



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:14 PM UTC

PDB ID : 7ZH8 / pdb_00007zh8
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 wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

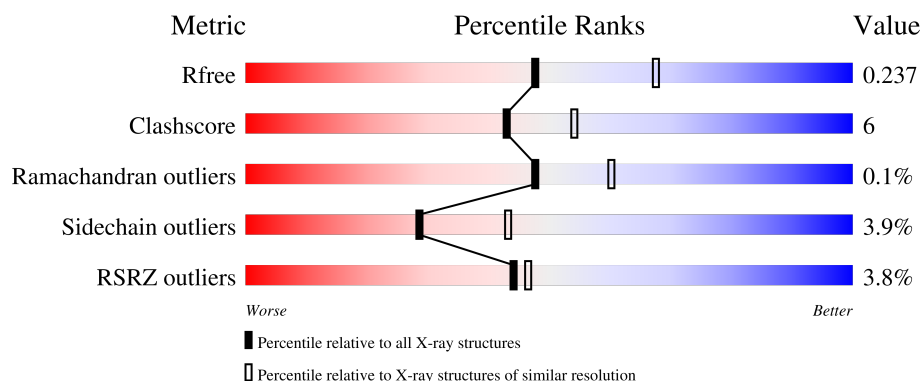
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 ≥ 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	 3% 78% 12% • 9%
1	B	382	 3% 79% 11% • 9%
1	C	382	 4% 77% 12% • 9%
1	D	382	 3% 76% 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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CL	C	513	-	-	X	-

2 Entry composition

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

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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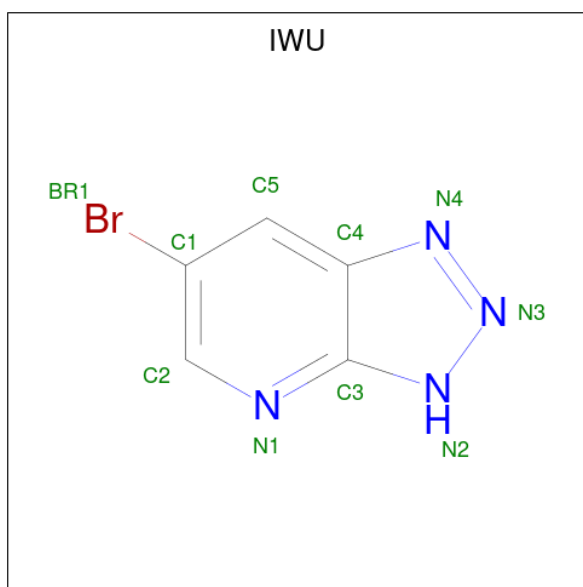
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A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	104	MET	-	initiating methionine	UNP Q13627
B	105	HIS	-	expression tag	UNP Q13627
B	106	HIS	-	expression tag	UNP Q13627
B	107	HIS	-	expression tag	UNP Q13627
B	108	HIS	-	expression 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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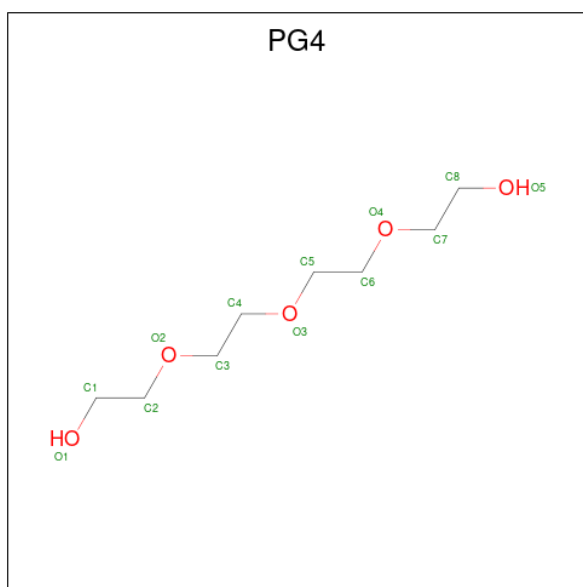
Chain	Residue	Modelled	Actual	Comment	Reference
C	121	LEU	-	expression tag	UNP Q13627
C	122	TYR	-	expression tag	UNP Q13627
C	123	PHE	-	expression tag	UNP Q13627
C	124	GLN	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627
D	104	MET	-	initiating methionine	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 (CCD ID: IWU) (formula: $C_5H_3BrN_4$) (labeled as "Ligand of Interest" by depositor).



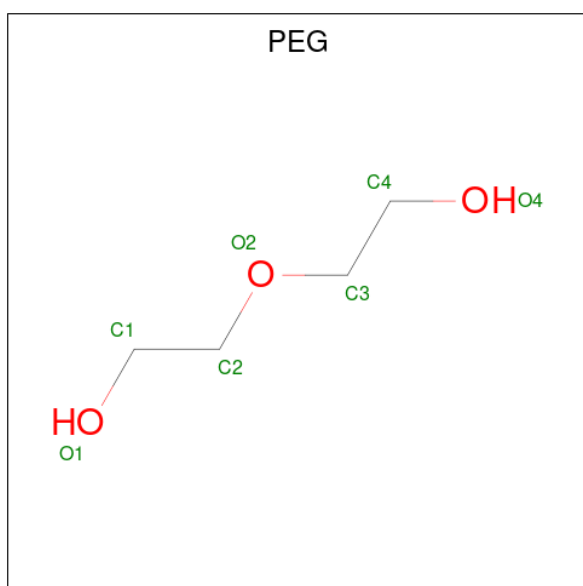
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	N	0	0
			10	1	5	4		
2	A	1	Total	Br	C	N	0	0
			10	1	5	4		
2	B	1	Total	Br	C	N	0	0
			10	1	5	4		
2	B	1	Total	Br	C	N	0	0
			10	1	5	4		
2	C	1	Total	Br	C	N	0	0
			10	1	5	4		
2	C	1	Total	Br	C	N	0	0
			10	1	5	4		
2	D	1	Total	Br	C	N	0	0
			10	1	5	4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

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



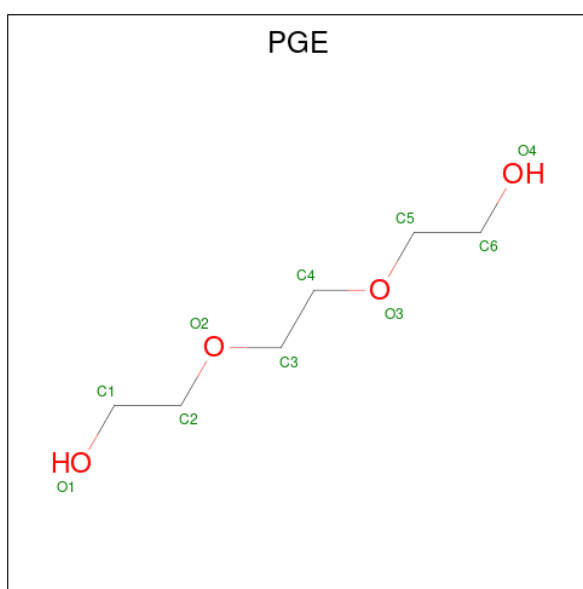
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

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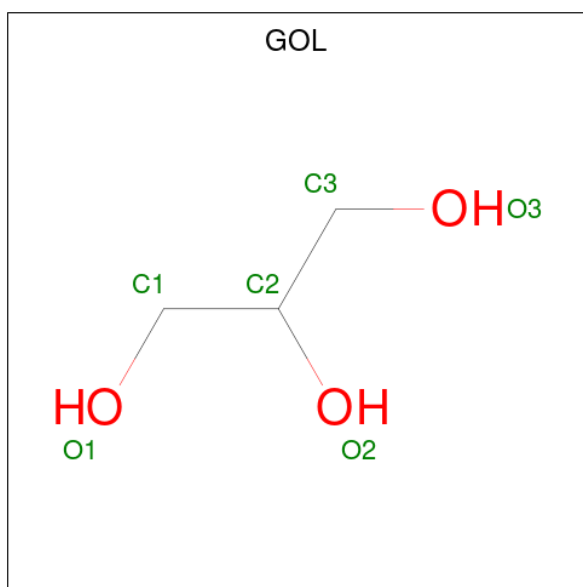
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



