



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 PM UTC

PDB ID : 7C2V / pdb_00007c2v
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 : 4-5-2 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

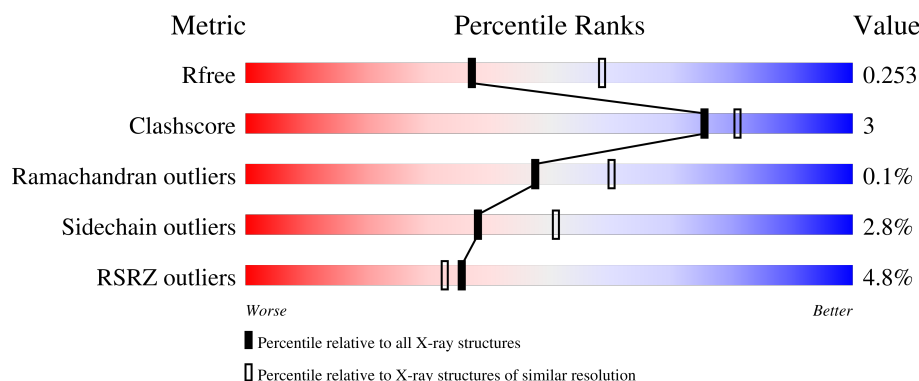
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (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	3% 89% 7% . .
1	B	300	4% 87% 8% 5%
1	C	300	7% 86% 7% . 6%
1	D	300	4% 84% 11% 5%

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.

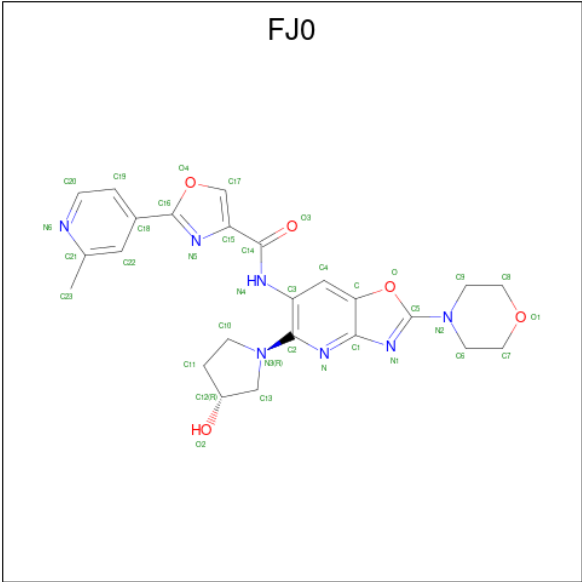
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

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

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 (CCD ID: FJ0) (formula: C₂₄H₂₅N₇O₅) (labeled as "Ligand of Interest" by depositor).



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

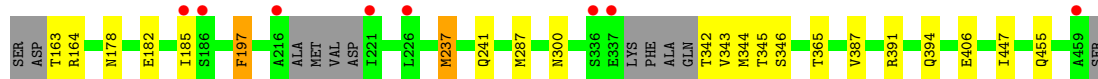
- Molecule 3 is water.

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

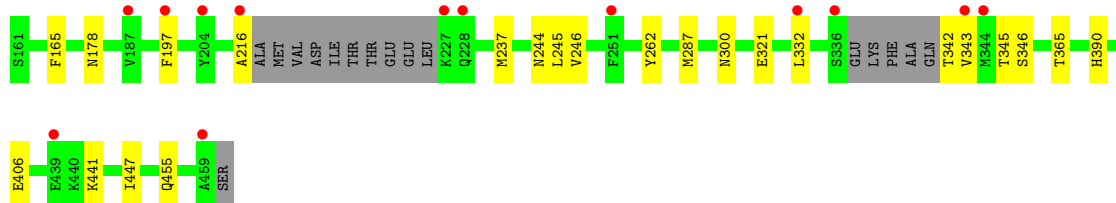
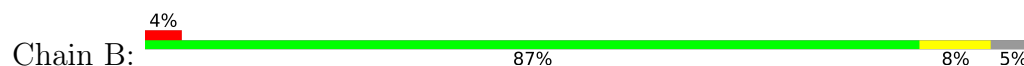
3 Residue-property plots [i](#)

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.

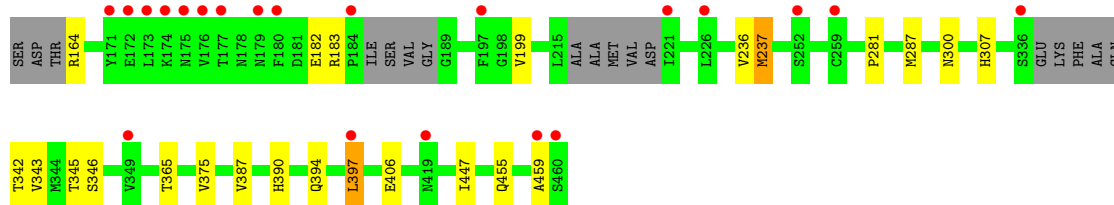
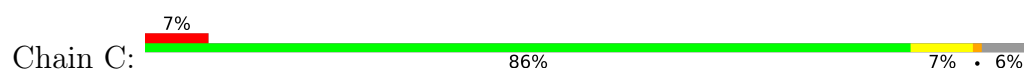
- Molecule 1: Interleukin-1 receptor-associated kinase 4



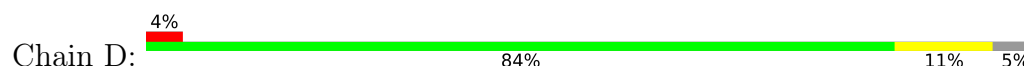
- Molecule 1: Interleukin-1 receptor-associated kinase 4

