Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 07:49 am GMT

PDB ID	:	8BSU
Title	:	Crystal structure of the kainate receptor GluK3-H523A ligand binding domain in complex with kainate and the positive allosteric modulator BPAM344 at 2.9A resolution
Authors	:	Venskutonyte, R.; Frydenvang, K.; Kastrup, J.S.
Deposited on	:	2022-11-26
Resolution	:	2.90 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

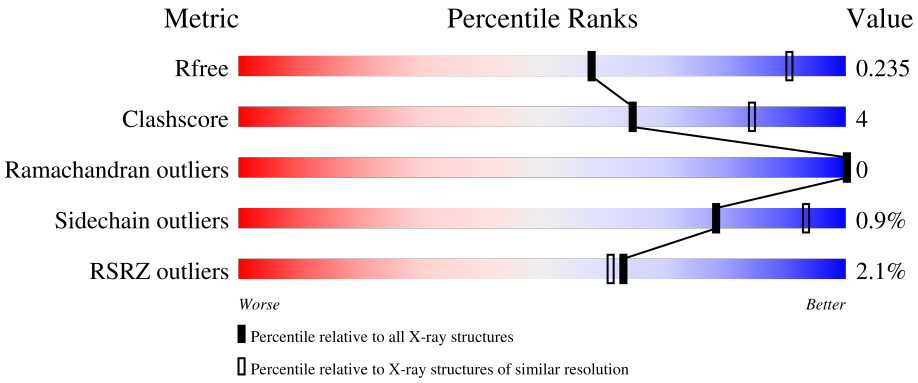
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	258	4% 88% 10% ·
1	B	258	84% 11% ·
1	C	258	2% 87% 11% ·
1	D	258	2% 81% 16% ·

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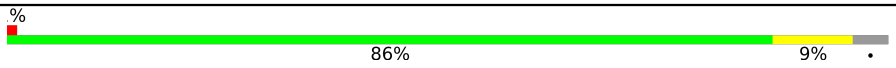
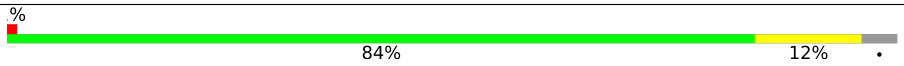
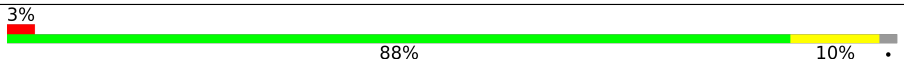
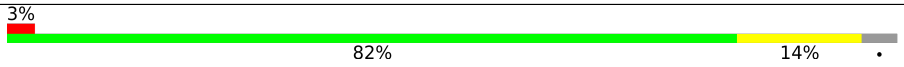
Mol	Chain	Length	Quality of chain
1	E	258	
1	F	258	
1	G	258	
1	H	258	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16506 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 Glutamate receptor ionotropic, kainate 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	2	0
			2008	1284	331	381	12			
1	B	247	Total	C	N	O	S	0	2	0
			1977	1267	326	373	11			
1	C	252	Total	C	N	O	S	0	1	0
			2002	1280	331	379	12			
1	D	253	Total	C	N	O	S	0	1	0
			2013	1286	335	380	12			
1	E	247	Total	C	N	O	S	0	3	0
			1988	1275	330	372	11			
1	F	248	Total	C	N	O	S	0	2	0
			1985	1272	329	373	11			
1	G	253	Total	C	N	O	S	0	1	0
			2013	1286	335	380	12			
1	H	248	Total	C	N	O	S	0	1	0
			1985	1271	330	373	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P42264
A	2	PRO	-	expression tag	UNP P42264
A	3	GLY	-	expression tag	UNP P42264
A	95	ALA	HIS	engineered mutation	UNP P42264
A	119	GLY	-	linker	UNP P42264
A	120	THR	-	linker	UNP P42264
B	1	GLY	-	expression tag	UNP P42264
B	2	PRO	-	expression tag	UNP P42264
B	3	GLY	-	expression tag	UNP P42264
B	95	ALA	HIS	engineered mutation	UNP P42264
B	119	GLY	-	linker	UNP P42264
B	120	THR	-	linker	UNP P42264
C	1	GLY	-	expression tag	UNP P42264

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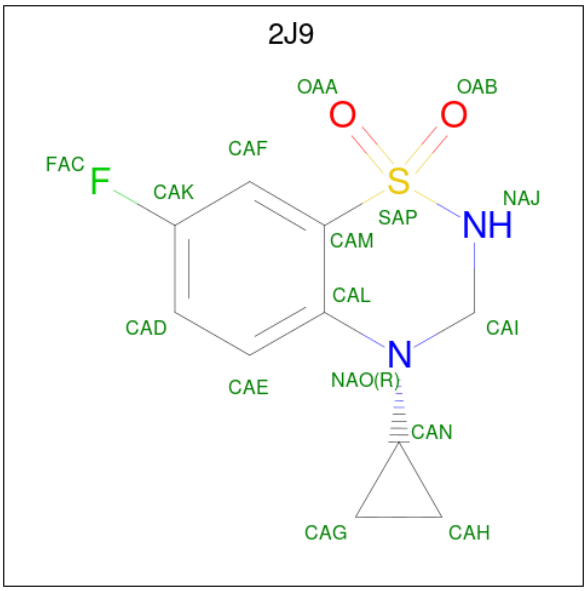
Chain	Residue	Modelled	Actual	Comment	Reference
C	2	PRO	-	expression tag	UNP P42264
C	3	GLY	-	expression tag	UNP P42264
C	95	ALA	HIS	engineered mutation	UNP P42264
C	119	GLY	-	linker	UNP P42264
C	120	THR	-	linker	UNP P42264
D	1	GLY	-	expression tag	UNP P42264
D	2	PRO	-	expression tag	UNP P42264
D	3	GLY	-	expression tag	UNP P42264
D	95	ALA	HIS	engineered mutation	UNP P42264
D	119	GLY	-	linker	UNP P42264
D	120	THR	-	linker	UNP P42264
E	1	GLY	-	expression tag	UNP P42264
E	2	PRO	-	expression tag	UNP P42264
E	3	GLY	-	expression tag	UNP P42264
E	95	ALA	HIS	engineered mutation	UNP P42264
E	119	GLY	-	linker	UNP P42264
E	120	THR	-	linker	UNP P42264
F	1	GLY	-	expression tag	UNP P42264
F	2	PRO	-	expression tag	UNP P42264
F	3	GLY	-	expression tag	UNP P42264
F	95	ALA	HIS	engineered mutation	UNP P42264
F	119	GLY	-	linker	UNP P42264
F	120	THR	-	linker	UNP P42264
G	1	GLY	-	expression tag	UNP P42264
G	2	PRO	-	expression tag	UNP P42264
G	3	GLY	-	expression tag	UNP P42264
G	95	ALA	HIS	engineered mutation	UNP P42264
G	119	GLY	-	linker	UNP P42264
G	120	THR	-	linker	UNP P42264
H	1	GLY	-	expression tag	UNP P42264
H	2	PRO	-	expression tag	UNP P42264
H	3	GLY	-	expression tag	UNP P42264
H	95	ALA	HIS	engineered mutation	UNP P42264
H	119	GLY	-	linker	UNP P42264
H	120	THR	-	linker	UNP P42264

- Molecule 2 is 4-cyclopropyl-7-fluoro-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide (three-letter code: 2J9) (formula: $C_{10}H_{11}FN_2O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			16	10	1	2	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			16	10	1	2	2	1		
2	C	1	Total	C	F	N	O	S	0	0
			16	10	1	2	2	1		
2	D	1	Total	C	F	N	O	S	0	0
			16	10	1	2	2	1		
2	E	1	Total	C	F	N	O	S	0	0
			16	10	1	2	2	1		
2	E	1	Total	C	F	N	O	S	0	0
			16	10	1	2	2	1		
2	F	1	Total	C	F	N	O	S	0	0
			16	10	1	2	2	1		
2	G	1	Total	C	F	N	O	S	0	0
			16	10	1	2	2	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	1
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	2
			2	2		
3	D	2	Total	Zn	0	2
			2	2		

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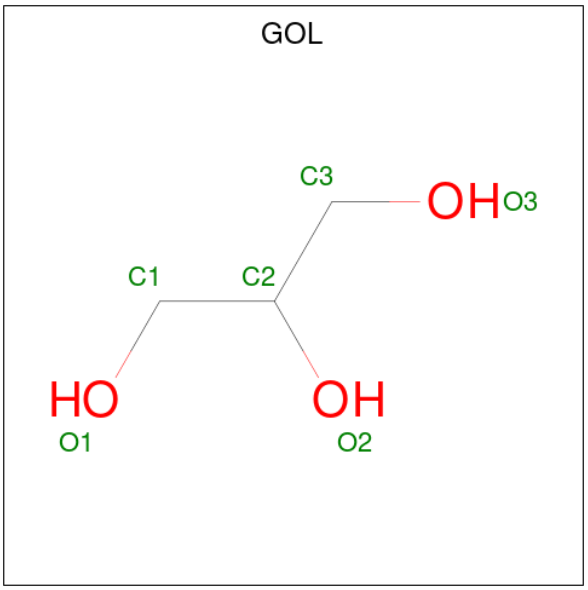
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	6	Total Zn 6 6	0	6
3	F	2	Total Zn 2 2	0	2
3	G	2	Total Zn 2 2	0	2
3	H	2	Total Zn 2 2	0	2

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0

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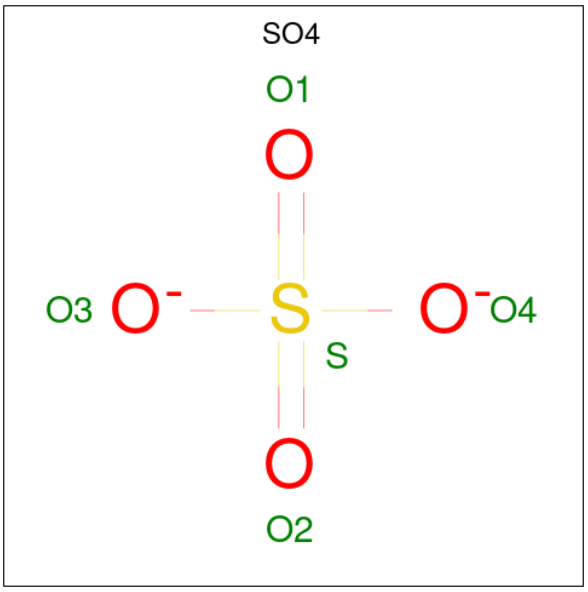
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

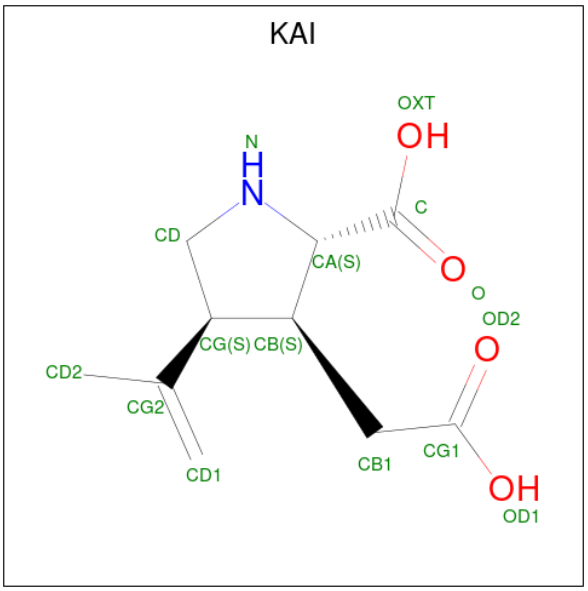
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0
5	B	4	Total Cl 4 4	0	0
5	C	4	Total Cl 4 4	0	0
5	E	1	Total Cl 1 1	0	0
5	F	4	Total Cl 4 4	0	0
5	G	3	Total Cl 3 3	0	0
5	H	3	Total Cl 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



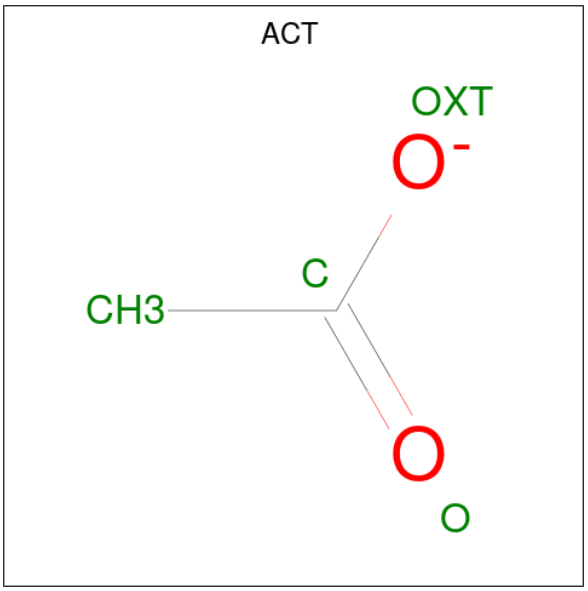
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0

- Molecule 7 is 3-(CARBOXYMETHYL)-4-ISOPROPENYLPROLINE (three-letter code: KAI) (formula: $C_{10}H_{15}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			15	10	1	4		
7	B	1	Total	C	N	O	0	0
			15	10	1	4		
7	C	1	Total	C	N	O	0	0
			15	10	1	4		
7	D	1	Total	C	N	O	0	0
			15	10	1	4		
7	E	1	Total	C	N	O	0	0
			15	10	1	4		
7	F	1	Total	C	N	O	0	0
			15	10	1	4		
7	G	1	Total	C	N	O	0	0
			15	10	1	4		
7	H	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	F	1	Total C O 4 2 2	0	0

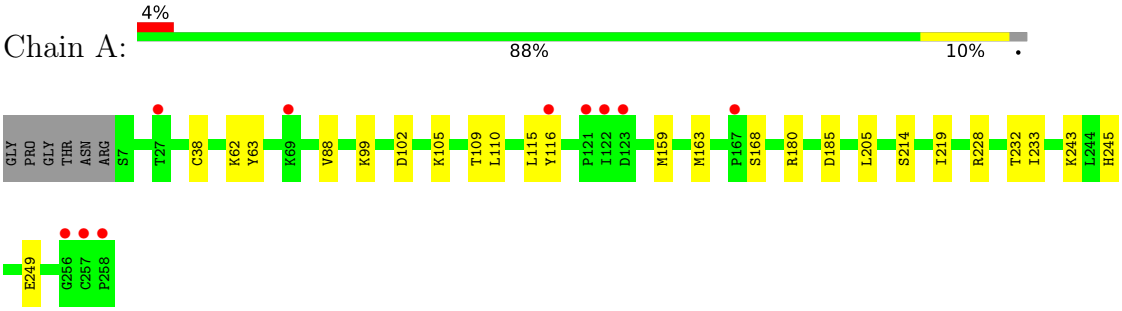
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	8	Total O 8 8	0	0
9	B	14	Total O 14 14	0	0
9	C	19	Total O 19 19	0	0
9	D	24	Total O 24 24	0	1
9	E	17	Total O 17 17	0	0
9	F	11	Total O 11 11	0	0
9	G	10	Total O 10 10	0	0
9	H	12	Total O 12 12	0	0

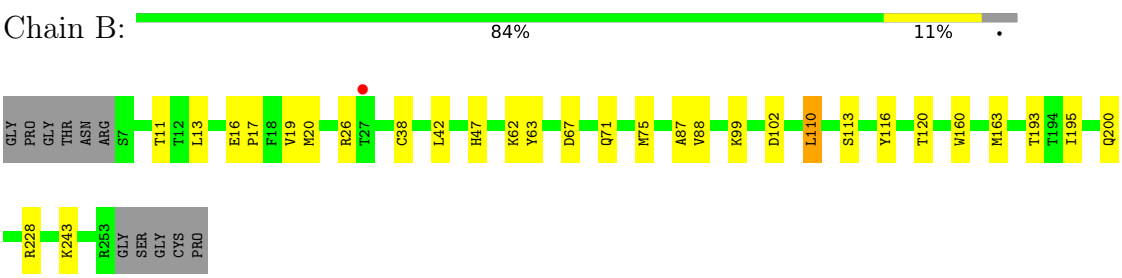
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

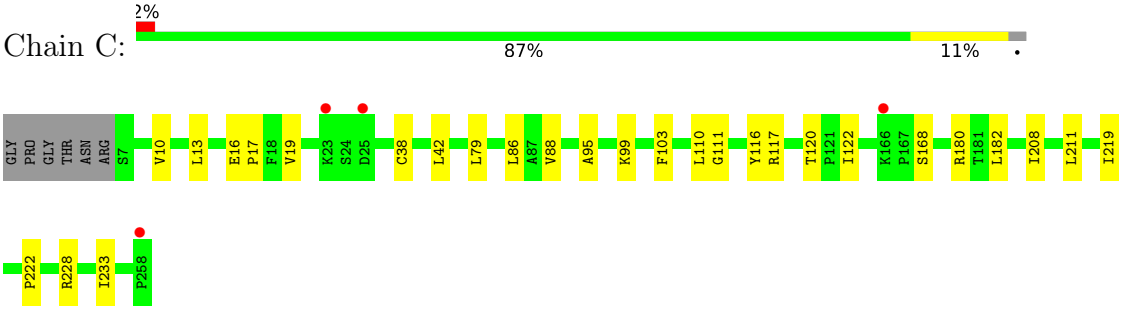
• Molecule 1: Glutamate receptor ionotropic, kainate 3



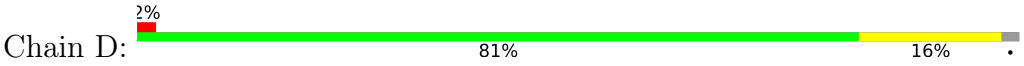
• Molecule 1: Glutamate receptor ionotropic, kainate 3

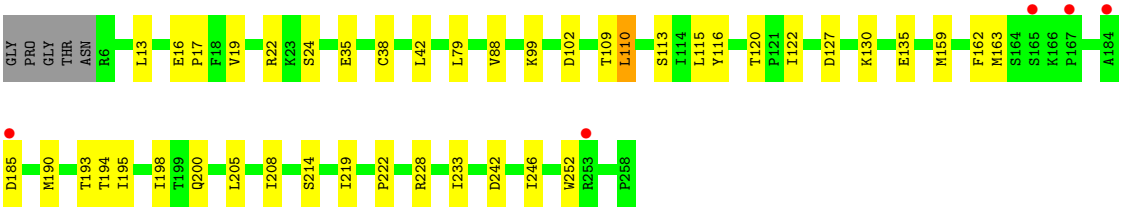


• Molecule 1: Glutamate receptor ionotropic, kainate 3

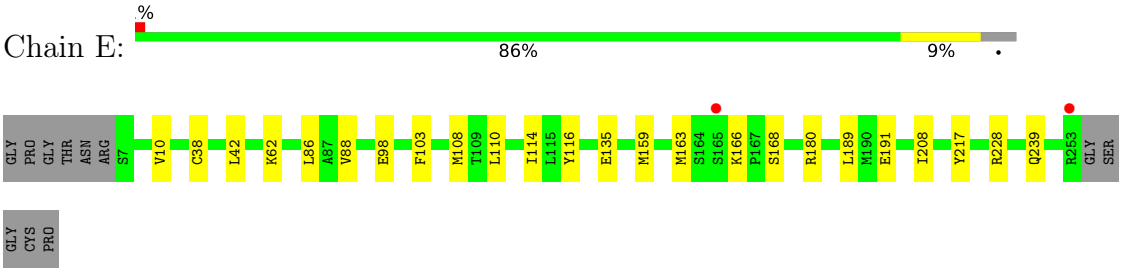


• Molecule 1: Glutamate receptor ionotropic, kainate 3

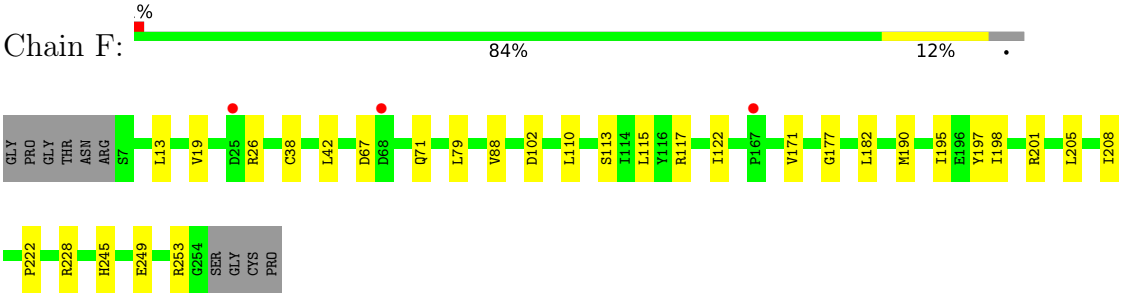




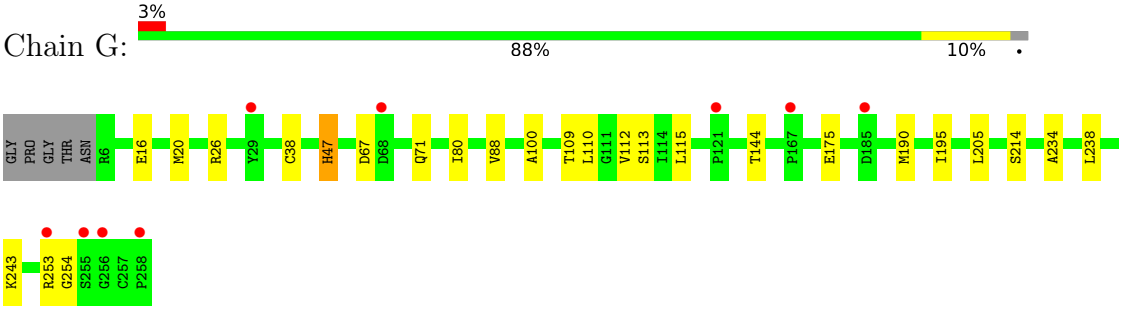
• Molecule 1: Glutamate receptor ionotropic, kainate 3



