



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2022 – 06:16 pm GMT

PDB ID : 7PE6
Title : Crystal structure of Lymnaea stagnalis Acetylcholine-binding protein (Ls-AChBP) Q55R/M114V double mutant complexed with Flupyrimin
Authors : Montgomery, M.G.
Deposited on : 2021-08-09
Resolution : 2.01 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

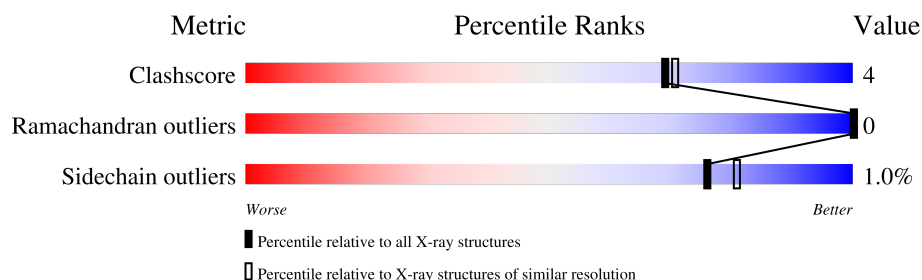
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AaA	210	94% • 5%
1	BaB	210	94% • •
1	CaC	210	91% • 6%
1	DaD	210	93% • 5%
1	EaE	210	93% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8246 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	200	Total	C	N	O	S	0	0	0
			1600	1003	275	318	4			
1	BaB	202	Total	C	N	O	S	0	0	0
			1613	1010	280	319	4			
1	CaC	197	Total	C	N	O	S	0	0	0
			1577	991	272	310	4			
1	DaD	199	Total	C	N	O	S	0	0	0
			1592	999	274	315	4			
1	EaE	200	Total	C	N	O	S	0	1	0
			1605	1009	275	317	4			

There are 20 discrepancies between the modelled and reference sequences:

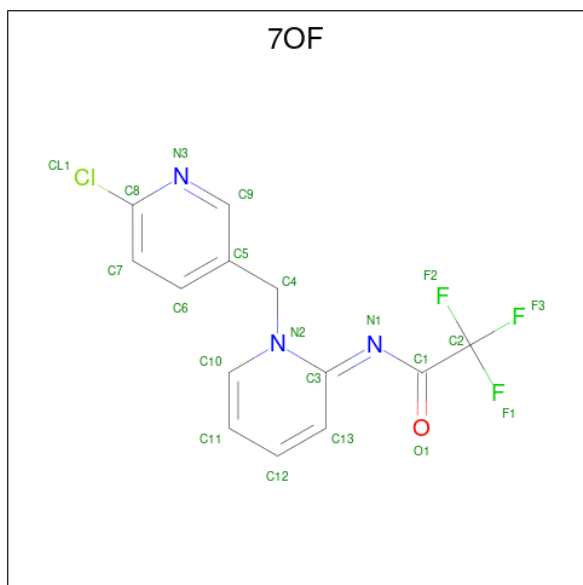
Chain	Residue	Modelled	Actual	Comment	Reference
AaA	1	ALA	-	expression tag	UNP P58154
AaA	55	ARG	GLN	engineered mutation	UNP P58154
AaA	66	ASP	ASN	engineered mutation	UNP P58154
AaA	114	VAL	MET	engineered mutation	UNP P58154
BaB	1	ALA	-	expression tag	UNP P58154
BaB	55	ARG	GLN	engineered mutation	UNP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

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Chain	Residue	Modelled	Actual	Comment	Reference
EaE	114	VAL	MET	engineered mutation	UNP P58154

- Molecule 2 is ({N} {E})- {N}-[1-[(6-chloranilpyridin-3-yl)methyl]pyridin-2-ylidene]-2,2,2-tris(fluoranyl)ethanamide (three-letter code: 7OF) (formula: C₁₃H₉ClF₃N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AaA	1	Total	C	Cl	F	N	O	0	0
			21	13	1	3	3	1		
2	BaB	1	Total	C	Cl	F	N	O	0	0
			21	13	1	3	3	1		
2	CaC	1	Total	C	Cl	F	N	O	0	0
			21	13	1	3	3	1		
2	DaD	1	Total	C	Cl	F	N	O	0	1
			42	26	2	6	6	2		
2	EaE	1	Total	C	Cl	F	N	O	0	1
			42	26	2	6	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AaA	29	Total	O	0	0
			29	29		
3	BaB	17	Total	O	0	0
			17	17		
3	CaC	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	DaD	21	Total	O	0	0
			21	21		
3	EaE	36	Total	O	0	0
			36	36		

