	8,11,11	1.28	0	7,15,15	1.72	2 (28%)

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
7	EPE	D	505	-	-	5/6/14/19	1/1/1/1
2	IWU	D	502	-	-	-	0/2/2/2
6	GOL	B	506	-	-	4/4/4/4	-
4	PEG	C	506	-	-	2/4/4/4	-
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	B	508	-	-	4/4/4/4	-
5	PGE	D	504	-	-	2/7/7/7	-
7	EPE	C	510	-	-	3/6/14/19	0/1/1/1
3	PG4	A	502	-	-	2/10/10/10	-
4	PEG	D	503	-	-	1/4/4/4	-
8	1PE	B	509	-	-	6/13/13/13	-
4	PEG	B	504	-	-	2/4/4/4	-
4	PEG	C	501	-	-	2/4/4/4	-
2	IWU	C	502	-	-	-	0/2/2/2
6	GOL	B	503	-	-	4/4/4/4	-
2	IWU	A	501	-	-	-	0/2/2/2
6	GOL	B	507	-	-	2/4/4/4	-
2	IWU	B	502	-	-	-	0/2/2/2
5	PGE	A	505	-	-	4/7/7/7	-
2	IWU	B	501	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	A	506	-	-	5/7/7/7	-
5	PGE	C	509	-	-	6/7/7/7	-
6	GOL	C	507	-	-	2/4/4/4	-
6	GOL	C	508	-	-	1/4/4/4	-
3	PG4	C	503	-	-	3/10/10/10	-
4	PEG	C	505	-	-	3/4/4/4	-
7	EPE	B	510	-	-	2/6/14/19	0/1/1/1
2	IWU	A	503	-	-	-	0/2/2/2
4	PEG	A	504	-	-	2/4/4/4	-
6	GOL	B	505	-	-	0/4/4/4	-
8	1PE	A	509	-	-	2/13/13/13	-
2	IWU	D	501	-	-	-	0/2/2/2
7	EPE	A	508	-	-	1/6/16/19	0/1/1/1
2	IWU	C	504	-	-	-	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	510	EPE	O2S-S	3.89	1.56	1.45
7	D	505	EPE	O3S-S	2.92	1.58	1.47
7	B	510	EPE	O3S-S	2.54	1.56	1.47
7	A	508	EPE	O3S-S	2.37	1.56	1.47
6	B	505	GOL	C1-C2	2.10	1.60	1.51
2	A	501	IWU	C3-N1	-2.10	1.34	1.37
2	B	501	IWU	C3-N1	-2.08	1.34	1.37
2	D	501	IWU	C3-N1	-2.02	1.34	1.37
2	C	502	IWU	C3-N1	-2.02	1.34	1.37
2	C	502	IWU	C2-N1	2.01	1.35	1.31

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	510	EPE	O2S-S-C10	-4.32	101.71	106.92
7	C	510	EPE	O3S-S-O1S	3.05	118.73	111.27
2	A	501	IWU	C1-C5-C4	-2.97	115.42	118.55
6	B	507	GOL	O1-C1-C2	-2.76	96.96	110.20
2	C	504	IWU	C1-C5-C4	-2.74	115.66	118.55
2	B	502	IWU	C1-C5-C4	-2.65	115.76	118.55
2	D	501	IWU	C1-C5-C4	-2.56	115.85	118.55
2	B	501	IWU	C1-C5-C4	-2.40	116.02	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	507	GOL	C3-C2-C1	-2.40	102.39	111.70
2	D	502	IWU	C1-C5-C4	-2.32	116.10	118.55
2	D	502	IWU	C5-C4-C3	-2.31	118.79	121.12
2	D	501	IWU	C5-C4-C3	-2.30	118.81	121.12
2	B	501	IWU	C5-C4-N4	2.27	134.19	130.51
7	A	508	EPE	O3S-S-O2S	-2.26	105.74	111.27
2	B	501	IWU	C5-C4-C3	-2.26	118.84	121.12
7	B	510	EPE	O3S-S-O2S	-2.24	105.80	111.27
2	C	502	IWU	C1-C5-C4	-2.24	116.19	118.55
2	D	501	IWU	C5-C4-N4	2.23	134.12	130.51
2	A	501	IWU	C5-C4-N4	2.19	134.06	130.51
2	C	502	IWU	C5-C4-C3	-2.14	118.96	121.12
2	A	503	IWU	C5-C4-C3	-2.12	118.99	121.12
2	A	501	IWU	C5-C4-C3	-2.10	119.00	121.12
2	A	503	IWU	C1-C5-C4	-2.09	116.35	118.55
2	D	502	IWU	C5-C4-N4	2.08	133.89	130.51
2	C	504	IWU	C5-C4-C3	-2.06	119.05	121.12
2	C	502	IWU	C5-C4-N4	2.04	133.82	130.51

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	503	GOL	C1-C2-C3-O3
6	B	503	GOL	O2-C2-C3-O3
6	B	506	GOL	C1-C2-C3-O3
6	B	508	GOL	O1-C1-C2-C3
6	B	508	GOL	C1-C2-C3-O3
7	A	508	EPE	S-C10-C9-N1
7	B	510	EPE	C10-C9-N1-C6
7	C	510	EPE	C10-C9-N1-C2
7	C	510	EPE	C10-C9-N1-C6
7	D	505	EPE	C10-C9-N1-C2
4	C	505	PEG	C4-C3-O2-C2
5	A	505	PGE	O2-C3-C4-O3
6	B	503	GOL	O1-C1-C2-O2
4	B	504	PEG	O1-C1-C2-O2
5	C	509	PGE	O3-C5-C6-O4
7	D	505	EPE	C9-C10-S-O3S
8	B	509	1PE	OH5-C14-C24-OH4
6	B	503	GOL	O1-C1-C2-C3
6	B	506	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	C	507	GOL	C1-C2-C3-O3
5	A	505	PGE	O1-C1-C2-O2
6	B	506	GOL	O1-C1-C2-O2
6	B	506	GOL	O2-C2-C3-O3
6	B	508	GOL	O1-C1-C2-O2
6	B	508	GOL	O2-C2-C3-O3
6	C	507	GOL	O2-C2-C3-O3
5	A	506	PGE	O2-C3-C4-O3
5	C	509	PGE	O2-C3-C4-O3
5	D	504	PGE	O2-C3-C4-O3
4	C	506	PEG	O1-C1-C2-O2
4	D	503	PEG	O2-C3-C4-O4
5	A	506	PGE	O3-C5-C6-O4
8	B	509	1PE	OH4-C13-C23-OH3
6	A	507	GOL	O1-C1-C2-O2
8	A	509	1PE	OH5-C14-C24-OH4
8	B	509	1PE	OH7-C16-C26-OH6
3	C	503	PG4	O3-C5-C6-O4
3	C	503	PG4	O1-C1-C2-O2
7	D	505	EPE	C10-C9-N1-C6
3	A	502	PG4	O1-C1-C2-O2
8	B	509	1PE	C12-C22-OH3-C23
5	C	509	PGE	C1-C2-O2-C3
4	A	504	PEG	C1-C2-O2-C3
5	A	506	PGE	C6-C5-O3-C4
5	D	504	PGE	C6-C5-O3-C4
5	C	509	PGE	C3-C4-O3-C5
5	C	509	PGE	C6-C5-O3-C4
5	A	506	PGE	C3-C4-O3-C5
4	C	501	PEG	C4-C3-O2-C2
6	B	507	GOL	O1-C1-C2-O2
5	A	506	PGE	O1-C1-C2-O2
4	C	501	PEG	C1-C2-O2-C3
7	D	505	EPE	C9-C10-S-O1S
7	D	505	EPE	C9-C10-S-O2S
3	C	503	PG4	C3-C4-O3-C5
4	C	505	PEG	O1-C1-C2-O2
5	A	505	PGE	C1-C2-O2-C3
4	A	504	PEG	C4-C3-O2-C2
4	C	506	PEG	C1-C2-O2-C3
5	C	509	PGE	C4-C3-O2-C2
6	A	507	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	505	PEG	O2-C3-C4-O4
5	A	505	PGE	C6-C5-O3-C4
8	A	509	1PE	OH4-C13-C23-OH3
3	A	502	PG4	O4-C7-C8-O5
4	B	504	PEG	C1-C2-O2-C3
6	B	507	GOL	O1-C1-C2-C3
6	C	508	GOL	O1-C1-C2-C3
8	B	509	1PE	C13-C23-OH3-C22
8	B	509	1PE	C24-C14-OH5-C25
7	C	510	EPE	S-C10-C9-N1
7	B	510	EPE	C10-C9-N1-C2

