



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2026 – 04:24 pm BST

PDB ID : 9T1V / pdb_00009t1v
Title : Crystal Structure of 17 bound to the PH domain of Btk
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Deposited on : 2025-10-22
Resolution : 2.41 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	:	1.8.4, CSD as541be (2020)
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

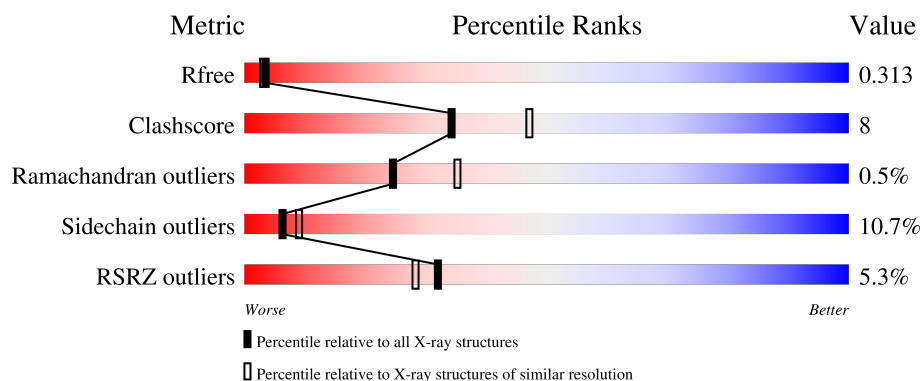
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	169	<div> <div>8%</div> <div>70% 22% • 7%</div> </div>
1	B	169	<div> <div>2%</div> <div>63% 22% • 11%</div> </div>
1	C	169	<div> <div>5%</div> <div>67% 21% • 8%</div> </div>
1	D	169	<div> <div>5%</div> <div>65% 25% • 7%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5404 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.

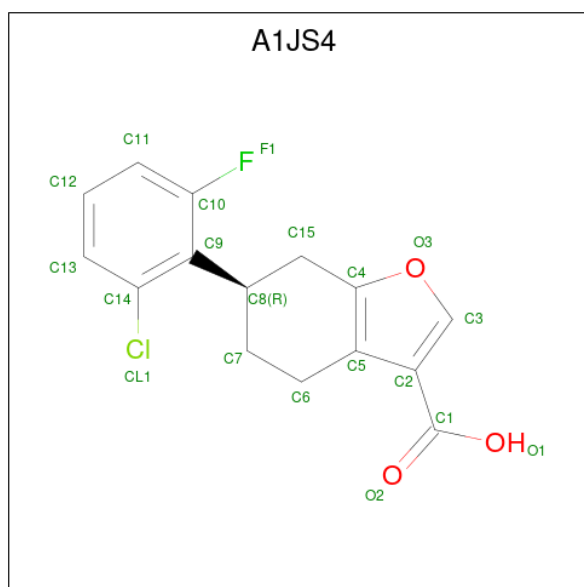
- Molecule 1 is a protein called Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	1	0
			1325	851	230	238	6			
1	B	150	Total	C	N	O	S	0	1	0
			1262	817	217	223	5			
1	C	156	Total	C	N	O	S	0	0	0
			1295	836	220	233	6			
1	D	158	Total	C	N	O	S	0	0	0
			1317	851	226	235	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	SER	CYS	engineered mutation	UNP Q06187
B	145	SER	CYS	engineered mutation	UNP Q06187
C	145	SER	CYS	engineered mutation	UNP Q06187
D	145	SER	CYS	engineered mutation	UNP Q06187

- Molecule 2 is (6 {R})-6-(2-chloranyl-6-fluoranyl-phenyl)-4,5,6,7-tetrahydro-1-benzofuran-3-carboxylic acid (CCD ID: A1JS4) (formula: C₁₅H₁₂ClFO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	O	0	0
			20	15	1	1	3		
2	B	1	Total	C	Cl	F	O	0	0
			20	15	1	1	3		
2	C	1	Total	C	Cl	F	O	0	0
			20	15	1	1	3		
2	D	1	Total	C	Cl	F	O	0	0
			20	15	1	1	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

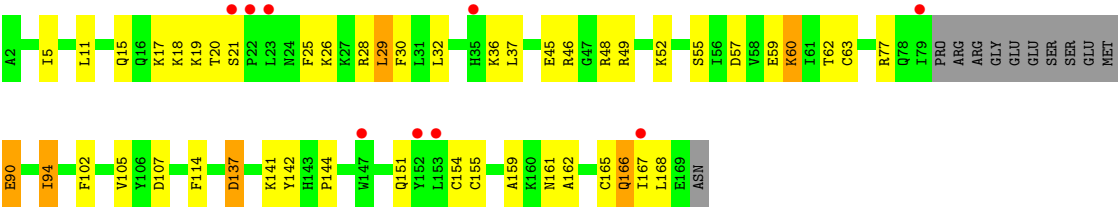
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total 31	O 31	0	0
5	B	30	Total 30	O 30	0	0
5	C	33	Total 33	O 33	0	0
5	D	24	Total 24	O 24	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	66.82Å 66.28Å 79.26Å 90.00° 99.95° 90.00°	Depositor
Resolution (Å)	55.24 – 2.41 55.24 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.5 (55.24-2.41) 99.5 (55.24-2.41)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, R_{free}	0.263 , 0.329 0.272 , 0.313	Depositor DCC
R_{free} test set	1360 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5404	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% 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: MG, A1JS4, ZN