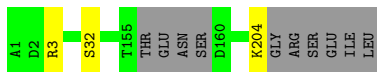
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS failed to run properly.

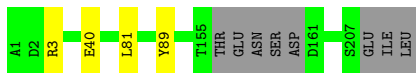
- Molecule 1: Acetylcholine-binding protein

Chain AaA:  94% 5%



- Molecule 1: Acetylcholine-binding protein

Chain BaB:  94% 5%



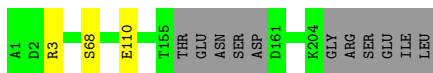
- Molecule 1: Acetylcholine-binding protein

Chain CaC:  91% 6%



- Molecule 1: Acetylcholine-binding protein

Chain DaD:  93% 5%



- Molecule 1: Acetylcholine-binding protein

Chain EaE:  93% 5%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	74.04Å 74.04Å 350.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.12 – 2.01	Depositor
% Data completeness (in resolution range)	99.9 (64.12-2.01)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.191 , 0.227	Depositor
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.527	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.098 for h,-h-k,-l	Xtriage
Total number of atoms	8246	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7OF

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	0.82	0/1635	0.96	3/2231 (0.1%)
1	BaB	0.81	0/1648	0.97	2/2247 (0.1%)
1	CaC	0.78	0/1612	0.93	2/2199 (0.1%)
1	DaD	0.82	0/1627	0.99	3/2220 (0.1%)
1	EaE	0.85	1/1644 (0.1%)	0.98	2/2243 (0.1%)
All	All	0.81	1/8166 (0.0%)	0.97	12/11140 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EaE	196	GLU	CD-OE2	5.93	1.32	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DaD	3	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	DaD	3	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	AaA	3	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	EaE	3	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	AaA	3	ARG	CG-CD-NE	-6.26	98.65	111.80
1	AaA	204	LYS	CA-C-O	-5.85	107.81	120.10
1	DaD	110	GLU	CB-CA-C	5.70	121.80	110.40
1	CaC	204	LYS	CA-C-O	-5.42	108.71	120.10
1	CaC	3	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	EaE	3	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	BaB	89	TYR	CB-CG-CD1	5.14	124.08	121.00
1	BaB	3	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	AaA	1600	0	1552	0	0
1	BaB	1613	0	1567	0	0
1	CaC	1577	0	1535	0	0
1	DaD	1592	0	1546	0	0
1	EaE	1605	0	1558	0	0
2	AaA	21	0	0	0	0
2	BaB	21	0	0	0	0
2	CaC	21	0	0	0	0
2	DaD	42	0	0	0	0
2	EaE	42	0	0	0	0
3	AaA	29	0	0	0	0
3	BaB	17	0	0	0	0
3	CaC	9	0	0	0	0
3	DaD	21	0	0	0	0
3	EaE	36	0	0	0	0
All	All	8246	0	7758	0	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.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AaA	196/210 (93%)	193 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BaB	198/210 (94%)	195 (98%)	3 (2%)	0	100	100
1	CaC	193/210 (92%)	192 (100%)	1 (0%)	0	100	100
1	DaD	195/210 (93%)	194 (100%)	1 (0%)	0	100	100
1	EaE	197/210 (94%)	196 (100%)	1 (0%)	0	100	100
All	All	979/1050 (93%)	970 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AaA	186/195 (95%)	185 (100%)	1 (0%)	88	92
1	BaB	187/195 (96%)	185 (99%)	2 (1%)	73	78
1	CaC	183/195 (94%)	180 (98%)	3 (2%)	62	67
1	DaD	185/195 (95%)	184 (100%)	1 (0%)	88	92
1	EaE	186/195 (95%)	184 (99%)	2 (1%)	73	78
All	All	927/975 (95%)	918 (99%)	9 (1%)	76	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AaA	32	SER
1	BaB	40	GLU
1	BaB	81	LEU
1	CaC	32	SER
1	CaC	153	ASP
1	CaC	177	THR
1	DaD	68	SER
1	EaE	68	SER
1	EaE	177	THR

