



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2024 – 01:21 pm BST

PDB ID : 8R8E
Title : DYRK1a in Complex with 2-Cyclopentyl-7-iodo-1H-indole-3-carbonitrile
Authors : Stahlecker, J.; Dammann, M.; Stehle, T.; Boeckler, F.M.
Deposited on : 2023-11-29
Resolution : 2.22 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

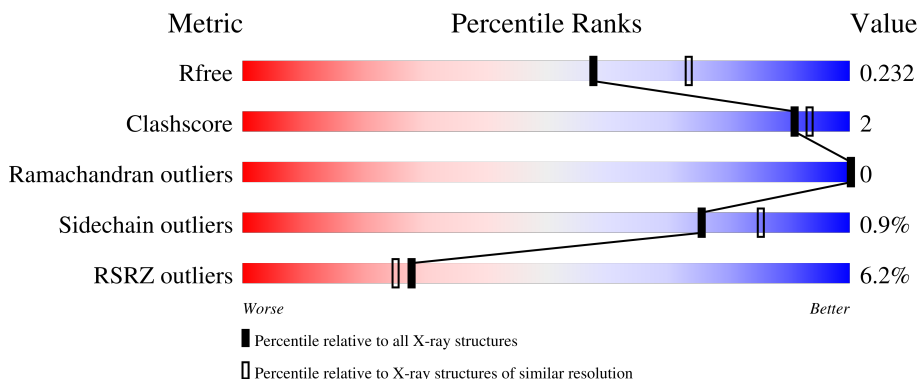
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

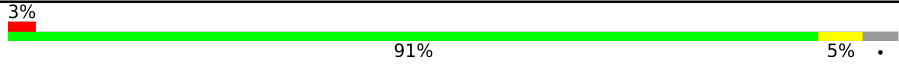
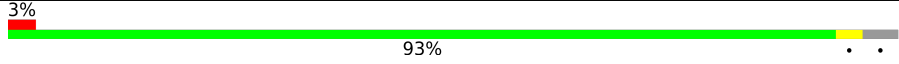
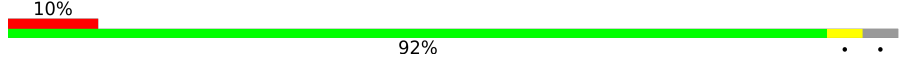
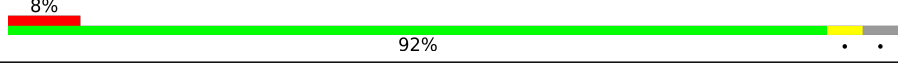
The reported resolution of this entry is 2.22 Å.

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}	164625	7167 (2.24-2.20)
Clashscore	180529	8096 (2.24-2.20)
Ramachandran outliers	177936	8010 (2.24-2.20)
Sidechain outliers	177891	8011 (2.24-2.20)
RSRZ outliers	164620	7166 (2.24-2.20)

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	361	 3% 91% 5%
1	B	361	 3% 93%
1	C	361	 10% 92%
2	D	361	 8% 92%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 12068 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	347	2808	1802	480	508	1	17	0	0	0
1	B	347	2819	1811	484	507	1	16	0	1	0
1	C	346	2701	1741	454	488	1	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627

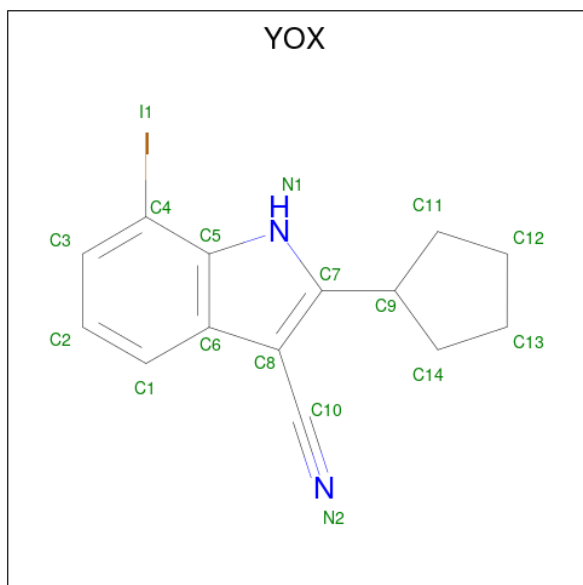
- Molecule 2 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	346	2768	1779	474	498	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

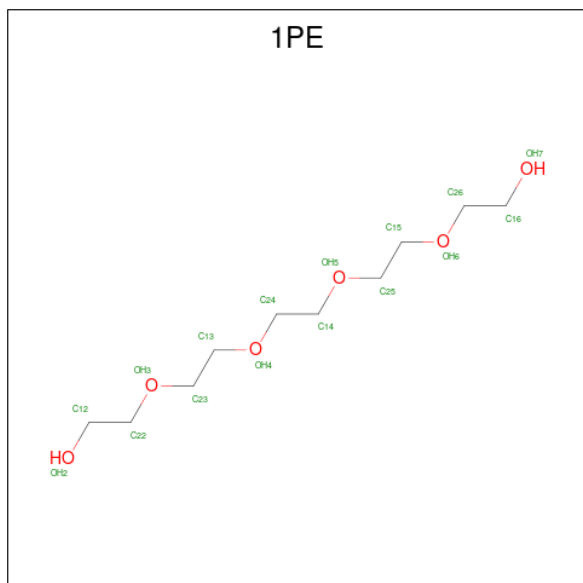
Chain	Residue	Modelled	Actual	Comment	Reference
D	125	SER	-	expression tag	UNP Q13627
D	126	MET	-	expression tag	UNP Q13627

- Molecule 3 is 2-cyclopentyl-7-iodanyl-1 {H}-indole-3-carbonitrile (three-letter code: YOX) (formula: C₁₄H₁₃IN₂) (labeled as "Ligand of Interest" by depositor).



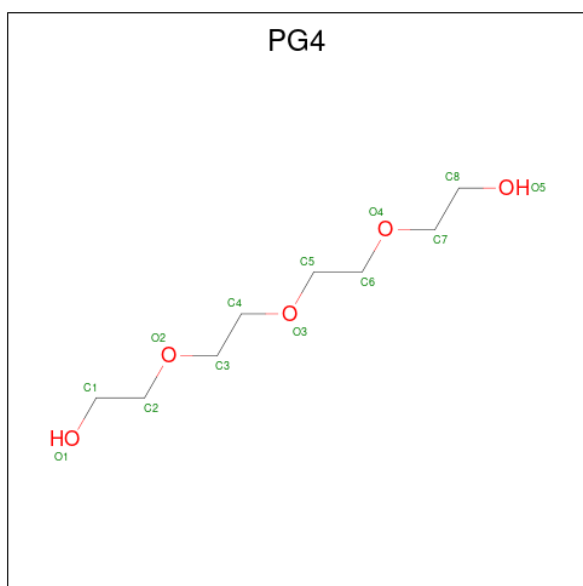
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	I	N	0	0
			17	14	1	2		
3	B	1	Total	C	I	N	0	0
			17	14	1	2		
3	C	1	Total	C	I	N	0	0
			17	14	1	2		
3	D	1	Total	C	I	N	0	0
			17	14	1	2		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



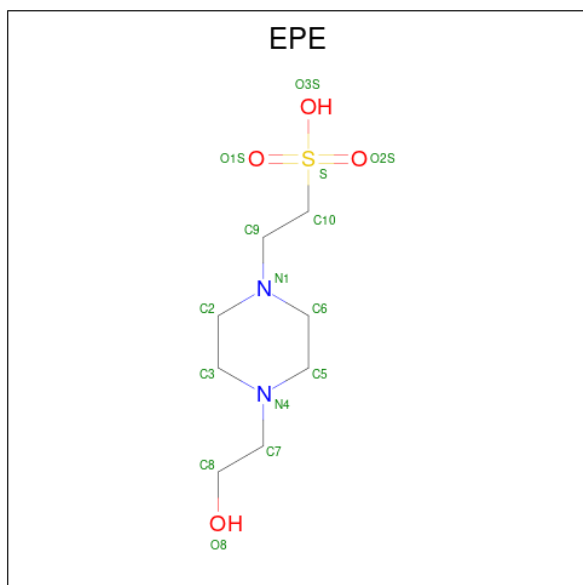
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	C	1	Total	C	O	0	0
			16	10	6		
4	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



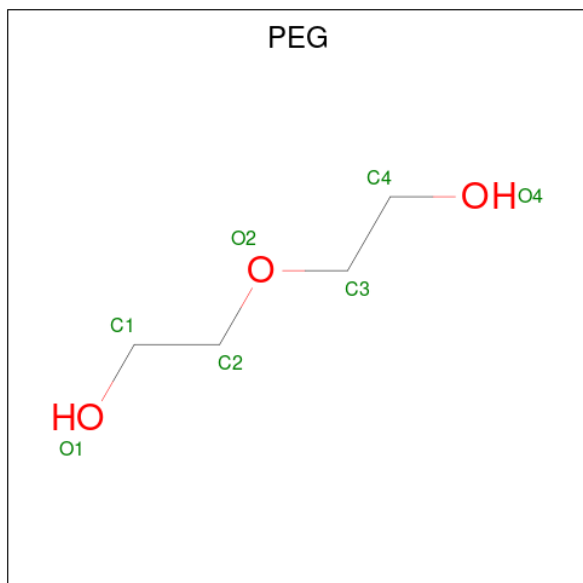
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



