



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2022 – 06:12 pm GMT

PDB ID : 7PDR
Title : Crystal structure of Lymnaea stagnalis Acetylcholine-binding protein (Ls-AChBP) Q55R/M114V double mutant complexed with Dichloromezotiaz
Authors : Montgomery, M.G.
Deposited on : 2021-08-06
Resolution : 2.33 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 : 2.26
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

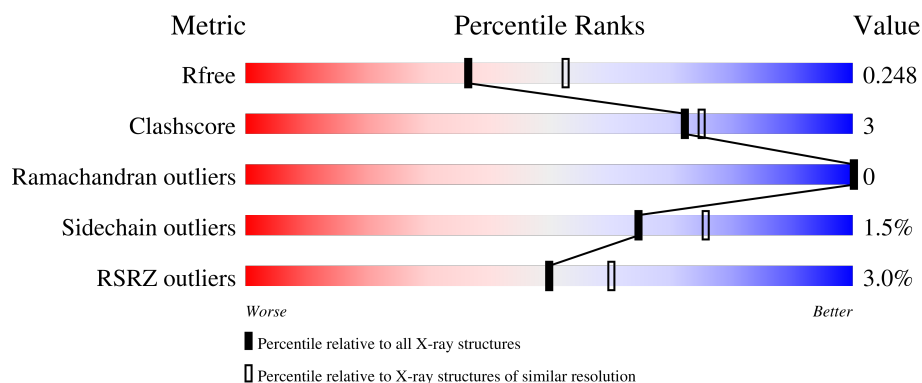
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AaA	210	<div> <div>3%</div> <div>90%</div> <div>7%</div> </div>
1	BaB	210	<div> <div>2%</div> <div>92%</div> <div>5%</div> </div>
1	CaC	210	<div> <div>4%</div> <div>92%</div> <div>6%</div> </div>
1	DaD	210	<div> <div>2%</div> <div>92%</div> <div>6%</div> </div>
1	EaE	210	<div> <div>2%</div> <div>92%</div> <div>5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8090 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	196	Total	C	N	O	S	0	1	0
			1569	987	267	311	4			
1	BaB	200	Total	C	N	O	S	0	1	0
			1602	1005	278	315	4			
1	CaC	197	Total	C	N	O	S	0	0	0
			1573	989	269	311	4			
1	DaD	198	Total	C	N	O	S	0	0	0
			1584	995	273	312	4			
1	EaE	199	Total	C	N	O	S	0	0	0
			1588	997	274	313	4			

There are 20 discrepancies between the modelled and reference sequences:

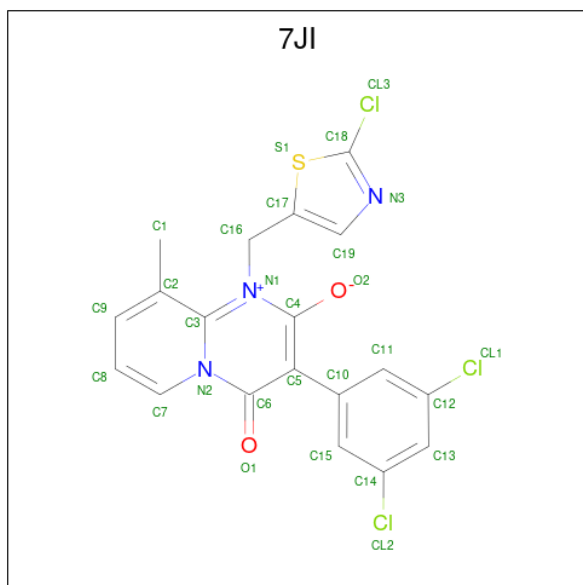
Chain	Residue	Modelled	Actual	Comment	Reference
AaA	1	ALA	-	expression tag	UNP P58154
AaA	55	ARG	GLN	engineered mutation	UNP P58154
AaA	66	ASP	ASN	engineered mutation	UNP P58154
AaA	114	VAL	MET	engineered mutation	UNP P58154
BaB	1	ALA	-	expression tag	UNP P58154
BaB	55	ARG	GLN	engineered mutation	UNP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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is 3-[3,5-bis(chloranyl)phenyl]-1-[(2-chloranyl-1,3-thiazol-5-yl)methyl]-9-methyl-pyrido[1,2-a]pyrimidine-2,4-dione (three-letter code: 7JI) (formula: C₁₉H₁₂Cl₃N₃O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	BaB	1	Total 28	C 19	Cl 3	N 3	O 2	S 1	0	0
2	CaC	1	Total 28	C 19	Cl 3	N 3	O 2	S 1	0	0
2	DaD	1	Total 28	C 19	Cl 3	N 3	O 2	S 1	0	0
2	EaE	1	Total 28	C 19	Cl 3	N 3	O 2	S 1	0	0
2	EaE	1	Total 28	C 19	Cl 3	N 3	O 2	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AaA	8	Total	O	0	0
			8	8		
3	BaB	4	Total	O	0	0
			4	4		
3	CaC	4	Total	O	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	DaD	4	Total	O	0	0
			4	4		
3	EaE	14	Total	O	0	0
			14	14		