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](#)

7 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	7OF	CaC	301	-	21,22,22	0.94	1 (4%)	24,31,31	0.89	0
2	7OF	EaE	301[A]	-	21,22,22	0.93	1 (4%)	24,31,31	0.87	0
2	7OF	AaA	301	-	21,22,22	0.85	0	24,31,31	0.86	0
2	7OF	BaB	301	-	21,22,22	0.98	0	24,31,31	0.88	0
2	7OF	EaE	301[B]	-	21,22,22	0.91	0	24,31,31	0.86	0
2	7OF	DaD	301[A]	-	21,22,22	1.09	2 (9%)	24,31,31	0.86	0
2	7OF	DaD	301[B]	-	21,22,22	0.88	0	24,31,31	0.88	0

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	7OF	CaC	301	-	-	3/11/14/14	0/2/2/2
2	7OF	EaE	301[A]	-	-	0/11/14/14	0/2/2/2
2	7OF	AaA	301	-	-	0/11/14/14	0/2/2/2
2	7OF	BaB	301	-	-	2/11/14/14	0/2/2/2
2	7OF	EaE	301[B]	-	-	2/11/14/14	0/2/2/2
2	7OF	DaD	301[A]	-	-	0/11/14/14	0/2/2/2
2	7OF	DaD	301[B]	-	-	2/11/14/14	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DaD	301[A]	7OF	C2-C1	2.40	1.56	1.53
2	DaD	301[A]	7OF	C3-N1	2.19	1.37	1.31
2	EaE	301[A]	7OF	C3-N1	2.04	1.37	1.31
2	CaC	301	7OF	C2-C1	2.02	1.56	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