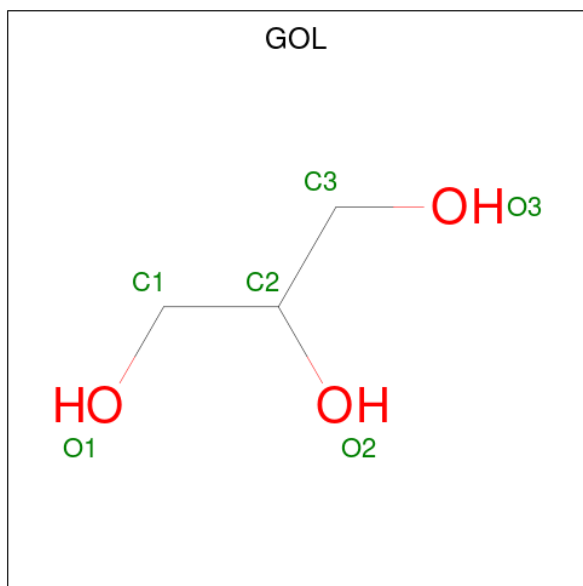
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
6	A	1	Total	12	6	2	3	1	0	0
6	B	1	Total	13	7	2	3	1	0	0
6	B	1	Total	15	8	2	4	1	0	0
6	C	1	Total	15	8	2	4	1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



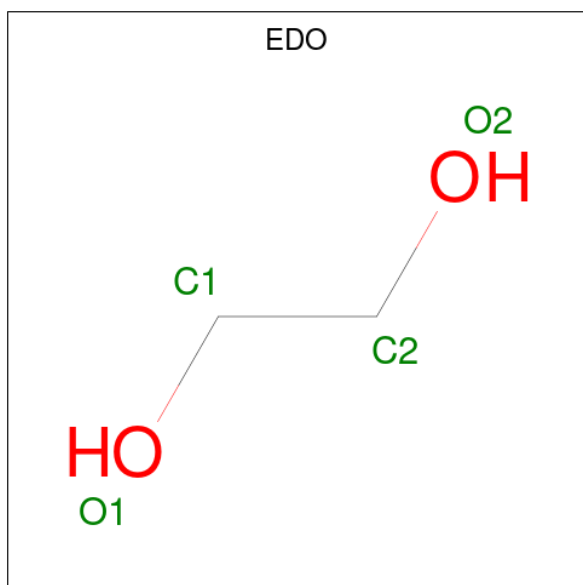
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

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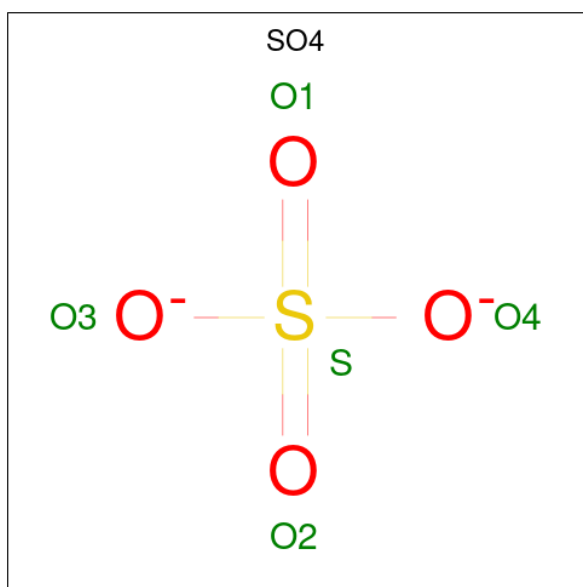
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



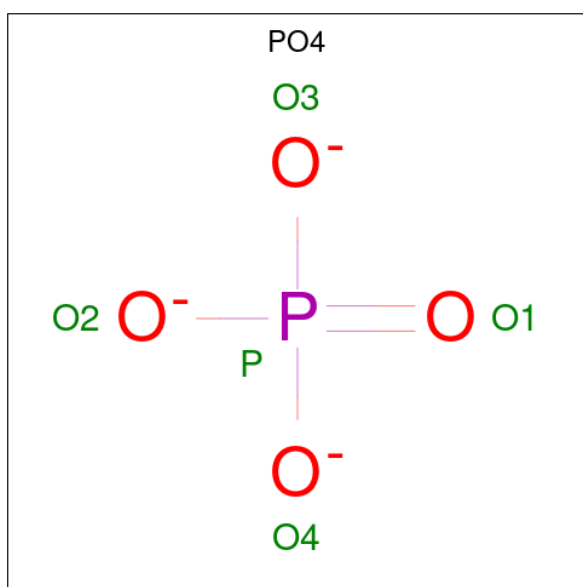
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10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

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

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	O	P	0	0
			5	4	1		

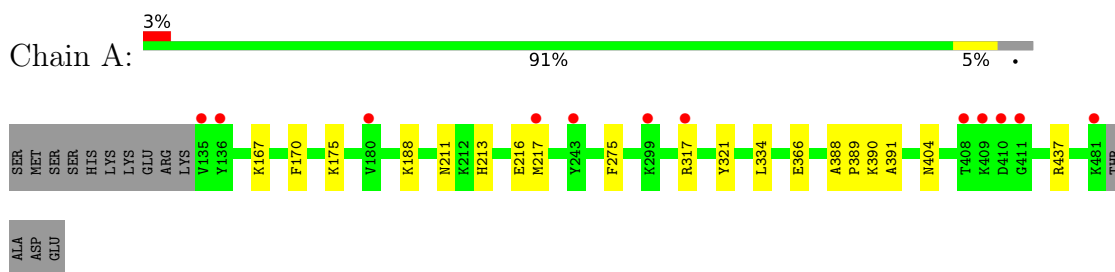
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	207	Total	O	0	0
			207	207		
12	B	158	Total	O	0	0
			158	158		
12	C	86	Total	O	0	0
			86	86		
12	D	67	Total	O	0	0
			67	67		

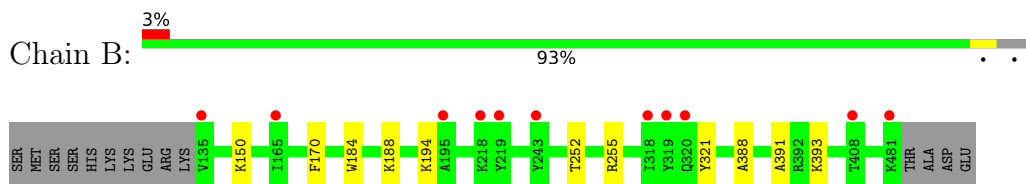
3 Residue-property plots [i](#)

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.

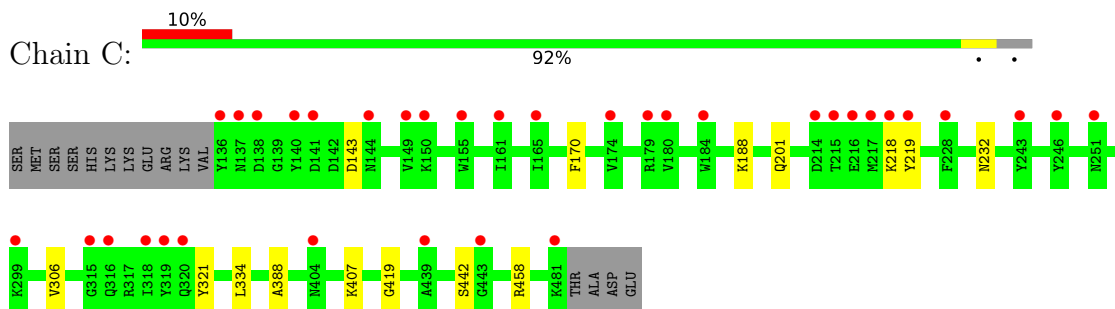
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



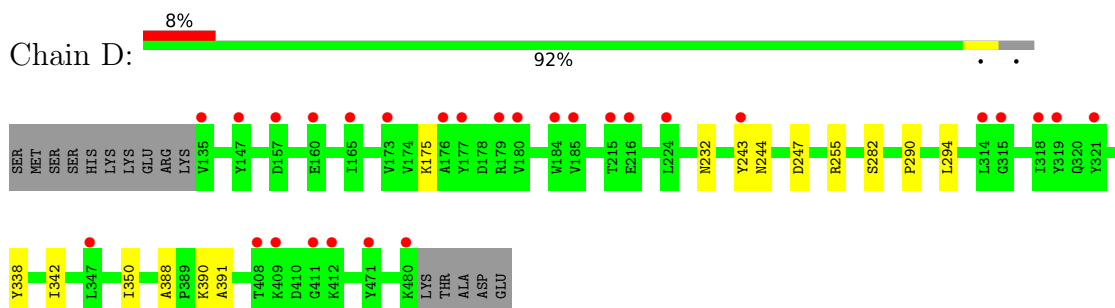
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



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



- Molecule 2: 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	244.24Å 64.47Å 147.33Å 90.00° 115.58° 90.00°	Depositor
Resolution (Å)	49.08 – 2.22 49.08 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.08-2.22) 99.7 (49.08-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.22Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.234 0.197 , 0.232	Depositor DCC
R_{free} test set	1536 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtrriage
Anisotropy	0.270	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12068	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.56% 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: PTR, YOX, PO4, PG4, SO4, 1PE, PEG, GOL, EDO, EPE

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	0.40	0/2857	0.62	0/3859
1	B	0.38	0/2870	0.62	0/3874
1	C	0.34	0/2748	0.58	0/3722
2	D	0.34	0/2834	0.59	0/3834
All	All	0.37	0/11309	0.60	0/15289

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	2808	0	2753	13	0
1	B	2819	0	2780	7	0
1	C	2701	0	2582	8	0
2	D	2768	0	2706	8	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	0	0
4	A	32	0	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	22	2	0
4	C	16	0	22	1	0
4	D	13	0	17	1	0
5	A	13	0	18	0	0
6	A	12	0	12	1	0
6	B	28	0	29	1	0
6	C	15	0	17	0	0
7	A	14	0	20	1	0
7	B	7	0	10	0	0
8	A	18	0	24	0	0
8	B	18	0	24	1	0
8	C	18	0	24	1	0
8	D	12	0	16	1	0
9	A	8	0	12	1	0
9	B	12	0	18	0	0
9	C	4	0	6	1	0
10	A	40	0	0	1	0
10	B	25	0	0	1	0
10	C	25	0	0	0	0
10	D	35	0	0	0	0
11	D	5	0	0	0	0
12	A	207	0	0	2	0
12	B	158	0	0	1	0
12	C	86	0	0	1	0
12	D	67	0	0	0	0
All	All	12068	0	11156	37	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 2.