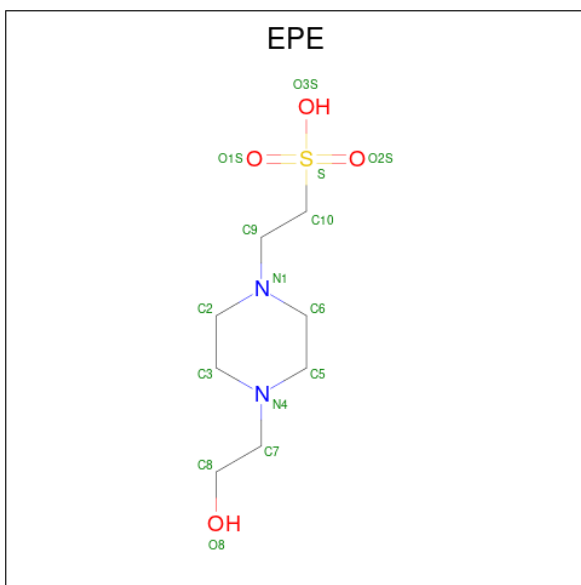
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



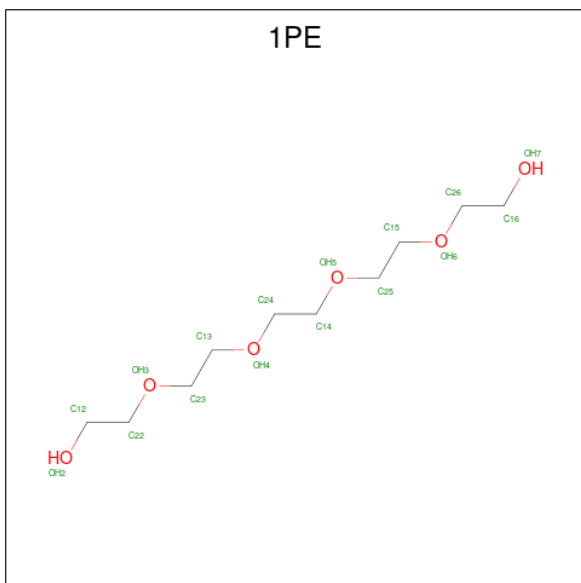
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



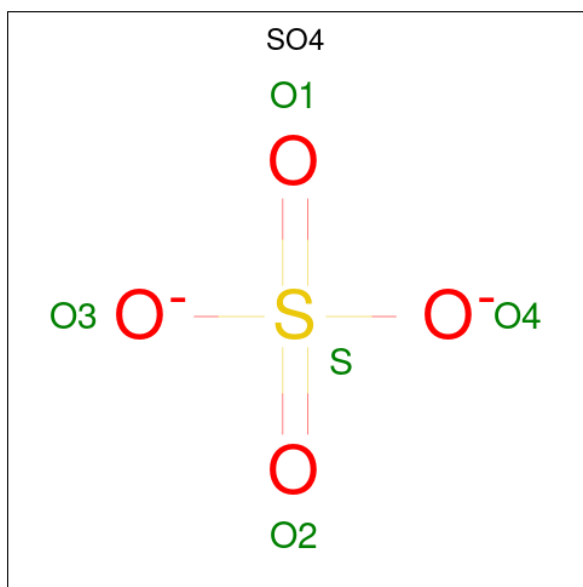
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			13	7	2	3	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
7	C	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
7	D	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

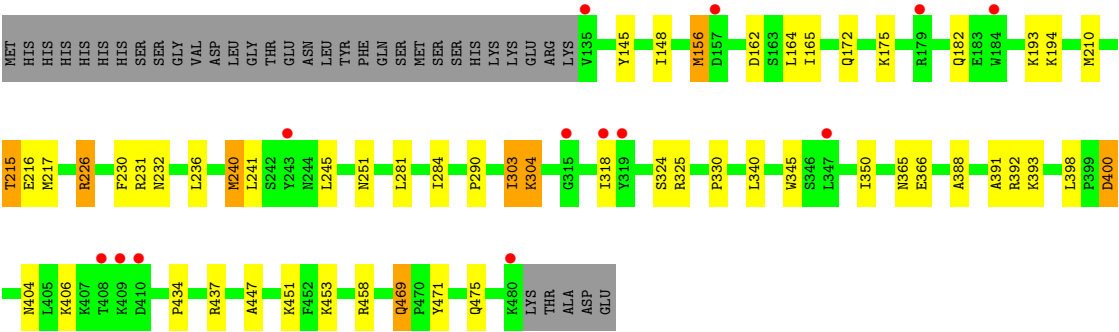
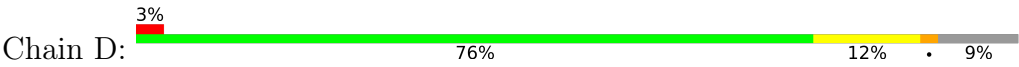
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total	Cl	0	0
			3	3		
10	B	1	Total	Cl	0	0
			1	1		
10	C	1	Total	Cl	0	0
			1	1		

- Molecule 11 is water.

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



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.199 , 0.235 0.199 , 0.237	Depositor DCC
R_{free} test set	1487 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: IWU, EPE, PTR, CL, PEG, GOL, 1PE, PGE, PG4, SO4

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	0.52	0/2887	0.66	0/3896
1	B	0.47	0/2859	0.62	0/3860
1	C	0.38	0/2813	0.57	0/3807
1	D	0.37	0/2834	0.55	0/3829
All	All	0.44	0/11393	0.60	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	38	0
1	B	2810	0	2779	36	0
1	C	2764	0	2676	30	0
1	D	2785	0	2734	31	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	6	0
8	A	16	0	22	2	0
8	B	16	0	22	6	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	10	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	141	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.

The worst 5 of 141 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: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
1:A:267:GLN:NE2	11:A:601:HOH:O	2.26	0.69

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%)	36	46
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%)	48	60

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%)	36	53
1	B	298/339 (88%)	289 (97%)	9 (3%)	36	53
1	C	286/339 (84%)	277 (97%)	9 (3%)	35	52
1	D	292/339 (86%)	273 (94%)	19 (6%)	15	22
All	All	1178/1356 (87%)	1132 (96%)	46 (4%)	28	43

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	156	MET
1	D	236	LEU
1	D	182	GLN
1	D	217	MET
1	D	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	182	GLN
1	D	232	ASN
1	D	371	ASN
1	D	267	GLN
1	C	213	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	321	1	15,16,17	0.82	0	17,22,24	1.03	0
1	PTR	A	321	1	15,16,17	0.79	0	17,22,24	1.15	1 (5%)
1	PTR	C	321	1	15,16,17	0.76	0	17,22,24	0.94	1 (5%)
1	PTR	B	321	1	15,16,17	0.86	0	17,22,24	1.49	4 (23%)

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	D	321	1	-	1/10/11/13	0/1/1/1
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1
1	PTR	C	321	1	-	1/10/11/13	0/1/1/1
1	PTR	B	321	1	-	1/10/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	PTR	CB-CG-CD2	-3.14	115.06	120.90
1	C	321	PTR	OH-P-O1P	-2.21	102.12	109.48
1	B	321	PTR	OH-P-O1P	-2.20	102.14	109.48
1	B	321	PTR	CB-CG-CD1	2.19	124.98	120.90
1	A	321	PTR	P-OH-CZ	2.16	131.58	123.88