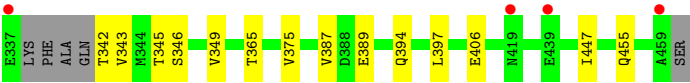


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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 30.00 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.44) 98.8 (30.00-2.44)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.45Å)	Xtriage
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 (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.9	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	0.95	EDS
Total number of atoms	9538	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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	0.69	0/2279	0.88	2/3070 (0.1%)
1	B	0.70	0/2242	0.88	2/3019 (0.1%)
1	C	0.71	0/2235	0.89	1/3009 (0.0%)
1	D	0.72	0/2257	0.88	2/3040 (0.1%)
All	All	0.71	0/9013	0.88	7/12138 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	GLU	CA-CB-CG	6.42	126.94	114.10
1	A	344	MET	CA-CB-CG	6.34	126.78	114.10
1	B	165	PHE	N-CA-C	5.42	117.14	108.41
1	A	406	GLU	N-CA-C	5.41	119.18	112.47
1	C	406	GLU	N-CA-C	5.28	119.01	112.47
1	B	406	GLU	N-CA-C	5.23	118.95	112.47
1	D	406	GLU	N-CA-C	5.21	118.93	112.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	12	0
1	B	2235	0	2192	11	0
1	C	2232	0	2188	10	0
1	D	2253	0	2212	23	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	0	0
3	D	120	0	0	10	0
All	All	9538	0	8826	54	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 (54) 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:D:177:THR:O	3:D:2101:HOH:O	1.71	1.07
1:A:287[B]:MET:HA	1:A:287[B]:MET:HE3	1.55	0.87
1:A:287[B]:MET:HE3	1:A:287[B]:MET:CA	2.08	0.81
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	0.80
1:B:237:MET:HE3	1:B:262:TYR:HE1	1.51	0.73
1:C:375:VAL:HG22	1:C:397:LEU:CD1	2.21	0.70
1:B:237:MET:HE1	1:B:246:VAL:HG23	1.74	0.68
1:D:237:MET:HE3	1:D:262:TYR:HE2	1.62	0.65
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:A:237:MET:HA	1:A:237:MET:HE2	1.89	0.54
1:B:216:ALA:CA	3:B:2149:HOH:O	2.54	0.54
1:A:197:PHE:CD1	1:A:197:PHE:N	2.76	0.54
1:D:237:MET:HE1	1:D:246:VAL:HG23	1.89	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:A:287[B]:MET:CA	1:A:287[B]:MET:CE	2.85	0.51
1:B:237:MET:HE3	1:B:262:TYR:CE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ASN:O	1:B:245:LEU:HD12	2.11	0.50
1:D:287:MET:HE2	1:D:323:PHE:CB	2.41	0.50
1:C:237:MET:HE2	1:C:237:MET:HA	1.93	0.50
1:D:287:MET:HE2	1:D:323:PHE:HB2	1.94	0.50
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
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:B:237:MET:HE1	1:B:246:VAL:CG2	2.44	0.46
1:C:287:MET:HA	1:C:287:MET:HE2	1.99	0.45
1:B:287[A]:MET:HA	1:B:287[A]:MET:HE2	1.98	0.44
1:D:287:MET:HE1	1:D:290:LYS:HD3	1.99	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: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 ⓘ

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	282/300 (94%)	269 (95%)	13 (5%)	0	100	100
1	B	278/300 (93%)	262 (94%)	16 (6%)	0	100	100
1	C	273/300 (91%)	259 (95%)	13 (5%)	1 (0%)	30	36
1	D	278/300 (93%)	265 (95%)	13 (5%)	0	100	100
All	All	1111/1200 (93%)	1055 (95%)	55 (5%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	459	ALA

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	248/258 (96%)	240 (97%)	8 (3%)	34	46
1	B	243/258 (94%)	238 (98%)	5 (2%)	47	60
1	C	243/258 (94%)	234 (96%)	9 (4%)	30	41
1	D	246/258 (95%)	241 (98%)	5 (2%)	48	62
All	All	980/1032 (95%)	953 (97%)	27 (3%)	38	51

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	182	GLU
1	A	185	ILE
1	A	197	PHE
1	A	237	MET

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Mol	Chain	Res	Type
1	A	343	VAL
1	A	365	THR
1	A	455	GLN
1	B	178	ASN
1	B	343	VAL
1	B	365	THR
1	B	441	LYS
1	B	455	GLN
1	C	164	ARG
1	C	182	GLU
1	C	183	ARG
1	C	199	VAL
1	C	237	MET
1	C	343	VAL
1	C	365	THR
1	C	397	LEU
1	C	455	GLN
1	D	178	ASN
1	D	343	VAL
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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	207	ASN
1	A	241	GLN
1	A	419	ASN
1	A	451	GLN
1	B	229	GLN
1	B	451	GLN
1	B	452	GLN
1	C	166	HIS
1	C	175	ASN
1	C	178	ASN
1	C	229	GLN
1	C	286	HIS
1	C	307	HIS
1	C	419	ASN
1	C	451	GLN

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Mol	Chain	Res	Type
1	D	166	HIS
1	D	229	GLN
1	D	390	HIS
1	D	419	ASN
1	D	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	SEP	C	346	1	8,9,10	0.66	0	7,12,14	1.71	2 (28%)
1	SEP	B	346	1	8,9,10	0.62	0	7,12,14	1.53	1 (14%)
1	SEP	A	346	1	8,9,10	0.69	0	7,12,14	1.48	1 (14%)
1	TPO	C	345	1	8,10,11	1.13	1 (12%)	10,14,16	1.09	1 (10%)
1	SEP	D	346	1	8,9,10	0.67	0	7,12,14	1.54	1 (14%)
1	TPO	C	342	1	8,10,11	1.18	1 (12%)	10,14,16	1.45	1 (10%)
1	TPO	A	345	1	8,10,11	1.25	1 (12%)	10,14,16	1.36	1 (10%)
1	TPO	D	345	1	8,10,11	0.86	0	10,14,16	1.01	1 (10%)
1	TPO	B	345	1	8,10,11	0.96	0	10,14,16	1.10	1 (10%)
1	TPO	D	342	1	8,10,11	0.91	0	10,14,16	1.29	1 (10%)
1	TPO	B	342	1	8,10,11	0.89	0	10,14,16	1.31	1 (10%)
1	TPO	A	342	1	8,10,11	1.23	1 (12%)	10,14,16	1.65	1 (10%)

