Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 01:15 pm GMT

PDB ID	:	7PD6
Title	:	Crystal structure of Lymnaea stagnalis Acetylcholine-binding protein (Ls-AChBP) Q55R/M114V double mutant complexed with Sulfoxaflor
Authors	:	Montgomery, M.G.
Deposited on	:	2021-08-04
Resolution	:	2.00 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:

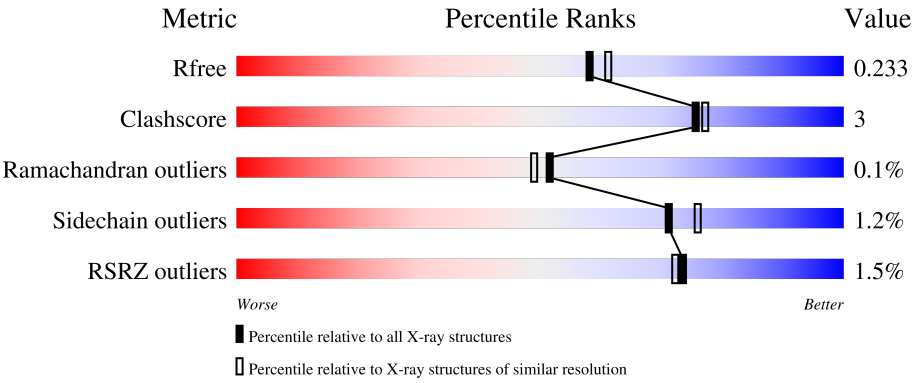
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.00 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.



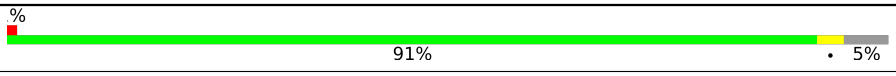
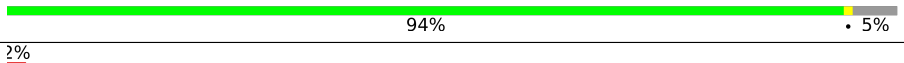
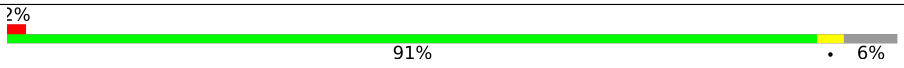
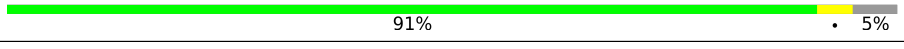
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	AaA	210	2% 90% · 6%
1	BaB	210	3% 94% · ·
1	CaC	210	2% 92% · ·
1	DaD	210	% 94% · 5%
1	EaE	210	2% 92% · 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FaF	210	
1	GaG	210	
1	HaH	210	
1	IaI	210	
1	JJJ	210	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16566 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AaA	197	Total	C	N	O	S	0	1	0
			1577	991	268	314	4			
1	BaB	203	Total	C	N	O	S	0	3	0
			1642	1030	282	326	4			
1	CaC	201	Total	C	N	O	S	0	2	0
			1614	1011	277	322	4			
1	DaD	200	Total	C	N	O	S	0	0	0
			1600	1003	278	315	4			
1	EaE	199	Total	C	N	O	S	0	3	0
			1603	1007	274	318	4			
1	FaF	199	Total	C	N	O	S	0	2	0
			1604	1005	277	318	4			
1	GaG	200	Total	C	N	O	S	0	1	0
			1607	1007	275	321	4			
1	HaH	198	Total	C	N	O	S	0	4	0
			1602	1008	276	314	4			
1	IaI	200	Total	C	N	O	S	0	3	0
			1613	1015	278	316	4			
1	JJJ	196	Total	C	N	O	S	0	3	0
			1592	1002	277	309	4			

There are 40 discrepancies between the modelled and reference sequences:

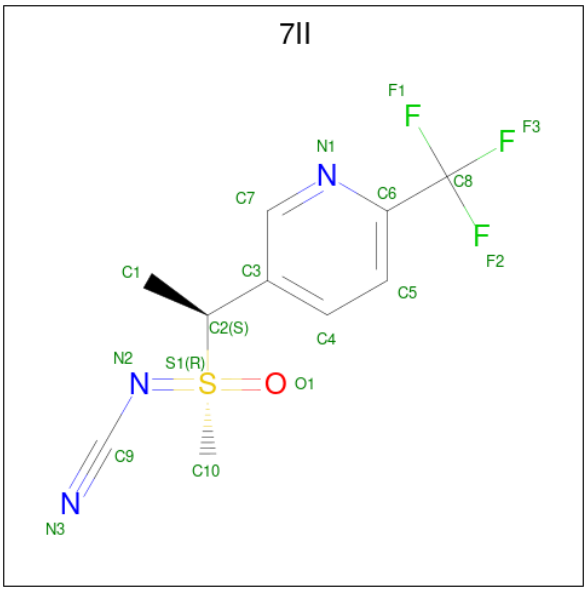
Chain	Residue	Modelled	Actual	Comment	Reference
AaA	1	ALA	-	expression tag	UNP P58154
AaA	55	ARG	GLN	engineered mutation	UNP P58154
AaA	66	ASP	ASN	engineered mutation	UNP P58154
AaA	114	VAL	MET	engineered mutation	UNP P58154
BaB	1	ALA	-	expression tag	UNP P58154
BaB	55	ARG	GLN	engineered mutation	UNP P58154
BaB	66	ASP	ASN	engineered mutation	UNP P58154
BaB	114	VAL	MET	engineered mutation	UNP P58154
CaC	1	ALA	-	expression tag	UNP P58154

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CaC	55	ARG	GLN	engineered mutation	UNP P58154
CaC	66	ASP	ASN	engineered mutation	UNP P58154
CaC	114	VAL	MET	engineered mutation	UNP P58154
DaD	1	ALA	-	expression tag	UNP P58154
DaD	55	ARG	GLN	engineered mutation	UNP P58154
DaD	66	ASP	ASN	engineered mutation	UNP P58154
DaD	114	VAL	MET	engineered mutation	UNP P58154
EaE	1	ALA	-	expression tag	UNP P58154
EaE	55	ARG	GLN	engineered mutation	UNP P58154
EaE	66	ASP	ASN	engineered mutation	UNP P58154
EaE	114	VAL	MET	engineered mutation	UNP P58154
FaF	1	ALA	-	expression tag	UNP P58154
FaF	55	ARG	GLN	engineered mutation	UNP P58154
FaF	66	ASP	ASN	engineered mutation	UNP P58154
FaF	114	VAL	MET	engineered mutation	UNP P58154
GaG	1	ALA	-	expression tag	UNP P58154
GaG	55	ARG	GLN	engineered mutation	UNP P58154
GaG	66	ASP	ASN	engineered mutation	UNP P58154
GaG	114	VAL	MET	engineered mutation	UNP P58154
HaH	1	ALA	-	expression tag	UNP P58154
HaH	55	ARG	GLN	engineered mutation	UNP P58154
HaH	66	ASP	ASN	engineered mutation	UNP P58154
HaH	114	VAL	MET	engineered mutation	UNP P58154
IaI	1	ALA	-	expression tag	UNP P58154
IaI	55	ARG	GLN	engineered mutation	UNP P58154
IaI	66	ASP	ASN	engineered mutation	UNP P58154
IaI	114	VAL	MET	engineered mutation	UNP P58154
JJJ	1	ALA	-	expression tag	UNP P58154
JJJ	55	ARG	GLN	engineered mutation	UNP P58154
JJJ	66	ASP	ASN	engineered mutation	UNP P58154
JJJ	114	VAL	MET	engineered mutation	UNP P58154

- Molecule 2 is Sulfoxaflor (three-letter code: 7II) (formula: $C_{10}H_{10}F_3N_3OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AaA	1	Total	C	F	N	O	S	0	0
			18	10	3	3	1	1		
2	BaB	1	Total	C	F	N	O	S	0	0
			18	10	3	3	1	1		
2	CaC	1	Total	C	F	N	O	S	0	0
			18	10	3	3	1	1		
2	DaD	1	Total	C	F	N	O	S	0	0
			18	10	3	3	1	1		
2	EaE	1	Total	C	F	N	O	S	0	0
			18	10	3	3	1	1		
2	FaF	1	Total	C	F	N	O	S	0	0
			18	10	3	3	1	1		
2	FaF	1	Total	C	F	N	O	S	0	0
			18	10	3	3	1	1		
2	GaG	1	Total	C	F	N	O	S	0	0
			18	10	3	3	1	1		
2	HaH	1	Total	C	F	N	O	S	0	0
			18	10	3	3	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AaA	36	Total	O	0	0
			36	36		
3	BaB	41	Total	O	0	0
			41	41		
3	CaC	53	Total	O	0	0
			53	53		

Continued on next page...

Continued from previous page...

