



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:13 AM UTC

PDB ID : 6H4Q / pdb_00006h4q
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 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

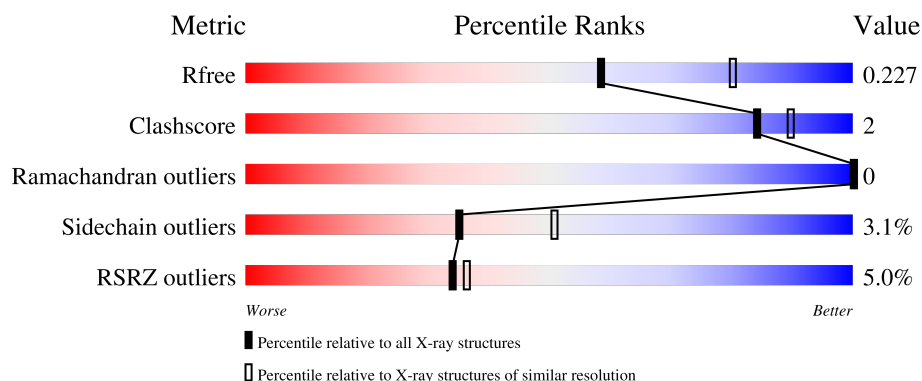
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (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 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	360	2% 88% 6% • 6%
1	B	360	4% 89% 7% • •
1	C	360	6% 89% 6% •
1	D	360	6% 90% 5% • •

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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			

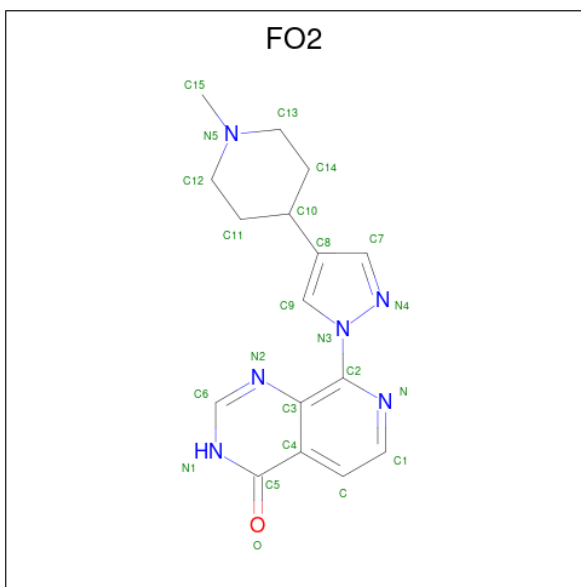
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	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 (CCD ID: FO2) (formula: C₁₆H₁₈N₆O) (labeled as "Ligand of Interest" by depositor).



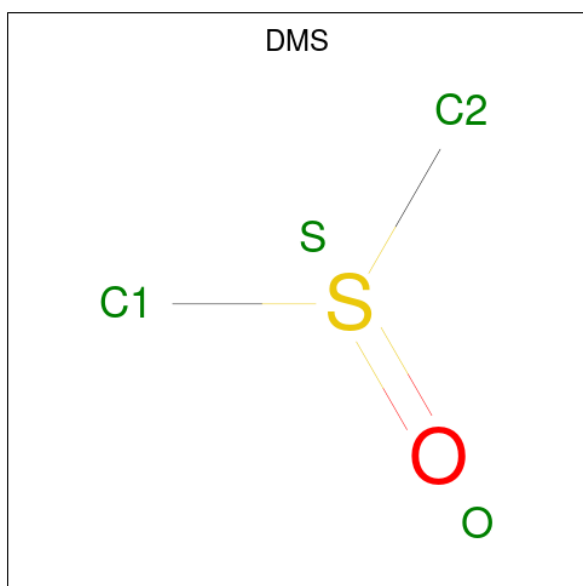
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	16	6	1		
3	B	1	Total	C	N	O	0	0
			23	16	6	1		
3	C	1	Total	C	N	O	0	0
			23	16	6	1		
3	D	1	Total	C	N	O	0	0
			23	16	6	1		

- Molecule 4 is GLYCEROL (CCD ID: 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 (CCD ID: DMS) (formula: C₂H₆OS).