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	SEP	C	346	1	-	2/6/8/10	-
1	SEP	B	346	1	-	2/6/8/10	-
1	SEP	A	346	1	-	2/6/8/10	-
1	TPO	C	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	2/6/8/10	-
1	TPO	C	342	1	-	1/9/11/13	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	D	342	1	-	1/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	P-OG1	3.03	1.64	1.59
1	A	342	TPO	P-OG1	2.97	1.64	1.59
1	C	342	TPO	P-OG1	2.80	1.64	1.59
1	C	345	TPO	P-OG1	2.32	1.63	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	TPO	P-OG1-CB	-3.79	113.04	123.33
1	A	342	TPO	P-OG1-CB	-3.69	113.31	123.33
1	B	342	TPO	P-OG1-CB	-3.23	114.54	123.33
1	D	342	TPO	P-OG1-CB	-3.22	114.58	123.33
1	A	346	SEP	OG-CB-CA	3.11	111.17	108.14
1	A	345	TPO	P-OG1-CB	-2.68	116.04	123.33
1	C	346	SEP	O3P-P-OG	-2.67	99.70	106.67
1	D	346	SEP	OG-CB-CA	2.64	110.71	108.14
1	C	345	TPO	P-OG1-CB	-2.49	116.57	123.33
1	C	346	SEP	OG-CB-CA	2.39	110.47	108.14
1	B	346	SEP	OG-CB-CA	2.27	110.36	108.14
1	B	345	TPO	P-OG1-CB	-2.08	117.68	123.33
1	D	345	TPO	P-OG1-CB	-2.02	117.83	123.33

There are no chirality outliers.

All (26) 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	A	346	SEP	C-CA-CB-OG
1	B	345	TPO	N-CA-CB-OG1
1	B	346	SEP	N-CA-CB-OG
1	B	346	SEP	C-CA-CB-OG
1	C	345	TPO	N-CA-CB-OG1
1	C	346	SEP	N-CA-CB-OG
1	C	346	SEP	C-CA-CB-OG
1	D	345	TPO	N-CA-CB-OG1
1	D	346	SEP	N-CA-CB-OG
1	D	346	SEP	C-CA-CB-OG
1	D	342	TPO	C-CA-CB-CG2
1	B	345	TPO	CB-OG1-P-O1P
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	C-CA-CB-CG2
1	A	345	TPO	O-C-CA-CB
1	B	342	TPO	C-CA-CB-CG2
1	B	345	TPO	O-C-CA-CB
1	C	342	TPO	C-CA-CB-CG2
1	C	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB
1	D	345	TPO	CB-OG1-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](#)

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	A	2001	-	40,41,41	3.07	13 (32%)	46,59,59	2.49	13 (28%)
2	FJ0	B	2001	-	40,41,41	2.92	12 (30%)	46,59,59	2.34	12 (26%)
2	FJ0	C	2001	-	40,41,41	2.99	15 (37%)	46,59,59	2.18	13 (28%)
2	FJ0	D	2001	-	40,41,41	2.96	13 (32%)	46,59,59	2.37	14 (30%)

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	A	2001	-	-	5/20/37/37	0/6/6/6
2	FJ0	B	2001	-	-	4/20/37/37	0/6/6/6
2	FJ0	C	2001	-	-	4/20/37/37	0/6/6/6
2	FJ0	D	2001	-	-	2/20/37/37	0/6/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FJ0	O-C	-9.65	1.22	1.38
2	C	2001	FJ0	O-C	-9.46	1.23	1.38
2	B	2001	FJ0	O-C	-9.45	1.23	1.38
2	D	2001	FJ0	O-C	-8.90	1.24	1.38
2	A	2001	FJ0	O4-C17	-8.37	1.22	1.37
2	D	2001	FJ0	O4-C17	-8.07	1.22	1.37
2	C	2001	FJ0	O4-C17	-7.98	1.23	1.37
2	D	2001	FJ0	O4-C16	-7.35	1.22	1.36
2	B	2001	FJ0	O4-C17	-7.27	1.24	1.37
2	B	2001	FJ0	O4-C16	-7.13	1.23	1.36
2	A	2001	FJ0	O4-C16	-7.05	1.23	1.36
2	C	2001	FJ0	O-C5	-6.89	1.24	1.37
2	B	2001	FJ0	O-C5	-6.68	1.25	1.37
2	A	2001	FJ0	O-C5	-6.44	1.25	1.37
2	C	2001	FJ0	O4-C16	-6.22	1.24	1.36
2	D	2001	FJ0	O-C5	-5.95	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FJ0	C5-N2	4.84	1.43	1.34
2	D	2001	FJ0	C5-N2	4.73	1.43	1.34
2	B	2001	FJ0	C-C1	-4.54	1.33	1.40
2	A	2001	FJ0	C-C1	-4.44	1.33	1.40
2	C	2001	FJ0	C16-N5	4.01	1.35	1.30
2	C	2001	FJ0	C1-N1	-3.99	1.31	1.38
2	B	2001	FJ0	C5-N2	3.76	1.41	1.34
2	C	2001	FJ0	C5-N2	3.75	1.41	1.34
2	A	2001	FJ0	C1-N1	-3.73	1.32	1.38
2	C	2001	FJ0	C-C1	-3.71	1.34	1.40
2	B	2001	FJ0	C16-N5	3.69	1.35	1.30
2	D	2001	FJ0	C2-N	3.56	1.38	1.34
2	A	2001	FJ0	C15-N5	-3.44	1.31	1.38
2	D	2001	FJ0	C16-N5	3.31	1.34	1.30
2	D	2001	FJ0	C5-N1	3.21	1.36	1.30
2	D	2001	FJ0	C-C1	-3.14	1.35	1.40
2	B	2001	FJ0	C1-N1	-3.06	1.33	1.38
2	D	2001	FJ0	C1-N1	-3.05	1.33	1.38
2	C	2001	FJ0	C2-N	2.97	1.38	1.34
2	D	2001	FJ0	C2-N3	2.93	1.44	1.37
2	C	2001	FJ0	C17-C15	2.93	1.37	1.34
2	C	2001	FJ0	C2-N3	2.79	1.44	1.37
2	B	2001	FJ0	C2-N3	2.74	1.44	1.37
2	A	2001	FJ0	C16-N5	2.58	1.33	1.30
2	D	2001	FJ0	C15-N5	-2.41	1.33	1.38
2	C	2001	FJ0	C15-N5	-2.40	1.33	1.38
2	A	2001	FJ0	C2-N3	2.37	1.43	1.37
2	C	2001	FJ0	C21-N6	2.36	1.39	1.34
2	A	2001	FJ0	C17-C15	2.33	1.37	1.34
2	D	2001	FJ0	C21-N6	2.19	1.38	1.34
2	A	2001	FJ0	C21-N6	2.18	1.38	1.34
2	B	2001	FJ0	C20-N6	2.16	1.39	1.34
2	B	2001	FJ0	C21-N6	2.13	1.38	1.34
2	B	2001	FJ0	C17-C15	2.08	1.36	1.34
2	A	2001	FJ0	C14-N4	2.05	1.39	1.35
2	C	2001	FJ0	C5-N1	2.03	1.34	1.30
2	C	2001	FJ0	C20-N6	2.02	1.38	1.34