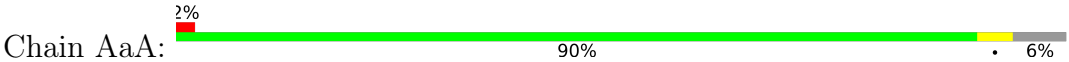
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	DaD	32	Total O 32 32	0	0
3	EaE	16	Total O 16 16	0	0
3	FaF	35	Total O 35 35	0	0
3	GaG	24	Total O 24 24	0	0
3	HaH	27	Total O 27 27	0	0
3	IaI	46	Total O 46 46	0	1
3	JJJ	40	Total O 40 40	0	0

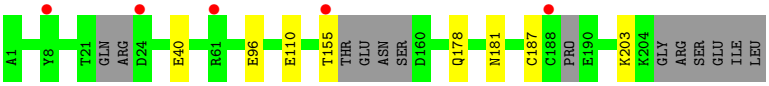
3 Residue-property plots (i)

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: Acetylcholine-binding protein

Chain AaA:



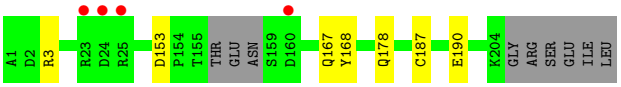


• Molecule 1: Acetylcholine-binding protein

Chain BaB:

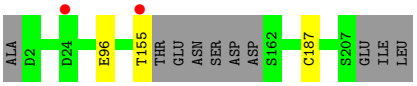
• Molecule 1: Acetylcholine-binding protein

Chain CaC:



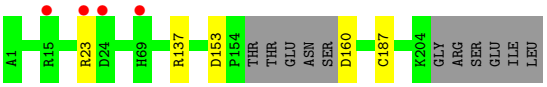
• Molecule 1: Acetylcholine-binding protein

Chain DaD:



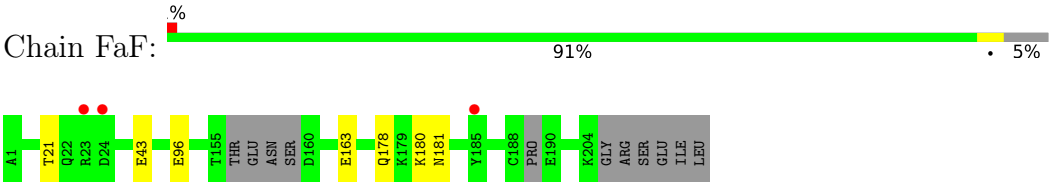
• Molecule 1: Acetylcholine-binding protein

Chain EaE:



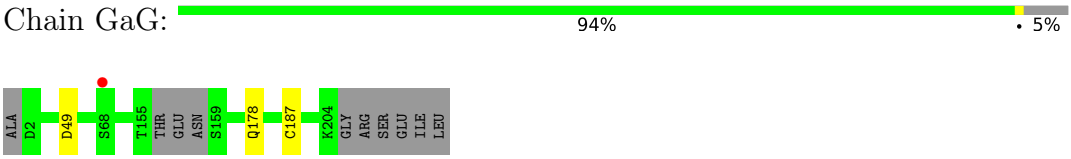
• Molecule 1: Acetylcholine-binding protein

Chain FaF:



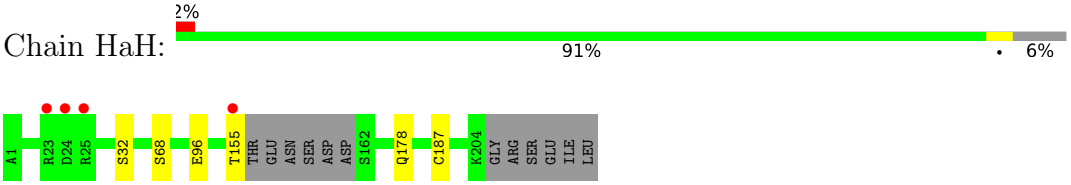
• Molecule 1: Acetylcholine-binding protein

Chain GaG:



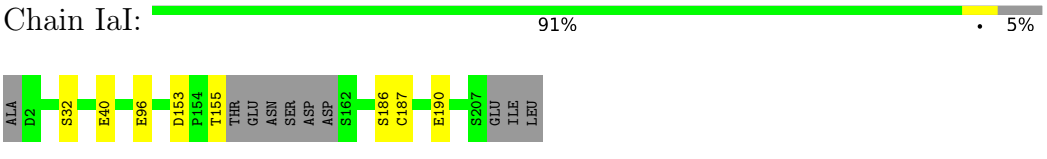
• Molecule 1: Acetylcholine-binding protein

Chain HaH:



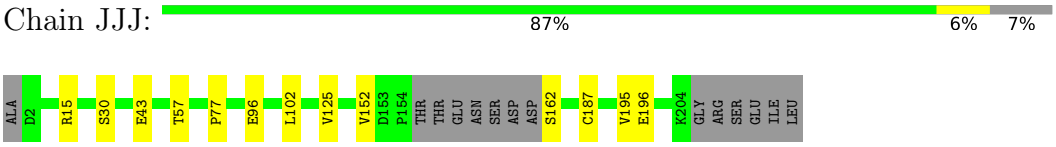
• Molecule 1: Acetylcholine-binding protein

Chain IaI:



• Molecule 1: Acetylcholine-binding protein

Chain JJJ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.89Å 74.37Å 130.06Å 90.00° 101.64° 90.00°	Depositor
Resolution (Å)	127.38 – 2.00 127.38 – 1.79	Depositor EDS
% Data completeness (in resolution range)	77.4 (127.38-2.00) 57.7 (127.38-1.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.206 , 0.231 0.212 , 0.233	Depositor DCC
R_{free} test set	5715 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 26.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16566	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 42.73 % 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 1.9546e-04. 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: 7II

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	AaA	0.86	3/1612 (0.2%)	0.98	1/2197 (0.0%)
1	BaB	0.83	0/1687	1.03	3/2305 (0.1%)
1	CaC	0.83	2/1655 (0.1%)	1.01	4/2258 (0.2%)
1	DaD	0.80	1/1635 (0.1%)	0.95	0/2229
1	EaE	0.78	0/1647	0.94	0/2247
1	FaF	0.85	3/1643 (0.2%)	1.01	2/2238 (0.1%)
1	GaG	0.77	0/1645	0.98	2/2244 (0.1%)
1	HaH	0.77	1/1649 (0.1%)	0.93	1/2249 (0.0%)
1	IaI	0.82	2/1655 (0.1%)	0.95	0/2258
1	JJJ	0.85	3/1636 (0.2%)	0.97	1/2230 (0.0%)
All	All	0.82	15/16464 (0.1%)	0.98	14/22455 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AaA	0	1
1	CaC	0	1
1	DaD	0	1
1	EaE	0	2
1	GaG	0	1
1	HaH	0	1
1	IaI	0	1
1	JJJ	0	1
All	All	0	9

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DaD	96	GLU	CD-OE2	8.14	1.34	1.25
1	AaA	40	GLU	CD-OE1	7.75	1.34	1.25
1	FaF	96	GLU	CD-OE1	6.72	1.33	1.25
1	CaC	190	GLU	CD-OE1	6.56	1.32	1.25
1	JJJ	96	GLU	CD-OE1	6.56	1.32	1.25
1	IaI	96	GLU	CD-OE2	6.29	1.32	1.25
1	AaA	96	GLU	CD-OE1	6.21	1.32	1.25
1	FaF	96	GLU	CD-OE2	6.17	1.32	1.25
1	AaA	110	GLU	CD-OE1	6.11	1.32	1.25
1	IaI	190	GLU	CD-OE1	5.73	1.31	1.25
1	CaC	153	ASP	CG-OD2	5.36	1.37	1.25
1	HaH	96	GLU	CD-OE2	5.34	1.31	1.25
1	JJJ	196	GLU	CD-OE2	5.31	1.31	1.25
1	FaF	163	GLU	CD-OE1	5.29	1.31	1.25
1	JJJ	196	GLU	CD-OE1	5.24	1.31	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BaB	168	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	CaC	168	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	BaB	11	ARG	CB-CG-CD	5.90	126.94	111.60
1	CaC	3	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	FaF	178	GLN	CB-CG-CD	5.79	126.64	111.60
1	GaG	178	GLN	CB-CG-CD	5.66	126.31	111.60
1	HaH	178	GLN	CB-CG-CD	5.51	125.93	111.60
1	CaC	178	GLN	CB-CG-CD	5.51	125.92	111.60
1	AaA	178	GLN	CB-CG-CD	5.26	125.28	111.60
1	FaF	21	THR	CA-CB-OG1	-5.25	97.96	109.00
1	CaC	153	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	BaB	184	THR	CA-CB-CG2	5.17	119.64	112.40
1	JJJ	15	ARG	CG-CD-NE	5.03	122.35	111.80
1	GaG	49	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AaA	187	CYS	Peptide
1	CaC	187	CYS	Peptide
1	DaD	187	CYS	Peptide
1	EaE	160	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	EaE	187	CYS	Peptide
1	GaG	187	CYS	Peptide
1	HaH	187	CYS	Peptide
1	IaI	187	CYS	Peptide
1	JJJ	187	CYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AaA	1577	0	1529	0	0
1	BaB	1642	0	1600	0	0
1	CaC	1614	0	1566	0	0
1	DaD	1600	0	1555	0	0
1	EaE	1603	0	1562	0	0
1	FaF	1604	0	1560	0	0
1	GaG	1607	0	1553	0	0
1	HaH	1602	0	1574	0	0
1	IaI	1613	0	1572	0	0
1	JJJ	1592	0	1562	4	0
2	AaA	18	0	0	0	0
2	BaB	18	0	0	0	0
2	CaC	18	0	0	0	0
2	DaD	18	0	0	0	0
2	EaE	18	0	0	0	0
2	FaF	36	0	0	0	0
2	GaG	18	0	0	0	0
2	HaH	18	0	0	0	0
3	AaA	36	0	0	0	0
3	BaB	41	0	0	0	0
3	CaC	53	0	0	0	0
3	DaD	32	0	0	0	0
3	EaE	16	0	0	0	0
3	FaF	35	0	0	0	0
3	GaG	24	0	0	0	0
3	HaH	27	0	0	0	0
3	IaI	46	0	0	0	0
3	JJJ	40	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16566	0	15633	4	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 (4) 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:JJJ:43:GLU:HG2	1:JJJ:125:VAL:HG12	1.72	0.72
1:JJJ:152[B]:VAL:HG12	1:JJJ:195:VAL:HG23	1.91	0.52
1:JJJ:77:PRO:HA	1:JJJ:102:LEU:HD23	1.98	0.45
1:JJJ:30:SER:HB3	1:JJJ:57:THR:OG1	2.19	0.43