All (1) ring outliers are listed below:

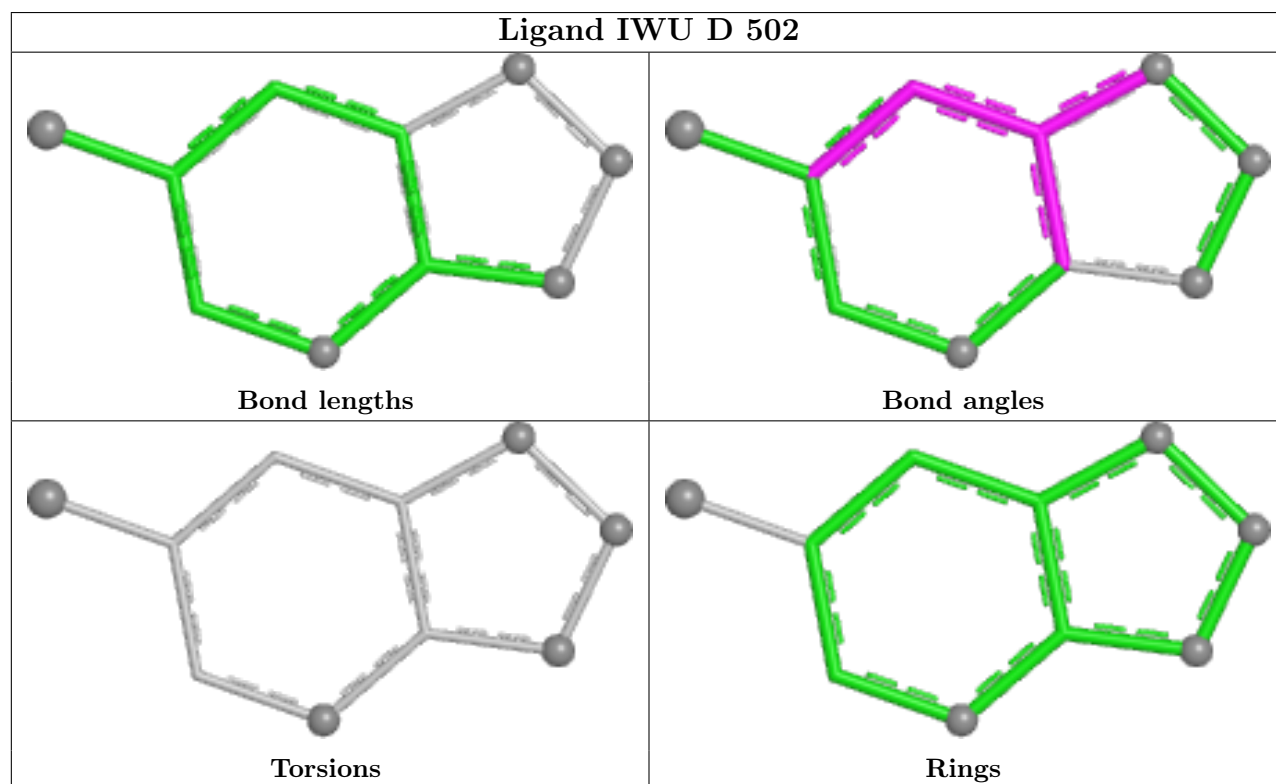
Mol	Chain	Res	Type	Atoms
7	D	505	EPE	C2-C3-C5-C6-N1-N4

20 monomers are involved in 39 short contacts:

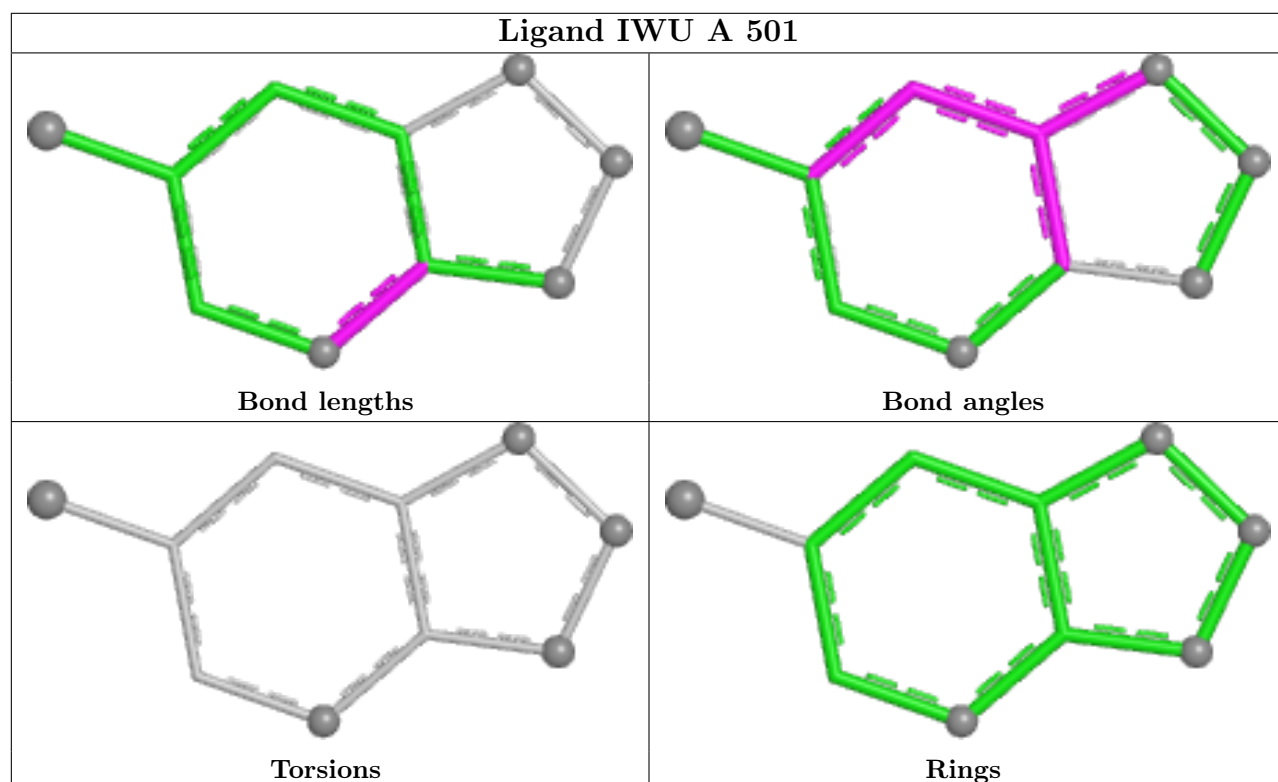
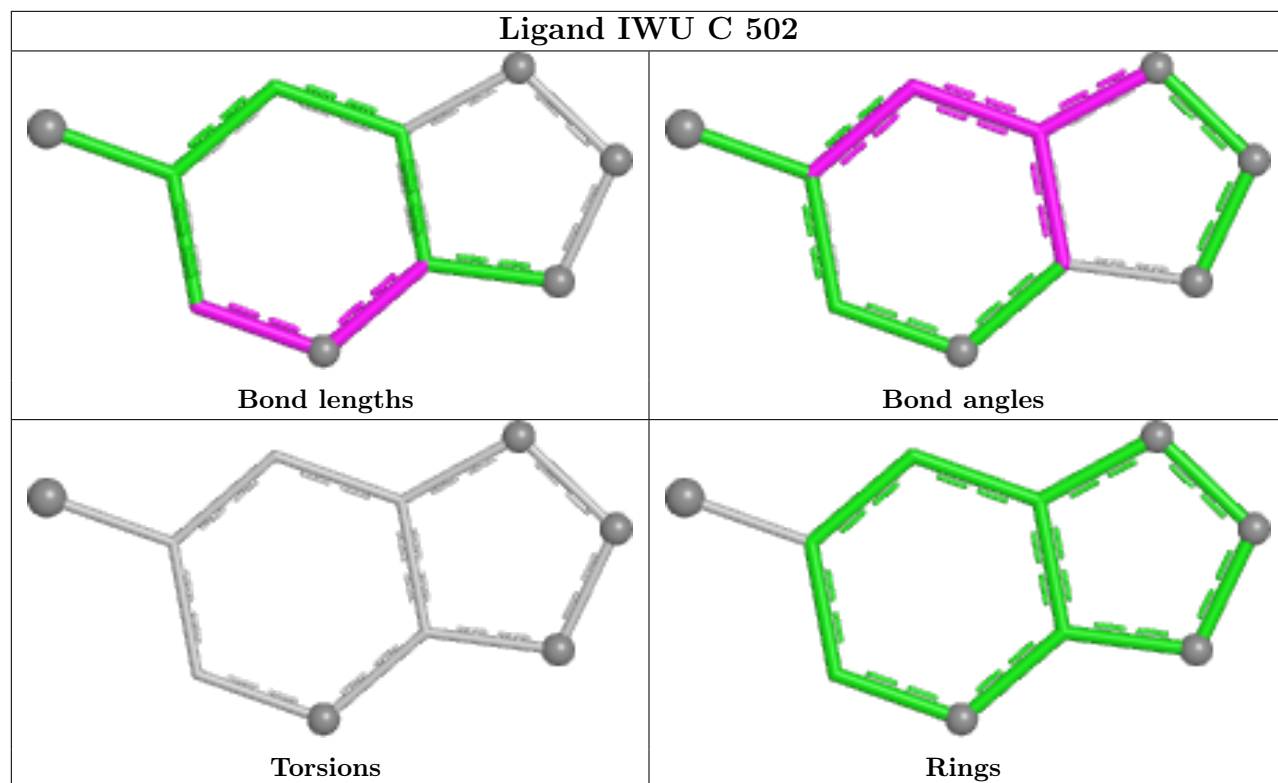
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	505	EPE	5	0
2	D	502	IWU	1	0
6	B	506	GOL	1	0
6	A	507	GOL	1	0
7	C	510	EPE	4	0
8	B	509	1PE	4	0
9	D	507	SO4	1	0
4	B	504	PEG	1	0
6	B	503	GOL	2	0
6	B	507	GOL	1	0
9	A	511	SO4	1	0
5	A	506	PGE	1	0
5	C	509	PGE	1	0
7	B	510	EPE	5	0
8	A	509	1PE	1	0
4	A	504	PEG	3	0
6	B	505	GOL	2	0
2	D	501	IWU	1	0
7	A	508	EPE	2	0
2	C	504	IWU	3	0

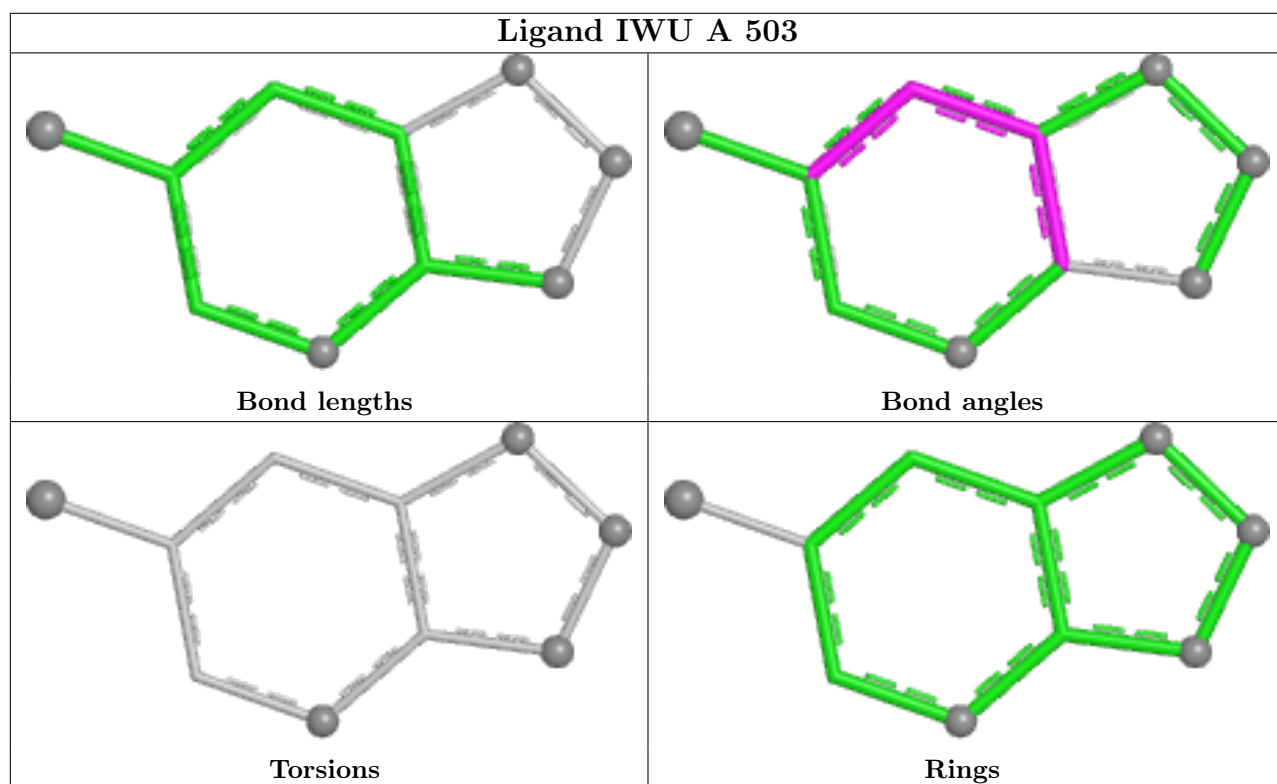
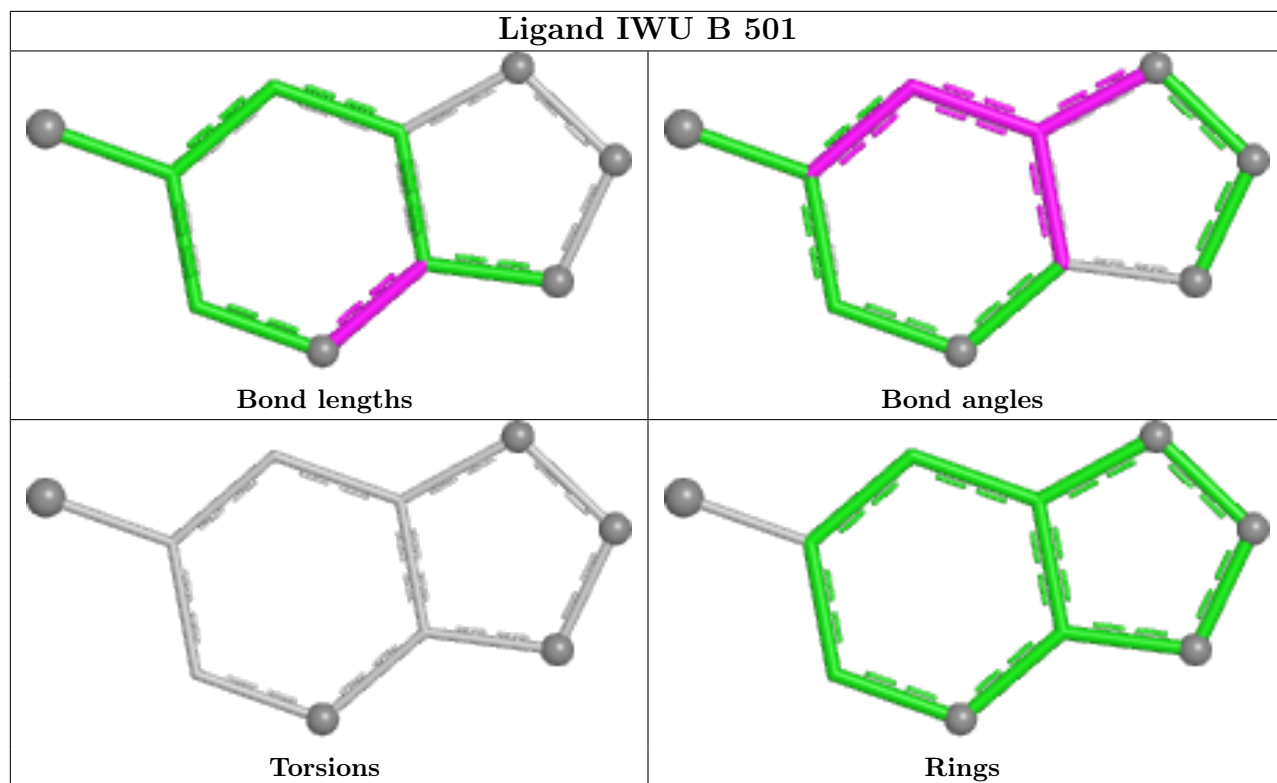
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

