Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:31 PM BST

PDB ID	:	6B2Q
Title	:	Dual Inhibition of the Essential Protein Kinases A and B in Mycobacterium tuberculosis
Authors	:	Zuccola, H.J.
Deposited on	:	2017-09-20
Resolution	:	2.88 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

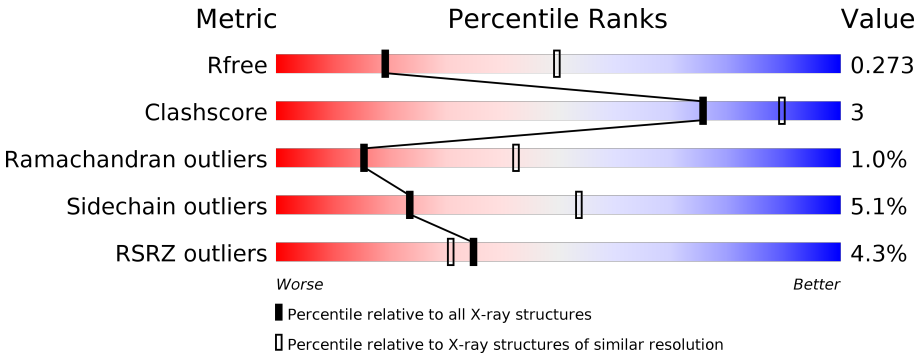
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	317	70% 12% 17%
1	B	317	2% 75% 9% 16%
1	C	317	5% 73% 10% 16%
1	D	317	7% 71% 11% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8162 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 Serine/threonine-protein kinase PknA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	P	S	0	0	0
			1990	1250	370	363	1	6			
1	B	267	Total	C	N	O	P	S	0	0	0
			2024	1272	375	368	1	8			
1	C	265	Total	C	N	O	P	S	0	1	0
			2023	1269	380	367	1	6			
1	D	260	Total	C	N	O	P	S	0	1	0
			1993	1253	373	359	1	7			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP A5TY85
A	-19	GLY	-	expression tag	UNP A5TY85
A	-18	SER	-	expression tag	UNP A5TY85
A	-17	SER	-	expression tag	UNP A5TY85
A	-16	HIS	-	expression tag	UNP A5TY85
A	-15	HIS	-	expression tag	UNP A5TY85
A	-14	HIS	-	expression tag	UNP A5TY85
A	-13	HIS	-	expression tag	UNP A5TY85
A	-12	HIS	-	expression tag	UNP A5TY85
A	-11	HIS	-	expression tag	UNP A5TY85
A	-10	SER	-	expression tag	UNP A5TY85
A	-9	SER	-	expression tag	UNP A5TY85
A	-8	GLY	-	expression tag	UNP A5TY85
A	-7	LEU	-	expression tag	UNP A5TY85
A	-6	VAL	-	expression tag	UNP A5TY85
A	-5	PRO	-	expression tag	UNP A5TY85
A	-4	ARG	-	expression tag	UNP A5TY85
A	-3	GLY	-	expression tag	UNP A5TY85
A	-2	SER	-	expression tag	UNP A5TY85
A	-1	LEU	-	expression tag	UNP A5TY85
A	0	HIS	-	expression tag	UNP A5TY85

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP A5TY85
B	-19	GLY	-	expression tag	UNP A5TY85
B	-18	SER	-	expression tag	UNP A5TY85
B	-17	SER	-	expression tag	UNP A5TY85
B	-16	HIS	-	expression tag	UNP A5TY85
B	-15	HIS	-	expression tag	UNP A5TY85
B	-14	HIS	-	expression tag	UNP A5TY85
B	-13	HIS	-	expression tag	UNP A5TY85
B	-12	HIS	-	expression tag	UNP A5TY85
B	-11	HIS	-	expression tag	UNP A5TY85
B	-10	SER	-	expression tag	UNP A5TY85
B	-9	SER	-	expression tag	UNP A5TY85
B	-8	GLY	-	expression tag	UNP A5TY85
B	-7	LEU	-	expression tag	UNP A5TY85
B	-6	VAL	-	expression tag	UNP A5TY85
B	-5	PRO	-	expression tag	UNP A5TY85
B	-4	ARG	-	expression tag	UNP A5TY85
B	-3	GLY	-	expression tag	UNP A5TY85
B	-2	SER	-	expression tag	UNP A5TY85
B	-1	LEU	-	expression tag	UNP A5TY85
B	0	HIS	-	expression tag	UNP A5TY85
C	-20	MET	-	expression tag	UNP A5TY85
C	-19	GLY	-	expression tag	UNP A5TY85
C	-18	SER	-	expression tag	UNP A5TY85
C	-17	SER	-	expression tag	UNP A5TY85
C	-16	HIS	-	expression tag	UNP A5TY85
C	-15	HIS	-	expression tag	UNP A5TY85
C	-14	HIS	-	expression tag	UNP A5TY85
C	-13	HIS	-	expression tag	UNP A5TY85
C	-12	HIS	-	expression tag	UNP A5TY85
C	-11	HIS	-	expression tag	UNP A5TY85
C	-10	SER	-	expression tag	UNP A5TY85
C	-9	SER	-	expression tag	UNP A5TY85
C	-8	GLY	-	expression tag	UNP A5TY85
C	-7	LEU	-	expression tag	UNP A5TY85
C	-6	VAL	-	expression tag	UNP A5TY85
C	-5	PRO	-	expression tag	UNP A5TY85
C	-4	ARG	-	expression tag	UNP A5TY85
C	-3	GLY	-	expression tag	UNP A5TY85
C	-2	SER	-	expression tag	UNP A5TY85
C	-1	LEU	-	expression tag	UNP A5TY85
C	0	HIS	-	expression tag	UNP A5TY85

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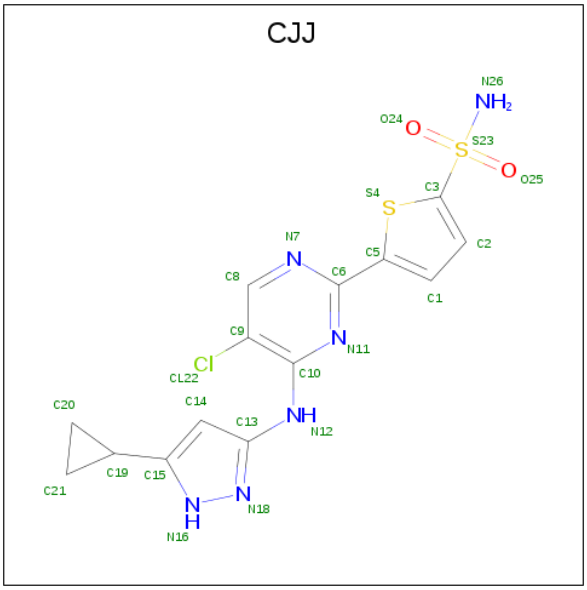
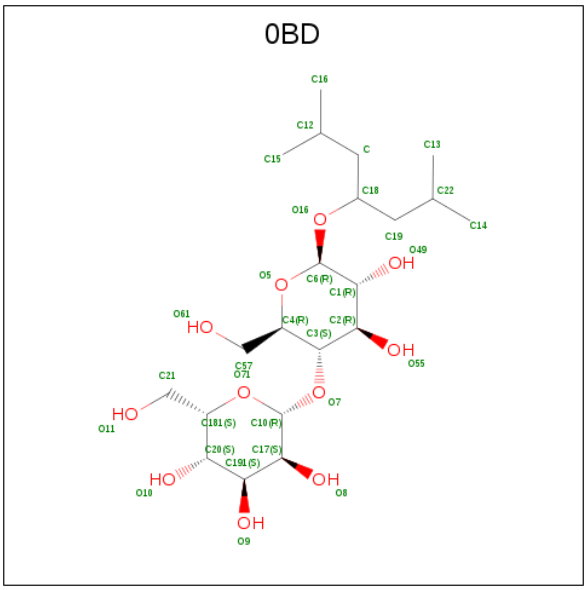
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP A5TY85
D	-19	GLY	-	expression tag	UNP A5TY85
D	-18	SER	-	expression tag	UNP A5TY85
D	-17	SER	-	expression tag	UNP A5TY85
D	-16	HIS	-	expression tag	UNP A5TY85
D	-15	HIS	-	expression tag	UNP A5TY85
D	-14	HIS	-	expression tag	UNP A5TY85
D	-13	HIS	-	expression tag	UNP A5TY85
D	-12	HIS	-	expression tag	UNP A5TY85
D	-11	HIS	-	expression tag	UNP A5TY85
D	-10	SER	-	expression tag	UNP A5TY85
D	-9	SER	-	expression tag	UNP A5TY85
D	-8	GLY	-	expression tag	UNP A5TY85
D	-7	LEU	-	expression tag	UNP A5TY85
D	-6	VAL	-	expression tag	UNP A5TY85
D	-5	PRO	-	expression tag	UNP A5TY85
D	-4	ARG	-	expression tag	UNP A5TY85
D	-3	GLY	-	expression tag	UNP A5TY85
D	-2	SER	-	expression tag	UNP A5TY85
D	-1	LEU	-	expression tag	UNP A5TY85
D	0	HIS	-	expression tag	UNP A5TY85