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	C	321	PTR	2	0
1	B	321	PTR	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
4	PEG	A	504	-	6,6,6	0.16	0	5,5,5	0.16	0
9	SO4	D	508	-	4,4,4	0.26	0	6,6,6	0.28	0
2	IWU	A	501	-	11,11,11	0.94	1 (9%)	13,15,15	1.61	1 (7%)
3	PG4	C	503	-	12,12,12	0.25	0	11,11,11	0.41	0
7	EPE	A	508	-	13,13,15	0.81	1 (7%)	17,18,20	0.98	1 (5%)
2	IWU	D	502	-	11,11,11	0.87	1 (9%)	13,15,15	1.40	2 (15%)
6	GOL	B	507	-	5,5,5	1.28	0	5,5,5	1.92	2 (40%)
5	PGE	D	504	-	9,9,9	0.40	0	8,8,8	0.30	0
9	SO4	A	510	-	4,4,4	0.29	0	6,6,6	0.19	0
9	SO4	B	513	-	4,4,4	0.31	0	6,6,6	0.29	0
2	IWU	D	501	-	11,11,11	0.83	1 (9%)	13,15,15	1.49	2 (15%)
9	SO4	D	507	-	4,4,4	0.32	0	6,6,6	0.17	0
4	PEG	D	503	-	6,6,6	0.22	0	5,5,5	0.08	0
6	GOL	B	508	-	5,5,5	0.92	0	5,5,5	1.01	0
5	PGE	A	506	-	9,9,9	0.45	0	8,8,8	0.69	0
6	GOL	B	503	-	5,5,5	1.02	0	5,5,5	0.84	0
4	PEG	C	505	-	6,6,6	0.30	0	5,5,5	0.24	0
5	PGE	A	505	-	9,9,9	0.49	0	8,8,8	0.40	0
4	PEG	C	501	-	6,6,6	0.33	0	5,5,5	0.20	0
4	PEG	B	504	-	6,6,6	0.32	0	5,5,5	0.12	0
6	GOL	C	508	-	5,5,5	0.97	0	5,5,5	1.05	0
9	SO4	A	513	-	4,4,4	0.42	0	6,6,6	0.71	0
7	EPE	D	505	-	12,12,15	0.87	1 (8%)	15,16,20	0.90	1 (6%)
9	SO4	B	511	-	4,4,4	0.23	0	6,6,6	0.42	0
9	SO4	A	514	-	4,4,4	0.33	0	6,6,6	0.20	0
2	IWU	C	502	-	11,11,11	0.84	1 (9%)	13,15,15	1.47	2 (15%)
6	GOL	C	507	-	5,5,5	0.81	0	5,5,5	1.03	0
2	IWU	C	504	-	11,11,11	0.83	1 (9%)	13,15,15	1.56	2 (15%)
2	IWU	B	502	-	11,11,11	0.86	1 (9%)	13,15,15	1.49	3 (23%)
9	SO4	C	511	-	4,4,4	0.18	0	6,6,6	0.37	0
4	PEG	C	506	-	6,6,6	0.15	0	5,5,5	0.15	0
6	GOL	B	505	-	5,5,5	1.13	1 (20%)	5,5,5	1.15	0
2	IWU	A	503	-	11,11,11	1.02	1 (9%)	13,15,15	1.38	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	506	-	5,5,5	0.88	0	5,5,5	0.92	0
7	EPE	B	510	-	12,12,15	0.77	1 (8%)	15,16,20	0.86	1 (6%)
2	IWU	B	501	-	11,11,11	0.77	1 (9%)	13,15,15	1.63	2 (15%)
5	PGE	C	509	-	9,9,9	0.37	0	8,8,8	0.53	0
9	SO4	B	512	-	4,4,4	0.32	0	6,6,6	0.15	0
9	SO4	D	506	-	4,4,4	0.27	0	6,6,6	0.34	0
7	EPE	C	510	-	12,12,15	1.21	1 (8%)	15,16,20	1.29	2 (13%)
3	PG4	A	502	-	12,12,12	0.20	0	11,11,11	0.49	0
9	SO4	C	512	-	4,4,4	0.26	0	6,6,6	0.32	0
9	SO4	A	512	-	4,4,4	0.40	0	6,6,6	0.50	0
8	1PE	A	509	-	15,15,15	0.27	0	14,14,14	0.29	0
8	1PE	B	509	-	15,15,15	0.24	0	14,14,14	0.22	0
6	GOL	A	507	-	5,5,5	1.02	0	5,5,5	1.17	0
9	SO4	A	511	-	4,4,4	0.70	0	6,6,6	0.86	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
4	PEG	A	504	-	-	2/4/4/4	-
2	IWU	A	501	-	-	-	0/2/2/2
3	PG4	C	503	-	-	3/10/10/10	-
7	EPE	A	508	-	-	1/6/16/19	0/1/1/1
2	IWU	D	502	-	-	-	0/2/2/2
6	GOL	B	507	-	-	2/4/4/4	-
5	PGE	D	504	-	-	2/7/7/7	-
2	IWU	D	501	-	-	-	0/2/2/2
4	PEG	D	503	-	-	1/4/4/4	-
6	GOL	B	508	-	-	4/4/4/4	-
5	PGE	A	506	-	-	5/7/7/7	-
6	GOL	B	503	-	-	4/4/4/4	-
4	PEG	C	505	-	-	3/4/4/4	-
5	PGE	A	505	-	-	4/7/7/7	-
4	PEG	C	501	-	-	2/4/4/4	-
4	PEG	B	504	-	-	3/4/4/4	-
6	GOL	C	508	-	-	0/4/4/4	-
7	EPE	D	505	-	-	5/6/14/19	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IWU	C	502	-	-	-	0/2/2/2
6	GOL	C	507	-	-	2/4/4/4	-
2	IWU	C	504	-	-	-	0/2/2/2
2	IWU	B	502	-	-	-	0/2/2/2
4	PEG	C	506	-	-	2/4/4/4	-
6	GOL	B	505	-	-	0/4/4/4	-
2	IWU	A	503	-	-	-	0/2/2/2
6	GOL	B	506	-	-	4/4/4/4	-
7	EPE	B	510	-	-	2/6/14/19	0/1/1/1
2	IWU	B	501	-	-	-	0/2/2/2
5	PGE	C	509	-	-	6/7/7/7	-
7	EPE	C	510	-	-	3/6/14/19	0/1/1/1
3	PG4	A	502	-	-	2/10/10/10	-
8	1PE	A	509	-	-	2/13/13/13	-
8	1PE	B	509	-	-	6/13/13/13	-
6	GOL	A	507	-	-	1/4/4/4	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	510	EPE	O2S-S	4.04	1.56	1.45
2	A	503	IWU	C4-C3	-3.07	1.38	1.41
2	A	501	IWU	C4-C3	-2.97	1.38	1.41
7	D	505	EPE	O3S-S	2.87	1.58	1.47
2	D	502	IWU	C4-C3	-2.58	1.38	1.41

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	IWU	C3-N2-N3	-4.71	108.56	111.18
2	A	501	IWU	C3-N2-N3	-4.36	108.76	111.18
2	C	504	IWU	C3-N2-N3	-4.34	108.77	111.18
2	D	501	IWU	C3-N2-N3	-4.10	108.91	111.18
2	C	502	IWU	C3-N2-N3	-4.00	108.96	111.18

There are no chirality outliers.

5 of 71 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

All (1) ring outliers are listed below:

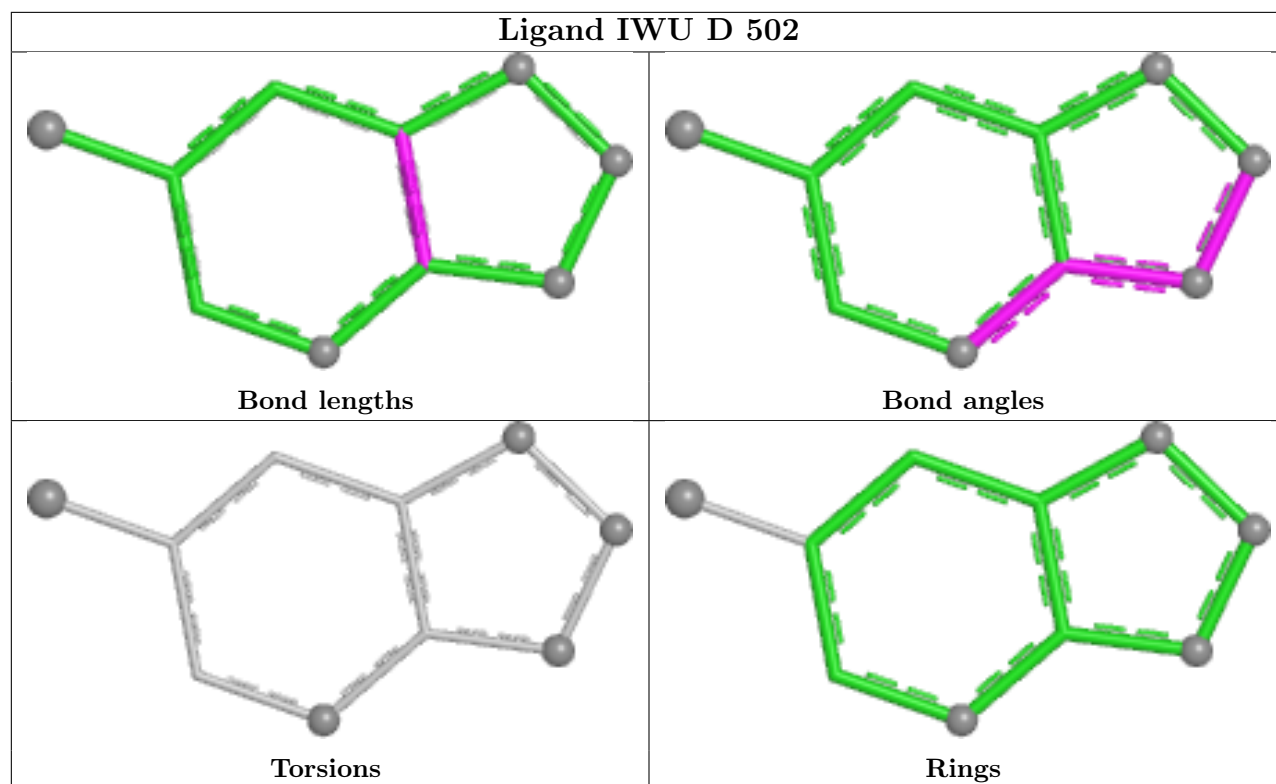
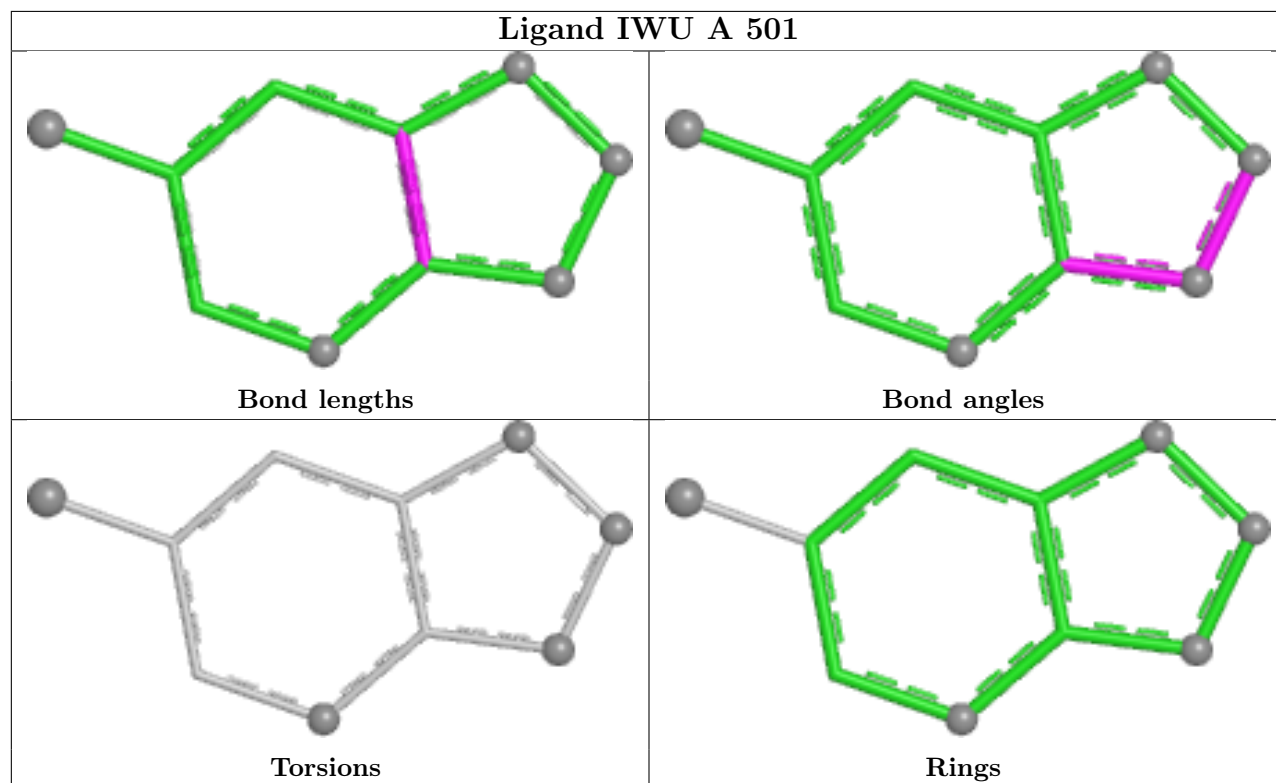
Mol	Chain	Res	Type	Atoms
7	D	505	EPE	C2-C3-C5-C6-N1-N4

20 monomers are involved in 43 short contacts:

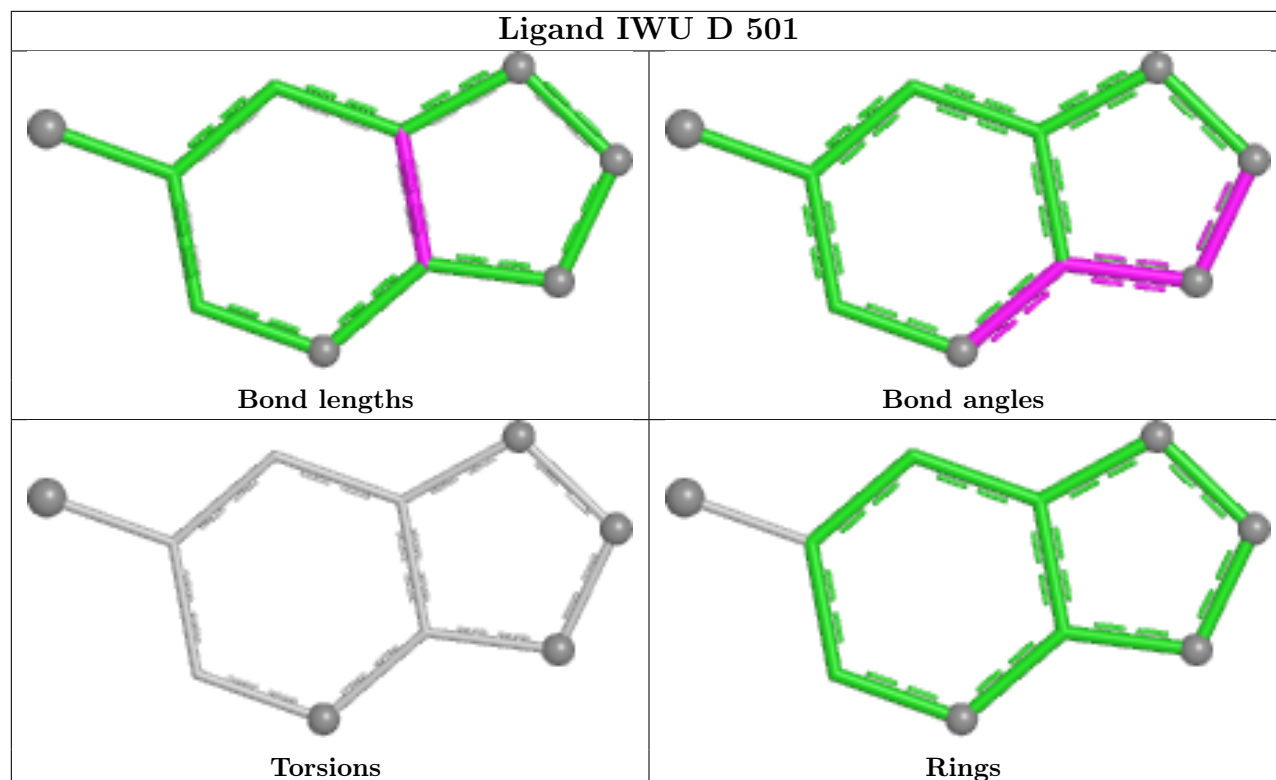
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	PEG	3	0
7	A	508	EPE	2	0
2	D	502	IWU	1	0
6	B	507	GOL	1	0
2	D	501	IWU	1	0
9	D	507	SO4	1	0
5	A	506	PGE	1	0
6	B	503	GOL	2	0
4	B	504	PEG	1	0
7	D	505	EPE	6	0
2	C	504	IWU	3	0
6	B	505	GOL	2	0
6	B	506	GOL	1	0
7	B	510	EPE	5	0
5	C	509	PGE	1	0
7	C	510	EPE	4	0
8	A	509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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