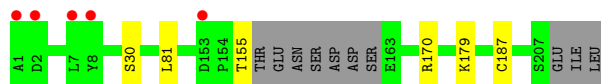
3 Residue-property plots [i](#)

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.

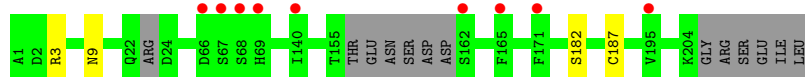
- Molecule 1: Acetylcholine-binding protein



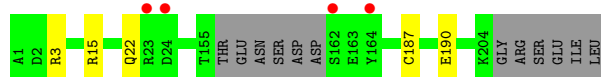
- Molecule 1: Acetylcholine-binding protein



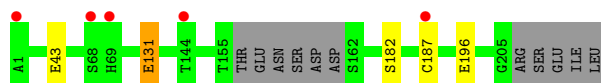
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	74.04Å 74.04Å 350.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.23 – 2.33 60.23 – 2.33	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.23-2.33) 100.0 (60.23-2.33)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.217 , 0.245 0.221 , 0.248	Depositor DCC
R_{free} test set	2310 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.073 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8090	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: 7JI

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	0.80	0/1606	0.97	2/2190 (0.1%)
1	BaB	0.80	0/1640	0.97	1/2236 (0.0%)
1	CaC	0.78	0/1607	0.92	1/2192 (0.0%)
1	DaD	0.80	0/1619	0.95	2/2209 (0.1%)
1	EaE	0.88	3/1623 (0.2%)	0.97	0/2214
All	All	0.81	3/8095 (0.0%)	0.96	6/11041 (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	BaB	0	1
1	CaC	0	1
1	DaD	0	1
1	EaE	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EaE	196	GLU	CD-OE2	5.29	1.31	1.25
1	EaE	43	GLU	CD-OE1	5.22	1.31	1.25
1	EaE	131	GLU	CD-OE1	5.18	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CaC	3	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	AaA	3	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	AaA	3	ARG	CG-CD-NE	-6.37	98.42	111.80
1	BaB	170	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	DaD	3	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	DaD	15	ARG	NE-CZ-NH1	-5.18	117.71	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

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	1569	0	1525	0	0
1	BaB	1602	0	1563	0	0
1	CaC	1573	0	1528	0	0
1	DaD	1584	0	1542	0	0
1	EaE	1588	0	1545	0	0
2	BaB	28	0	0	0	0
2	CaC	28	0	0	0	0
2	DaD	28	0	0	0	0
2	EaE	56	0	0	0	0
3	AaA	8	0	0	0	0
3	BaB	4	0	0	0	0
3	CaC	4	0	0	0	0
3	DaD	4	0	0	0	0
3	EaE	14	0	0	0	0
All	All	8090	0	7703	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 3.

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	191/210 (91%)	191 (100%)	0	0	100	100
1	BaB	197/210 (94%)	195 (99%)	2 (1%)	0	100	100
1	CaC	191/210 (91%)	191 (100%)	0	0	100	100
1	DaD	194/210 (92%)	193 (100%)	1 (0%)	0	100	100
1	EaE	195/210 (93%)	194 (100%)	1 (0%)	0	100	100
All	All	968/1050 (92%)	964 (100%)	4 (0%)	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	183/195 (94%)	179 (98%)	4 (2%)	52	63
1	BaB	186/195 (95%)	182 (98%)	4 (2%)	52	63
1	CaC	183/195 (94%)	181 (99%)	2 (1%)	73	83
1	DaD	184/195 (94%)	182 (99%)	2 (1%)	73	83
1	EaE	184/195 (94%)	182 (99%)	2 (1%)	73	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	920/975 (94%)	906 (98%)	14 (2%)	65	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AaA	59	SER
1	AaA	131	GLU
1	AaA	161	ASP
1	AaA	182	SER
1	BaB	30	SER
1	BaB	81	LEU
1	BaB	155	THR
1	BaB	179	LYS
1	CaC	9	ASN
1	CaC	182	SER
1	DaD	22	GLN
1	DaD	190	GLU
1	EaE	131	GLU
1	EaE	182	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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	7JI	EaE	302	-	24,31,31	1.74	3 (12%)	28,46,46	1.98	7 (25%)
2	7JI	CaC	301	-	24,31,31	1.76	3 (12%)	28,46,46	1.99	7 (25%)
2	7JI	DaD	301	-	24,31,31	1.76	3 (12%)	28,46,46	1.97	7 (25%)
2	7JI	EaE	301	-	24,31,31	1.74	3 (12%)	28,46,46	1.97	7 (25%)
2	7JI	BaB	301	-	24,31,31	1.75	3 (12%)	28,46,46	2.02	7 (25%)