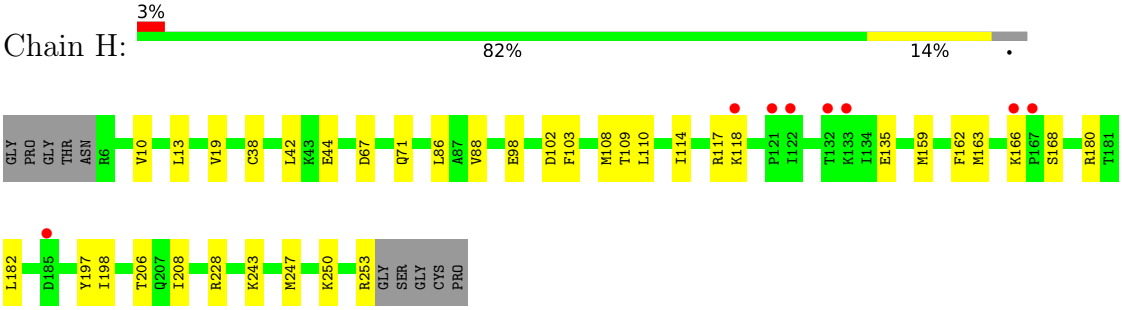
• Molecule 1: Glutamate receptor ionotropic, kainate 3



• Molecule 1: Glutamate receptor ionotropic, kainate 3



• Molecule 1: Glutamate receptor ionotropic, kainate 3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.14Å 100.56Å 132.83Å 90.00° 103.93° 90.00°	Depositor
Resolution (Å)	45.33 – 2.90 45.32 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.33-2.90) 99.8 (45.32-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.207 , 0.234 0.206 , 0.235	Depositor DCC
R_{free} test set	2383 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16506	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9683e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ZN, CL, KAI, GOL, SO4, ACT, 2J9

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	0.24	0/2053	0.47	0/2764
1	B	0.24	0/2021	0.47	0/2722
1	C	0.25	0/2044	0.47	0/2752
1	D	0.24	0/2055	0.48	0/2766
1	E	0.24	0/2037	0.46	0/2744
1	F	0.24	0/2030	0.47	0/2734
1	G	0.25	0/2055	0.48	0/2766
1	H	0.24	0/2026	0.47	0/2728
All	All	0.24	0/16321	0.47	0/21976

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	2008	0	2026	18	0
1	B	1977	0	2004	18	0
1	C	2002	0	2020	15	0
1	D	2013	0	2033	27	0
1	E	1988	0	2013	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1985	0	2009	15	0
1	G	2013	0	2033	17	0
1	H	1985	0	2012	19	0
2	A	16	0	10	2	0
2	B	16	0	10	0	0
2	C	16	0	10	0	0
2	D	16	0	10	1	0
2	E	32	0	20	1	0
2	F	16	0	10	1	0
2	G	16	0	10	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	6	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	6	0	8	2	0
4	B	6	0	8	2	0
4	C	12	0	16	0	0
4	D	12	0	16	1	0
4	E	36	0	48	2	0
4	H	6	0	8	1	0
5	A	3	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	E	1	0	0	0	0
5	F	4	0	0	0	0
5	G	3	0	0	0	0
5	H	3	0	0	0	0
6	A	10	0	0	0	0
6	B	5	0	0	1	0
6	D	10	0	0	1	0
6	E	5	0	0	0	0
6	G	5	0	0	1	0
6	H	5	0	0	0	0
7	A	15	0	13	0	0
7	B	15	0	13	0	0
7	C	15	0	13	0	0
7	D	15	0	13	0	0
7	E	15	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	15	0	13	0	0
7	G	15	0	13	0	0
7	H	15	0	13	0	0
8	A	4	0	3	0	0
8	B	4	0	3	0	0
8	F	4	0	3	0	0
9	A	8	0	0	0	0
9	B	14	0	0	0	0
9	C	19	0	0	0	0
9	D	24	0	0	0	0
9	E	17	0	0	0	0
9	F	11	0	0	0	0
9	G	10	0	0	0	0
9	H	12	0	0	0	0
All	All	16506	0	16447	135	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 4.

All (135) 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:63:TYR:H	4:B:304:GOL:H11	1.42	0.84
1:A:63:TYR:H	4:A:304:GOL:H31	1.50	0.76
1:F:102:ASP:HB3	1:F:228:ARG:HD3	1.66	0.76
1:C:168:SER:O	1:C:180:ARG:NH1	2.20	0.74
1:H:168:SER:O	1:H:180:ARG:NH1	2.21	0.73
1:F:190:MET:HE3	1:F:195:ILE:HG12	1.73	0.69
1:B:26:ARG:NH1	6:B:309:SO4:O4	2.27	0.68
1:F:42:LEU:HD13	1:F:88:VAL:HG21	1.78	0.65
1:A:233:ILE:HD13	1:D:99:LYS:HG2	1.79	0.63
1:C:116:TYR:HE2	1:C:120:THR:HG21	1.64	0.63
1:D:190:MET:HE3	1:D:195:ILE:HG12	1.81	0.62
1:F:117:ARG:HH21	1:F:182:LEU:HA	1.66	0.61
1:G:26:ARG:NH1	6:G:307:SO4:O4	2.33	0.60
1:E:135:GLU:OE2	1:E:166:LYS:NZ	2.27	0.60
1:E:42:LEU:HD13	1:E:88:VAL:HG21	1.83	0.60
1:A:245:HIS:NE2	1:A:249[A]:GLU:OE2	2.34	0.59
1:G:190:MET:HE3	1:G:195:ILE:HG12	1.85	0.58
1:C:117:ARG:NH2	1:C:182:LEU:O	2.34	0.57
1:E:108:MET:HG3	4:E:313:GOL:H12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:ASP:HB3	1:H:228:ARG:HD2	1.87	0.56
1:G:80:ILE:HD11	1:G:100:ALA:HB1	1.88	0.56
1:D:42:LEU:HD13	1:D:88:VAL:HG21	1.87	0.55
1:B:243:LYS:HD3	1:H:243:LYS:HE3	1.89	0.55
1:D:102:ASP:HB3	1:D:228:ARG:HD2	1.87	0.55
1:E:168:SER:O	1:E:180:ARG:NH1	2.39	0.55
1:H:108:MET:HA	4:H:303:GOL:H2	1.87	0.55
1:D:200:GLN:NE2	1:D:252:TRP:O	2.41	0.54
1:D:116:TYR:HB3	1:D:208:ILE:HD13	1.89	0.54
1:H:117:ARG:NH2	1:H:182:LEU:O	2.32	0.54
1:E:116:TYR:HB3	1:E:208:ILE:HD13	1.90	0.53
1:E:38:CYS:HB3	1:E:88:VAL:HG12	1.91	0.53
1:F:113:SER:HB3	1:F:195:ILE:HD12	1.91	0.53
1:C:10:VAL:HG22	1:C:86:LEU:HB2	1.92	0.52
1:H:118:LYS:HG2	1:H:206:THR:HB	1.92	0.52
1:E:191:GLU:OE1	1:E:217:TYR:OH	2.19	0.52
1:B:67:ASP:OD1	1:B:71:GLN:N	2.43	0.51
1:C:103:PHE:O	1:C:228:ARG:NH1	2.38	0.51
1:B:113:SER:HB3	1:B:195:ILE:HD12	1.92	0.51
1:A:38:CYS:HB3	1:A:88:VAL:HG12	1.93	0.51
1:D:127:ASP:HA	1:D:130:LYS:HE2	1.94	0.50
1:F:79:LEU:HD22	1:F:222:PRO:HD3	1.93	0.50
1:H:135:GLU:OE2	1:H:166:LYS:NZ	2.34	0.50
1:F:201:ARG:NH2	1:F:253:ARG:O	2.44	0.50
1:A:99:LYS:HG2	1:D:233:ILE:HD13	1.94	0.50
1:A:109:THR:HG23	2:A:301:2J9:H4	1.94	0.50
1:B:62:LYS:HA	4:B:304:GOL:H31	1.93	0.50
1:F:38:CYS:HB3	1:F:88:VAL:HG12	1.94	0.49
1:E:10:VAL:HG22	1:E:86:LEU:HB2	1.93	0.49
1:D:194:THR:O	1:D:198:ILE:HG13	2.13	0.49
1:H:159:MET:O	1:H:163:MET:HG3	2.13	0.49
1:D:116:TYR:OH	1:D:185:ASP:OD1	2.26	0.49
1:G:253:ARG:HG2	1:G:254:GLY:H	1.78	0.49
1:D:135:GLU:HG3	1:D:162:PHE:HE1	1.77	0.48
1:G:67:ASP:OD1	1:G:71:GLN:N	2.43	0.48
1:B:102:ASP:HB3	1:B:228:ARG:HD2	1.96	0.48
1:A:243:LYS:HE2	1:G:243:LYS:HE2	1.96	0.48
1:B:99:LYS:HG2	1:C:233:ILE:HD13	1.94	0.48
1:D:115:LEU:HD22	1:D:190:MET:HE1	1.95	0.48
1:C:38:CYS:HB3	1:C:88:VAL:HG12	1.95	0.48
1:C:88:VAL:HG22	1:C:219:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:LEU:HD22	1:G:190:MET:HE1	1.95	0.47
1:A:105:LYS:HG3	1:A:232:THR:HG23	1.96	0.47
1:E:62:LYS:HB3	4:E:311:GOL:H2	1.96	0.47
1:G:112:VAL:HG22	1:G:144:THR:HG22	1.95	0.47
1:A:102:ASP:HB3	1:A:228:ARG:HD2	1.97	0.47
1:G:113:SER:HB3	1:G:195:ILE:HD12	1.97	0.47
1:B:38:CYS:HB3	1:B:88:VAL:HG12	1.96	0.47
1:C:79:LEU:HD22	1:C:222:PRO:HD3	1.97	0.47
2:E:302:2J9:H4	1:H:109:THR:HG23	1.95	0.47
1:H:42:LEU:HD13	1:H:88:VAL:HG21	1.96	0.47
1:A:88:VAL:HG22	1:A:219:ILE:HD12	1.97	0.46
1:D:38:CYS:HB3	1:D:88:VAL:HG12	1.97	0.46
1:D:115:LEU:HD21	1:D:205:LEU:HD13	1.97	0.46
1:A:116:TYR:OH	1:A:185:ASP:OD1	2.26	0.46
1:G:16:GLU:HG2	1:G:20:MET:HG2	1.97	0.46
1:D:24:SER:OG	6:D:307:SO4:O3	2.34	0.45
2:A:301:2J9:H1	1:D:214:SER:HB3	1.98	0.45
1:B:16:GLU:HG2	1:B:20:MET:HG2	1.99	0.45
1:H:38:CYS:HB3	1:H:88:VAL:HG12	1.98	0.45
1:D:120:THR:HG22	1:D:122:ILE:H	1.82	0.45
1:H:10:VAL:HG22	1:H:86:LEU:HB2	1.97	0.45
1:B:160:TRP:HA	1:B:163:MET:HE3	1.98	0.45
1:F:245[B]:HIS:NE2	1:F:249:GLU:OE2	2.49	0.45
1:A:245:HIS:CE1	1:G:47[B]:HIS:HE1	2.35	0.45
1:B:116:TYR:CD2	1:B:120:THR:HG21	2.52	0.45
1:F:122:ILE:HG22	1:F:208:ILE:HG21	1.98	0.44
1:A:168:SER:O	1:A:180:ARG:NH1	2.50	0.44
1:F:171:VAL:HG11	1:F:177:GLY:HA2	1.99	0.44
1:H:13:LEU:O	1:H:19:VAL:HB	2.17	0.44
1:E:159:MET:O	1:E:163:MET:HG3	2.17	0.44
1:F:67:ASP:OD1	1:F:71:GLN:N	2.51	0.44
1:A:115:LEU:HD11	1:A:205:LEU:HB3	2.00	0.44
1:G:38:CYS:HB3	1:G:88:VAL:HG12	1.99	0.44
1:H:114:ILE:HB	1:H:208:ILE:HB	2.00	0.44
1:F:197:TYR:HD2	1:F:198:ILE:HD12	1.82	0.44
1:H:197:TYR:HD2	1:H:198:ILE:HD12	1.83	0.44
1:C:111:GLY:HA3	1:C:211:LEU:HD23	2.00	0.43
1:D:79:LEU:HD22	1:D:222:PRO:HD3	2.00	0.43
1:G:109:THR:HG23	2:G:301:2J9:H4	1.99	0.43
1:C:95:ALA:O	1:C:99:LYS:HG3	2.18	0.43
1:H:98:GLU:OE1	1:H:103:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ILE:HG22	1:C:208:ILE:HG21	2.00	0.43
1:B:16:GLU:HA	1:B:17:PRO:HA	1.79	0.43
1:H:44:GLU:HG3	1:H:247:MET:HE1	2.00	0.43
1:A:214:SER:HB3	2:D:301:2J9:H1	2.00	0.43
1:A:243:LYS:HE2	1:G:243:LYS:CE	2.48	0.43
1:D:13:LEU:O	1:D:19:VAL:HB	2.19	0.43
1:D:113:SER:HB3	1:D:195:ILE:HD12	2.00	0.43
1:G:115:LEU:HD11	1:G:205:LEU:HB3	2.01	0.43
2:F:301:2J9:H1	1:G:214:SER:HB3	2.00	0.43
1:D:22:ARG:HG3	1:D:35:GLU:HB3	2.01	0.42
1:A:159:MET:O	1:A:163:MET:HG3	2.18	0.42
1:C:16:GLU:HA	1:C:17:PRO:HA	1.82	0.42
1:D:110:LEU:HB3	1:D:193:THR:HG23	2.02	0.42
1:D:16:GLU:HA	1:D:17:PRO:HA	1.83	0.42
1:D:159:MET:O	1:D:163:MET:HG3	2.20	0.42
1:E:98:GLU:OE1	1:E:103:PHE:HB2	2.20	0.42
1:D:242:ASP:O	1:D:246:ILE:HG13	2.20	0.42
1:B:110:LEU:HB3	1:B:193:THR:HG23	2.01	0.41
1:F:115:LEU:HD11	1:F:205:LEU:HB3	2.02	0.41
1:F:13:LEU:O	1:F:19:VAL:HB	2.20	0.41
1:B:42:LEU:HD13	1:B:88:VAL:HG21	2.01	0.41
1:C:13:LEU:O	1:C:19:VAL:HB	2.21	0.41
1:D:88:VAL:HG22	1:D:219:ILE:HD12	2.01	0.41
1:C:42:LEU:HD13	1:C:88:VAL:HG21	2.02	0.41
1:D:109:THR:H	4:D:305:GOL:H2	1.86	0.41
1:H:135:GLU:HG2	1:H:162:PHE:HZ	1.86	0.41
1:E:114:ILE:HG13	1:E:189:LEU:HD13	2.03	0.40
1:A:62:LYS:HA	4:A:304:GOL:H11	2.04	0.40
1:E:103:PHE:O	1:E:228:ARG:NH1	2.47	0.40
1:H:67:ASP:OD1	1:H:71:GLN:N	2.50	0.40
1:B:13:LEU:O	1:B:19:VAL:HB	2.21	0.40
1:B:75:MET:HE2	1:B:87:ALA:HB1	2.03	0.40
1:B:11:THR:HG23	1:B:75:MET:HE3	2.03	0.40
1:G:234:ALA:O	1:G:238:LEU:HG	2.22	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	252/258 (98%)	247 (98%)	5 (2%)	0	100	100
1	B	247/258 (96%)	244 (99%)	3 (1%)	0	100	100
1	C	251/258 (97%)	246 (98%)	5 (2%)	0	100	100
1	D	252/258 (98%)	249 (99%)	3 (1%)	0	100	100
1	E	248/258 (96%)	245 (99%)	3 (1%)	0	100	100
1	F	248/258 (96%)	245 (99%)	3 (1%)	0	100	100
1	G	252/258 (98%)	248 (98%)	4 (2%)	0	100	100
1	H	247/258 (96%)	240 (97%)	7 (3%)	0	100	100
All	All	1997/2064 (97%)	1964 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/220 (99%)	217 (100%)	1 (0%)	88	96
1	B	215/220 (98%)	211 (98%)	4 (2%)	57	84
1	C	217/220 (99%)	216 (100%)	1 (0%)	88	96
1	D	218/220 (99%)	217 (100%)	1 (0%)	88	96
1	E	216/220 (98%)	214 (99%)	2 (1%)	78	93
1	F	215/220 (98%)	213 (99%)	2 (1%)	78	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	218/220 (99%)	214 (98%)	4 (2%)	59 85
1	H	215/220 (98%)	212 (99%)	3 (1%)	67 89
All	All	1732/1760 (98%)	1714 (99%)	18 (1%)	78 92

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	B	47[A]	HIS
1	B	47[B]	HIS
1	B	110	LEU
1	B	200	GLN
1	C	110	LEU
1	D	110	LEU
1	E	110	LEU
1	E	239	GLN
1	F	26	ARG
1	F	110	LEU
1	G	47[A]	HIS
1	G	47[B]	HIS
1	G	110	LEU
1	G	175	GLU
1	H	110	LEU
1	H	250	LYS
1	H	253	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	200	GLN
1	E	204	ASN
1	G	245	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 82 ligands modelled in this entry, 42 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
4	GOL	E	312	-	5,5,5	0.87	0	5,5,5	1.01	0
2	2J9	E	301	-	17,18,18	3.36	7 (41%)	23,28,28	5.37	10 (43%)
8	ACT	A	311	3	3,3,3	1.36	0	3,3,3	1.52	0
4	GOL	B	304	-	5,5,5	0.90	0	5,5,5	0.96	0
2	2J9	A	301	-	17,18,18	3.34	7 (41%)	23,28,28	5.19	9 (39%)
4	GOL	H	303	-	5,5,5	0.90	0	5,5,5	0.96	0
7	KAI	E	317	-	13,15,15	1.37	2 (15%)	14,21,21	1.07	0
6	SO4	H	307	-	4,4,4	0.15	0	6,6,6	0.07	0
6	SO4	D	307	-	4,4,4	0.14	0	6,6,6	0.06	0
7	KAI	G	308	-	13,15,15	1.39	2 (15%)	14,21,21	1.06	0
2	2J9	C	301	-	17,18,18	3.31	7 (41%)	23,28,28	5.03	8 (34%)
4	GOL	E	311	-	5,5,5	0.91	0	5,5,5	1.02	0
6	SO4	D	306	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	G	307	-	4,4,4	0.14	0	6,6,6	0.08	0
7	KAI	F	308	-	13,15,15	1.41	1 (7%)	14,21,21	0.99	0
4	GOL	A	304	-	5,5,5	0.91	0	5,5,5	0.98	0
7	KAI	H	308	-	13,15,15	1.39	1 (7%)	14,21,21	0.95	0
4	GOL	D	304	-	5,5,5	0.92	0	5,5,5	1.01	0
4	GOL	C	304	-	5,5,5	0.95	0	5,5,5	0.95	0
4	GOL	E	314	-	5,5,5	0.93	0	5,5,5	0.99	0
4	GOL	E	309	-	5,5,5	1.00	0	5,5,5	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	KAI	C	310	-	13,15,15	1.40	1 (7%)	14,21,21	0.89	0
8	ACT	B	311	-	3,3,3	1.34	0	3,3,3	1.54	0
2	2J9	G	301	-	17,18,18	3.37	7 (41%)	23,28,28	5.22	9 (39%)
6	SO4	A	308	-	4,4,4	0.14	0	6,6,6	0.05	0
2	2J9	F	301	-	17,18,18	3.38	7 (41%)	23,28,28	5.16	9 (39%)
4	GOL	E	310	-	5,5,5	0.99	0	5,5,5	0.97	0
6	SO4	B	309	-	4,4,4	0.14	0	6,6,6	0.07	0
2	2J9	E	302	-	17,18,18	3.36	7 (41%)	23,28,28	5.19	9 (39%)
4	GOL	E	313	-	5,5,5	0.93	0	5,5,5	0.98	0
4	GOL	C	305	-	5,5,5	0.90	0	5,5,5	0.98	0
2	2J9	D	301	-	17,18,18	3.37	7 (41%)	23,28,28	5.07	10 (43%)
6	SO4	E	316	-	4,4,4	0.14	0	6,6,6	0.07	0
7	KAI	A	310	-	13,15,15	1.39	1 (7%)	14,21,21	0.91	0
8	ACT	F	309	3	3,3,3	1.33	0	3,3,3	1.39	0
4	GOL	D	305	-	5,5,5	0.90	0	5,5,5	1.01	0
7	KAI	B	310	-	13,15,15	1.40	2 (15%)	14,21,21	0.95	0
7	KAI	D	308	-	13,15,15	1.39	2 (15%)	14,21,21	0.95	0
6	SO4	A	309	-	4,4,4	0.13	0	6,6,6	0.06	0
2	2J9	B	301	-	17,18,18	3.41	7 (41%)	23,28,28	5.25	9 (39%)

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
4	GOL	E	312	-	-	0/4/4/4	-
2	2J9	E	301	-	-	1/4/22/22	0/3/3/3
4	GOL	B	304	-	-	2/4/4/4	-
2	2J9	A	301	-	-	1/4/22/22	0/3/3/3
4	GOL	H	303	-	-	2/4/4/4	-
7	KAI	E	317	-	-	1/12/25/25	0/1/1/1
7	KAI	G	308	-	-	2/12/25/25	0/1/1/1
2	2J9	C	301	-	-	1/4/22/22	0/3/3/3
4	GOL	E	311	-	-	0/4/4/4	-
7	KAI	F	308	-	-	1/12/25/25	0/1/1/1
4	GOL	A	304	-	-	0/4/4/4	-
7	KAI	H	308	-	-	4/12/25/25	0/1/1/1
4	GOL	D	304	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	304	-	-	4/4/4/4	-
4	GOL	E	314	-	-	0/4/4/4	-
4	GOL	E	309	-	-	0/4/4/4	-
7	KAI	C	310	-	-	0/12/25/25	0/1/1/1
2	2J9	G	301	-	-	1/4/22/22	0/3/3/3
2	2J9	F	301	-	-	1/4/22/22	0/3/3/3
4	GOL	E	310	-	-	1/4/4/4	-
2	2J9	E	302	-	-	1/4/22/22	0/3/3/3
4	GOL	E	313	-	-	0/4/4/4	-
4	GOL	C	305	-	-	0/4/4/4	-
2	2J9	D	301	-	-	1/4/22/22	0/3/3/3
7	KAI	A	310	-	-	2/12/25/25	0/1/1/1
4	GOL	D	305	-	-	0/4/4/4	-
7	KAI	B	310	-	-	0/12/25/25	0/1/1/1
7	KAI	D	308	-	-	2/12/25/25	0/1/1/1
2	2J9	B	301	-	-	1/4/22/22	0/3/3/3