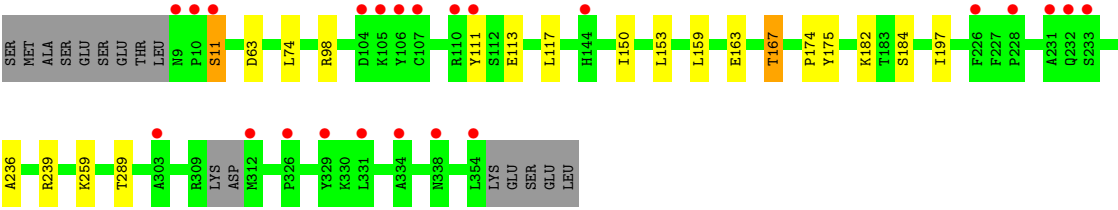
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Cl	0	0
			1	1		
6	D	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 46.20 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.20-2.31) 100.0 (46.20-2.31)	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)	0.36 , 67.9	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	0.93	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, DMS, FO2, ZN, 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	0.90	0/2848	1.25	3/3867 (0.1%)
1	B	0.88	0/2887	1.22	1/3928 (0.0%)
1	C	0.85	0/2838	1.23	6/3862 (0.2%)
1	D	0.87	0/2843	1.23	1/3870 (0.0%)
All	All	0.88	0/11416	1.23	11/15527 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	SER	N-CA-C	6.95	120.30	109.52
1	A	184	SER	N-CA-C	6.74	119.97	109.52
1	C	184	SER	N-CA-C	6.25	119.20	109.52
1	B	184	SER	N-CA-C	5.61	118.22	109.52
1	C	23	GLU	CA-C-N	5.36	128.00	120.28
1	C	23	GLU	C-N-CA	5.36	128.00	120.28
1	A	8	LEU	CA-C-N	5.32	128.57	122.83
1	A	8	LEU	C-N-CA	5.32	128.57	122.83
1	C	8	LEU	CA-C-N	5.20	128.44	122.83
1	C	8	LEU	C-N-CA	5.20	128.44	122.83
1	C	189	THR	N-CA-C	-5.10	102.64	110.14

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	13	0
1	B	2801	0	2585	15	0
1	C	2753	0	2542	14	0
1	D	2757	0	2538	8	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
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	1	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	49	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 (49) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:ASN:CG	1:B:15:MET:HE3	2.29	0.57
1:A:100:ILE:HG22	1:A:180:MET:HE1	1.88	0.54
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
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:A:63:ASP:CG	1:A:98:ARG:HH12	2.20	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:A:258:ASP:HA	5:A:406:DMS:H23	1.97	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:A:249:MET:HA	1:A:249:MET:HE2	1.97	0.45
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:C:150:ILE:HG22	1:C:174:PRO:HB3	1.99	0.44
1:D:63:ASP:CG	1:D:98:ARG:HH12	2.26	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:B:63:ASP:CG	1:B:98[A]:ARG:HH12	2.27	0.42
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:HD22	1:C:8:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:THR:HB	4:C:404:GOL:H11	2.03	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	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 [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	277/316 (88%)	269 (97%)	8 (3%)	37	53
1	B	278/316 (88%)	268 (96%)	10 (4%)	31	45
1	C	268/316 (85%)	260 (97%)	8 (3%)	36	52
1	D	275/316 (87%)	266 (97%)	9 (3%)	33	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1098/1264 (87%)	1063 (97%)	35 (3%)	35 50