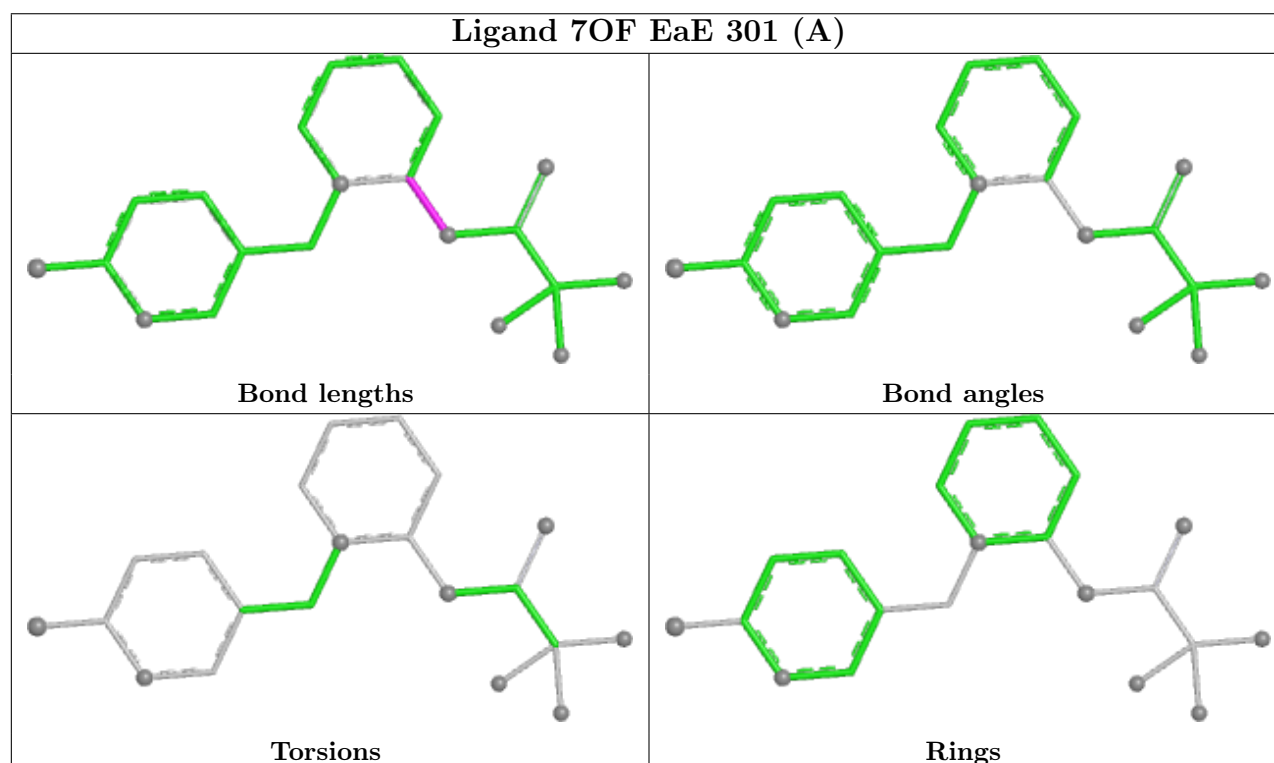
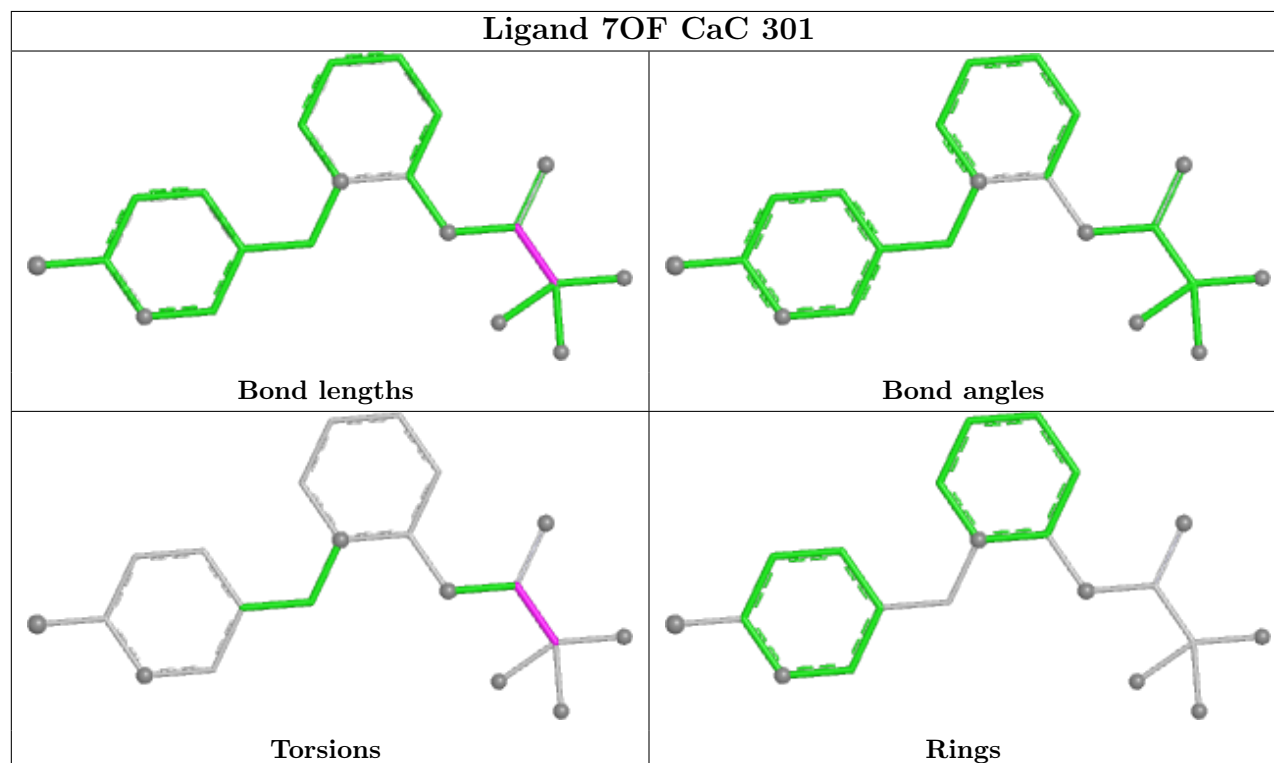
Mol	Chain	Res	Type	Atoms
2	CaC	301	7OF	O1-C1-C2-F2
2	CaC	301	7OF	O1-C1-C2-F1
2	CaC	301	7OF	O1-C1-C2-F3
2	BaB	301	7OF	N2-C4-C5-C6
2	EaE	301[B]	7OF	N2-C4-C5-C6
2	EaE	301[B]	7OF	N2-C4-C5-C9
2	BaB	301	7OF	N2-C4-C5-C9
2	DaD	301[B]	7OF	N2-C4-C5-C6
2	DaD	301[B]	7OF	N2-C4-C5-C9

