



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:25 am BST

PDB ID : 6H4Q
Title : Crystal structure of human KDM4A in complex with compound 34a
Authors : Le Bihan, Y.V.; van Montfort, R.L.M.
Deposited on : 2018-07-23
Resolution : 2.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

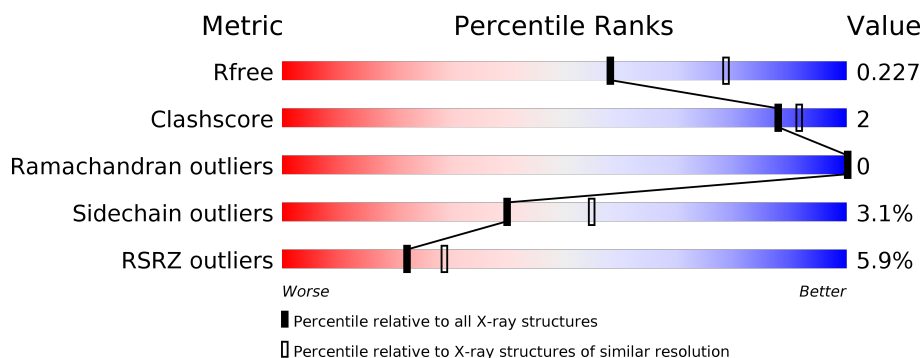
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	360	<div> <div>3%</div> <div>89%</div> <div>5% • 6%</div> </div>
1	B	360	<div> <div>4%</div> <div>90%</div> <div>7% •</div> </div>
1	C	360	<div> <div>7%</div> <div>89%</div> <div>6% •</div> </div>
1	D	360	<div> <div>8%</div> <div>91%</div> <div>• • •</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	404	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12206 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 Lysine-specific demethylase 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	6	1
			2762	1798	452	496	16			
1	B	350	Total	C	N	O	S	0	3	0
			2801	1815	460	511	15			
1	C	345	Total	C	N	O	S	0	3	0
			2753	1793	448	498	14			
1	D	344	Total	C	N	O	S	0	3	0
			2757	1783	455	504	15			

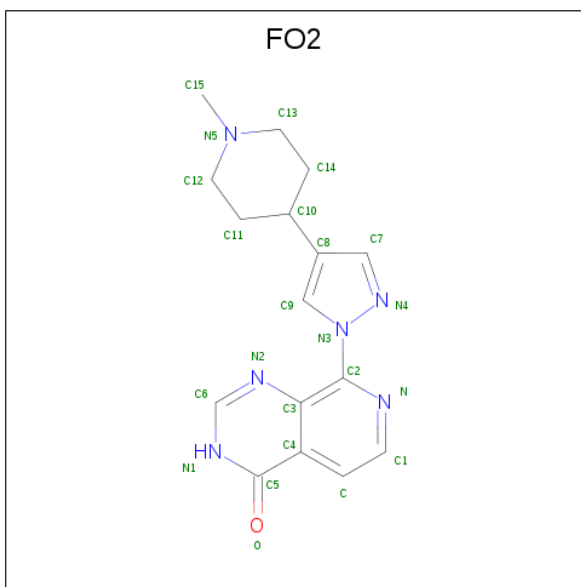
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O75164
B	0	SER	-	expression tag	UNP O75164
C	0	SER	-	expression tag	UNP O75164
D	0	SER	-	expression tag	UNP O75164

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 8-[4-(1-methylpiperidin-4-yl)pyrazol-1-yl]-3 {H}-pyrido[3,4-d]pyrimidin-4-one (three-letter code: FO2) (formula: C₁₆H₁₈N₆O) (labeled as "Ligand of Interest" by author).



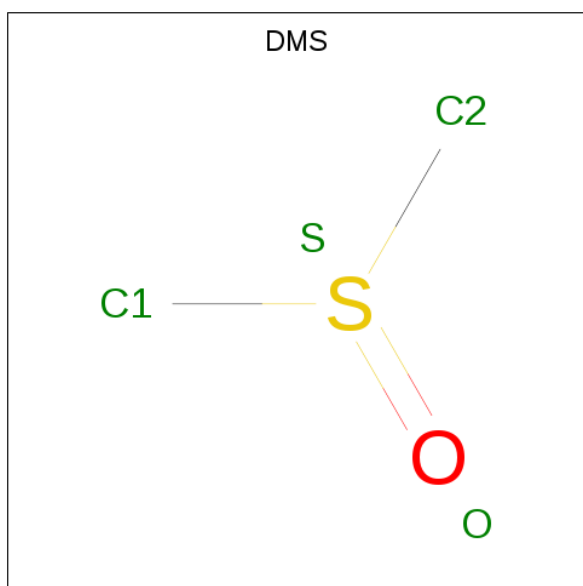
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	16	6	1		
3	B	1	Total	C	N	O	0	0
			23	16	6	1		
3	C	1	Total	C	N	O	0	0
			23	16	6	1		
3	D	1	Total	C	N	O	0	0
			23	16	6	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