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	182	LYS
1	A	249	MET
1	B	13	ARG
1	B	63	ASP
1	B	74	LEU
1	B	81	LEU
1	B	161	GLU
1	B	175	TYR
1	B	182	LYS
1	B	184	SER
1	B	289	THR
1	B	309	ARG
1	C	8	LEU
1	C	63	ASP
1	C	74	LEU
1	C	175	TYR
1	C	182	LYS
1	C	184	SER
1	C	251	LYS
1	C	309	ARG
1	D	11	SER
1	D	74	LEU
1	D	113	GLU
1	D	159	LEU
1	D	163	GLU
1	D	167	THR
1	D	175	TYR
1	D	182	LYS
1	D	289	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	137	ASN
1	A	144	HIS
1	A	215	HIS
1	B	78	GLN
1	B	84	GLN
1	B	102	ASN
1	C	26	ASN
1	C	84	GLN
1	C	128	ASN
1	C	215	HIS
1	D	26	ASN
1	D	144	HIS
1	D	215	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
3	FO2	A	403	2	25,26,26	0.65	1 (4%)	30,37,37	0.85	1 (3%)
5	DMS	B	405	-	3,3,3	0.26	0	3,3,3	0.58	0
4	GOL	C	404	-	5,5,5	0.14	0	5,5,5	0.55	0
3	FO2	C	403	2	25,26,26	0.63	0	30,37,37	0.79	1 (3%)
3	FO2	B	403	2	25,26,26	0.71	1 (4%)	30,37,37	0.86	1 (3%)
4	GOL	A	405	-	5,5,5	0.50	0	5,5,5	1.03	1 (20%)
4	GOL	D	404	-	5,5,5	0.16	0	5,5,5	0.25	0
5	DMS	A	406	-	3,3,3	0.28	0	3,3,3	0.15	0
3	FO2	D	403	2	25,26,26	0.73	1 (4%)	30,37,37	0.87	2 (6%)
4	GOL	B	404	-	5,5,5	0.32	0	5,5,5	0.42	0
4	GOL	A	404	-	5,5,5	0.24	0	5,5,5	0.60	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
3	FO2	A	403	2	-	4/8/18/18	0/4/4/4
4	GOL	C	404	-	-	0/4/4/4	-
3	FO2	C	403	2	-	5/8/18/18	0/4/4/4
3	FO2	B	403	2	-	4/8/18/18	0/4/4/4
4	GOL	A	405	-	-	2/4/4/4	-
4	GOL	D	404	-	-	0/4/4/4	-
3	FO2	D	403	2	-	4/8/18/18	0/4/4/4
4	GOL	B	404	-	-	4/4/4/4	-
4	GOL	A	404	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	FO2	C5-N1	-2.71	1.33	1.38
3	B	403	FO2	C5-N1	-2.42	1.33	1.38
3	A	403	FO2	C5-N1	-2.39	1.33	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	FO2	C3-C2-N	3.25	125.30	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	FO2	C3-C2-N	2.81	124.39	118.55
3	C	403	FO2	C3-C2-N	2.49	123.71	118.55
3	D	403	FO2	C3-C2-N	2.24	123.19	118.55
4	A	405	GOL	C3-C2-C1	2.22	119.92	111.80
3	D	403	FO2	C10-C8-C9	2.20	131.67	127.47

There are no chirality outliers.

All (27) torsion outliers are listed below:

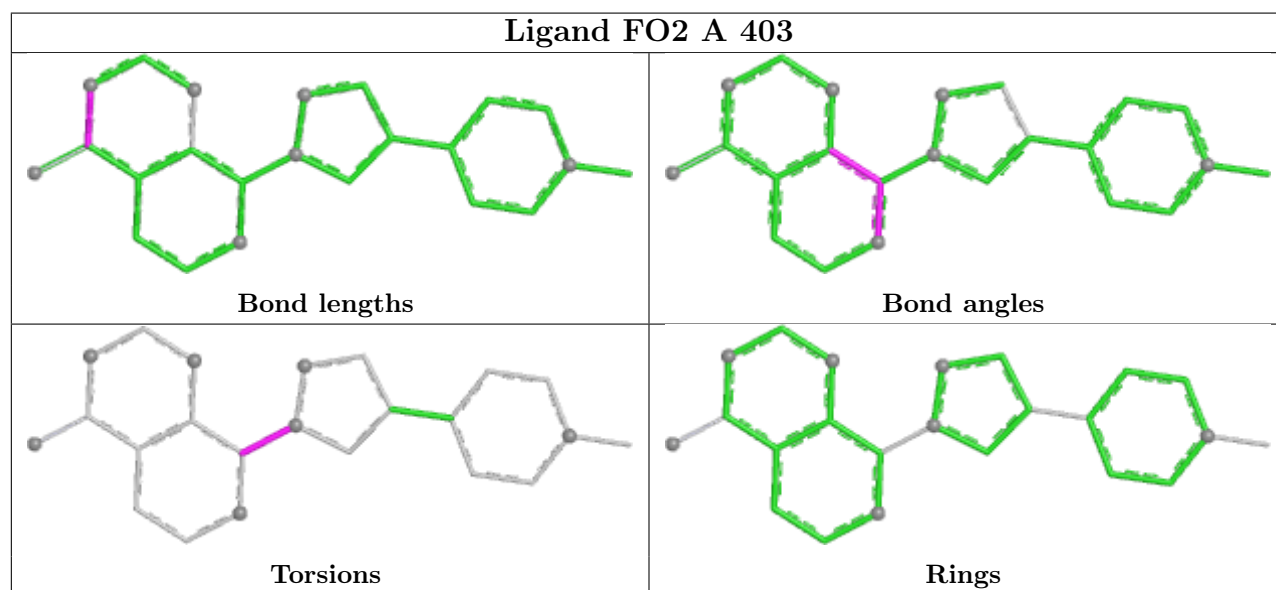
Mol	Chain	Res	Type	Atoms
3	A	403	FO2	C3-C2-N3-N4
3	A	403	FO2	C3-C2-N3-C9
3	A	403	FO2	N-C2-N3-N4
3	A	403	FO2	N-C2-N3-C9
3	B	403	FO2	C3-C2-N3-N4
3	B	403	FO2	C3-C2-N3-C9
3	B	403	FO2	N-C2-N3-N4
3	B	403	FO2	N-C2-N3-C9
3	C	403	FO2	C3-C2-N3-N4
3	C	403	FO2	C3-C2-N3-C9
3	D	403	FO2	C3-C2-N3-N4
3	D	403	FO2	C3-C2-N3-C9
3	D	403	FO2	N-C2-N3-N4
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	A	404	GOL	O1-C1-C2-C3
4	A	404	GOL	C1-C2-C3-O3
4	B	404	GOL	C1-C2-C3-O3
4	A	404	GOL	O2-C2-C3-O3
3	C	403	FO2	N-C2-N3-C9
3	D	403	FO2	N-C2-N3-C9
3	C	403	FO2	N-C2-N3-N4
4	B	404	GOL	O2-C2-C3-O3
4	A	405	GOL	O1-C1-C2-C3
4	A	405	GOL	C1-C2-C3-O3
3	C	403	FO2	C11-C10-C8-C9

There are no ring outliers.

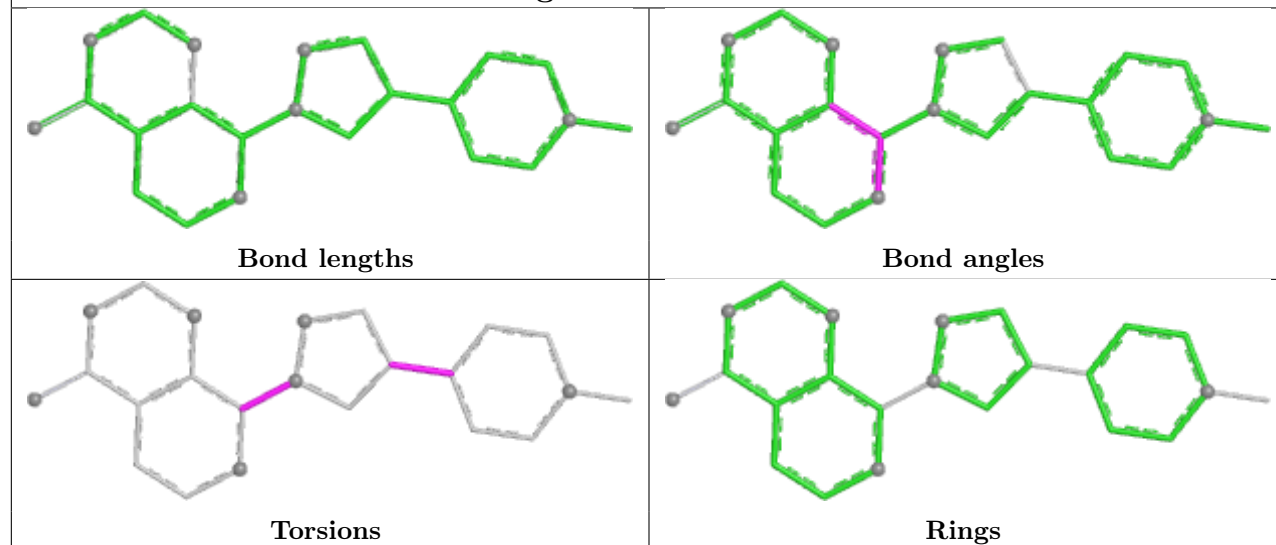
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	GOL	3	0
3	B	403	FO2	1	0
4	A	405	GOL	1	0
5	A	406	DMS	1	0
4	B	404	GOL	4	0
4	A	404	GOL	3	0