- Molecule 2 is 5-{5-chloro-4-[(5-cyclopropyl-1H-pyrazol-3-yl)amino]pyrimidin-2-yl}thiophene -2-sulfonamide (three-letter code: CJJ) (formula: $C_{14}H_{13}ClN_6O_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			25	14	1	6	2	2		
2	B	1	Total	C	Cl	N	O	S	0	0
			25	14	1	6	2	2		
2	C	1	Total	C	Cl	N	O	S	0	0
			25	14	1	6	2	2		
2	D	1	Total	C	Cl	N	O	S	0	0
			25	14	1	6	2	2		

- Molecule 3 is 3-methyl-1-(2-methylpropyl)butyl 4-O-beta-L-gulopyranosyl-beta-D-glucopyranoside (three-letter code: 0BD) (formula: $C_{21}H_{40}O_{11}$).



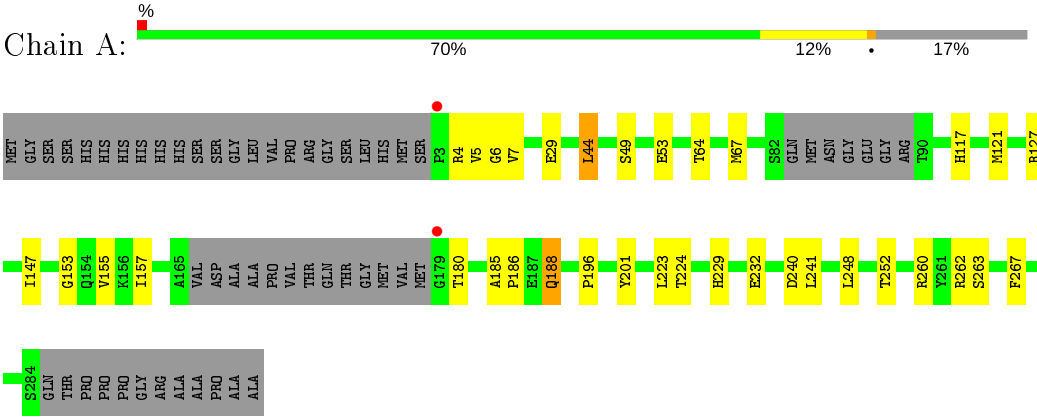
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			32	21	11		

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.

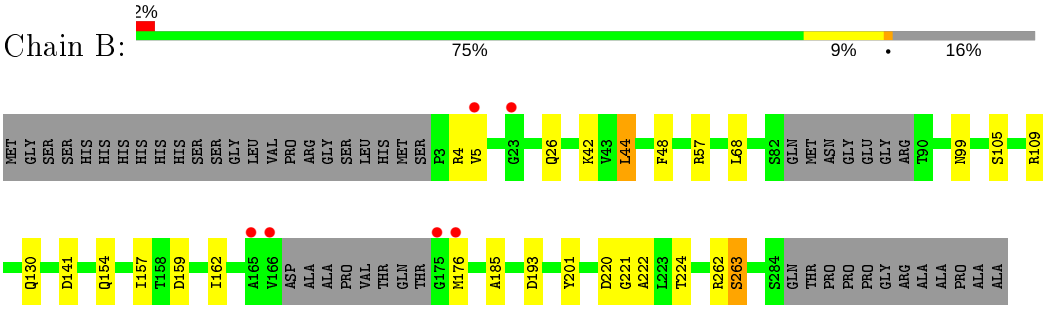
- Molecule 1: Serine/threonine-protein kinase PknA

Chain A:



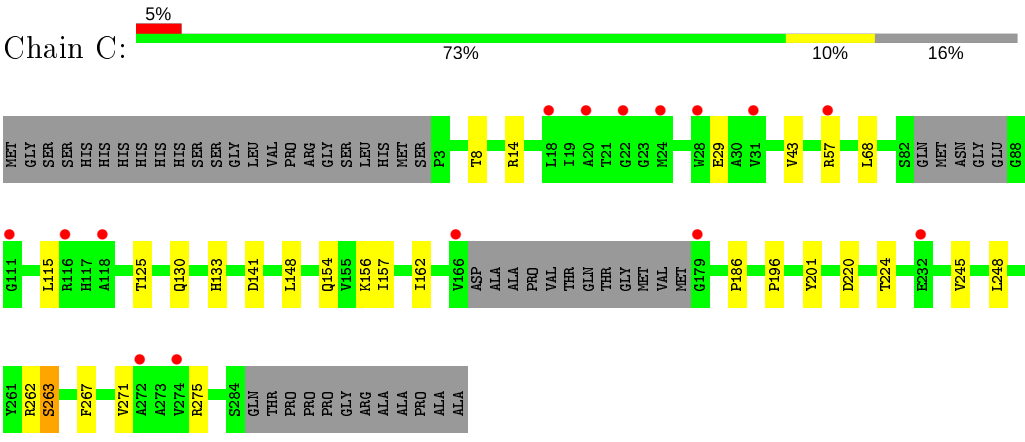
- Molecule 1: Serine/threonine-protein kinase PknA

Chain B:



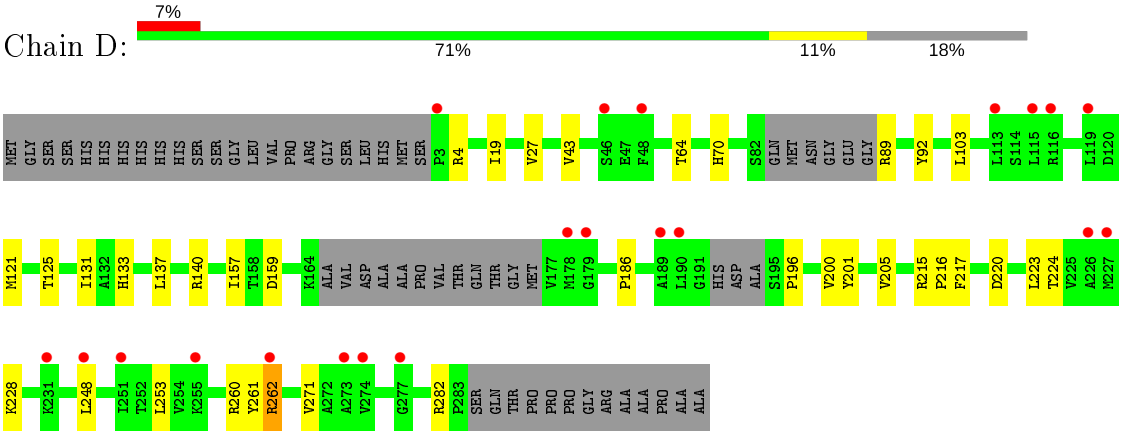
- Molecule 1: Serine/threonine-protein kinase PknA