There are no ring outliers.

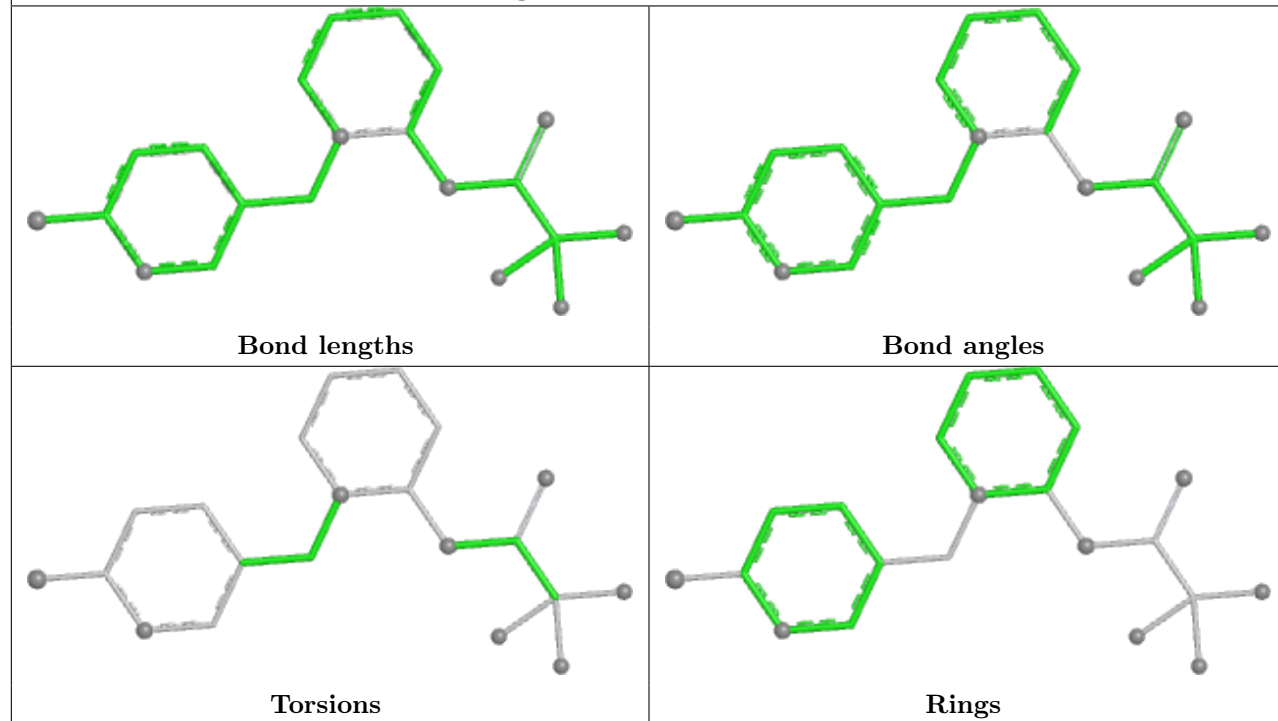
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