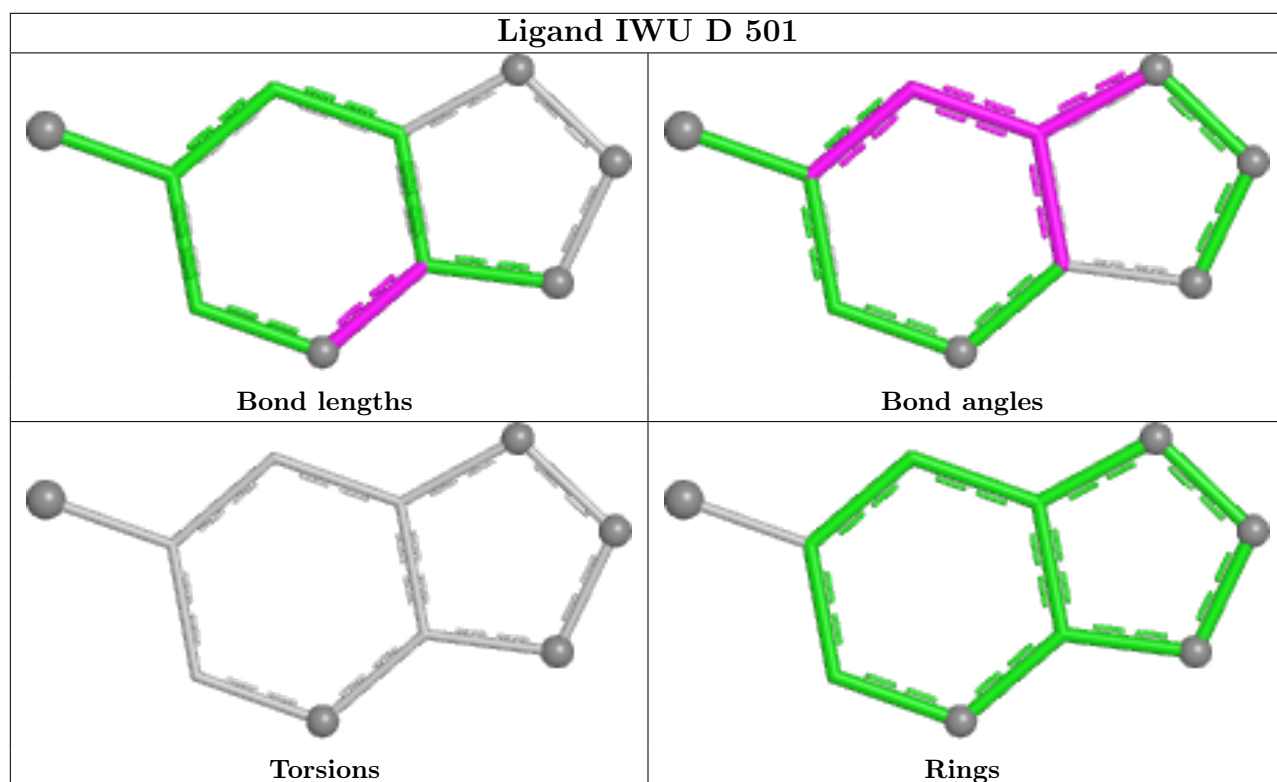
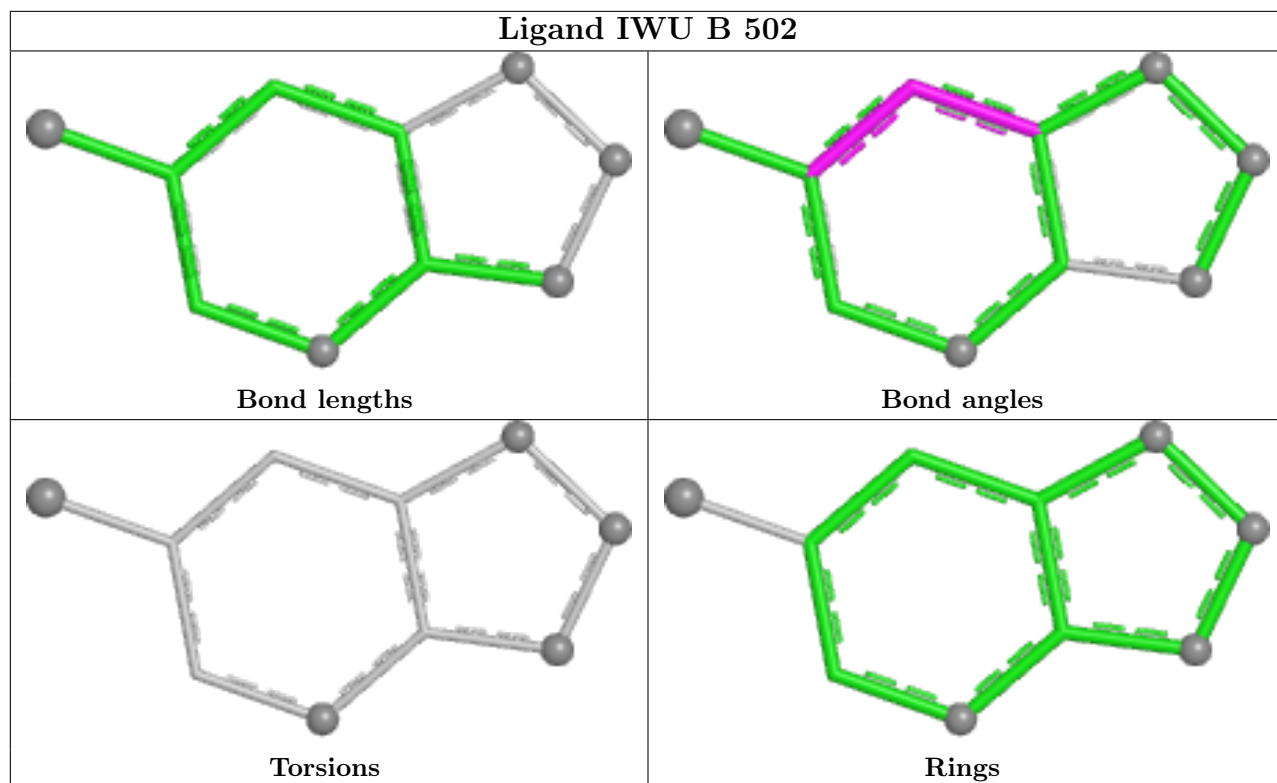
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

