



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 09:55 PM JST

PDB ID : 7C2V
Title : Crystal Structure of IRAK4 kinase in complex with the inhibitor CA-4948
Authors : Krishnamurthy, N.R.; Robert, B.
Deposited on : 2020-05-09
Resolution : 2.44 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

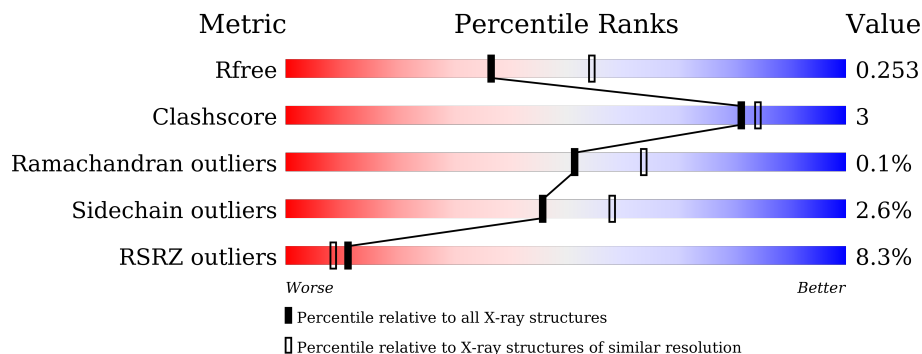
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	300	
1	B	300	
1	C	300	
1	D	300	

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
1	SEP	A	346	-	-	-	X
1	SEP	B	346	-	-	-	X
1	SEP	C	346	-	-	-	X
1	SEP	D	346	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9538 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.

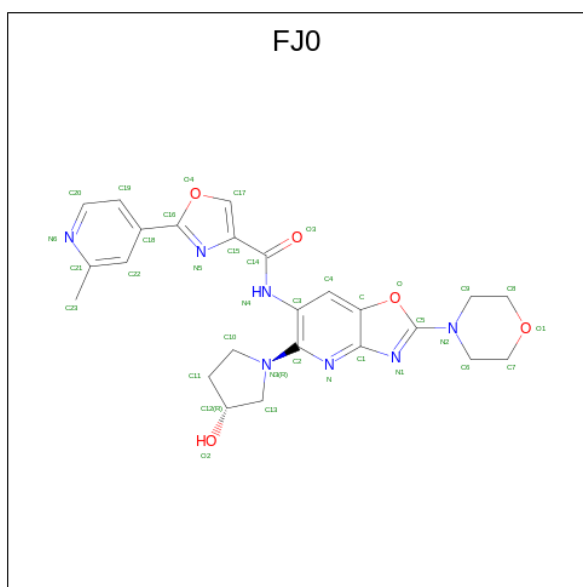
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	289	2272	1423	382	449	3	15	0	1	2
1	B	284	2235	1400	377	440	3	15	0	2	3
1	C	283	2232	1398	376	441	3	14	0	0	1
1	D	286	2253	1410	380	446	3	14	0	0	2

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	SER	-	expression tag	UNP Q9NWZ3
B	161	SER	-	expression tag	UNP Q9NWZ3
C	161	SER	-	expression tag	UNP Q9NWZ3
D	161	SER	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 2-(2-methylpyridin-4-yl)-N-[2-morpholin-4-yl-5-[(3R)-3-oxidanylpyrrolidin-1-yl]-[1,3]oxazolo[4,5-b]pyridin-6-yl]-1,3-oxazole-4-carboxamide (three-letter code: FJ0) (formula: C₂₄H₂₅N₇O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	36	24	7	5	0	0
2	B	1	36	24	7	5	0	0
2	C	1	36	24	7	5	0	0
2	D	1	36	24	7	5	0	0

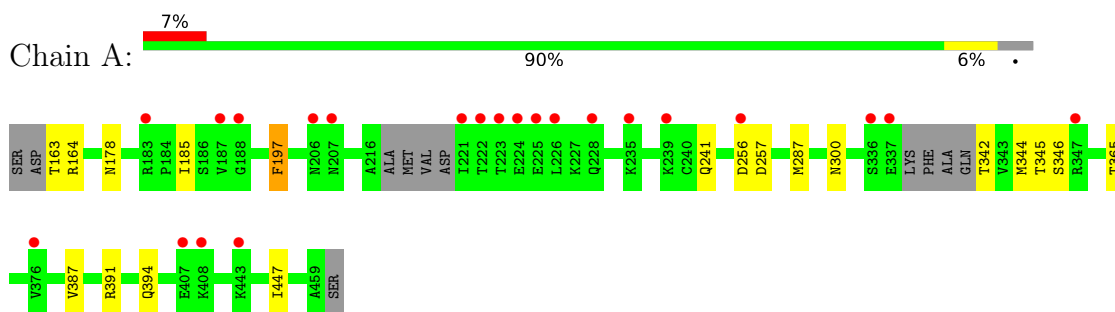
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	86	86	86	0	0
3	B	94	94	94	0	0
3	C	102	102	102	0	0
3	D	120	120	120	0	0

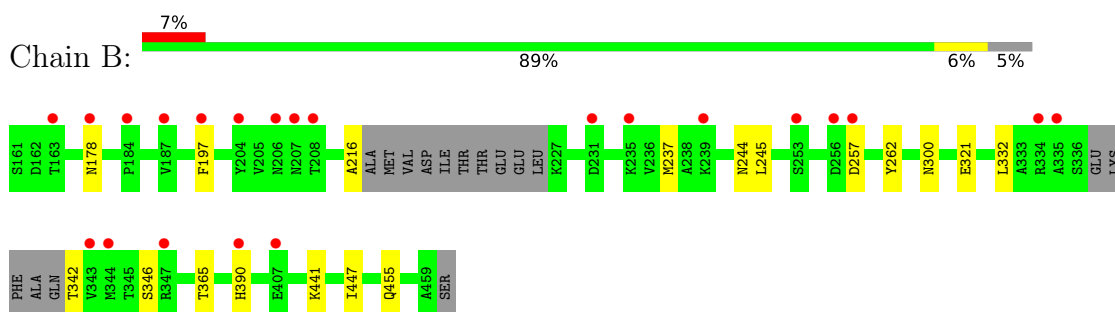
3 Residue-property plots [i](#)

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.