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	AaA	190/210 (90%)	190 (100%)	0	0	100	100
1	BaB	204/210 (97%)	202 (99%)	1 (0%)	1 (0%)	29	23
1	CaC	199/210 (95%)	197 (99%)	2 (1%)	0	100	100
1	DaD	196/210 (93%)	195 (100%)	1 (0%)	0	100	100
1	EaE	198/210 (94%)	198 (100%)	0	0	100	100
1	FaF	195/210 (93%)	195 (100%)	0	0	100	100
1	GaG	197/210 (94%)	197 (100%)	0	0	100	100
1	HaH	198/210 (94%)	197 (100%)	1 (0%)	0	100	100
1	IaI	198/210 (94%)	197 (100%)	1 (0%)	0	100	100
1	JJJ	195/210 (93%)	195 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1970/2100 (94%)	1963 (100%)	6 (0%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BaB	155	THR

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	AaA	184/195 (94%)	181 (98%)	3 (2%)	62 67
1	BaB	193/195 (99%)	191 (99%)	2 (1%)	76 81
1	CaC	189/195 (97%)	188 (100%)	1 (0%)	88 92
1	DaD	186/195 (95%)	185 (100%)	1 (0%)	88 92
1	EaE	188/195 (96%)	185 (98%)	3 (2%)	62 67
1	FaF	187/195 (96%)	184 (98%)	3 (2%)	62 67
1	GaG	188/195 (96%)	188 (100%)	0	100 100
1	HaH	188/195 (96%)	185 (98%)	3 (2%)	62 67
1	IaI	188/195 (96%)	183 (97%)	5 (3%)	44 46
1	JJJ	186/195 (95%)	185 (100%)	1 (0%)	88 92
All	All	1877/1950 (96%)	1855 (99%)	22 (1%)	71 76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AaA	155	THR
1	AaA	181	ASN
1	AaA	203	LYS
1	BaB	170	ARG
1	BaB	181	ASN
1	CaC	167	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DaD	155	THR
1	EaE	23	ARG
1	EaE	137	ARG
1	EaE	153	ASP
1	FaF	43	GLU
1	FaF	180	LYS
1	FaF	181	ASN
1	HaH	32	SER
1	HaH	68	SER
1	HaH	155	THR
1	IaI	32	SER
1	IaI	40	GLU
1	IaI	153	ASP
1	IaI	155	THR
1	IaI	186	SER
1	JJJ	162	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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)

9 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	7II	FaF	302	-	16,18,18	1.34	2 (12%)	19,27,27	2.83	2 (10%)
2	7II	BaB	301	-	16,18,18	2.16	1 (6%)	19,27,27	2.70	6 (31%)
2	7II	AaA	301	-	16,18,18	0.69	0	19,27,27	2.45	2 (10%)
2	7II	FaF	301	-	16,18,18	0.65	0	19,27,27	1.67	2 (10%)
2	7II	GaG	301	-	16,18,18	0.48	0	19,27,27	1.77	2 (10%)
2	7II	HaH	301	-	16,18,18	0.64	0	19,27,27	1.00	2 (10%)
2	7II	EaE	301	-	16,18,18	0.51	0	19,27,27	1.82	3 (15%)
2	7II	CaC	301	-	16,18,18	0.85	0	19,27,27	1.63	4 (21%)
2	7II	DaD	301	-	16,18,18	0.90	1 (6%)	19,27,27	1.47	3 (15%)

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	7II	FaF	302	-	-	4/14/20/20	0/1/1/1
2	7II	BaB	301	-	-	4/14/20/20	0/1/1/1
2	7II	AaA	301	-	-	4/14/20/20	0/1/1/1
2	7II	FaF	301	-	-	0/14/20/20	0/1/1/1
2	7II	GaG	301	-	-	3/14/20/20	0/1/1/1
2	7II	HaH	301	-	-	1/14/20/20	0/1/1/1
2	7II	EaE	301	-	-	2/14/20/20	0/1/1/1
2	7II	CaC	301	-	-	2/14/20/20	0/1/1/1
2	7II	DaD	301	-	-	2/14/20/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BaB	301	7II	C9-N3	8.28	1.36	1.15
2	FaF	302	7II	C9-N3	4.25	1.26	1.15
2	FaF	302	7II	C2-S1	2.67	1.83	1.80
2	DaD	301	7II	C9-N3	2.66	1.22	1.15

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	FaF	302	7II	C10-S1-C2	11.09	119.61	105.06
2	BaB	301	7II	C10-S1-C2	10.21	118.45	105.06
2	AaA	301	7II	C10-S1-C2	9.43	117.43	105.06
2	GaG	301	7II	C10-S1-C2	5.26	111.97	105.06
2	FaF	301	7II	C10-S1-C2	5.13	111.80	105.06
2	EaE	301	7II	C10-S1-C2	4.82	111.39	105.06
2	CaC	301	7II	C1-C2-S1	4.31	112.93	107.48
2	DaD	301	7II	C10-S1-C2	4.15	110.50	105.06
2	EaE	301	7II	C1-C2-S1	3.90	112.41	107.48
2	EaE	301	7II	O1-S1-C10	-3.68	103.76	109.01
2	CaC	301	7II	C10-S1-C2	3.37	109.48	105.06
2	GaG	301	7II	C1-C2-S1	3.36	111.73	107.48
2	FaF	301	7II	C5-C4-C3	-3.08	118.10	121.20
2	DaD	301	7II	O1-S1-C10	-3.04	104.68	109.01
2	BaB	301	7II	C4-C3-C2	2.73	125.06	120.54
2	FaF	302	7II	C4-C3-C2	2.71	125.02	120.54
2	DaD	301	7II	C1-C2-S1	2.54	110.69	107.48
2	AaA	301	7II	C8-C6-N1	2.50	117.61	114.61
2	BaB	301	7II	O1-S1-C10	2.46	112.51	109.01
2	CaC	301	7II	C5-C4-C3	-2.41	118.77	121.20
2	HaH	301	7II	C1-C2-S1	2.29	110.38	107.48
2	CaC	301	7II	O1-S1-C10	2.19	112.12	109.01
2	BaB	301	7II	C10-S1-N2	-2.17	98.68	107.49
2	BaB	301	7II	C1-C2-S1	2.11	110.14	107.48
2	HaH	301	7II	C10-S1-C2	-2.10	102.31	105.06
2	BaB	301	7II	C1-C2-C3	-2.01	111.33	114.84

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AaA	301	7II	C1-C2-C3-C4
2	AaA	301	7II	C1-C2-C3-C7
2	AaA	301	7II	S1-C2-C3-C4
2	BaB	301	7II	C1-C2-C3-C4
2	BaB	301	7II	C1-C2-C3-C7
2	BaB	301	7II	S1-C2-C3-C4
2	CaC	301	7II	C1-C2-S1-O1
2	CaC	301	7II	C1-C2-S1-C10
2	DaD	301	7II	C1-C2-S1-O1
2	DaD	301	7II	C1-C2-S1-C10
2	EaE	301	7II	C1-C2-S1-C10
2	FaF	302	7II	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