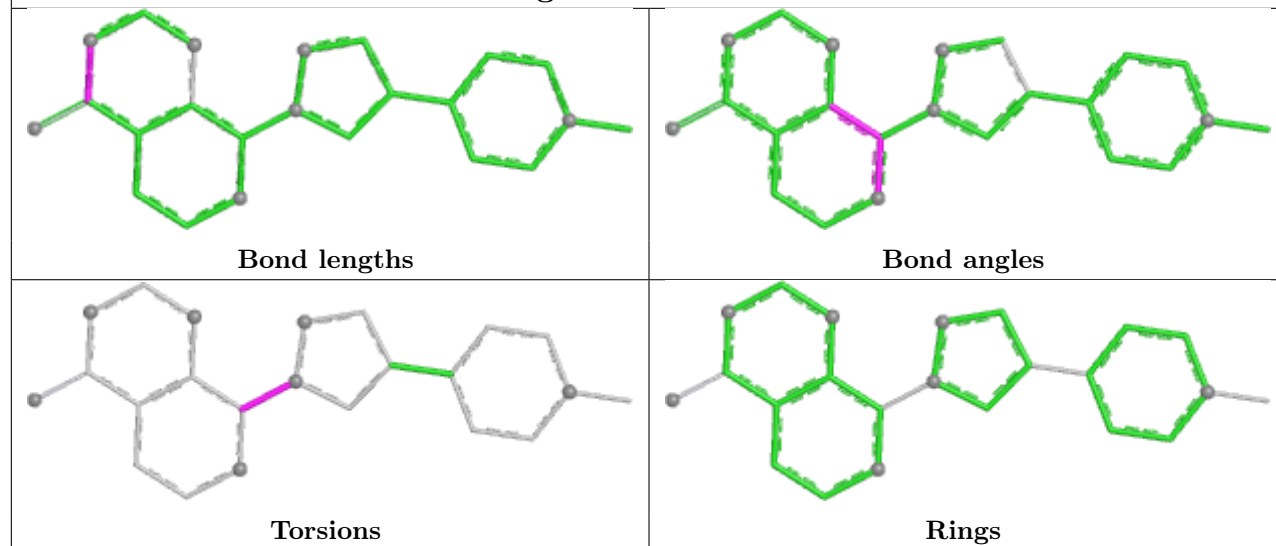
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