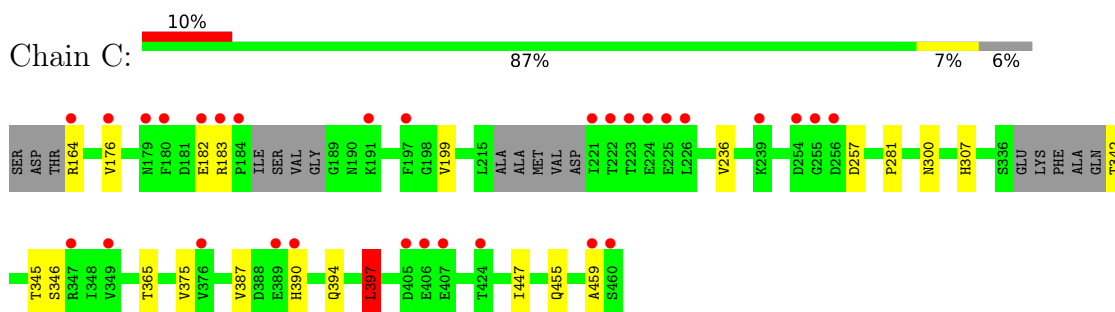
- Molecule 1: Interleukin-1 receptor-associated kinase 4



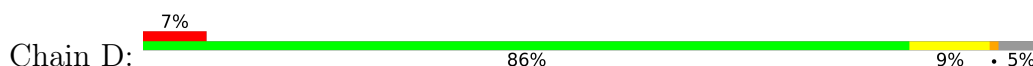
- Molecule 1: Interleukin-1 receptor-associated kinase 4

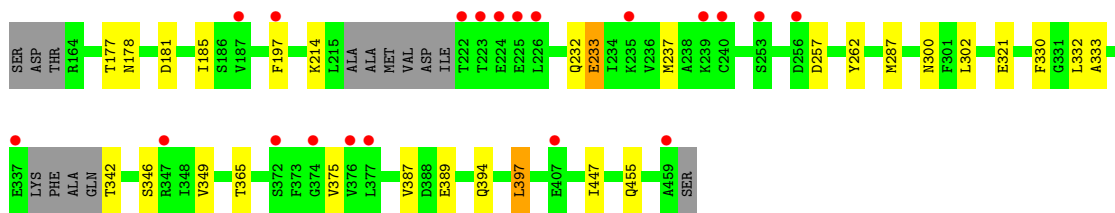


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.76Å 138.59Å 87.36Å 90.00° 124.50° 90.00°	Depositor
Resolution (Å)	30.00 – 2.44 29.90 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.44) 98.9 (29.90-2.44)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.196 , 0.253 0.203 , 0.253	Depositor DCC
R_{free} test set	2535 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	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	9538	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.93% 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: FJ0, SEP, TPO

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	0.53	0/2279	0.72	1/3070 (0.0%)
1	B	0.52	0/2242	0.70	0/3019
1	C	0.54	0/2235	0.73	3/3009 (0.1%)
1	D	0.54	0/2257	0.71	2/3040 (0.1%)
All	All	0.53	0/9013	0.72	6/12138 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	MET	CA-CB-CG	7.93	126.78	113.30
1	C	397	LEU	CA-CB-CG	6.65	130.60	115.30
1	D	233	GLU	CA-CB-CG	6.16	126.94	113.40
1	D	397	LEU	CA-CB-CG	5.77	128.57	115.30
1	C	397	LEU	CB-CA-C	-5.07	100.57	110.20
1	C	176	VAL	CB-CA-C	-5.05	101.80	111.40

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	2272	0	2234	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2235	0	2192	7	0
1	C	2232	0	2188	8	0
1	D	2253	0	2212	19	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	0	0
3	A	86	0	0	2	0
3	B	94	0	0	2	0
3	C	102	0	0	1	0
3	D	120	0	0	10	0
All	All	9538	0	8826	46	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 3.

All (46) 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:287[B]:MET:SD	3:C:2163:HOH:O	1.96	1.22
1:D:177:THR:O	3:D:2101:HOH:O	1.71	1.07
1:D:330:PHE:O	3:D:2102:HOH:O	1.99	0.81
1:D:214:LYS:NZ	3:D:2103:HOH:O	2.14	0.76
1:A:287[B]:MET:HA	1:A:287[B]:MET:HE3	1.68	0.74
1:C:375:VAL:HG22	1:C:397:LEU:CD1	2.21	0.70
1:A:287[B]:MET:HA	1:A:287[B]:MET:CE	2.32	0.60
1:C:281:PRO:HD3	1:D:321:GLU:HG3	1.86	0.57
1:D:197:PHE:HE2	1:D:332:LEU:HD21	1.70	0.57
1:D:333:ALA:N	3:D:2102:HOH:O	2.38	0.56
1:D:181:ASP:CB	3:D:2101:HOH:O	2.53	0.56
1:D:375:VAL:HG22	1:D:397:LEU:HD23	1.88	0.55
1:B:216:ALA:CA	3:B:2149:HOH:O	2.54	0.54
1:A:287[B]:MET:HE3	1:A:287[B]:MET:CA	2.35	0.54
1:A:287[B]:MET:CE	1:A:287[B]:MET:CA	2.85	0.54
1:A:197:PHE:CD1	1:A:197:PHE:N	2.76	0.54
1:B:321:GLU:HG2	3:B:2174:HOH:O	2.08	0.53
1:B:390:HIS:O	1:C:390:HIS:O	2.27	0.52
1:B:244:ASN:O	1:B:245:LEU:HD12	2.11	0.50
1:D:237:MET:HE3	1:D:262:TYR:HE2	1.79	0.48
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.96	0.48
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:HG21	1:A:241:GLN:HE22	1.80	0.47
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.96	0.47
1:D:181:ASP:HB2	3:D:2101:HOH:O	2.11	0.47
1:A:164:ARG:NH1	3:A:2109:HOH:O	2.46	0.47
1:D:197:PHE:CE2	1:D:332:LEU:HD21	2.49	0.47
1:A:197:PHE:N	1:A:197:PHE:HD1	2.14	0.46
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.97	0.46
1:A:287[B]:MET:HB3	1:A:287[B]:MET:HE2	1.73	0.44
1:D:232:GLN:HG3	3:D:2102:HOH:O	2.17	0.44
1:A:391:ARG:HD3	3:A:2140:HOH:O	2.18	0.43
1:D:232:GLN:CG	3:D:2102:HOH:O	2.67	0.43
1:B:197:PHE:HE2	1:B:332:LEU:HD21	1.85	0.42
1:A:163:THR:OG1	1:A:241:GLN:NE2	2.52	0.42
1:D:287:MET:HG3	3:D:2214:HOH:O	2.19	0.42
1:C:375:VAL:CG2	1:C:397:LEU:CD1	2.96	0.42
1:C:236:VAL:HG22	1:C:307:HIS:CE1	2.55	0.41
1:B:237:MET:HE3	1:B:262:TYR:HE1	1.85	0.41
1:D:302:LEU:HD11	1:D:330:PHE:HE1	1.85	0.41
1:C:387:VAL:HA	1:C:394:GLN:O	2.21	0.41
1:D:387:VAL:HA	1:D:394:GLN:O	2.20	0.41
1:A:387:VAL:HA	1:A:394:GLN:O	2.21	0.41
1:D:185:ILE:HG22	3:D:2185:HOH:O	2.20	0.41
1:D:332:LEU:HD22	1:D:349:VAL:HG21	2.02	0.40
1:C:375:VAL:CG2	1:C:397:LEU:HD11	2.51	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	282/300 (94%)	269 (95%)	13 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	278/300 (93%)	262 (94%)	16 (6%)	0	100	100
1	C	273/300 (91%)	259 (95%)	13 (5%)	1 (0%)	34	41
1	D	278/300 (93%)	265 (95%)	13 (5%)	0	100	100
All	All	1111/1200 (93%)	1055 (95%)	55 (5%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	459	ALA