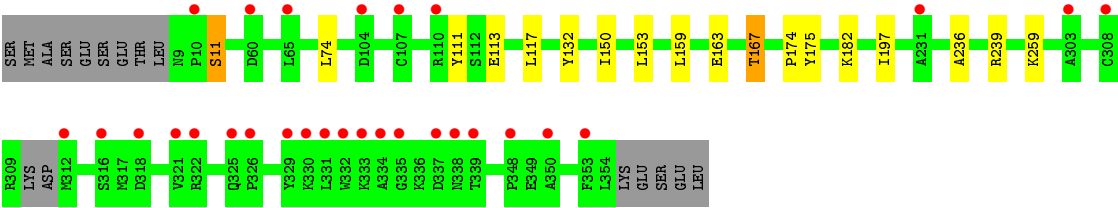
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	311	Total 318	O 318	0	7
7	B	257	Total 261	O 261	0	4
7	C	230	Total 231	O 231	0	1
7	D	183	Total 183	O 183	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.42Å 101.80Å 142.11Å 90.00° 99.55° 90.00°	Depositor
Resolution (Å)	46.20 – 2.31 43.50 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.20-2.31) 100.0 (43.50-2.31)	Depositor EDS
R_{merge}	0.97	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.32Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.173 , 0.213 0.183 , 0.227	Depositor DCC
R_{free} test set	3430 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12206	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.71% 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, ZN, DMS, FO2, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/2848	0.69	0/3867
1	B	0.53	0/2887	0.67	0/3928
1	C	0.52	0/2838	0.68	0/3862
1	D	0.51	0/2843	0.66	0/3870
All	All	0.53	0/11416	0.67	0/15527

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	2762	0	2589	10	0
1	B	2801	0	2585	14	0
1	C	2753	0	2542	14	0
1	D	2757	0	2538	7	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	0	0	1	0
3	C	23	0	0	0	0
3	D	23	0	0	0	0
4	A	12	0	16	4	0
4	B	6	0	8	4	0
4	C	6	0	8	3	0
4	D	6	0	8	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	318	0	0	2	0
7	B	261	0	0	0	0
7	C	231	0	0	2	0
7	D	183	0	0	3	0
All	All	12206	0	10306	44	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 (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:TRP:HE1	4:B:404:GOL:H31	1.07	1.09
1:A:126:THR:HB	4:A:404:GOL:H2	1.46	0.98
1:B:181:TRP:HE1	4:B:404:GOL:C3	1.79	0.95
1:B:181:TRP:NE1	4:B:404:GOL:H31	1.89	0.86
1:B:9:ASN:HB2	1:B:15:MET:HE1	1.68	0.75
1:C:153:LEU:HD11	1:C:197:ILE:HG21	1.74	0.68
1:A:76[B]:THR:HA	4:A:404:GOL:H31	1.78	0.65
1:A:76[A]:THR:HA	4:A:404:GOL:H31	1.79	0.65
1:C:126:THR:HB	4:C:404:GOL:H32	1.80	0.64
1:D:153:LEU:HD11	1:D:197:ILE:HG21	1.79	0.64
1:D:11:SER:HB2	7:D:636:HOH:O	2.01	0.60
1:B:153:LEU:HD11	1:B:197:ILE:HG21	1.91	0.53
1:B:124:ASN:HB3	4:B:404:GOL:H12	1.91	0.53
1:A:158:ASP:OD1	4:A:405:GOL:H31	2.08	0.53
1:C:333[B]:LYS:HD2	7:C:650:HOH:O	2.10	0.51
1:A:82:PHE:HB2	1:A:244[A]:LEU:HB2	1.91	0.51
1:D:150:ILE:HG22	1:D:174:PRO:HB3	1.93	0.50
1:B:150:ILE:HG22	1:B:174:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ALA:HB1	1:B:239:ARG:HG3	1.94	0.49
1:A:153:LEU:HD11	1:A:197:ILE:HG21	1.94	0.49
1:B:82:PHE:HB2	1:B:244:LEU:HB2	1.94	0.48
1:C:126:THR:CB	4:C:404:GOL:H32	2.43	0.48
1:A:236:ALA:HB1	1:A:239:ARG:HG3	1.96	0.47
1:C:236:ALA:HB1	1:C:239:ARG:HG3	1.96	0.47
1:D:167:THR:HB	7:D:596:HOH:O	2.15	0.47
1:D:236:ALA:HB1	1:D:239:ARG:HG3	1.98	0.46
1:B:81:LEU:HD13	1:B:249:MET:HG3	1.97	0.46
1:C:55:PRO:HG3	1:C:199:TYR:CE2	2.51	0.45
1:D:111:TYR:CD1	1:D:117:LEU:HD13	2.52	0.45
1:B:144:HIS:HB3	1:C:333[B]:LYS:HB3	1.99	0.44
1:A:63:ASP:CG	1:A:98:ARG:HH12	2.20	0.44
1:C:150:ILE:HG22	1:C:174:PRO:HB3	1.99	0.44
1:A:43:GLY:HA3	7:A:501:HOH:O	2.18	0.44
1:C:210:SER:HB2	7:C:540:HOH:O	2.18	0.43
1:C:56:ARG:HD2	1:C:140:LEU:O	2.19	0.43
1:B:144:HIS:HB3	1:C:333[A]:LYS:HB3	2.00	0.43
1:C:82:PHE:HB2	1:C:244:LEU:HB2	1.99	0.43
1:D:259:LYS:HB2	7:D:576:HOH:O	2.18	0.43
1:A:144:HIS:HD2	7:A:757:HOH:O	2.01	0.42
3:B:403:FO2:C9	3:B:403:FO2:N2	2.83	0.42
1:C:8:LEU:HA	1:C:8:LEU:HD22	1.89	0.42
1:B:169:GLU:HA	1:B:173:THR:OG1	2.21	0.41
1:B:125:LEU:HD12	1:B:244:LEU:HD13	2.02	0.40
1:C:126:THR:HB	4:C:404:GOL:H11	2.03	0.40