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	FJ0	C17-O4-C16	7.97	111.22	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	FJ0	C17-O4-C16	7.80	111.07	104.30
2	B	2001	FJ0	C17-O4-C16	7.52	110.83	104.30
2	D	2001	FJ0	C17-O4-C16	6.94	110.33	104.30
2	A	2001	FJ0	O-C5-N1	-6.05	110.89	116.47
2	A	2001	FJ0	C12-C13-N3	-5.99	96.82	103.44
2	D	2001	FJ0	C12-C13-N3	-5.60	97.26	103.44
2	B	2001	FJ0	C15-N5-C16	-5.34	101.81	105.53
2	B	2001	FJ0	C13-N3-C2	-5.29	108.21	123.60
2	D	2001	FJ0	O-C5-N1	-4.78	112.06	116.47
2	D	2001	FJ0	C17-C15-N5	-4.56	105.75	109.15
2	B	2001	FJ0	N-C2-N3	-4.37	108.54	116.77
2	B	2001	FJ0	O-C5-N1	-4.27	112.53	116.47
2	A	2001	FJ0	N-C2-N3	-4.16	108.93	116.77
2	C	2001	FJ0	C15-N5-C16	-4.09	102.68	105.53
2	C	2001	FJ0	O-C5-N1	-4.01	112.77	116.47
2	D	2001	FJ0	C19-C20-N6	-4.01	119.06	123.97
2	A	2001	FJ0	O-C-C4	3.97	133.30	124.95
2	A	2001	FJ0	C15-N5-C16	-3.87	102.83	105.53
2	D	2001	FJ0	C13-N3-C2	-3.74	112.71	123.60
2	A	2001	FJ0	C-O-C5	3.71	110.10	103.96
2	B	2001	FJ0	C19-C20-N6	-3.69	119.46	123.97
2	C	2001	FJ0	O-C-C4	3.64	132.61	124.95
2	C	2001	FJ0	N-C2-N3	-3.62	109.94	116.77
2	B	2001	FJ0	O-C-C4	3.51	132.33	124.95
2	A	2001	FJ0	C10-N3-C2	-3.51	113.51	123.53
2	C	2001	FJ0	C12-C13-N3	-3.50	99.58	103.44
2	D	2001	FJ0	N-C2-N3	-3.48	110.21	116.77
2	B	2001	FJ0	C3-C2-N	-3.45	117.48	123.32
2	D	2001	FJ0	C15-N5-C16	-3.27	103.25	105.53
2	A	2001	FJ0	C19-C20-N6	-3.25	119.99	123.97
2	D	2001	FJ0	O-C-C4	3.23	131.74	124.95
2	D	2001	FJ0	C3-C2-N	-3.21	117.90	123.32
2	C	2001	FJ0	C-O-C5	3.17	109.20	103.96
2	D	2001	FJ0	C3-N4-C14	3.06	135.37	126.84
2	B	2001	FJ0	C-O-C5	3.06	109.02	103.96
2	D	2001	FJ0	C-O-C5	3.05	109.01	103.96
2	C	2001	FJ0	C19-C20-N6	-2.94	120.37	123.97
2	A	2001	FJ0	C13-N3-C2	-2.93	115.07	123.60
2	C	2001	FJ0	C3-C2-N	-2.90	118.41	123.32
2	C	2001	FJ0	C10-N3-C2	-2.90	115.25	123.53
2	B	2001	FJ0	C3-N4-C14	2.68	134.30	126.84
2	C	2001	FJ0	O4-C16-N5	-2.63	111.20	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	FJ0	C3-C2-N	-2.52	119.06	123.32
2	C	2001	FJ0	C17-C15-N5	-2.47	107.31	109.15
2	B	2001	FJ0	C19-C18-C22	2.45	122.08	119.25
2	A	2001	FJ0	O4-C16-N5	-2.39	111.46	114.07
2	D	2001	FJ0	O4-C16-N5	-2.21	111.66	114.07
2	B	2001	FJ0	C17-C15-N5	-2.15	107.55	109.15
2	C	2001	FJ0	C13-N3-C2	-2.14	117.37	123.60
2	D	2001	FJ0	C14-C15-N5	2.03	124.50	120.67
2	A	2001	FJ0	C17-C15-N5	-2.01	107.65	109.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

