



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:24 AM UTC

PDB ID : 8R8E / pdb_00008r8e
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 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

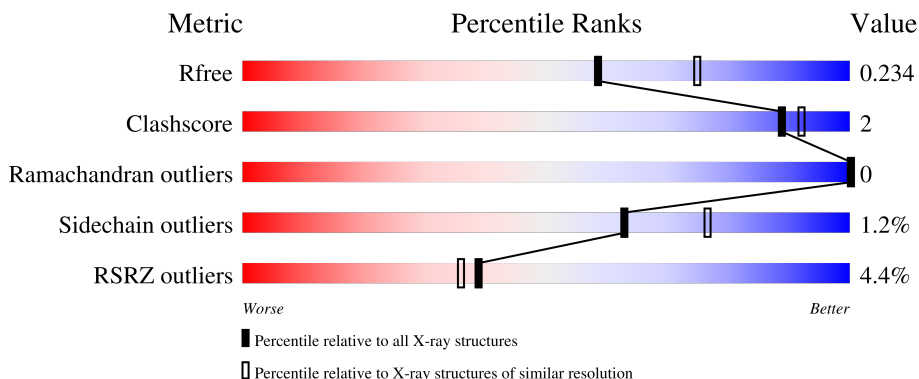
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (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% 90% 6% .
1	B	361	3% 92% . .
1	C	361	7% 91% . .
2	D	361	3% 91% 5% .

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
1	A	347	Total	C	N	O	P	S	0	0	0
			2808	1802	480	508	1	17			
1	B	347	Total	C	N	O	P	S	0	1	0
			2819	1811	484	507	1	16			
1	C	346	Total	C	N	O	P	S	0	0	0
			2701	1741	454	488	1	17			

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

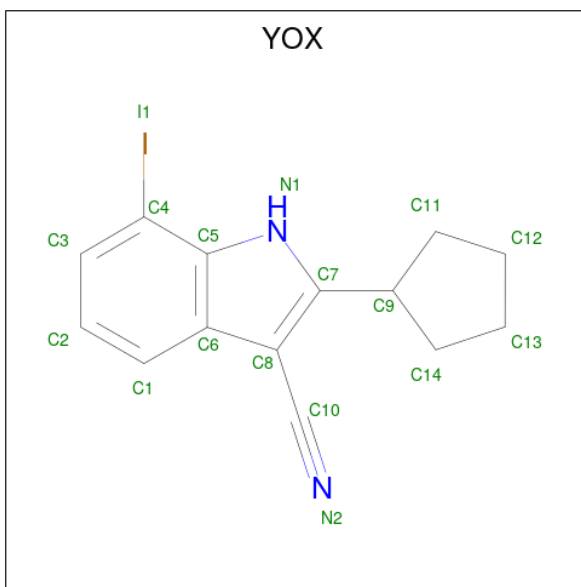
- Molecule 2 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

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

There are 2 discrepancies between the modelled and reference sequences:

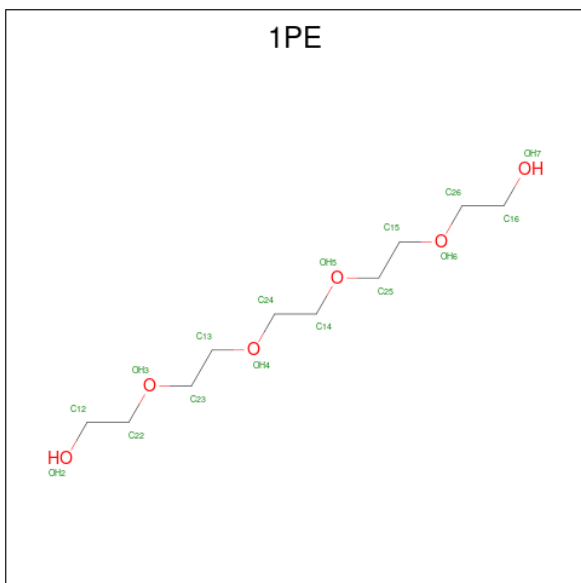
Chain	Residue	Modelled	Actual	Comment	Reference
D	125	SER	-	expression tag	UNP Q13627
D	126	MET	-	expression tag	UNP Q13627

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



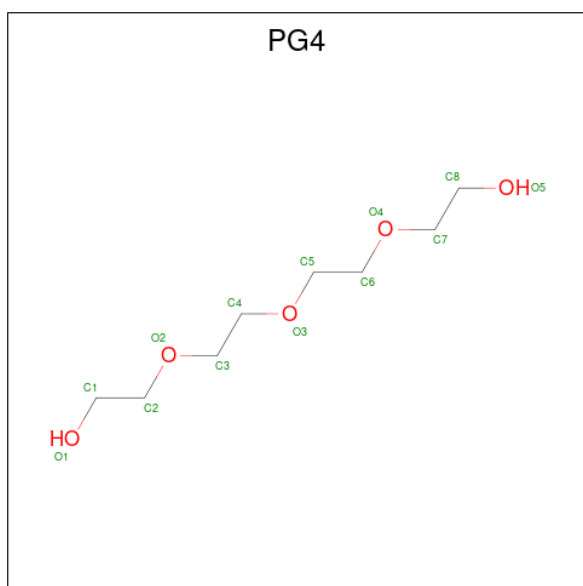
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	I	N	0	0
			17	14	1	2		
3	B	1	Total	C	I	N	0	0
			17	14	1	2		
3	C	1	Total	C	I	N	0	0
			17	14	1	2		
3	D	1	Total	C	I	N	0	0
			17	14	1	2		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



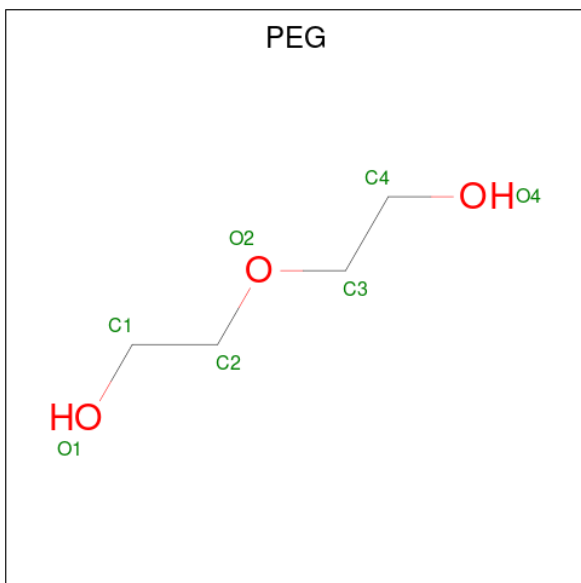
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