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	2J9	OAB-SAP	8.73	1.53	1.43
2	B	301	2J9	OAB-SAP	8.68	1.53	1.43
2	E	302	2J9	OAB-SAP	8.68	1.53	1.43
2	F	301	2J9	OAB-SAP	8.67	1.53	1.43
2	E	301	2J9	OAB-SAP	8.63	1.53	1.43
2	C	301	2J9	OAB-SAP	8.59	1.53	1.43
2	D	301	2J9	OAB-SAP	8.54	1.53	1.43
2	A	301	2J9	OAB-SAP	8.54	1.53	1.43
2	B	301	2J9	OAA-SAP	8.49	1.53	1.43
2	G	301	2J9	OAA-SAP	8.45	1.53	1.43
2	D	301	2J9	OAA-SAP	8.42	1.53	1.43
2	E	301	2J9	OAA-SAP	8.39	1.53	1.43
2	F	301	2J9	OAA-SAP	8.35	1.53	1.43
2	E	302	2J9	OAA-SAP	8.35	1.53	1.43
2	A	301	2J9	OAA-SAP	8.33	1.53	1.43
2	C	301	2J9	OAA-SAP	8.11	1.52	1.43
2	F	301	2J9	CAN-NAO	3.19	1.53	1.47
2	B	301	2J9	CAN-NAO	3.17	1.53	1.47
2	D	301	2J9	CAN-NAO	3.16	1.53	1.47
2	C	301	2J9	CAN-NAO	3.15	1.53	1.47
2	A	301	2J9	CAN-NAO	3.05	1.53	1.47
2	E	301	2J9	CAN-NAO	3.01	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	302	2J9	CAN-NAO	3.01	1.53	1.47
2	G	301	2J9	CAN-NAO	2.99	1.52	1.47
2	D	301	2J9	CAL-CAM	2.95	1.43	1.40
2	B	301	2J9	CAL-CAM	2.94	1.43	1.40
2	E	302	2J9	CAL-CAM	2.92	1.43	1.40
2	D	301	2J9	CAH-CAN	2.91	1.55	1.48
2	F	301	2J9	CAH-CAN	2.89	1.55	1.48
2	F	301	2J9	CAL-CAM	2.89	1.43	1.40
2	B	301	2J9	CAH-CAN	2.86	1.55	1.48
2	A	301	2J9	CAH-CAN	2.83	1.55	1.48
2	C	301	2J9	CAH-CAN	2.81	1.55	1.48
2	G	301	2J9	CAL-CAM	2.81	1.43	1.40
2	G	301	2J9	CAH-CAN	2.80	1.55	1.48
2	E	301	2J9	CAH-CAN	2.80	1.54	1.48
2	A	301	2J9	CAL-CAM	2.80	1.43	1.40
2	E	302	2J9	CAH-CAN	2.78	1.54	1.48
2	E	301	2J9	CAL-CAM	2.74	1.43	1.40
2	C	301	2J9	CAL-CAM	2.67	1.43	1.40
7	G	308	KAI	CA-C	2.65	1.56	1.52
7	D	308	KAI	CA-C	2.64	1.56	1.52
7	B	310	KAI	CA-C	2.63	1.56	1.52
7	A	310	KAI	CA-C	2.58	1.56	1.52
7	F	308	KAI	CA-C	2.57	1.56	1.52
7	E	317	KAI	CA-C	2.50	1.56	1.52
7	C	310	KAI	CA-C	2.50	1.56	1.52
7	H	308	KAI	CA-C	2.46	1.56	1.52
2	B	301	2J9	CAG-CAN	2.42	1.54	1.48
2	C	301	2J9	CAG-CAN	2.42	1.54	1.48
2	F	301	2J9	CAG-CAN	2.41	1.54	1.48
2	D	301	2J9	CAG-CAN	2.40	1.54	1.48
2	E	301	2J9	CAG-CAN	2.39	1.54	1.48
2	E	302	2J9	CAG-CAN	2.37	1.54	1.48
2	A	301	2J9	CAG-CAN	2.35	1.54	1.48
2	G	301	2J9	CAG-CAN	2.31	1.53	1.48
2	E	302	2J9	CAF-CAK	2.18	1.41	1.37
2	B	301	2J9	CAF-CAK	2.16	1.41	1.37
2	E	301	2J9	CAF-CAK	2.11	1.41	1.37
2	G	301	2J9	CAF-CAK	2.11	1.41	1.37
2	A	301	2J9	CAF-CAK	2.09	1.41	1.37
2	F	301	2J9	CAF-CAK	2.09	1.41	1.37
2	C	301	2J9	CAF-CAK	2.05	1.41	1.37
7	E	317	KAI	CB1-CB	2.04	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	2J9	CAF-CAK	2.04	1.41	1.37
7	B	310	KAI	CB1-CB	2.02	1.56	1.53
7	D	308	KAI	CB1-CB	2.02	1.56	1.53
7	G	308	KAI	CB1-CB	2.01	1.56	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	2J9	CAI-NAO-CAL	23.10	120.59	110.25
2	B	301	2J9	CAI-NAO-CAL	22.14	120.16	110.25
2	G	301	2J9	CAI-NAO-CAL	22.07	120.13	110.25
2	E	302	2J9	CAI-NAO-CAL	21.88	120.04	110.25
2	A	301	2J9	CAI-NAO-CAL	21.69	119.96	110.25
2	F	301	2J9	CAI-NAO-CAL	21.55	119.90	110.25
2	D	301	2J9	CAI-NAO-CAL	21.06	119.67	110.25
2	C	301	2J9	CAI-NAO-CAL	20.23	119.31	110.25
2	C	301	2J9	OAB-SAP-OAA	-8.67	109.61	118.46
2	F	301	2J9	OAB-SAP-OAA	-8.19	110.10	118.46
2	D	301	2J9	OAB-SAP-OAA	-8.11	110.19	118.46
2	A	301	2J9	OAB-SAP-OAA	-7.90	110.40	118.46
2	B	301	2J9	OAB-SAP-OAA	-7.85	110.45	118.46
2	G	301	2J9	OAB-SAP-OAA	-7.78	110.52	118.46
2	E	302	2J9	OAB-SAP-OAA	-7.70	110.60	118.46
2	E	301	2J9	OAB-SAP-OAA	-7.69	110.61	118.46
2	C	301	2J9	CAM-SAP-NAJ	6.39	107.43	102.37
2	E	302	2J9	CAM-SAP-NAJ	6.11	107.20	102.37
2	A	301	2J9	CAM-SAP-NAJ	5.71	106.89	102.37
2	D	301	2J9	CAM-SAP-NAJ	5.65	106.84	102.37
2	G	301	2J9	CAM-SAP-NAJ	5.64	106.84	102.37
2	B	301	2J9	CAM-SAP-NAJ	5.59	106.79	102.37
2	F	301	2J9	CAM-SAP-NAJ	5.14	106.44	102.37
2	E	301	2J9	CAM-SAP-NAJ	4.79	106.16	102.37
2	C	301	2J9	CAM-CAL-NAO	-3.28	118.86	121.57
2	D	301	2J9	CAF-CAM-SAP	-3.06	117.31	119.82
2	C	301	2J9	CAF-CAM-SAP	-2.99	117.36	119.82
2	F	301	2J9	OAA-SAP-NAJ	2.95	110.67	107.92
2	F	301	2J9	CAF-CAM-SAP	-2.90	117.44	119.82
2	E	302	2J9	CAM-CAL-NAO	-2.87	119.20	121.57
2	A	301	2J9	OAA-SAP-NAJ	2.80	110.54	107.92
2	B	301	2J9	OAA-SAP-NAJ	2.80	110.53	107.92
2	E	301	2J9	CAF-CAM-SAP	-2.79	117.53	119.82
2	A	301	2J9	CAM-CAL-NAO	-2.78	119.28	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	2J9	CAM-CAL-NAO	-2.77	119.29	121.57
2	B	301	2J9	CAK-CAF-CAM	2.72	118.71	116.86
2	A	301	2J9	CAK-CAF-CAM	2.69	118.69	116.86
2	C	301	2J9	CAK-CAF-CAM	2.66	118.67	116.86
2	B	301	2J9	CAM-CAL-NAO	-2.64	119.39	121.57
2	F	301	2J9	CAK-CAF-CAM	2.63	118.65	116.86
2	B	301	2J9	CAF-CAM-SAP	-2.61	117.68	119.82
2	G	301	2J9	CAM-CAL-NAO	-2.59	119.43	121.57
2	G	301	2J9	CAK-CAF-CAM	2.58	118.61	116.86
2	A	301	2J9	CAF-CAM-SAP	-2.58	117.71	119.82
2	E	302	2J9	CAK-CAF-CAM	2.54	118.59	116.86
2	C	301	2J9	OAA-SAP-NAJ	2.54	110.29	107.92
2	E	301	2J9	CAK-CAF-CAM	2.52	118.58	116.86
2	F	301	2J9	CAM-CAL-NAO	-2.43	119.56	121.57
2	D	301	2J9	CAK-CAF-CAM	2.41	118.50	116.86
2	G	301	2J9	OAA-SAP-NAJ	2.39	110.15	107.92
2	E	301	2J9	OAA-SAP-NAJ	2.39	110.15	107.92
2	E	302	2J9	OAA-SAP-NAJ	2.32	110.09	107.92
2	G	301	2J9	CAF-CAM-SAP	-2.29	117.94	119.82
2	D	301	2J9	OAB-SAP-NAJ	2.27	110.04	107.92
2	B	301	2J9	CAD-CAK-CAF	-2.23	120.39	123.29
2	E	301	2J9	CAM-CAL-NAO	-2.22	119.74	121.57
2	F	301	2J9	CAD-CAK-CAF	-2.19	120.44	123.29
2	E	302	2J9	CAF-CAM-SAP	-2.19	118.02	119.82
2	E	301	2J9	CAD-CAK-CAF	-2.19	120.45	123.29
2	A	301	2J9	CAD-CAK-CAF	-2.18	120.46	123.29
2	B	301	2J9	CAE-CAD-CAK	2.17	120.61	118.36
2	F	301	2J9	CAE-CAD-CAK	2.16	120.59	118.36
2	D	301	2J9	OAA-SAP-NAJ	2.14	109.92	107.92
2	G	301	2J9	CAD-CAK-CAF	-2.12	120.53	123.29
2	C	301	2J9	CAD-CAK-CAF	-2.11	120.55	123.29
2	E	301	2J9	CAE-CAD-CAK	2.08	120.52	118.36
2	G	301	2J9	CAE-CAD-CAK	2.08	120.51	118.36
2	E	301	2J9	OAB-SAP-NAJ	2.07	109.85	107.92
2	E	302	2J9	CAE-CAD-CAK	2.06	120.50	118.36
2	D	301	2J9	CAE-CAD-CAK	2.05	120.48	118.36
2	E	302	2J9	CAD-CAK-CAF	-2.05	120.63	123.29
2	D	301	2J9	CAD-CAK-CAF	-2.02	120.67	123.29
2	A	301	2J9	CAE-CAD-CAK	2.00	120.44	118.36

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	2J9	CAH-CAN-NAO-CAL
2	B	301	2J9	CAH-CAN-NAO-CAL
2	C	301	2J9	CAH-CAN-NAO-CAL
2	D	301	2J9	CAH-CAN-NAO-CAL
2	E	301	2J9	CAH-CAN-NAO-CAL
2	E	302	2J9	CAH-CAN-NAO-CAL
2	F	301	2J9	CAH-CAN-NAO-CAL
2	G	301	2J9	CAH-CAN-NAO-CAL
4	C	304	GOL	C1-C2-C3-O3
4	C	304	GOL	O1-C1-C2-C3
4	H	303	GOL	C1-C2-C3-O3
4	C	304	GOL	O2-C2-C3-O3
4	B	304	GOL	O1-C1-C2-C3
7	E	317	KAI	CA-CB-CB1-CG1
7	G	308	KAI	O-C-CA-N
4	H	303	GOL	O2-C2-C3-O3
7	G	308	KAI	OXT-C-CA-N
4	E	310	GOL	C1-C2-C3-O3
7	A	310	KAI	CB-CB1-CG1-OD1
4	B	304	GOL	O1-C1-C2-O2
4	C	304	GOL	O1-C1-C2-O2
7	D	308	KAI	CB-CB1-CG1-OD1
7	H	308	KAI	O-C-CA-CB
7	A	310	KAI	CB-CB1-CG1-OD2
7	D	308	KAI	CB-CB1-CG1-OD2
7	H	308	KAI	CB-CB1-CG1-OD1
7	F	308	KAI	CA-CB-CB1-CG1
7	H	308	KAI	CA-CB-CB1-CG1
7	H	308	KAI	OXT-C-CA-CB

There are no ring outliers.

14 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	304	GOL	2	0
2	A	301	2J9	2	0
4	H	303	GOL	1	0
6	D	307	SO4	1	0
4	E	311	GOL	1	0
6	G	307	SO4	1	0
4	A	304	GOL	2	0
2	G	301	2J9	1	0
2	F	301	2J9	1	0

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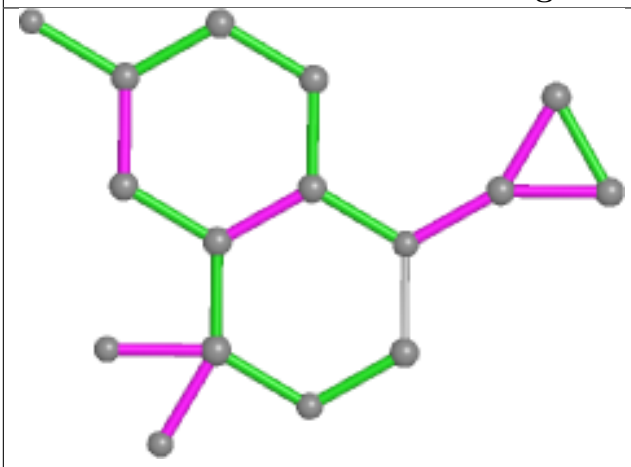
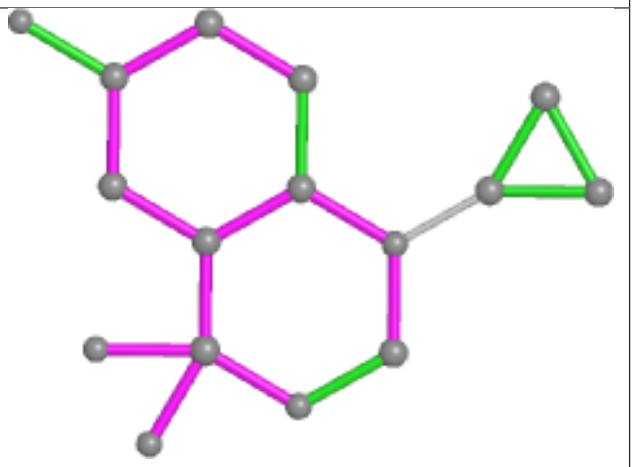
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	309	SO4	1	0
2	E	302	2J9	1	0
4	E	313	GOL	1	0
2	D	301	2J9	1	0
4	D	305	GOL	1	0

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 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.