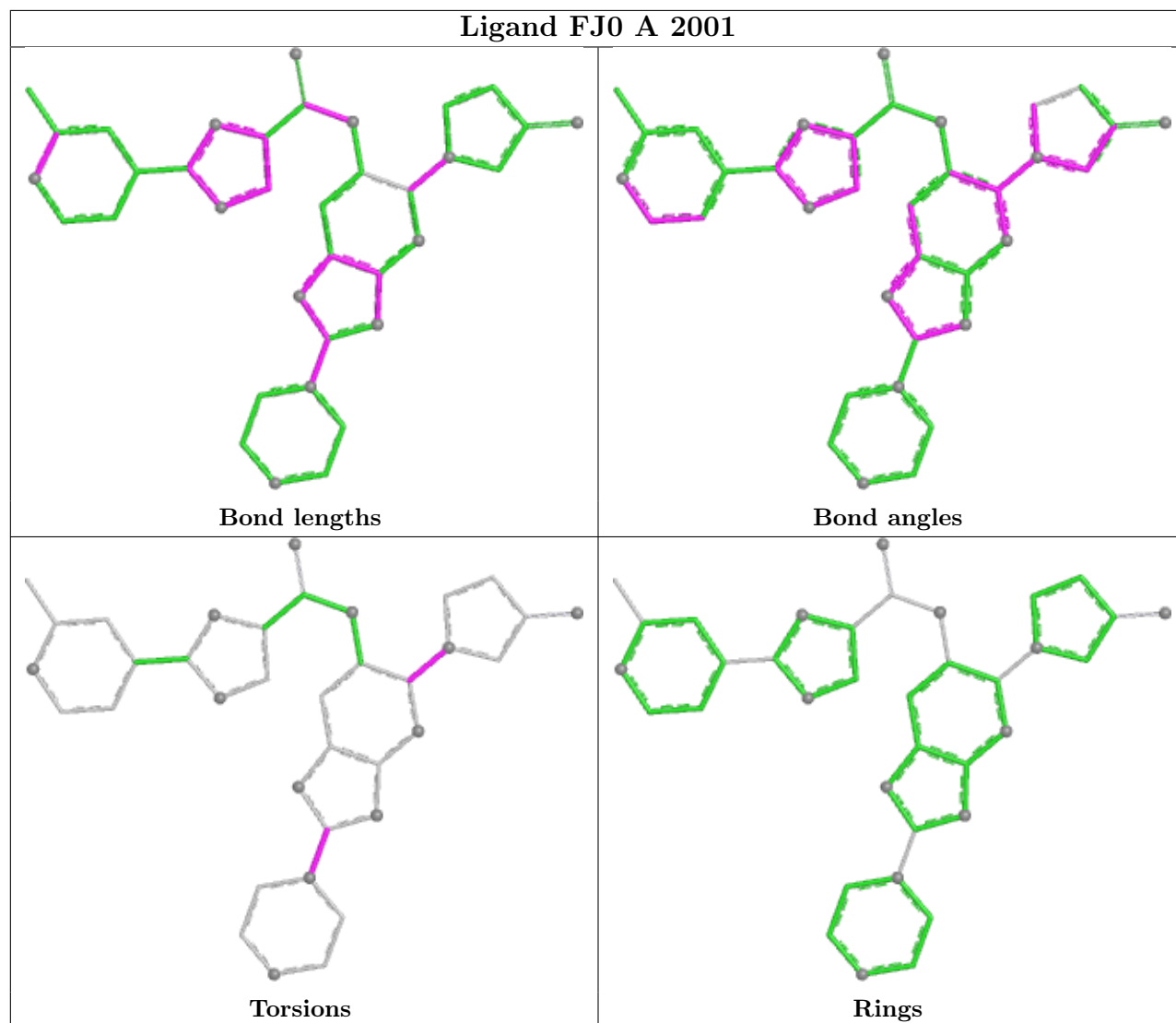
Mol	Chain	Res	Type	Atoms
2	A	2001	FJ0	C3-C2-N3-C10
2	A	2001	FJ0	C3-C2-N3-C13
2	A	2001	FJ0	N-C2-N3-C10
2	A	2001	FJ0	N-C2-N3-C13
2	B	2001	FJ0	C3-C2-N3-C13
2	B	2001	FJ0	N-C2-N3-C13
2	C	2001	FJ0	C3-C2-N3-C10
2	C	2001	FJ0	C3-C2-N3-C13
2	C	2001	FJ0	N-C2-N3-C10
2	C	2001	FJ0	N-C2-N3-C13
2	D	2001	FJ0	C3-C2-N3-C13
2	D	2001	FJ0	N-C2-N3-C13
2	B	2001	FJ0	C3-C2-N3-C10
2	B	2001	FJ0	N-C2-N3-C10
2	A	2001	FJ0	O-C5-N2-C6

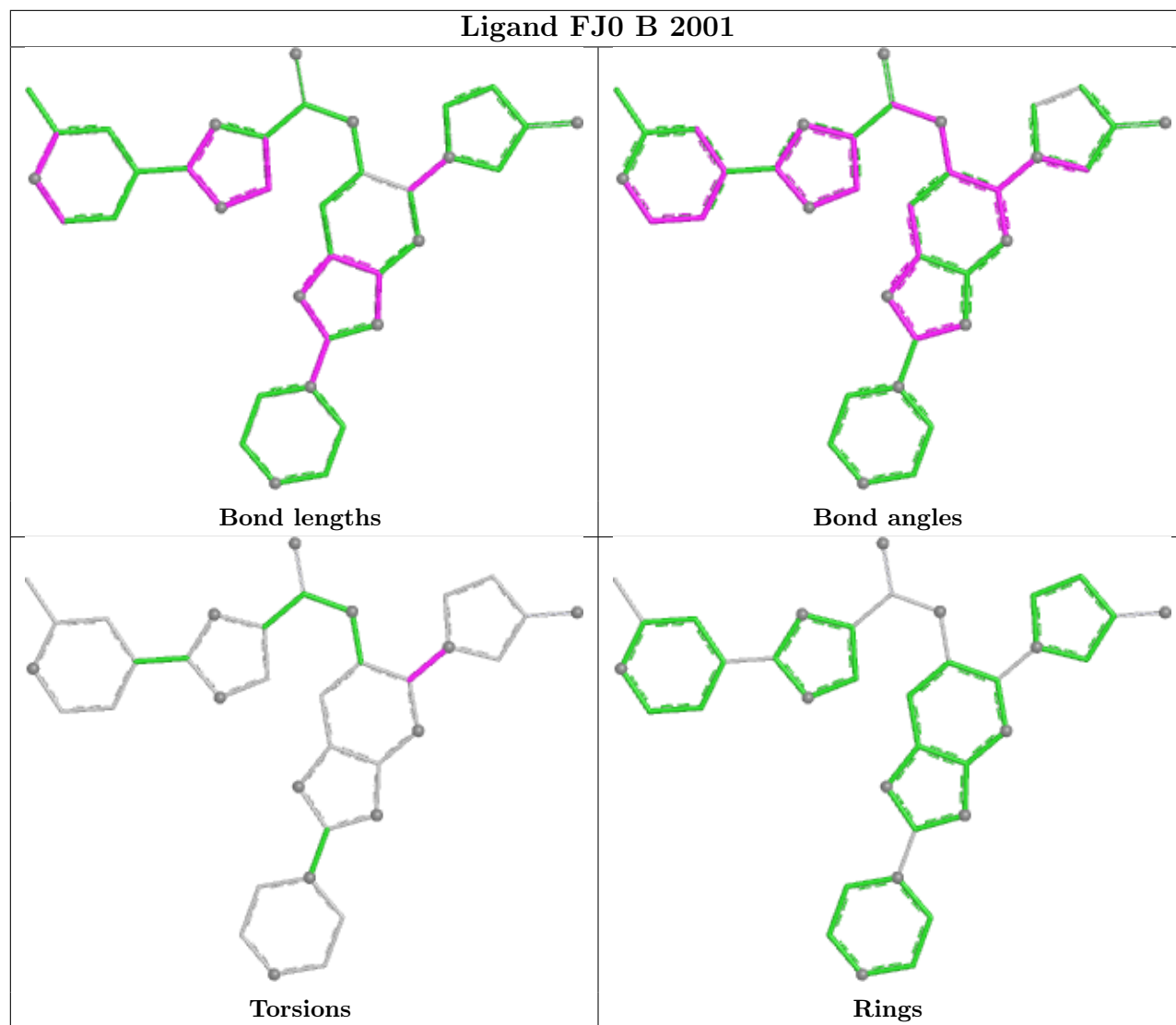
There are no ring outliers.