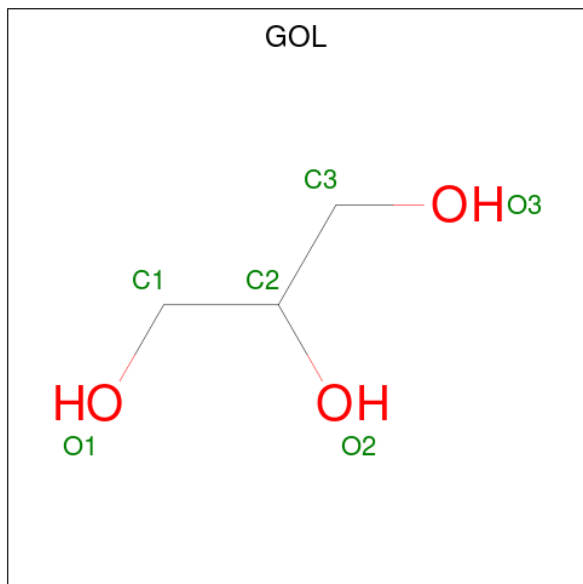
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
6	B	1	Total	C	N	O	S	0	0
			13	7	2	3	1		
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



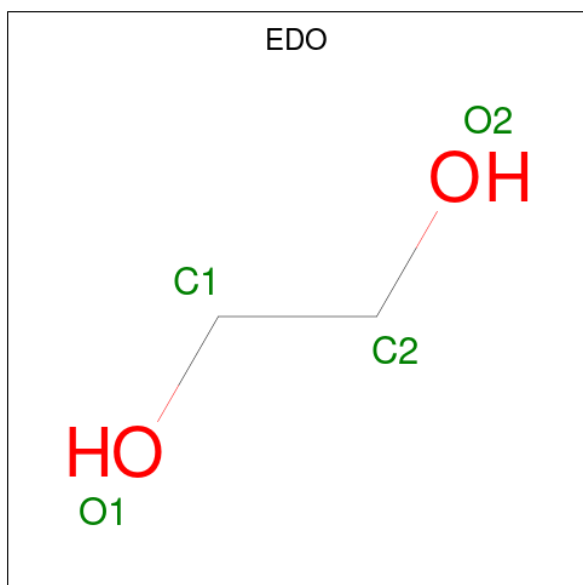
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total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

Continued on next page...

Continued from previous page...

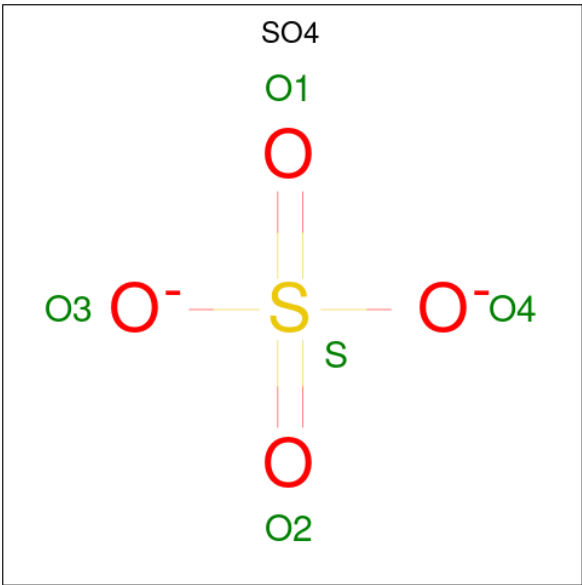
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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 (CCD ID: SO4) (formula: O_4S).



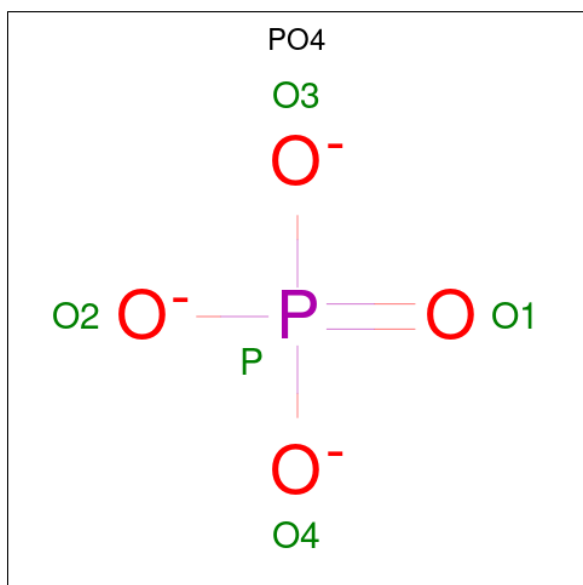
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10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

Continued on next page...

Continued from previous page...

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

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

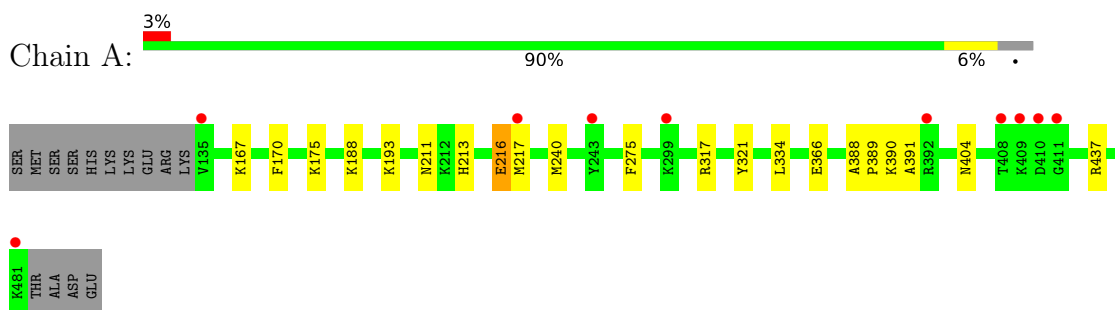
- Molecule 12 is water.

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		

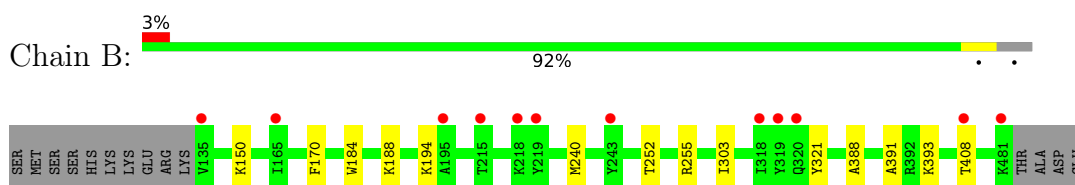
3 Residue-property plots [i](#)

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.