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	0.77	0/1358	1.06	2/1831 (0.1%)
1	B	0.74	0/1293	1.06	0/1744
1	C	0.72	0/1326	1.06	4/1789 (0.2%)
1	D	0.68	0/1349	1.02	3/1819 (0.2%)
All	All	0.72	0/5326	1.05	9/7183 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	1
All	All	0	6

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	GLU	CA-C-N	6.51	128.91	120.44
1	C	118	GLU	C-N-CA	6.51	128.91	120.44
1	D	90	GLU	CA-C-N	6.32	129.03	120.38
1	D	90	GLU	C-N-CA	6.32	129.03	120.38
1	C	146	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	102	PHE	CA-CB-CG	5.84	119.64	113.80
1	C	102	PHE	CA-CB-CG	5.81	119.61	113.80
1	D	102	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	92	ILE	N-CA-C	-5.29	106.12	113.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	81	ARG	Sidechain
1	A	82	ARG	Sidechain
1	B	123	ARG	Sidechain
1	B	13	ARG	Sidechain
1	C	13	ARG	Sidechain

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	1325	0	1315	18	0
1	B	1262	0	1260	20	0
1	C	1295	0	1293	21	0
1	D	1317	0	1327	23	0
2	A	20	0	0	1	0
2	B	20	0	0	3	0
2	C	20	0	0	1	0
2	D	20	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	0	0	0
5	B	30	0	0	0	0
5	C	33	0	0	0	0
5	D	24	0	0	0	0
All	All	5404	0	5195	80	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 8.