All (37) 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:A:366:GLU:HG3	6:A:504:EPE:H101	1.71	0.71
1:B:194:LYS:HD2	8:B:504:GOL:H12	1.84	0.60
2:D:388:ALA:HB3	2:D:391:ALA:HB2	1.88	0.56
1:C:334:LEU:HB3	1:C:388:ALA:HB1	1.88	0.54
1:B:170:PHE:CD1	1:B:188:LYS:HE3	2.45	0.52
1:C:201:GLN:NE2	12:C:602:HOH:O	2.42	0.51
2:D:243:TYR:HB3	2:D:247:ASP:HB2	1.95	0.48
1:C:201:GLN:OE1	4:C:503:1PE:H262	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.93	0.48
1:A:216:GLU:H	1:A:216:GLU:CD	2.16	0.48
2:D:175:LYS:HD2	4:D:503:1PE:H242	1.96	0.48
1:A:217:MET:HB3	1:A:275:PHE:HB2	1.94	0.47
1:A:437:ARG:NE	10:A:518:SO4:O4	2.40	0.47
1:C:419:GLY:HA3	8:C:506:GOL:H2	1.96	0.47
1:A:389:PRO:HA	7:A:506:PEG:H12	1.98	0.46
1:C:218:LYS:HE3	1:C:219:TYR:CZ	2.51	0.46
1:B:393:LYS:HD2	6:B:503:EPE:H91	1.98	0.45
2:D:290:PRO:HD3	2:D:350:ILE:HG12	1.99	0.45
2:D:338:TYR:HB2	2:D:342:ILE:HG21	1.99	0.45
1:B:184:TRP:CZ2	4:B:501:1PE:H252	2.50	0.45
1:A:334:LEU:HB3	1:A:388:ALA:HB1	1.99	0.44
1:A:404:ASN:ND2	12:A:622:HOH:O	2.51	0.43
4:B:501:1PE:OH2	4:B:501:1PE:OH7	2.36	0.43
1:A:211:ASN:ND2	12:A:601:HOH:O	2.44	0.43
2:D:390:LYS:HB3	2:D:390:LYS:HE2	1.92	0.42
2:D:244:ASN:HA	2:D:294:LEU:HA	2.02	0.42
1:A:170:PHE:CD1	1:A:188:LYS:HE3	2.55	0.42
1:C:458:ARG:HH11	9:C:507:EDO:H12	1.85	0.42
1:A:167:LYS:H	9:A:509:EDO:H21	1.85	0.41
1:A:388:ALA:HB3	1:A:391:ALA:HB2	2.01	0.41
1:A:390:LYS:HB3	1:A:390:LYS:HE2	1.87	0.41
2:D:282:SER:HB2	8:D:502:GOL:H31	2.01	0.41
1:A:175:LYS:HD3	4:A:505:1PE:H122	2.02	0.41
1:B:150:LYS:NZ	12:B:622:HOH:O	2.54	0.40
1:B:255:ARG:NH1	10:B:512:SO4:O3	2.54	0.40
1:C:170:PHE:CD2	1:C:188:LYS:HE3	2.56	0.40
1:C:218:LYS:HE3	1:C:219:TYR:OH	2.22	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	344/361 (95%)	330 (96%)	14 (4%)	0	100	100
1	B	345/361 (96%)	332 (96%)	13 (4%)	0	100	100
1	C	343/361 (95%)	332 (97%)	11 (3%)	0	100	100
2	D	344/361 (95%)	329 (96%)	15 (4%)	0	100	100
All	All	1376/1444 (95%)	1323 (96%)	53 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	296/320 (92%)	294 (99%)	2 (1%)	81	89
1	B	298/320 (93%)	297 (100%)	1 (0%)	91	95
1	C	272/320 (85%)	267 (98%)	5 (2%)	54	67
2	D	291/321 (91%)	289 (99%)	2 (1%)	81	89
All	All	1157/1281 (90%)	1147 (99%)	10 (1%)	75	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	317	ARG
1	B	252	THR
1	C	143	ASP
1	C	232	ASN
1	C	306	VAL
1	C	407	LYS
1	C	442	SER
2	D	232	ASN
2	D	255	ARG

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	198	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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	B	321	1	15,16,17	1.22	1 (6%)	19,22,24	0.87	2 (10%)
1	PTR	A	321	1	15,16,17	1.08	1 (6%)	19,22,24	1.00	3 (15%)
1	PTR	C	321	1	15,16,17	1.23	2 (13%)	19,22,24	0.90	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	B	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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	PTR	OH-CZ	-3.90	1.31	1.40
1	C	321	PTR	OH-CZ	-3.81	1.32	1.40
1	A	321	PTR	OH-CZ	-3.35	1.33	1.40
1	C	321	PTR	P-OH	2.26	1.62	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	PTR	O2P-P-OH	3.11	114.96	105.24
1	B	321	PTR	P-OH-CZ	2.45	131.60	123.75
1	A	321	PTR	CG-CB-CA	2.26	118.67	114.10
1	A	321	PTR	P-OH-CZ	2.22	130.86	123.75
1	A	321	PTR	O3P-P-O2P	2.04	115.42	107.64
1	B	321	PTR	CG-CB-CA	2.03	118.20	114.10

There are no chirality outliers.