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	248/258 (96%)	242 (98%)	6 (2%)	49	61
1	B	243/258 (94%)	238 (98%)	5 (2%)	53	66
1	C	243/258 (94%)	235 (97%)	8 (3%)	38	49
1	D	246/258 (95%)	240 (98%)	6 (2%)	49	61
All	All	980/1032 (95%)	955 (97%)	25 (3%)	46	58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	185	ILE
1	A	197	PHE
1	A	256	ASP
1	A	257	ASP
1	A	365	THR
1	B	178	ASN
1	B	257	ASP
1	B	365	THR
1	B	441	LYS

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Mol	Chain	Res	Type
1	B	455	GLN
1	C	164	ARG
1	C	182	GLU
1	C	183	ARG
1	C	199	VAL
1	C	257	ASP
1	C	365	THR
1	C	397	LEU
1	C	455	GLN
1	D	178	ASN
1	D	233	GLU
1	D	257	ASP
1	D	365	THR
1	D	389	GLU
1	D	455	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	B	207	ASN
1	B	229	GLN
1	B	452	GLN
1	C	175	ASN
1	C	207	ASN
1	C	307	HIS
1	D	229	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 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	TPO	C	345	1	8,10,11	1.11	1 (12%)	10,14,16	1.00	1 (10%)
1	TPO	B	342	1	8,10,11	0.88	0	10,14,16	1.21	1 (10%)
1	TPO	A	345	1	8,10,11	1.21	1 (12%)	10,14,16	1.25	1 (10%)
1	TPO	B	345	1	8,10,11	0.94	0	10,14,16	1.02	0
1	SEP	A	346	1	8,9,10	0.68	0	8,12,14	1.39	1 (12%)
1	TPO	A	342	1	8,10,11	1.20	1 (12%)	10,14,16	1.49	1 (10%)
1	SEP	B	346	1	8,9,10	0.60	0	8,12,14	1.52	1 (12%)
1	TPO	D	345	1	8,10,11	0.85	0	10,14,16	0.94	0
1	TPO	C	342	1	8,10,11	1.14	1 (12%)	10,14,16	1.32	1 (10%)
1	TPO	D	342	1	8,10,11	0.90	0	10,14,16	1.20	1 (10%)
1	SEP	C	346	1	8,9,10	0.64	0	8,12,14	1.69	2 (25%)
1	SEP	D	346	1	8,9,10	0.66	0	8,12,14	1.49	1 (12%)

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	TPO	C	345	1	-	3/9/11/13	-
1	TPO	B	342	1	-	0/9/11/13	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	5/9/11/13	-
1	SEP	A	346	1	-	1/5/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	1/5/8/10	-
1	TPO	D	345	1	-	4/9/11/13	-
1	TPO	C	342	1	-	0/9/11/13	-
1	TPO	D	342	1	-	1/9/11/13	-
1	SEP	C	346	1	-	1/5/8/10	-
1	SEP	D	346	1	-	1/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	P-OG1	2.93	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	TPO	P-OG1	2.87	1.64	1.59
1	C	342	TPO	P-OG1	2.72	1.64	1.59
1	C	345	TPO	P-OG1	2.27	1.63	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	TPO	P-OG1-CB	-3.37	113.04	123.21
1	A	342	TPO	P-OG1-CB	-3.28	113.31	123.21
1	A	346	SEP	OG-CB-CA	3.11	111.17	108.14
1	B	342	TPO	P-OG1-CB	-2.87	114.54	123.21
1	D	342	TPO	P-OG1-CB	-2.86	114.58	123.21
1	C	346	SEP	O3P-P-OG	-2.64	99.70	106.73
1	D	346	SEP	OG-CB-CA	2.64	110.71	108.14
1	C	346	SEP	OG-CB-CA	2.39	110.47	108.14
1	A	345	TPO	P-OG1-CB	-2.37	116.04	123.21
1	B	346	SEP	OG-CB-CA	2.27	110.36	108.14
1	C	345	TPO	P-OG1-CB	-2.20	116.57	123.21

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	346	SEP	N-CA-CB-OG
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	CB-OG1-P-O1P
1	B	346	SEP	N-CA-CB-OG
1	C	345	TPO	N-CA-CB-OG1
1	C	346	SEP	N-CA-CB-OG
1	D	345	TPO	N-CA-CB-OG1
1	D	346	SEP	N-CA-CB-OG
1	D	345	TPO	CB-OG1-P-O1P
1	D	342	TPO	C-CA-CB-CG2
1	A	345	TPO	CA-CB-OG1-P
1	B	345	TPO	CA-CB-OG1-P
1	C	345	TPO	CA-CB-OG1-P
1	D	345	TPO	CA-CB-OG1-P
1	A	342	TPO	CB-OG1-P-O2P
1	B	345	TPO	CB-OG1-P-O3P
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	C	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	FJ0	B	2001	-	32,41,41	1.31	4 (12%)	34,59,59	2.96	9 (26%)
2	FJ0	A	2001	-	32,41,41	1.39	5 (15%)	34,59,59	2.52	5 (14%)
2	FJ0	C	2001	-	32,41,41	1.53	4 (12%)	34,59,59	2.33	7 (20%)
2	FJ0	D	2001	-	32,41,41	1.59	3 (9%)	34,59,59	2.38	10 (29%)