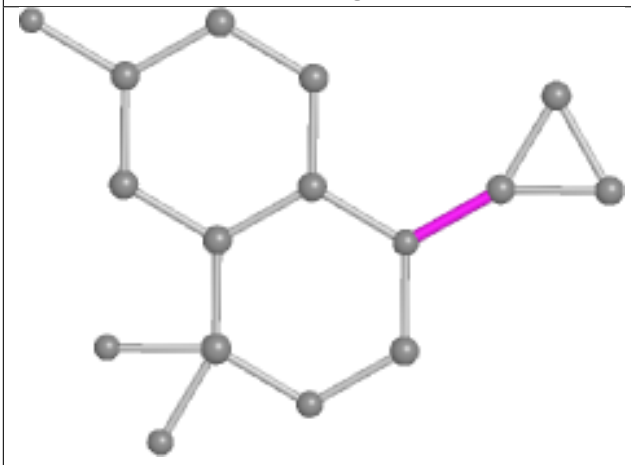
Ligand 2J9 E 301



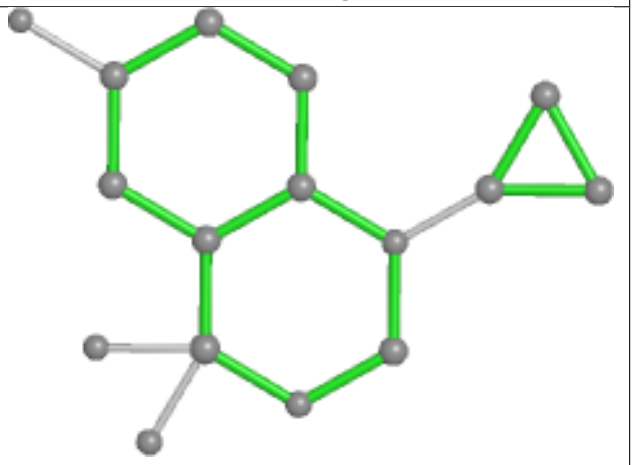
Bond lengths



Bond angles

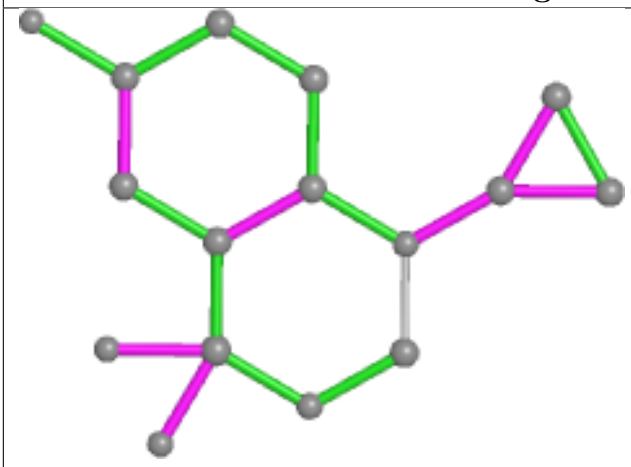


Torsions

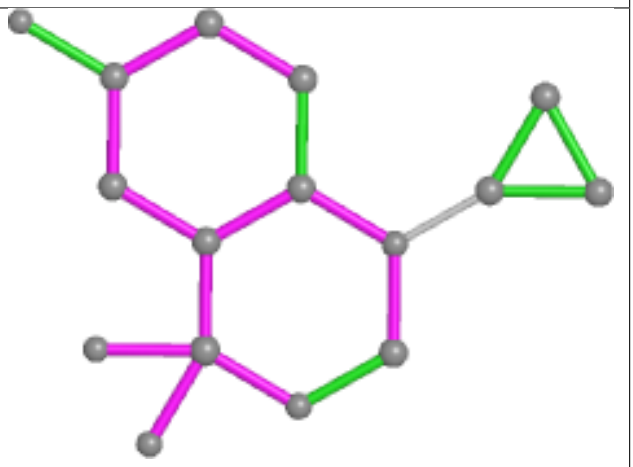


Rings

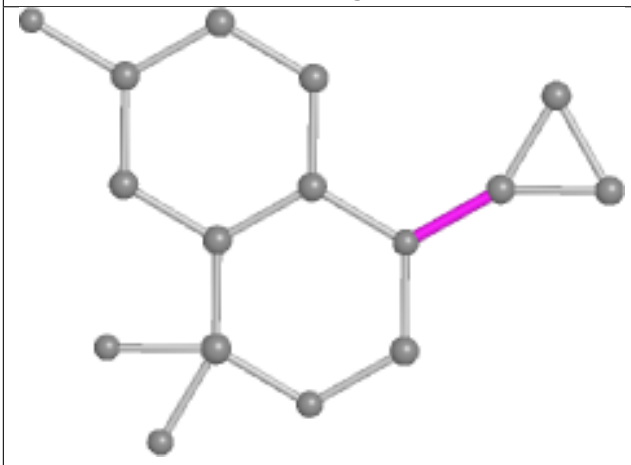
Ligand 2J9 A 301



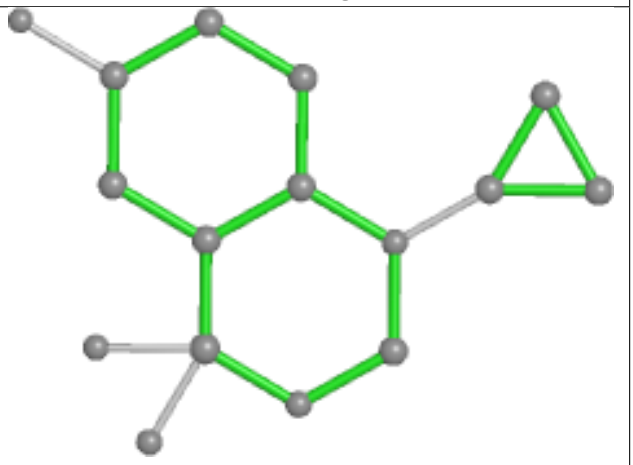
Bond lengths



Bond angles

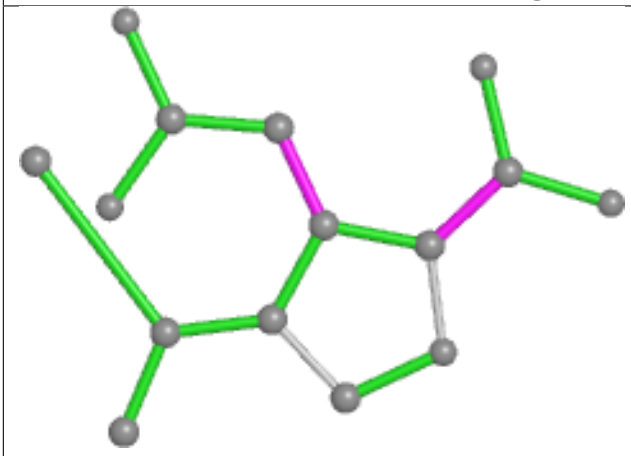


Torsions

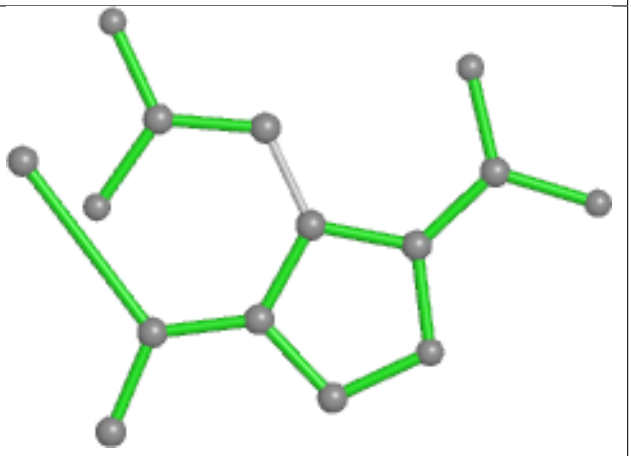


Rings

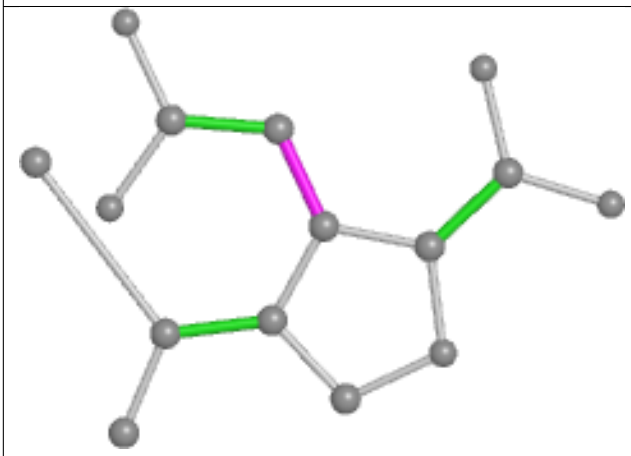
Ligand KAI E 317



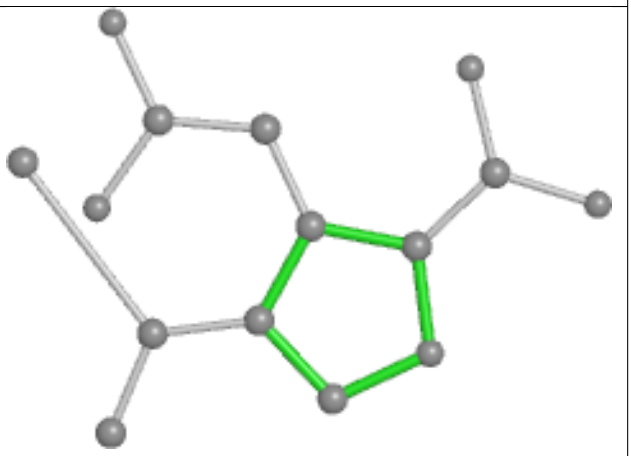
Bond lengths



Bond angles

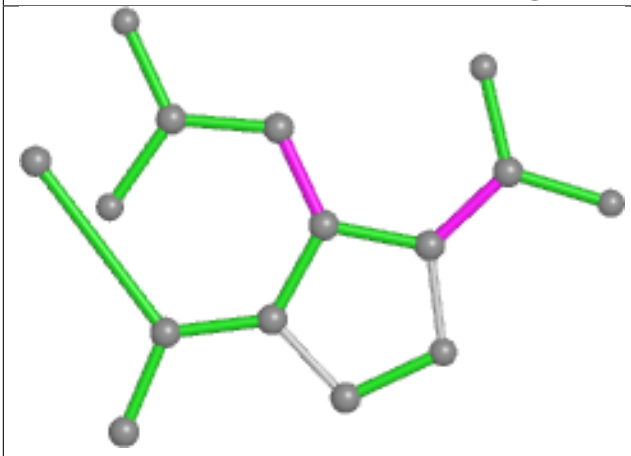


Torsions



Rings

Ligand KAI G 308



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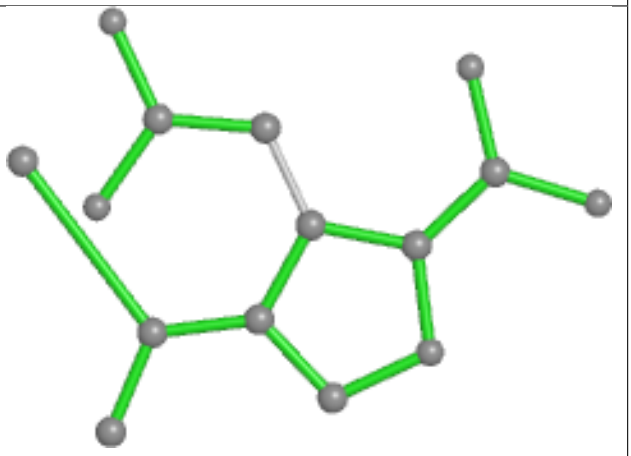

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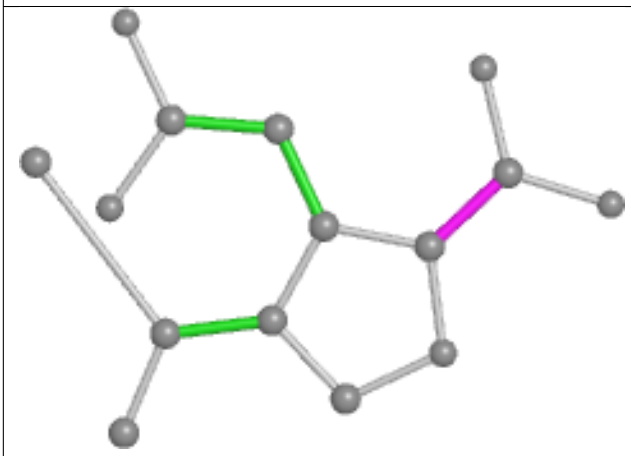

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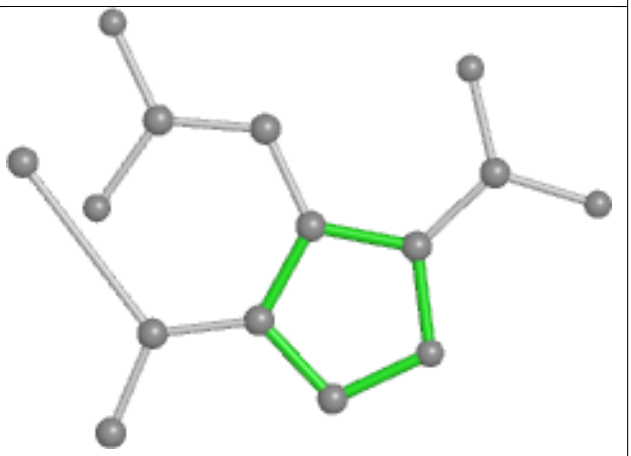
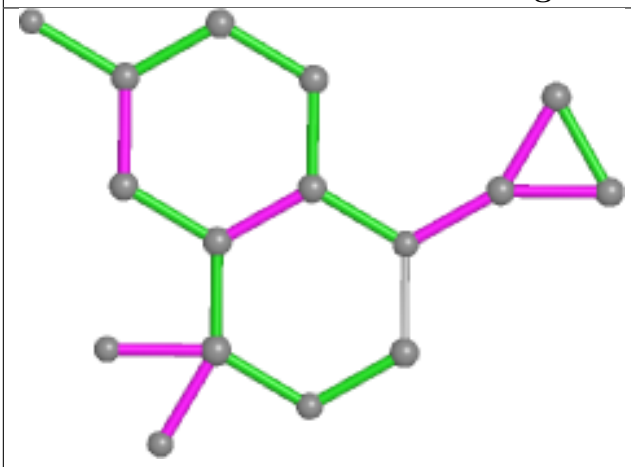


Rings

Ligand 2J9 C 301



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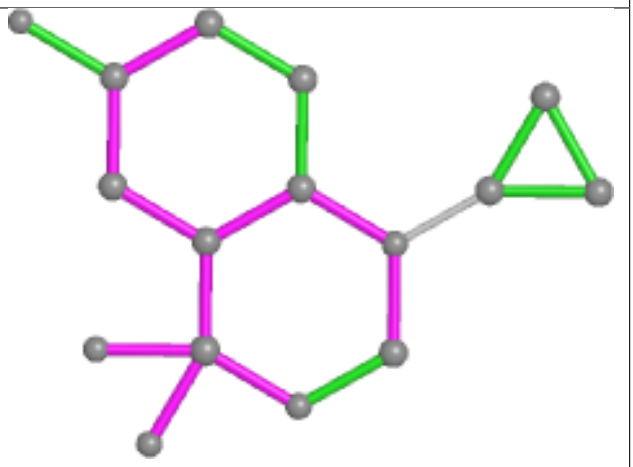
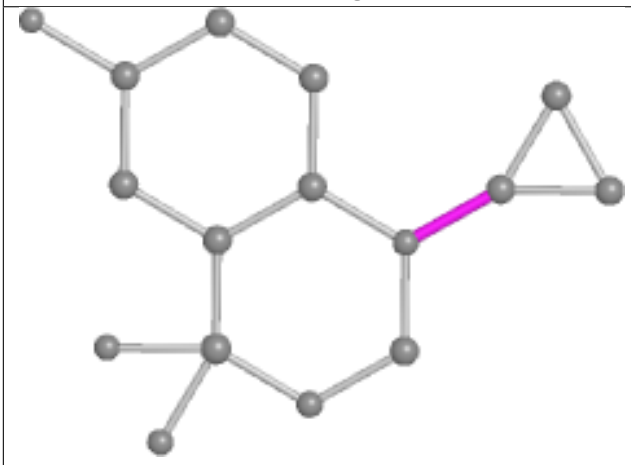


Bond angles



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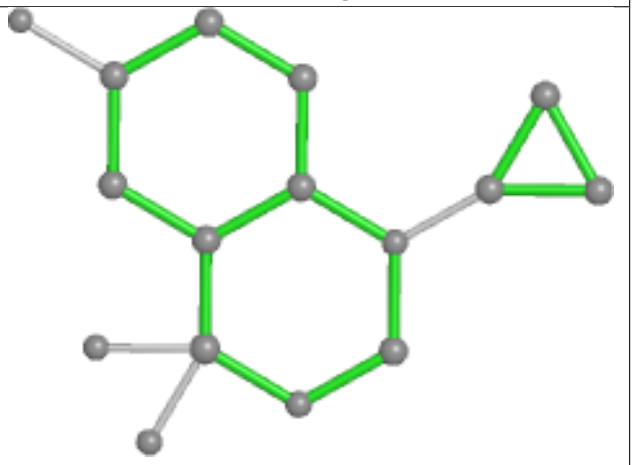
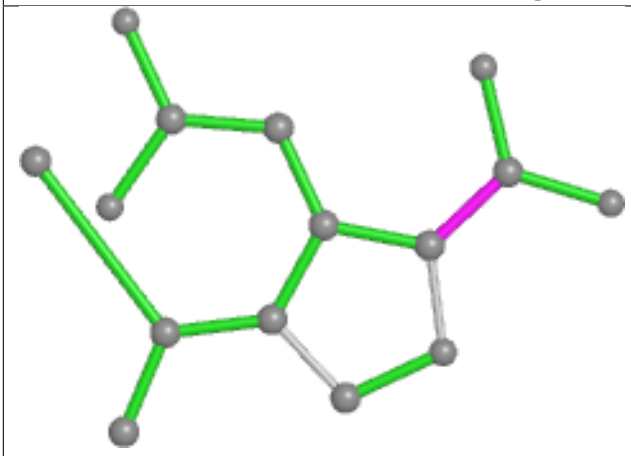


Rings

Ligand KAI F 308



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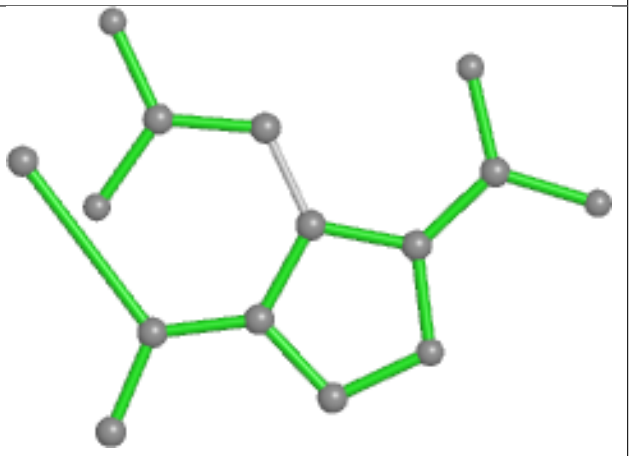
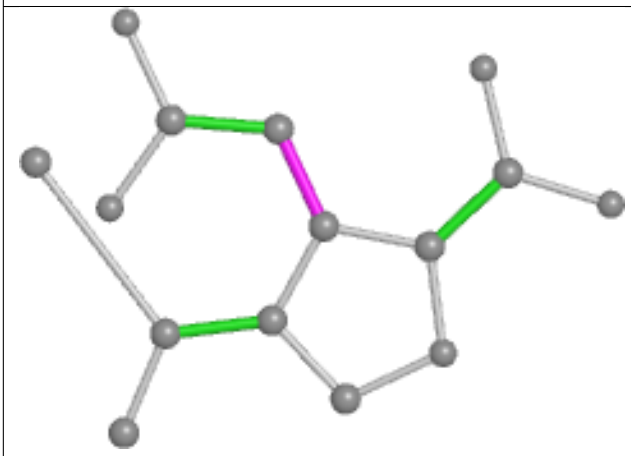


Bond angles



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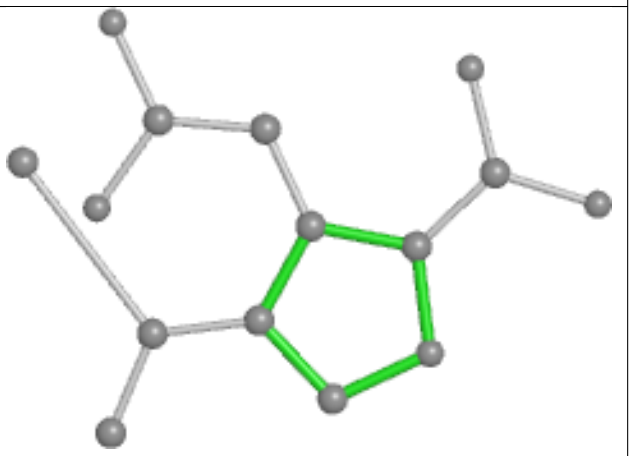
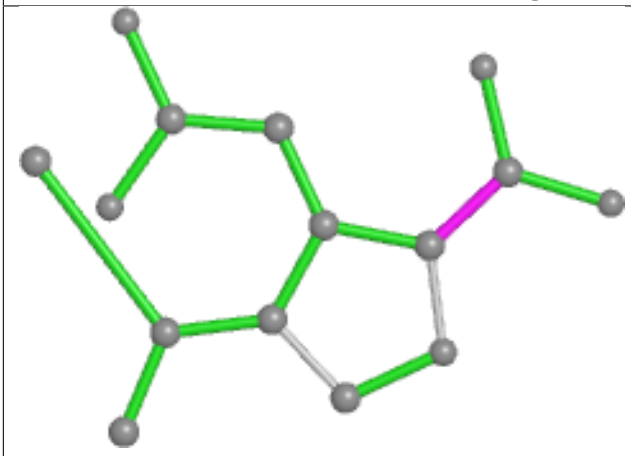
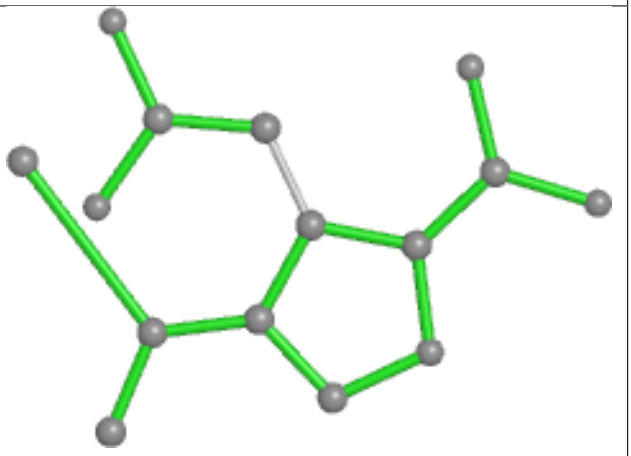


Rings

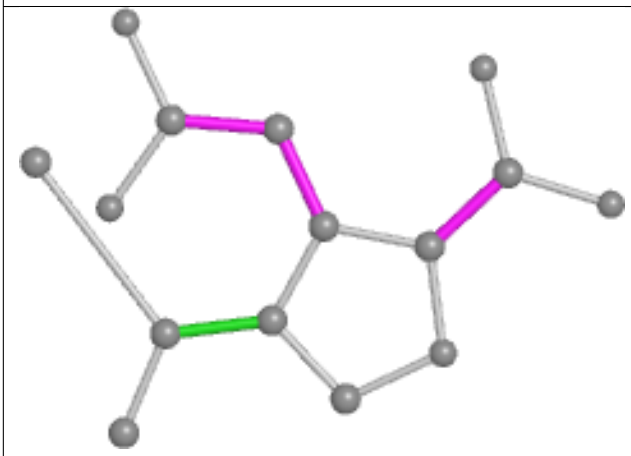
Ligand KAI H 308



Bond lengths



Bond angles



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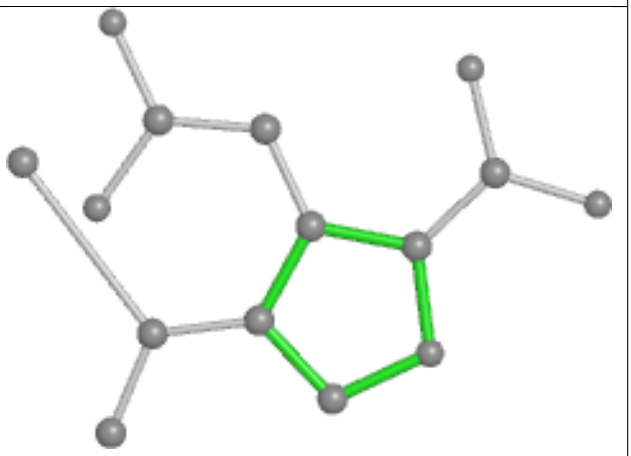
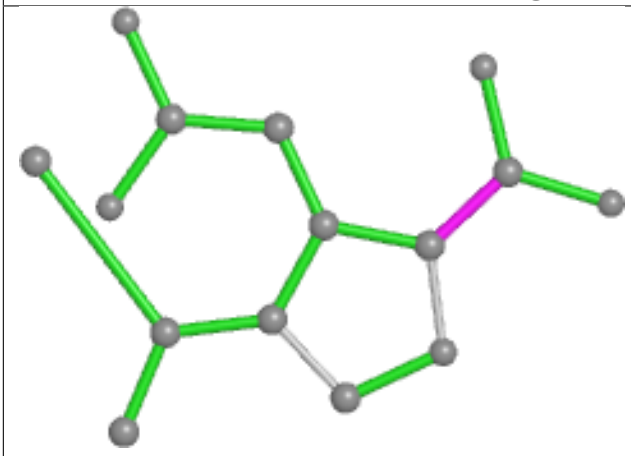


Rings

Ligand KAI C 310



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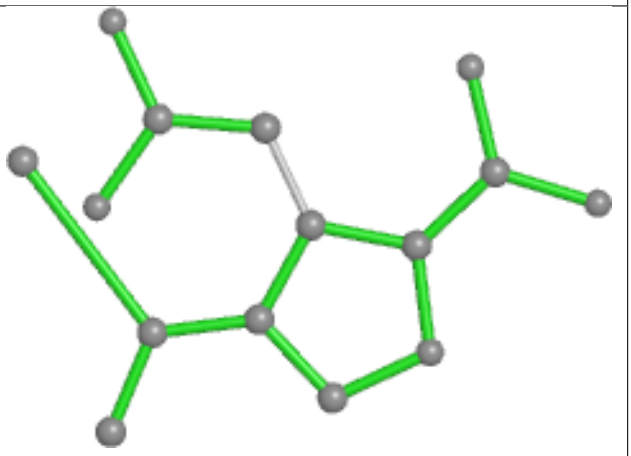
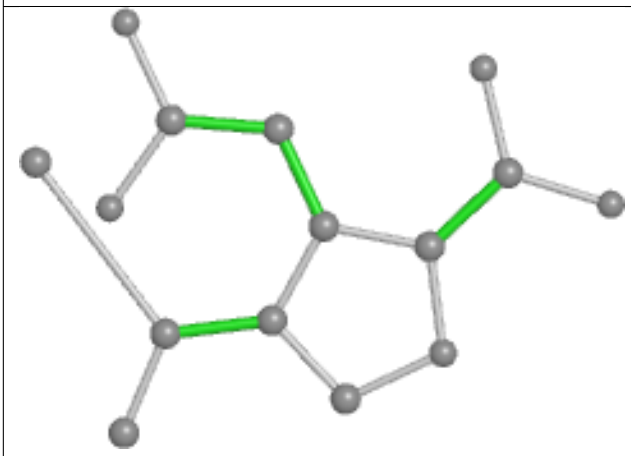