All (3) 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	CZ-OH-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 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	$\# Z > 2$
6	EPE	B	505	-	15,15,15	0.97	1 (6%)	18,20,20	2.21	5 (27%)
10	SO4	A	519	-	4,4,4	0.16	0	6,6,6	0.10	0
4	1PE	A	505	-	15,15,15	0.17	0	14,14,14	0.10	0
7	PEG	A	506	-	6,6,6	0.28	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	A	509	-	3,3,3	0.49	0	2,2,2	0.46	0
10	SO4	B	516	-	4,4,4	0.16	0	6,6,6	0.13	0
10	SO4	B	514	-	4,4,4	0.12	0	6,6,6	0.11	0
9	EDO	C	507	-	3,3,3	0.43	0	2,2,2	0.66	0
3	YOX	C	502	-	13,19,19	0.59	0	19,27,27	1.37	3 (15%)
8	GOL	C	506	-	5,5,5	0.88	0	5,5,5	0.94	0
8	GOL	D	502	-	5,5,5	0.80	0	5,5,5	0.90	0
8	GOL	C	501	-	5,5,5	1.21	1 (20%)	5,5,5	0.72	0
10	SO4	D	508	-	4,4,4	0.18	0	6,6,6	0.06	0
10	SO4	D	510	-	4,4,4	0.15	0	6,6,6	0.12	0
10	SO4	A	514	-	4,4,4	0.17	0	6,6,6	0.34	0
5	PG4	A	503	-	12,12,12	0.14	0	11,11,11	0.62	0
10	SO4	A	515	-	4,4,4	0.11	0	6,6,6	0.31	0
4	1PE	A	502	-	15,15,15	0.20	0	14,14,14	0.20	0
10	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.24	0
10	SO4	C	511	-	4,4,4	0.16	0	6,6,6	0.38	0
4	1PE	B	501	-	15,15,15	0.20	0	14,14,14	0.23	0
8	GOL	A	507	-	5,5,5	1.06	0	5,5,5	0.81	0
6	EPE	B	503	-	13,13,15	1.10	1 (7%)	16,18,20	3.33	9 (56%)
3	YOX	B	502	-	13,19,19	0.61	0	19,27,27	1.51	5 (26%)
8	GOL	B	507	-	5,5,5	1.06	1 (20%)	5,5,5	0.82	0
8	GOL	B	509	-	5,5,5	0.97	0	5,5,5	1.04	0
9	EDO	B	508	-	3,3,3	0.39	0	2,2,2	0.64	0
9	EDO	A	510	-	3,3,3	0.54	0	2,2,2	0.15	0
9	EDO	B	506	-	3,3,3	0.38	0	2,2,2	0.67	0
10	SO4	A	513	-	4,4,4	0.17	0	6,6,6	0.19	0
8	GOL	A	511	-	5,5,5	0.82	0	5,5,5	1.10	0
10	SO4	A	516	-	4,4,4	0.20	0	6,6,6	0.33	0
10	SO4	D	507	-	4,4,4	0.13	0	6,6,6	0.10	0
8	GOL	C	505	-	5,5,5	0.83	0	5,5,5	0.93	0
11	PO4	D	512	-	4,4,4	0.87	0	6,6,6	0.60	0
8	GOL	A	508	-	5,5,5	0.83	0	5,5,5	0.90	0
10	SO4	C	509	-	4,4,4	0.14	0	6,6,6	0.22	0
10	SO4	A	520	-	4,4,4	0.16	0	6,6,6	0.16	0
10	SO4	D	511	-	4,4,4	0.19	0	6,6,6	0.12	0
10	SO4	C	510	-	4,4,4	0.18	0	6,6,6	0.17	0
10	SO4	B	512	-	4,4,4	0.17	0	6,6,6	0.14	0
7	PEG	A	512	-	6,6,6	0.16	0	5,5,5	0.19	0
6	EPE	C	504	-	15,15,15	0.97	1 (6%)	18,20,20	2.02	6 (33%)
8	GOL	B	504	-	5,5,5	1.22	1 (20%)	5,5,5	0.92	0
3	YOX	D	501	-	13,19,19	0.57	0	19,27,27	1.76	7 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SO4	D	506	-	4,4,4	0.21	0	6,6,6	0.35	0
4	1PE	C	503	-	15,15,15	0.19	0	14,14,14	0.27	0
10	SO4	B	513	-	4,4,4	0.25	0	6,6,6	0.33	0
8	GOL	D	504	-	5,5,5	0.95	0	5,5,5	0.87	0
6	EPE	A	504	-	12,12,15	1.12	1 (8%)	14,16,20	3.33	5 (35%)
3	YOX	A	501	-	13,19,19	0.76	0	19,27,27	1.53	4 (21%)
10	SO4	C	512	-	4,4,4	0.16	0	6,6,6	0.14	0
10	SO4	D	509	-	4,4,4	0.13	0	6,6,6	0.17	0
10	SO4	B	515	-	4,4,4	0.14	0	6,6,6	0.22	0
7	PEG	B	510	-	6,6,6	0.16	0	5,5,5	0.06	0
9	EDO	B	511	-	3,3,3	0.50	0	2,2,2	0.42	0
10	SO4	A	518	-	4,4,4	0.23	0	6,6,6	0.23	0
10	SO4	A	517	-	4,4,4	0.18	0	6,6,6	0.13	0
4	1PE	D	503	-	12,12,15	0.16	0	11,11,14	0.20	0
10	SO4	C	508	-	4,4,4	0.19	0	6,6,6	0.32	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
6	EPE	B	505	-	-	4/9/19/19	0/1/1/1
4	1PE	A	505	-	-	5/13/13/13	-
7	PEG	A	506	-	-	2/4/4/4	-
9	EDO	A	509	-	-	1/1/1/1	-
9	EDO	C	507	-	-	0/1/1/1	-
3	YOX	C	502	-	-	0/0/13/13	0/3/3/3
8	GOL	C	506	-	-	2/4/4/4	-
8	GOL	D	502	-	-	0/4/4/4	-
8	GOL	C	501	-	-	2/4/4/4	-
5	PG4	A	503	-	-	9/10/10/10	-
4	1PE	A	502	-	-	4/13/13/13	-
4	1PE	B	501	-	-	4/13/13/13	-
8	GOL	A	507	-	-	4/4/4/4	-
6	EPE	B	503	-	-	1/6/16/19	0/1/1/1
3	YOX	B	502	-	-	0/0/13/13	0/3/3/3
8	GOL	B	507	-	-	0/4/4/4	-
8	GOL	B	509	-	-	4/4/4/4	-
9	EDO	B	508	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	510	-	-	1/1/1/1	-
9	EDO	B	506	-	-	1/1/1/1	-
8	GOL	A	511	-	-	0/4/4/4	-
8	GOL	C	505	-	-	0/4/4/4	-
8	GOL	A	508	-	-	2/4/4/4	-
7	PEG	A	512	-	-	2/4/4/4	-
6	EPE	C	504	-	-	6/9/19/19	0/1/1/1
8	GOL	B	504	-	-	1/4/4/4	-
3	YOX	D	501	-	-	0/0/13/13	0/3/3/3
4	1PE	C	503	-	-	6/13/13/13	-
8	GOL	D	504	-	-	2/4/4/4	-
6	EPE	A	504	-	-	1/6/14/19	0/1/1/1
3	YOX	A	501	-	-	0/0/13/13	0/3/3/3
7	PEG	B	510	-	-	2/4/4/4	-
9	EDO	B	511	-	-	1/1/1/1	-
4	1PE	D	503	-	-	5/10/10/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	503	EPE	C10-S	3.54	1.82	1.77
6	C	504	EPE	C10-S	3.30	1.82	1.77
6	B	505	EPE	C10-S	3.08	1.81	1.77
6	A	504	EPE	C10-S	2.97	1.81	1.77
8	C	501	GOL	C3-C2	2.09	1.60	1.51
8	B	507	GOL	O2-C2	-2.08	1.37	1.43
8	B	504	GOL	C3-C2	2.04	1.60	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	504	EPE	O2S-S-C10	10.94	120.09	106.92
6	B	503	EPE	C5-N4-C3	7.14	119.51	109.52
6	B	503	EPE	C7-N4-C3	6.88	120.95	110.66
6	B	503	EPE	C7-N4-C5	5.89	119.47	110.66
6	B	505	EPE	C7-N4-C3	4.41	122.50	111.23
6	C	504	EPE	C5-N4-C3	4.40	118.73	108.83
6	B	505	EPE	O1S-S-C10	4.17	111.93	106.92
6	B	505	EPE	O2S-S-C10	4.01	111.74	106.92
6	C	504	EPE	C7-N4-C3	3.54	120.29	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	YOX	C11-C9-C7	3.39	119.30	114.38
6	C	504	EPE	C7-N4-C5	3.35	119.80	111.23
6	B	505	EPE	C5-N4-C3	3.28	116.21	108.83
6	C	504	EPE	O2S-S-C10	3.19	110.76	106.92
6	A	504	EPE	C5-N4-C3	3.15	119.40	110.34
6	B	503	EPE	O1S-S-C10	3.15	110.71	106.92
6	A	504	EPE	C3-C2-N1	3.14	115.44	110.94
3	C	502	YOX	C8-C7-N1	-2.87	108.05	111.55
3	A	501	YOX	C8-C7-C9	-2.86	125.20	129.87
3	D	501	YOX	C8-C7-N1	-2.86	108.07	111.55
3	B	502	YOX	C8-C7-N1	-2.70	108.27	111.55
3	A	501	YOX	C11-C9-C7	2.63	118.20	114.38
3	A	501	YOX	C7-N1-C5	2.60	110.04	104.41
3	C	502	YOX	C7-N1-C5	2.57	109.96	104.41
6	B	503	EPE	C6-N1-C2	2.56	114.59	108.83
6	C	504	EPE	O3S-S-C10	2.55	109.89	105.77
3	D	501	YOX	C7-N1-C5	2.54	109.90	104.41
3	B	502	YOX	C7-N1-C5	2.53	109.88	104.41
3	A	501	YOX	C8-C7-N1	-2.50	108.51	111.55
3	D	501	YOX	C8-C7-C9	-2.48	125.83	129.87
6	B	503	EPE	C5-C6-N1	2.45	115.66	110.64
6	C	504	EPE	O1S-S-C10	2.41	109.81	106.92
3	B	502	YOX	C8-C7-C9	-2.32	126.08	129.87
6	B	503	EPE	O2S-S-C10	2.28	109.66	106.92
6	B	505	EPE	C6-C5-N4	-2.24	106.05	110.64
3	C	502	YOX	C7-C8-C10	-2.20	124.17	127.33
3	B	502	YOX	C14-C9-C7	2.15	117.50	114.38
6	B	503	EPE	C6-C5-N4	2.13	113.21	110.80
3	D	501	YOX	C8-C10-N2	-2.09	173.28	177.31
3	B	502	YOX	C11-C9-C7	2.06	117.36	114.38
6	A	504	EPE	C9-N1-C2	-2.04	106.01	111.23
6	A	504	EPE	O2S-S-O1S	-2.04	106.88	113.95
3	D	501	YOX	C7-C8-C10	-2.02	124.43	127.33
6	B	503	EPE	O3S-S-C10	2.01	109.02	105.77
3	D	501	YOX	C12-C11-C9	-2.01	101.08	104.71

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	504	EPE	S-C10-C9-N1
6	B	503	EPE	S-C10-C9-N1

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Mol	Chain	Res	Type	Atoms
6	B	505	EPE	C9-C10-S-O1S
6	B	505	EPE	C9-C10-S-O3S
6	C	504	EPE	C10-C9-N1-C6
6	C	504	EPE	C8-C7-N4-C3
6	C	504	EPE	C9-C10-S-O1S
6	C	504	EPE	C9-C10-S-O3S
8	A	507	GOL	O1-C1-C2-C3
8	A	508	GOL	O1-C1-C2-C3
8	B	509	GOL	O1-C1-C2-C3
8	B	509	GOL	C1-C2-C3-O3
8	C	506	GOL	O1-C1-C2-C3
8	D	504	GOL	C1-C2-C3-O3
7	A	506	PEG	C4-C3-O2-C2
4	C	503	1PE	C25-C15-OH6-C26
4	C	503	1PE	OH5-C14-C24-OH4
8	B	509	GOL	O1-C1-C2-O2
4	A	505	1PE	OH2-C12-C22-OH3
5	A	503	PG4	O4-C7-C8-O5
7	A	506	PEG	O1-C1-C2-O2
4	D	503	1PE	OH5-C14-C24-OH4
4	A	502	1PE	OH7-C16-C26-OH6
4	A	505	1PE	OH7-C16-C26-OH6
5	A	503	PG4	O1-C1-C2-O2
8	A	507	GOL	C1-C2-C3-O3
8	C	501	GOL	O1-C1-C2-C3
4	B	501	1PE	OH7-C16-C26-OH6
8	A	507	GOL	O2-C2-C3-O3
8	B	509	GOL	O2-C2-C3-O3
8	C	506	GOL	O1-C1-C2-O2
8	D	504	GOL	O2-C2-C3-O3
9	A	509	EDO	O1-C1-C2-O2
9	B	511	EDO	O1-C1-C2-O2
5	A	503	PG4	O2-C3-C4-O3
4	D	503	1PE	OH4-C13-C23-OH3
8	A	508	GOL	O1-C1-C2-O2
4	A	505	1PE	OH5-C14-C24-OH4
4	B	501	1PE	OH5-C14-C24-OH4
7	B	510	PEG	C4-C3-O2-C2
5	A	503	PG4	C3-C4-O3-C5
5	A	503	PG4	C8-C7-O4-C6
4	C	503	1PE	C13-C23-OH3-C22
4	B	501	1PE	C25-C15-OH6-C26