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
2	FJ0	B	2001	-	-	4/10/37/37	0/6/6/6
2	FJ0	A	2001	-	-	4/10/37/37	0/6/6/6
2	FJ0	C	2001	-	-	4/10/37/37	0/6/6/6
2	FJ0	D	2001	-	-	2/10/37/37	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	FJ0	C2-N	6.41	1.38	1.31
2	C	2001	FJ0	C2-N	5.75	1.38	1.31
2	B	2001	FJ0	C2-N	4.66	1.36	1.31
2	A	2001	FJ0	C2-N	4.11	1.36	1.31
2	D	2001	FJ0	C2-N3	2.87	1.44	1.37
2	C	2001	FJ0	C2-N3	2.73	1.44	1.37
2	B	2001	FJ0	C2-N3	2.68	1.44	1.37
2	A	2001	FJ0	C4-C3	2.42	1.42	1.37
2	C	2001	FJ0	C21-N6	2.35	1.39	1.34
2	A	2001	FJ0	C2-N3	2.34	1.43	1.37
2	D	2001	FJ0	C21-N6	2.17	1.38	1.34
2	A	2001	FJ0	C21-N6	2.17	1.38	1.34
2	B	2001	FJ0	C20-N6	2.14	1.39	1.34
2	B	2001	FJ0	C21-N6	2.11	1.38	1.34
2	A	2001	FJ0	C15-N5	-2.06	1.31	1.37
2	C	2001	FJ0	C20-N6	2.01	1.38	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	FJ0	N-C2-N3	-12.76	108.54	117.62
2	A	2001	FJ0	N-C2-N3	-12.21	108.93	117.62
2	C	2001	FJ0	N-C2-N3	-10.79	109.94	117.62
2	D	2001	FJ0	N-C2-N3	-10.41	110.21	117.62
2	B	2001	FJ0	C13-N3-C2	-5.31	108.21	123.61
2	B	2001	FJ0	C18-C22-C21	-4.79	118.09	120.23
2	C	2001	FJ0	C11-C10-N3	-4.05	98.60	103.35
2	D	2001	FJ0	C19-C20-N6	-3.94	119.06	123.96
2	D	2001	FJ0	C13-N3-C2	-3.76	112.71	123.61
2	B	2001	FJ0	C19-C20-N6	-3.62	119.46	123.96
2	B	2001	FJ0	C10-C11-C12	-3.60	99.53	104.17
2	A	2001	FJ0	C10-N3-C2	-3.50	113.51	123.54
2	B	2001	FJ0	C11-C10-N3	-3.42	99.34	103.35
2	B	2001	FJ0	C2-N-C1	3.35	122.14	117.29
2	A	2001	FJ0	C19-C20-N6	-3.19	119.99	123.96
2	D	2001	FJ0	C3-N4-C14	3.08	135.37	126.93
2	A	2001	FJ0	C13-N3-C2	-2.94	115.07	123.61
2	C	2001	FJ0	C10-N3-C2	-2.89	115.25	123.54
2	C	2001	FJ0	C19-C20-N6	-2.89	120.37	123.96
2	B	2001	FJ0	C19-C18-C22	2.77	122.08	118.16
2	B	2001	FJ0	C3-N4-C14	2.69	134.30	126.93
2	D	2001	FJ0	C10-N3-C13	-2.62	104.78	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	FJ0	C2-N-C1	2.53	120.96	117.29
2	A	2001	FJ0	C2-N-C1	2.52	120.94	117.29
2	D	2001	FJ0	C10-C11-C12	-2.50	100.95	104.17
2	C	2001	FJ0	C10-C11-C12	-2.34	101.16	104.17
2	D	2001	FJ0	C2-N-C1	2.21	120.49	117.29
2	C	2001	FJ0	C13-N3-C2	-2.15	117.37	123.61
2	D	2001	FJ0	C22-C21-N6	-2.04	119.68	121.66
2	D	2001	FJ0	C7-C6-N2	2.03	113.77	110.02
2	D	2001	FJ0	C8-C9-N2	2.01	113.72	110.02

There are no chirality outliers.

All (14) torsion outliers are listed below:

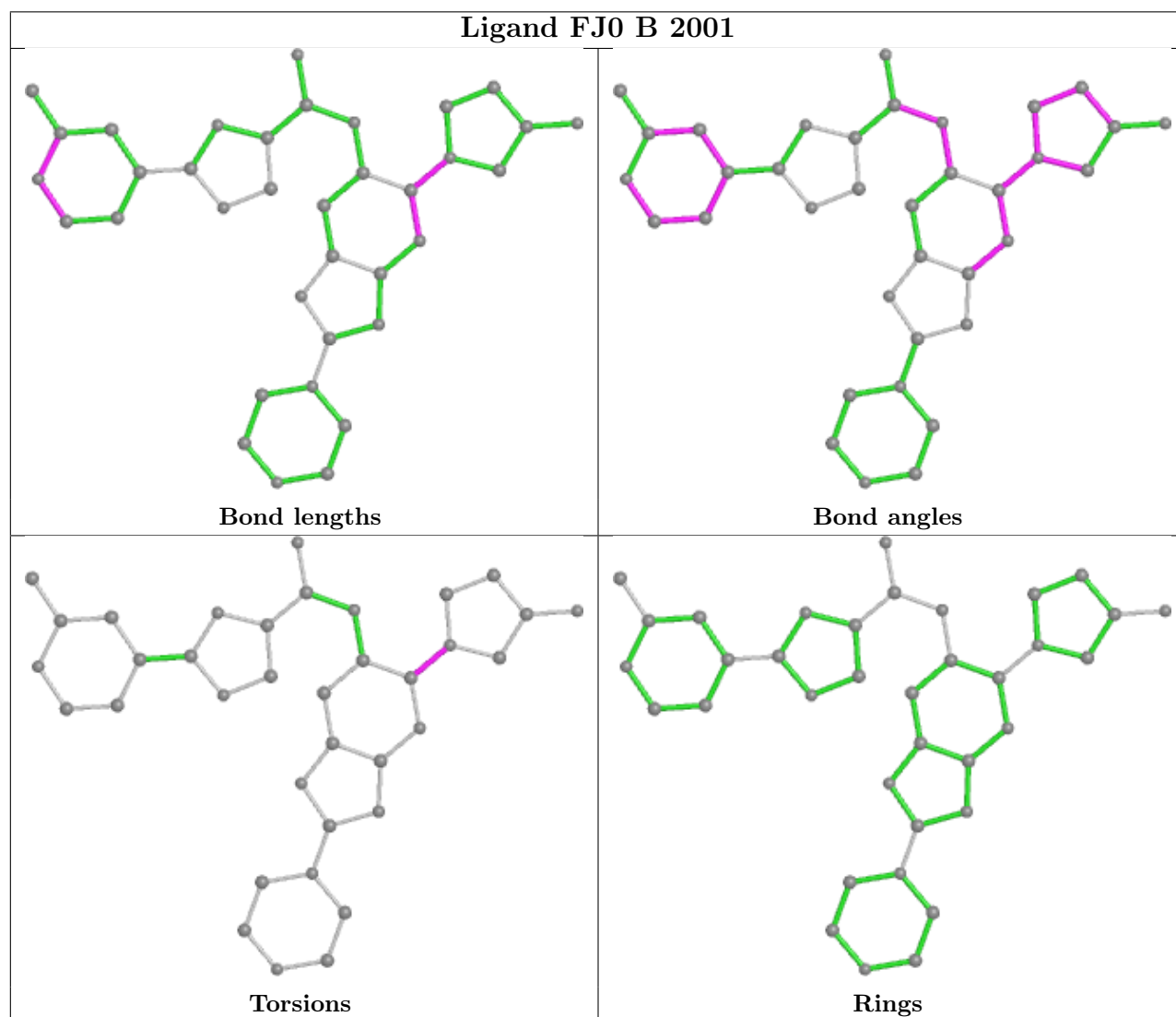
Mol	Chain	Res	Type	Atoms
2	A	2001	FJ0	C3-C2-N3-C10
2	A	2001	FJ0	C3-C2-N3-C13
2	A	2001	FJ0	N-C2-N3-C10
2	A	2001	FJ0	N-C2-N3-C13
2	B	2001	FJ0	C3-C2-N3-C13
2	B	2001	FJ0	N-C2-N3-C13
2	C	2001	FJ0	C3-C2-N3-C10
2	C	2001	FJ0	C3-C2-N3-C13
2	C	2001	FJ0	N-C2-N3-C10
2	C	2001	FJ0	N-C2-N3-C13
2	D	2001	FJ0	C3-C2-N3-C13
2	D	2001	FJ0	N-C2-N3-C13
2	B	2001	FJ0	C3-C2-N3-C10
2	B	2001	FJ0	N-C2-N3-C10