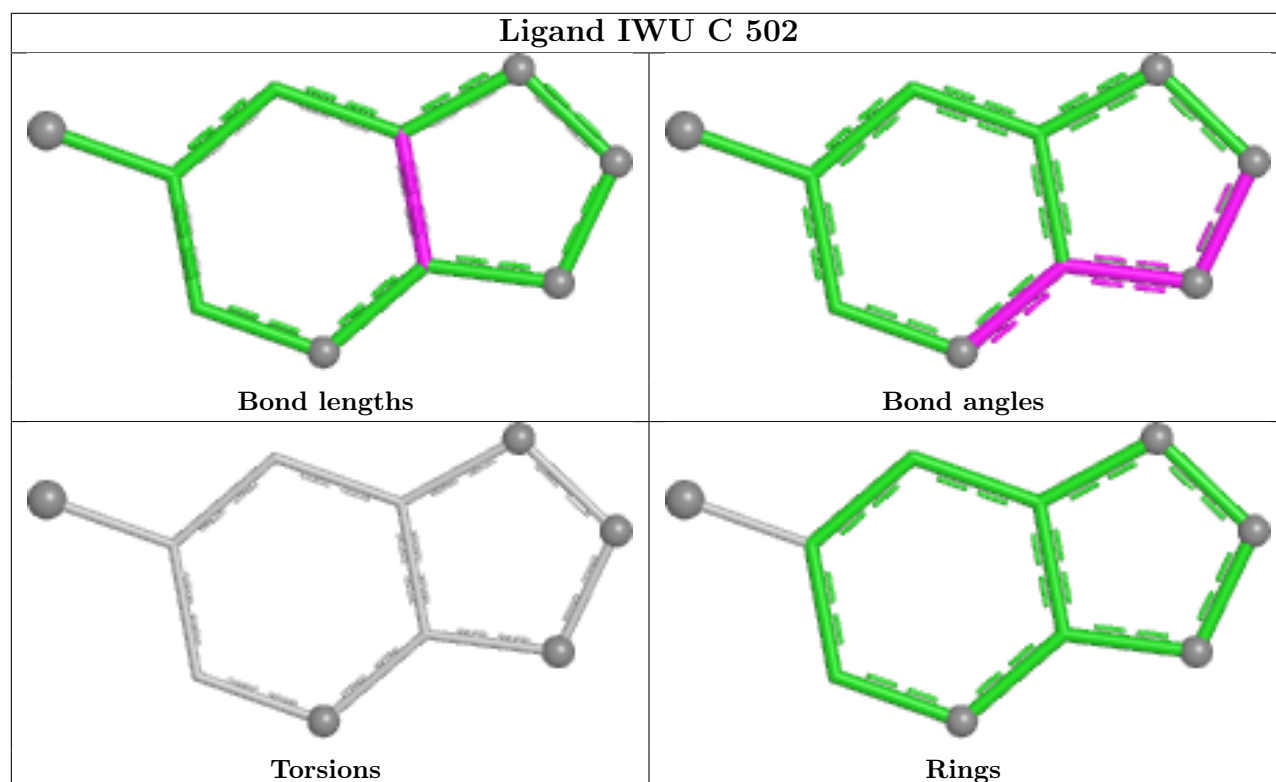
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