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	7JI	EaE	302	-	-	1/7/8/8	0/4/4/4
2	7JI	CaC	301	-	-	1/7/8/8	0/4/4/4
2	7JI	DaD	301	-	-	1/7/8/8	0/4/4/4
2	7JI	EaE	301	-	-	1/7/8/8	0/4/4/4
2	7JI	BaB	301	-	-	0/7/8/8	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CaC	301	7JI	C6-N2	6.86	1.49	1.37
2	DaD	301	7JI	C6-N2	6.85	1.49	1.37
2	BaB	301	7JI	C6-N2	6.80	1.49	1.37
2	EaE	302	7JI	C6-N2	6.78	1.49	1.37
2	EaE	301	7JI	C6-N2	6.77	1.49	1.37
2	CaC	301	7JI	C4-N1	3.24	1.43	1.38
2	BaB	301	7JI	C4-N1	3.20	1.43	1.38
2	EaE	302	7JI	C4-N1	3.13	1.43	1.38
2	EaE	301	7JI	C4-N1	3.11	1.43	1.38
2	DaD	301	7JI	C4-N1	3.08	1.43	1.38
2	DaD	301	7JI	O2-C4	-2.98	1.23	1.32
2	EaE	302	7JI	O2-C4	-2.97	1.23	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CaC	301	7JI	O2-C4	-2.97	1.23	1.32
2	EaE	301	7JI	O2-C4	-2.97	1.23	1.32
2	BaB	301	7JI	O2-C4	-2.95	1.23	1.32

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CaC	301	7JI	C1-C2-C3	4.91	124.79	120.03
2	EaE	301	7JI	C1-C2-C3	4.88	124.77	120.03
2	BaB	301	7JI	C1-C2-C3	4.88	124.76	120.03
2	DaD	301	7JI	C1-C2-C3	4.88	124.76	120.03
2	EaE	302	7JI	C1-C2-C3	4.74	124.63	120.03
2	BaB	301	7JI	C7-N2-C6	-4.38	114.77	119.36
2	DaD	301	7JI	C7-N2-C6	-4.23	114.92	119.36
2	CaC	301	7JI	C7-N2-C6	-4.19	114.97	119.36
2	EaE	302	7JI	C7-N2-C6	-4.17	115.00	119.36
2	BaB	301	7JI	C16-N1-C4	-4.15	112.78	117.86
2	EaE	301	7JI	C7-N2-C6	-4.03	115.14	119.36
2	DaD	301	7JI	C16-N1-C4	-3.92	113.06	117.86
2	EaE	302	7JI	C16-N1-C4	-3.90	113.09	117.86
2	EaE	301	7JI	C16-N1-C4	-3.78	113.23	117.86
2	CaC	301	7JI	C16-N1-C4	-3.56	113.50	117.86
2	BaB	301	7JI	C10-C5-C6	-3.53	117.92	122.44
2	CaC	301	7JI	C10-C5-C6	-3.47	118.00	122.44
2	EaE	302	7JI	C17-C16-N1	3.39	117.11	112.88
2	EaE	302	7JI	C19-C17-S1	-3.35	108.67	112.00
2	EaE	301	7JI	C17-C16-N1	3.34	117.04	112.88
2	CaC	301	7JI	C19-C17-S1	-3.26	108.76	112.00
2	BaB	301	7JI	C19-C17-S1	-3.23	108.79	112.00
2	DaD	301	7JI	C19-C17-S1	-3.22	108.80	112.00
2	EaE	301	7JI	C19-C17-S1	-3.22	108.80	112.00
2	EaE	301	7JI	C10-C5-C6	-3.19	118.35	122.44
2	CaC	301	7JI	C17-C16-N1	3.14	116.80	112.88
2	EaE	302	7JI	C10-C5-C6	-2.99	118.61	122.44
2	DaD	301	7JI	C17-C16-N1	2.94	116.55	112.88
2	BaB	301	7JI	C17-C16-N1	2.83	116.41	112.88
2	DaD	301	7JI	C10-C5-C6	-2.80	118.85	122.44
2	DaD	301	7JI	C5-C6-N2	-2.60	115.67	119.29
2	EaE	302	7JI	C5-C6-N2	-2.55	115.74	119.29
2	BaB	301	7JI	C5-C6-N2	-2.48	115.84	119.29
2	EaE	301	7JI	C5-C6-N2	-2.46	115.87	119.29
2	CaC	301	7JI	C5-C6-N2	-2.36	116.01	119.29

There are no chirality outliers.