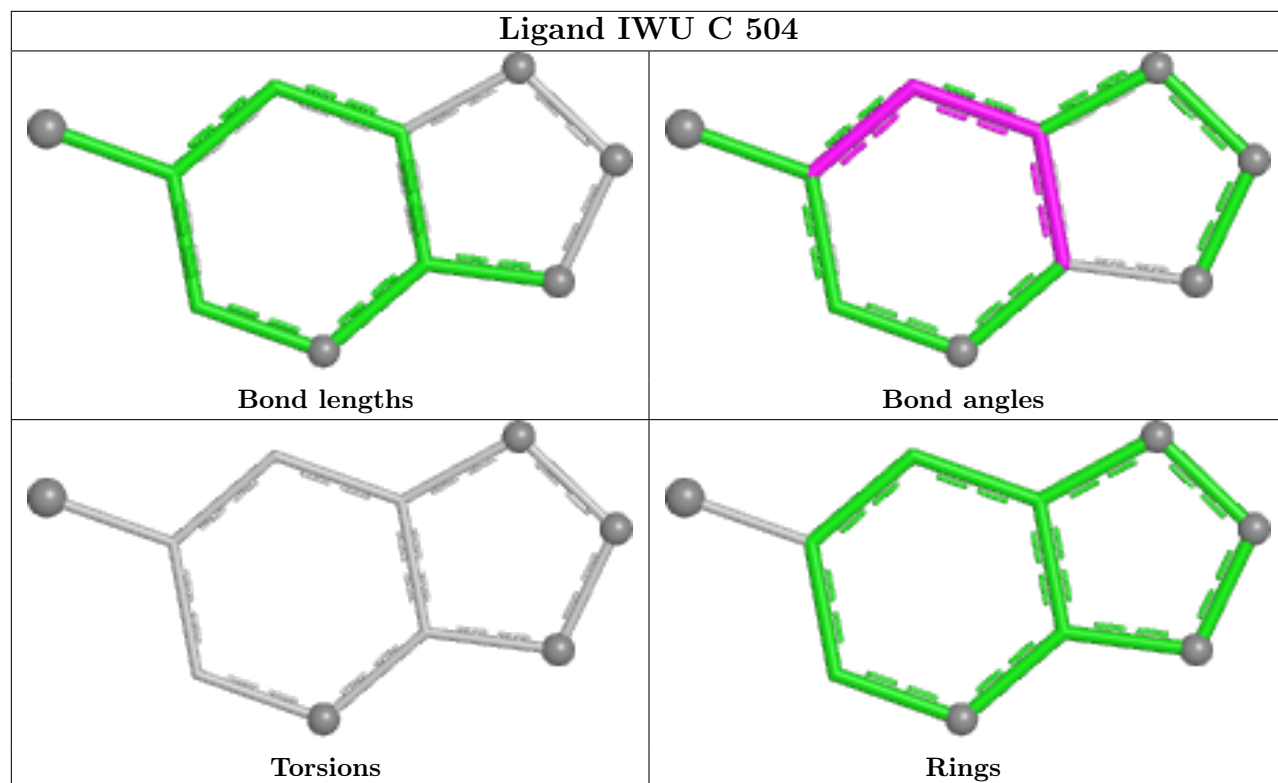












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	347/382 (90%)	-0.02	3 (0%) 84 88	30, 43, 70, 104	0
1	B	346/382 (90%)	-0.06	4 (1%) 79 83	36, 48, 73, 99	0
1	C	345/382 (90%)	0.10	17 (4%) 29 36	42, 63, 100, 114	0
1	D	345/382 (90%)	0.17	14 (4%) 37 44	46, 66, 92, 114	0
All	All	1383/1528 (90%)	0.05	38 (2%) 54 62	30, 56, 91, 114	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	440	GLY	4.4
1	D	398	LEU	4.0
1	C	140	TYR	3.9
1	C	243	TYR	3.9
1	B	408	THR	3.6
1	D	155	TRP	3.6
1	C	157	ASP	3.5
1	C	138	ASP	3.4
1	A	135	VAL	3.4
1	D	409	LYS	3.3
1	A	215	THR	3.1
1	C	241	LEU	3.1
1	D	401	GLY	3.1
1	B	243	TYR	2.9
1	D	399	PRO	2.7
1	C	443	GLY	2.7
1	D	403	TRP	2.6
1	C	298	PRO	2.5
1	C	440	GLY	2.5
1	C	152	GLY	2.4
1	C	238	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	150	LYS	2.3
1	D	138	ASP	2.3
1	B	242	SER	2.2
1	D	381	PRO	2.2
1	C	219	TYR	2.2
1	D	136	TYR	2.2
1	C	411	GLY	2.1
1	D	140	TYR	2.1
1	C	155	TRP	2.1
1	C	215	THR	2.1
1	A	360	LEU	2.1
1	C	432	GLY	2.1
1	D	400	ASP	2.1
1	C	439	ALA	2.0
1	D	318	ILE	2.0
1	B	318	ILE	2.0
1	C	148	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PTR	C	321	16/17	0.91	0.12	72,80,87,92	0
1	PTR	D	321	16/17	0.91	0.20	66,76,82,82	0
1	PTR	B	321	16/17	0.92	0.14	61,68,72,76	0
1	PTR	A	321	16/17	0.96	0.13	44,58,59,60	0