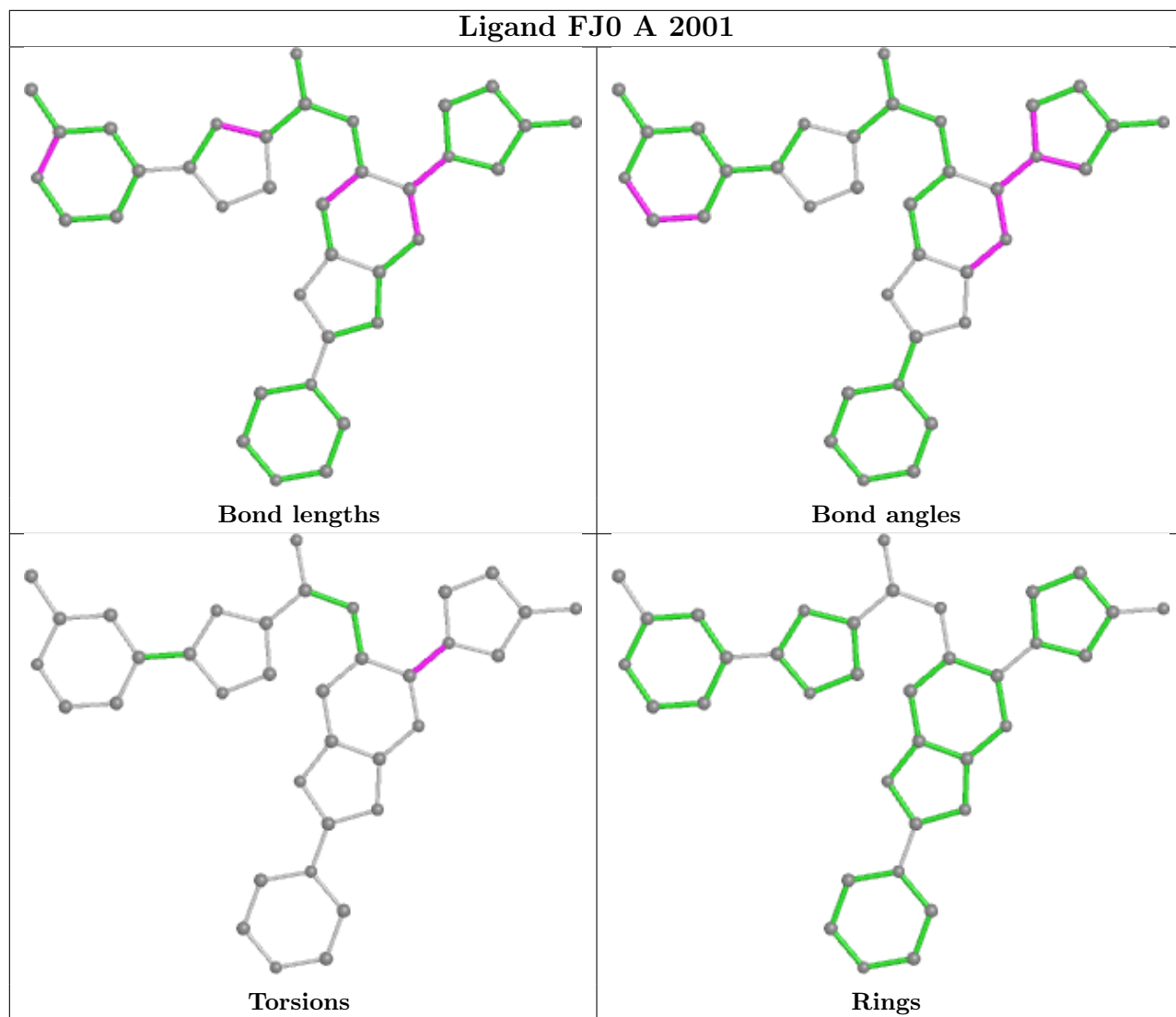
There are no ring outliers.