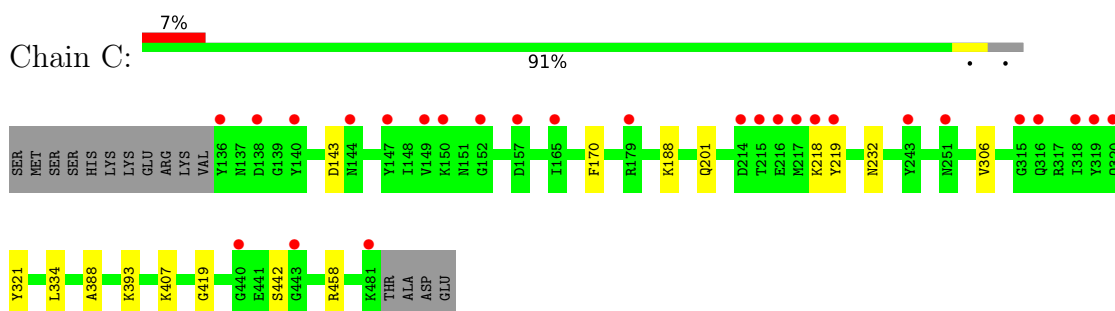
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



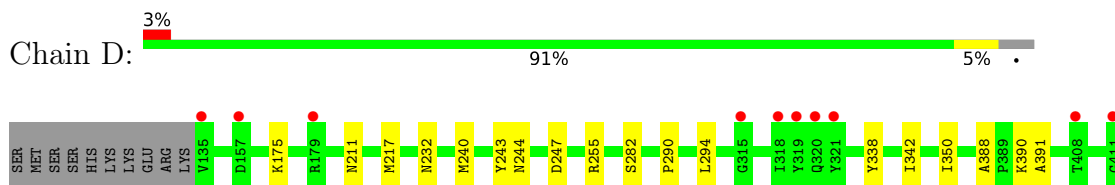
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

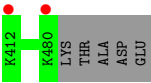


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- 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)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.234 0.200 , 0.234	Depositor DCC
R_{free} test set	1536 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12068	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage'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: GOL, 1PE, PEG, EDO, PTR, EPE, PO4, SO4, PG4, YOX

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	0.34	0/2857	0.53	0/3859
1	B	0.32	0/2870	0.55	0/3874
1	C	0.27	0/2748	0.51	0/3722
2	D	0.26	0/2834	0.51	0/3834
All	All	0.30	0/11309	0.53	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	14	0
1	B	2819	0	2780	8	0
1	C	2701	0	2582	9	0
2	D	2768	0	2706	10	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	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	22	3	0
4	C	16	0	22	1	0
4	D	13	0	17	2	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	1	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	42	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.

The worst 5 of 42 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
2:D:240:MET:HE2	4:D:503:1PE:H241	1.75	0.68
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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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%)	292 (99%)	4 (1%)	59	73
1	B	298/320 (93%)	295 (99%)	3 (1%)	68	80
1	C	272/320 (85%)	267 (98%)	5 (2%)	51	66
2	D	291/321 (91%)	289 (99%)	2 (1%)	76	86
All	All	1157/1281 (90%)	1143 (99%)	14 (1%)	63	76

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	143	ASP
1	C	232	ASN
2	D	255	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	442	SER
2	D	232	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	227	HIS
2	D	223	HIS
1	C	232	ASN
2	D	469	GLN
2	D	201	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	321	1	15,16,17	1.06	1 (6%)	17,22,24	0.88	1 (5%)
1	PTR	B	321	1	15,16,17	1.19	1 (6%)	17,22,24	0.73	1 (5%)
1	PTR	C	321	1	15,16,17	1.18	1 (6%)	17,22,24	0.92	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	A	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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	PTR	OH-CZ	-3.94	1.31	1.40
1	C	321	PTR	OH-CZ	-3.85	1.32	1.40
1	A	321	PTR	OH-CZ	-3.40	1.33	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	PTR	O2P-P-OH	3.26	114.96	105.32
1	B	321	PTR	P-OH-CZ	2.17	131.60	123.88
1	A	321	PTR	O3P-P-O2P	2.03	115.42	107.80

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	$\# Z > 2$
10	SO4	B	516	-	4,4,4	0.28	0	6,6,6	0.15	0
9	EDO	A	509	-	3,3,3	0.46	0	2,2,2	0.49	0
9	EDO	A	510	-	3,3,3	0.50	0	2,2,2	0.20	0
6	EPE	B	505	-	15,15,15	0.97	1 (6%)	19,20,20	2.01	7 (36%)
8	GOL	D	502	-	5,5,5	0.83	0	5,5,5	0.96	0
10	SO4	B	514	-	4,4,4	0.23	0	6,6,6	0.11	0
4	1PE	A	505	-	15,15,15	0.16	0	14,14,14	0.10	0
10	SO4	C	511	-	4,4,4	0.23	0	6,6,6	0.39	0
10	SO4	A	520	-	4,4,4	0.28	0	6,6,6	0.16	0
10	SO4	D	508	-	4,4,4	0.29	0	6,6,6	0.06	0
3	YOX	B	502	-	18,19,19	0.55	0	21,27,27	1.11	1 (4%)
5	PG4	A	503	-	12,12,12	0.13	0	11,11,11	0.61	0
9	EDO	C	507	-	3,3,3	0.40	0	2,2,2	0.68	0
9	EDO	B	511	-	3,3,3	0.48	0	2,2,2	0.45	0
6	EPE	C	504	-	15,15,15	0.97	1 (6%)	19,20,20	1.87	5 (26%)
10	SO4	A	514	-	4,4,4	0.28	0	6,6,6	0.36	0
10	SO4	A	517	-	4,4,4	0.30	0	6,6,6	0.08	0
8	GOL	C	505	-	5,5,5	0.86	0	5,5,5	1.01	0
4	1PE	D	503	-	12,12,15	0.16	0	11,11,14	0.20	0
4	1PE	A	502	-	15,15,15	0.19	0	14,14,14	0.20	0
8	GOL	A	508	-	5,5,5	0.86	0	5,5,5	0.97	0
10	SO4	A	513	-	4,4,4	0.29	0	6,6,6	0.17	0
10	SO4	C	509	-	4,4,4	0.26	0	6,6,6	0.18	0
3	YOX	A	501	-	18,19,19	0.61	0	21,27,27	1.26	1 (4%)
7	PEG	A	512	-	6,6,6	0.16	0	5,5,5	0.20	0
10	SO4	D	505	-	4,4,4	0.23	0	6,6,6	0.22	0
10	SO4	C	512	-	4,4,4	0.27	0	6,6,6	0.10	0
4	1PE	B	501	-	15,15,15	0.20	0	14,14,14	0.23	0
10	SO4	A	518	-	4,4,4	0.34	0	6,6,6	0.18	0
8	GOL	B	507	-	5,5,5	1.09	1 (20%)	5,5,5	0.88	0
10	SO4	D	507	-	4,4,4	0.25	0	6,6,6	0.06	0
6	EPE	B	503	-	13,13,15	1.10	1 (7%)	17,18,20	2.73	6 (35%)
3	YOX	C	502	-	18,19,19	0.54	0	21,27,27	0.96	1 (4%)
4	1PE	C	503	-	15,15,15	0.19	0	14,14,14	0.27	0
7	PEG	A	506	-	6,6,6	0.28	0	5,5,5	0.34	0
8	GOL	C	506	-	5,5,5	0.93	0	5,5,5	1.01	0
10	SO4	C	510	-	4,4,4	0.30	0	6,6,6	0.20	0
10	SO4	B	512	-	4,4,4	0.29	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SO4	D	509	-	4,4,4	0.25	0	6,6,6	0.16	0
9	EDO	B	508	-	3,3,3	0.35	0	2,2,2	0.66	0
10	SO4	D	510	-	4,4,4	0.27	0	6,6,6	0.14	0
8	GOL	B	504	-	5,5,5	1.29	1 (20%)	5,5,5	0.98	0
10	SO4	A	516	-	4,4,4	0.32	0	6,6,6	0.31	0
8	GOL	A	511	-	5,5,5	0.84	0	5,5,5	1.19	0
10	SO4	A	519	-	4,4,4	0.28	0	6,6,6	0.12	0
8	GOL	D	504	-	5,5,5	1.00	0	5,5,5	0.94	0
10	SO4	D	506	-	4,4,4	0.32	0	6,6,6	0.30	0
9	EDO	B	506	-	3,3,3	0.35	0	2,2,2	0.68	0
8	GOL	B	509	-	5,5,5	1.00	0	5,5,5	1.12	0
8	GOL	C	501	-	5,5,5	1.29	1 (20%)	5,5,5	0.77	0
10	SO4	B	513	-	4,4,4	0.36	0	6,6,6	0.27	0
10	SO4	B	515	-	4,4,4	0.26	0	6,6,6	0.22	0
10	SO4	D	511	-	4,4,4	0.30	0	6,6,6	0.09	0
6	EPE	A	504	-	12,12,15	1.11	1 (8%)	15,16,20	2.69	4 (26%)
8	GOL	A	507	-	5,5,5	1.11	0	5,5,5	0.86	0
10	SO4	A	515	-	4,4,4	0.23	0	6,6,6	0.29	0
11	PO4	D	512	-	4,4,4	0.91	0	6,6,6	0.63	0
3	YOX	D	501	-	18,19,19	0.54	0	21,27,27	1.25	1 (4%)
7	PEG	B	510	-	6,6,6	0.16	0	5,5,5	0.06	0
10	SO4	C	508	-	4,4,4	0.30	0	6,6,6	0.30	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
9	EDO	A	509	-	-	1/1/1/1	-
9	EDO	A	510	-	-	1/1/1/1	-
6	EPE	B	505	-	-	4/9/19/19	0/1/1/1
8	GOL	D	502	-	-	0/4/4/4	-
4	1PE	A	505	-	-	5/13/13/13	-
3	YOX	B	502	-	-	1/2/13/13	0/3/3/3
5	PG4	A	503	-	-	8/10/10/10	-
9	EDO	C	507	-	-	0/1/1/1	-
9	EDO	B	511	-	-	1/1/1/1	-
6	EPE	C	504	-	-	6/9/19/19	0/1/1/1
8	GOL	C	505	-	-	0/4/4/4	-
4	1PE	D	503	-	-	5/10/10/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	A	502	-	-	4/13/13/13	-
8	GOL	A	508	-	-	2/4/4/4	-
3	YOX	A	501	-	-	1/2/13/13	0/3/3/3
7	PEG	A	512	-	-	2/4/4/4	-
4	1PE	B	501	-	-	4/13/13/13	-
8	GOL	B	507	-	-	0/4/4/4	-
6	EPE	B	503	-	-	1/6/16/19	0/1/1/1
3	YOX	C	502	-	-	1/2/13/13	0/3/3/3
4	1PE	C	503	-	-	5/13/13/13	-
7	PEG	A	506	-	-	2/4/4/4	-
8	GOL	C	506	-	-	2/4/4/4	-
9	EDO	B	508	-	-	1/1/1/1	-
8	GOL	B	504	-	-	1/4/4/4	-
8	GOL	A	511	-	-	0/4/4/4	-
8	GOL	D	504	-	-	2/4/4/4	-
9	EDO	B	506	-	-	1/1/1/1	-
8	GOL	B	509	-	-	4/4/4/4	-
8	GOL	C	501	-	-	2/4/4/4	-
6	EPE	A	504	-	-	1/6/14/19	0/1/1/1
8	GOL	A	507	-	-	4/4/4/4	-
3	YOX	D	501	-	-	1/2/13/13	0/3/3/3
7	PEG	B	510	-	-	2/4/4/4	-