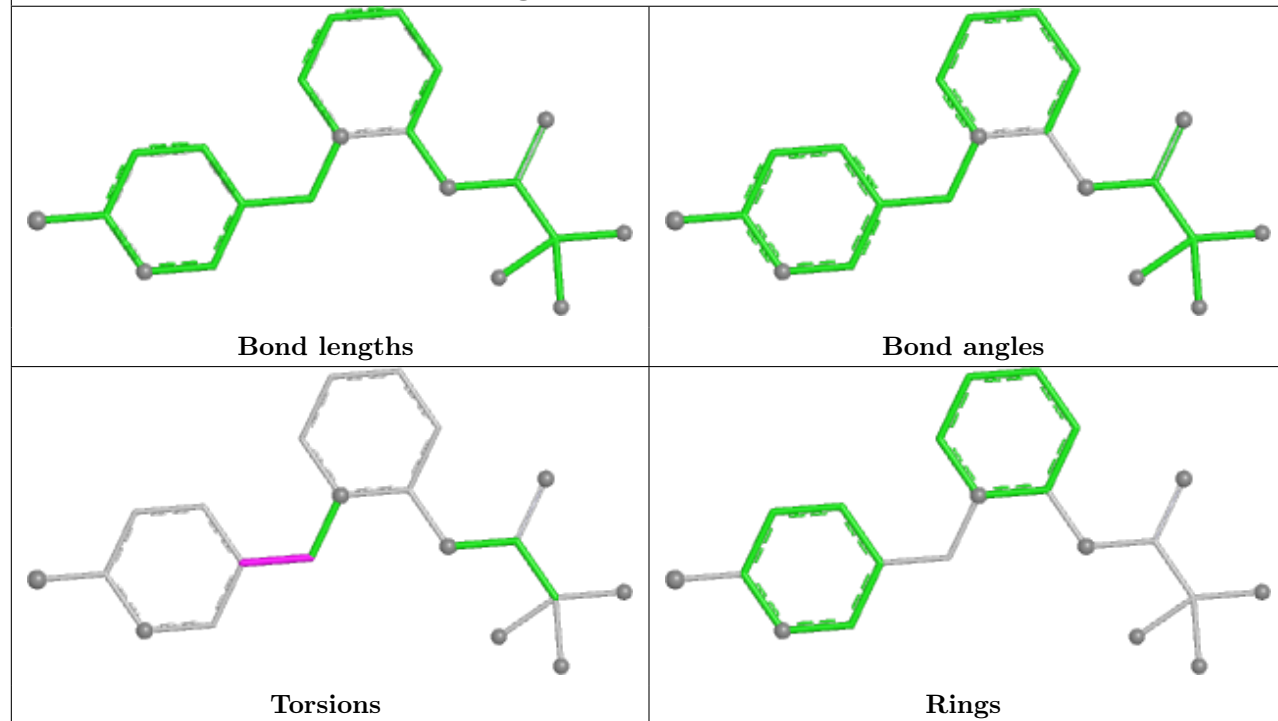
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