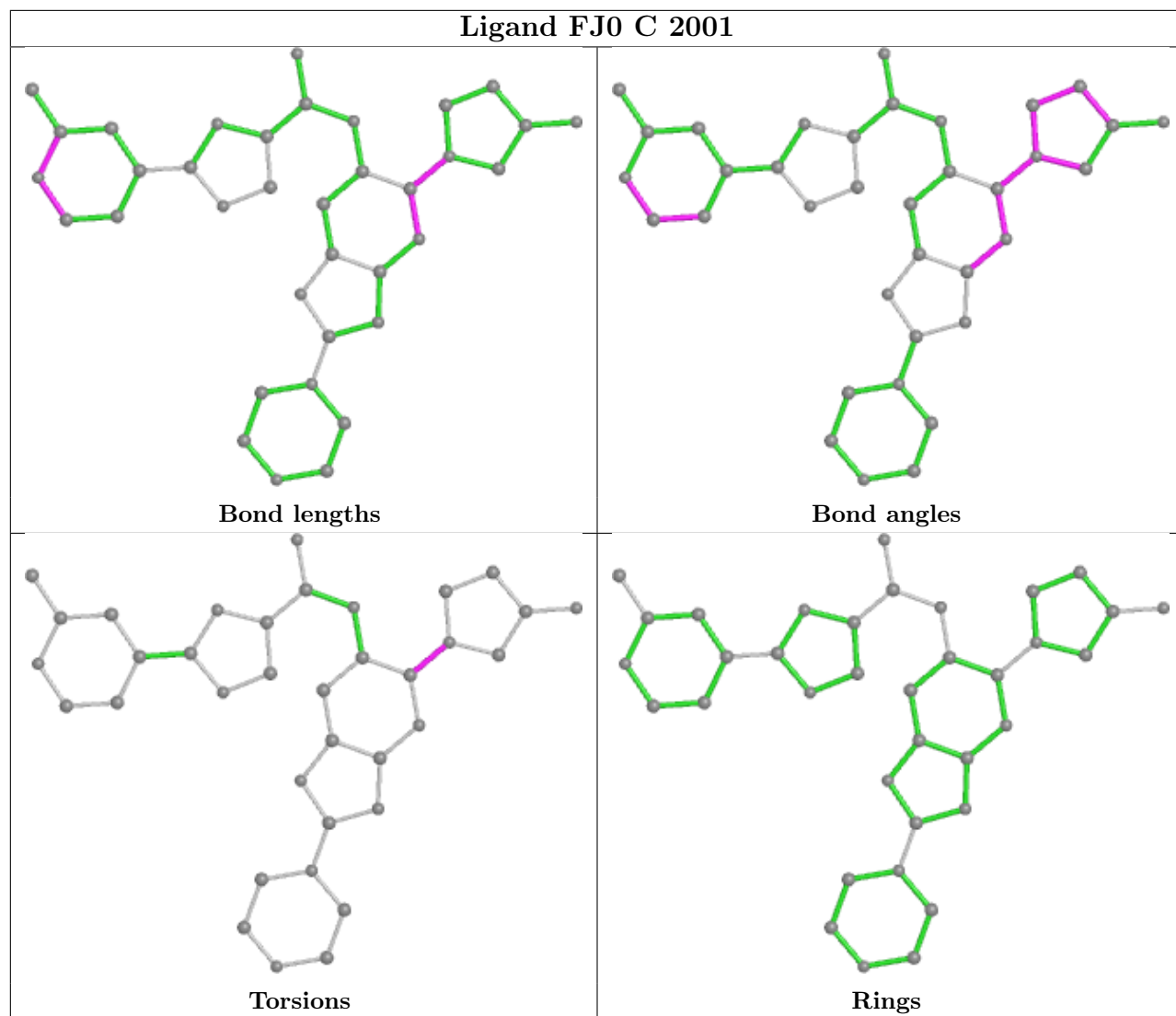
No monomer is involved in short contacts.