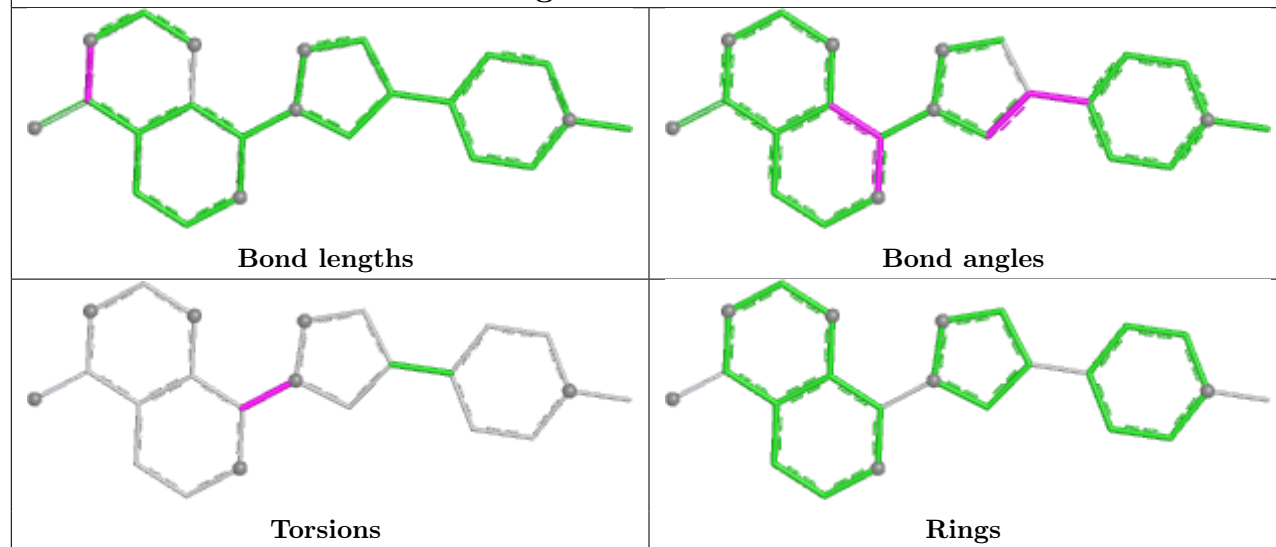
Ligand FO2 C 403



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%)	-0.32	7 (2%) 63 66	4, 20, 46, 86	6 (1%)
1	B	350/360 (97%)	0.02	16 (4%) 37 40	4, 28, 65, 103	3 (0%)
1	C	345/360 (95%)	0.11	23 (6%) 24 26	5, 29, 67, 84	3 (0%)
1	D	344/360 (95%)	0.32	23 (6%) 24 26	7, 35, 69, 86	3 (0%)
All	All	1377/1440 (95%)	0.03	69 (5%) 34 36	4, 27, 66, 103	15 (1%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	354	LEU	5.1
1	C	333[A]	LYS	4.6
1	A	309	ARG	4.2
1	B	309	ARG	4.2
1	C	354	LEU	4.0
1	D	10	PRO	3.6
1	C	338	ASN	3.5
1	B	112	SER	3.3
1	B	5	SER	3.1
1	B	304	VAL	3.1
1	A	312	MET	3.1
1	B	333	LYS	3.1
1	D	11	SER	3.0
1	D	9	ASN	3.0
1	D	231	ALA	2.9
1	D	111	TYR	2.9
1	D	105	LYS	2.9
1	A	308	CYS	2.8
1	B	329	TYR	2.8
1	C	235	GLU	2.8
1	C	231	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	112	SER	2.7
1	D	226	PHE	2.7
1	A	170	GLY	2.7
1	D	312	MET	2.7
1	B	354	LEU	2.6
1	D	110	ARG	2.6
1	B	331	LEU	2.6
1	D	232	GLN	2.6
1	B	226	PHE	2.6
1	C	309	ARG	2.5
1	D	334	ALA	2.5
1	C	304	VAL	2.5
1	D	338	ASN	2.5
1	D	303	ALA	2.5
1	B	230	SER	2.4
1	B	312	MET	2.4
1	B	313	VAL	2.4
1	C	312	MET	2.4
1	C	334	ALA	2.4
1	B	307	SER	2.4
1	A	307	SER	2.3
1	C	307	SER	2.3
1	D	331	LEU	2.3
1	C	351	ALA	2.3
1	C	313	VAL	2.3
1	D	326	PRO	2.3
1	C	229	GLY	2.2
1	D	107	CYS	2.2
1	C	163	GLU	2.2
1	C	335	GLY	2.2
1	C	228	PRO	2.2
1	C	232	GLN	2.2
1	D	233	SER	2.2
1	B	63	ASP	2.1
1	D	104	ASP	2.1
1	A	313	VAL	2.1
1	D	144	HIS	2.1
1	C	303	ALA	2.1
1	D	106	TYR	2.1
1	D	329	TYR	2.1
1	C	225	GLY	2.1
1	C	332	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	62	ILE	2.0
1	C	168	ILE	2.0
1	D	228	PRO	2.0
1	C	111	TYR	2.0
1	C	336	LYS	2.0
1	B	334	ALA	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 oligosaccharides 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
5	DMS	B	405	4/4	0.75	0.25	38,40,42,43	4
6	CL	C	405	1/1	0.81	0.22	78,78,78,78	0
4	GOL	B	404	6/6	0.84	0.15	15,21,21,22	6
4	GOL	A	405	6/6	0.87	0.16	8,15,16,19	6
5	DMS	A	406	4/4	0.88	0.21	72,72,73,73	4
6	CL	D	405	1/1	0.89	0.14	57,57,57,57	0
4	GOL	C	404	6/6	0.90	0.13	3,10,13,15	6
4	GOL	D	404	6/6	0.92	0.10	4,12,14,14	6
3	FO2	C	403	23/23	0.95	0.09	6,14,34,34	23
3	FO2	D	403	23/23	0.95	0.09	13,17,24,24	23
3	FO2	A	403	23/23	0.96	0.09	3,9,29,30	23
3	FO2	B	403	23/23	0.96	0.08	5,15,33,34	23
4	GOL	A	404	6/6	0.97	0.09	3,4,6,6	6
2	ZN	D	401	1/1	0.99	0.02	22,22,22,22	0
2	ZN	D	402	1/1	0.99	0.08	34,34,34,34	1
2	ZN	A	402	1/1	0.99	0.03	16,16,16,16	1
2	ZN	B	402	1/1	0.99	0.03	23,23,23,23	1