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	338/360 (94%)	331 (98%)	7 (2%)	0	100	100
1	B	349/360 (97%)	344 (99%)	5 (1%)	0	100	100
1	C	344/360 (96%)	336 (98%)	8 (2%)	0	100	100
1	D	343/360 (95%)	336 (98%)	7 (2%)	0	100	100
All	All	1374/1440 (95%)	1347 (98%)	27 (2%)	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	277/316 (88%)	268 (97%)	9 (3%)	39	53
1	B	278/316 (88%)	269 (97%)	9 (3%)	39	53
1	C	268/316 (85%)	260 (97%)	8 (3%)	41	56
1	D	275/316 (87%)	266 (97%)	9 (3%)	38	52
All	All	1098/1264 (87%)	1063 (97%)	35 (3%)	40	53

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	65	LEU
1	A	74	LEU
1	A	76[A]	THR
1	A	76[B]	THR
1	A	112	SER
1	A	132	TYR
1	A	182	LYS
1	A	249	MET
1	B	13	ARG
1	B	63	ASP
1	B	74	LEU
1	B	81	LEU

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Mol	Chain	Res	Type
1	B	132	TYR
1	B	161	GLU
1	B	175	TYR
1	B	182	LYS
1	B	184	SER
1	C	8	LEU
1	C	63	ASP
1	C	74	LEU
1	C	132	TYR
1	C	175	TYR
1	C	182	LYS
1	C	184	SER
1	C	251	LYS
1	D	11	SER
1	D	74	LEU
1	D	113	GLU
1	D	132	TYR
1	D	159	LEU
1	D	163	GLU
1	D	167	THR
1	D	175	TYR
1	D	182	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	144	HIS
1	B	128	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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	GOL	D	404	-	5,5,5	0.16	0	5,5,5	0.26	0
3	FO2	B	403	2	24,26,26	1.04	1 (4%)	27,37,37	1.83	7 (25%)
4	GOL	B	404	-	5,5,5	0.31	0	5,5,5	0.40	0
4	GOL	A	404	-	5,5,5	0.24	0	5,5,5	0.59	0
5	DMS	A	406	-	3,3,3	0.28	0	3,3,3	0.15	0
4	GOL	A	405	-	5,5,5	0.49	0	5,5,5	0.98	1 (20%)
3	FO2	D	403	2	24,26,26	0.93	1 (4%)	27,37,37	1.90	7 (25%)
5	DMS	B	405	-	3,3,3	0.27	0	3,3,3	0.57	0
3	FO2	A	403	2	24,26,26	1.05	1 (4%)	27,37,37	1.86	8 (29%)
3	FO2	C	403	2	24,26,26	0.90	1 (4%)	27,37,37	1.90	7 (25%)
4	GOL	C	404	-	5,5,5	0.14	0	5,5,5	0.54	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	GOL	D	404	-	-	0/4/4/4	-
3	FO2	B	403	2	-	0/0/18/18	0/4/4/4
4	GOL	B	404	-	-	4/4/4/4	-
4	GOL	A	404	-	-	4/4/4/4	-
4	GOL	A	405	-	-	2/4/4/4	-
3	FO2	D	403	2	-	0/0/18/18	0/4/4/4
3	FO2	A	403	2	-	0/0/18/18	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FO2	C	403	2	-	0/0/18/18	0/4/4/4
4	GOL	C	404	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	FO2	C2-N	4.05	1.34	1.31
3	A	403	FO2	C2-N	3.81	1.34	1.31
3	D	403	FO2	C2-N	3.36	1.33	1.31
3	C	403	FO2	C2-N	2.76	1.33	1.31