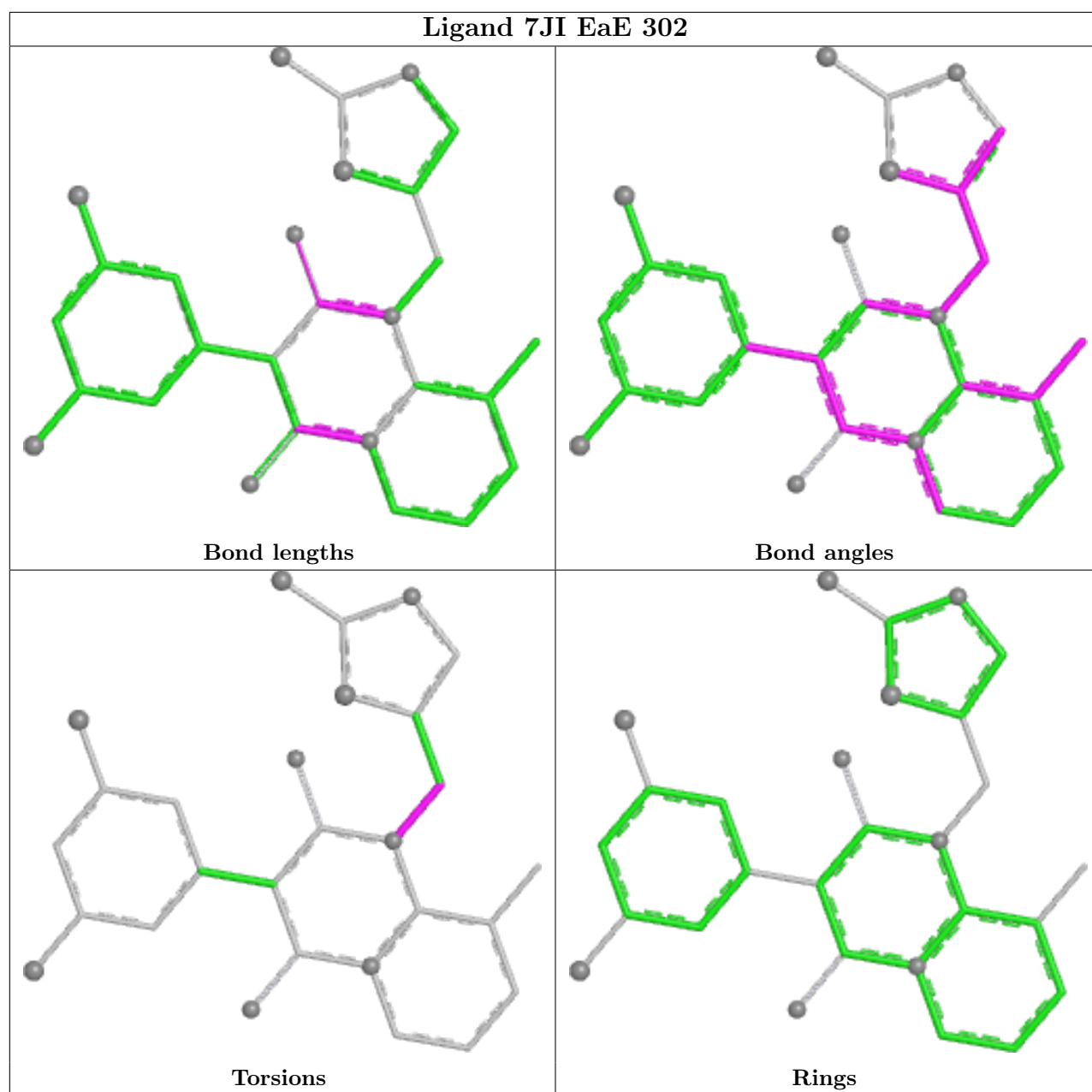
All (4) torsion outliers are listed below:

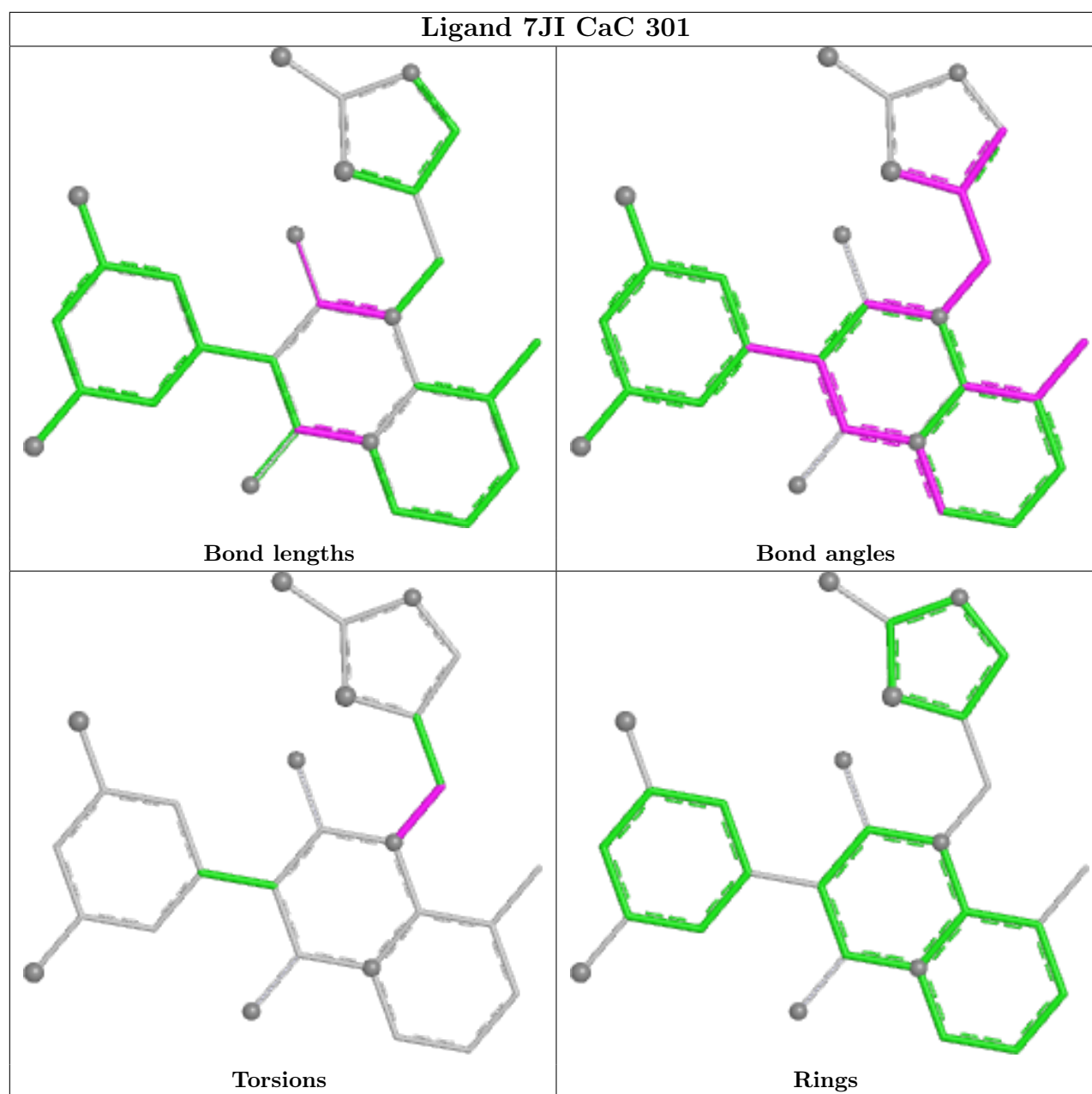
Mol	Chain	Res	Type	Atoms
2	EaE	302	7JI	C17-C16-N1-C3
2	CaC	301	7JI	C17-C16-N1-C3
2	DaD	301	7JI	C17-C16-N1-C3
2	EaE	301	7JI	C17-C16-N1-C3

There are no ring outliers.