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Mol	Chain	Res	Type	Atoms
8	A	507	GOL	O1-C1-C2-O2
8	C	501	GOL	O1-C1-C2-O2
5	A	503	PG4	C6-C5-O3-C4
7	A	512	PEG	C4-C3-O2-C2
4	C	503	1PE	C24-C14-OH5-C25
4	C	503	1PE	C15-C25-OH5-C14
4	D	503	1PE	C24-C14-OH5-C25
6	B	505	EPE	C9-C10-S-O2S
6	C	504	EPE	C9-C10-S-O2S
4	D	503	1PE	C16-C26-OH6-C15
6	C	504	EPE	C8-C7-N4-C5
7	B	510	PEG	O2-C3-C4-O4
5	A	503	PG4	C4-C3-O2-C2
4	B	501	1PE	OH4-C13-C23-OH3
7	A	512	PEG	O2-C3-C4-O4
5	A	503	PG4	C5-C6-O4-C7
4	A	505	1PE	C15-C25-OH5-C14
4	A	502	1PE	C13-C23-OH3-C22
4	A	502	1PE	OH2-C12-C22-OH3
6	B	505	EPE	C8-C7-N4-C5
9	B	508	EDO	O1-C1-C2-O2
8	B	504	GOL	C1-C2-C3-O3
4	A	502	1PE	OH4-C13-C23-OH3
4	D	503	1PE	OH7-C16-C26-OH6
9	A	510	EDO	O1-C1-C2-O2
9	B	506	EDO	O1-C1-C2-O2
5	A	503	PG4	O3-C5-C6-O4
4	A	505	1PE	C16-C26-OH6-C15
4	C	503	1PE	OH6-C15-C25-OH5

There are no ring outliers.

14 monomers are involved in 15 short contacts:

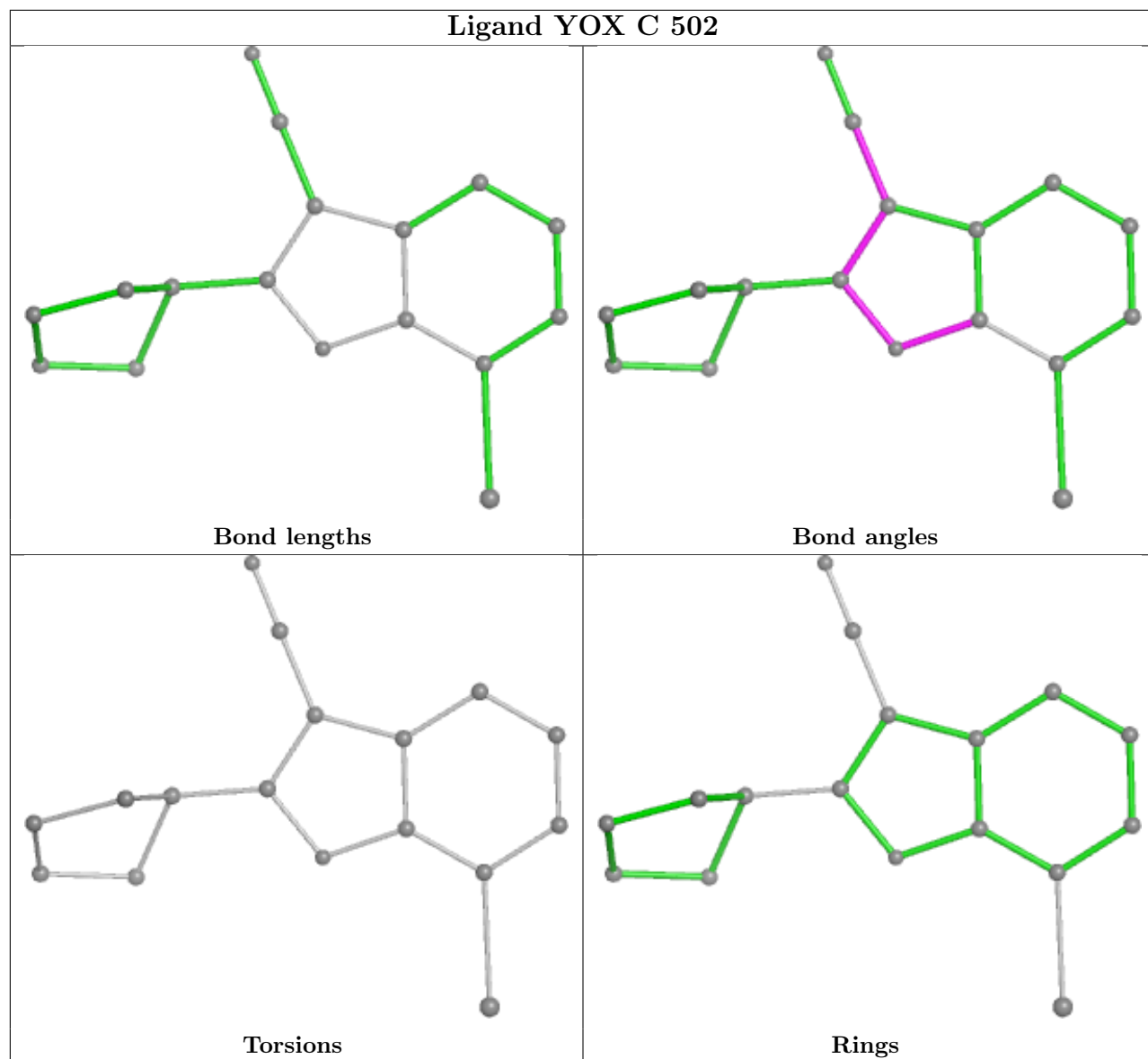
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	1PE	1	0
7	A	506	PEG	1	0
9	A	509	EDO	1	0
9	C	507	EDO	1	0
8	C	506	GOL	1	0
8	D	502	GOL	1	0
4	B	501	1PE	2	0
6	B	503	EPE	1	0