Chain C:



• Molecule 1: Serine/threonine-protein kinase PknA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	79.06Å 227.43Å 158.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.72 – 2.88 113.72 – 2.55	Depositor EDS
% Data completeness (in resolution range)	94.7 (113.72-2.88) 81.9 (113.72-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.55Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.230 , 0.263 0.231 , 0.273	Depositor DCC
R_{free} test set	2004 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	63.0	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8162	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CJJ, TPO, 0BD

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	0.44	0/2019	0.66	0/2736
1	B	0.43	0/2053	0.64	0/2781
1	C	0.42	0/2052	0.60	0/2779
1	D	0.43	0/2020	0.62	0/2733
All	All	0.43	0/8144	0.63	0/11029

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1990	0	2025	15	0
1	B	2024	0	2064	8	0
1	C	2023	0	2062	15	0
1	D	1993	0	2041	13	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	0	0
2	D	25	0	0	0	0
3	A	32	0	40	3	0
All	All	8162	0	8232	51	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 (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:THR:HG23	1:B:157:ILE:HD11	1.62	0.80
1:D:125:THR:HG23	1:D:157:ILE:HD11	1.70	0.72
1:C:125:THR:HG23	1:C:157:ILE:HD11	1.76	0.67
1:C:98:VAL:HG11	1:C:156:LYS:HG3	1.86	0.57
1:A:201:TYR:HD2	1:A:260:ARG:NH1	2.03	0.55
1:A:153:GLY:CA	3:A:302:0BD:H13B	2.38	0.53
1:A:130:GLN:OE1	1:A:263:SER:HB3	2.08	0.52
1:C:248:LEU:HD21	1:C:271:VAL:HG22	1.91	0.52
1:A:153:GLY:HA2	3:A:302:0BD:H13B	1.91	0.52
1:B:105:SER:O	1:B:109:ARG:HG3	2.10	0.51
1:D:103:LEU:HD22	1:D:121:MET:HE1	1.93	0.51
1:B:26:GLN:O	1:B:42:LYS:HA	2.11	0.50
1:C:133:HIS:CG	1:C:196:PRO:HB3	2.47	0.50
1:D:200:VAL:HG11	1:D:261:TYR:HB2	1.95	0.49
1:A:270:ALA:HA	1:A:281:PRO:HD2	1.95	0.48
1:B:57:ARG:HE	1:B:162:ILE:HG22	1.78	0.48
1:D:43:VAL:HG12	1:D:92:TYR:HB3	1.94	0.48
1:B:130:GLN:OE1	1:B:263:SER:HB3	2.13	0.48
1:D:205:VAL:HG22	1:D:253:LEU:HD21	1.96	0.48
1:A:252:THR:HG21	1:A:267:PHE:CE1	2.49	0.47
1:C:8:THR:HA	1:C:14[B]:ARG:HA	1.97	0.47
1:D:64:THR:HG23	1:D:137:LEU:HD22	1.95	0.47
1:D:248:LEU:HD21	1:D:271:VAL:HG22	1.96	0.47
1:A:147:ILE:HG23	1:A:155:VAL:HG13	1.97	0.47
1:B:141:ASP:HB2	1:B:162:ILE:HD11	1.97	0.47
1:A:201:TYR:CD2	1:A:260:ARG:NH1	2.83	0.46
1:D:186:PRO:HD3	1:D:201:TYR:CZ	2.51	0.46
1:D:70:HIS:HB2	1:D:131:ILE:HG13	1.98	0.45
1:A:133:HIS:CG	1:A:196:PRO:HB3	2.52	0.45
1:C:201:TYR:HB2	1:C:260:ARG:HE	1.82	0.45
1:C:130:GLN:OE1	1:C:263:SER:HB3	2.16	0.44
1:A:248:LEU:HD21	1:A:271:VAL:HG22	1.99	0.44
1:C:141:ASP:HB2	1:C:162:ILE:HD11	1.98	0.44
1:A:44:LEU:HD13	1:A:49:SER:HA	2.00	0.44
1:B:44:LEU:HD22	1:B:48:PHE:HB2	2.00	0.43
1:A:117:HIS:CE1	3:A:302:0BD:H15A	2.54	0.43
1:C:57:ARG:HH21	1:C:162:ILE:HG22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:PHE:CD1	1:D:228:LYS:HB3	2.53	0.43
1:C:201:TYR:HB2	1:C:260:ARG:NE	2.33	0.43
1:C:148:LEU:HB2	1:C:156:LYS:HB2	1.99	0.43
1:C:252:THR:HG21	1:C:267:PHE:CE1	2.54	0.43
1:C:8:THR:HA	1:C:14[A]:ARG:HA	2.01	0.42
1:A:186:PRO:HG3	1:A:229:HIS:O	2.20	0.42
1:D:196:PRO:HB2	1:D:262:ARG:O	2.20	0.42
1:A:64:THR:O	1:A:67:MET:HB3	2.20	0.42
1:C:186:PRO:HG2	1:C:255:LYS:HA	2.01	0.42
1:B:185:ALA:HA	1:B:201:TYR:CD1	2.55	0.42
1:C:115:LEU:HD22	1:C:245:VAL:HG21	2.02	0.41
1:D:19:ILE:HD12	1:D:27:VAL:HG12	2.03	0.41
1:A:185:ALA:HB3	1:A:188:GLN:HB2	2.03	0.40
1:D:133:HIS:CD2	1:D:196:PRO:HB3	2.57	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	255/317 (80%)	243 (95%)	9 (4%)	3 (1%)	13	38
1	B	260/317 (82%)	247 (95%)	9 (4%)	4 (2%)	10	32
1	C	259/317 (82%)	246 (95%)	12 (5%)	1 (0%)	34	64
1	D	252/317 (80%)	241 (96%)	9 (4%)	2 (1%)	19	48
All	All	1026/1268 (81%)	977 (95%)	39 (4%)	10 (1%)	15	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	VAL

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Mol	Chain	Res	Type
1	B	222	ALA
1	B	263	SER
1	C	263	SER
1	A	6	GLY
1	A	7	VAL
1	B	159	ASP
1	D	159	ASP
1	D	216	PRO
1	B	221	GLY

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	206/248 (83%)	192 (93%)	14 (7%)	16	40
1	B	210/248 (85%)	199 (95%)	11 (5%)	23	53
1	C	209/248 (84%)	201 (96%)	8 (4%)	33	65
1	D	207/248 (84%)	198 (96%)	9 (4%)	29	60
All	All	832/992 (84%)	790 (95%)	42 (5%)	24	54

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	29	GLU
1	A	44	LEU
1	A	53	GLU
1	A	121	MET
1	A	127	ARG
1	A	157	ILE
1	A	180	THR
1	A	188	GLN
1	A	223	LEU
1	A	232	GLU
1	A	240	ASP

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	262	ARG
1	B	4	ARG
1	B	5	VAL
1	B	44	LEU
1	B	68	LEU
1	B	99	ASN
1	B	121	MET
1	B	154	GLN
1	B	176	MET
1	B	193	ASP
1	B	220	ASP
1	B	262	ARG
1	C	29	GLU
1	C	43	VAL
1	C	68	LEU
1	C	104	ASN
1	C	154	GLN
1	C	220	ASP
1	C	262	ARG
1	C	275	ARG
1	D	4	ARG
1	D	89	ARG
1	D	140	ARG
1	D	215	ARG
1	D	220	ASP
1	D	223	LEU
1	D	260	ARG
1	D	262	ARG
1	D	282	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	B	146	ASN
1	C	146	ASN
1	D	146	ASN
1	D	188	GLN
1	D	244	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	A	224	1	8,10,11	1.72	1 (12%)	10,14,16	1.16	2 (20%)
1	TPO	B	224	1	8,10,11	1.11	1 (12%)	10,14,16	1.06	1 (10%)
1	TPO	C	224	1	8,10,11	1.41	1 (12%)	10,14,16	1.51	2 (20%)
1	TPO	D	224	1	8,10,11	1.33	1 (12%)	10,14,16	1.18	2 (20%)