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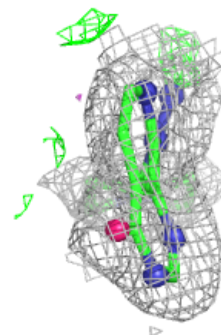
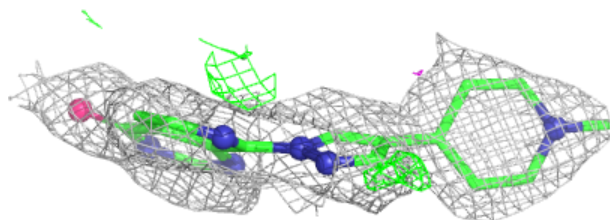
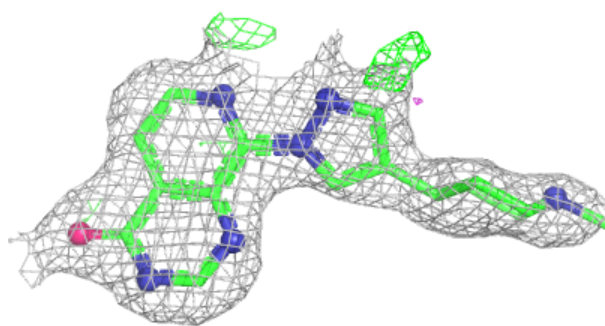
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	402	1/1	0.99	0.04	41,41,41,41	1
2	ZN	A	401	1/1	1.00	0.02	17,17,17,17	0
2	ZN	C	401	1/1	1.00	0.02	24,24,24,24	0
2	ZN	B	401	1/1	1.00	0.02	20,20,20,20	0

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.