## 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(Å <sup>2</sup> )	Q<0.9
10	CL	A	516	1/1	0.73	0.35	75,75,75,75	0
6	GOL	C	508	6/6	0.78	0.18	85,93,96,97	0
7	EPE	A	508	13/15	0.80	0.36	65,75,89,96	0
4	PEG	B	504	7/7	0.81	0.34	60,65,72,72	0
5	PGE	D	504	10/10	0.82	0.14	73,84,90,91	0
5	PGE	C	509	10/10	0.83	0.15	58,73,79,83	0
6	GOL	B	505	6/6	0.84	0.25	75,76,77,80	0
4	PEG	D	503	7/7	0.85	0.22	71,76,79,81	0
5	PGE	A	506	10/10	0.85	0.16	45,58,73,77	0
7	EPE	B	510	12/15	0.86	0.23	67,77,88,88	0
6	GOL	B	503	6/6	0.87	0.13	50,55,62,63	0
9	SO4	A	514	5/5	0.87	0.28	80,80,92,98	0
9	SO4	D	508	5/5	0.87	0.21	90,93,108,120	0
3	PG4	C	503	13/13	0.87	0.13	56,61,71,72	0
6	GOL	B	506	6/6	0.88	0.14	68,72,76,78	0
6	GOL	B	508	6/6	0.88	0.41	67,69,72,73	0
8	1PE	B	509	16/16	0.89	0.14	57,63,72,73	0
6	GOL	C	507	6/6	0.89	0.34	65,70,73,78	0
4	PEG	C	505	7/7	0.89	0.14	53,60,63,69	0
7	EPE	D	505	12/15	0.89	0.17	59,81,92,95	0
7	EPE	C	510	12/15	0.90	0.19	71,82,94,95	0
6	GOL	B	507	6/6	0.90	0.26	43,52,63,64	0
5	PGE	A	505	10/10	0.90	0.12	48,62,67,70	0
4	PEG	A	504	7/7	0.91	0.19	54,62,67,71	0
9	SO4	A	511	5/5	0.91	0.15	51,54,76,83	0
9	SO4	A	513	5/5	0.91	0.22	74,76,82,91	0
4	PEG	C	501	7/7	0.92	0.14	48,56,61,61	0
10	CL	A	517	1/1	0.92	0.09	73,73,73,73	0
6	GOL	A	507	6/6	0.93	0.20	58,63,65,68	0
9	SO4	D	507	5/5	0.93	0.20	80,92,99,111	0
9	SO4	A	510	5/5	0.93	0.25	90,96,104,108	0
2	IWU	B	502	10/10	0.93	0.09	38,42,46,75	0
2	IWU	D	502	10/10	0.93	0.10	57,66,70,95	0
10	CL	B	514	1/1	0.93	0.24	76,76,76,76	0
2	IWU	C	504	10/10	0.94	0.10	53,60,63,93	0
8	1PE	A	509	16/16	0.94	0.14	55,63,67,67	0
4	PEG	C	506	7/7	0.94	0.09	72,74,75,77	0
2	IWU	A	503	10/10	0.94	0.11	38,44,46,74	0
10	CL	C	513	1/1	0.94	0.06	85,85,85,85	0
2	IWU	C	502	10/10	0.95	0.09	60,66,70,88	0
10	CL	A	515	1/1	0.95	0.10	69,69,69,69	0
9	SO4	C	512	5/5	0.96	0.13	64,74,77,77	0
3	PG4	A	502	13/13	0.96	0.14	32,43,53,55	0