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	A	224	1	-	1/9/11/13	-
1	TPO	B	224	1	-	1/9/11/13	-
1	TPO	C	224	1	-	1/9/11/13	-
1	TPO	D	224	1	-	2/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	TPO	P-OG1	-4.24	1.51	1.59
1	C	224	TPO	P-OG1	-3.55	1.52	1.59
1	D	224	TPO	P-OG1	-2.81	1.54	1.59
1	B	224	TPO	P-OG1	-2.17	1.55	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	224	TPO	P-OG1-CB	-3.65	112.19	123.21
1	D	224	TPO	P-OG1-CB	-2.41	115.93	123.21
1	B	224	TPO	P-OG1-CB	-2.26	116.39	123.21
1	A	224	TPO	P-OG1-CB	-2.11	116.82	123.21
1	A	224	TPO	O-C-CA	-2.10	119.26	124.78
1	D	224	TPO	O-C-CA	-2.06	119.38	124.78
1	C	224	TPO	O-C-CA	-2.01	119.52	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	224	TPO	O-C-CA-CB
1	D	224	TPO	CB-OG1-P-O3P
1	A	224	TPO	O-C-CA-CB
1	B	224	TPO	O-C-CA-CB
1	D	224	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)

5 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	CJJ	D	300	-	24,28,28	1.22	2 (8%)	25,42,42	2.13	11 (44%)
2	CJJ	C	300	-	24,28,28	1.14	3 (12%)	25,42,42	2.25	11 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CJJ	B	300	-	24,28,28	1.19	2 (8%)	25,42,42	2.17	11 (44%)
3	0BD	A	302	-	33,33,33	0.32	0	45,47,47	1.09	2 (4%)
2	CJJ	A	301	-	24,28,28	1.20	3 (12%)	25,42,42	2.31	10 (40%)

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	CJJ	D	300	-	-	2/6/20/20	0/4/4/4
2	CJJ	C	300	-	-	4/6/20/20	0/4/4/4
2	CJJ	B	300	-	-	2/6/20/20	0/4/4/4
3	0BD	A	302	-	-	4/20/60/60	0/2/2/2
2	CJJ	A	301	-	-	2/6/20/20	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CJJ	S23-N26	3.30	1.66	1.60
2	D	300	CJJ	S23-N26	3.13	1.66	1.60
2	B	300	CJJ	S23-N26	3.03	1.66	1.60
2	C	300	CJJ	S23-N26	2.95	1.66	1.60
2	A	301	CJJ	C14-C15	-2.20	1.35	1.39
2	B	300	CJJ	C3-S4	2.16	1.76	1.72
2	C	300	CJJ	C3-S4	2.15	1.76	1.72
2	C	300	CJJ	C14-C15	-2.14	1.35	1.39
2	D	300	CJJ	C3-S4	2.14	1.76	1.72
2	A	301	CJJ	C3-S4	2.11	1.76	1.72

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	CJJ	C21-C19-C15	-4.56	114.97	120.33
3	A	302	0BD	O16-C18-C19	4.56	116.50	108.18
2	C	300	CJJ	C21-C19-C15	-4.37	115.19	120.33
2	A	301	CJJ	N7-C6-N11	-4.27	121.07	125.25
2	C	300	CJJ	N7-C6-N11	-4.20	121.14	125.25
2	D	300	CJJ	N7-C6-N11	-3.97	121.36	125.25
2	A	301	CJJ	C9-C8-N7	-3.94	119.46	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	CJJ	C19-C15-N16	3.70	125.69	120.23
2	D	300	CJJ	C10-N11-C6	3.67	122.70	116.10
2	B	300	CJJ	C9-C8-N7	-3.59	119.75	122.84
2	B	300	CJJ	N7-C6-N11	-3.51	121.81	125.25
2	A	301	CJJ	C10-N11-C6	3.49	122.38	116.10
2	B	300	CJJ	C10-N11-C6	3.46	122.32	116.10
2	C	300	CJJ	C10-N11-C6	3.38	122.18	116.10
2	B	300	CJJ	C19-C15-N16	3.34	125.16	120.23
2	C	300	CJJ	C9-C8-N7	-3.26	120.04	122.84
2	A	301	CJJ	C8-N7-C6	3.17	120.41	116.22
2	D	300	CJJ	C9-C8-N7	-3.16	120.12	122.84
2	C	300	CJJ	C8-N7-C6	3.12	120.34	116.22
2	B	300	CJJ	C13-C14-C15	3.12	108.83	106.07
2	D	300	CJJ	C13-C14-C15	3.10	108.81	106.07
2	D	300	CJJ	C20-C19-C15	-3.06	116.73	120.33
2	A	301	CJJ	C19-C15-N16	2.99	124.64	120.23
2	B	300	CJJ	C14-C13-N18	-2.92	106.29	110.47
2	D	300	CJJ	C19-C15-N16	2.91	124.53	120.23
2	D	300	CJJ	C8-N7-C6	2.82	119.94	116.22
2	D	300	CJJ	C14-C13-N18	-2.79	106.47	110.47
2	B	300	CJJ	O25-S23-O24	2.79	123.34	118.76
2	D	300	CJJ	O25-S23-O24	2.64	123.09	118.76
2	A	301	CJJ	O25-S23-O24	2.62	123.07	118.76
2	C	300	CJJ	O25-S23-O24	2.61	123.05	118.76
2	C	300	CJJ	C13-N12-C10	-2.58	120.51	128.61
2	B	300	CJJ	C21-C19-C15	-2.53	117.36	120.33
2	B	300	CJJ	C8-N7-C6	2.53	119.56	116.22
2	A	301	CJJ	C8-C9-CL22	2.49	121.98	118.60
2	C	300	CJJ	C13-C14-C15	2.47	108.26	106.07
2	A	301	CJJ	C13-C14-C15	2.47	108.26	106.07
2	D	300	CJJ	C8-C9-C10	-2.46	118.17	120.00
2	A	301	CJJ	C14-C13-N18	-2.44	106.97	110.47
2	C	300	CJJ	C8-C9-C10	-2.32	118.27	120.00
2	D	300	CJJ	C14-C15-N16	-2.27	107.25	110.28
3	A	302	0BD	C-C18-C19	-2.13	108.27	112.50
2	C	300	CJJ	C14-C13-N18	-2.08	107.49	110.47
2	B	300	CJJ	C14-C15-N16	-2.05	107.54	110.28
2	B	300	CJJ	C5-C6-N11	-2.03	114.72	117.48

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	0BD	C20-C181-C21-O11
3	A	302	0BD	O71-C181-C21-O11
2	D	300	CJJ	C14-C15-C19-C20
2	D	300	CJJ	N16-C15-C19-C20
2	C	300	CJJ	N16-C15-C19-C21
2	B	300	CJJ	N16-C15-C19-C21
2	C	300	CJJ	N11-C10-N12-C13
3	A	302	0BD	C12-C-C18-O16
2	C	300	CJJ	C9-C10-N12-C13
2	C	300	CJJ	C14-C15-C19-C21
2	B	300	CJJ	C14-C15-C19-C21
2	A	301	CJJ	C14-C15-C19-C21
2	A	301	CJJ	N16-C15-C19-C21
3	A	302	0BD	C12-C-C18-C19

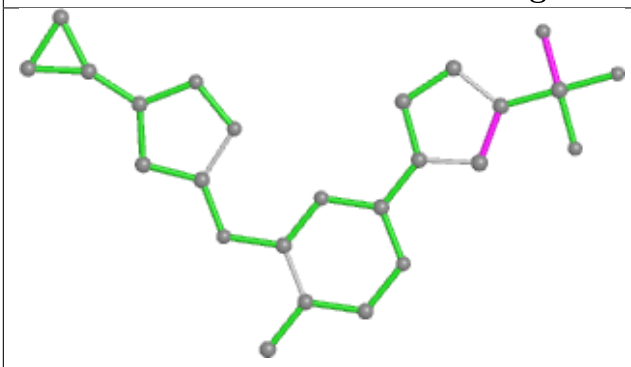
There are no ring outliers.