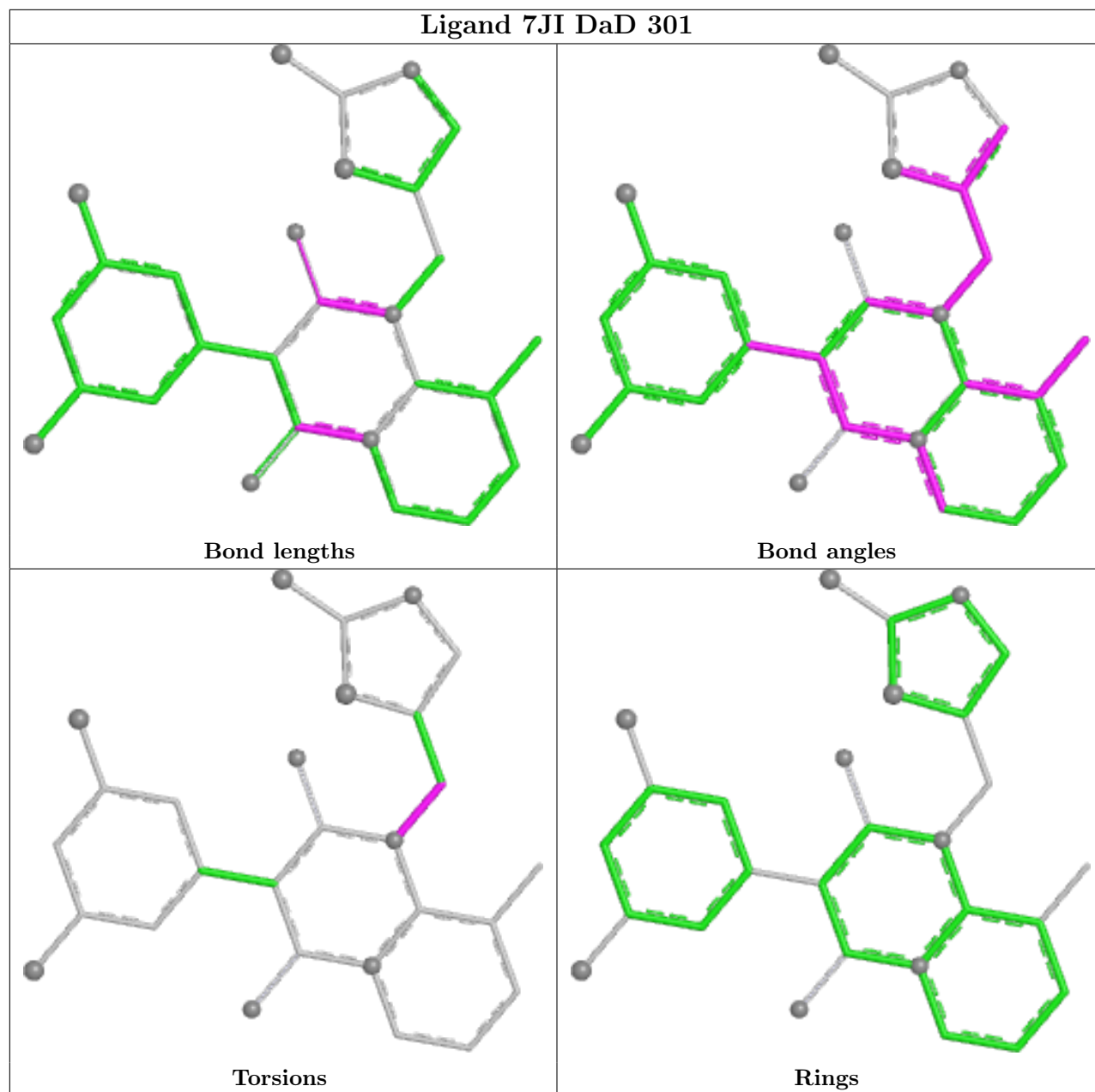
No monomer is involved in short contacts.