The worst 5 of 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	3.29	1.82	1.77
6	B	505	EPE	C10-S	3.06	1.81	1.77
6	A	504	EPE	C10-S	2.95	1.81	1.77
8	C	501	GOL	C3-C2	2.24	1.60	1.51

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	504	EPE	O2S-S-C10	8.84	120.09	106.73
6	B	503	EPE	C5-N4-C3	6.27	119.52	109.54
6	B	503	EPE	C7-N4-C3	5.41	120.94	110.63
6	B	503	EPE	C7-N4-C5	4.64	119.47	110.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	504	EPE	C5-N4-C3	4.59	118.73	108.84

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	YOX	N1-C7-C9-C14
3	B	502	YOX	N1-C7-C9-C14
3	D	501	YOX	N1-C7-C9-C11
6	A	504	EPE	S-C10-C9-N1
6	B	505	EPE	C9-C10-S-O1S

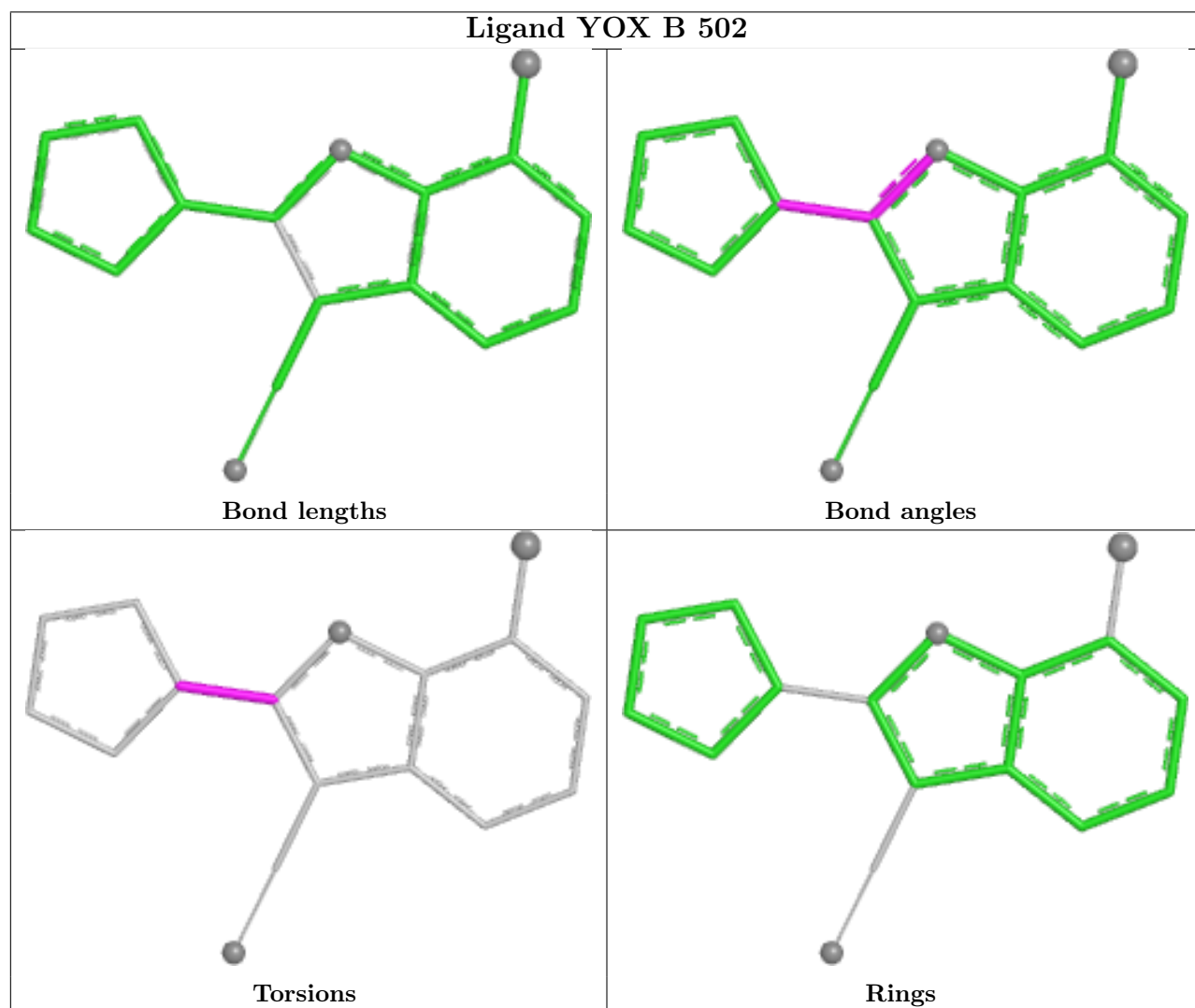
There are no ring outliers.