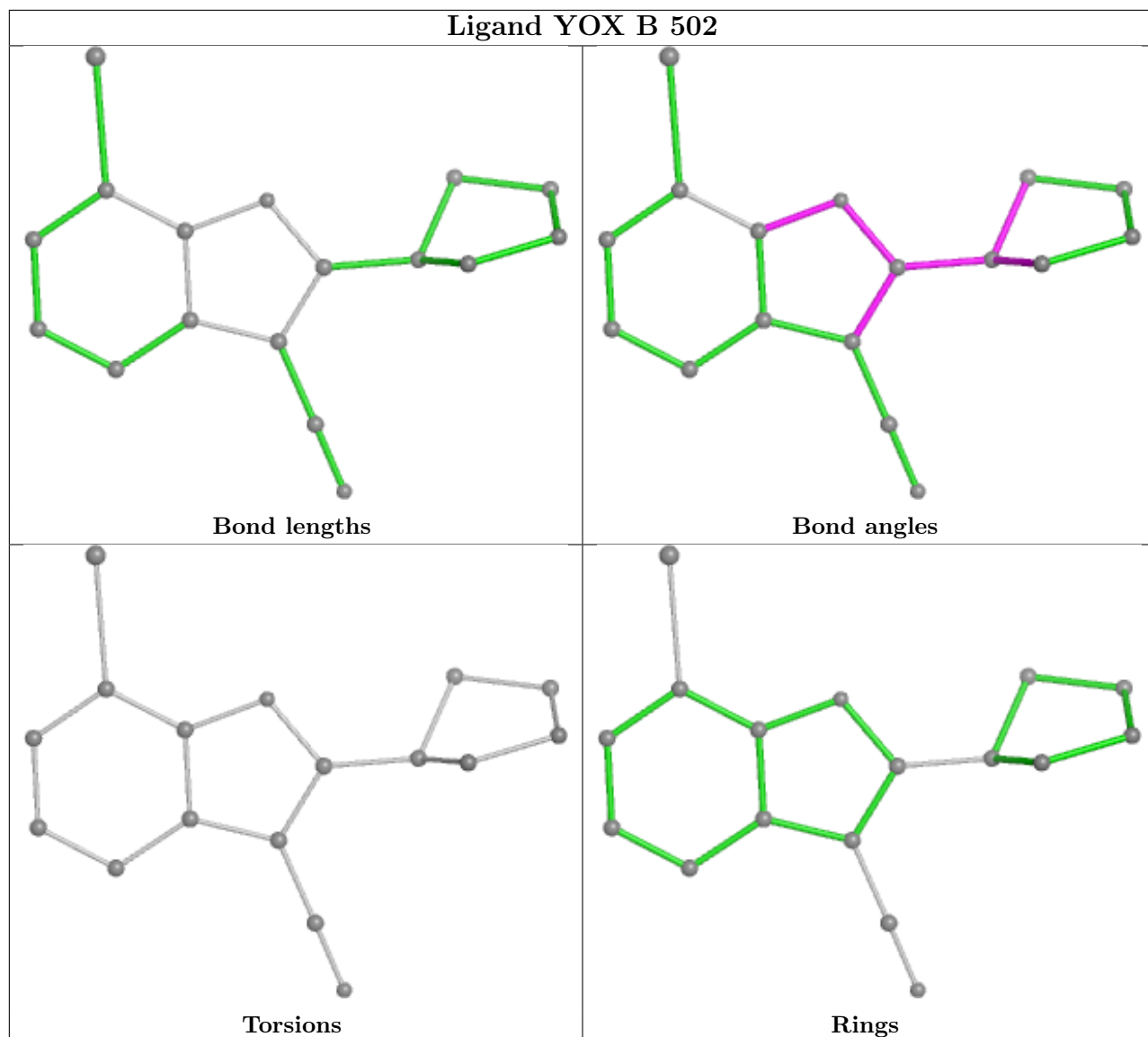
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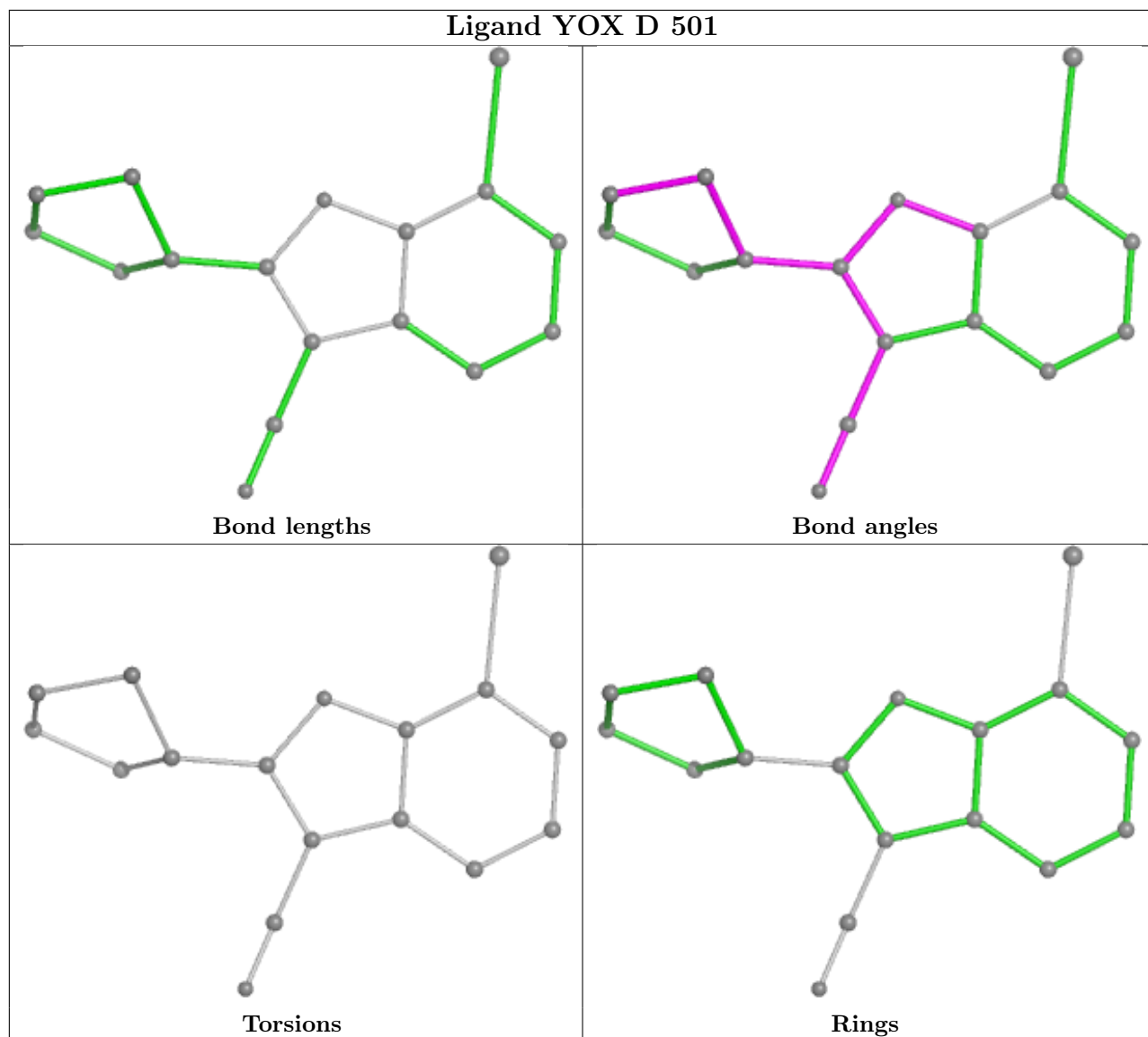
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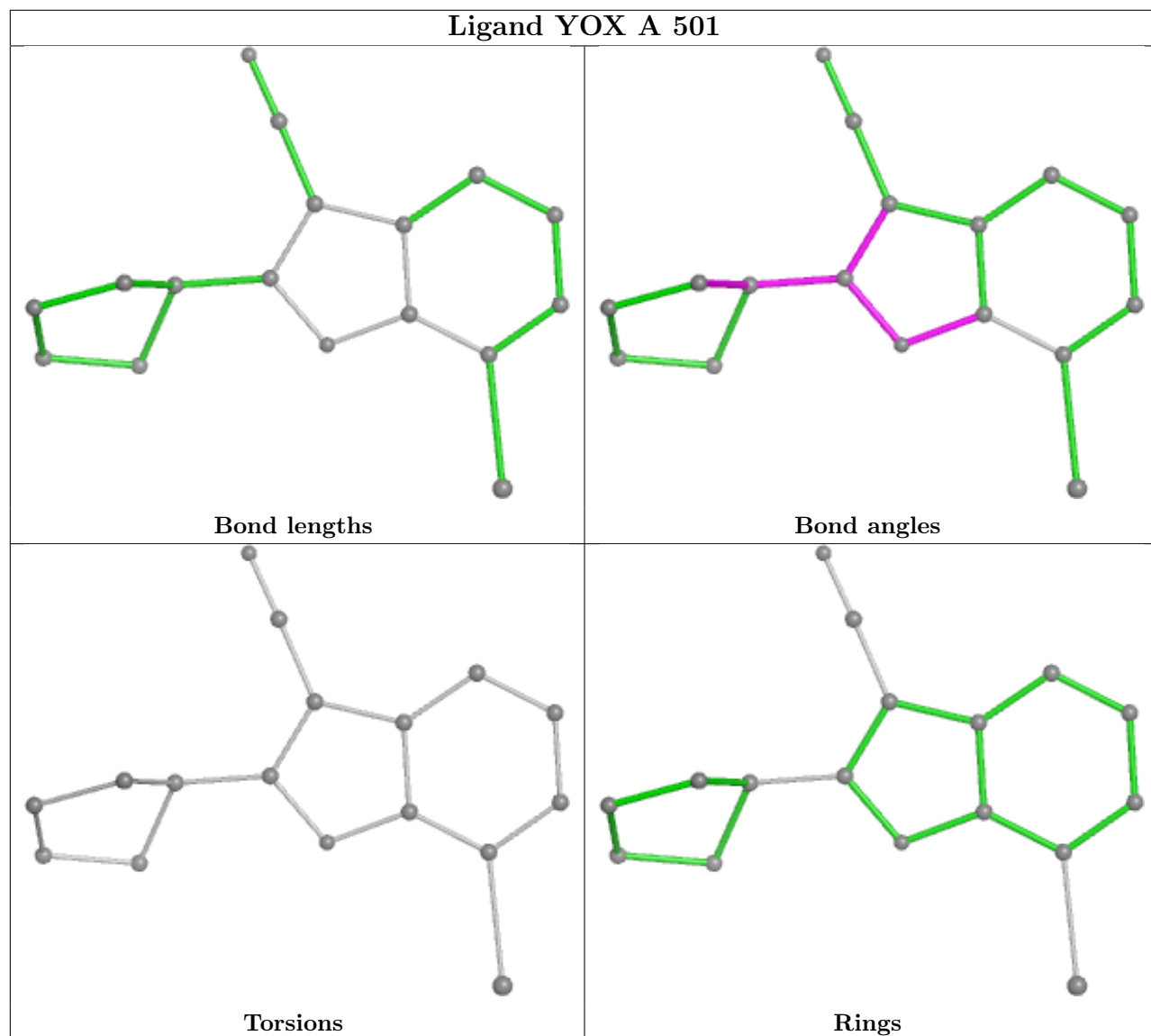
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	512	SO4	1	0
8	B	504	GOL	1	0
4	C	503	1PE	1	0
6	A	504	EPE	1	0
10	A	518	SO4	1	0
4	D	503	1PE	1	0

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.