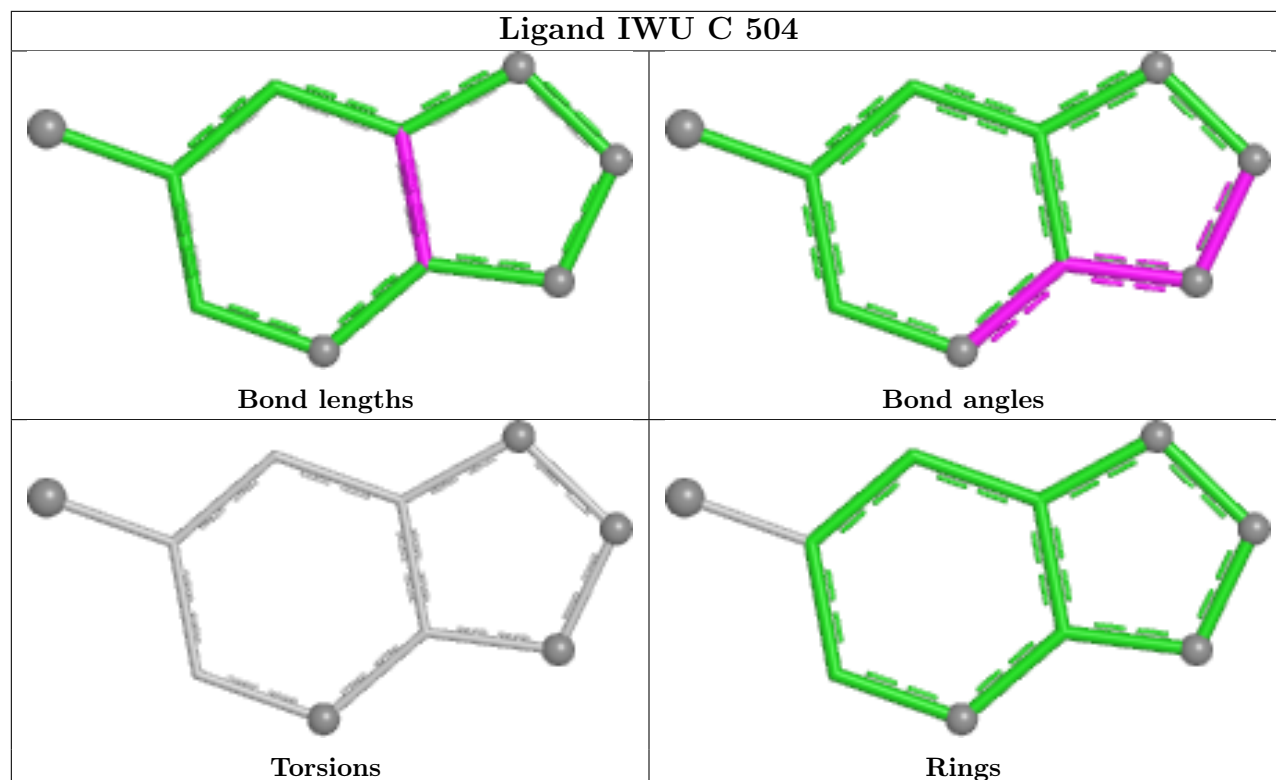
Ligand IWU D 501



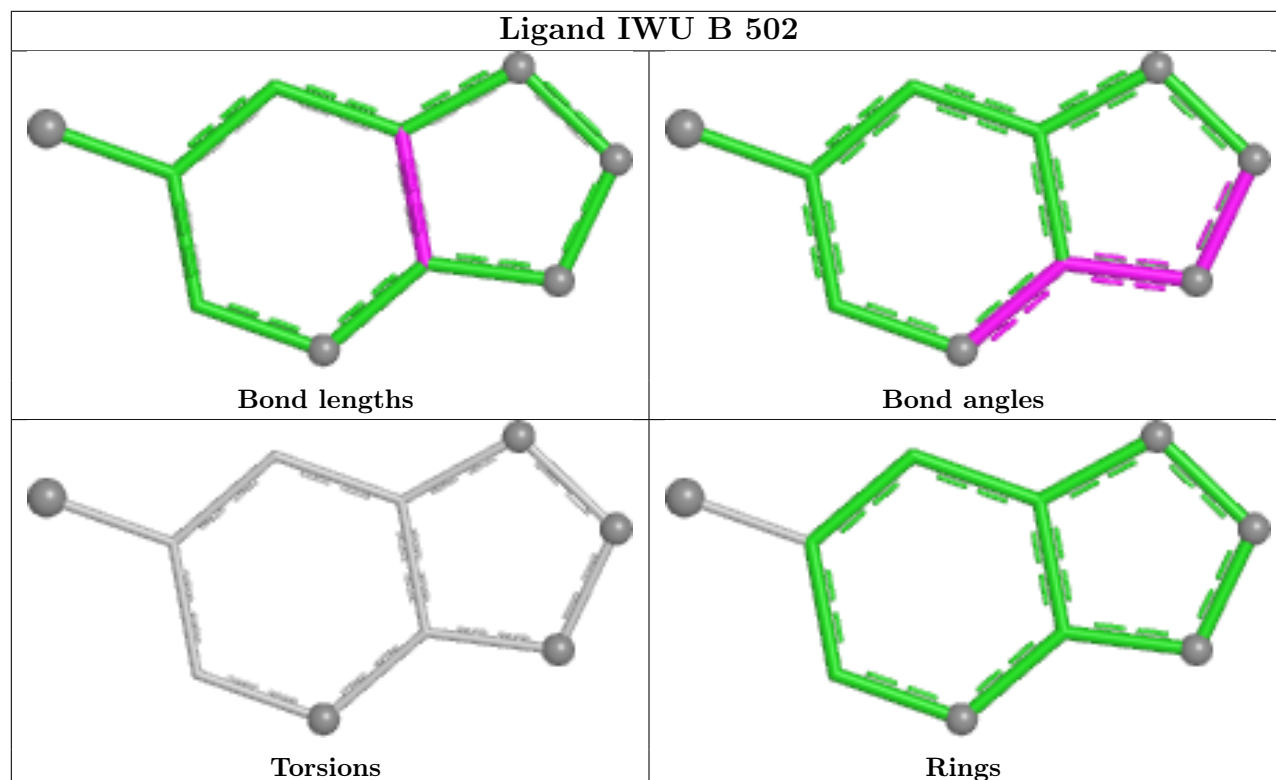
Ligand IWU C 502

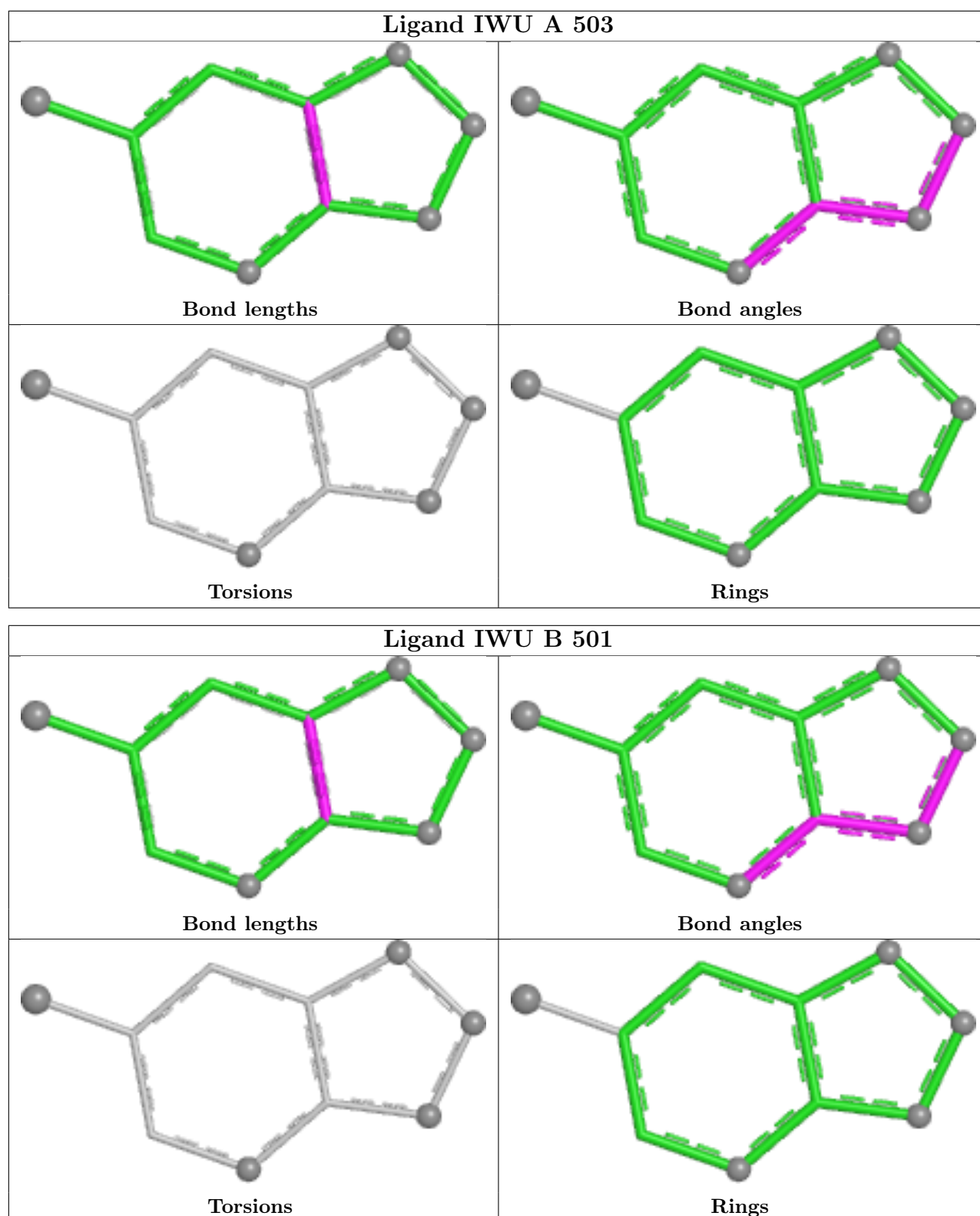


Ligand IWU C 504



Ligand IWU B 502





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	347/382 (90%)	0.00	10 (2%) 53 56	22, 43, 70, 104	1 (0%)
1	B	346/382 (90%)	0.06	12 (3%) 47 49	36, 48, 73, 99	0
1	C	345/382 (90%)	0.49	17 (4%) 35 36	38, 63, 100, 114	1 (0%)
1	D	345/382 (90%)	0.51	13 (3%) 44 46	46, 66, 92, 114	0
All	All	1383/1528 (90%)	0.26	52 (3%) 44 46	22, 56, 91, 114	2 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	482	THR	5.4
1	D	409	LYS	5.1
1	B	135	VAL	4.7
1	B	408	THR	4.6
1	D	480	LYS	4.1

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, 95th 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
1	PTR	C	321	16/17	0.87	0.13	72,80,87,92	0
1	PTR	D	321	16/17	0.88	0.15	66,76,82,82	0
1	PTR	B	321	16/17	0.91	0.11	61,68,72,76	0
1	PTR	A	321	16/17	0.94	0.09	44,58,59,60	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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
7	EPE	A	508	13/15	0.61	0.22	65,75,89,96	0
9	SO4	D	508	5/5	0.65	0.13	90,93,108,120	0
9	SO4	A	513	5/5	0.68	0.14	74,76,82,91	0
9	SO4	A	510	5/5	0.68	0.11	90,96,104,108	0
9	SO4	A	514	5/5	0.72	0.11	80,80,92,98	0
9	SO4	D	507	5/5	0.73	0.13	80,92,99,111	0
7	EPE	C	510	12/15	0.73	0.18	71,82,94,95	0
7	EPE	D	505	12/15	0.77	0.19	59,81,92,95	0
5	PGE	D	504	10/10	0.78	0.18	73,84,90,91	0
6	GOL	C	507	6/6	0.78	0.14	65,70,73,78	0
7	EPE	B	510	12/15	0.79	0.18	67,77,88,88	0
5	PGE	A	506	10/10	0.80	0.17	45,58,73,77	0
6	GOL	A	507	6/6	0.82	0.12	58,63,65,68	0
6	GOL	B	505	6/6	0.82	0.13	75,76,77,80	0
5	PGE	C	509	10/10	0.82	0.17	58,73,79,83	0
4	PEG	D	503	7/7	0.84	0.13	71,76,79,81	0
6	GOL	B	503	6/6	0.84	0.14	50,55,62,63	0
4	PEG	B	504	7/7	0.84	0.14	60,65,72,72	0
6	GOL	B	506	6/6	0.84	0.14	68,72,76,78	0
6	GOL	B	508	6/6	0.84	0.15	67,69,72,73	0
6	GOL	C	508	6/6	0.86	0.13	85,93,96,97	0
4	PEG	C	501	7/7	0.86	0.13	48,56,61,61	0
10	CL	A	516	1/1	0.86	0.14	75,75,75,75	0
9	SO4	A	511	5/5	0.87	0.15	51,54,76,83	0
4	PEG	C	505	7/7	0.87	0.13	53,60,63,69	0
6	GOL	B	507	6/6	0.89	0.22	43,52,63,64	0
9	SO4	B	512	5/5	0.90	0.08	66,69,76,86	0
4	PEG	A	504	7/7	0.90	0.11	54,62,67,71	0
5	PGE	A	505	10/10	0.90	0.14	48,62,67,70	0
4	PEG	C	506	7/7	0.90	0.11	72,74,75,77	0
9	SO4	B	513	5/5	0.91	0.15	57,64,73,76	0
8	1PE	B	509	16/16	0.91	0.12	57,63,72,73	0