Bond angles



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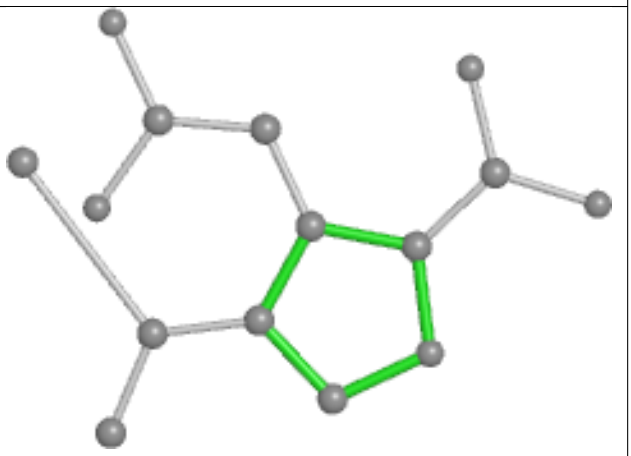
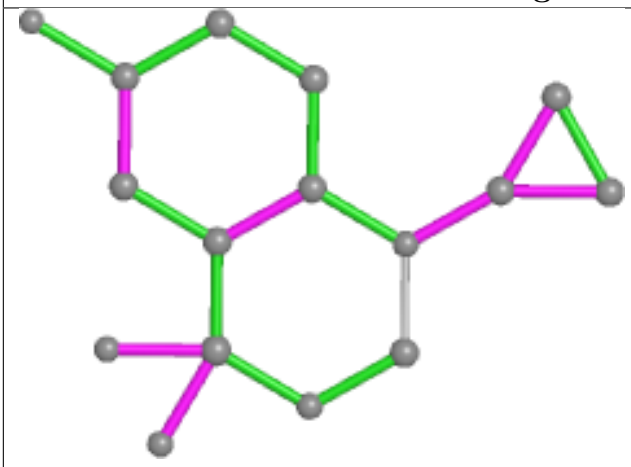


Rings

Ligand 2J9 G 301



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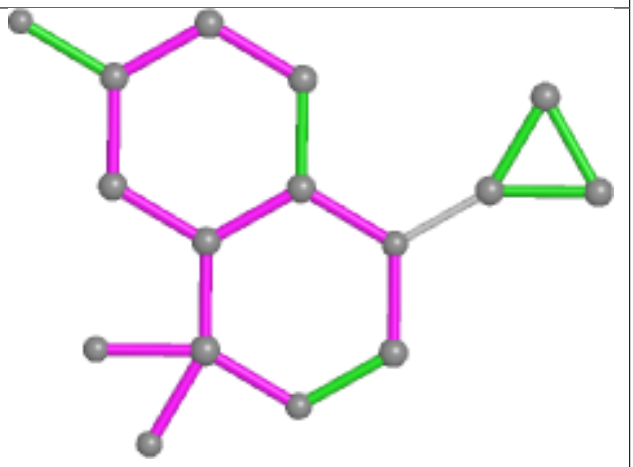
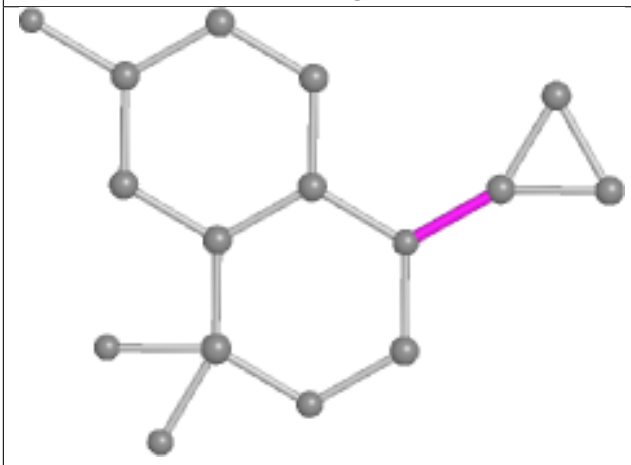


Bond angles



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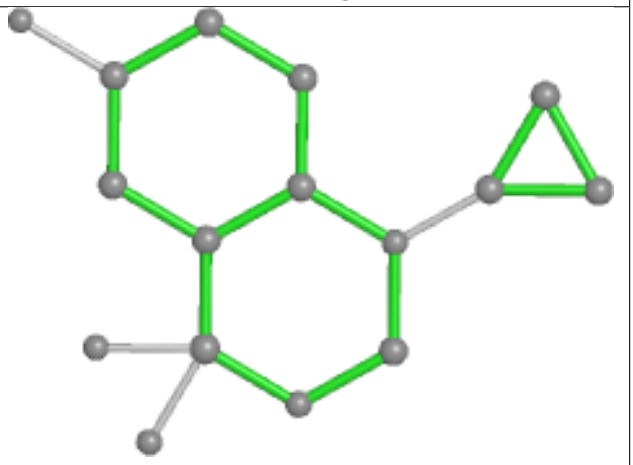
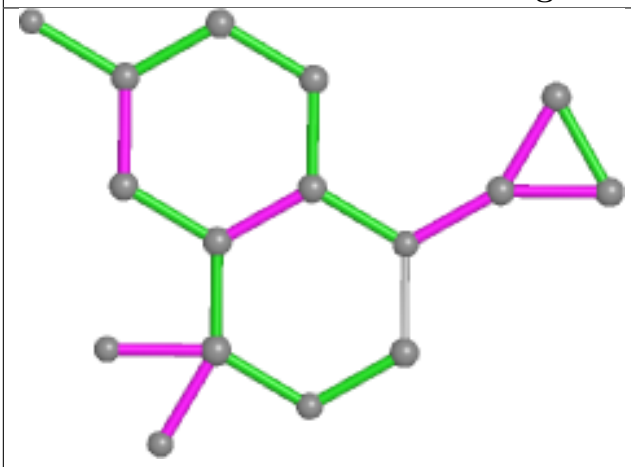


Rings

Ligand 2J9 F 301



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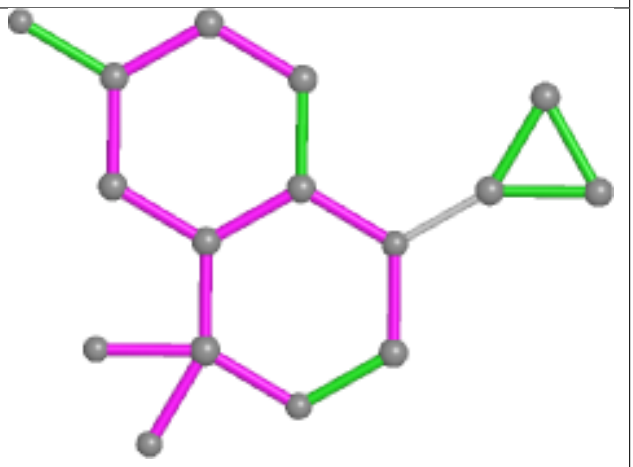
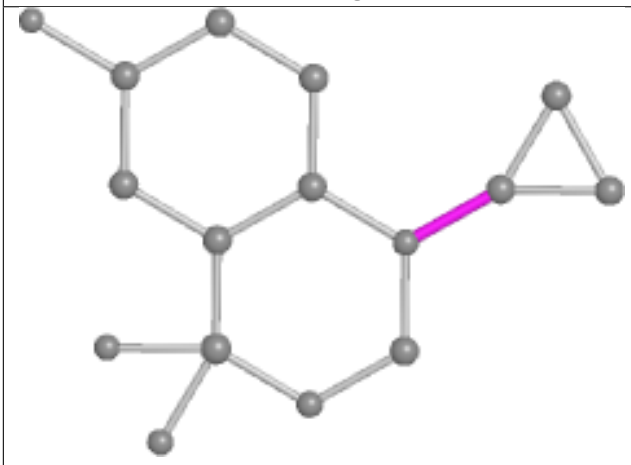
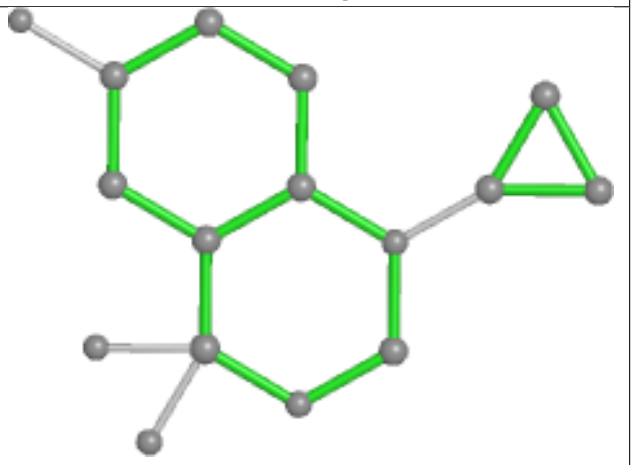


Bond angles

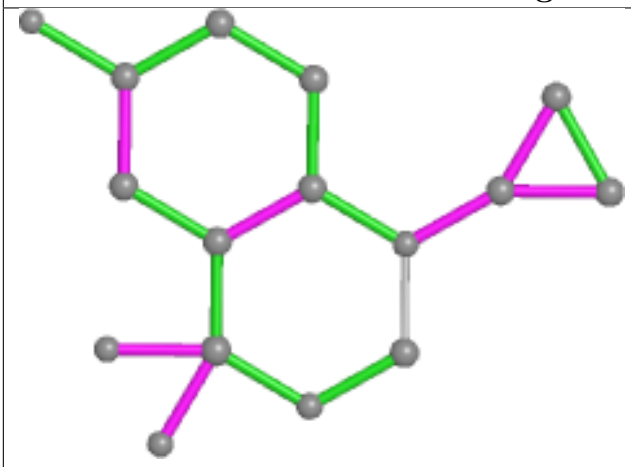


Torsions

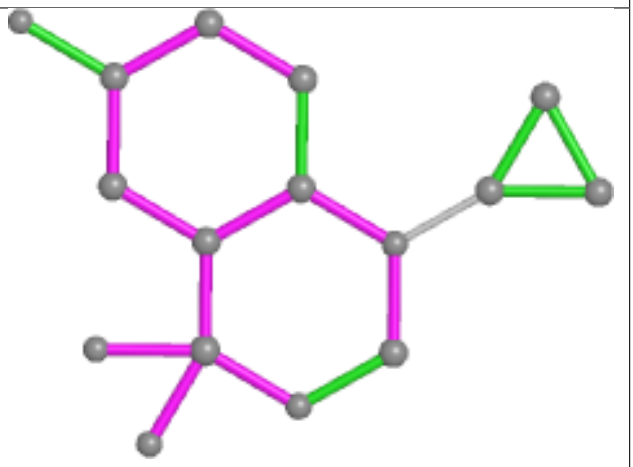


Rings

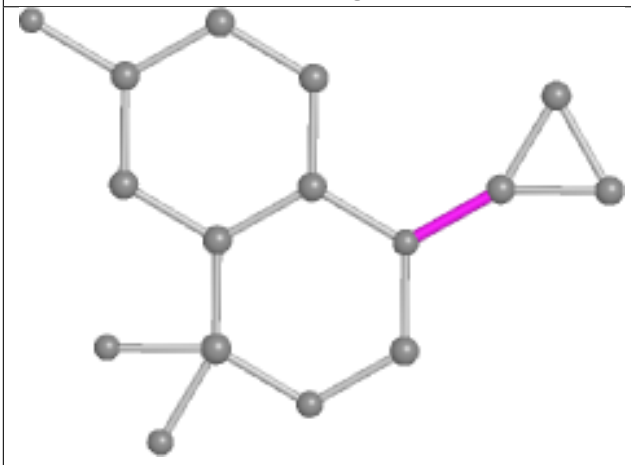
Ligand 2J9 E 302



Bond lengths



Bond angles



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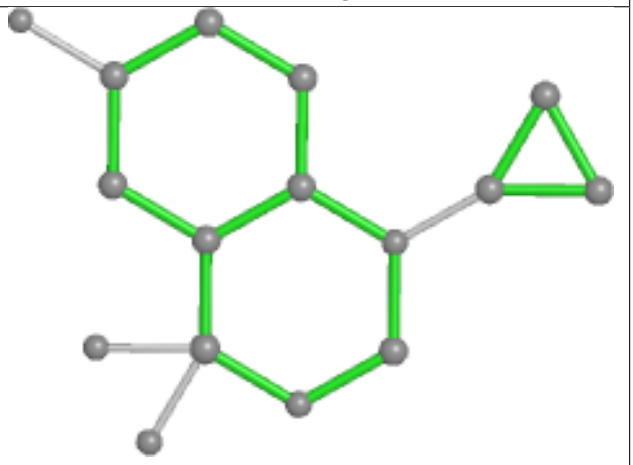
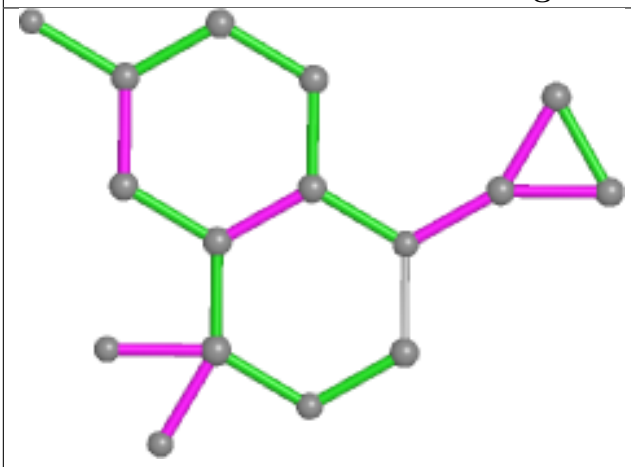


Rings

Ligand 2J9 D 301



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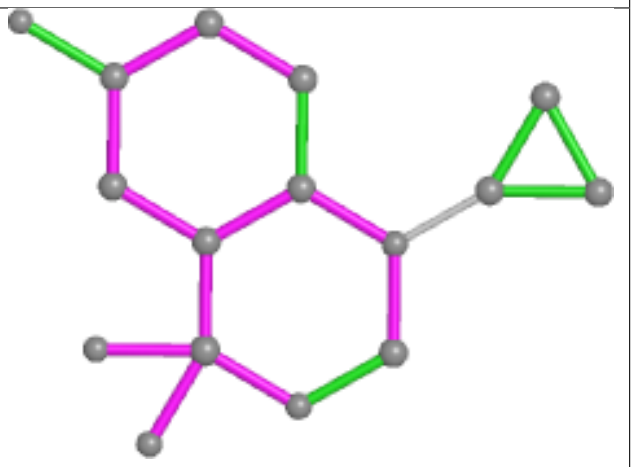
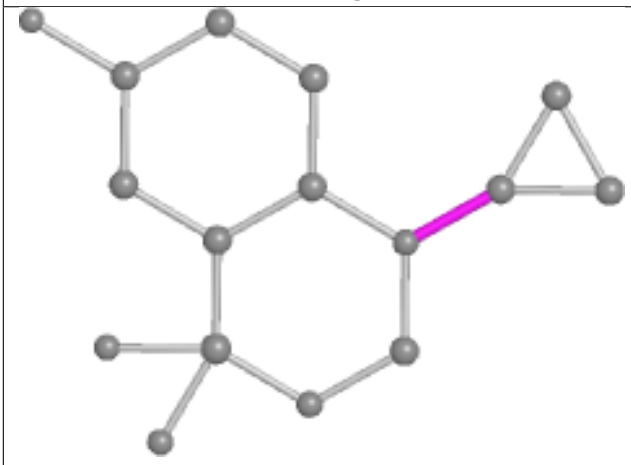
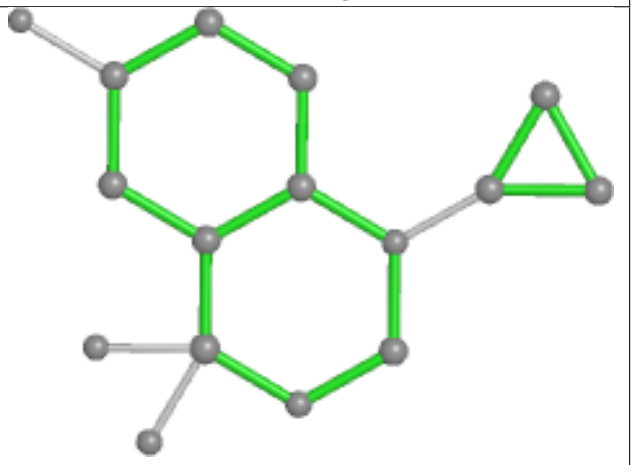


Bond angles

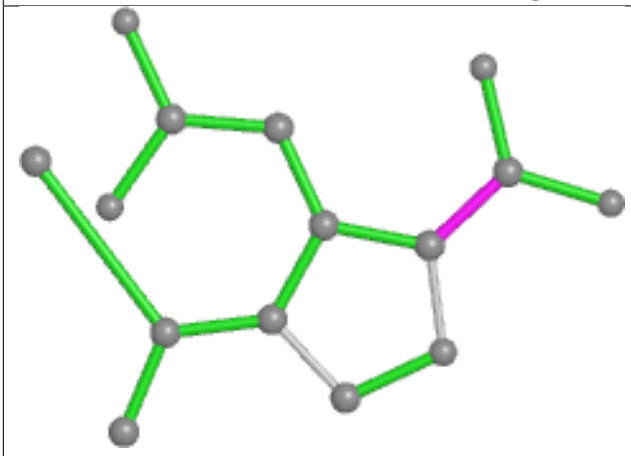


Torsions



Rings

Ligand KAI A 310



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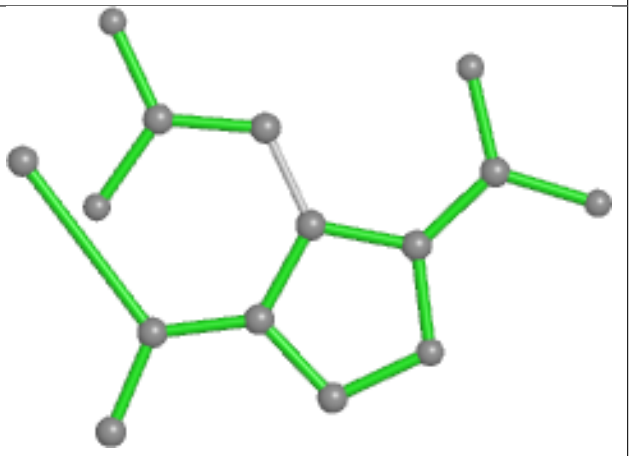
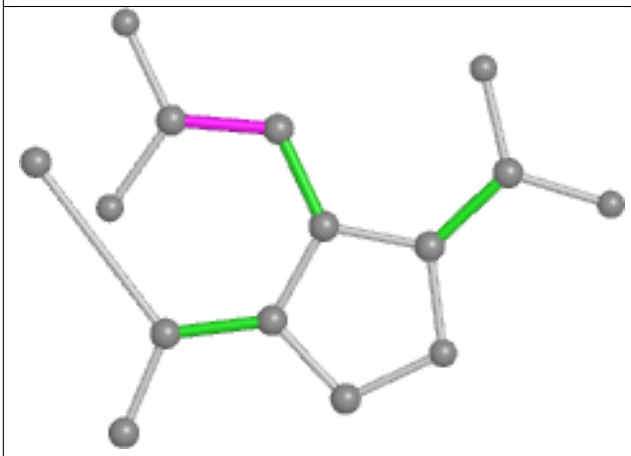
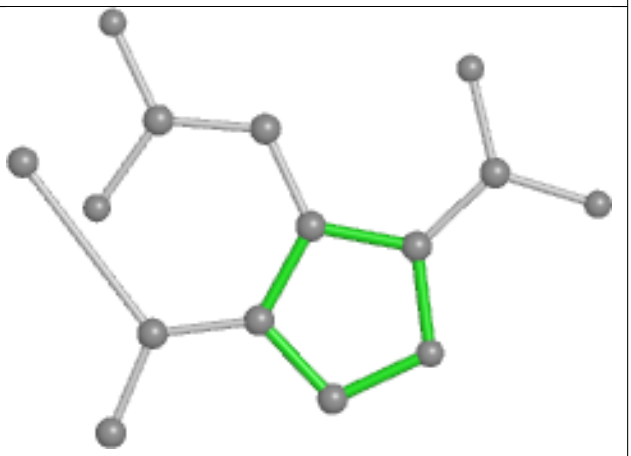