All (80) 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:C:34:VAL:HG23	1:C:35:HIS:CD2	2.01	0.96
1:C:34:VAL:HG23	1:C:35:HIS:HD2	1.46	0.81
1:A:34:VAL:HG23	1:A:35[B]:HIS:HD2	1.48	0.78
1:B:15:GLN:HA	2:B:201:A1JS4:CL1	2.21	0.78
1:B:126:HIS:HD2	1:B:127:GLN:NE2	1.91	0.67
1:A:14:SER:HB2	1:A:26:LYS:HG3	1.78	0.66
1:B:15:GLN:CA	2:B:201:A1JS4:CL1	2.83	0.63
1:D:29:LEU:HD12	1:D:49:ARG:HB3	1.82	0.62
1:A:155:CYS:HB2	1:A:157:GLN:HG3	1.84	0.60
1:D:26:LYS:HD3	1:D:28:ARG:NH2	2.18	0.59
1:A:105:VAL:HG22	1:A:110:PRO:HB3	1.85	0.59
1:A:64:VAL:HG21	1:A:128:LEU:HB3	1.85	0.58
1:D:52:LYS:HZ2	1:D:55:SER:HB2	1.68	0.58
1:B:98:PHE:HA	1:B:116:PRO:HA	1.85	0.58
1:C:155:CYS:HB3	1:C:165:CYS:HB3	1.85	0.58
1:D:52:LYS:NZ	1:D:55:SER:HB2	2.20	0.57
1:A:94:ILE:HG23	1:B:91:GLN:HG3	1.87	0.56
1:B:15:GLN:N	2:B:201:A1JS4:CL1	2.76	0.56
1:A:34:VAL:HG23	1:A:35[B]:HIS:CD2	2.35	0.56
1:A:155:CYS:HB3	1:A:165:CYS:HB3	1.88	0.55
1:D:144:PRO:HD3	1:D:166:GLN:HB2	1.90	0.54
1:B:12:LYS:HE3	1:B:39:TYR:CD2	2.43	0.53
1:C:159:ALA:HB3	1:C:162:ALA:HB2	1.90	0.53
1:B:155:CYS:HB3	1:B:165:CYS:HB3	1.91	0.53
1:A:12:LYS:NZ	1:A:39:TYR:CE2	2.78	0.52
1:C:12:LYS:HE3	1:C:28:ARG:HG3	1.90	0.52
1:D:11:LEU:HB3	1:D:114:PHE:HB2	1.91	0.52
1:B:144:PRO:HD2	1:B:165:CYS:SG	2.50	0.52
1:B:57:ASP:HB2	1:B:60:LYS:HD3	1.91	0.51
1:A:63:CYS:HB3	1:A:105:VAL:HB	1.92	0.51
1:B:37:LEU:HD23	1:B:56:ILE:HD12	1.93	0.50
1:C:15:GLN:HB2	2:C:201:A1JS4:CL1	2.50	0.49
1:B:123:ARG:HD2	1:B:123:ARG:HA	1.58	0.49
1:C:166:GLN:HG3	1:C:167:ILE:H	1.78	0.49
1:C:64:VAL:HG21	1:C:128:LEU:HB3	1.94	0.49
1:C:52:LYS:HZ2	1:C:55:SER:HB2	1.78	0.48
1:C:52:LYS:NZ	1:C:55:SER:HB2	2.28	0.48
1:B:67:VAL:HB	1:B:101:PRO:HB2	1.95	0.47
1:B:46:ARG:HB3	1:B:48:ARG:HE	1.79	0.47
1:C:91:GLN:HG3	1:D:94:ILE:HG23	1.96	0.47
1:D:141:LYS:HG2	1:D:167:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:THR:O	1:D:21:SER:C	2.57	0.47
1:D:52:LYS:NZ	1:D:55:SER:CB	2.78	0.47
1:B:24:ASN:ND2	1:B:26:LYS:NZ	2.62	0.47
1:D:52:LYS:HZ2	1:D:55:SER:CB	2.28	0.47
1:A:14:SER:O	2:A:201:A1JS4:CL1	2.70	0.46
1:D:46:ARG:NH1	1:D:48:ARG:NH1	2.63	0.46
1:A:39:TYR:CZ	1:A:54:GLY:HA3	2.51	0.46
1:D:25:PHE:CE1	1:D:77:ARG:NH1	2.84	0.45
1:B:126:HIS:CD2	1:B:127:GLN:NE2	2.79	0.44
1:A:12:LYS:HE2	1:A:39:TYR:CD2	2.52	0.44
1:B:46:ARG:HD2	1:B:48:ARG:HE	1.82	0.44
1:B:73:PRO:HG2	1:B:78:GLN:HG2	1.97	0.44
1:D:46:ARG:HH11	1:D:48:ARG:NH1	2.14	0.44
1:D:144:PRO:HD2	1:D:165:CYS:SG	2.57	0.44
1:A:98:PHE:HA	1:A:116:PRO:HA	1.99	0.43
1:C:29:LEU:HD12	1:C:49:ARG:HB3	2.00	0.43
1:C:105:VAL:HA	1:C:110:PRO:HA	2.00	0.43
1:C:46:ARG:HB2	1:C:48:ARG:HG2	2.00	0.43
1:C:58:VAL:HG13	1:C:132:ILE:HG22	2.01	0.43
1:D:30:PHE:HD2	1:D:37:LEU:HD11	1.84	0.43
1:C:157:GLN:OE1	1:C:162:ALA:HB1	2.19	0.43
1:D:159:ALA:HB3	1:D:162:ALA:HB2	2.01	0.43
1:D:5:ILE:HD12	1:D:32:LEU:HG	2.02	0.42
1:A:52:LYS:NZ	1:A:55:SER:HB2	2.34	0.42
1:B:12:LYS:HE3	1:B:39:TYR:CE2	2.54	0.42
1:C:168:LEU:HD12	1:C:168:LEU:HA	1.73	0.42
1:A:12:LYS:HE2	1:A:28:ARG:HG3	2.01	0.42
1:B:52:LYS:HE2	1:B:55:SER:HB2	2.00	0.42
1:C:26:LYS:HD3	1:C:26:LYS:HA	1.88	0.42
1:D:62:THR:HG22	1:D:137:ASP:HB2	2.03	0.41
1:A:80:PRO:HB3	1:A:97:ARG:HD2	2.02	0.41
1:D:155:CYS:HB3	1:D:165:CYS:HB3	2.02	0.41
1:A:14:SER:CB	1:A:26:LYS:HG3	2.48	0.41
1:D:57:ASP:HB2	1:D:60:LYS:HG3	2.02	0.41
1:D:63:CYS:HB3	1:D:105:VAL:HB	2.02	0.41
1:C:143:HIS:HA	1:C:165:CYS:SG	2.61	0.40
1:C:13:ARG:C	1:C:15:GLN:H	2.29	0.40
1:C:67:VAL:HG11	1:C:146:PHE:CD1	2.57	0.40
1:D:142:TYR:HB3	1:D:168:LEU:HD11	2.02	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	155/169 (92%)	144 (93%)	9 (6%)	2 (1%)	9	13
1	B	145/169 (86%)	138 (95%)	7 (5%)	0	100	100
1	C	150/169 (89%)	136 (91%)	14 (9%)	0	100	100
1	D	154/169 (91%)	147 (96%)	6 (4%)	1 (1%)	21	30
All	All	604/676 (89%)	565 (94%)	36 (6%)	3 (0%)	24	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	MET
1	A	91	GLN
1	D	15	GLN

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	148/158 (94%)	137 (93%)	11 (7%)	13	20
1	B	141/158 (89%)	120 (85%)	21 (15%)	3	3
1	C	146/158 (92%)	131 (90%)	15 (10%)	7	10
1	D	148/158 (94%)	132 (89%)	16 (11%)	6	9
All	All	583/632 (92%)	520 (89%)	63 (11%)	6	9

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	48	ARG
1	A	57	ASP
1	A	58	VAL
1	A	70	GLU
1	A	88	GLU
1	A	92	ILE
1	A	151	GLN
1	A	155	CYS
1	A	160	LYS
1	A	166	GLN
1	B	12	LYS
1	B	13	ARG
1	B	14	SER
1	B	15	GLN
1	B	26	LYS
1	B	35[A]	HIS
1	B	35[B]	HIS
1	B	59	GLU
1	B	71	LYS
1	B	90	GLU
1	B	107	ASP
1	B	108	GLU
1	B	118	GLU
1	B	119	GLU
1	B	120	LEU
1	B	140	GLN
1	B	141	LYS
1	B	151	GLN
1	B	160	LYS
1	B	167	ILE
1	B	168	LEU
1	C	12	LYS
1	C	15	GLN
1	C	23	LEU
1	C	29	LEU
1	C	45	GLU
1	C	94	ILE
1	C	107	ASP
1	C	108	GLU
1	C	119	GLU
1	C	141	LYS
1	C	151	GLN