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	FO2	C2-C3-C4	-5.37	114.44	119.59
3	C	403	FO2	C2-C3-C4	-4.96	114.83	119.59
3	B	403	FO2	C2-C3-C4	-4.62	115.16	119.59
3	D	403	FO2	C2-C3-C4	-4.57	115.21	119.59
3	D	403	FO2	C6-N1-C5	4.34	123.16	115.88
3	D	403	FO2	C-C4-C3	4.29	121.82	118.14
3	C	403	FO2	C6-N1-C5	4.25	123.00	115.88
3	A	403	FO2	C6-N1-C5	4.25	122.99	115.88
3	B	403	FO2	C6-N1-C5	4.19	122.89	115.88
3	C	403	FO2	C-C4-C3	4.16	121.70	118.14
3	B	403	FO2	C-C4-C3	3.88	121.46	118.14
3	A	403	FO2	C-C4-C3	3.51	121.14	118.14
3	D	403	FO2	C1-C-C4	-3.31	116.92	119.77
3	C	403	FO2	C1-C-C4	-3.09	117.10	119.77
3	B	403	FO2	C1-C-C4	-2.97	117.21	119.77
3	A	403	FO2	C6-N2-C3	2.46	116.72	114.81
3	D	403	FO2	C1-N-C2	2.44	118.61	115.90
3	A	403	FO2	C5-C4-C3	-2.43	118.15	119.98
3	B	403	FO2	C5-C4-C3	-2.32	118.23	119.98
3	C	403	FO2	N2-C6-N1	-2.27	125.13	128.68
3	A	403	FO2	C3-C2-N	2.27	125.30	118.92
3	D	403	FO2	C5-C4-C3	-2.25	118.29	119.98
3	D	403	FO2	N2-C6-N1	-2.18	125.27	128.68
3	B	403	FO2	N2-C6-N1	-2.18	125.28	128.68
3	C	403	FO2	C5-C4-C3	-2.17	118.35	119.98
3	A	403	FO2	C1-C-C4	-2.16	117.90	119.77
3	A	403	FO2	N2-C6-N1	-2.16	125.30	128.68
3	C	403	FO2	C1-N-C2	2.13	118.27	115.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	GOL	C3-C2-C1	2.11	119.92	111.70
3	B	403	FO2	C6-N2-C3	2.07	116.42	114.81

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	404	GOL	O1-C1-C2-O2
4	B	404	GOL	O1-C1-C2-C3
4	A	404	GOL	O1-C1-C2-O2
4	B	404	GOL	C1-C2-C3-O3
4	A	404	GOL	O1-C1-C2-C3
4	A	404	GOL	C1-C2-C3-O3
4	A	404	GOL	O2-C2-C3-O3
4	A	405	GOL	O1-C1-C2-C3
4	A	405	GOL	C1-C2-C3-O3
4	B	404	GOL	O2-C2-C3-O3

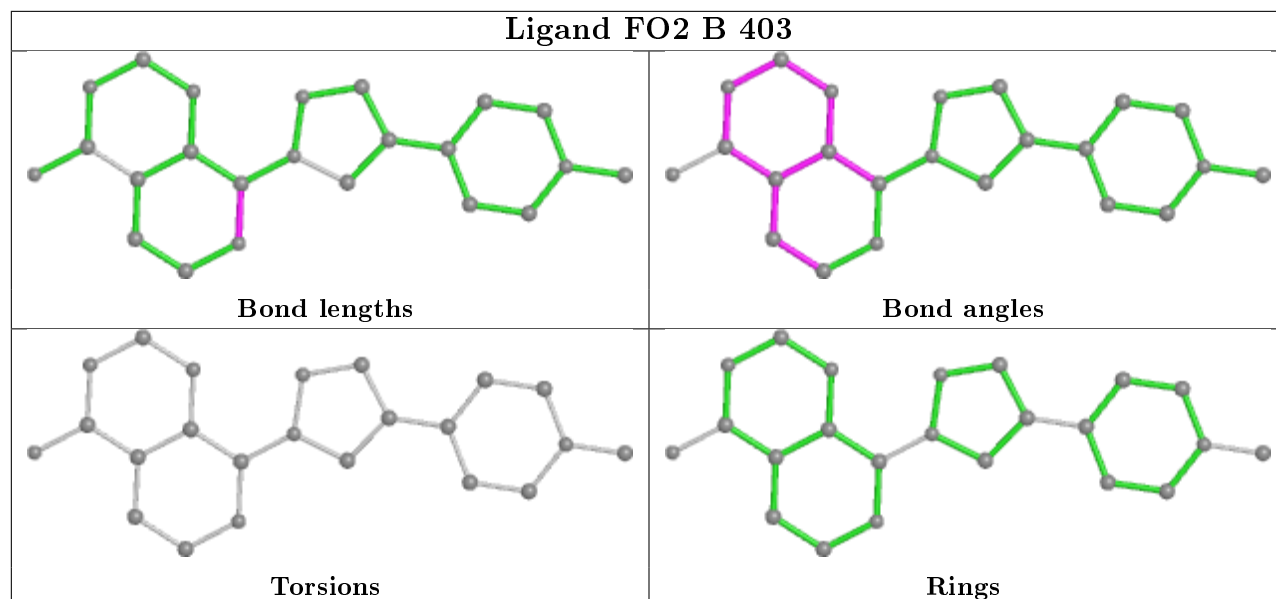
There are no ring outliers.