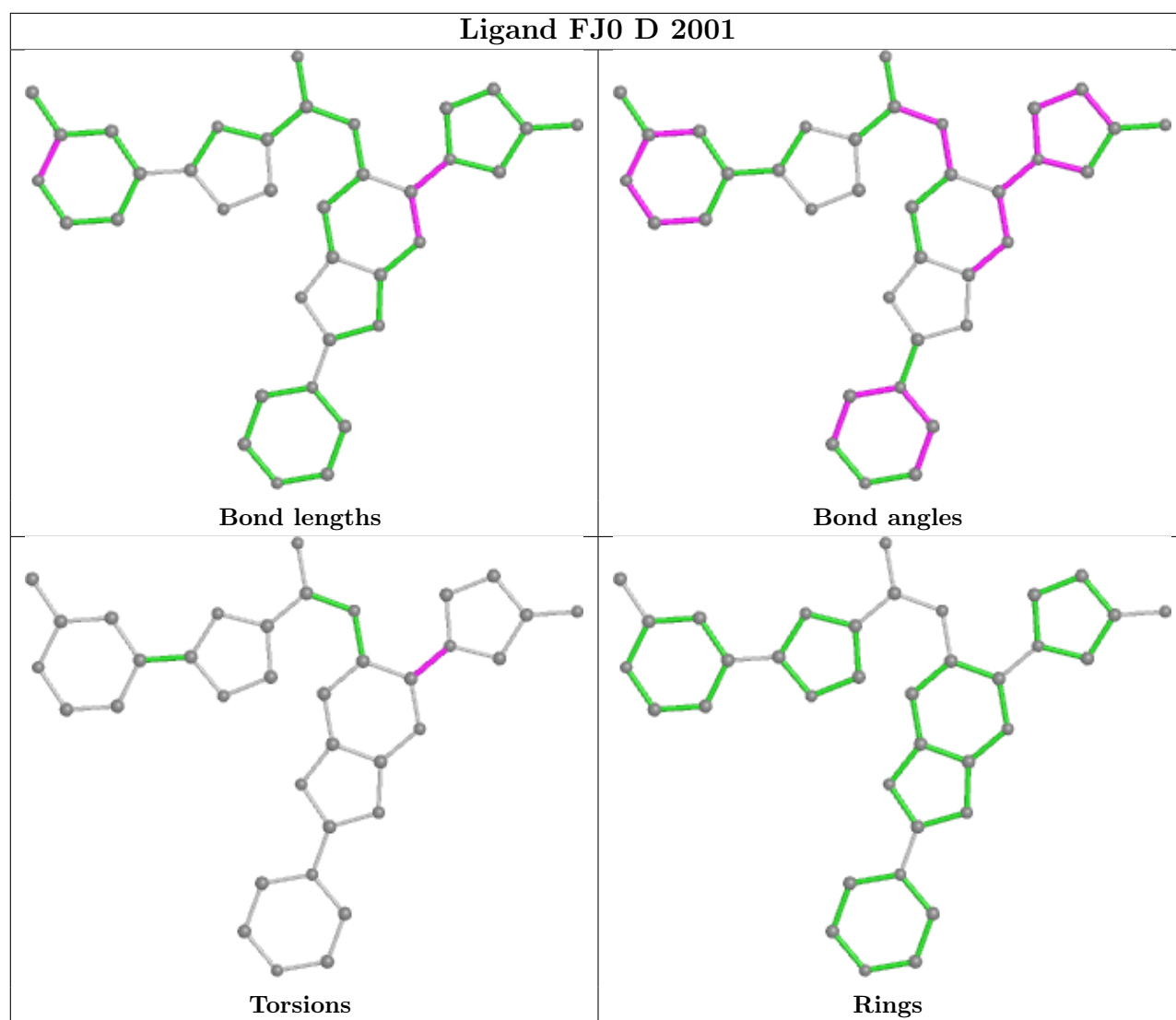
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	286/300 (95%)	0.26	22 (7%) 13 10	30, 59, 122, 181	0
1	B	281/300 (93%)	0.31	22 (7%) 13 10	29, 60, 116, 167	0
1	C	280/300 (93%)	0.43	30 (10%) 6 4	32, 60, 129, 173	0
1	D	283/300 (94%)	0.26	20 (7%) 16 12	31, 55, 112, 176	0
All	All	1130/1200 (94%)	0.31	94 (8%) 11 8	29, 58, 122, 181	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	GLU	9.9
1	B	207	ASN	8.9
1	D	222	THR	8.2
1	C	222	THR	8.1
1	D	223	THR	7.0
1	A	225	GLU	6.7
1	C	223	THR	6.7
1	C	459	ALA	6.5
1	C	460	SER	6.5
1	A	336	SER	6.4
1	D	197	PHE	6.0
1	C	224	GLU	5.7
1	C	256	ASP	5.4
1	A	222	THR	5.1
1	A	407	GLU	5.0
1	D	224	GLU	4.8
1	B	206	ASN	4.7
1	A	337	GLU	4.5
1	C	390	HIS	4.3
1	A	206	ASN	4.3
1	A	207	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	347	ARG	4.1
1	B	204	TYR	4.0
1	B	187	VAL	4.0
1	A	221	ILE	4.0
1	C	225	GLU	3.9
1	C	191	LYS	3.9
1	C	183	ARG	3.9
1	B	347	ARG	3.7
1	A	224	GLU	3.7
1	C	179	ASN	3.7
1	B	163	THR	3.7
1	C	221	ILE	3.6
1	A	228	GLN	3.6
1	C	164	ARG	3.5
1	C	255	GLY	3.4
1	B	343	VAL	3.4
1	A	187	VAL	3.3
1	B	208	THR	3.3
1	D	256	ASP	3.2
1	B	334	ARG	3.2
1	C	239	LYS	3.2
1	C	347	ARG	3.1
1	C	226	LEU	3.1
1	D	226	LEU	3.0
1	D	239	LYS	2.9
1	B	197	PHE	2.9
1	C	197	PHE	2.9
1	D	225	GLU	2.9
1	C	376	VAL	2.9
1	C	407	GLU	2.9
1	D	407	GLU	2.8
1	C	184	PRO	2.8
1	A	183	ARG	2.8
1	D	347	ARG	2.8
1	B	239	LYS	2.8
1	B	257	ASP	2.7
1	B	184	PRO	2.7
1	C	254	ASP	2.7
1	A	223	THR	2.7
1	A	188	GLY	2.6
1	D	376	VAL	2.6
1	B	390	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	407	GLU	2.5
1	C	182	GLU	2.5
1	A	256	ASP	2.4
1	A	226	LEU	2.4
1	D	459	ALA	2.4
1	D	377	LEU	2.4
1	D	187	VAL	2.4
1	D	253	SER	2.4
1	D	372	SER	2.3
1	D	240	CYS	2.3
1	B	253	SER	2.3
1	B	335	ALA	2.3
1	A	408	LYS	2.2
1	B	231	ASP	2.2
1	A	443	LYS	2.2
1	D	235	LYS	2.2
1	B	178	ASN	2.2
1	B	235	LYS	2.2
1	C	406	GLU	2.2
1	A	376	VAL	2.1
1	C	389	GLU	2.1
1	A	235	LYS	2.1
1	B	256	ASP	2.1
1	C	424	THR	2.1
1	B	344	MET	2.1
1	C	176	VAL	2.1
1	C	405	ASP	2.1
1	D	374	GLY	2.1
1	C	180	PHE	2.1
1	C	349	VAL	2.0
1	A	239	LYS	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	SEP	D	346	10/11	0.64	0.46	113,133,161,173	0
1	SEP	B	346	10/11	0.74	0.42	101,133,152,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	C	346	10/11	0.78	0.43	100,137,167,167	0
1	TPO	C	342	11/12	0.78	0.23	78,96,136,160	0
1	TPO	A	342	11/12	0.80	0.36	85,123,148,156	0
1	TPO	D	342	11/12	0.80	0.23	95,116,162,164	0
1	SEP	A	346	10/11	0.80	0.43	99,127,155,164	0
1	TPO	B	342	11/12	0.87	0.33	87,140,177,204	0
1	TPO	A	345	11/12	0.91	0.21	69,85,105,111	0
1	TPO	D	345	11/12	0.94	0.23	73,89,102,111	0
1	TPO	B	345	11/12	0.94	0.27	74,87,108,110	0
1	TPO	C	345	11/12	0.95	0.17	66,76,87,92	0