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Mol	Chain	Res	Type
1	C	156	SER
1	C	160	LYS
1	C	165	CYS
1	C	168	LEU
1	D	17	LYS
1	D	18	LYS
1	D	19	LYS
1	D	29	LEU
1	D	36	LYS
1	D	45	GLU
1	D	59	GLU
1	D	60	LYS
1	D	90	GLU
1	D	94	ILE
1	D	107	ASP
1	D	137	ASP
1	D	151	GLN
1	D	154	CYS
1	D	161	ASN
1	D	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	127	GLN
1	A	151	GLN
1	A	166	GLN
1	B	24	ASN
1	B	126	HIS
1	B	127	GLN
1	B	151	GLN
1	B	166	GLN
1	C	35	HIS
1	C	72	ASN
1	C	126	HIS
1	C	127	GLN
1	D	15	GLN
1	D	126	HIS
1	D	151	GLN
1	D	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	$\# Z > 2$
2	A1JS4	A	201	1	22,22,22	0.95	2 (9%)	23,32,32	1.34	2 (8%)
2	A1JS4	D	201	1	22,22,22	1.03	2 (9%)	23,32,32	1.43	4 (17%)
2	A1JS4	B	201	1	22,22,22	1.04	2 (9%)	23,32,32	1.30	3 (13%)
2	A1JS4	C	201	1	22,22,22	1.02	2 (9%)	23,32,32	1.21	1 (4%)

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	A1JS4	A	201	1	-	4/8/17/17	0/3/3/3
2	A1JS4	D	201	1	-	4/8/17/17	0/3/3/3
2	A1JS4	B	201	1	-	4/8/17/17	0/3/3/3
2	A1JS4	C	201	1	-	4/8/17/17	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	A1JS4	O1-C1	-3.48	1.20	1.30
2	C	201	A1JS4	O1-C1	-3.44	1.20	1.30
2	A	201	A1JS4	O1-C1	-3.33	1.20	1.30
2	D	201	A1JS4	O1-C1	-3.23	1.21	1.30
2	C	201	A1JS4	C2-C1	-2.68	1.44	1.48
2	B	201	A1JS4	C2-C1	-2.61	1.44	1.48
2	A	201	A1JS4	C2-C1	-2.17	1.45	1.48
2	D	201	A1JS4	C2-C1	-2.14	1.45	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	A1JS4	O3-C4-C15	3.66	123.64	119.84
2	B	201	A1JS4	O3-C4-C15	3.42	123.38	119.84
2	D	201	A1JS4	C7-C6-C5	-3.20	103.95	111.56
2	D	201	A1JS4	O3-C4-C15	3.18	123.14	119.84
2	C	201	A1JS4	O3-C4-C15	2.89	122.83	119.84
2	B	201	A1JS4	O1-C1-C2	2.21	121.32	115.83
2	D	201	A1JS4	O1-C1-C2	2.19	121.28	115.83
2	A	201	A1JS4	O1-C1-C2	2.08	121.00	115.83
2	B	201	A1JS4	O2-C1-C2	-2.06	117.94	122.46
2	D	201	A1JS4	O2-C1-C2	-2.06	117.94	122.46

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	A1JS4	O1-C1-C2-C5
2	A	201	A1JS4	O2-C1-C2-C5
2	A	201	A1JS4	O1-C1-C2-C3
2	A	201	A1JS4	O2-C1-C2-C3
2	B	201	A1JS4	O1-C1-C2-C5
2	B	201	A1JS4	O2-C1-C2-C5
2	B	201	A1JS4	O1-C1-C2-C3
2	B	201	A1JS4	O2-C1-C2-C3
2	C	201	A1JS4	O1-C1-C2-C5
2	C	201	A1JS4	O2-C1-C2-C5
2	C	201	A1JS4	O1-C1-C2-C3
2	C	201	A1JS4	O2-C1-C2-C3
2	D	201	A1JS4	O1-C1-C2-C5
2	D	201	A1JS4	O2-C1-C2-C5