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 [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	346/361 (95%)	-0.04	12 (3%) 47 44	32, 44, 71, 93	0
1	B	346/361 (95%)	0.13	11 (3%) 50 48	34, 50, 75, 91	1 (0%)
1	C	345/361 (95%)	0.70	35 (10%) 14 12	42, 63, 99, 110	0
2	D	346/361 (95%)	0.90	28 (8%) 19 17	49, 66, 92, 105	0
All	All	1383/1444 (95%)	0.42	86 (6%) 28 25	32, 57, 91, 110	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	321	TYR	4.6
1	A	411	GLY	4.5
1	C	215	THR	4.5
1	C	318	ILE	4.3
1	A	135	VAL	4.2
1	C	216	GLU	4.0
2	D	135	VAL	4.0
2	D	318	ILE	4.0
1	B	135	VAL	3.8
2	D	411	GLY	3.6
1	C	319	TYR	3.5
1	C	136	TYR	3.5
1	C	481	LYS	3.4
1	C	214	ASP	3.3
1	B	243	TYR	3.3
1	C	243	TYR	3.2
1	A	481	LYS	3.2
1	C	138	ASP	3.2
1	B	481	LYS	3.1
1	C	217	MET	3.1
2	D	319	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	251	ASN	3.0
1	C	315	GLY	3.0
1	A	410	ASP	3.0
1	C	150	LYS	3.0
1	A	409	LYS	3.0
1	C	219	TYR	2.9
1	C	218	LYS	2.9
1	C	179	ARG	2.9
1	A	243	TYR	2.9
2	D	215	THR	2.9
1	C	320	GLN	2.9
2	D	185	VAL	2.8
2	D	408	THR	2.8
2	D	412	LYS	2.8
1	C	149	VAL	2.8
1	C	180	VAL	2.8
2	D	180	VAL	2.7
1	B	319	TYR	2.7
1	B	218	LYS	2.7
1	A	136	TYR	2.7
1	B	195	ALA	2.7
1	A	408	THR	2.6
1	B	408	THR	2.6
2	D	471	TYR	2.6
1	B	219	TYR	2.5
2	D	315	GLY	2.5
1	A	299	LYS	2.5
2	D	177	TYR	2.4
2	D	243	TYR	2.4
2	D	157	ASP	2.4
2	D	480	LYS	2.4
1	C	246	TYR	2.4
2	D	165	ILE	2.4
2	D	179	ARG	2.4
2	D	409	LYS	2.3
1	B	320	GLN	2.3
1	C	140	TYR	2.3
1	C	439	ALA	2.3
2	D	184	TRP	2.3
2	D	216	GLU	2.3
2	D	314	LEU	2.3
1	C	174	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	228	PHE	2.3
1	B	165	ILE	2.3
2	D	224	LEU	2.2
1	C	184	TRP	2.2
1	A	217	MET	2.2
2	D	147	TYR	2.2
1	C	161	ILE	2.2
1	C	155	TRP	2.2
1	C	137	ASN	2.2
1	C	299	LYS	2.2
2	D	160	GLU	2.2
1	C	404	ASN	2.2
1	C	316	GLN	2.1
1	C	443	GLY	2.1
1	C	144	ASN	2.1
2	D	173	VAL	2.1
1	C	165	ILE	2.1
2	D	347	LEU	2.1
1	A	180	VAL	2.1
1	C	141	ASP	2.1
1	B	318	ILE	2.1
1	A	317	ARG	2.0
2	D	176	ALA	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, 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	0.79	0.14	68,73,83,89	0
1	PTR	B	321	16/17	0.88	0.14	55,67,70,76	0
1	PTR	A	321	16/17	0.91	0.11	49,57,64,66	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, 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
10	SO4	D	510	5/5	0.52	0.14	95,96,109,110	0
10	SO4	C	512	5/5	0.55	0.12	100,108,115,123	0
10	SO4	B	516	5/5	0.60	0.13	73,78,96,97	0
10	SO4	A	515	5/5	0.61	0.15	73,75,83,88	0
10	SO4	D	509	5/5	0.64	0.15	89,91,105,107	0
6	EPE	C	504	15/15	0.65	0.19	75,83,94,98	0
10	SO4	D	508	5/5	0.67	0.12	90,95,109,113	0
10	SO4	A	520	5/5	0.69	0.12	86,91,104,109	0
10	SO4	C	508	5/5	0.69	0.13	67,76,93,96	0
10	SO4	A	517	5/5	0.71	0.11	78,83,92,96	0
6	EPE	B	503	13/15	0.73	0.19	66,75,92,97	0
8	GOL	D	502	6/6	0.74	0.16	80,82,85,87	0
10	SO4	A	519	5/5	0.74	0.10	90,98,106,112	0
10	SO4	D	507	5/5	0.74	0.10	76,85,89,91	0
7	PEG	A	506	7/7	0.75	0.16	59,62,67,70	0
10	SO4	D	511	5/5	0.76	0.12	79,83,95,95	0
8	GOL	A	507	6/6	0.77	0.14	57,61,63,74	0
6	EPE	A	504	12/15	0.77	0.19	50,66,72,76	0
10	SO4	B	513	5/5	0.78	0.12	60,62,79,87	0
8	GOL	C	505	6/6	0.79	0.15	68,73,76,76	0
8	GOL	C	506	6/6	0.80	0.17	56,68,72,74	0
8	GOL	C	501	6/6	0.81	0.19	60,66,67,67	0
3	YOX	C	502	17/17	0.82	0.19	63,72,79,207	0
4	1PE	D	503	13/16	0.82	0.18	77,84,88,90	0
10	SO4	D	506	5/5	0.83	0.10	58,68,87,89	0
8	GOL	A	511	6/6	0.83	0.12	62,67,70,71	0
10	SO4	A	513	5/5	0.84	0.10	54,72,78,81	0
7	PEG	B	510	7/7	0.84	0.16	67,70,78,79	0
10	SO4	C	510	5/5	0.84	0.13	58,78,81,89	0
9	EDO	A	510	4/4	0.84	0.14	62,63,64,64	0
10	SO4	B	515	5/5	0.84	0.11	72,76,81,86	0
10	SO4	A	518	5/5	0.85	0.11	60,65,82,85	0
9	EDO	B	511	4/4	0.85	0.15	54,58,61,63	0
8	GOL	D	504	6/6	0.85	0.14	75,78,83,84	0
9	EDO	A	509	4/4	0.85	0.17	55,61,63,68	0
6	EPE	B	505	15/15	0.85	0.17	65,71,76,76	0
8	GOL	B	504	6/6	0.87	0.13	59,63,69,72	0

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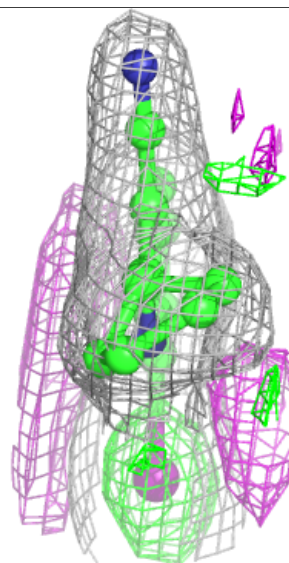
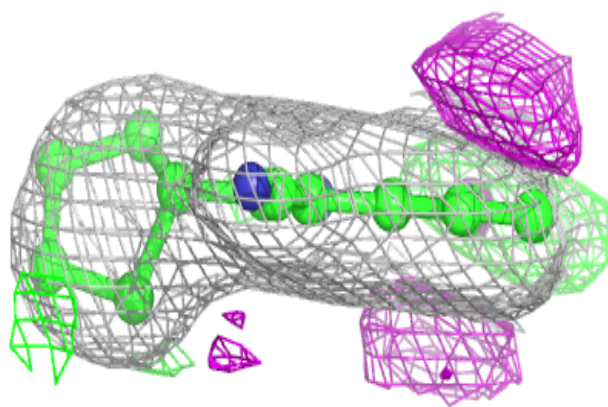
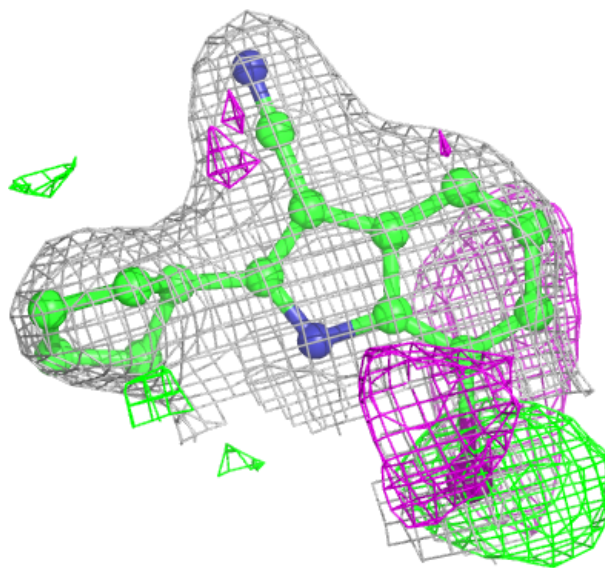
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	SO4	A	516	5/5	0.87	0.12	53,62,78,84	0
9	EDO	B	506	4/4	0.87	0.24	51,55,57,60	0
10	SO4	B	512	5/5	0.87	0.09	62,65,80,84	0
10	SO4	C	509	5/5	0.88	0.08	75,75,81,87	0
7	PEG	A	512	7/7	0.89	0.14	51,55,60,62	0
8	GOL	B	507	6/6	0.90	0.10	63,67,71,71	0
8	GOL	B	509	6/6	0.90	0.13	41,57,62,64	0
4	1PE	B	501	16/16	0.90	0.13	61,65,72,73	0
9	EDO	C	507	4/4	0.90	0.17	51,56,57,62	0
8	GOL	A	508	6/6	0.90	0.12	61,65,74,77	0
9	EDO	B	508	4/4	0.91	0.25	53,54,55,55	0
5	PG4	A	503	13/13	0.91	0.12	49,64,68,69	0
4	1PE	C	503	16/16	0.91	0.12	56,65,72,76	0
11	PO4	D	512	5/5	0.91	0.12	60,63,69,72	0
10	SO4	C	511	5/5	0.92	0.19	51,64,70,73	0
4	1PE	A	505	16/16	0.93	0.11	61,67,74,75	0
4	1PE	A	502	16/16	0.94	0.10	40,46,59,61	0
10	SO4	B	514	5/5	0.94	0.14	52,61,64,70	0
10	SO4	D	505	5/5	0.95	0.07	56,58,62,64	0
3	YOX	D	501	17/17	0.95	0.15	61,68,73,94	0
3	YOX	A	501	17/17	0.96	0.10	39,41,48,78	0
3	YOX	B	502	17/17	0.97	0.11	50,52,58,85	0
10	SO4	A	514	5/5	0.97	0.15	53,58,58,60	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.