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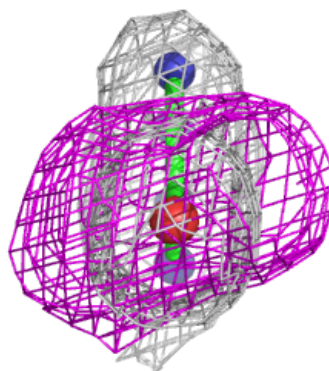
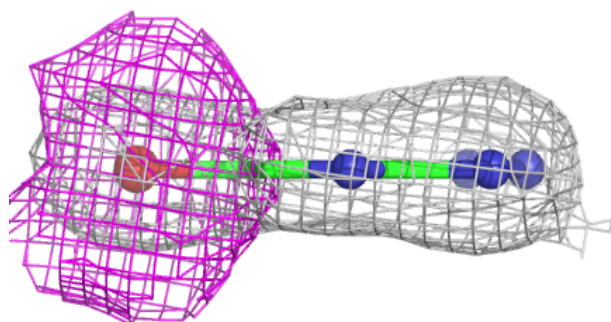
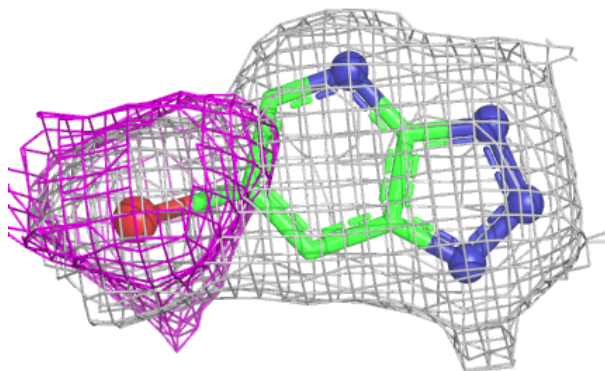
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	CL	A	517	1/1	0.91	0.11	73,73,73,73	0
2	IWU	B	502	10/10	0.92	0.11	38,42,46,75	0
2	IWU	D	502	10/10	0.92	0.11	57,66,70,95	0
3	PG4	C	503	13/13	0.92	0.12	56,61,71,72	0
10	CL	C	513	1/1	0.92	0.09	85,85,85,85	0
8	1PE	A	509	16/16	0.93	0.10	55,63,67,67	0
2	IWU	C	504	10/10	0.93	0.10	53,60,63,93	0
10	CL	B	514	1/1	0.93	0.16	76,76,76,76	0
10	CL	A	515	1/1	0.93	0.10	69,69,69,69	0
9	SO4	D	506	5/5	0.94	0.07	55,58,67,69	0
2	IWU	C	502	10/10	0.94	0.11	60,66,70,88	0
2	IWU	A	503	10/10	0.94	0.10	38,44,46,74	0
9	SO4	C	512	5/5	0.94	0.06	64,74,77,77	0
9	SO4	B	511	5/5	0.95	0.08	62,62,66,69	0
9	SO4	A	512	5/5	0.96	0.15	49,57,64,68	0
3	PG4	A	502	13/13	0.96	0.08	32,43,53,55	0
9	SO4	C	511	5/5	0.96	0.12	51,58,67,68	0
2	IWU	D	501	10/10	0.97	0.10	62,67,75,77	0
2	IWU	B	501	10/10	0.98	0.07	45,49,55,56	0
2	IWU	A	501	10/10	0.99	0.05	39,43,48,54	0

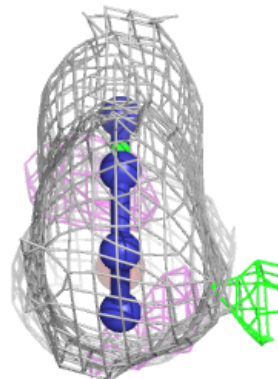
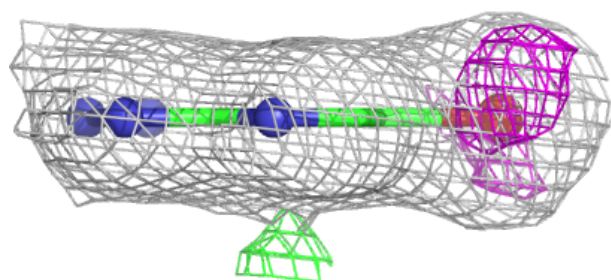
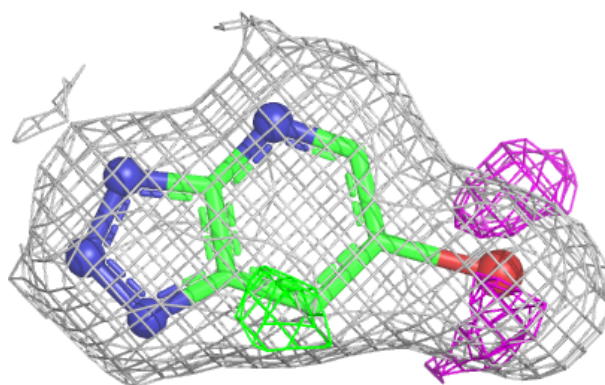
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IWU 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)

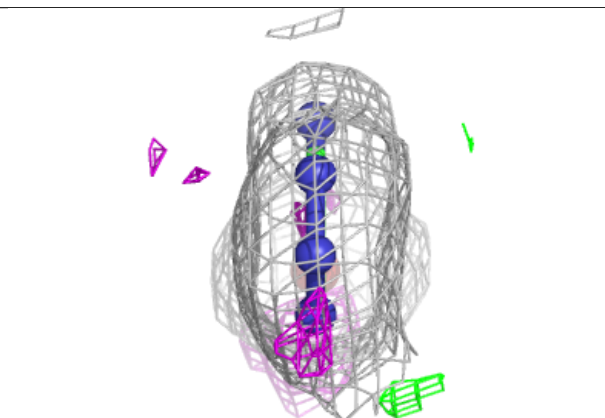
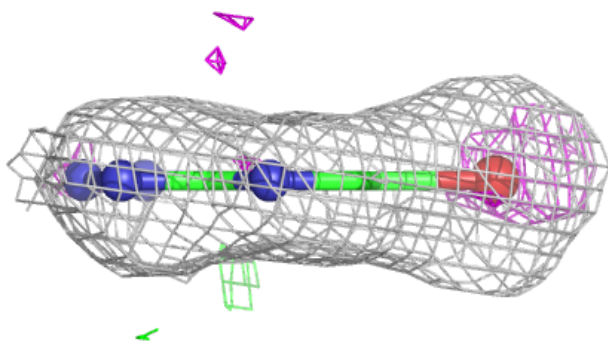
**Electron density around IWU D 502:**