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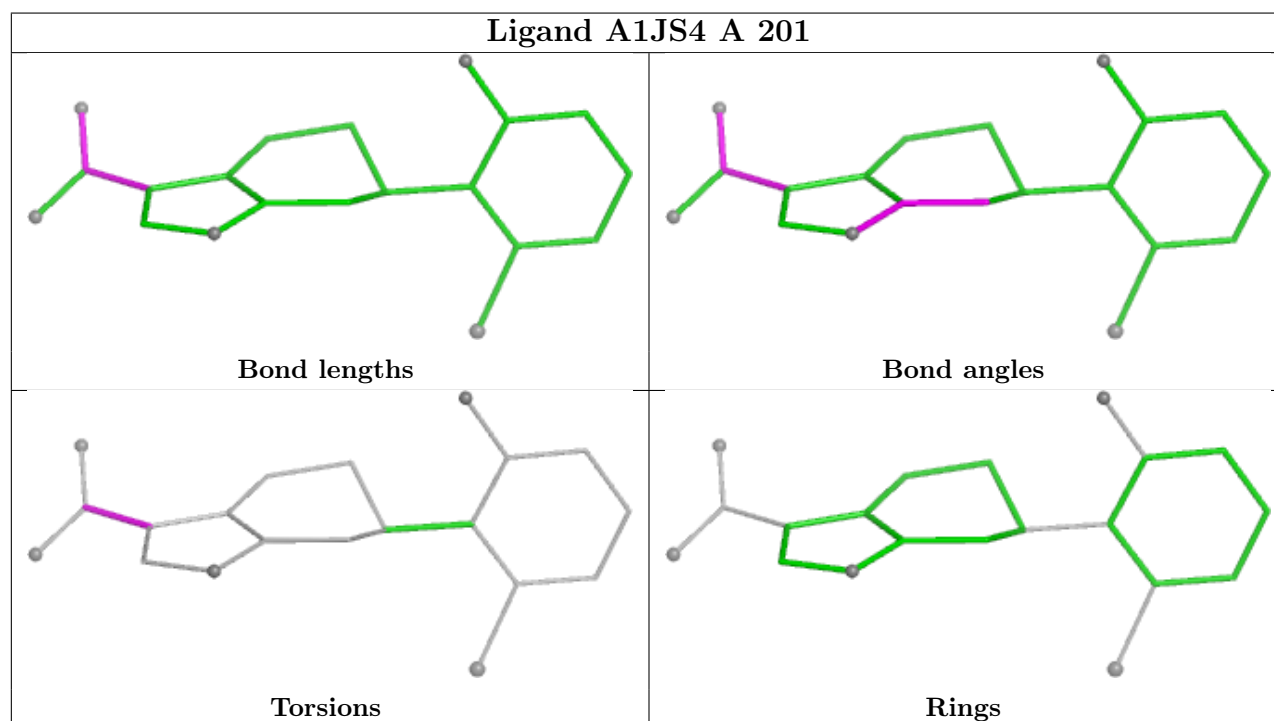
Mol	Chain	Res	Type	Atoms
2	D	201	A1JS4	O1-C1-C2-C3
2	D	201	A1JS4	O2-C1-C2-C3

There are no ring outliers.

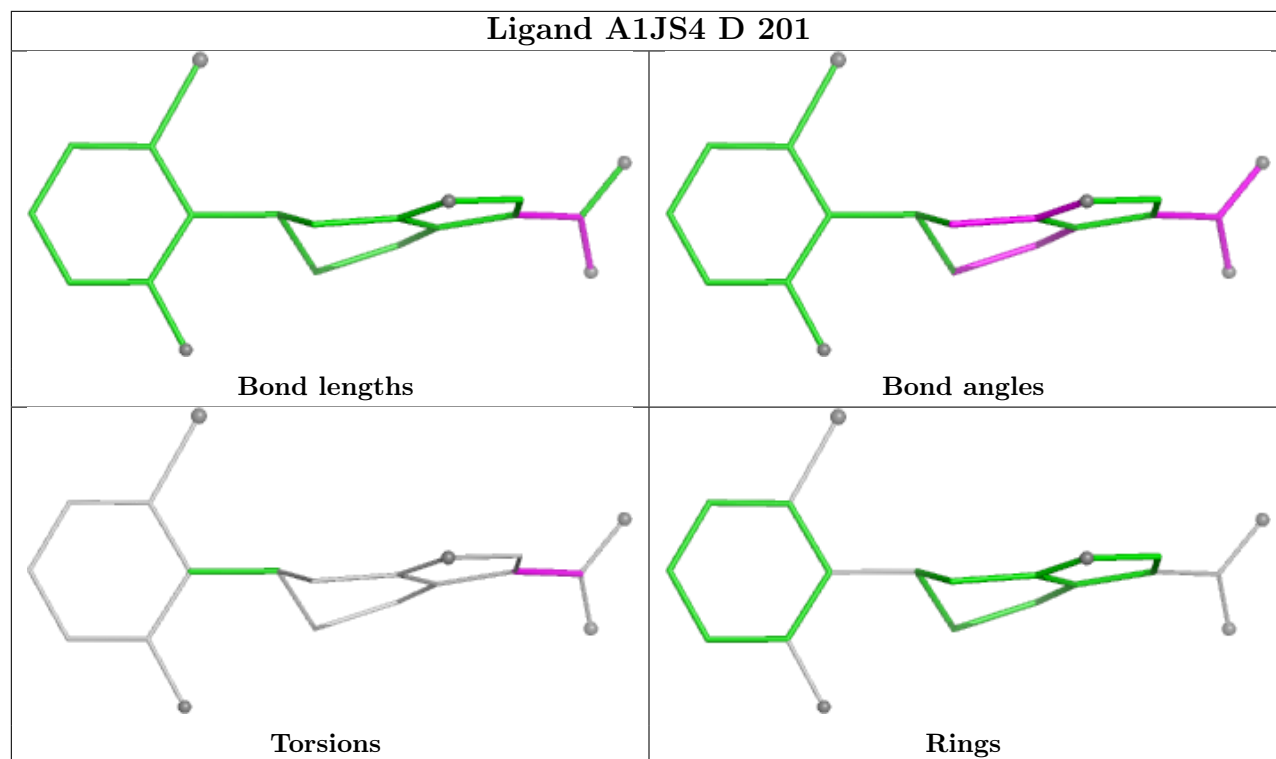
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	A1JS4	1	0
2	B	201	A1JS4	3	0
2	C	201	A1JS4	1	0