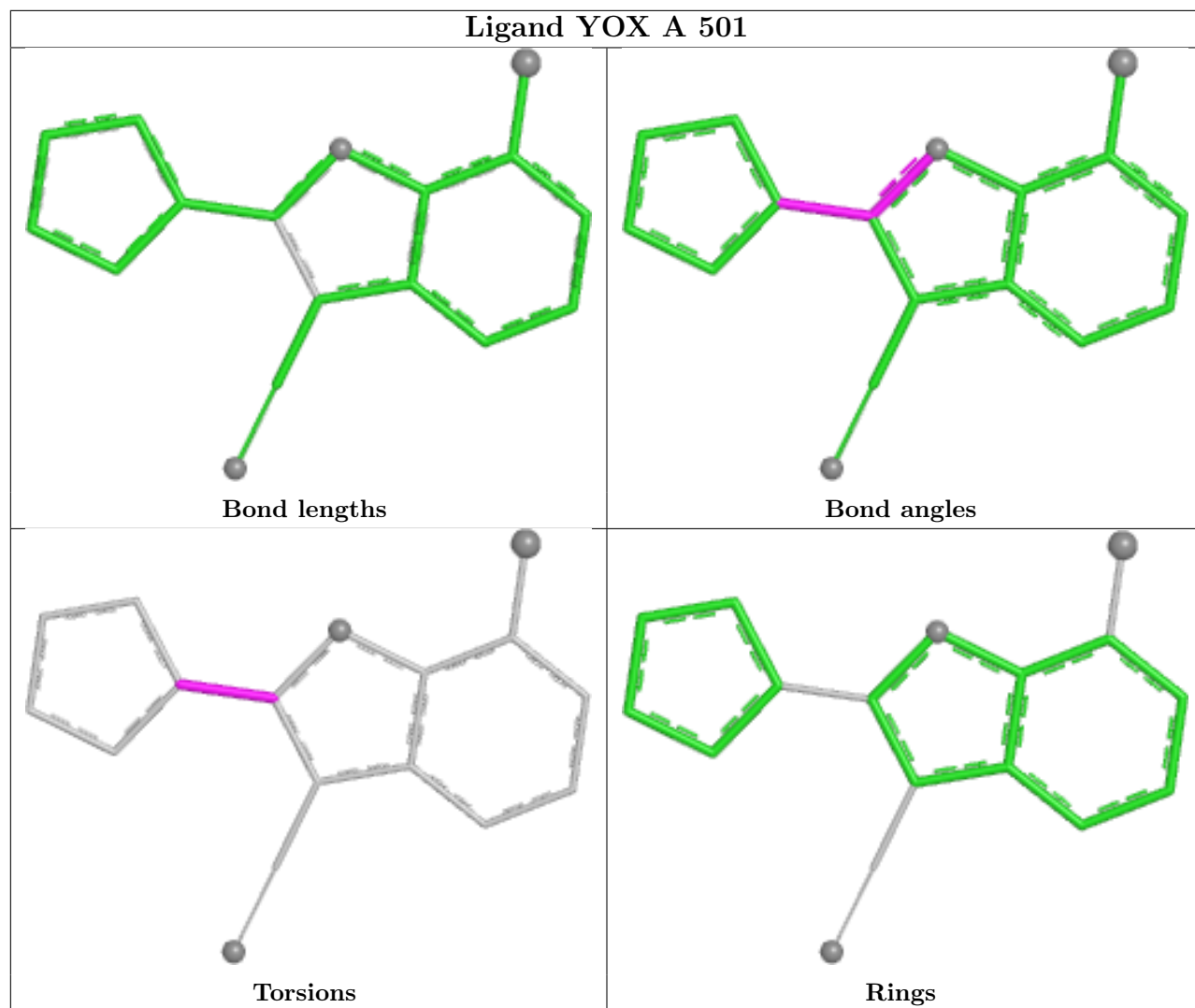
15 monomers are involved in 19 short contacts:

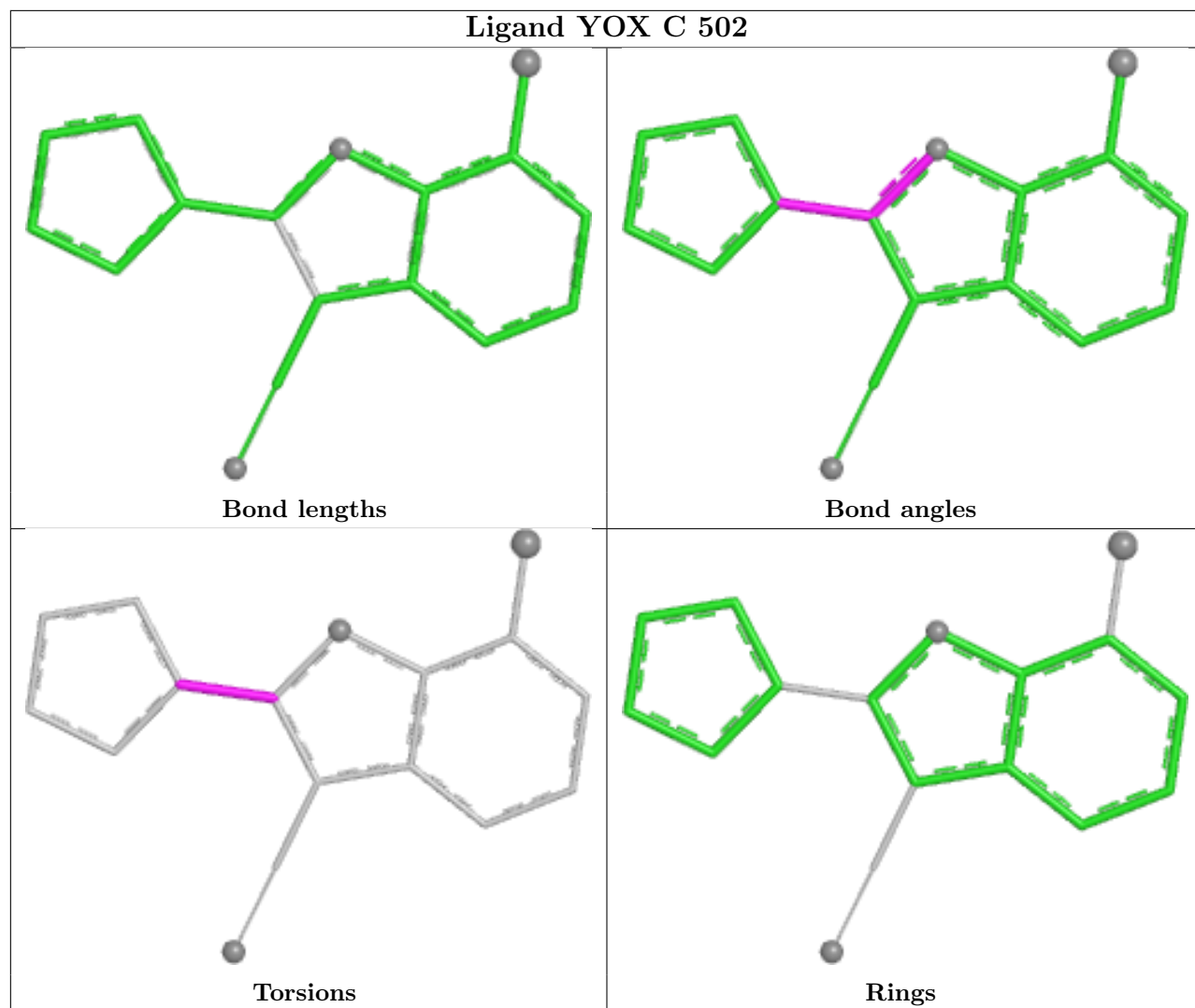
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	509	EDO	1	0
8	D	502	GOL	1	0
4	A	505	1PE	2	0
9	C	507	EDO	1	0
4	D	503	1PE	2	0
4	B	501	1PE	3	0
10	A	518	SO4	1	0
6	B	503	EPE	1	0
4	C	503	1PE	1	0
7	A	506	PEG	1	0
8	C	506	GOL	1	0
10	B	512	SO4	1	0
8	B	504	GOL	1	0
6	A	504	EPE	1	0
10	C	508	SO4	1	0

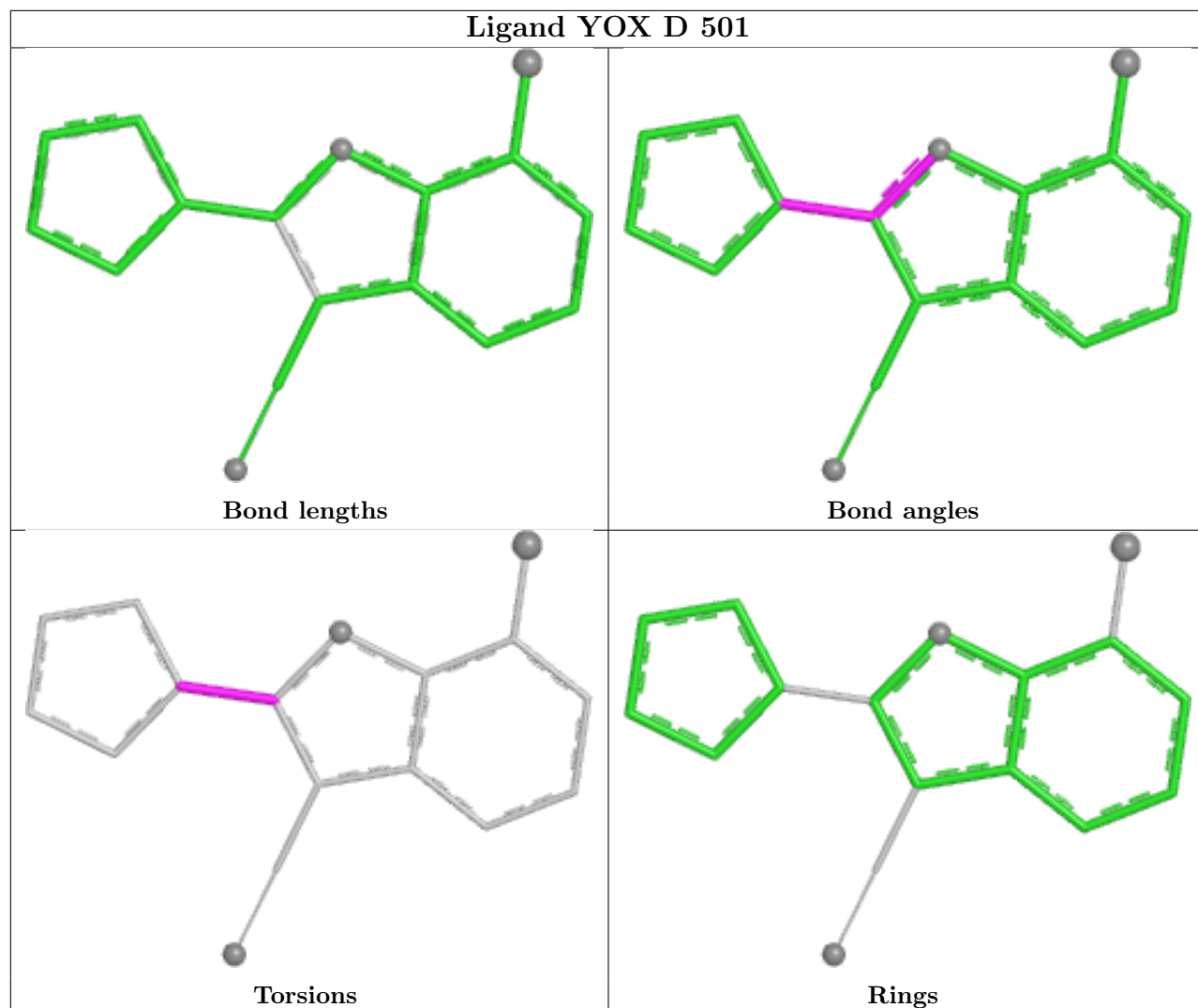
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.