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

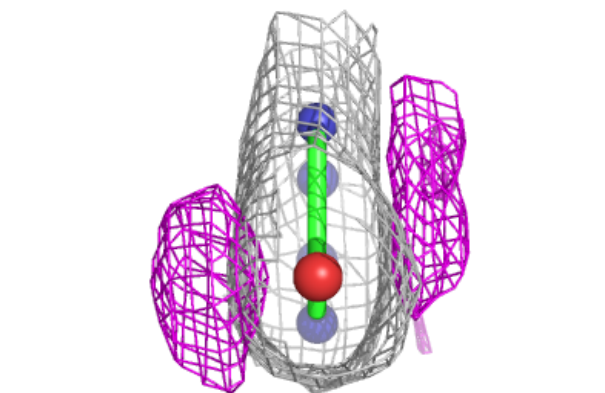
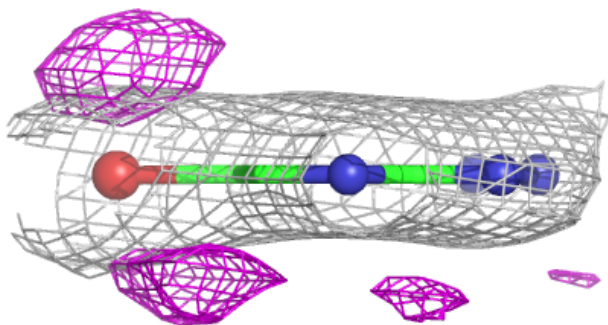
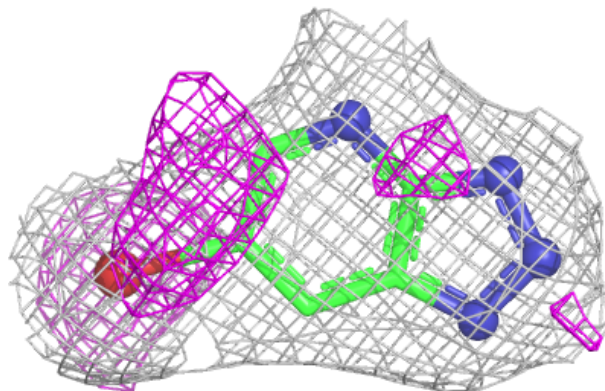


Electron density around IWU C 504:

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

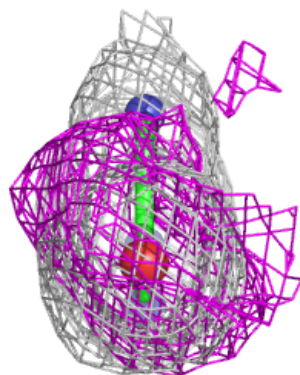
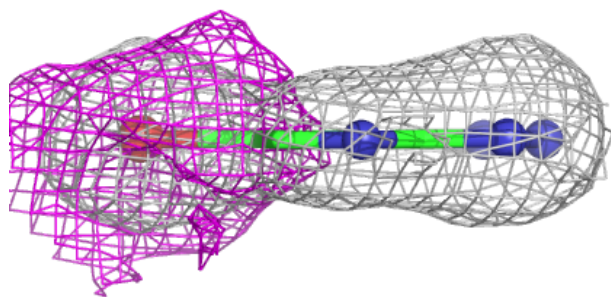
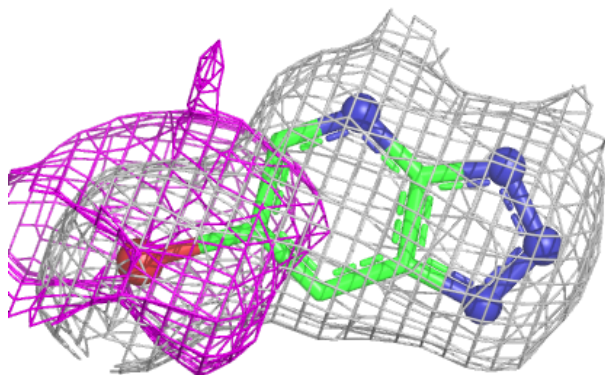
**Electron density around IWU C 502:**

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

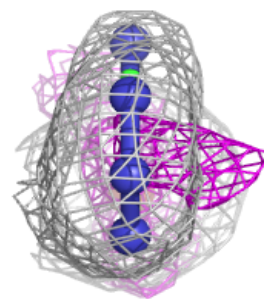
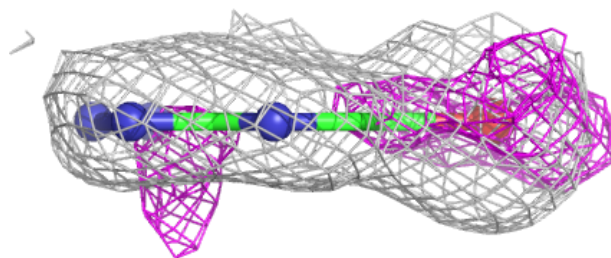
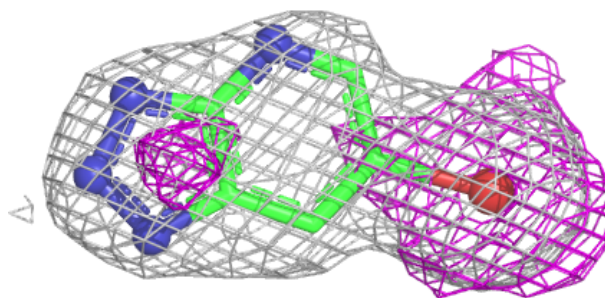


Electron density around IWU A 503:

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

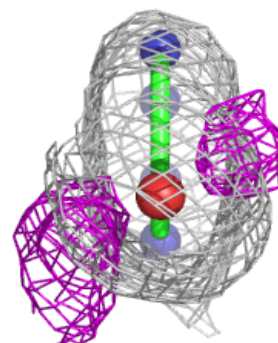
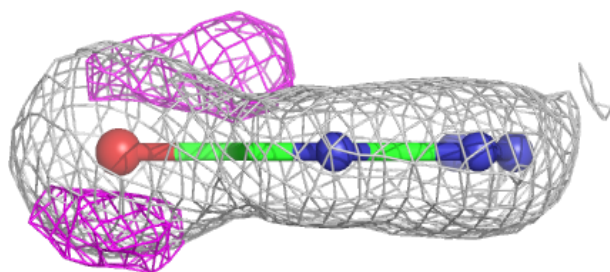
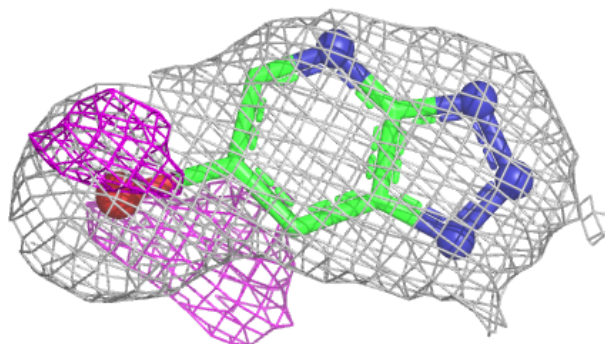
**Electron density around IWU D 501:**

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

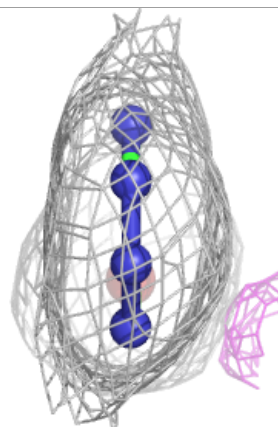
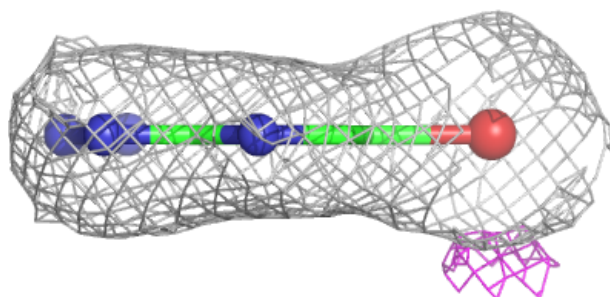
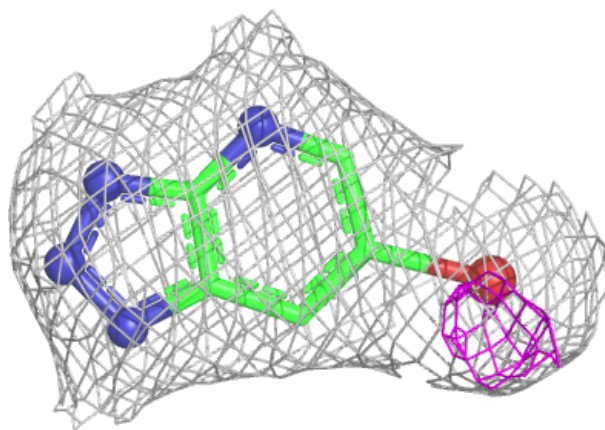


Electron density around IWU B 501:

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

**Electron density around 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.