5 monomers are involved in 12 short contacts:

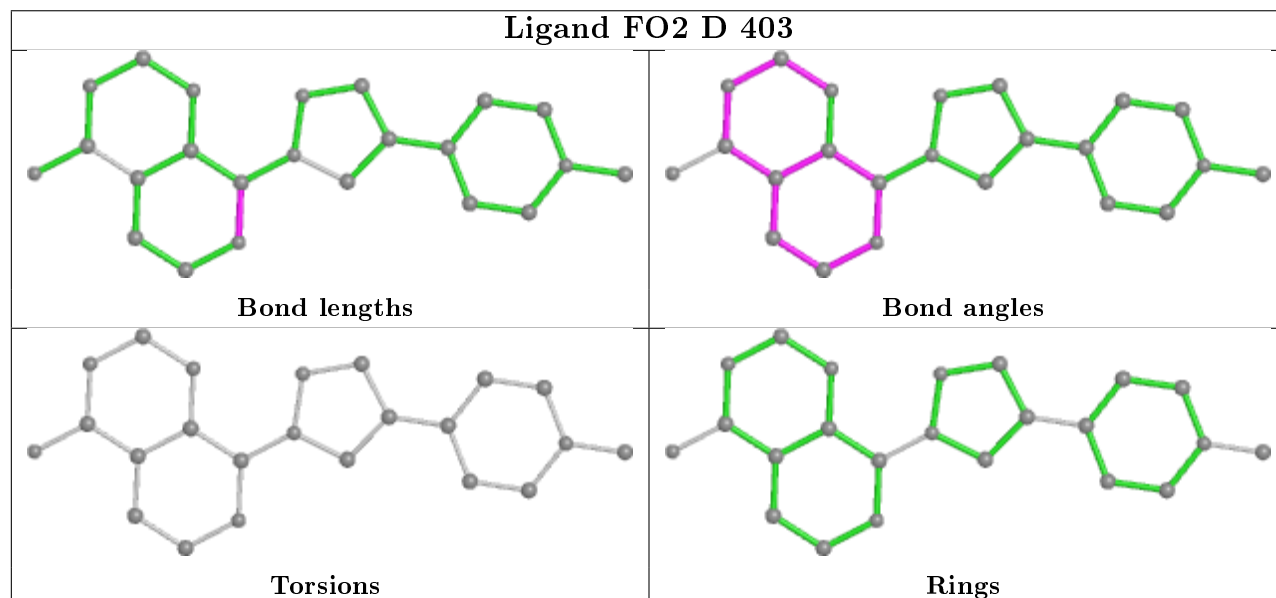
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	FO2	1	0
4	B	404	GOL	4	0
4	A	404	GOL	3	0
4	A	405	GOL	1	0
4	C	404	GOL	3	0