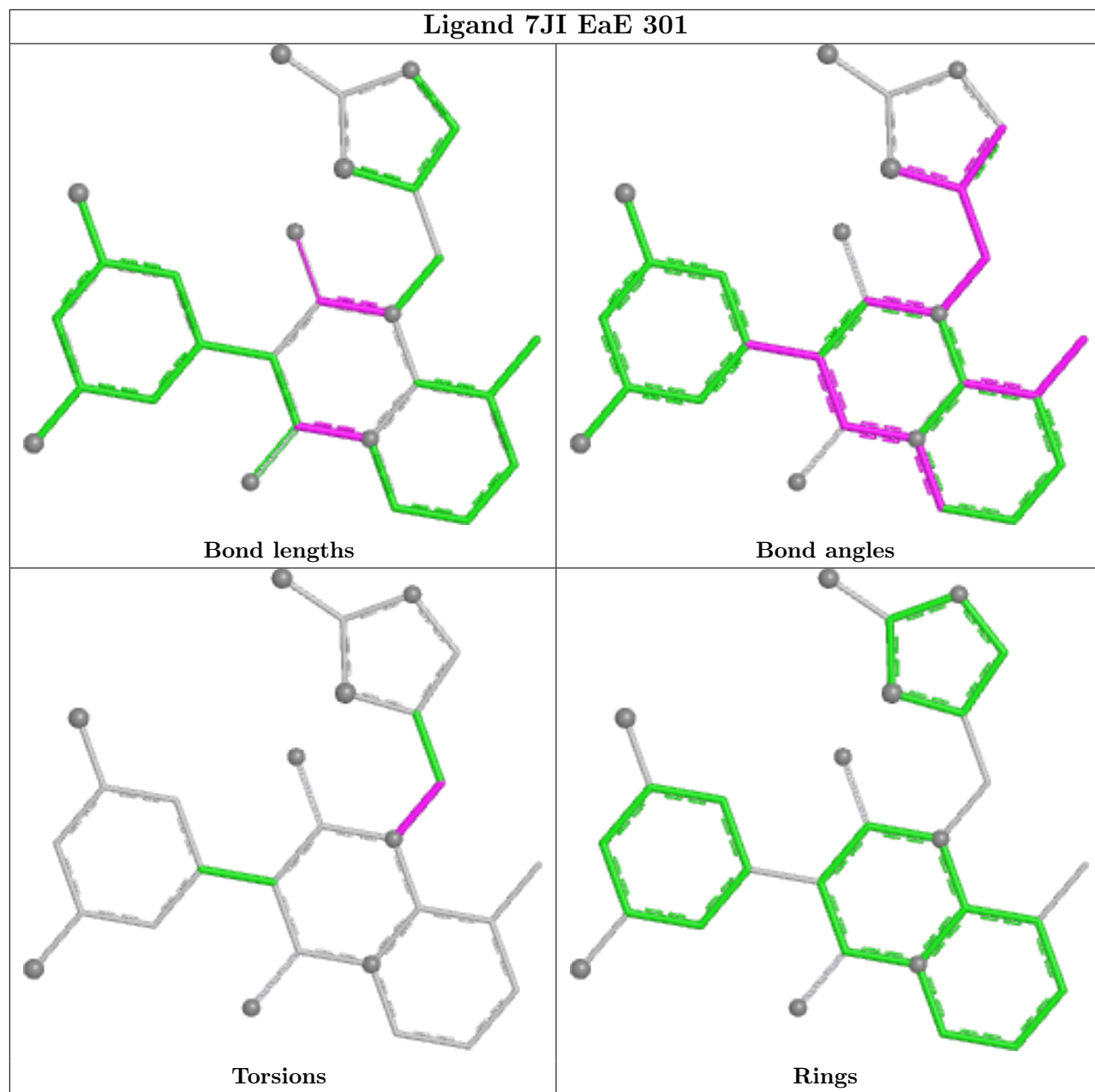
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