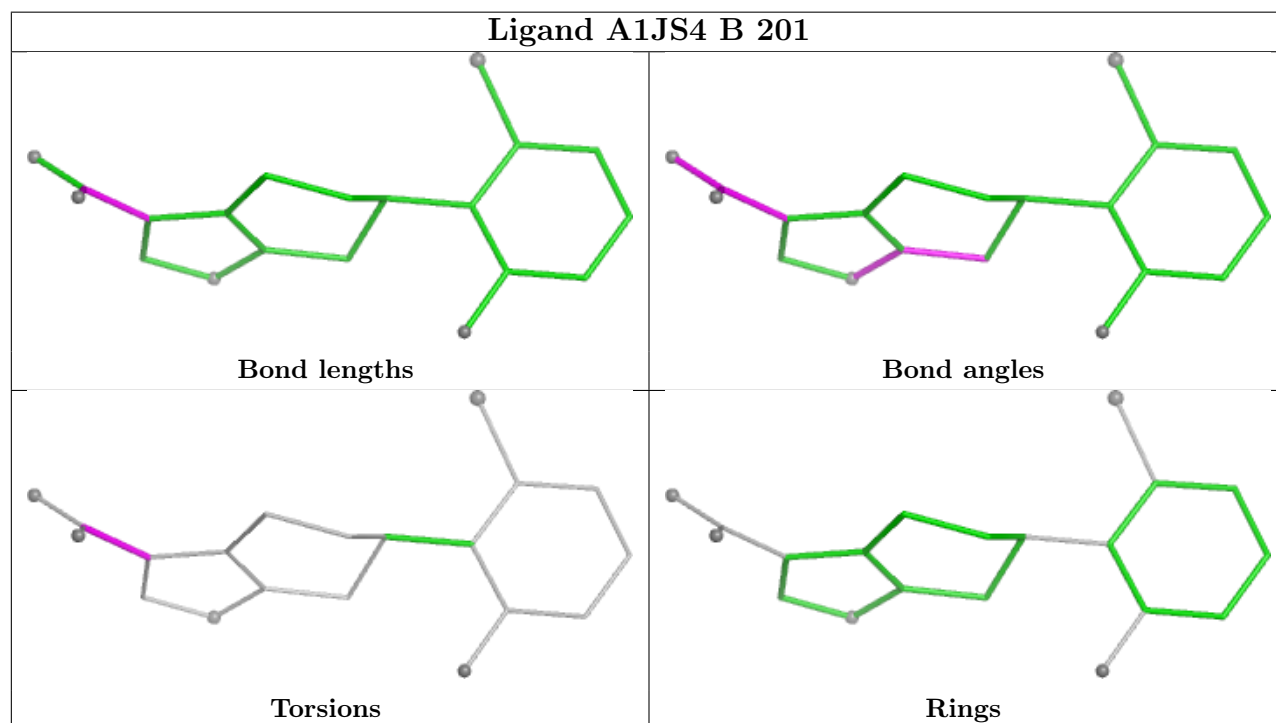
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