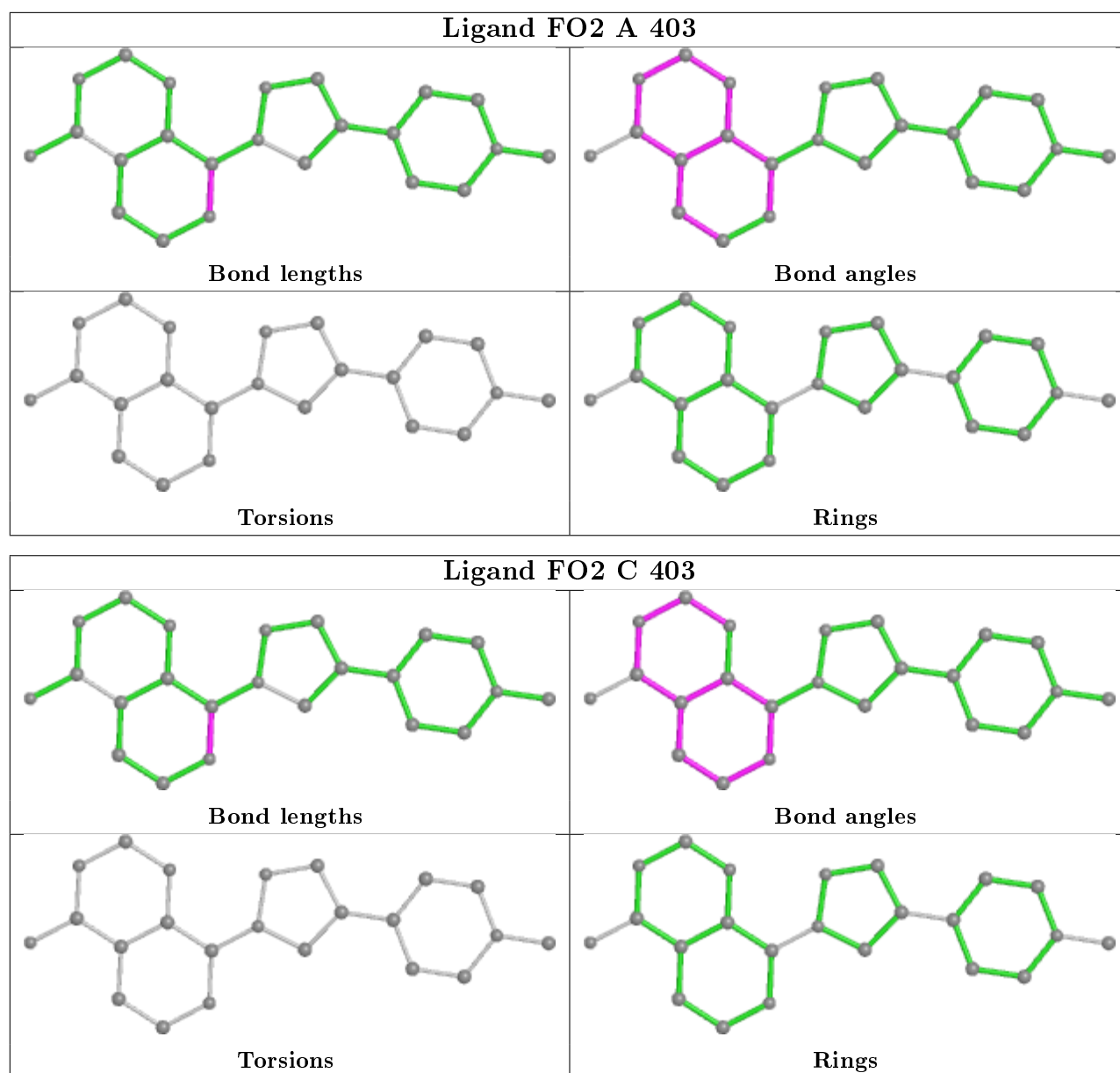
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FO2 B 403



Ligand FO2 D 403





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	338/360 (93%)	-0.09	12 (3%)	42 49	5, 20, 46, 86	0
1	B	350/360 (97%)	0.16	14 (4%)	38 45	6, 28, 65, 103	0
1	C	345/360 (95%)	0.30	26 (7%)	14 19	9, 29, 67, 84	0
1	D	344/360 (95%)	0.40	29 (8%)	11 15	11, 35, 69, 86	0
All	All	1377/1440 (95%)	0.19	81 (5%)	22 29	5, 27, 66, 103	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	334	ALA	7.4
1	B	5	SER	4.1
1	A	351	ALA	4.1
1	D	331	LEU	4.1
1	C	353	PHE	4.1
1	C	350	ALA	3.9
1	C	326	PRO	3.9
1	D	332	TRP	3.9
1	C	332	TRP	3.8
1	D	326	PRO	3.7
1	C	308	CYS	3.7
1	A	353	PHE	3.7
1	B	334	ALA	3.7
1	D	10	PRO	3.6
1	D	329	TYR	3.6
1	C	335	GLY	3.5
1	D	318	ASP	3.5
1	D	231	ALA	3.3
1	C	307	SER	3.3
1	C	8	LEU	3.3
1	C	333[A]	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	318	ASP	3.2
1	D	337	ASP	3.2
1	D	330	LYS	3.2
1	A	338	ASN	3.2
1	A	348	PRO	3.1
1	C	337	ASP	3.0
1	D	110	ARG	2.9
1	D	104	ASP	2.8
1	B	353	PHE	2.8
1	D	338	ASN	2.8
1	C	163	GLU	2.8
1	B	308	CYS	2.8
1	A	307	SER	2.7
1	B	159	LEU	2.7
1	C	330	LYS	2.7
1	A	335	GLY	2.7
1	D	335	GLY	2.7
1	C	321	VAL	2.7
1	C	227	PHE	2.7
1	A	312	MET	2.7
1	A	308	CYS	2.6
1	C	303	ALA	2.6
1	C	351	ALA	2.6
1	D	322	ARG	2.6
1	B	351	ALA	2.6
1	D	339	THR	2.6
1	C	304	VAL	2.5
1	D	350	ALA	2.4
1	C	336	LYS	2.4
1	D	316	SER	2.4
1	C	334	ALA	2.4
1	A	112	SER	2.4
1	B	304	VAL	2.4
1	B	309	ARG	2.3
1	C	324	PHE	2.3
1	C	354	LEU	2.3
1	D	107	CYS	2.3
1	D	308	CYS	2.3
1	A	352	GLU	2.3
1	B	350	ALA	2.3
1	D	303	ALA	2.3
1	B	324	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	312	MET	2.2
1	D	325	GLN	2.2
1	A	334	ALA	2.2
1	D	348	PRO	2.2
1	B	3	SER	2.1
1	D	321	VAL	2.1
1	D	60	ASP	2.1
1	C	327	GLU	2.1
1	C	339	THR	2.1
1	C	340	VAL	2.1
1	C	348	PRO	2.1
1	A	8	LEU	2.0
1	B	313	VAL	2.0
1	D	353	PHE	2.0
1	D	65	LEU	2.0
1	B	112	SER	2.0
1	B	60	ASP	2.0
1	D	333	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
4	GOL	B	404	6/6	0.77	0.29	15,21,21,22	6
6	CL	C	405	1/1	0.83	0.17	78,78,78,78	0
4	GOL	A	405	6/6	0.84	0.30	8,15,16,19	6
5	DMS	B	405	4/4	0.85	0.26	38,40,42,43	4
6	CL	D	405	1/1	0.86	0.11	57,57,57,57	0