6.3 Carbohydrates [i](#)

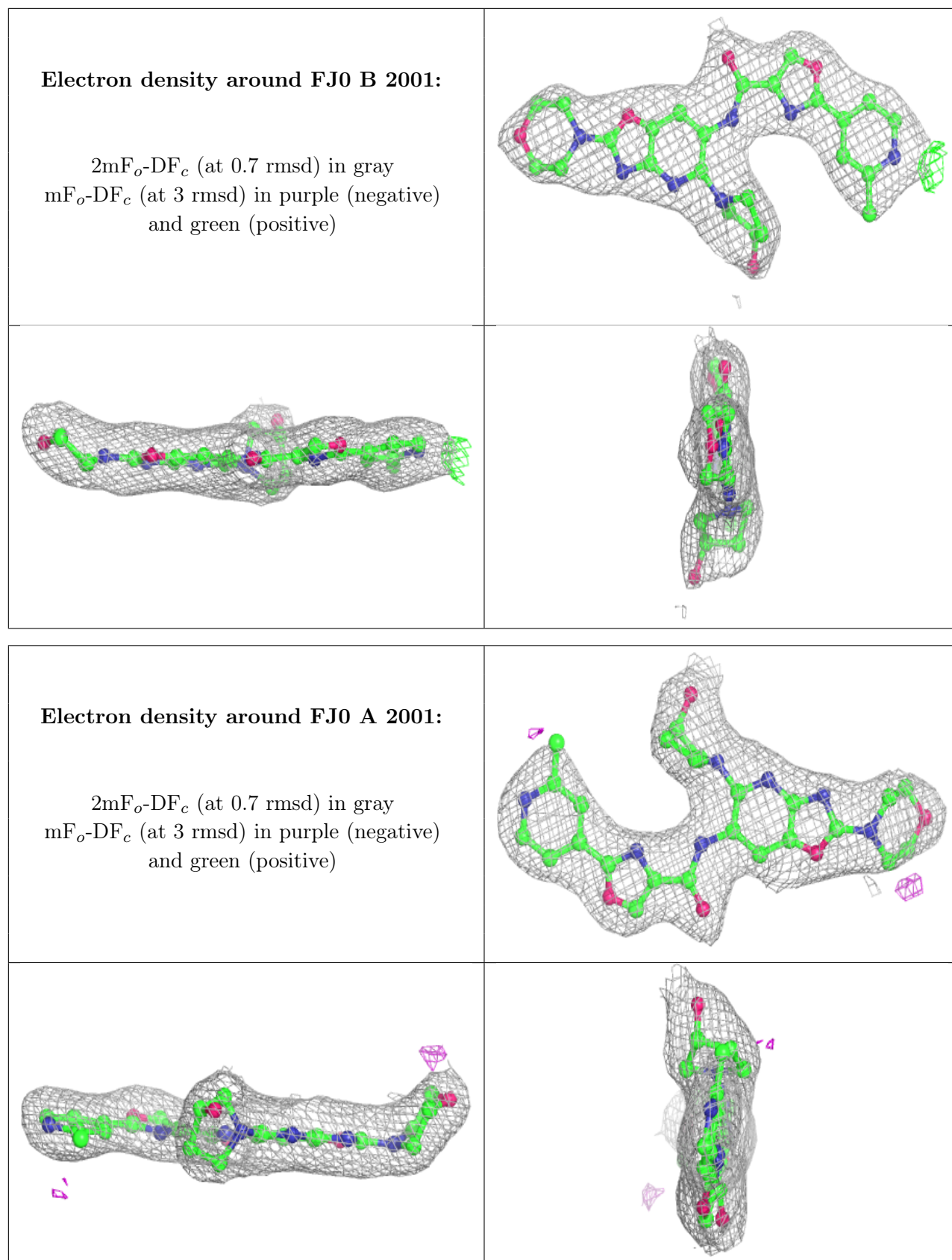
There are no monosaccharides in this entry.

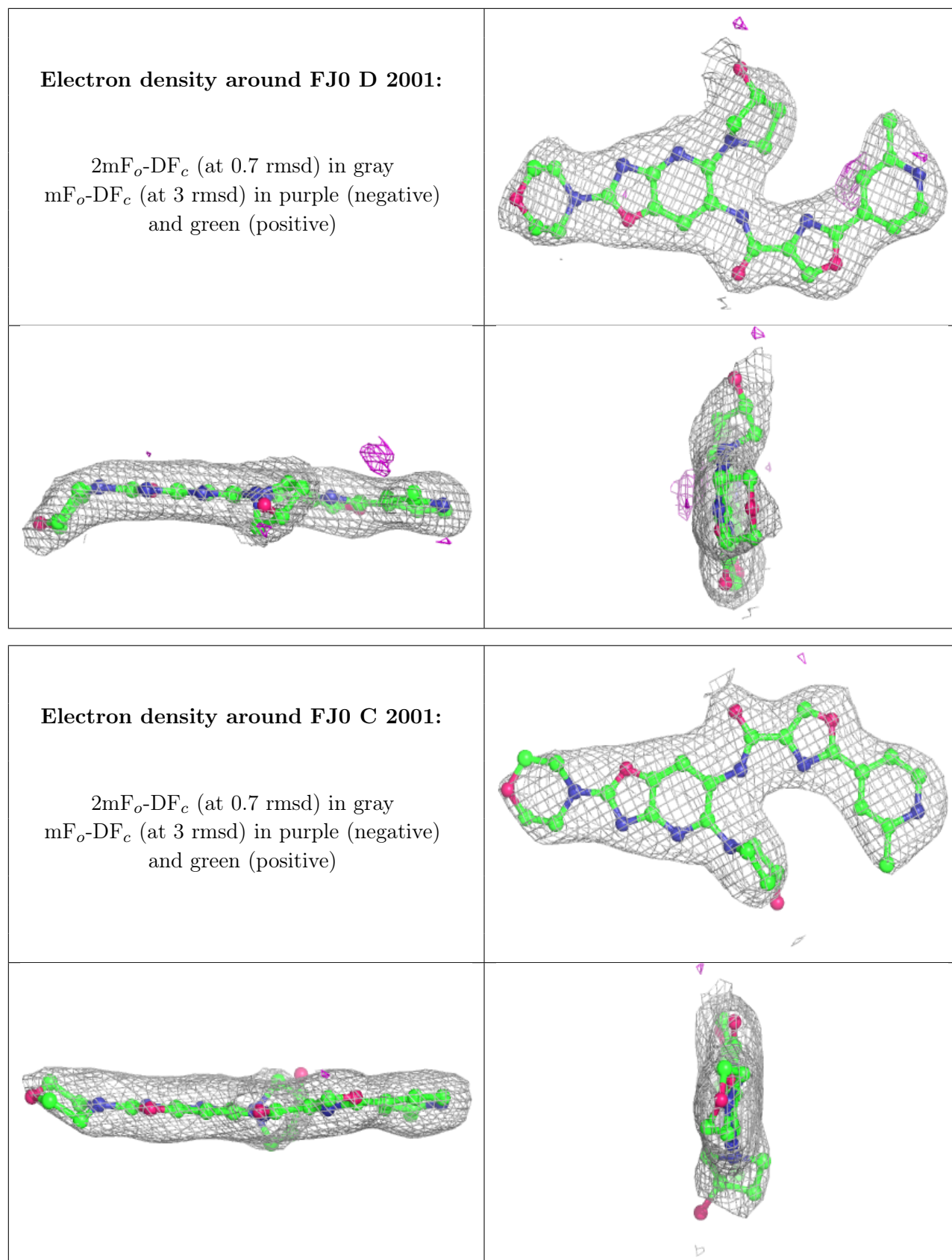
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	FJ0	B	2001	36/36	0.95	0.14	31,46,71,79	0
2	FJ0	A	2001	36/36	0.96	0.14	37,49,66,80	0
2	FJ0	D	2001	36/36	0.96	0.12	33,47,79,90	0
2	FJ0	C	2001	36/36	0.97	0.13	37,51,100,127	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.