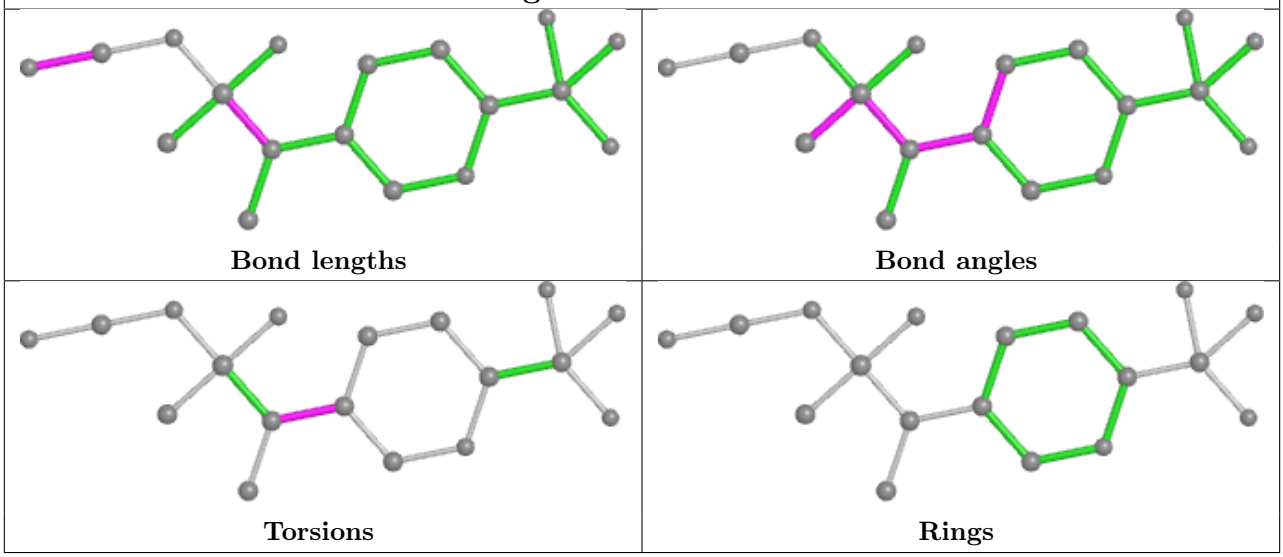
Mol	Chain	Res	Type	Atoms
2	FaF	302	7II	C1-C2-C3-C7
2	FaF	302	7II	S1-C2-C3-C4
2	GaG	301	7II	C1-C2-S1-O1
2	GaG	301	7II	C1-C2-S1-C10
2	AaA	301	7II	S1-C2-C3-C7
2	BaB	301	7II	S1-C2-C3-C7
2	FaF	302	7II	S1-C2-C3-C7
2	EaE	301	7II	C1-C2-S1-O1
2	GaG	301	7II	C3-C2-S1-O1
2	HaH	301	7II	C1-C2-S1-C10

There are no ring outliers.

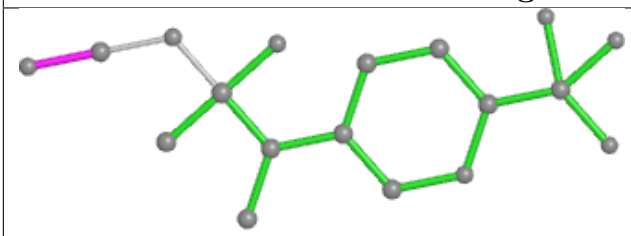
No monomer is involved in short contacts.