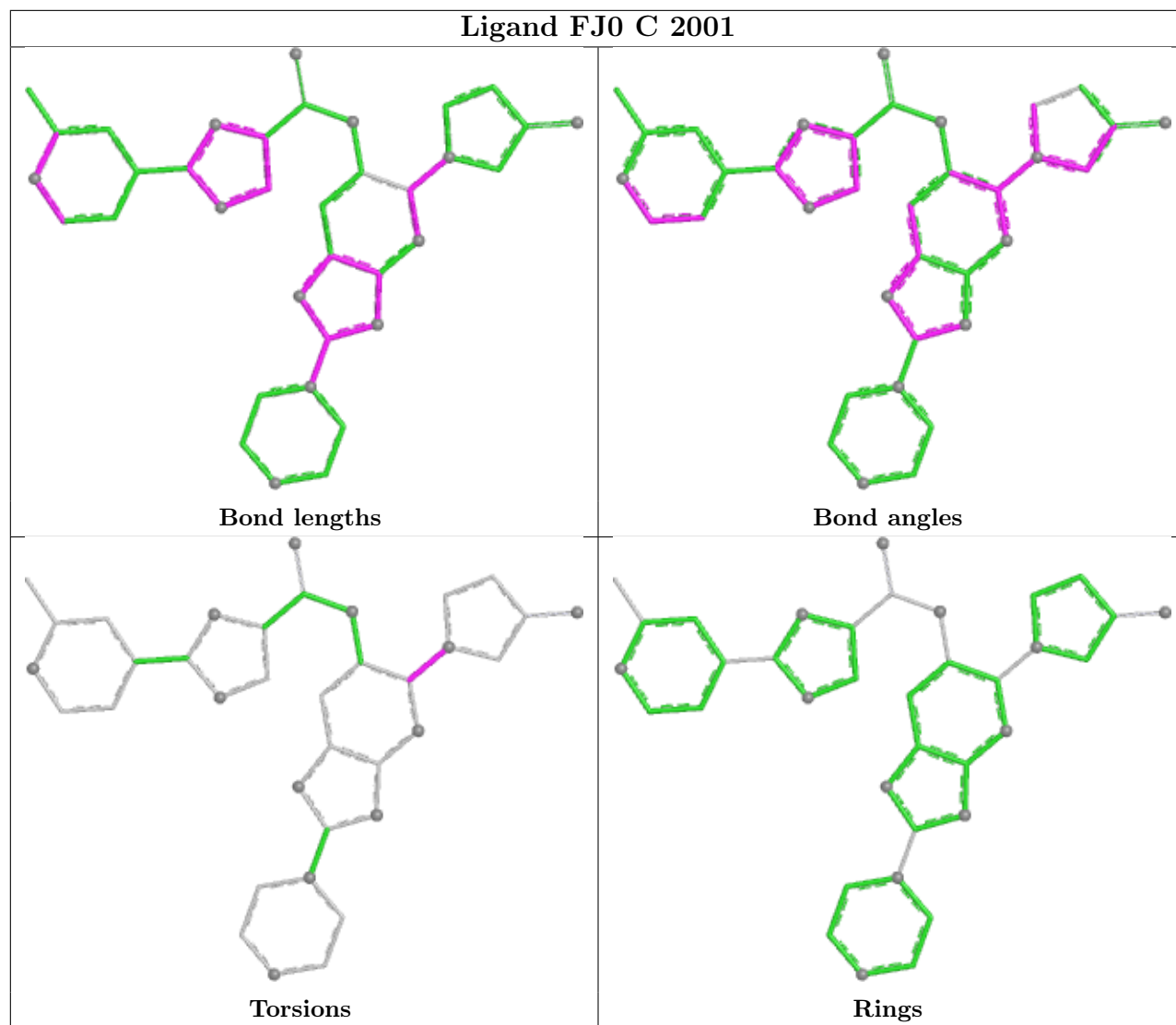
No monomer is involved in short contacts.