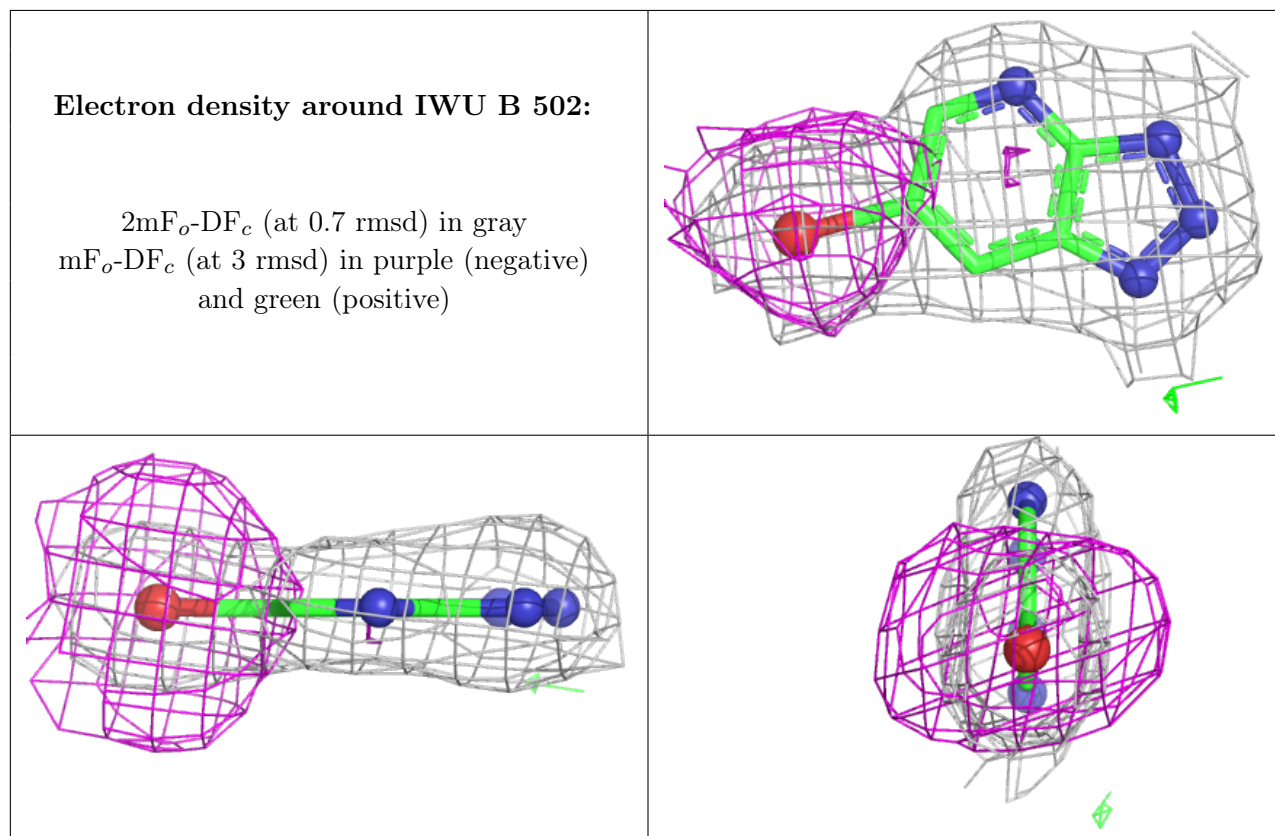
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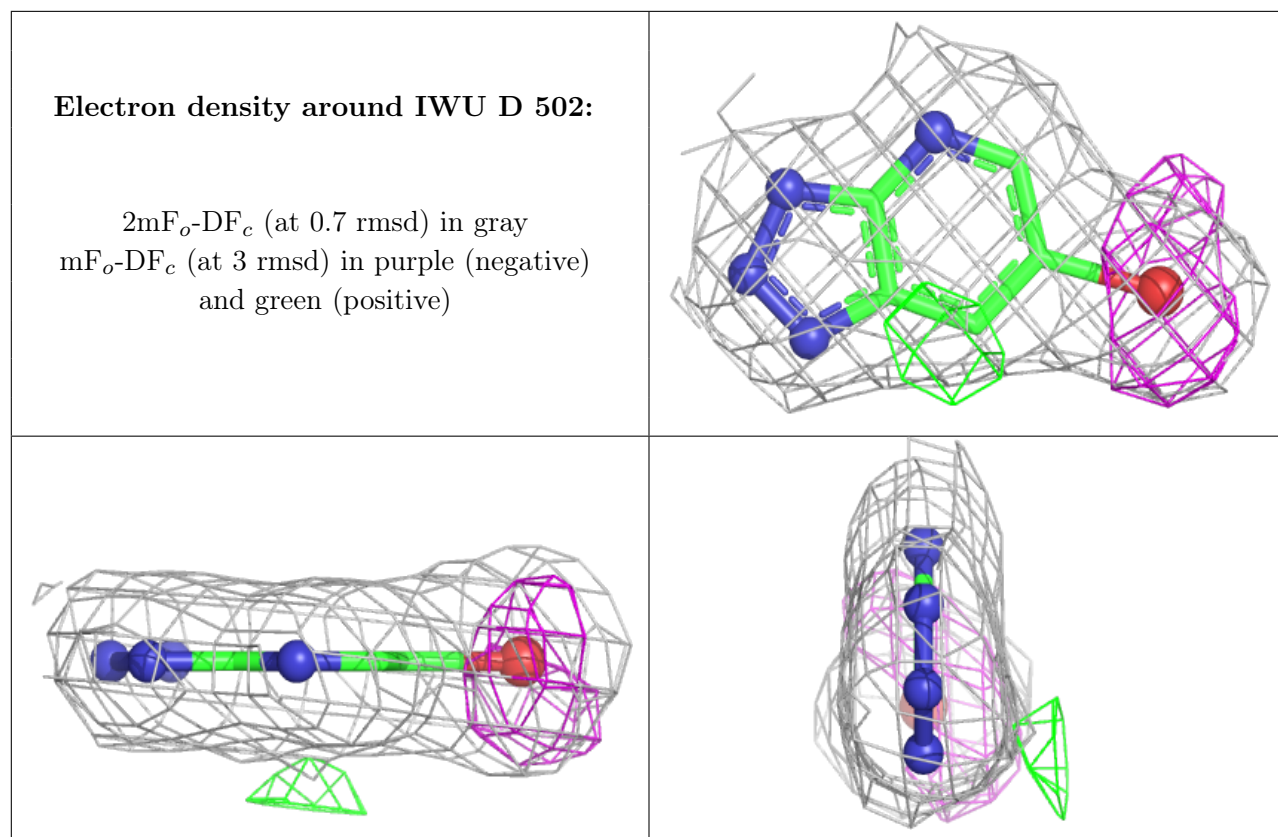
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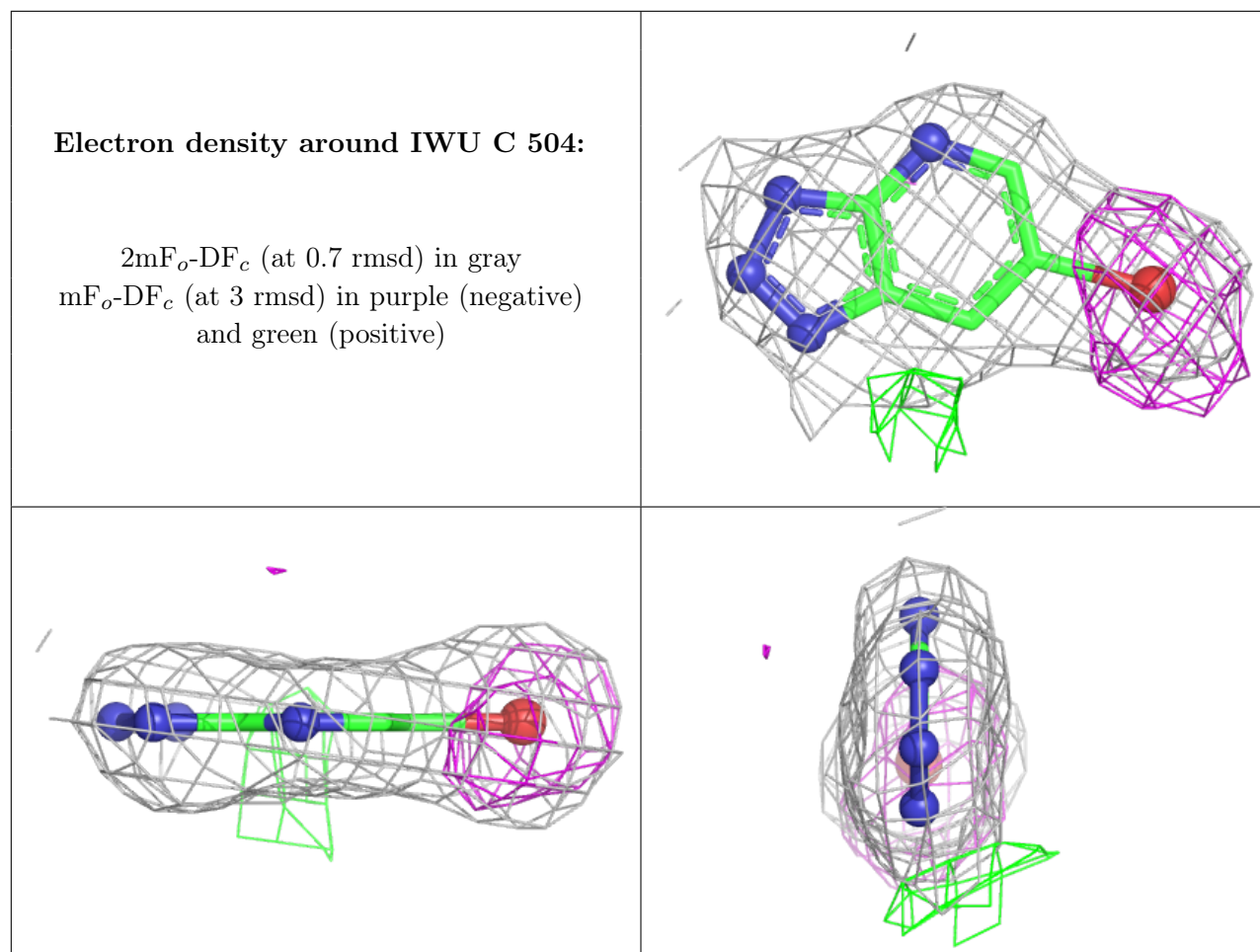
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	SO4	A	512	5/5	0.97	0.10	49,57,64,68	0
9	SO4	B	513	5/5	0.97	0.16	57,64,73,76	0
9	SO4	C	511	5/5	0.98	0.11	51,58,67,68	0
2	IWU	A	501	10/10	0.98	0.11	39,43,48,54	0
9	SO4	D	506	5/5	0.98	0.10	55,58,67,69	0
9	SO4	B	512	5/5	0.98	0.19	66,69,76,86	0
2	IWU	B	501	10/10	0.98	0.12	45,49,55,56	0
2	IWU	D	501	10/10	0.99	0.15	62,67,75,77	0
9	SO4	B	511	5/5	0.99	0.08	62,62,66,69	0

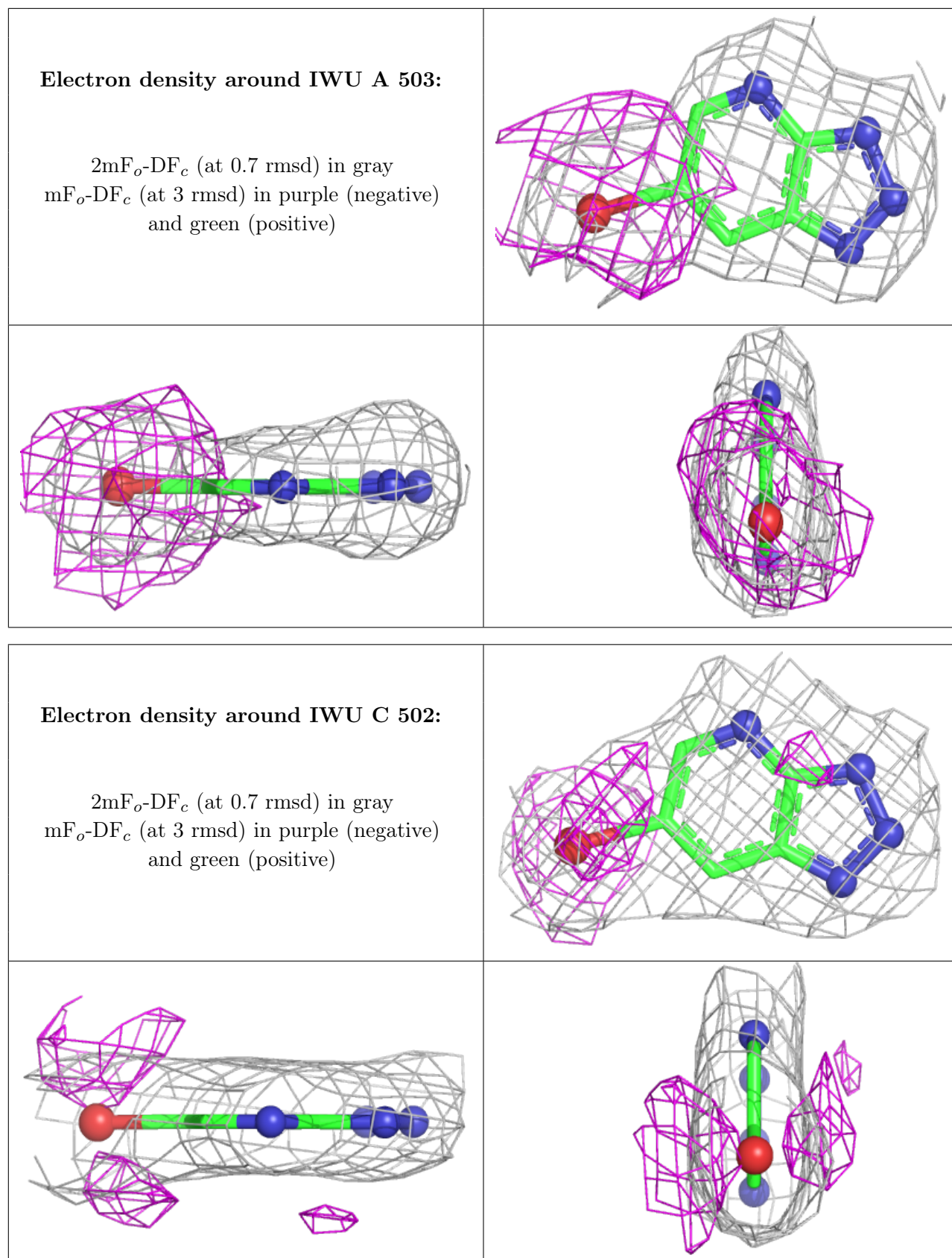
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