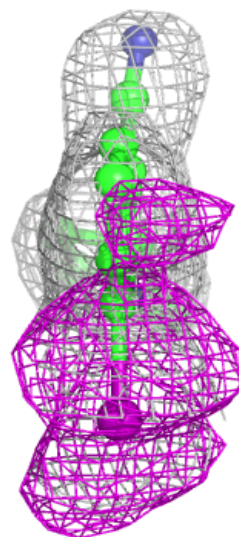
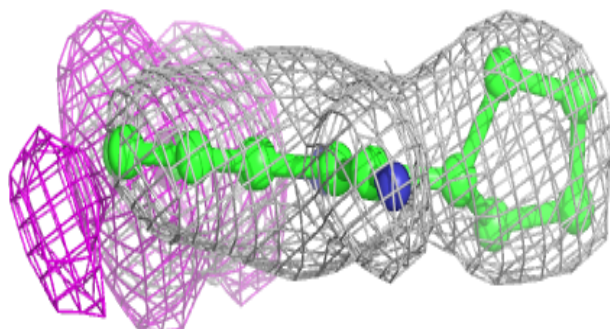
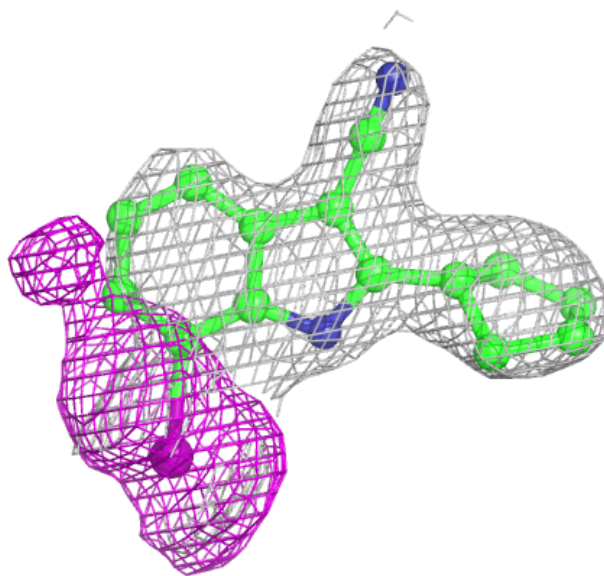
Electron density around YOX C 502:

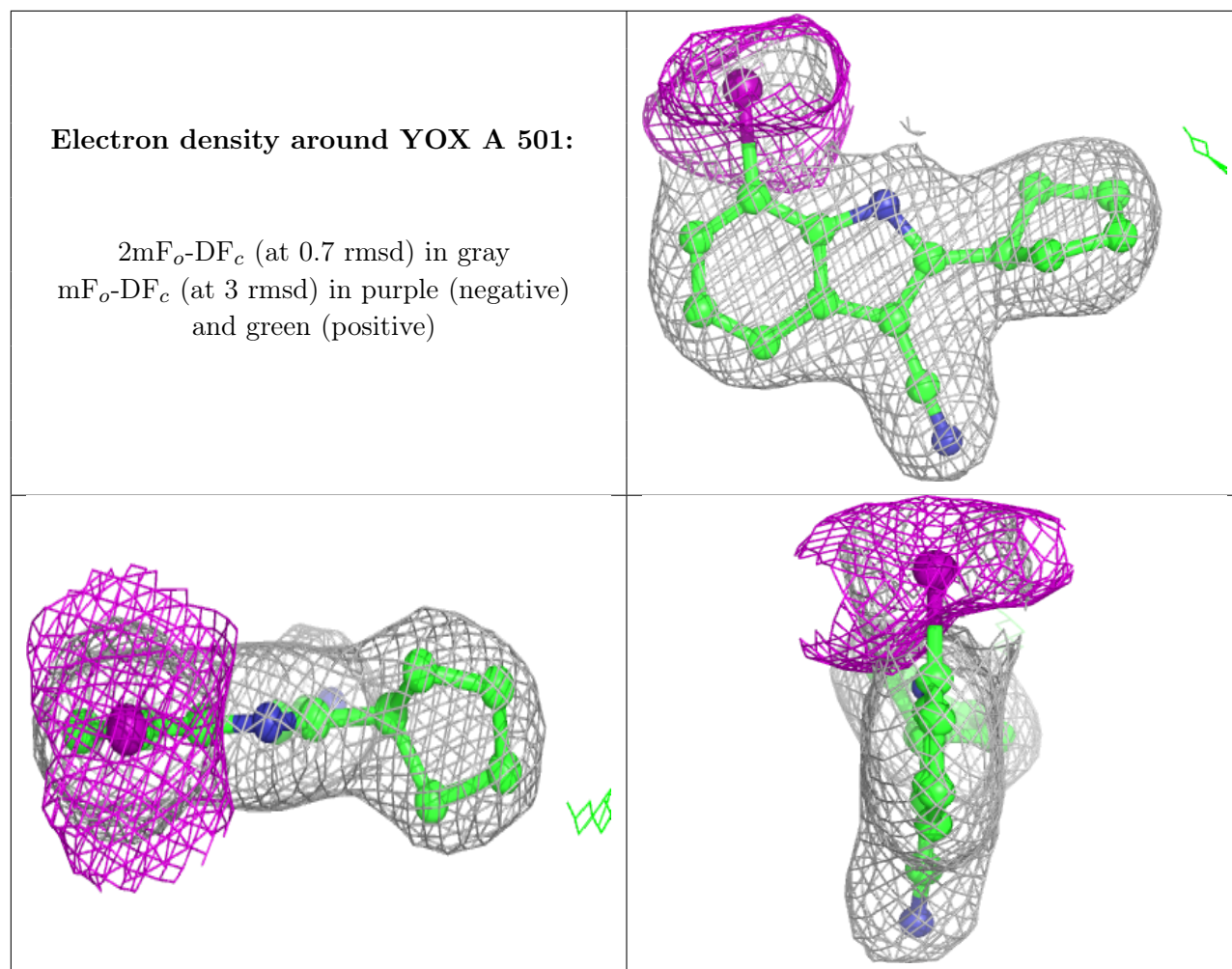
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

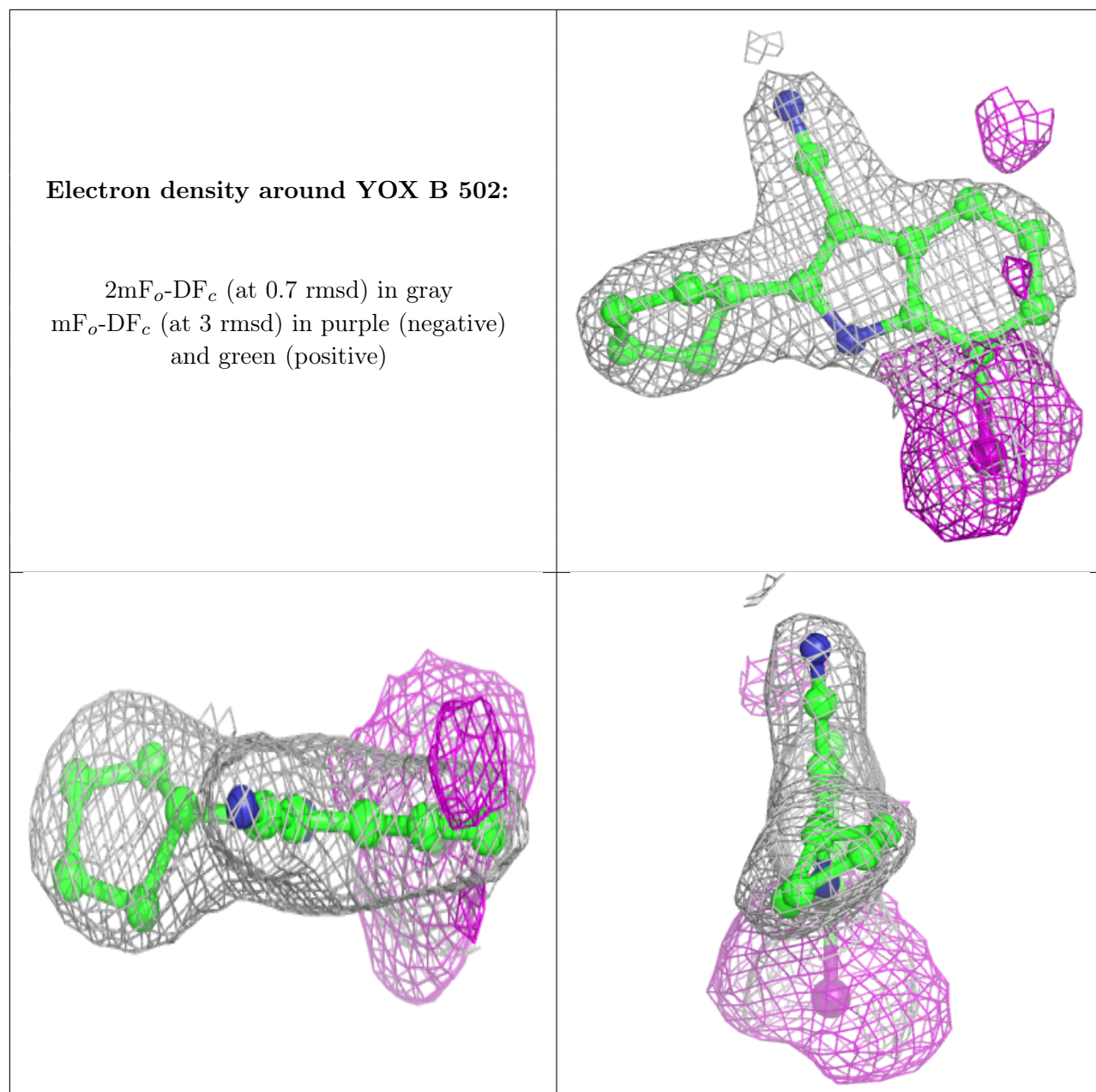


Electron density around YOX D 501:

$2mF_o-DF_c$ (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.