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%)	-0.11	10 (2%) 53 51	32, 44, 71, 93	0
1	B	346/361 (95%)	-0.01	12 (3%) 47 44	34, 50, 75, 91	1 (0%)
1	C	345/361 (95%)	0.41	27 (7%) 19 16	42, 63, 99, 110	0
2	D	346/361 (95%)	0.39	12 (3%) 47 44	49, 66, 92, 105	0
All	All	1383/1444 (95%)	0.17	61 (4%) 39 36	32, 57, 91, 110	1 (0%)

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	GLY	4.9
2	D	321	TYR	4.8
1	A	135	VAL	4.5
2	D	318	ILE	4.3
1	C	215	THR	4.3

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	0.15	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	0.92	0.11	49,57,64,66	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
10	SO4	D	510	5/5	0.56	0.13	95,96,109,110	0
10	SO4	C	512	5/5	0.61	0.11	100,108,115,123	0
10	SO4	B	516	5/5	0.61	0.13	73,78,96,97	0
10	SO4	A	515	5/5	0.63	0.15	73,75,83,88	0
10	SO4	D	509	5/5	0.67	0.15	89,91,105,107	0
10	SO4	A	520	5/5	0.68	0.13	86,91,104,109	0
6	EPE	C	504	15/15	0.69	0.18	75,83,94,98	0
10	SO4	D	508	5/5	0.69	0.12	90,95,109,113	0
10	SO4	A	519	5/5	0.71	0.11	90,98,106,112	0
6	EPE	B	503	13/15	0.72	0.20	66,75,92,97	0
10	SO4	C	508	5/5	0.72	0.13	67,76,93,96	0
10	SO4	A	517	5/5	0.72	0.10	78,83,92,96	0
8	GOL	D	502	6/6	0.75	0.15	80,82,85,87	0
10	SO4	D	507	5/5	0.76	0.10	76,85,89,91	0
10	SO4	B	513	5/5	0.76	0.12	60,62,79,87	0
7	PEG	A	506	7/7	0.77	0.16	59,62,67,70	0
8	GOL	A	507	6/6	0.78	0.15	57,61,63,74	0
6	EPE	A	504	12/15	0.78	0.19	50,66,72,76	0
10	SO4	D	511	5/5	0.79	0.12	79,83,95,95	0
8	GOL	C	505	6/6	0.81	0.15	68,73,76,76	0
7	PEG	B	510	7/7	0.82	0.17	67,70,78,79	0
9	EDO	A	510	4/4	0.82	0.15	62,63,64,64	0
8	GOL	C	506	6/6	0.82	0.17	56,68,72,74	0
10	SO4	D	506	5/5	0.83	0.10	58,68,87,89	0
3	YOX	C	502	17/17	0.83	0.19	63,72,79,207	0
8	GOL	C	501	6/6	0.83	0.18	60,66,67,67	0
9	EDO	B	511	4/4	0.84	0.15	54,58,61,63	0
10	SO4	C	510	5/5	0.84	0.12	58,78,81,89	0
10	SO4	A	518	5/5	0.84	0.12	60,65,82,85	0
4	1PE	D	503	13/16	0.85	0.17	77,84,88,90	0
8	GOL	A	511	6/6	0.86	0.11	62,67,70,71	0
10	SO4	A	513	5/5	0.86	0.10	54,72,78,81	0

Continued on next page...

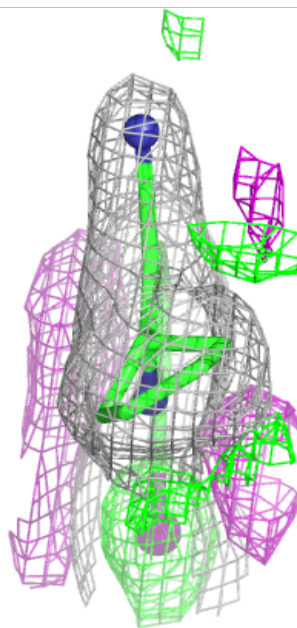
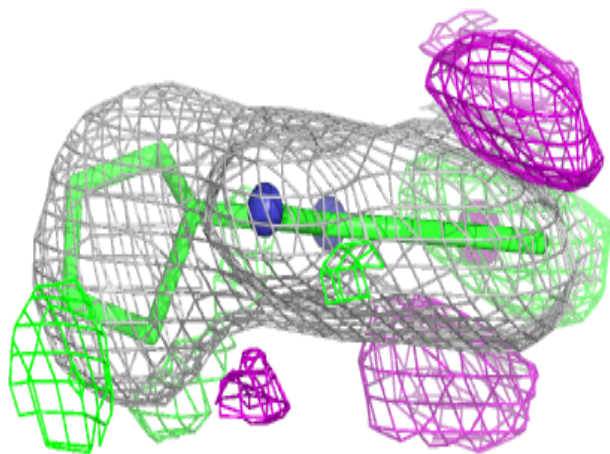
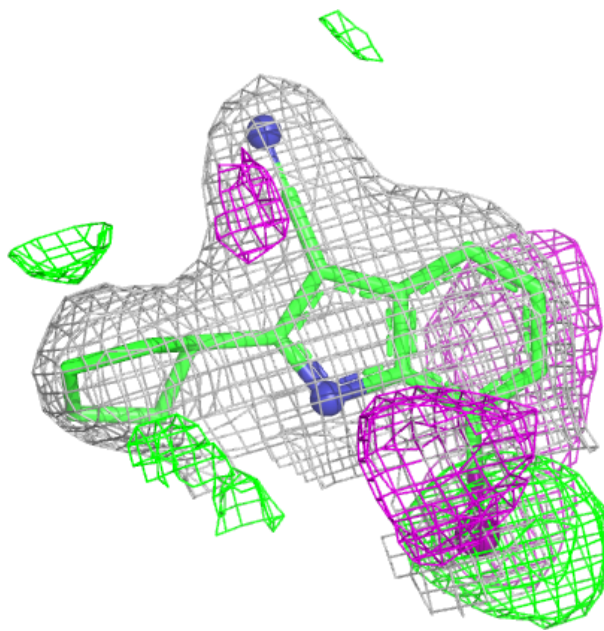
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EPE	B	505	15/15	0.86	0.17	65,71,76,76	0
9	EDO	B	506	4/4	0.86	0.26	51,55,57,60	0
10	SO4	B	515	5/5	0.86	0.10	72,76,81,86	0
9	EDO	A	509	4/4	0.87	0.16	55,61,63,68	0
8	GOL	B	504	6/6	0.87	0.14	59,63,69,72	0
8	GOL	D	504	6/6	0.88	0.13	75,78,83,84	0
10	SO4	C	509	5/5	0.89	0.07	75,75,81,87	0
9	EDO	C	507	4/4	0.89	0.18	51,56,57,62	0
10	SO4	A	516	5/5	0.89	0.11	53,62,78,84	0
4	1PE	B	501	16/16	0.90	0.13	61,65,72,73	0
7	PEG	A	512	7/7	0.90	0.13	51,55,60,62	0
5	PG4	A	503	13/13	0.90	0.12	49,64,68,69	0
8	GOL	B	507	6/6	0.90	0.10	63,67,71,71	0
10	SO4	B	512	5/5	0.90	0.08	62,65,80,84	0
9	EDO	B	508	4/4	0.90	0.23	53,54,55,55	0
8	GOL	A	508	6/6	0.91	0.11	61,65,74,77	0
8	GOL	B	509	6/6	0.91	0.12	41,57,62,64	0
11	PO4	D	512	5/5	0.91	0.11	60,63,69,72	0
4	1PE	A	505	16/16	0.92	0.12	61,67,74,75	0
4	1PE	C	503	16/16	0.93	0.12	56,65,72,76	0
10	SO4	C	511	5/5	0.93	0.20	51,64,70,73	0
4	1PE	A	502	16/16	0.94	0.10	40,46,59,61	0
3	YOX	D	501	17/17	0.95	0.14	61,68,73,94	0
10	SO4	B	514	5/5	0.95	0.13	52,61,64,70	0
10	SO4	D	505	5/5	0.96	0.06	56,58,62,64	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.