Bond angles

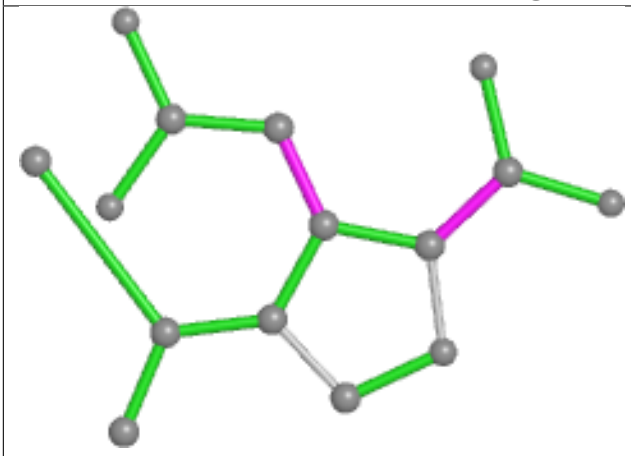


Torsions

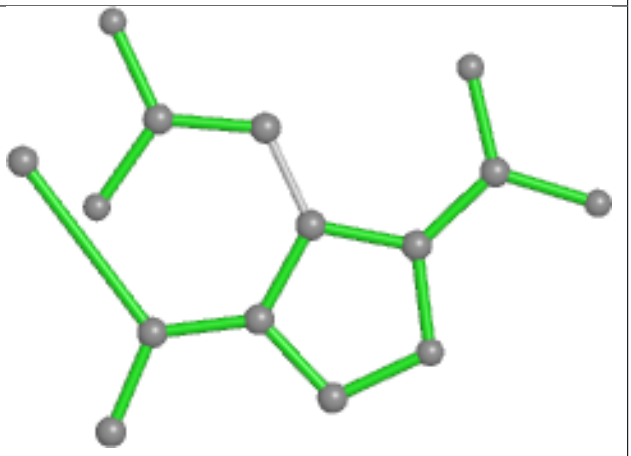


Rings

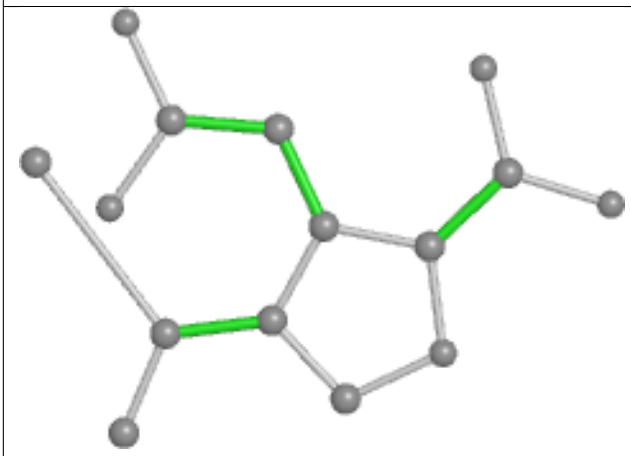
Ligand KAI B 310



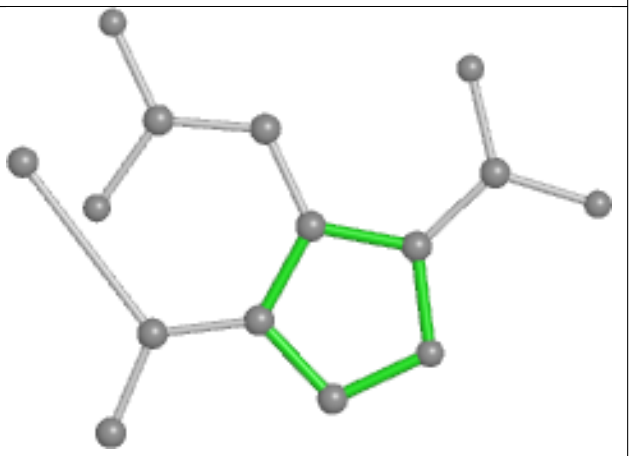
Bond lengths



Bond angles

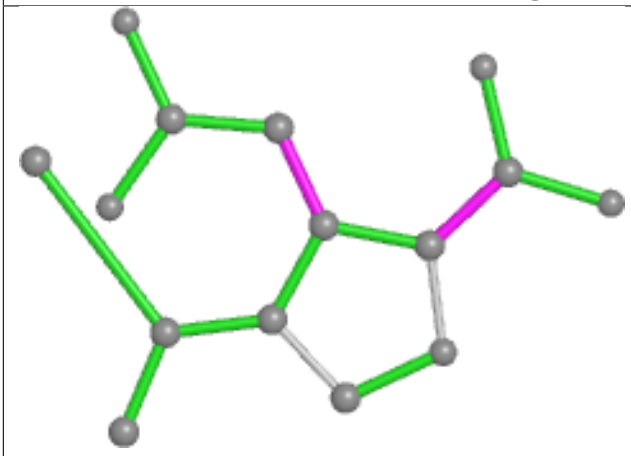


Torsions

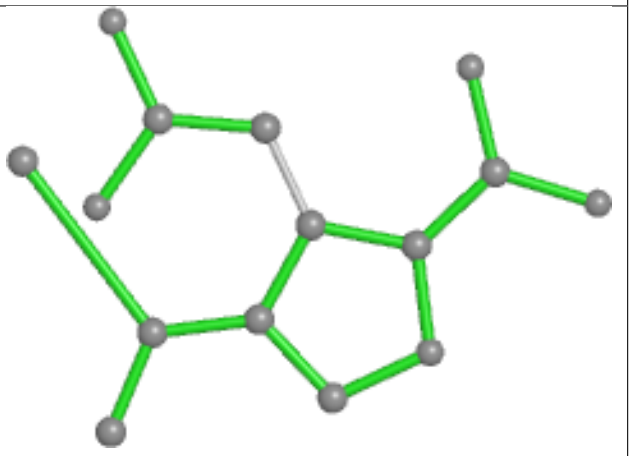


Rings

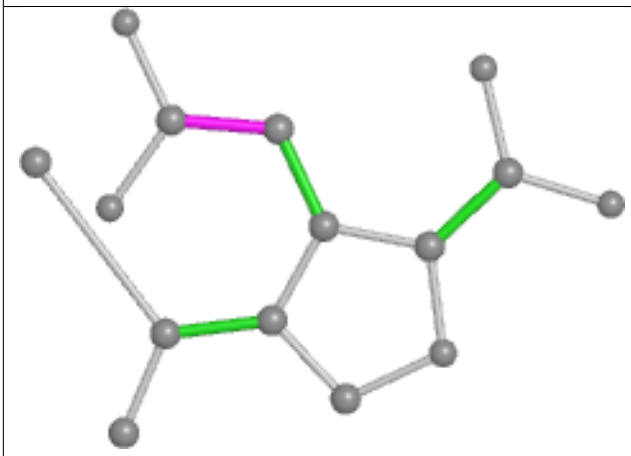
Ligand KAI D 308



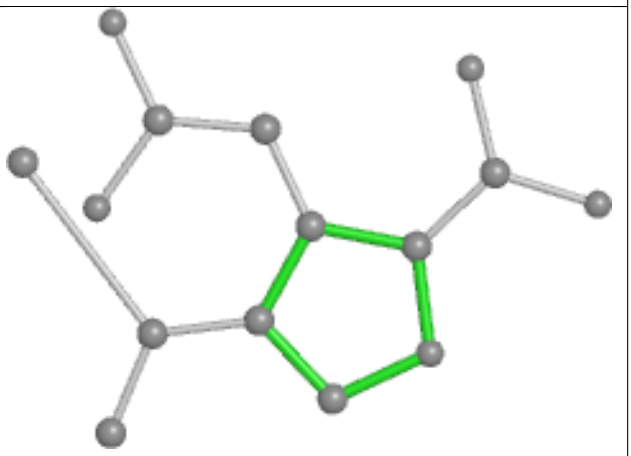
Bond lengths



Bond angles

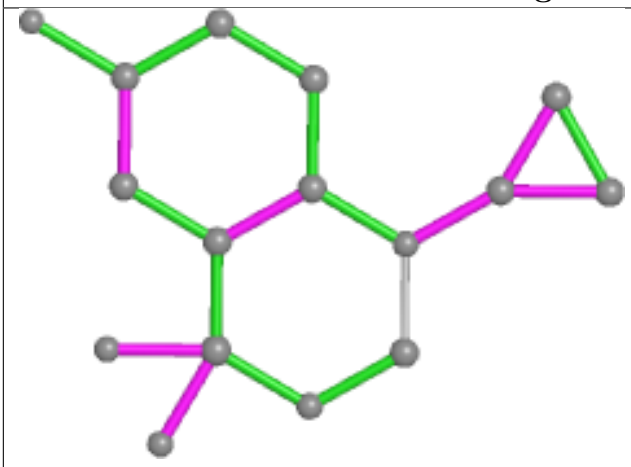


Torsions

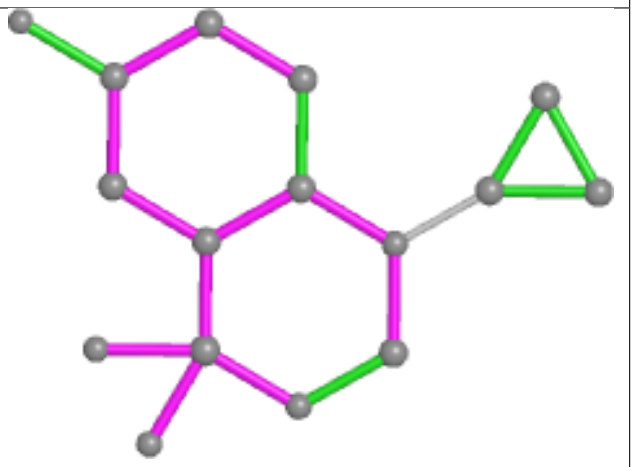


Rings

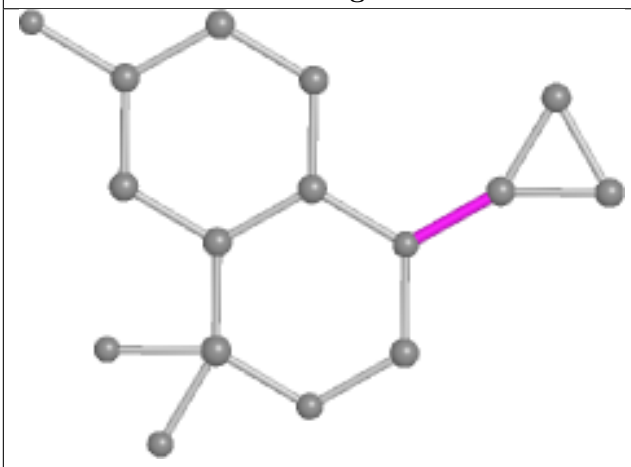
Ligand 2J9 B 301



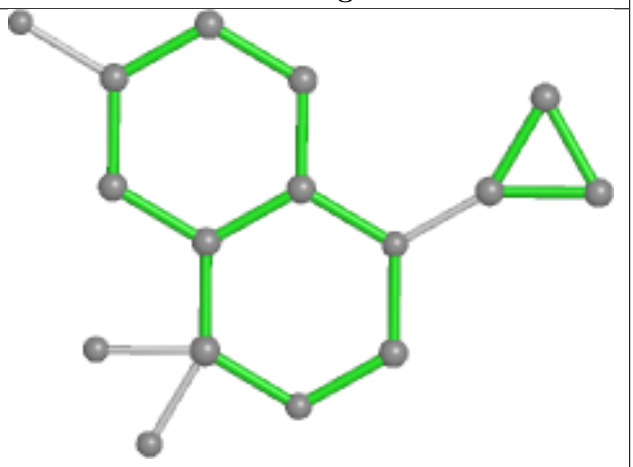
Bond lengths



Bond angles



Torsions



Rings

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	252/258 (97%)	0.05	10 (3%)	38	33	21, 36, 61, 68	0
1	B	247/258 (95%)	-0.22	1 (0%)	92	93	22, 31, 44, 58	0
1	C	252/258 (97%)	-0.05	4 (1%)	72	71	23, 37, 55, 75	0
1	D	253/258 (98%)	-0.14	5 (1%)	65	63	20, 30, 51, 60	0
1	E	247/258 (95%)	-0.13	2 (0%)	86	86	19, 29, 52, 58	0
1	F	248/258 (96%)	-0.08	3 (1%)	79	79	26, 36, 53, 74	0
1	G	253/258 (98%)	0.10	9 (3%)	42	37	28, 46, 61, 71	0
1	H	248/258 (96%)	-0.05	8 (3%)	47	43	19, 30, 56, 67	0
All	All	2000/2064 (96%)	-0.07	42 (2%)	63	61	19, 35, 57, 75	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	121	PRO	4.1
1	C	258	PRO	4.1
1	A	258	PRO	3.9
1	A	27	THR	3.8
1	F	25	ASP	3.8
1	C	23	LYS	3.8
1	A	116	TYR	3.7
1	A	257	CYS	3.6
1	F	68	ASP	3.5
1	D	167	PRO	3.4
1	G	256	GLY	3.4
1	A	256	GLY	3.3
1	G	258	PRO	3.1
1	A	122	ILE	3.0
1	G	167	PRO	2.8
1	C	25	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	121	PRO	2.6
1	H	167	PRO	2.6
1	E	253	ARG	2.6
1	H	132	THR	2.6
1	H	185	ASP	2.6
1	G	29	TYR	2.5
1	C	166	LYS	2.4
1	D	184	ALA	2.4
1	A	121	PRO	2.3
1	H	166	LYS	2.3
1	G	185	ASP	2.3
1	G	255	SER	2.3
1	D	185	ASP	2.3
1	H	122	ILE	2.3
1	H	133	LYS	2.3
1	G	68	ASP	2.2
1	A	69	LYS	2.2
1	B	27	THR	2.2
1	E	165	SER	2.1
1	H	118	LYS	2.1
1	D	165	SER	2.1
1	G	253	ARG	2.1
1	A	123	ASP	2.1
1	D	253	ARG	2.0
1	A	167	PRO	2.0
1	F	167	PRO	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 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
5	CL	F	306	1/1	0.62	0.21	47,47,47,47	0
3	ZN	C	303[A]	1/1	0.67	0.18	39,39,39,39	1
6	SO4	B	309	5/5	0.69	0.33	44,44,44,44	5
4	GOL	E	310	6/6	0.70	0.35	29,29,29,29	0
3	ZN	B	303	1/1	0.71	0.10	55,55,55,55	1
3	ZN	D	302[A]	1/1	0.75	0.10	45,45,45,45	1
4	GOL	E	312	6/6	0.77	0.34	30,30,30,30	0
3	ZN	G	303[A]	1/1	0.78	0.19	40,40,40,40	1
4	GOL	H	303	6/6	0.79	0.31	24,24,24,24	0
5	CL	C	309	1/1	0.79	0.25	69,69,69,69	0
3	ZN	F	302[B]	1/1	0.80	0.17	47,47,47,47	1
4	GOL	D	304	6/6	0.81	0.25	32,32,32,32	0
4	GOL	A	304	6/6	0.81	0.27	35,35,35,35	0
5	CL	B	308	1/1	0.81	0.23	48,48,48,48	0
6	SO4	G	307	5/5	0.81	0.20	54,54,54,54	0
8	ACT	F	309	4/4	0.81	0.22	44,44,44,44	0
8	ACT	A	311	4/4	0.83	0.21	44,44,44,44	0
4	GOL	C	305	6/6	0.83	0.27	37,37,37,37	0
5	CL	B	306	1/1	0.85	0.16	35,35,35,35	0
3	ZN	E	303[A]	1/1	0.85	0.10	38,38,38,38	1
3	ZN	F	303[A]	1/1	0.86	0.11	48,48,48,48	1
5	CL	C	308	1/1	0.86	0.09	35,35,35,35	0
6	SO4	E	316	5/5	0.87	0.20	40,40,40,40	5
4	GOL	C	304	6/6	0.87	0.31	27,27,27,27	0
6	SO4	A	308	5/5	0.88	0.30	32,32,32,32	5
4	GOL	B	304	6/6	0.88	0.23	33,33,33,33	0
4	GOL	E	314	6/6	0.88	0.50	47,47,47,47	0
8	ACT	B	311	4/4	0.89	0.20	34,34,34,34	0
3	ZN	E	304[B]	1/1	0.89	0.07	44,44,44,44	1
4	GOL	D	305	6/6	0.90	0.18	26,26,26,26	0
3	ZN	E	305[A]	1/1	0.90	0.14	47,47,47,47	1
5	CL	G	305	1/1	0.90	0.12	52,52,52,52	0
3	ZN	A	303	1/1	0.90	0.08	57,57,57,57	1
3	ZN	D	303[B]	1/1	0.90	0.20	44,44,44,44	1
4	GOL	E	313	6/6	0.91	0.22	26,26,26,26	0
3	ZN	E	308[A]	1/1	0.91	0.10	44,44,44,44	1
3	ZN	E	306[B]	1/1	0.92	0.16	29,29,29,29	1
5	CL	C	306	1/1	0.92	0.18	44,44,44,44	0
3	ZN	C	302[B]	1/1	0.92	0.13	39,39,39,39	1
4	GOL	E	311	6/6	0.92	0.18	30,30,30,30	0
7	KAI	C	310	15/15	0.92	0.21	29,29,29,29	0
5	CL	A	307	1/1	0.92	0.19	37,37,37,37	0
3	ZN	G	302[B]	1/1	0.92	0.15	40,40,40,40	1

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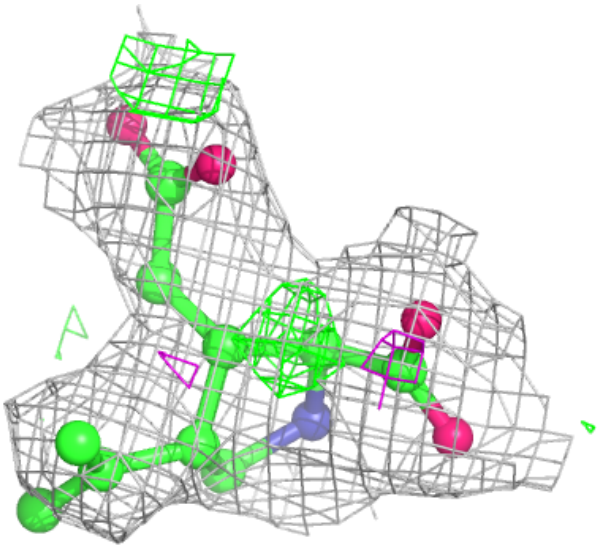
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	H	306	1/1	0.92	0.33	44,44,44,44	0
5	CL	C	307	1/1	0.93	0.24	52,52,52,52	0
5	CL	H	305	1/1	0.93	0.16	34,34,34,34	0
5	CL	F	305	1/1	0.93	0.13	34,34,34,34	0
7	KAI	D	308	15/15	0.93	0.17	26,26,26,26	0
7	KAI	E	317	15/15	0.93	0.18	25,25,25,25	0
3	ZN	H	302[B]	1/1	0.93	0.09	34,34,34,34	1
6	SO4	A	309	5/5	0.93	0.24	62,62,62,62	0
5	CL	G	304	1/1	0.93	0.10	47,47,47,47	0
5	CL	F	304	1/1	0.94	0.11	45,45,45,45	0
6	SO4	D	306	5/5	0.94	0.17	28,28,28,28	5
6	SO4	D	307	5/5	0.94	0.17	37,37,37,37	5
7	KAI	F	308	15/15	0.94	0.18	30,30,30,30	0
7	KAI	G	308	15/15	0.94	0.15	38,38,38,38	0
5	CL	A	306	1/1	0.94	0.14	51,51,51,51	0
4	GOL	E	309	6/6	0.94	0.26	27,27,27,27	0
7	KAI	B	310	15/15	0.94	0.21	26,26,26,26	0
3	ZN	A	302[A]	1/1	0.95	0.10	41,41,41,41	1
6	SO4	H	307	5/5	0.95	0.11	38,38,38,38	0
7	KAI	A	310	15/15	0.95	0.19	28,28,28,28	0
5	CL	B	307	1/1	0.95	0.32	51,51,51,51	0
3	ZN	H	301[A]	1/1	0.95	0.10	32,32,32,32	1
5	CL	B	305	1/1	0.95	0.12	32,32,32,32	0
7	KAI	H	308	15/15	0.96	0.15	26,26,26,26	0
5	CL	H	304	1/1	0.96	0.11	35,35,35,35	0
3	ZN	E	307[A]	1/1	0.96	0.12	29,29,29,29	1
5	CL	G	306	1/1	0.96	0.15	38,38,38,38	0
2	2J9	E	301	16/16	0.97	0.20	21,21,21,21	0
5	CL	F	307	1/1	0.97	0.12	34,34,34,34	0
2	2J9	G	301	16/16	0.97	0.19	26,26,26,26	0
2	2J9	B	301	16/16	0.98	0.17	23,23,23,23	0
2	2J9	C	301	16/16	0.98	0.18	22,22,22,22	0
5	CL	E	315	1/1	0.98	0.09	24,24,24,24	0
2	2J9	D	301	16/16	0.98	0.18	21,21,21,21	0
3	ZN	B	302	1/1	0.98	0.10	38,38,38,38	0
2	2J9	A	301	16/16	0.98	0.17	22,22,22,22	0
2	2J9	E	302	16/16	0.98	0.19	20,20,20,20	0
2	2J9	F	301	16/16	0.98	0.16	27,27,27,27	0
5	CL	A	305	1/1	0.99	0.07	25,25,25,25	0

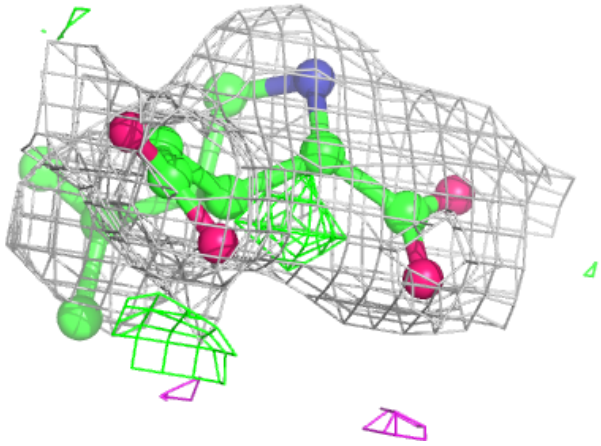
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

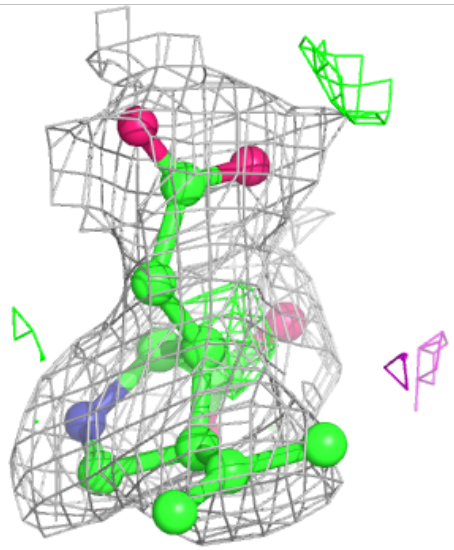
orientation to approximate a three-dimensional view.