1 monomer is involved in 3 short contacts:

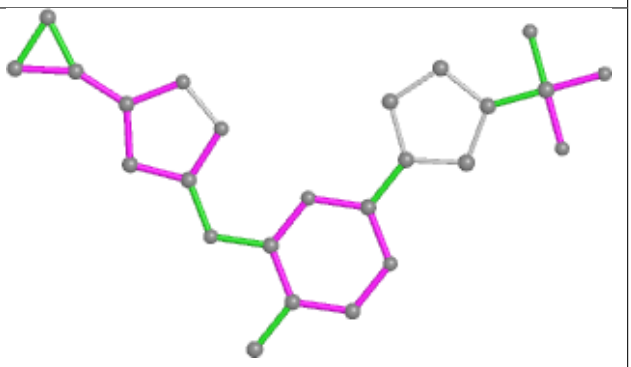
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	0BD	3	0

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

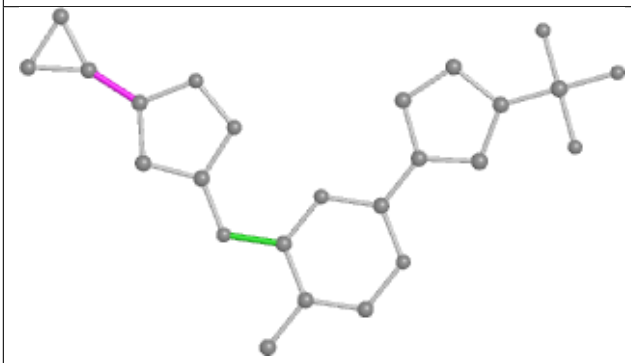
Ligand CJJ D 300



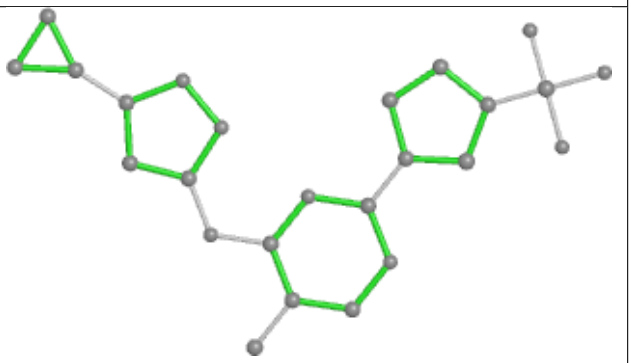
Bond lengths



Bond angles

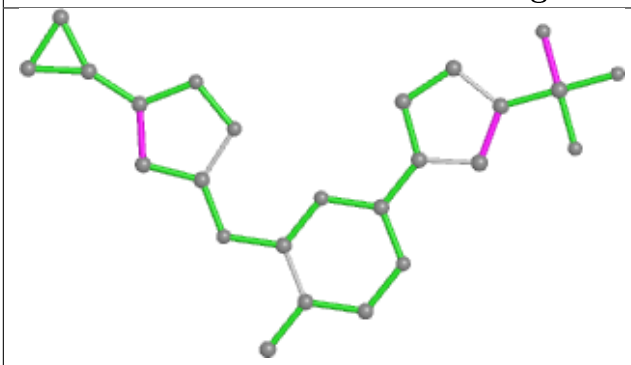


Torsions

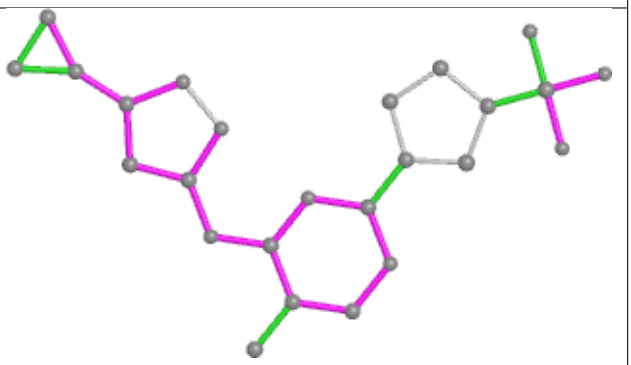


Rings

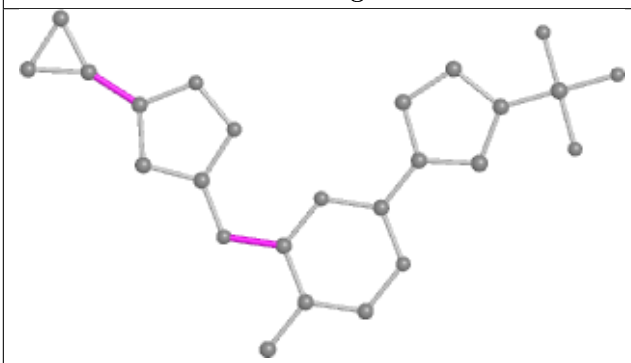
Ligand CJJ C 300



Bond lengths



Bond angles



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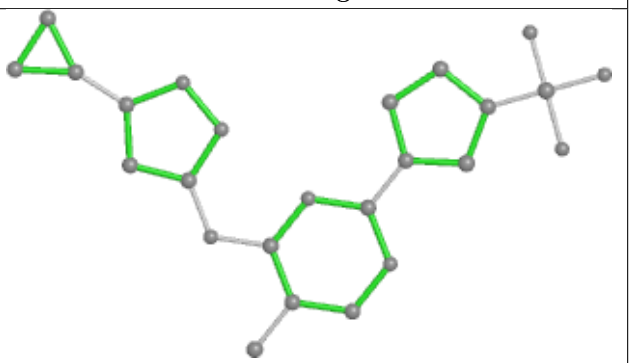
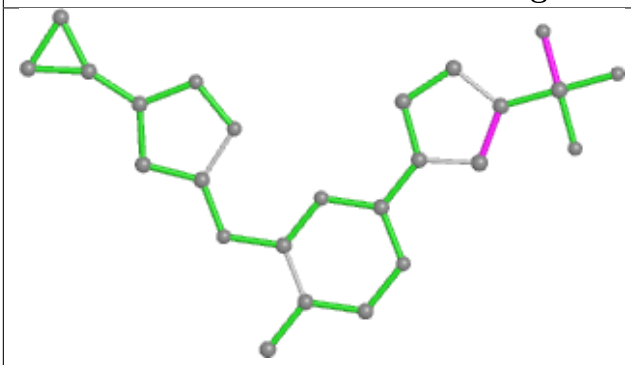
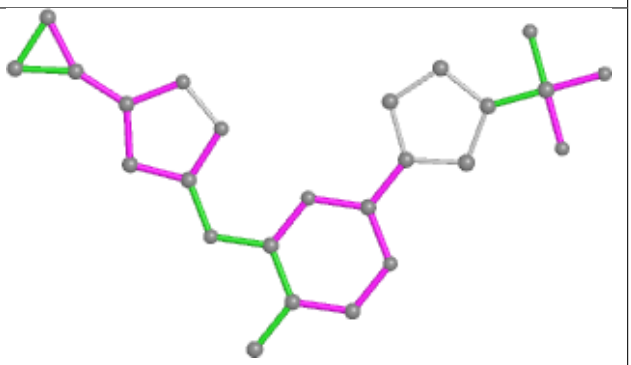