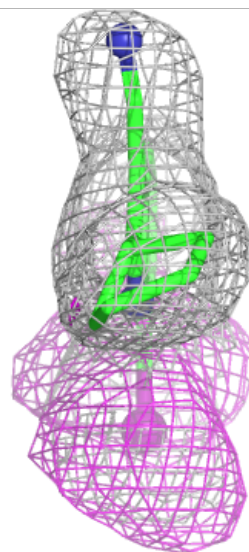
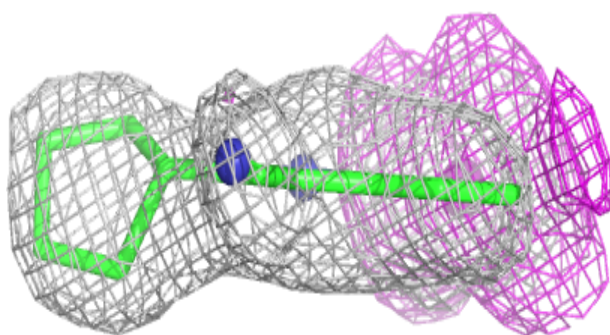
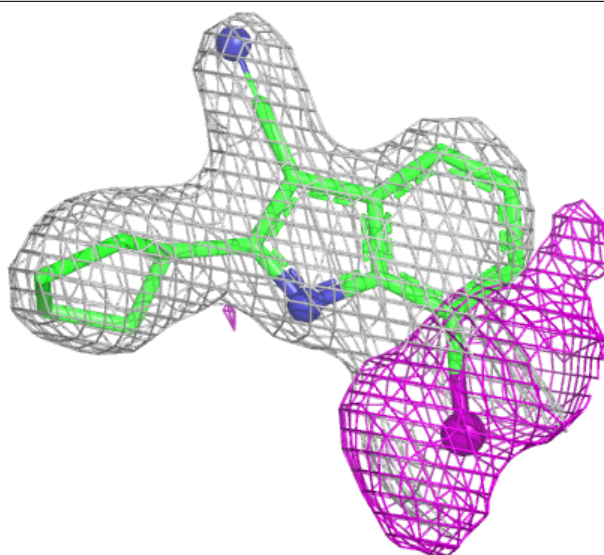
Electron density around YOX C 502:

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



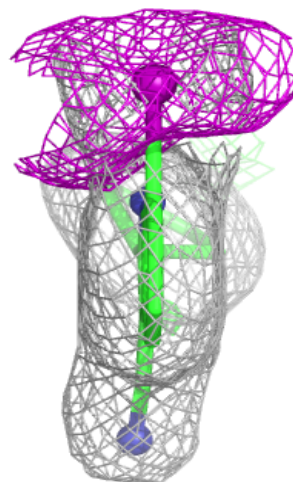
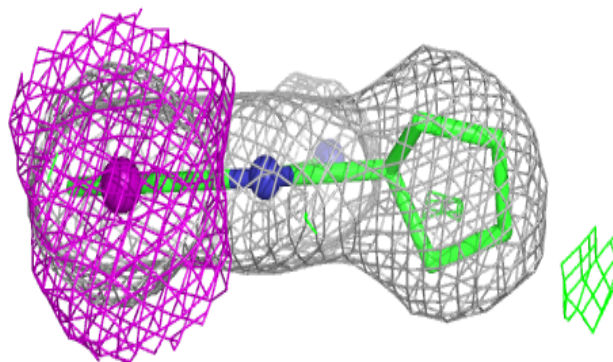
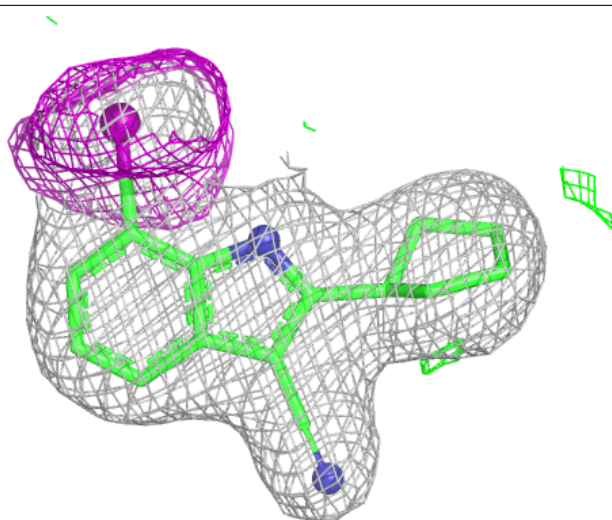
Electron density around YOX D 501:

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



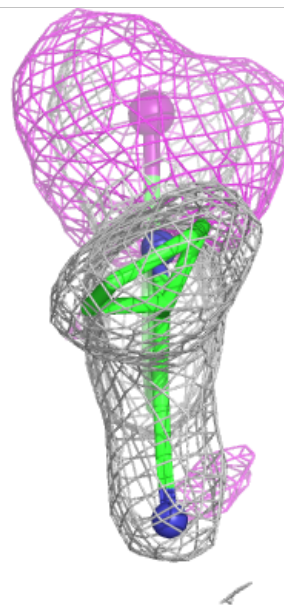
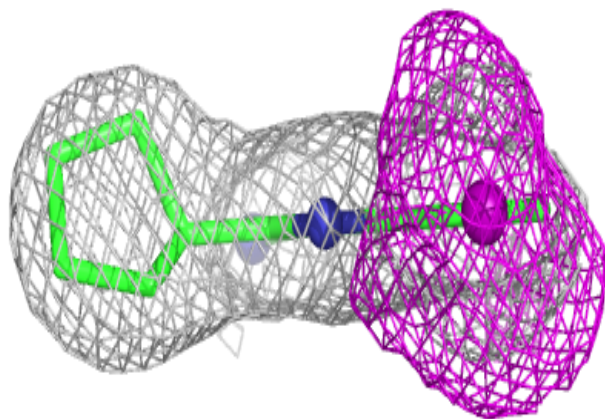
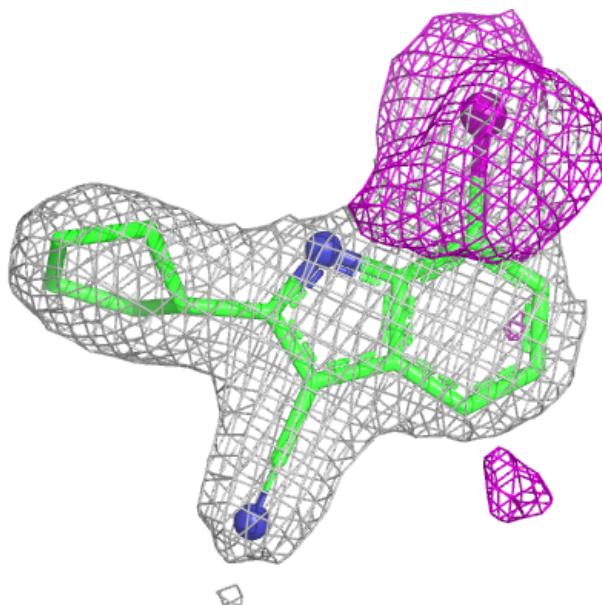
Electron density around YOX A 501:

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



Electron density around YOX 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.