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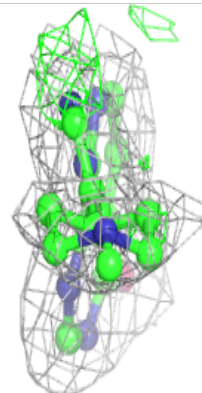
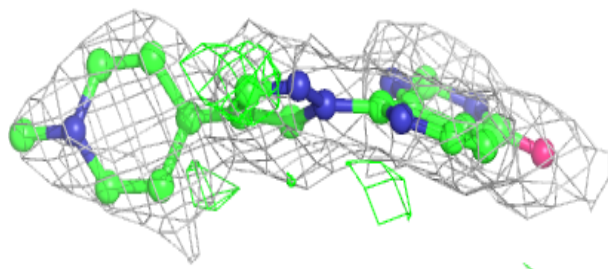
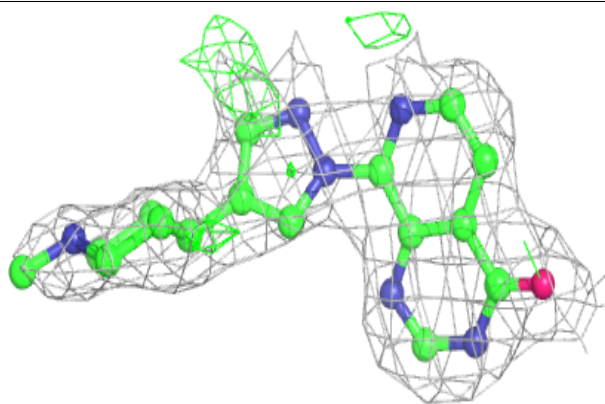
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	A	406	4/4	0.87	0.28	72,72,73,73	4
4	GOL	C	404	6/6	0.90	0.30	3,10,13,15	6
2	ZN	C	402	1/1	0.94	0.07	41,41,41,41	1
4	GOL	D	404	6/6	0.94	0.19	4,12,14,14	6
3	FO2	C	403	23/23	0.95	0.17	6,14,34,34	23
3	FO2	A	403	23/23	0.96	0.17	3,9,29,30	23
4	GOL	A	404	6/6	0.96	0.20	3,4,6,6	6
3	FO2	B	403	23/23	0.97	0.14	5,15,33,34	23
3	FO2	D	403	23/23	0.97	0.14	13,17,24,24	23
2	ZN	B	402	1/1	0.97	0.07	23,23,23,23	1
2	ZN	C	401	1/1	0.99	0.10	24,24,24,24	0
2	ZN	B	401	1/1	0.99	0.10	20,20,20,20	0
2	ZN	D	402	1/1	0.99	0.13	34,34,34,34	1
2	ZN	A	402	1/1	0.99	0.07	16,16,16,16	1
2	ZN	D	401	1/1	0.99	0.09	22,22,22,22	0
2	ZN	A	401	1/1	1.00	0.08	17,17,17,17	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.