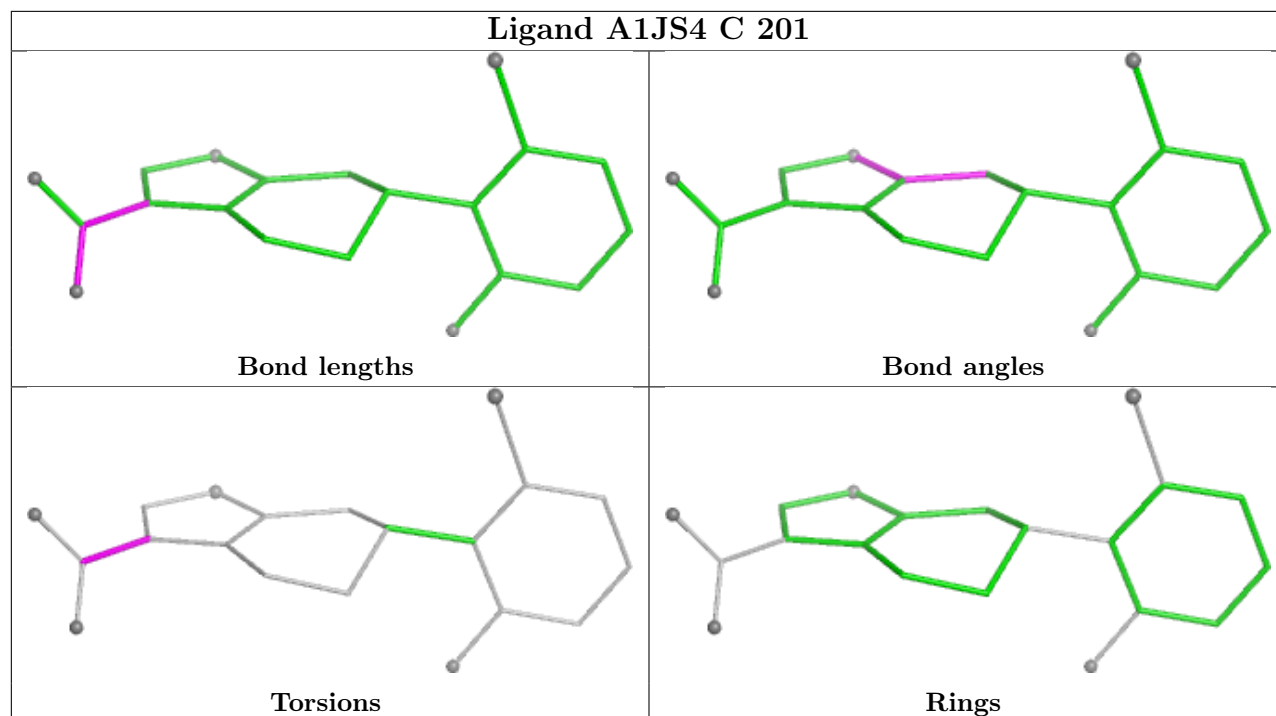


Ligand A1JS4 D 201



Ligand A1JS4 B 201





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	158/169 (93%)	0.64	13 (8%) 17 14	25, 52, 82, 92	1 (0%)
1	B	150/169 (88%)	0.55	3 (2%) 65 61	27, 51, 68, 92	1 (0%)
1	C	156/169 (92%)	0.84	8 (5%) 33 30	50, 67, 82, 98	0
1	D	158/169 (93%)	0.74	9 (5%) 29 25	48, 63, 88, 105	0
All	All	622/676 (92%)	0.69	33 (5%) 32 28	25, 59, 80, 105	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	SER	4.2
1	D	23	LEU	3.9
1	A	89	MET	3.6
1	A	13	ARG	3.3
1	D	22	PRO	3.2
1	C	104	VAL	3.1
1	C	23	LEU	3.1
1	B	23	LEU	3.0
1	A	83	GLY	2.9
1	A	91	GLN	2.9
1	A	81	ARG	2.9
1	A	109	GLY	2.9
1	D	147	TRP	2.8
1	D	21	SER	2.7
1	A	25	PHE	2.7
1	C	168	LEU	2.7
1	D	35	HIS	2.6
1	D	79	ILE	2.5
1	A	152	TYR	2.4
1	C	167	ILE	2.4
1	D	153	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	15	GLN	2.4
1	D	167	ILE	2.3
1	A	168	LEU	2.3
1	C	22	PRO	2.3
1	D	152	TYR	2.3
1	C	148	ILE	2.2
1	C	29	LEU	2.2
1	B	35[A]	HIS	2.2
1	A	148	ILE	2.2
1	A	80	PRO	2.2
1	B	168	LEU	2.1
1	A	166	GLN	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](#)

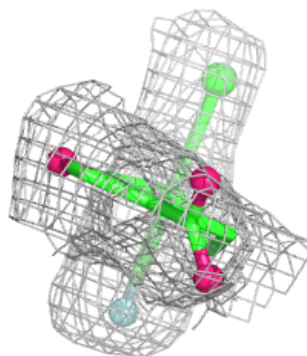
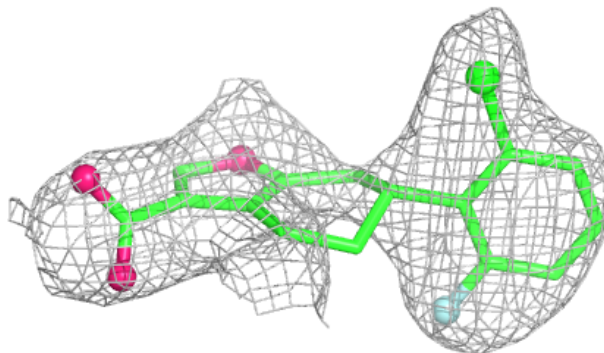
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1JS4	C	201	20/20	0.78	0.15	85,86,86,87	0
4	MG	A	203	1/1	0.82	0.07	22,22,22,22	0
3	ZN	A	202	1/1	0.83	0.25	23,23,23,23	0
2	A1JS4	A	201	20/20	0.83	0.13	72,73,74,75	0
2	A1JS4	B	201	20/20	0.84	0.11	62,64,66,68	0
2	A1JS4	D	201	20/20	0.88	0.10	77,78,80,80	0
4	MG	D	203	1/1	0.91	0.23	44,44,44,44	0
3	ZN	B	202	1/1	0.92	0.18	21,21,21,21	0
4	MG	C	203	1/1	0.92	0.15	41,41,41,41	0
3	ZN	C	202	1/1	0.92	0.14	35,35,35,35	0
3	ZN	D	202	1/1	0.97	0.09	41,41,41,41	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.