Electron density around KAI C 310:

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

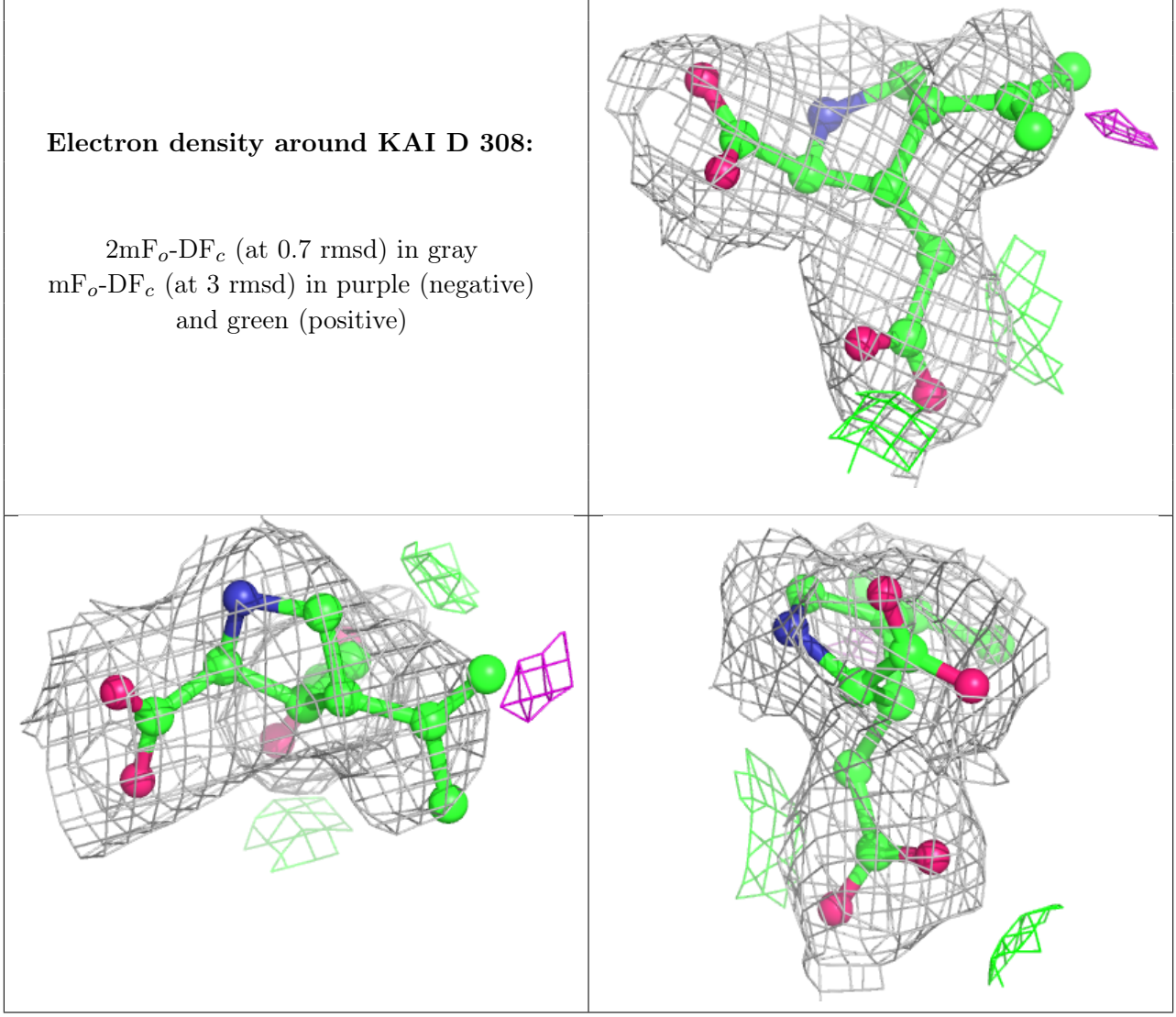






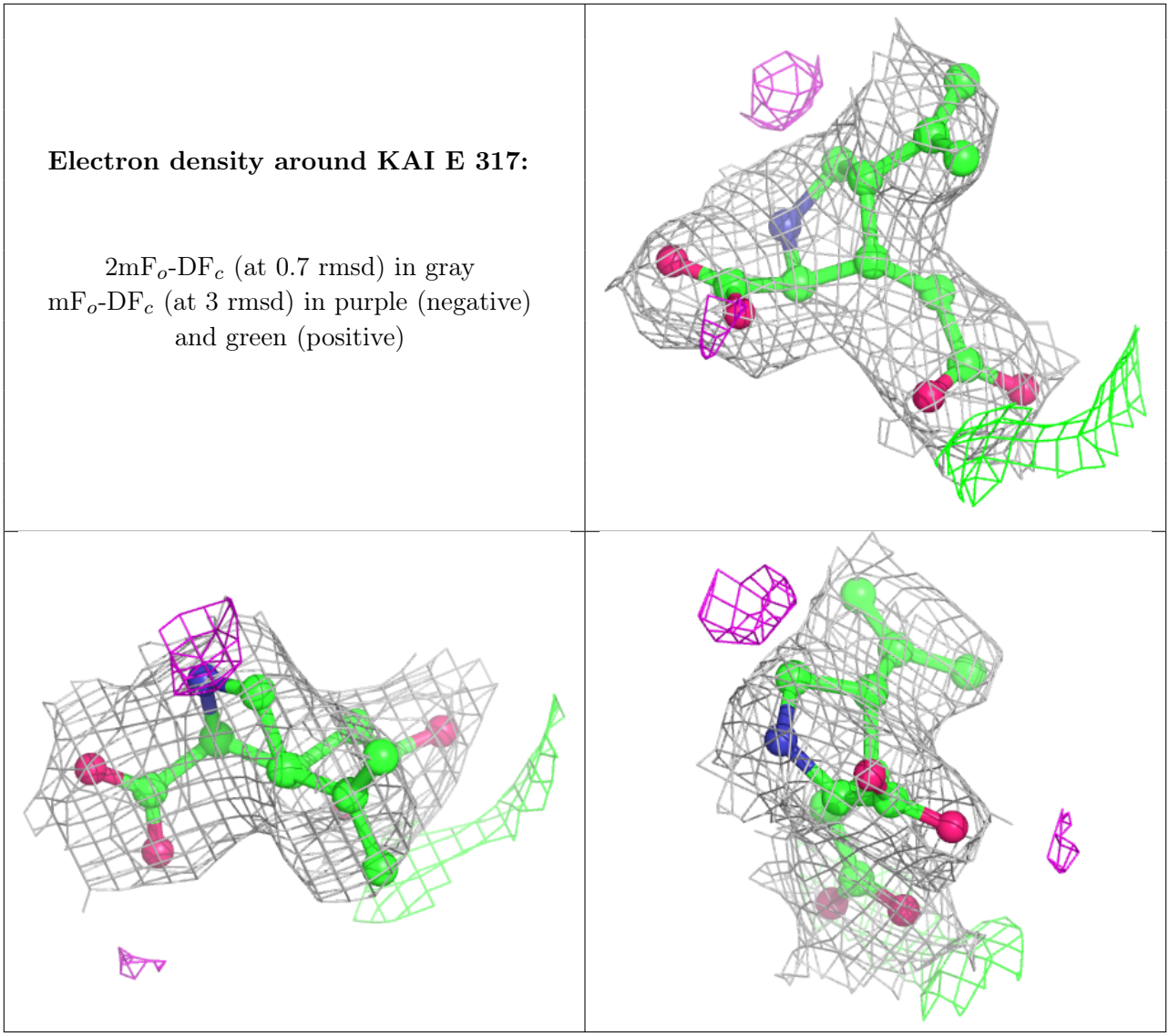
Electron density around KAI D 308:

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



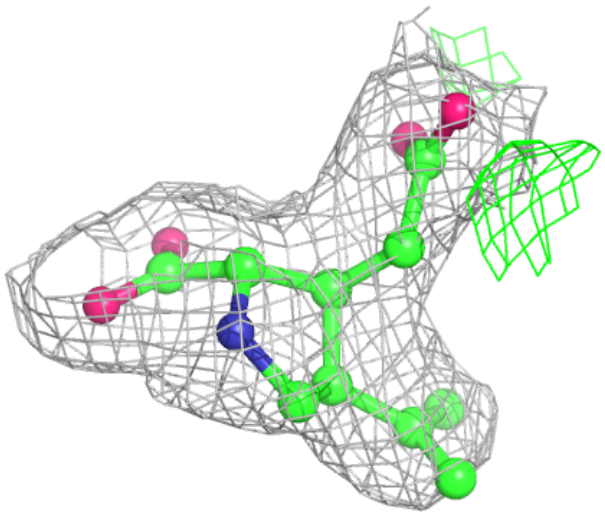
Electron density around KAI E 317:

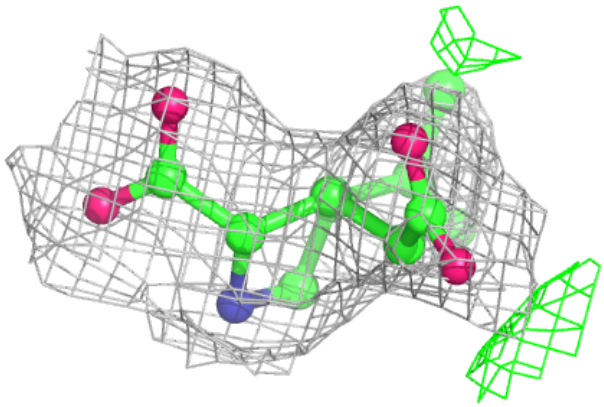
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

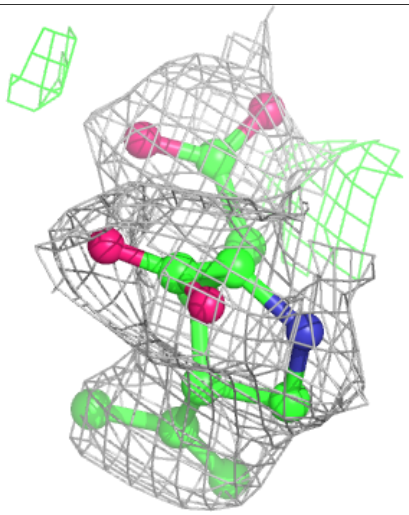


Electron density around KAI F 308:

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

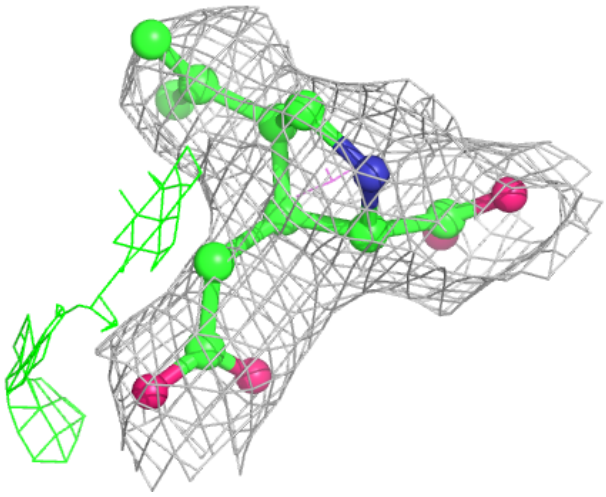


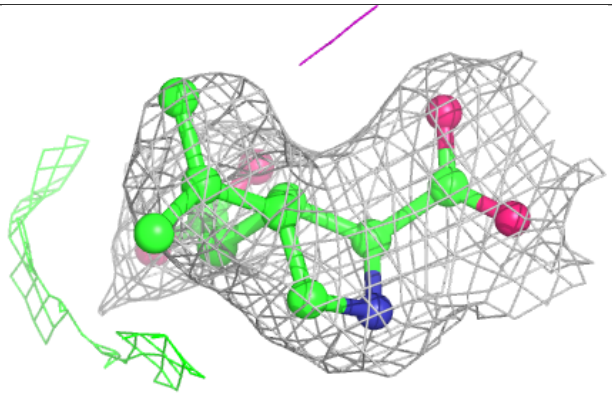


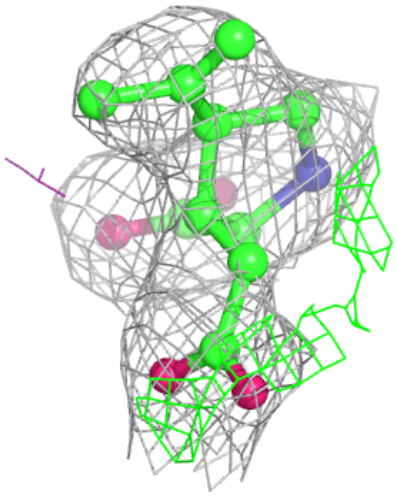


Electron density around KAI G 308:

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

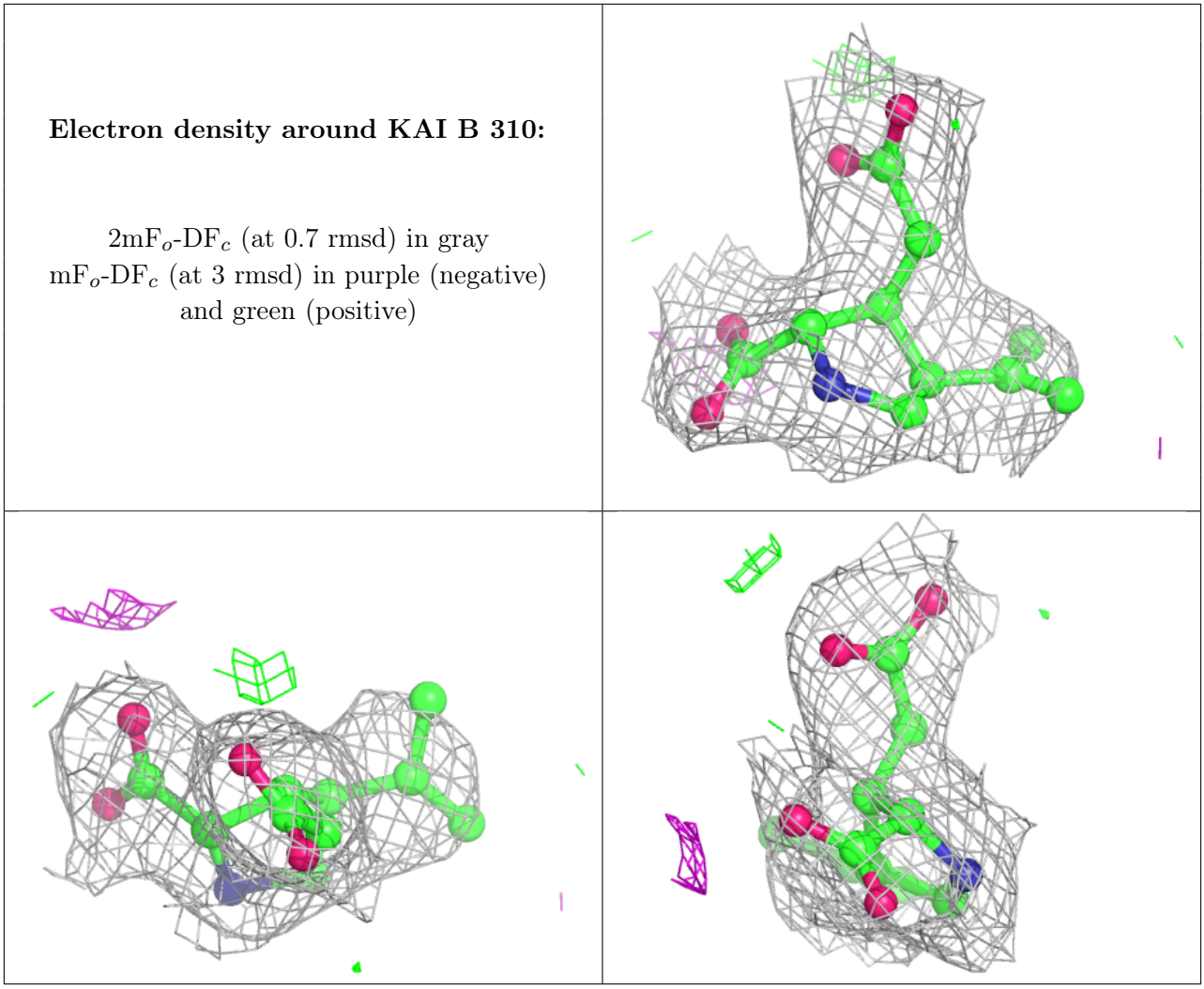






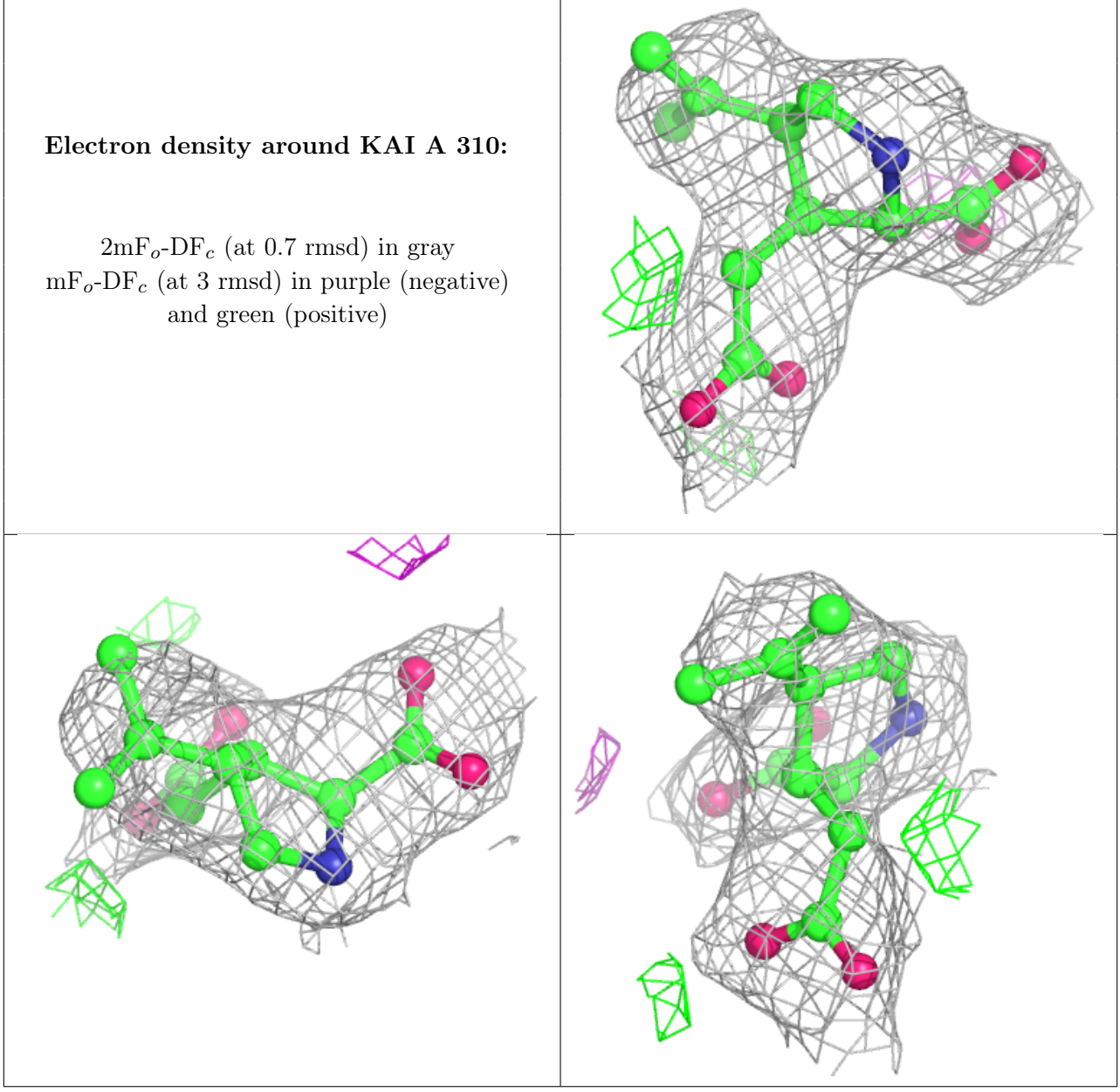
Electron density around KAI B 310:

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



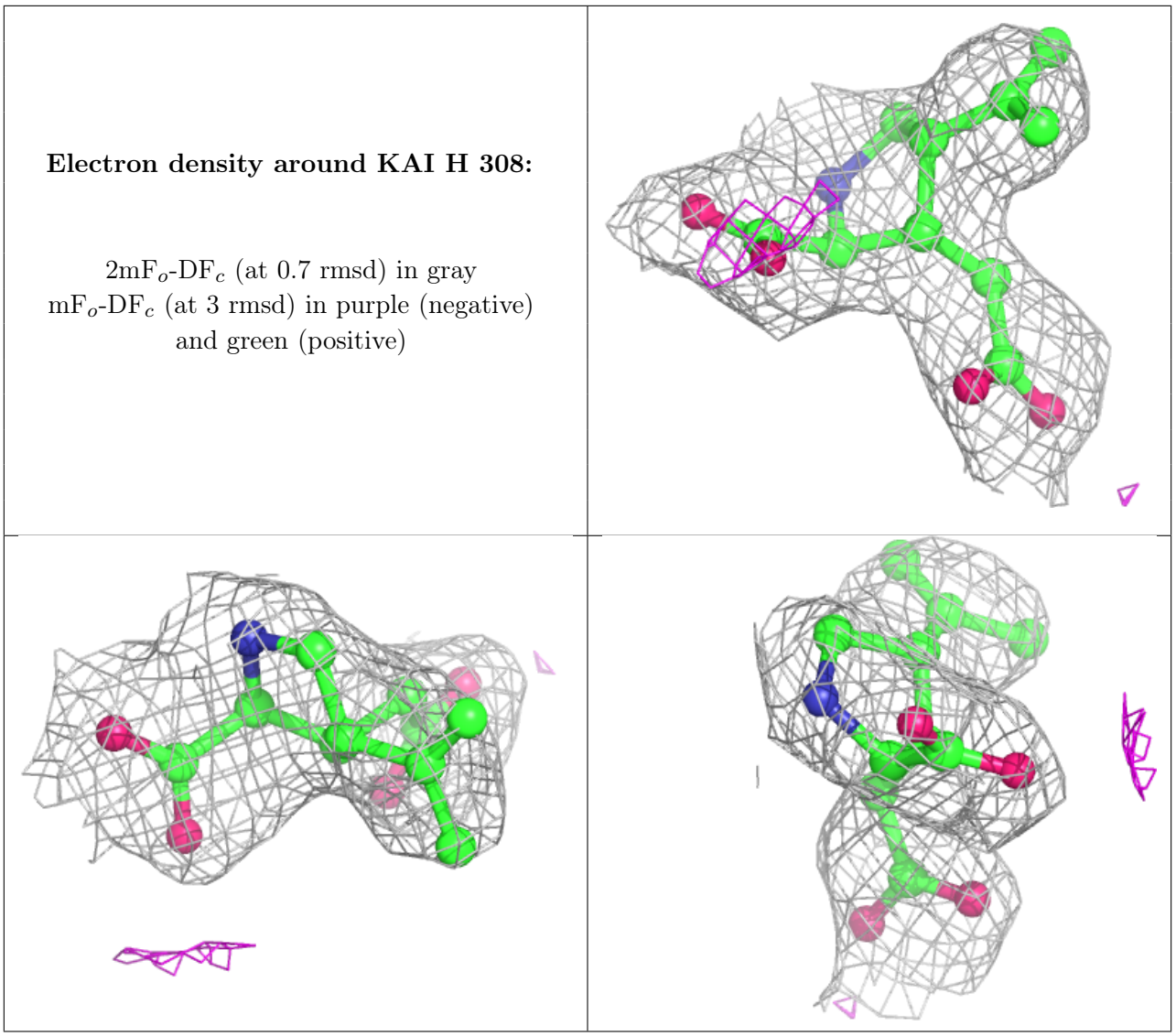
Electron density around KAI A 310:

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



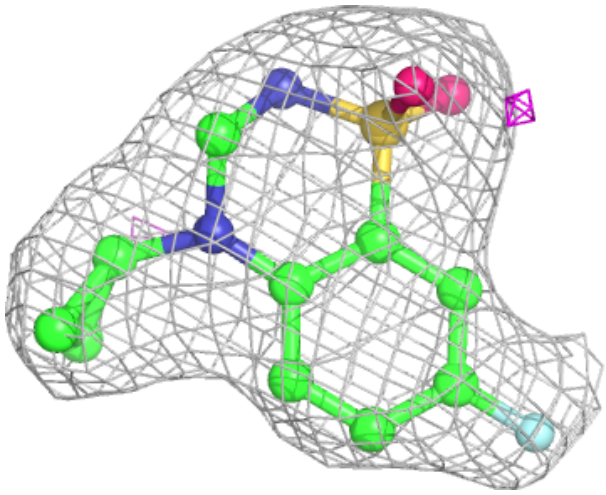
Electron density around KAI H 308:

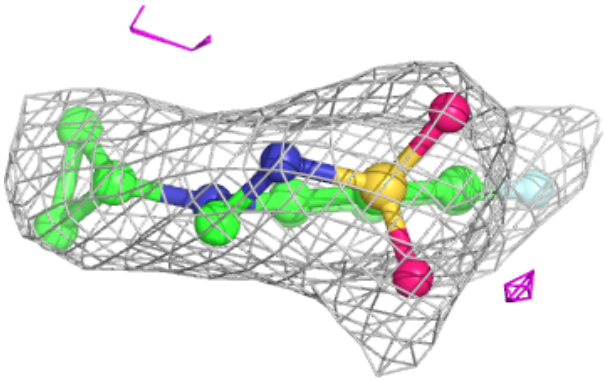
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

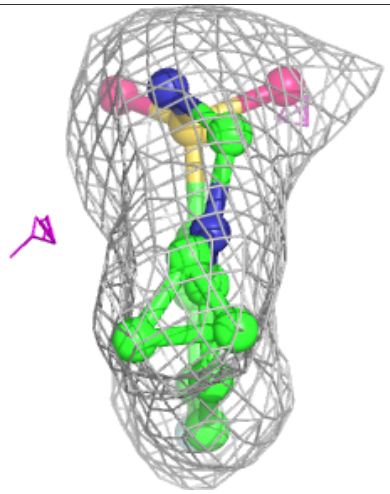


Electron density around 2J9 E 301:

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

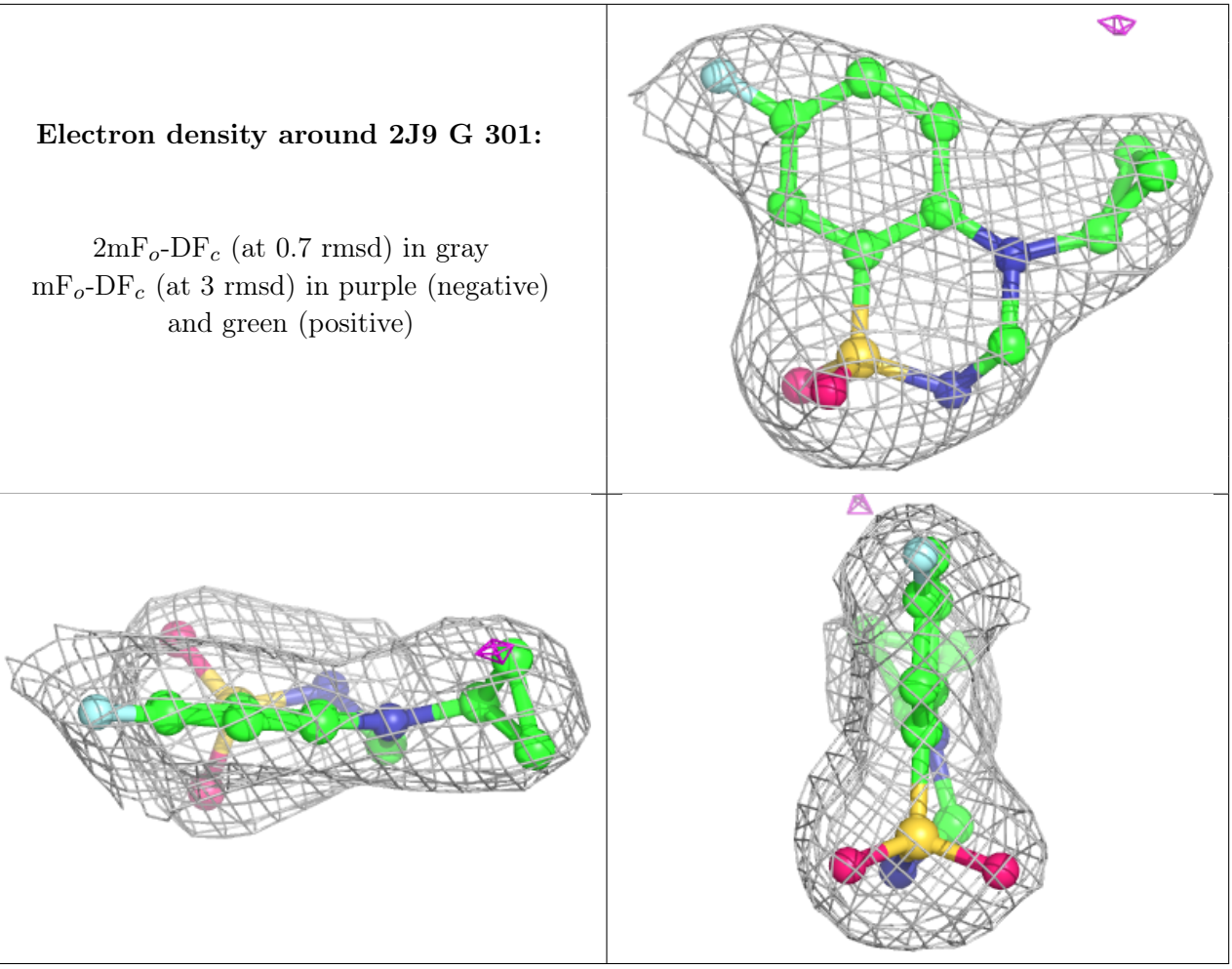






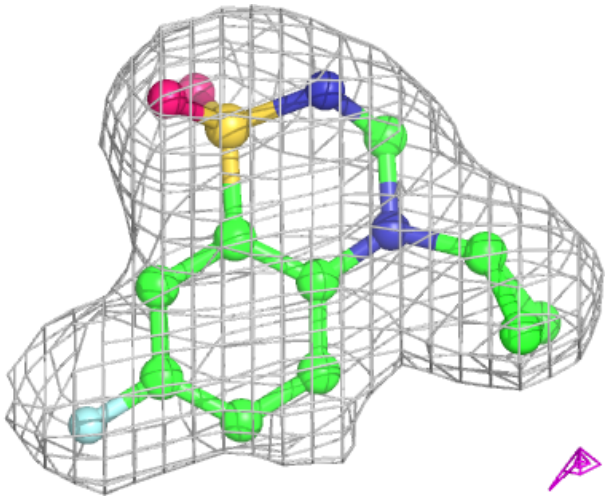
Electron density around 2J9 G 301:

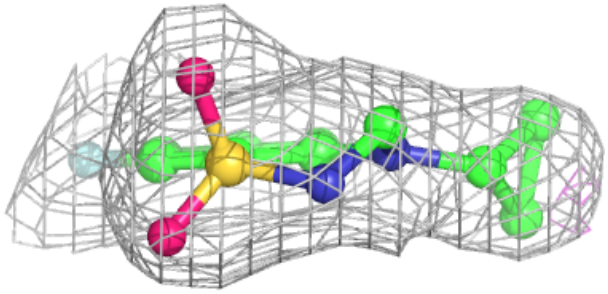
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

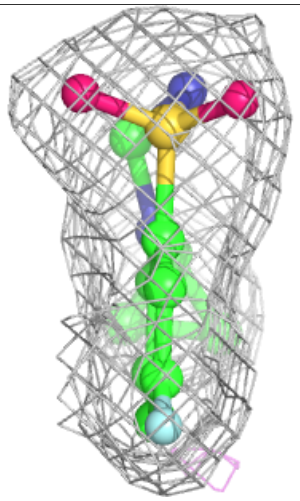


Electron density around 2J9 B 301:

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

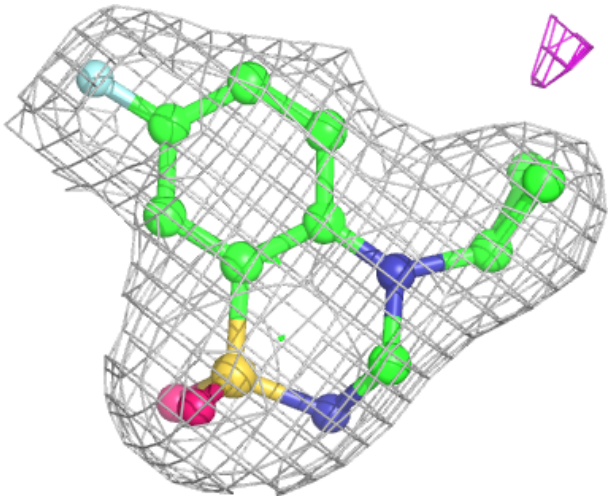


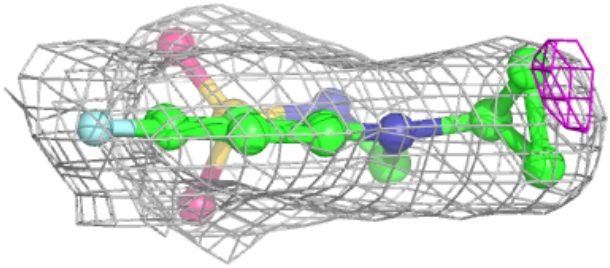


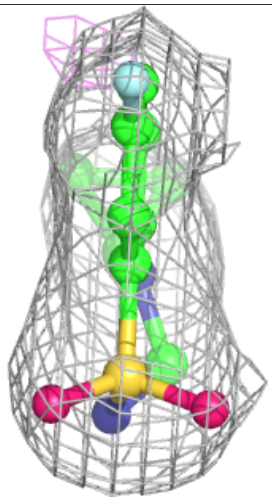


Electron density around 2J9 C 301:

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

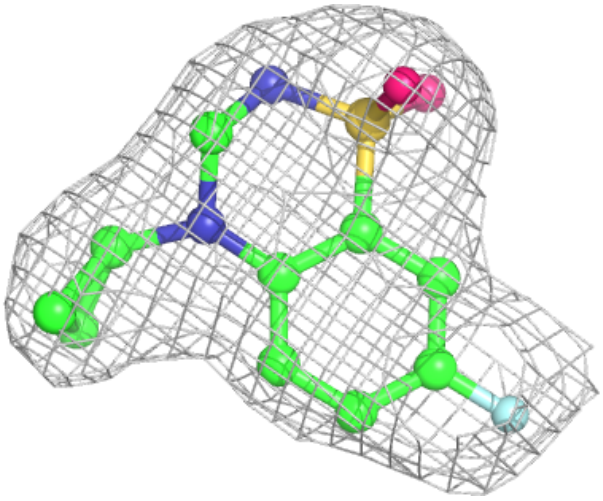


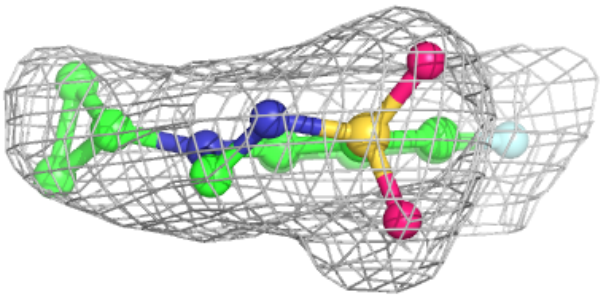


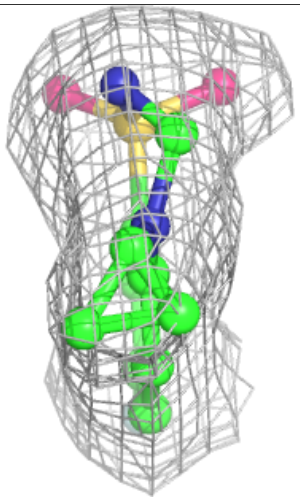


Electron density around 2J9 D 301:

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

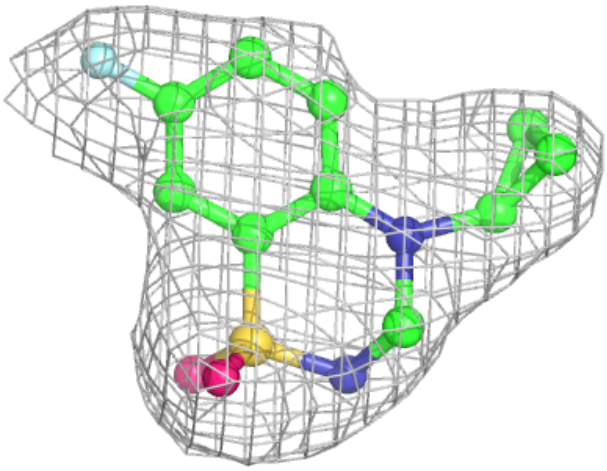


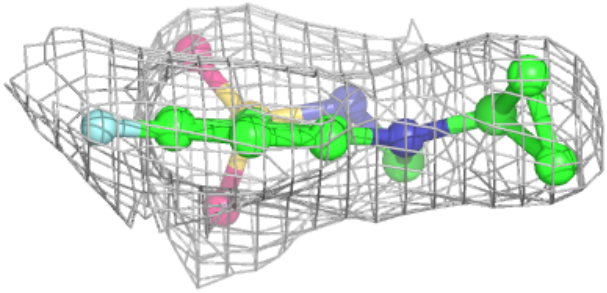


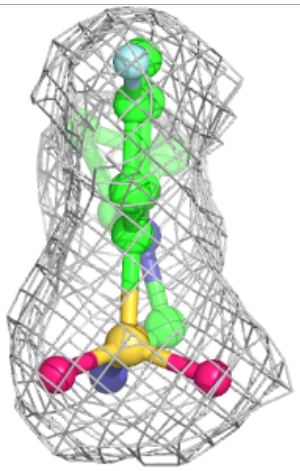


Electron density around 2J9 A 301:

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

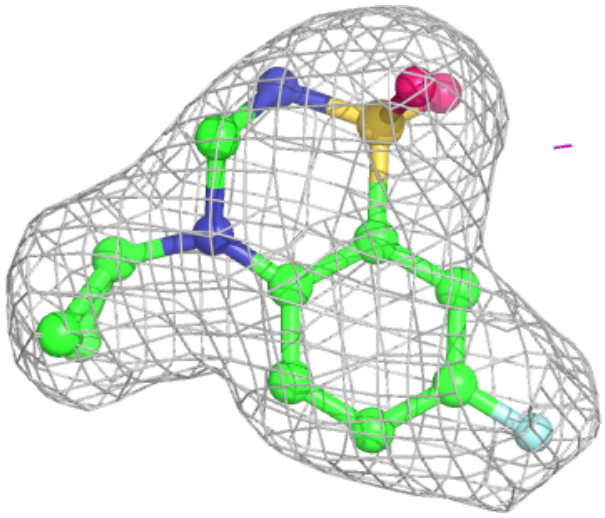


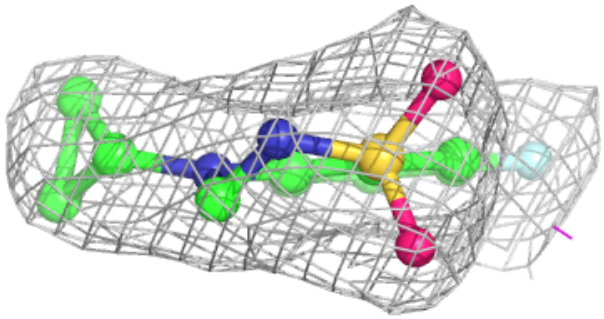


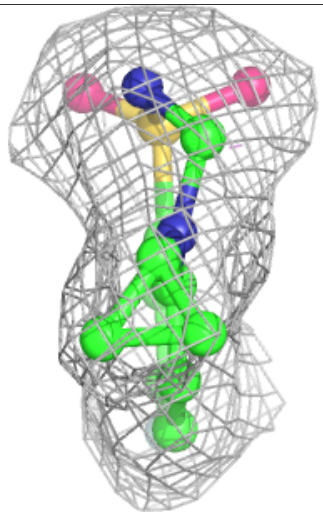


Electron density around 2J9 E 302:

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

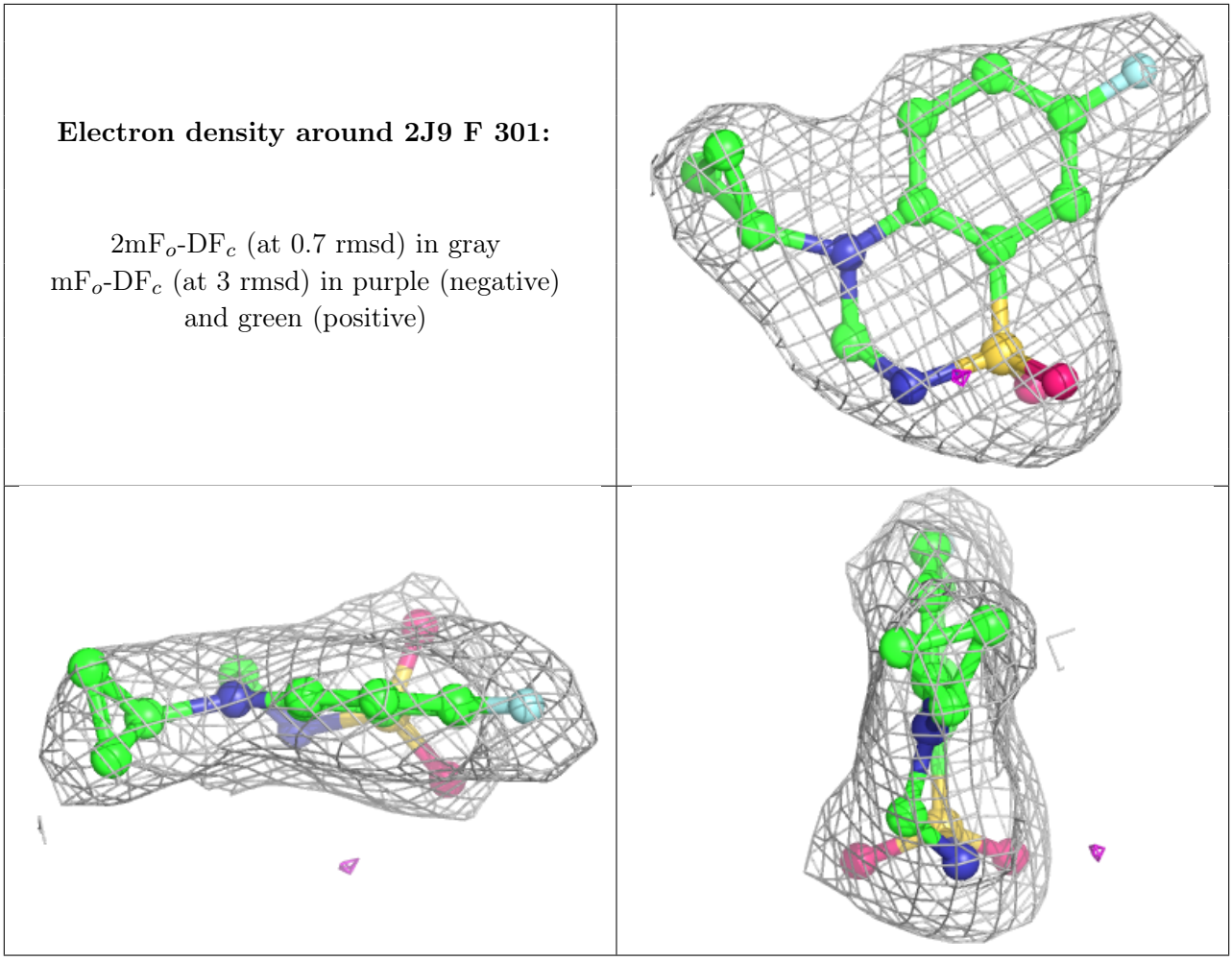






Electron density around 2J9 F 301:

$2mF_o$-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.