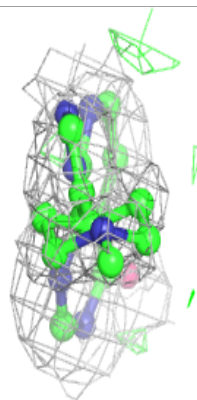
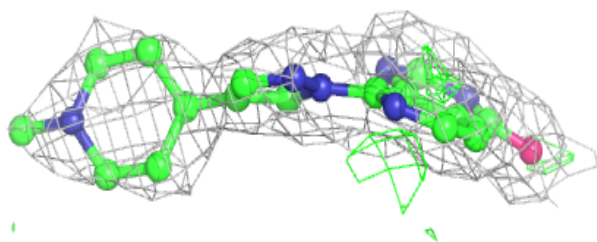
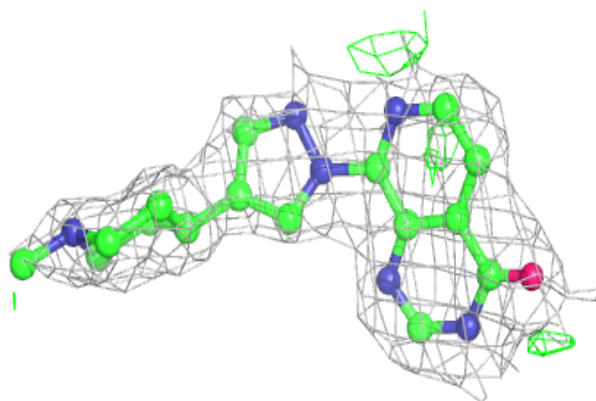
Electron density around FO2 C 403:

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

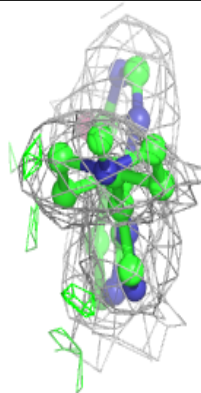
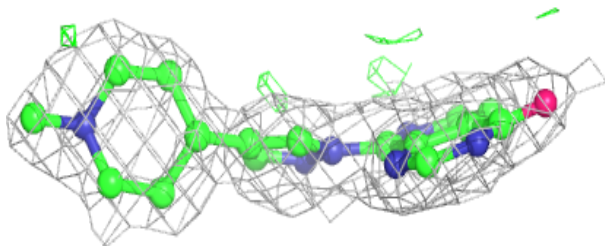
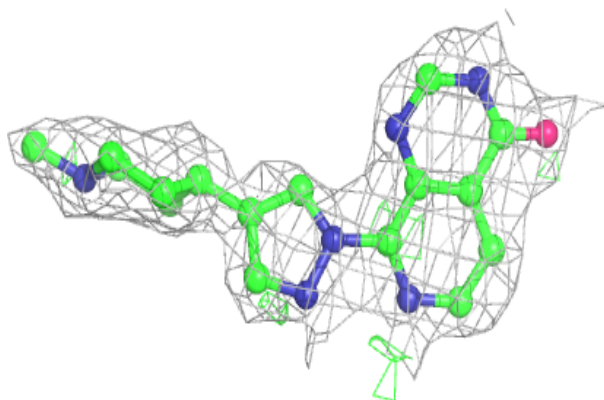


Electron density around FO2 A 403:

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

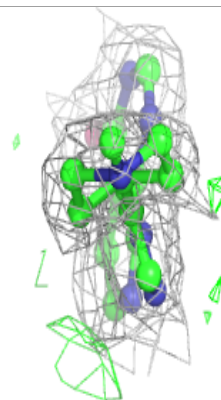
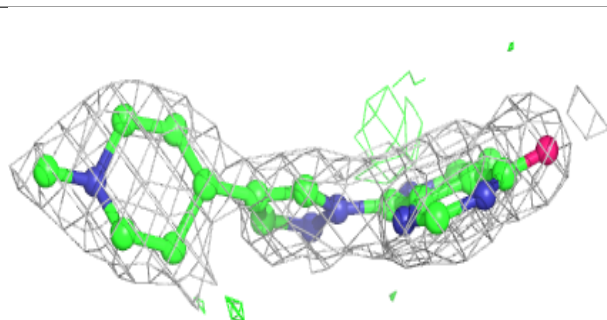
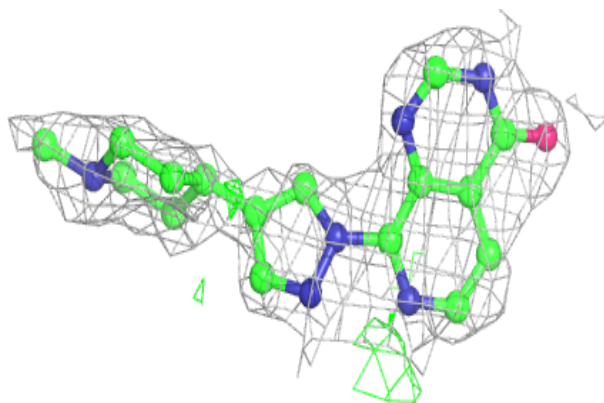
**Electron density around FO2 B 403:**

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



Electron density around FO2 D 403:

$2mF_o - DF_c$ (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.