Rings

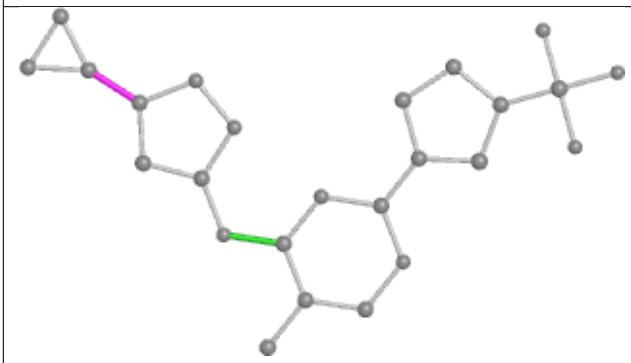
Ligand CJJ B 300



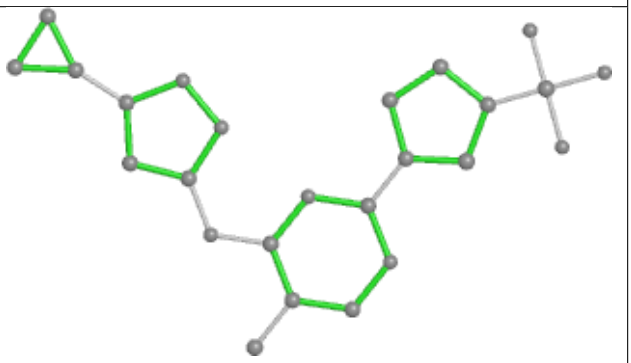
Bond lengths



Bond angles

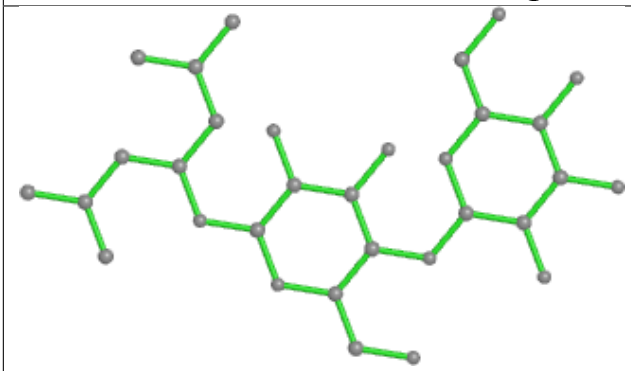


Torsions

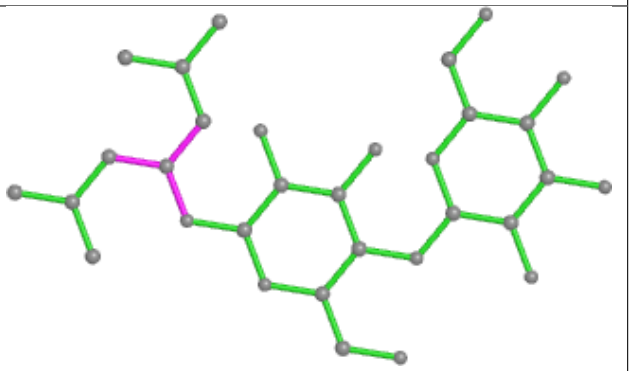


Rings

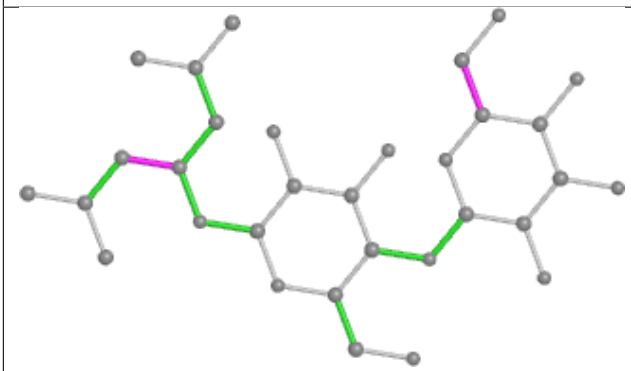
Ligand 0BD A 302



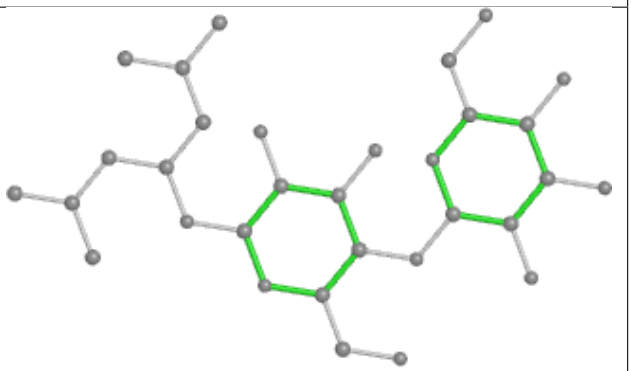
Bond lengths



Bond angles

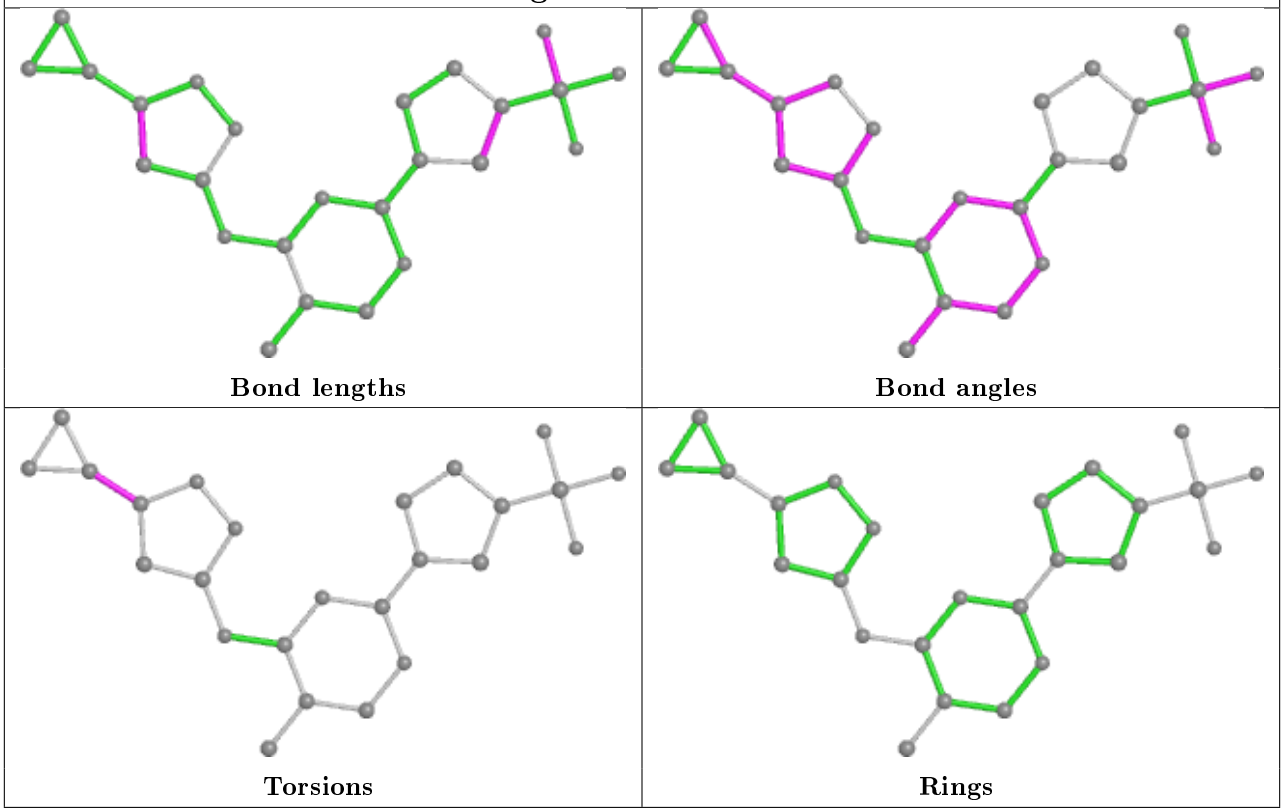


Torsions



Rings

Ligand CJJ A 301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	261/317 (82%)	-0.01	2 (0%)	86	86	41, 64, 91, 121	0
1	B	266/317 (83%)	0.26	6 (2%)	60	59	49, 80, 133, 168	0
1	C	264/317 (83%)	0.56	16 (6%)	21	17	65, 102, 135, 165	0
1	D	259/317 (81%)	0.64	21 (8%)	12	9	55, 101, 146, 175	0
All	All	1050/1268 (82%)	0.36	45 (4%)	35	31	41, 85, 136, 175	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	SER	4.3
1	D	251	ILE	4.1
1	B	175	GLY	4.0
1	C	179	GLY	3.9
1	D	115	LEU	3.7
1	C	274	VAL	3.6
1	D	231	LYS	3.6
1	D	113	LEU	3.5
1	B	165	ALA	3.5
1	C	20	ALA	3.4
1	B	23	GLY	3.4
1	D	178	MET	3.4
1	D	119	LEU	3.3
1	D	190	LEU	3.3
1	C	116	ARG	3.2
1	C	166	VAL	3.0
1	C	31	VAL	2.8
1	B	176	MET	2.8
1	C	272	ALA	2.8
1	D	3	PRO	2.8
1	C	111	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	248	LEU	2.6
1	D	262	ARG	2.6
1	D	48	PHE	2.6
1	D	179	GLY	2.6
1	D	116	ARG	2.6
1	D	255	LYS	2.6
1	A	3	PRO	2.5
1	D	274	VAL	2.5