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

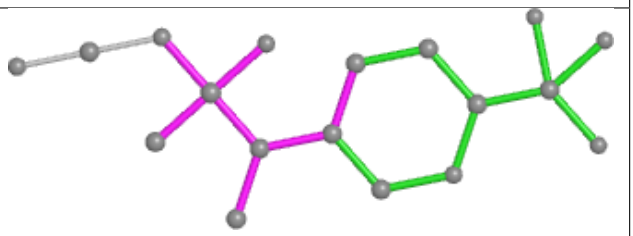
Ligand 7II FaF 302



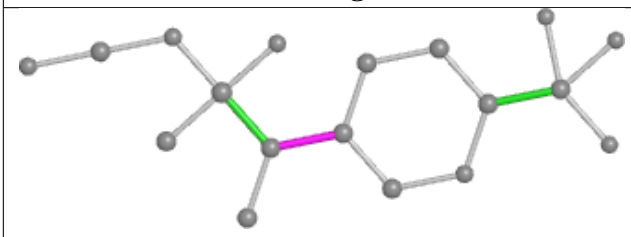
Ligand 7II BaB 301



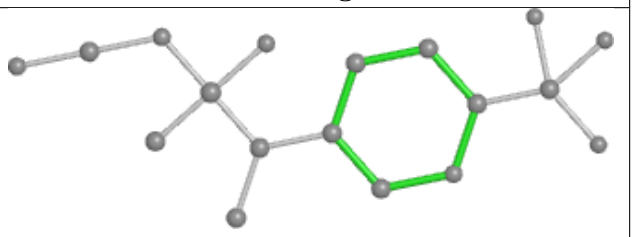
Bond lengths



Bond angles

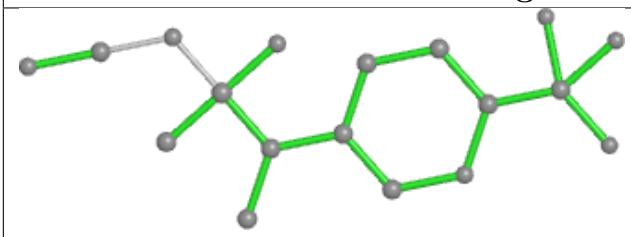


Torsions

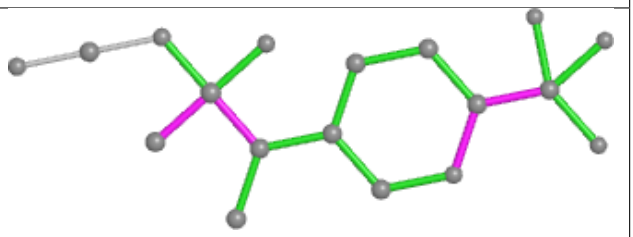


Rings

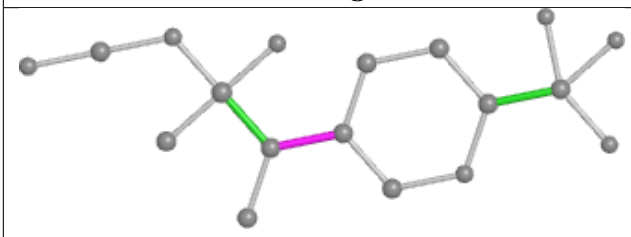
Ligand 7II AaA 301



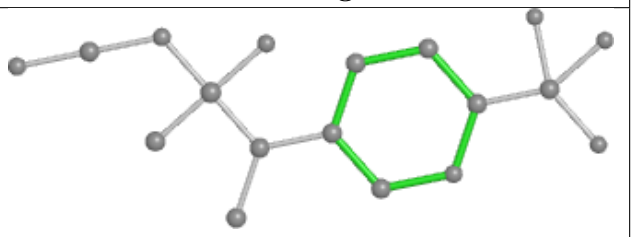
Bond lengths



Bond angles

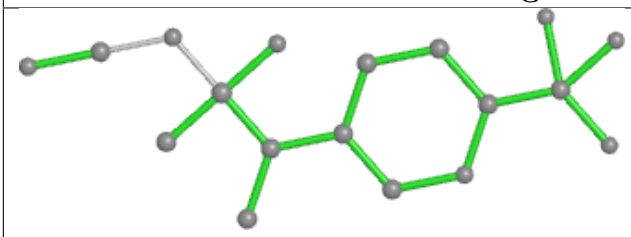


Torsions

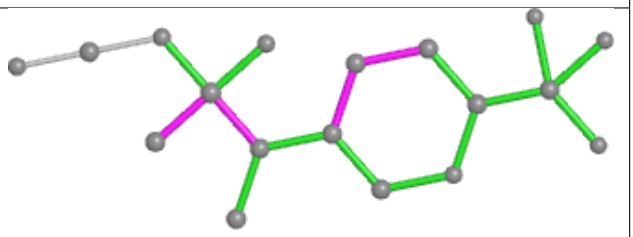


Rings

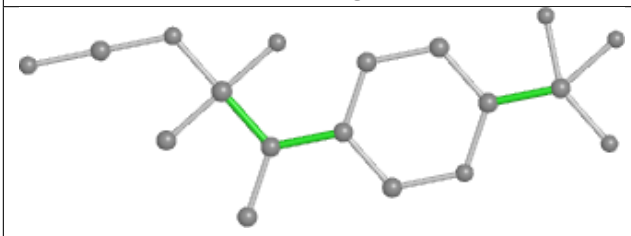
Ligand 7II FaF 301



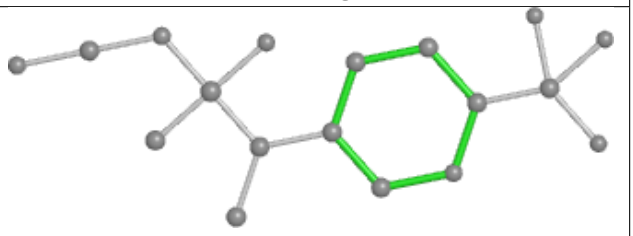
Bond lengths



Bond angles

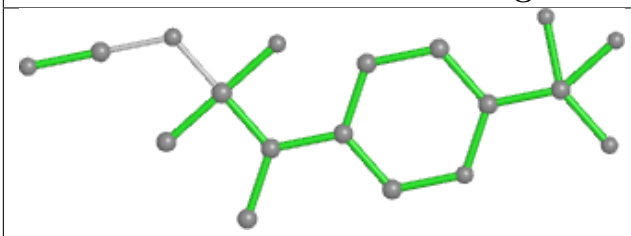


Torsions

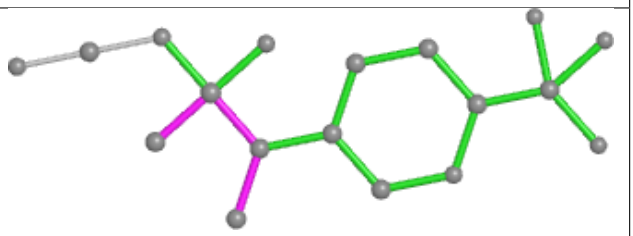


Rings

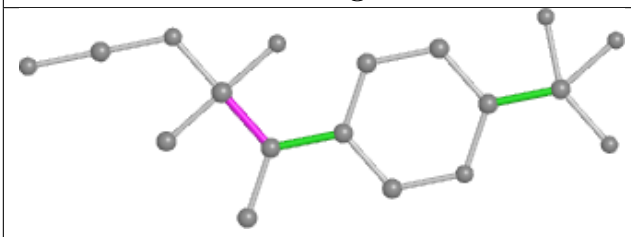
Ligand 7II GaG 301



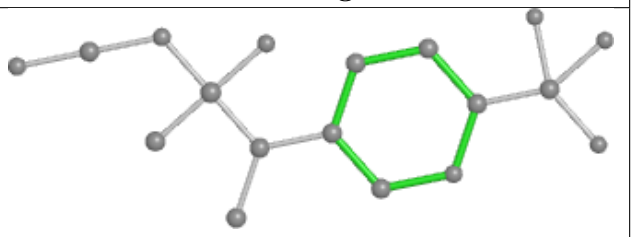
Bond lengths



Bond angles

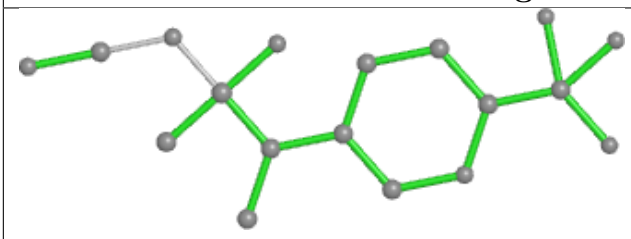


Torsions

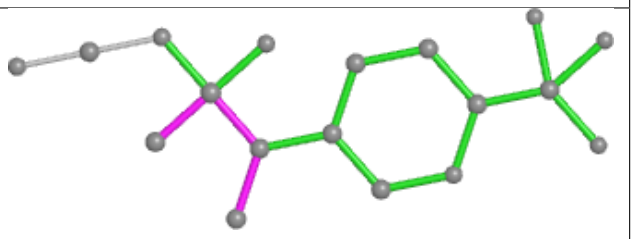


Rings

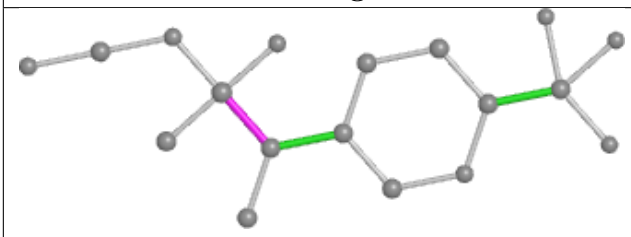
Ligand 7II HaH 301



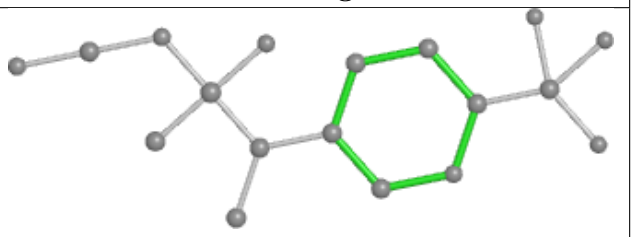
Bond lengths



Bond angles

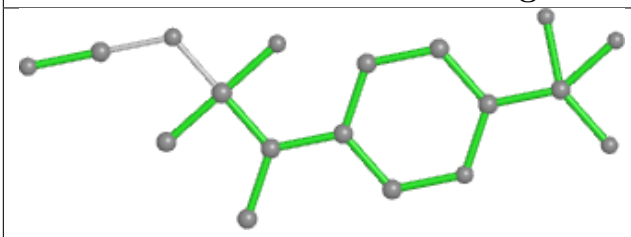


Torsions

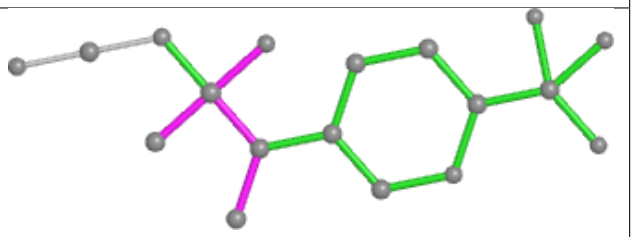


Rings

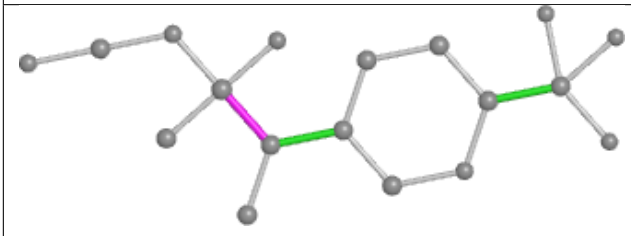
Ligand 7II EaE 301



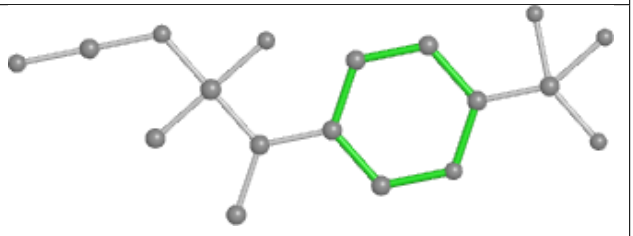
Bond lengths



Bond angles

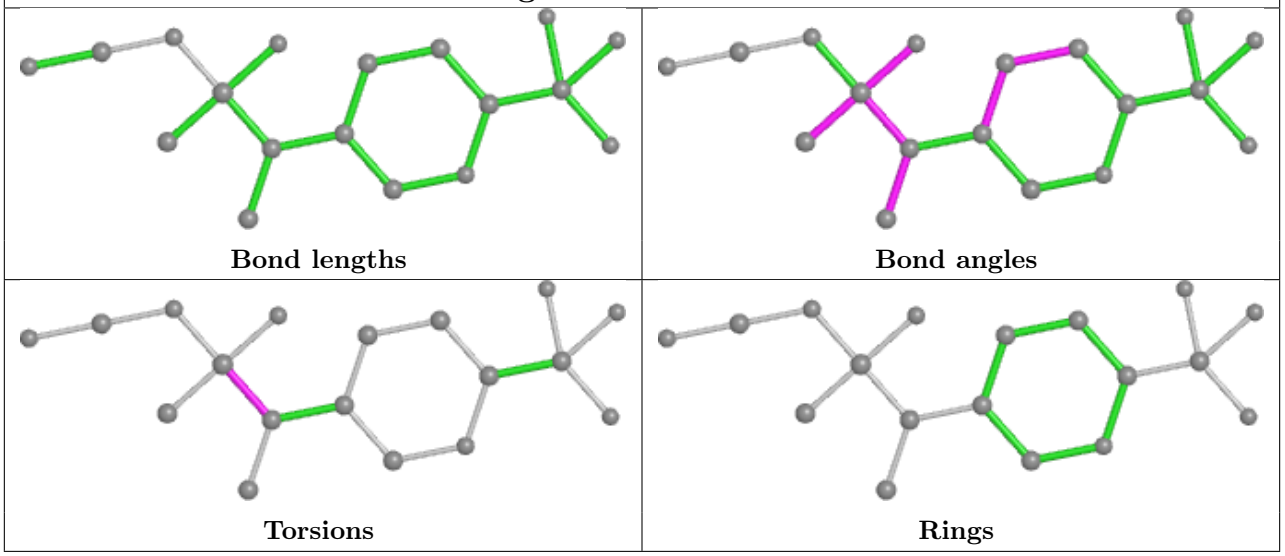


Torsions

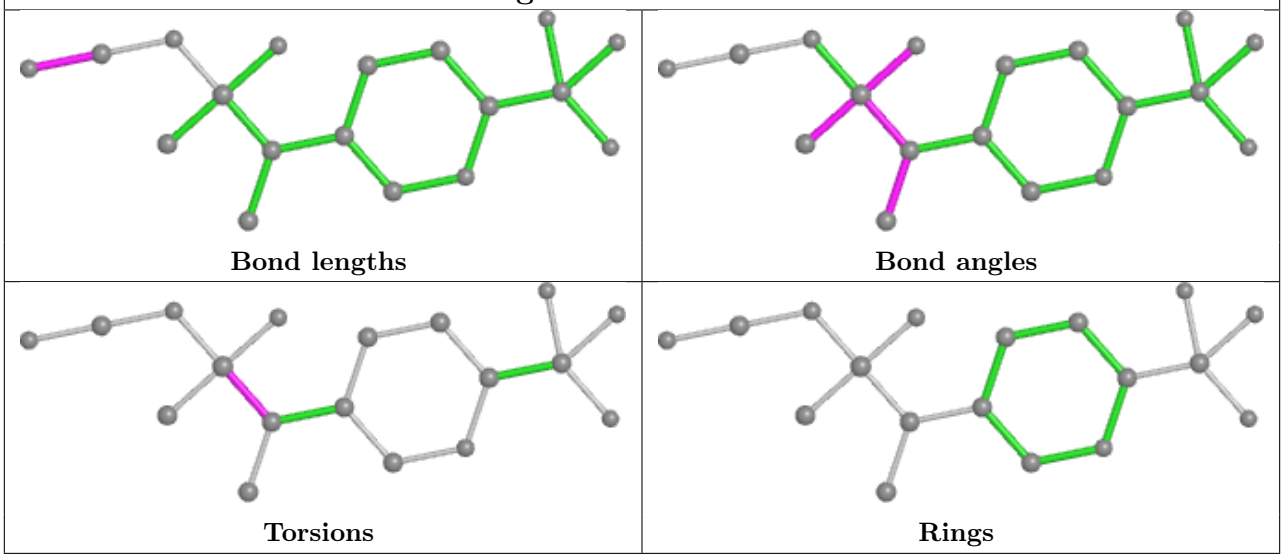


Rings

Ligand 7II CaC 301



Ligand 7II DaD 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AaA	197/210 (93%)	-0.30	5 (2%) 57 56	23, 40, 79, 114	0
1	BaB	203/210 (96%)	-0.27	6 (2%) 50 49	20, 35, 68, 87	0
1	CaC	201/210 (95%)	-0.36	4 (1%) 65 63	20, 33, 59, 82	0
1	DaD	200/210 (95%)	-0.42	2 (1%) 82 81	24, 38, 64, 82	0
1	EaE	199/210 (94%)	-0.12	4 (2%) 65 63	29, 52, 78, 94	0