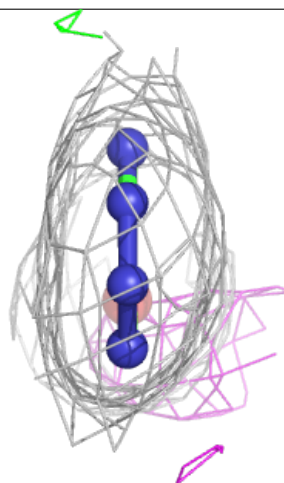
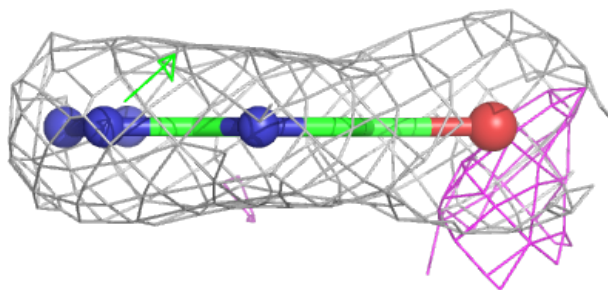
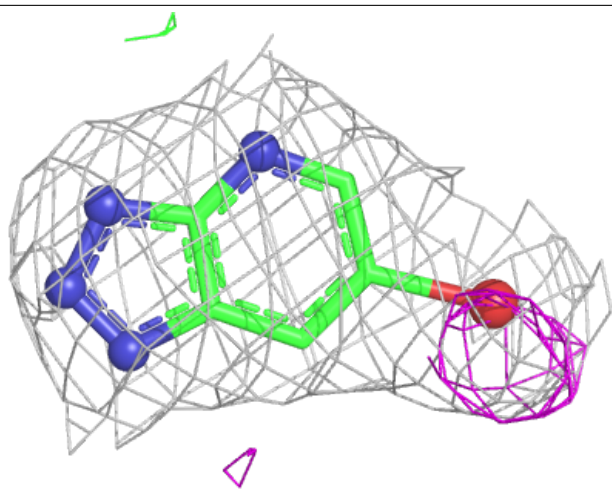


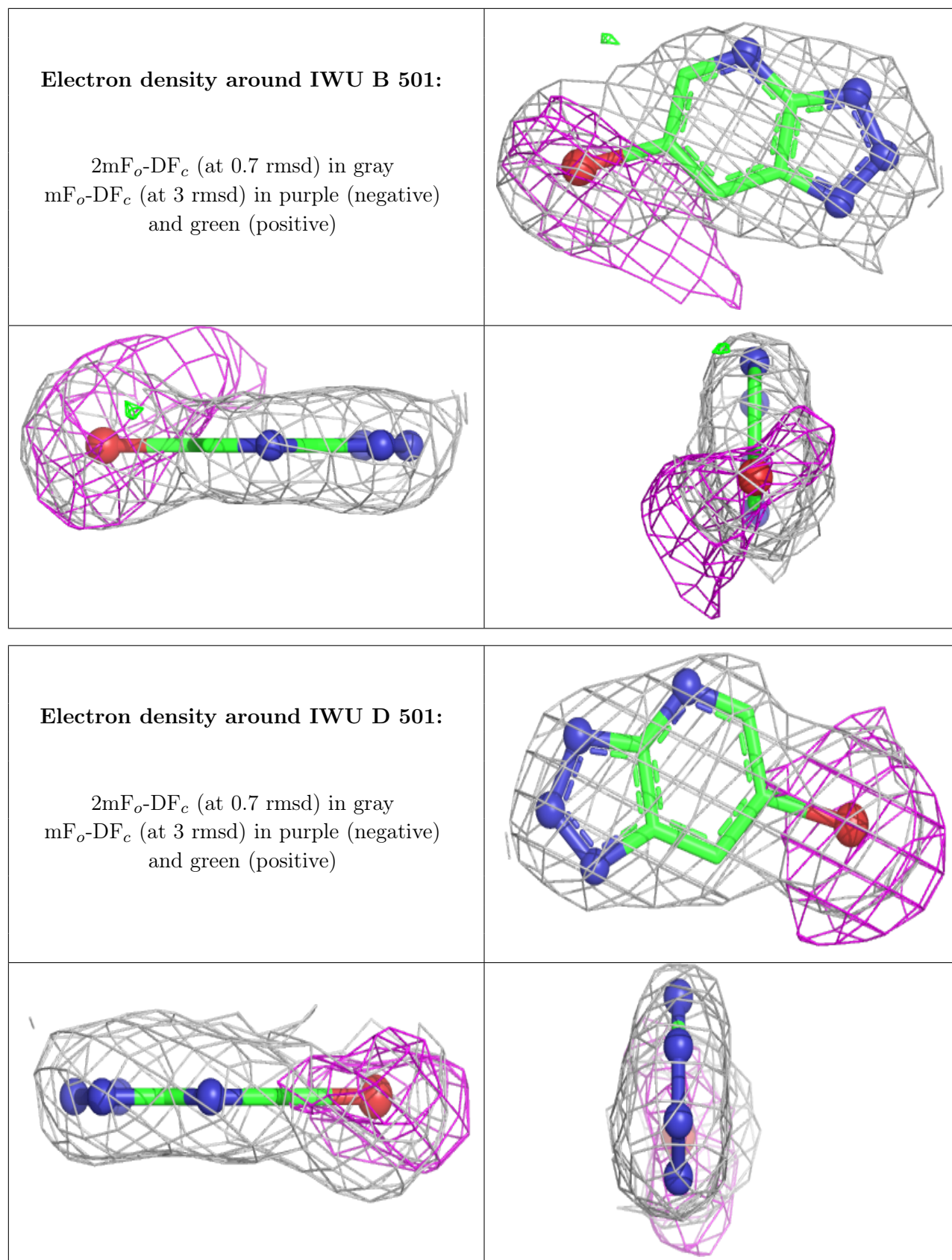




**Electron density around IWU A 501:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.