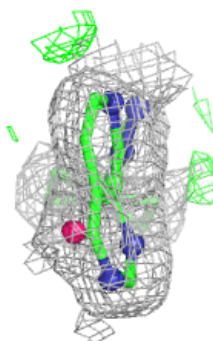
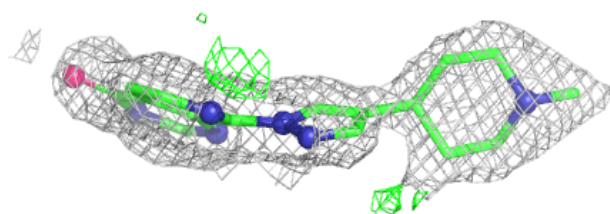
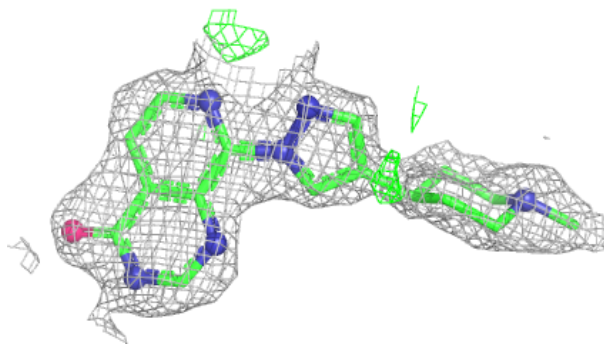
Electron density around FO2 C 403:

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

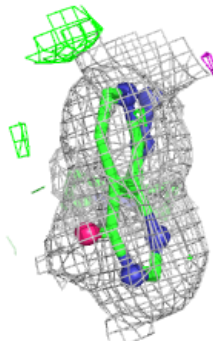
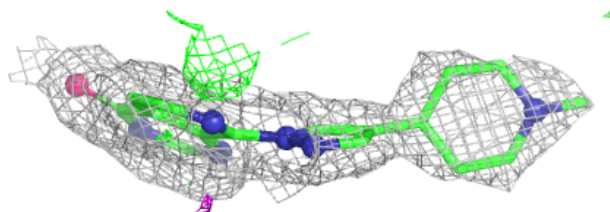
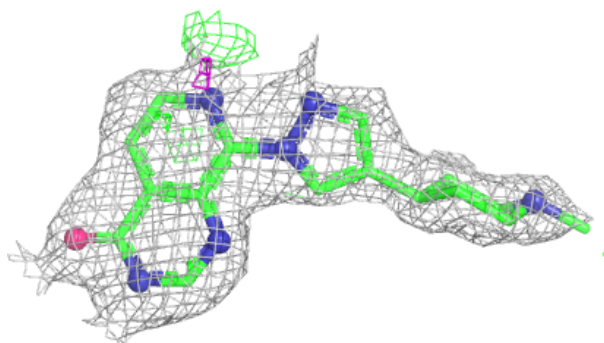


Electron density around FO2 D 403:

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

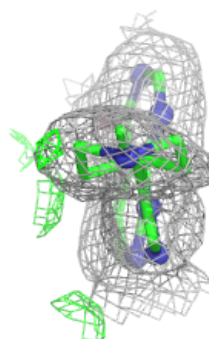
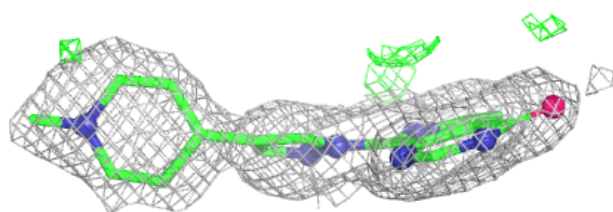
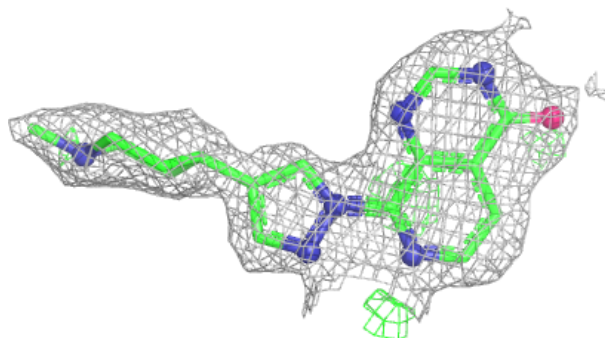
**Electron density around FO2 A 403:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.