1	FaF	199/210 (94%)	-0.34	3 (1%) 73 72	21, 34, 68, 92	0
1	GaG	200/210 (95%)	-0.25	1 (0%) 91 90	25, 44, 71, 92	0
1	HaH	198/210 (94%)	-0.30	4 (2%) 65 63	26, 40, 65, 90	0
1	IaI	200/210 (95%)	-0.40	0 100 100	23, 36, 60, 79	0
1	JJJ	196/210 (93%)	-0.45	0 100 100	21, 33, 50, 57	0
All	All	1993/2100 (94%)	-0.32	29 (1%) 73 72	20, 38, 70, 114	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	GaG	68	SER	5.1
1	HaH	23	ARG	4.5
1	DaD	155	THR	4.3
1	HaH	24	ASP	3.8
1	FaF	23	ARG	3.6
1	HaH	25	ARG	3.3
1	CaC	23	ARG	3.1
1	EaE	15	ARG	3.1
1	AaA	24	ASP	2.9
1	BaB	156	THR	2.8
1	FaF	24	ASP	2.7
1	CaC	24	ASP	2.7
1	EaE	24	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CaC	25	ARG	2.6
1	BaB	158	ASN	2.5
1	EaE	23	ARG	2.4
1	AaA	188	CYS	2.4
1	BaB	187	CYS	2.4
1	BaB	22	GLN	2.3
1	BaB	188	CYS	2.3
1	AaA	155	THR	2.2
1	CaC	160	ASP	2.2
1	EaE	69	HIS	2.2
1	BaB	24	ASP	2.2
1	AaA	8	TYR	2.1
1	FaF	185	TYR	2.1
1	HaH	155	THR	2.1
1	AaA	61	ARG	2.0
1	DaD	24	ASP	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
2	7II	EaE	301	18/18	0.81	0.17	45,51,77,77	0
2	7II	DaD	301	18/18	0.83	0.19	48,55,94,97	0
2	7II	FaF	302	18/18	0.85	0.16	46,52,72,76	0
2	7II	AaA	301	18/18	0.86	0.14	41,47,62,65	0
2	7II	HaH	301	18/18	0.87	0.17	37,44,80,82	0
2	7II	GaG	301	18/18	0.88	0.15	37,43,78,81	0
2	7II	FaF	301	18/18	0.88	0.14	26,31,55,59	0

Continued on next page...

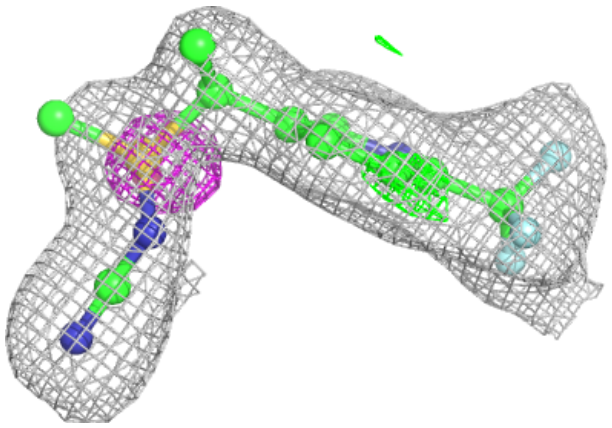
Continued from previous page...

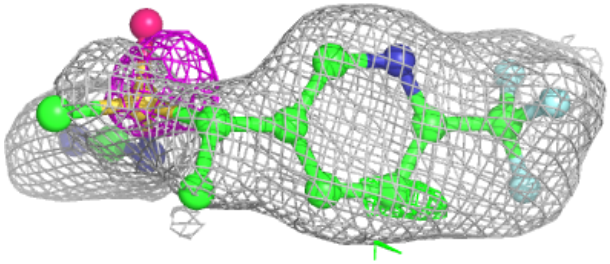
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	7II	BaB	301	18/18	0.91	0.14	36,47,74,78	0
2	7II	CaC	301	18/18	0.92	0.16	36,44,91,97	0

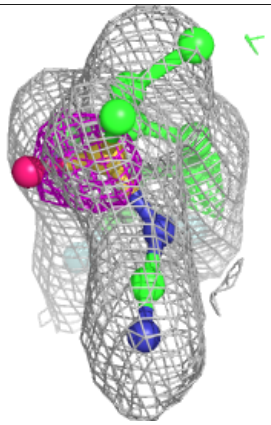
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7II EaE 301:

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

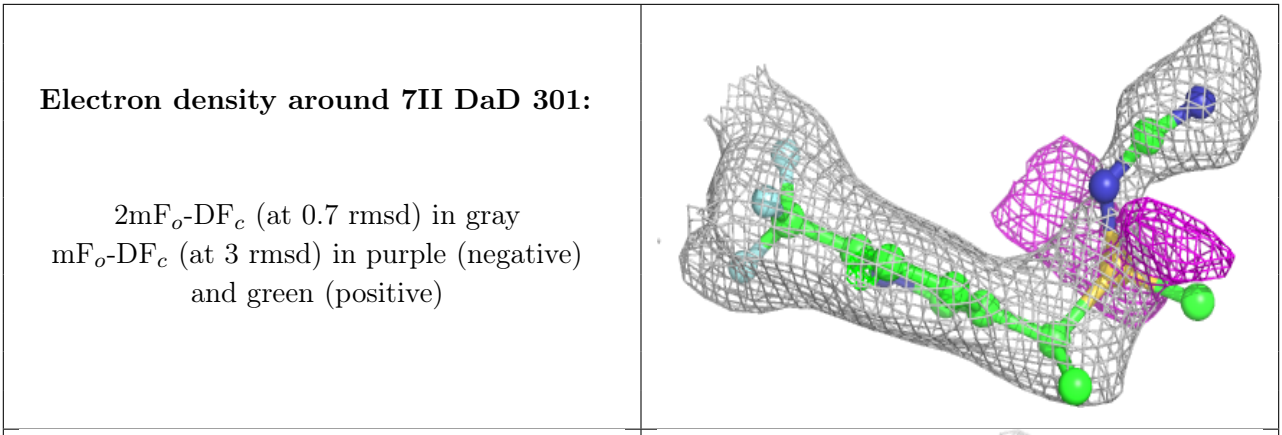






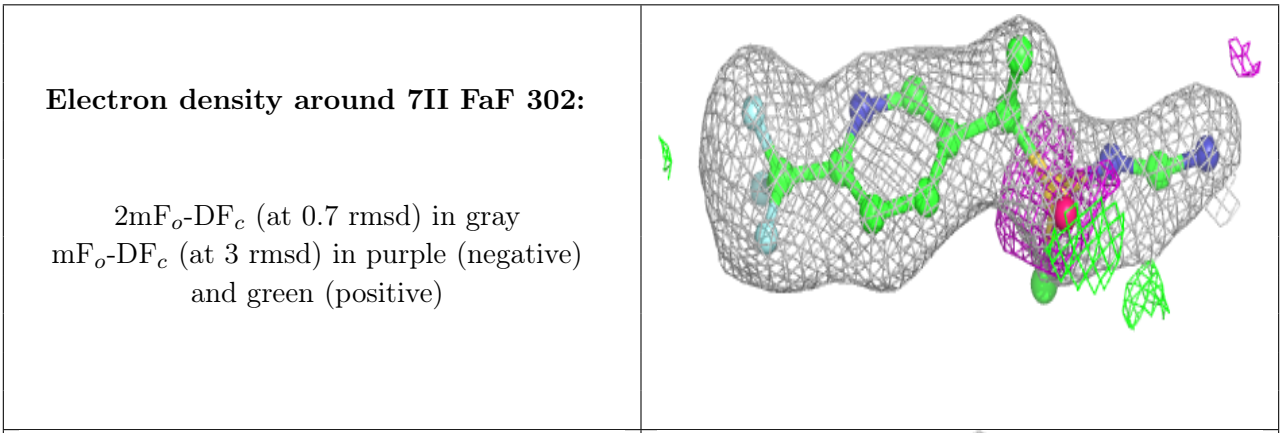
Electron density around 7II DaD 301:

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



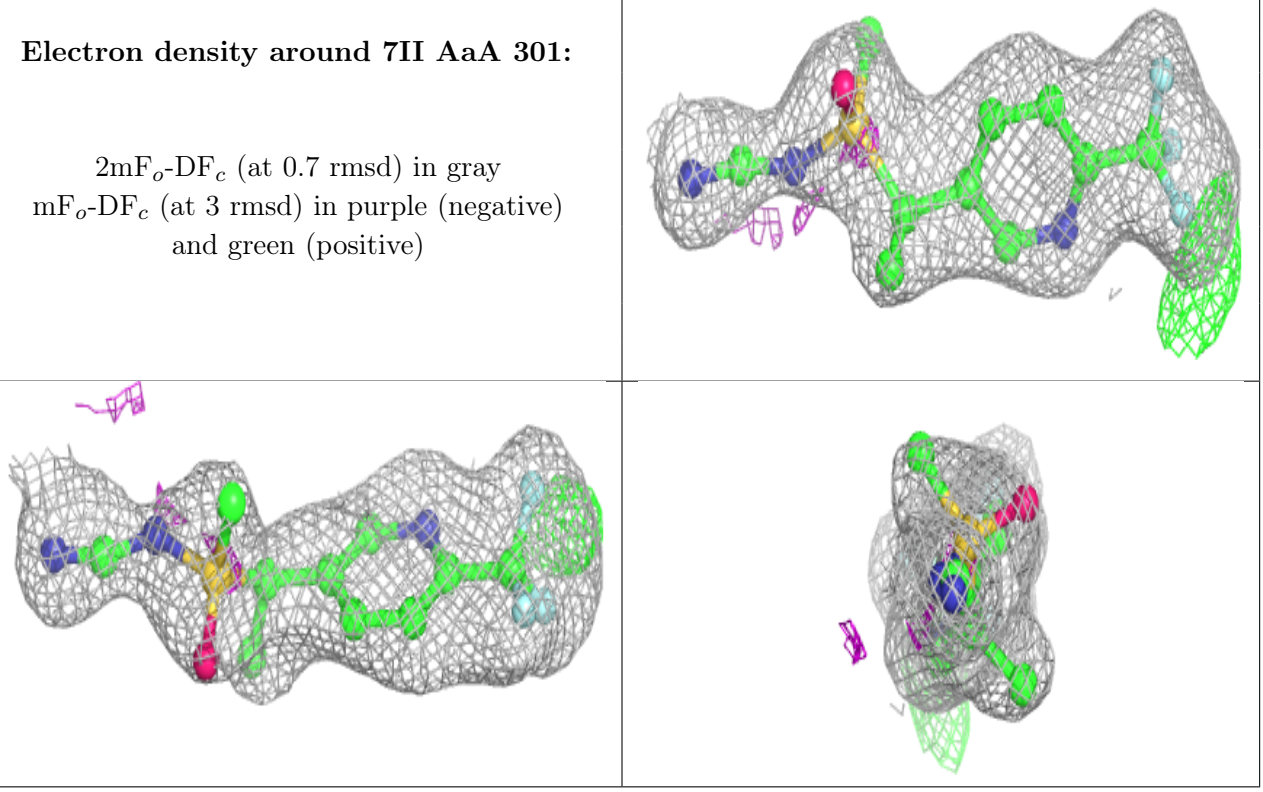
Electron density around 7II FaF 302:

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



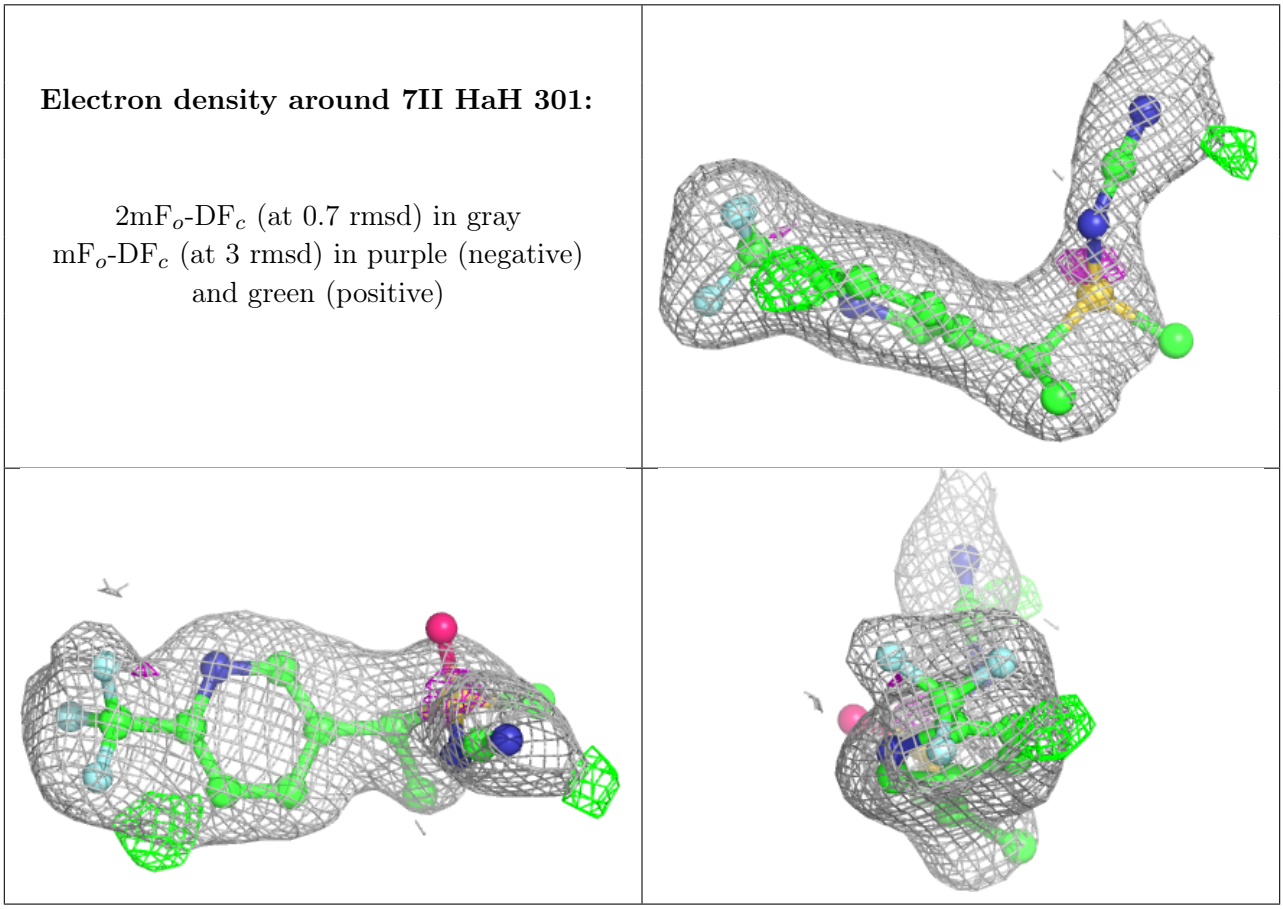
Electron density around 7II AaA 301:

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



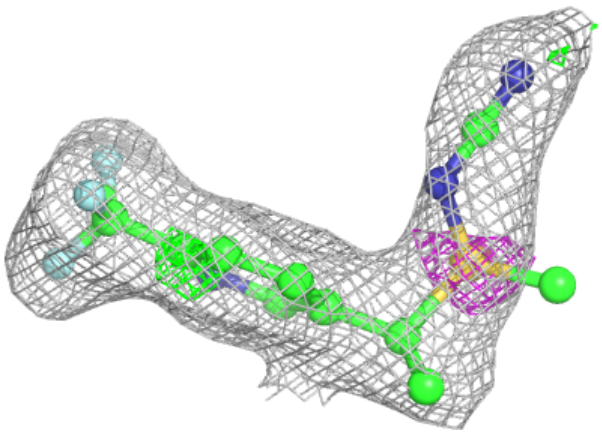
Electron density around 7II HaH 301:

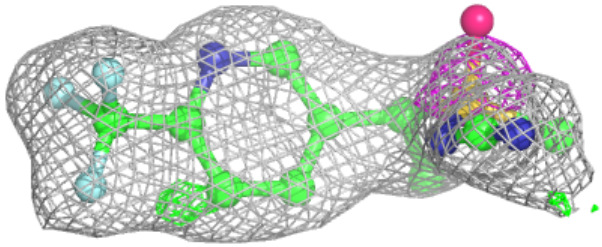
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