1	C	18	LEU	2.4
1	D	227	MET	2.4
1	A	179	GLY	2.4
1	B	5	VAL	2.4
1	C	28	TRP	2.4
1	C	232	GLU	2.4
1	D	277	GLY	2.4
1	C	22	GLY	2.4
1	D	189	ALA	2.4
1	C	57	ARG	2.3
1	C	118	ALA	2.3
1	B	166	VAL	2.3
1	C	24	MET	2.3
1	C	104	ASN	2.2
1	D	273	ALA	2.1
1	D	226	ALA	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, 95^{th} 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	TPO	D	224	11/12	0.95	0.18	108,109,113,119	0
1	TPO	C	224	11/12	0.96	0.19	100,106,117,118	0
1	TPO	A	224	11/12	0.98	0.18	65,68,75,76	0
1	TPO	B	224	11/12	0.98	0.17	63,65,72,74	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

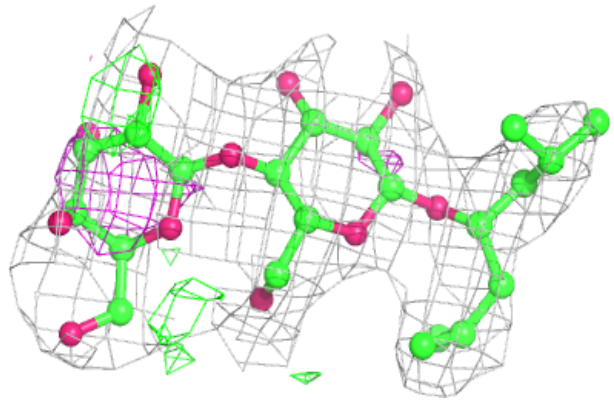
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

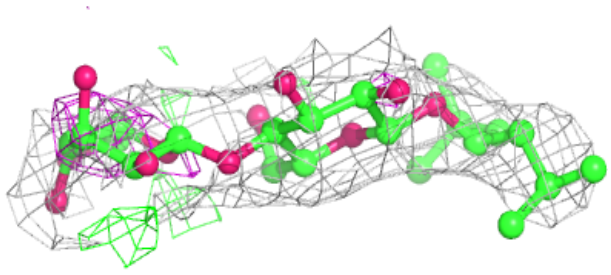
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	0BD	A	302	32/32	0.77	0.28	76,89,98,99	0
2	CJJ	C	300	25/25	0.83	0.31	116,143,146,148	0
2	CJJ	B	300	25/25	0.92	0.18	59,77,100,101	0
2	CJJ	D	300	25/25	0.92	0.22	65,91,100,102	0
2	CJJ	A	301	25/25	0.92	0.20	50,69,87,87	0

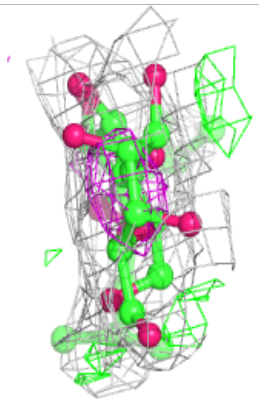
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0BD A 302:

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

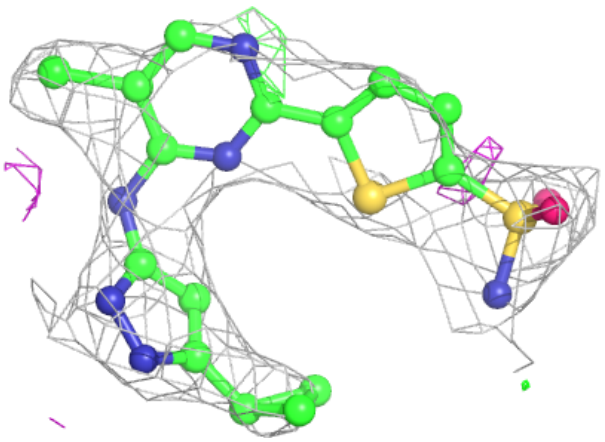


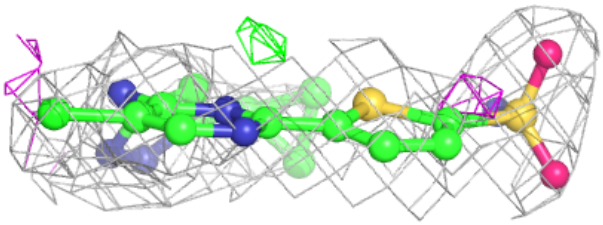


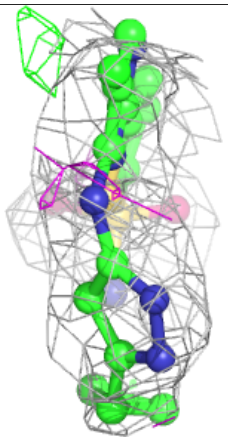


Electron density around CJJ C 300:

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

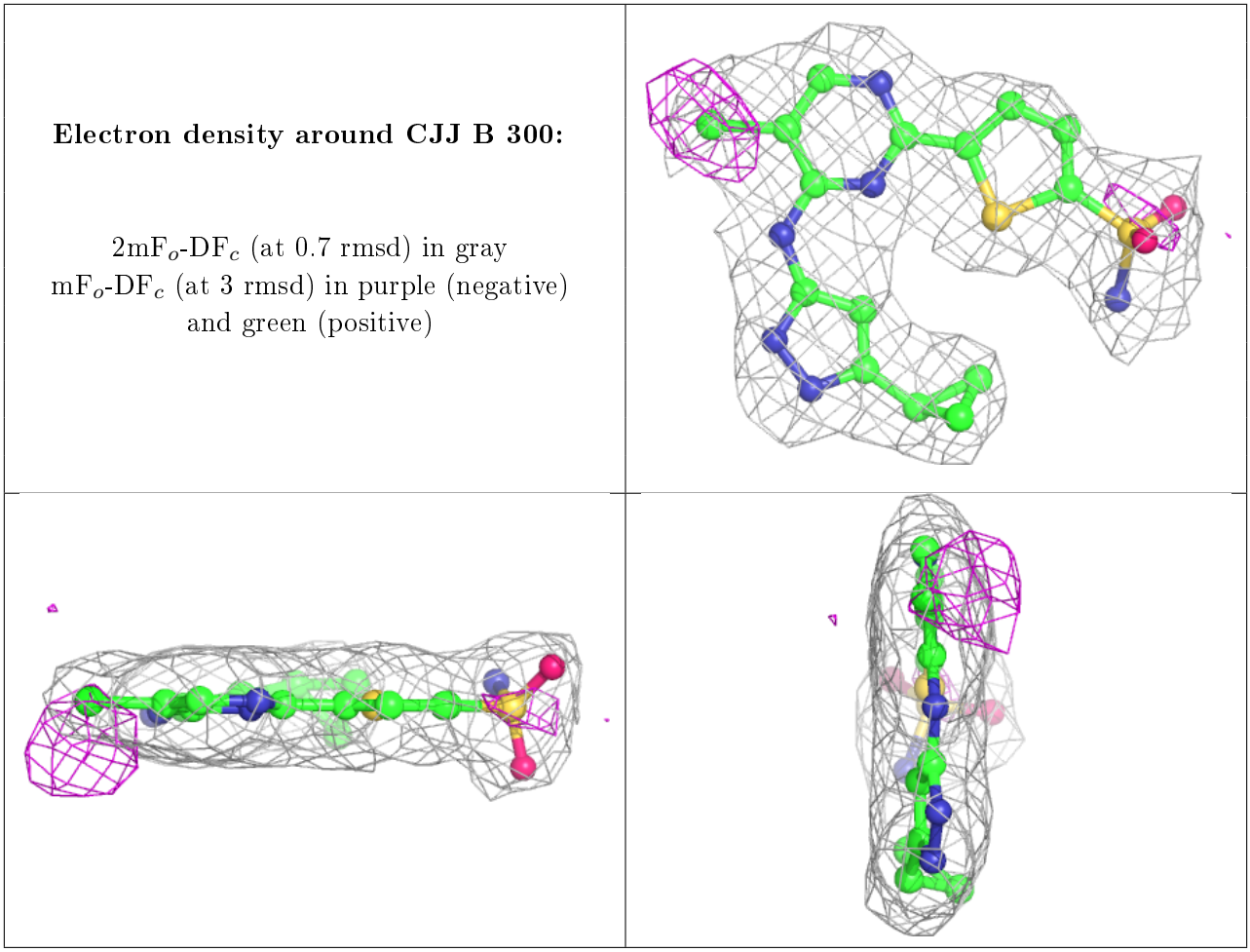






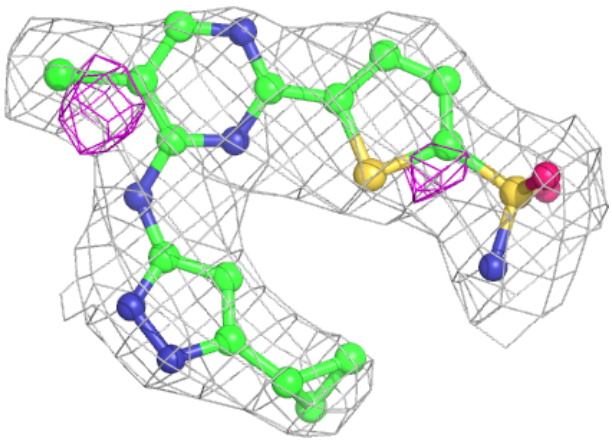
Electron density around CJJ B 300:

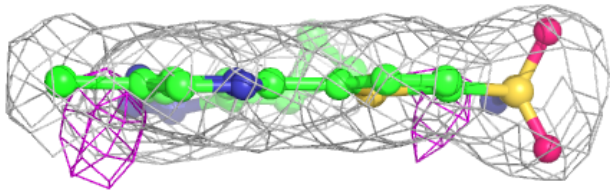
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

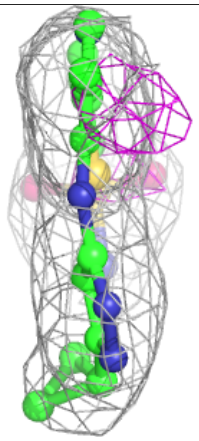


Electron density around CJJ D 300:

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

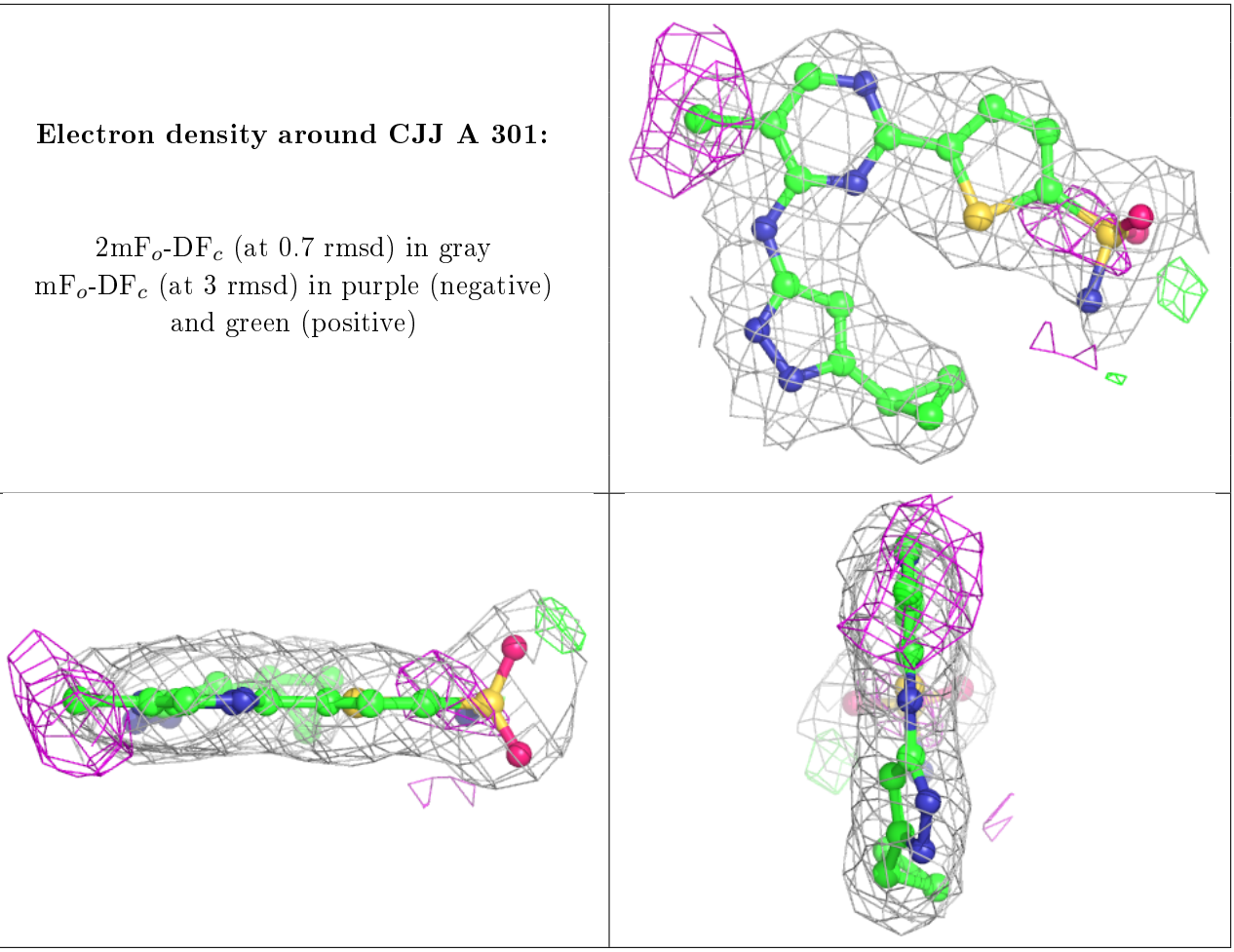






Electron density around CJJ A 301:

$2mF_o$-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

There are no such residues in this entry.