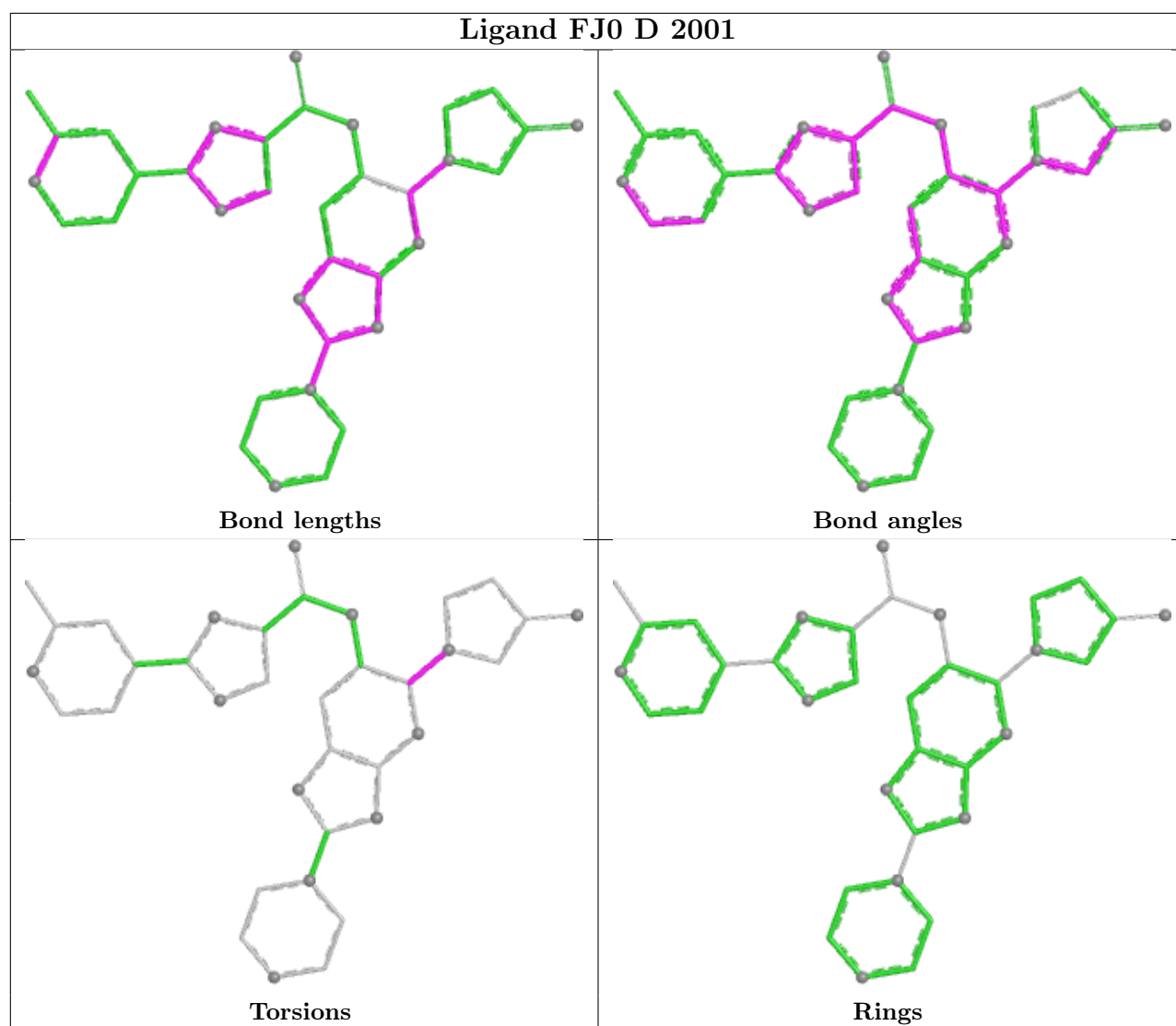
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	0.29	8 (2%) 55 54	27, 59, 122, 181	1 (0%)
1	B	281/300 (93%)	0.32	13 (4%) 37 34	20, 60, 116, 167	2 (0%)
1	C	280/300 (93%)	0.43	21 (7%) 20 17	32, 60, 129, 173	0
1	D	283/300 (94%)	0.25	12 (4%) 40 38	31, 55, 112, 176	0
All	All	1130/1200 (94%)	0.32	54 (4%) 35 33	20, 58, 122, 181	3 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	GLU	8.4
1	B	336	SER	6.7
1	D	337	GLU	5.7
1	B	459	ALA	5.1
1	C	336	SER	4.8
1	C	460	SER	4.8
1	C	184	PRO	4.6
1	C	176	VAL	4.1
1	A	185	ILE	3.8
1	A	459	ALA	3.8
1	A	216	ALA	3.8
1	D	459	ALA	3.5
1	C	197	PHE	3.3
1	D	197	PHE	3.2
1	A	336	SER	3.2
1	C	175	ASN	3.0
1	D	223	THR	2.9
1	C	174	LYS	2.8
1	D	226	LEU	2.8
1	B	251	PHE	2.7
1	B	343	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	221	ILE	2.6
1	C	180	PHE	2.6
1	C	179	ASN	2.6
1	D	335	ALA	2.6
1	B	204	TYR	2.6
1	C	252	SER	2.5
1	D	222	THR	2.5
1	B	197	PHE	2.5
1	A	221	ILE	2.4
1	C	226	LEU	2.4
1	C	171	TYR	2.4
1	C	172	GLU	2.4
1	C	173	LEU	2.3
1	C	259	CYS	2.3
1	D	439	GLU	2.3
1	C	177	THR	2.2
1	D	196	GLY	2.2
1	B	216	ALA	2.2
1	A	186	SER	2.2
1	B	228	GLN	2.2
1	B	227	LYS	2.2
1	B	332	LEU	2.1
1	B	187	VAL	2.1
1	C	459	ALA	2.1
1	D	419	ASN	2.1
1	C	397	LEU	2.1
1	B	439	GLU	2.1
1	D	229	GLN	2.1
1	C	349	VAL	2.1
1	B	344	MET	2.1
1	A	226	LEU	2.0
1	C	419	ASN	2.0
1	D	256	ASP	2.0

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

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($\text{\AA}^2$)	Q<0.9
1	SEP	B	346	10/11	0.47	0.14	101,133,152,154	0
1	SEP	D	346	10/11	0.58	0.13	113,133,161,173	0
1	SEP	A	346	10/11	0.61	0.13	99,127,155,164	0
1	SEP	C	346	10/11	0.65	0.13	100,137,167,167	0
1	TPO	D	342	11/12	0.67	0.17	95,116,162,164	0
1	TPO	C	342	11/12	0.78	0.16	78,96,136,160	0
1	TPO	A	342	11/12	0.79	0.15	85,123,148,156	0
1	TPO	B	342	11/12	0.81	0.15	87,140,177,204	0
1	TPO	A	345	11/12	0.90	0.10	69,85,105,111	0
1	TPO	D	345	11/12	0.92	0.11	73,89,102,111	0
1	TPO	C	345	11/12	0.93	0.10	66,76,87,92	0
1	TPO	B	345	11/12	0.94	0.10	74,87,108,110	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