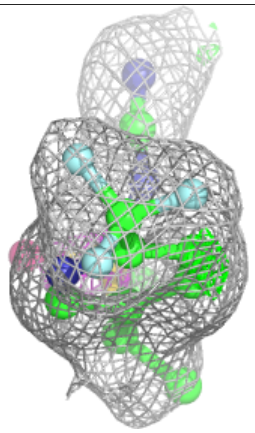


Electron density around 7II GaG 301:

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

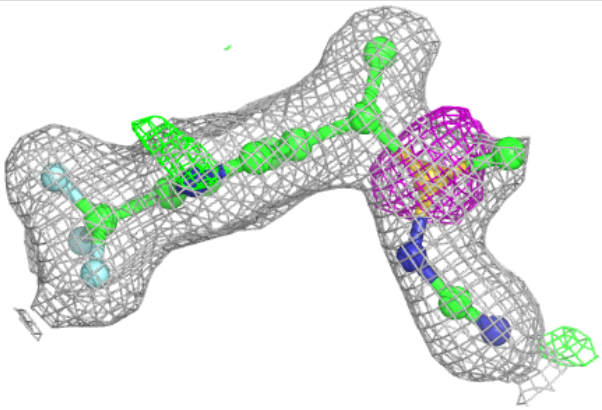


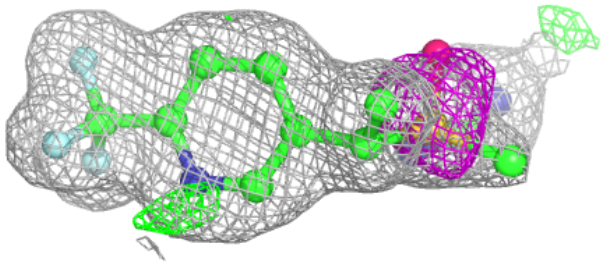


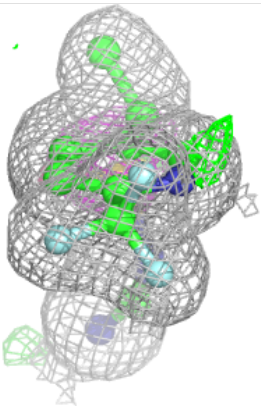


Electron density around 7II FaF 301:

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

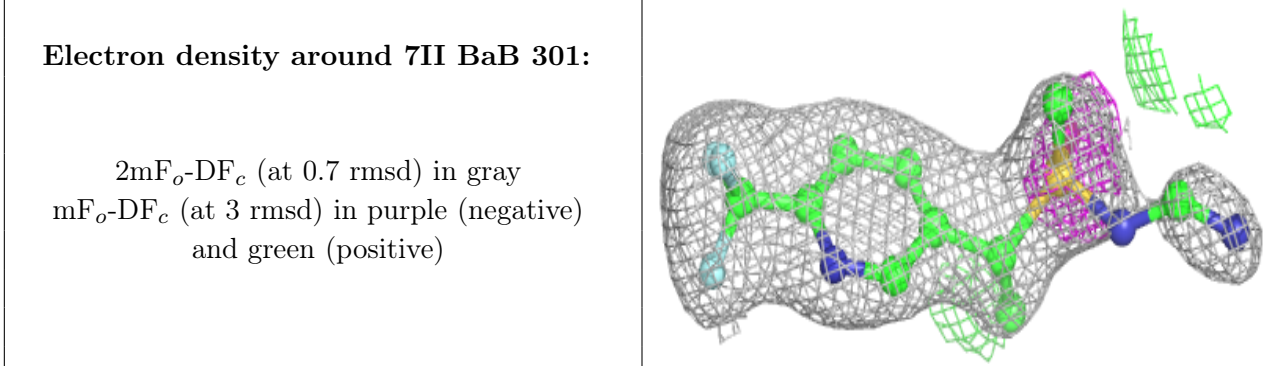


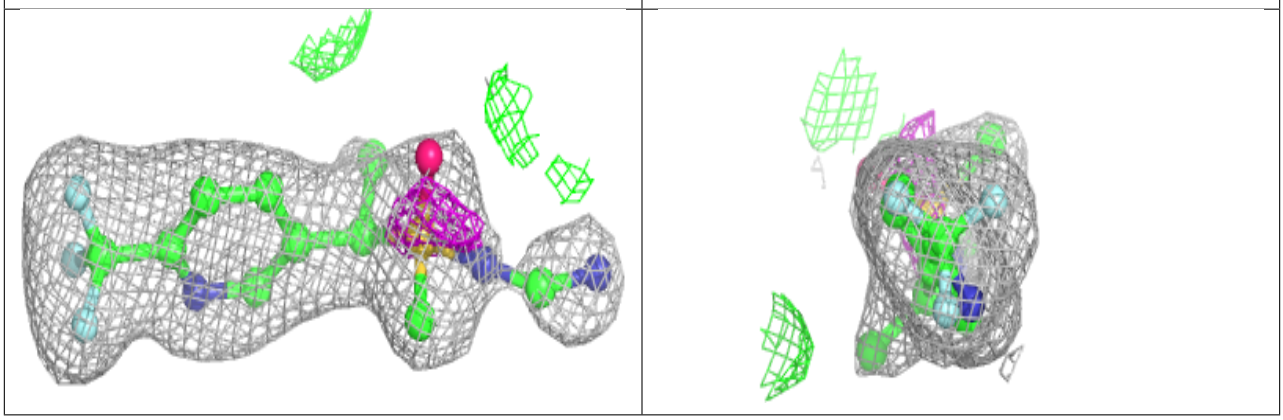




Electron density around 7II BaB 301:

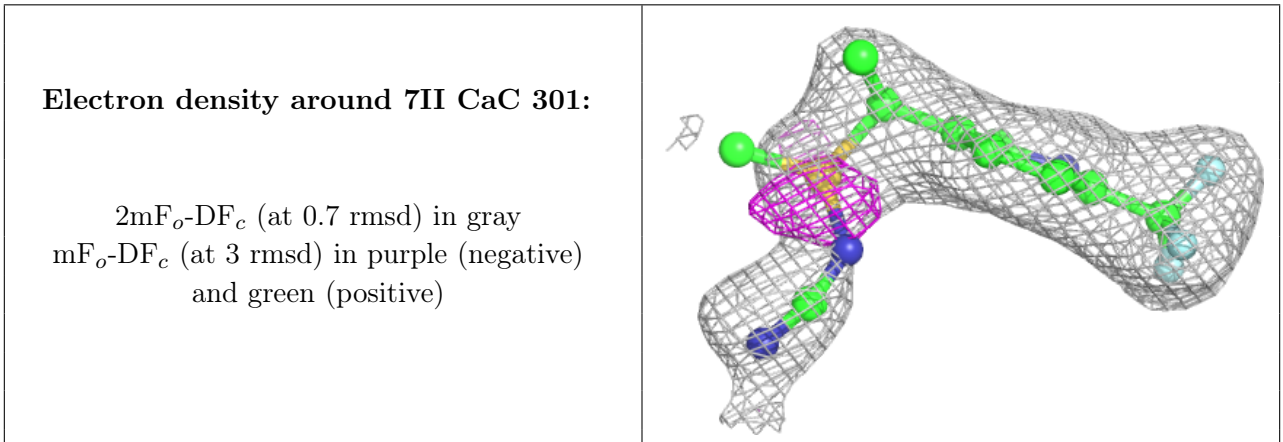
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

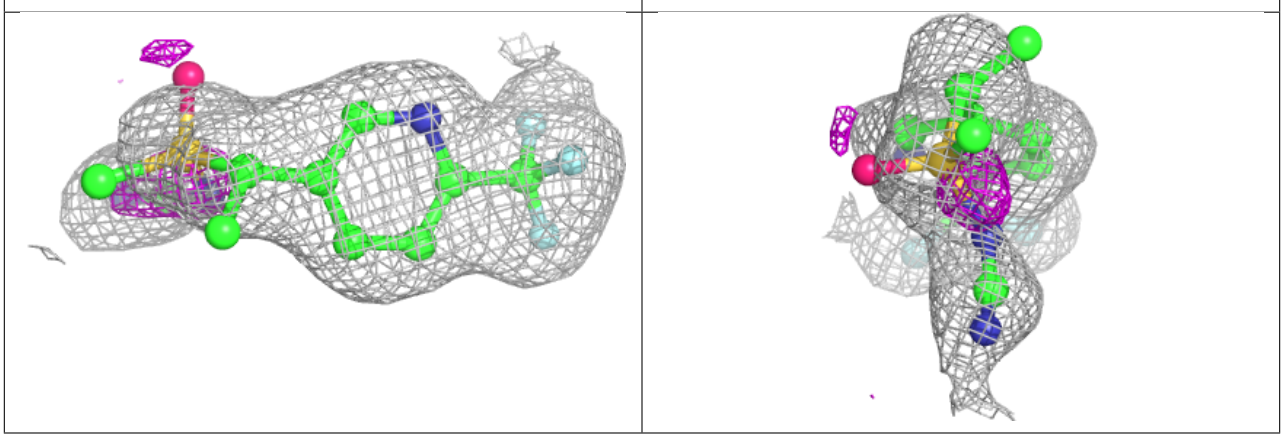




Electron density around 7II CaC 301:

$2mF_o$-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 (i)

There are no such residues in this entry.