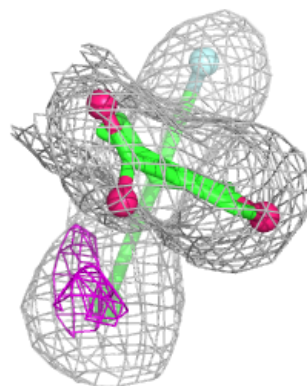
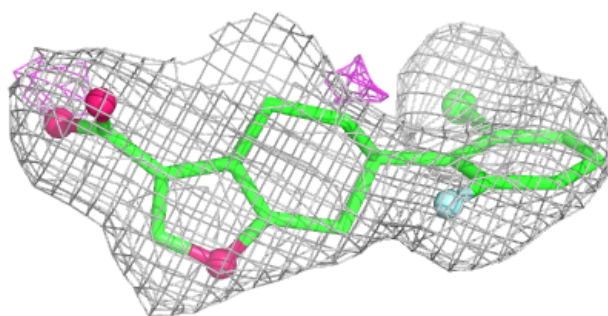
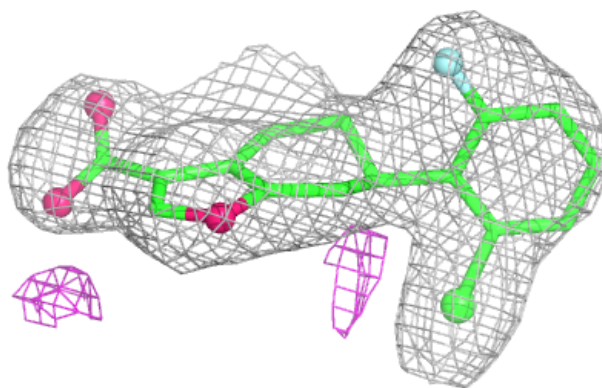
Electron density around A1JS4 C 201:

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

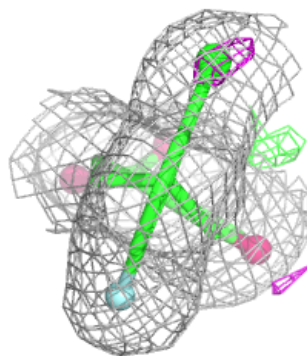
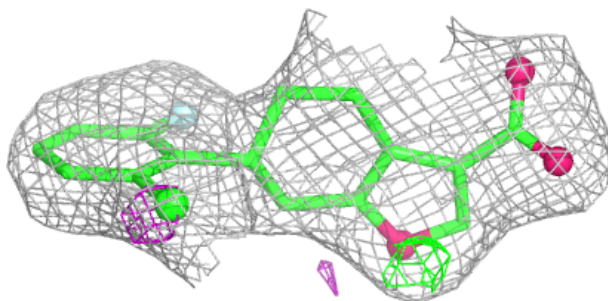
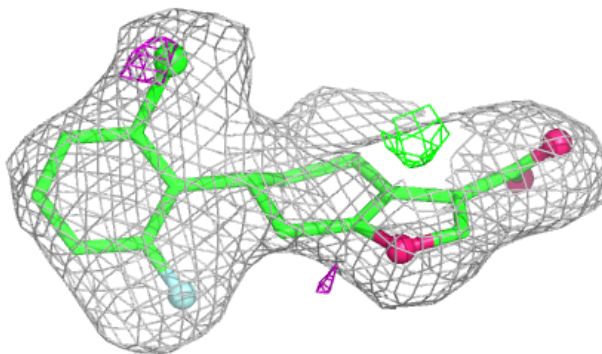


Electron density around A1JS4 A 201:

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

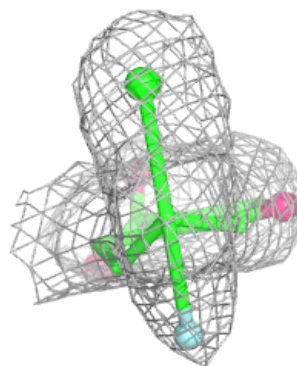
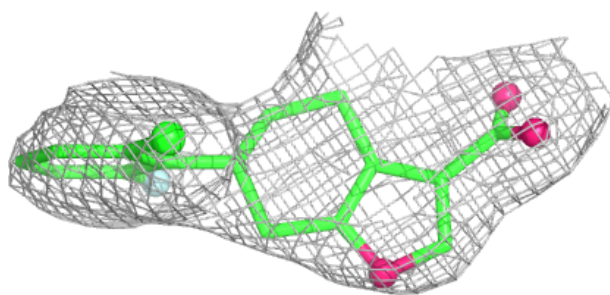
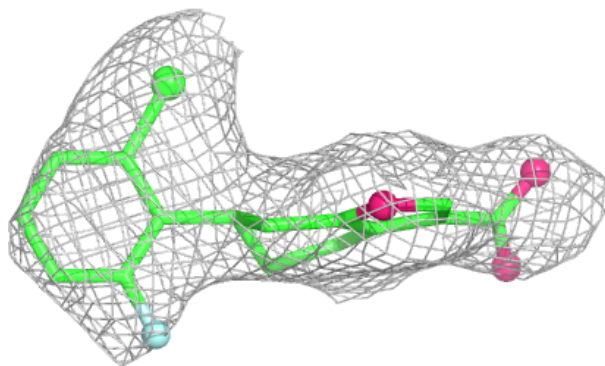
**Electron density around A1JS4 B 201:**

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



Electron density around A1JS4 D 201:

$2mF_o-DF_c$ (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.