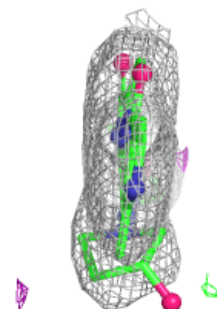
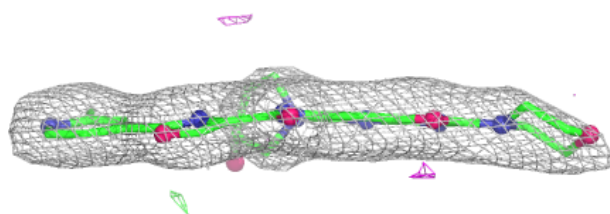
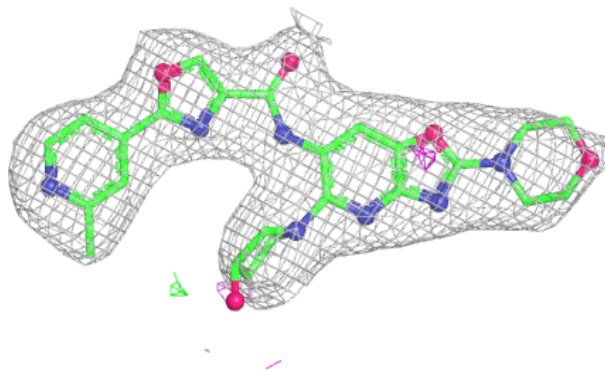
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FJ0	C	2001	36/36	0.94	0.10	37,51,100,127	0
2	FJ0	D	2001	36/36	0.94	0.09	33,47,79,90	0
2	FJ0	B	2001	36/36	0.95	0.09	31,46,71,79	0
2	FJ0	A	2001	36/36	0.96	0.08	37,49,66,80	0

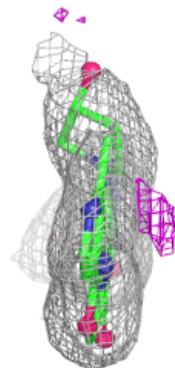
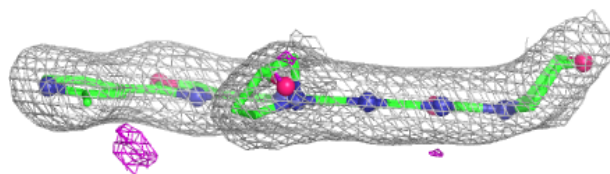
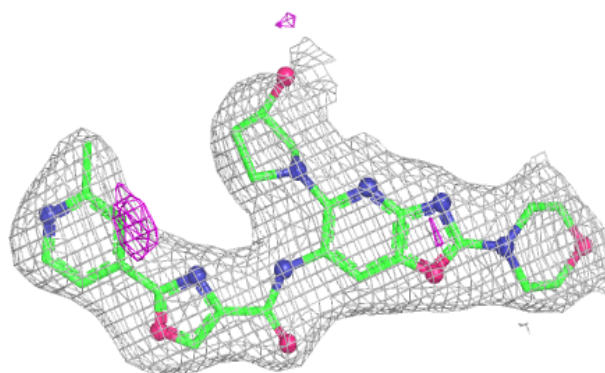
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FJ0 C 2001:

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

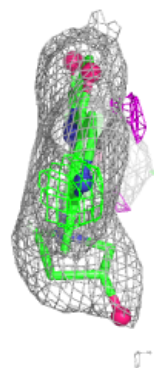
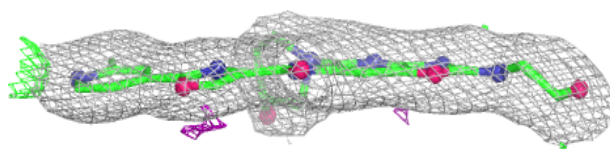
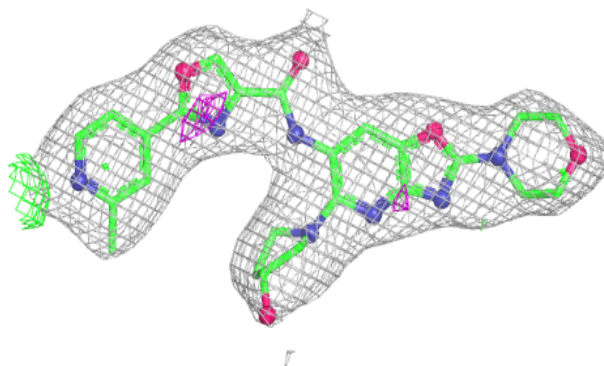
**Electron density around FJ0 D 2001:**

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

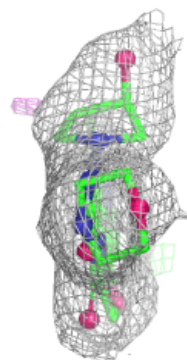
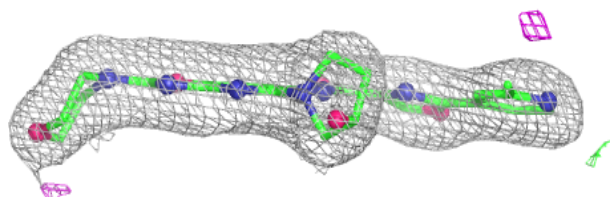
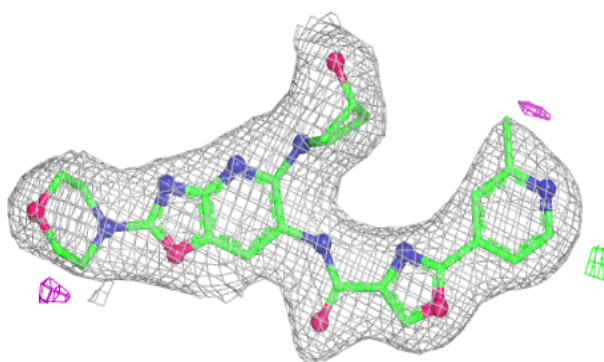


Electron density around FJ0 B 2001:

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

**Electron density around FJ0 A 2001:**

$2mF_o-DF_c$ (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.