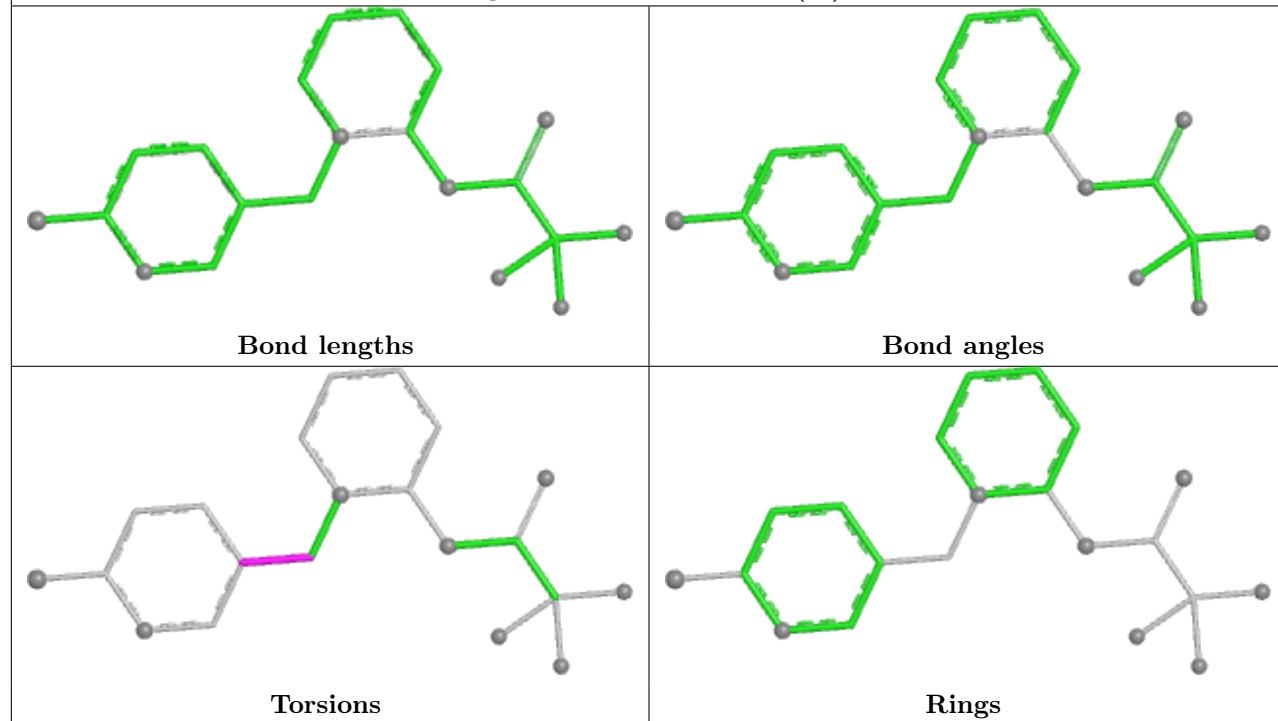
Ligand 7OF AaA 301



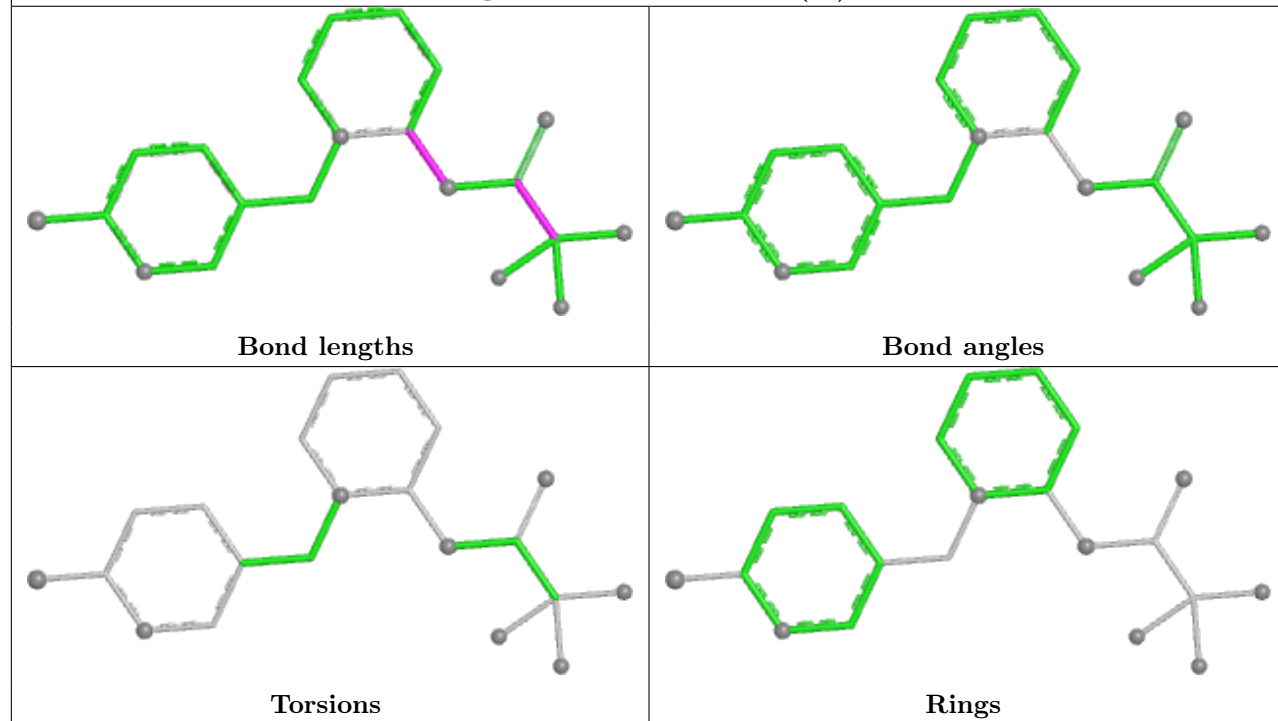
Ligand 7OF BaB 301

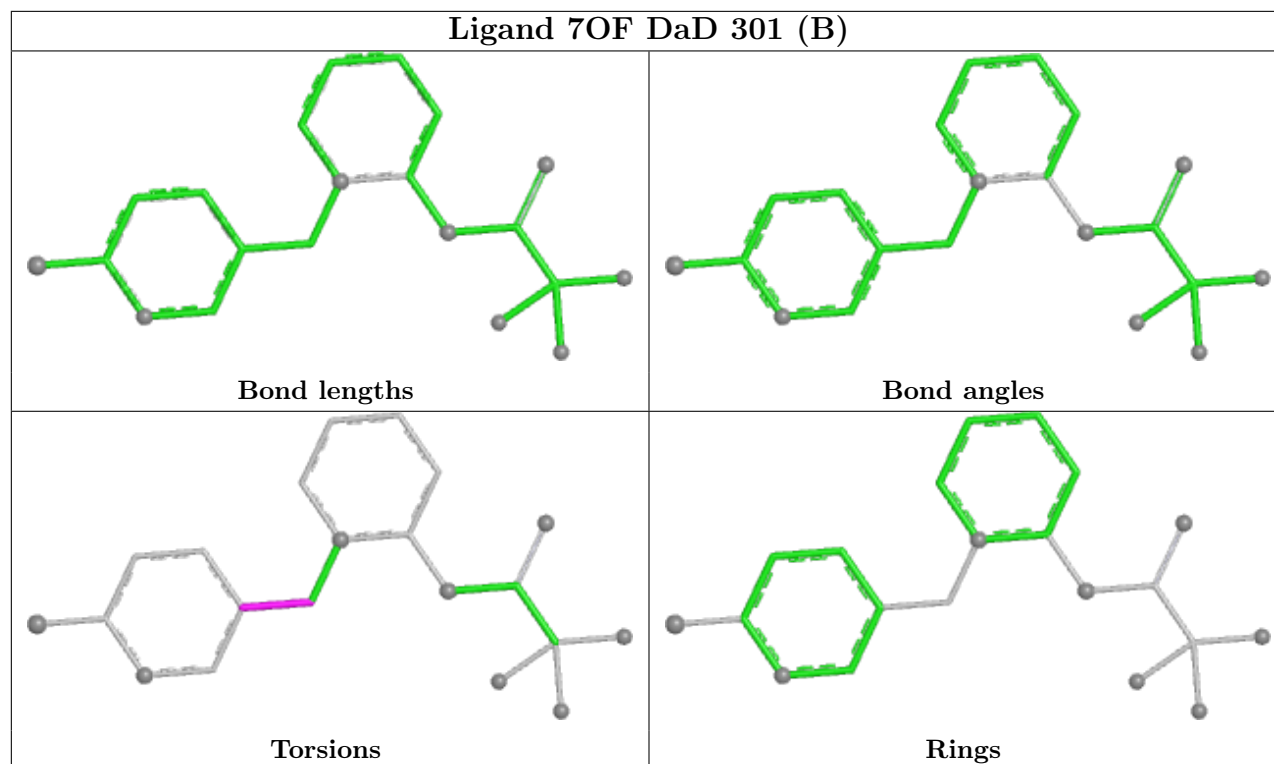


Ligand 7OF EaE 301 (B)



Ligand 7OF DaD 301 (A)





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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.