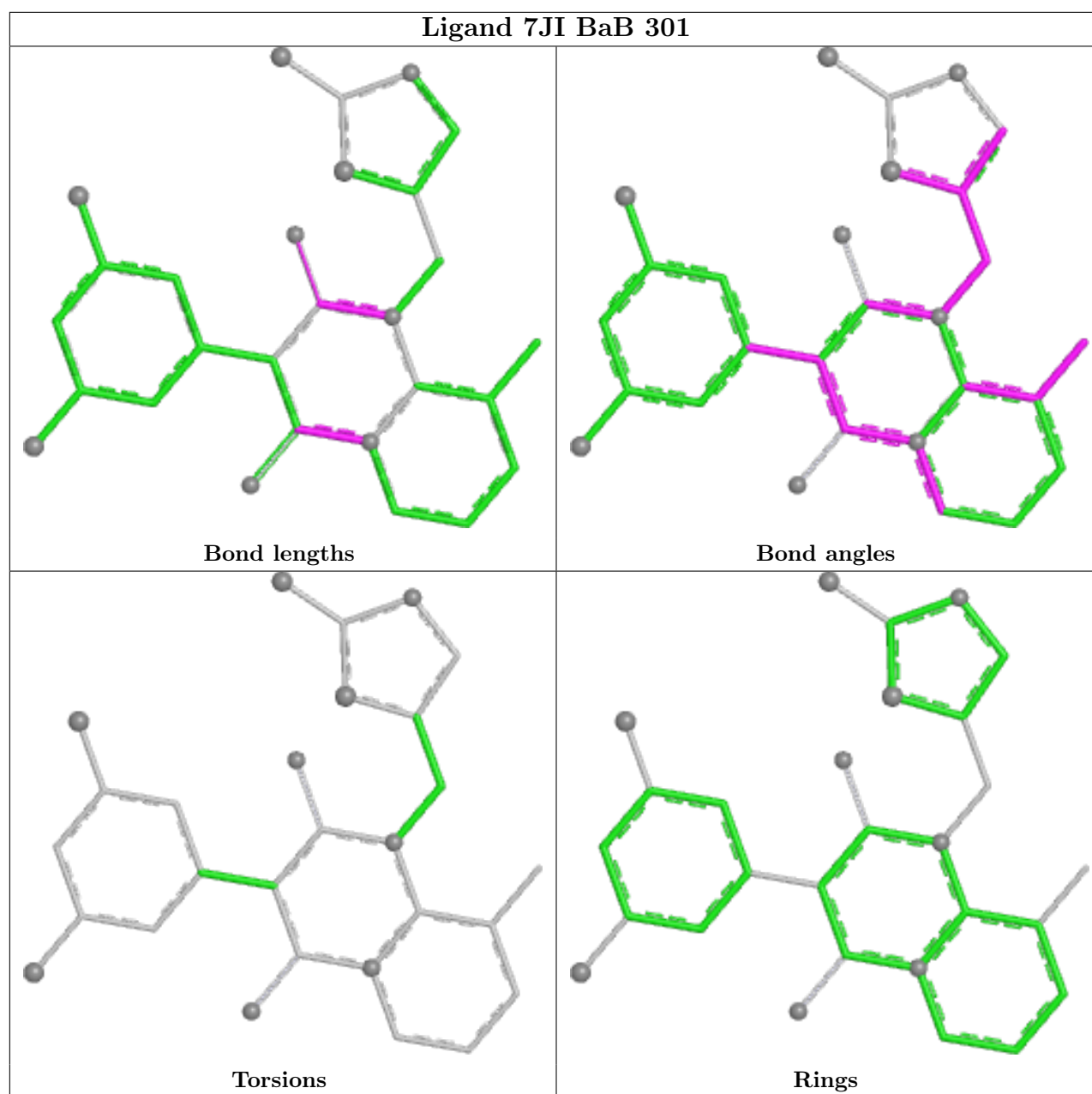




Ligand 7JI DaD 301







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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AaA	196/210 (93%)	0.39	7 (3%)	42	53	24, 34, 65, 101	0
1	BaB	200/210 (95%)	0.49	5 (2%)	57	66	27, 42, 71, 89	0
1	CaC	197/210 (93%)	0.58	9 (4%)	32	43	31, 43, 70, 91	0
1	DaD	198/210 (94%)	0.34	4 (2%)	65	74	24, 36, 62, 82	0
1	EaE	199/210 (94%)	0.24	5 (2%)	57	66	19, 29, 57, 68	0
All	All	990/1050 (94%)	0.41	30 (3%)	50	60	19, 37, 65, 101	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BaB	1	ALA	5.6
1	AaA	187	CYS	5.2
1	AaA	185	TYR	4.9
1	CaC	68	SER	4.7
1	CaC	67	SER	3.6
1	BaB	153	ASP	3.5
1	AaA	186	SER	3.3
1	DaD	24	ASP	3.2
1	EaE	187	CYS	3.1
1	CaC	171	PHE	3.1
1	AaA	112	LEU	3.0
1	BaB	2	ASP	3.0
1	EaE	69	HIS	2.9
1	AaA	7	LEU	2.8
1	CaC	195	VAL	2.8
1	EaE	68	SER	2.8
1	CaC	66	ASP	2.7
1	CaC	165	PHE	2.7
1	BaB	7	LEU	2.6
1	DaD	23	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CaC	140	ILE	2.5
1	AaA	19	ILE	2.3
1	DaD	164	TYR	2.3
1	EaE	144	THR	2.3
1	CaC	69	HIS	2.3
1	BaB	8	TYR	2.2
1	EaE	1	ALA	2.2
1	CaC	162	SER	2.1
1	AaA	148	ARG	2.1
1	DaD	162	SER	2.1

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](#)

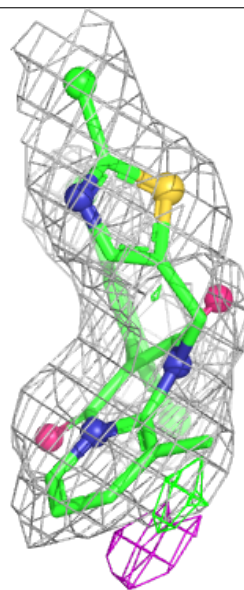
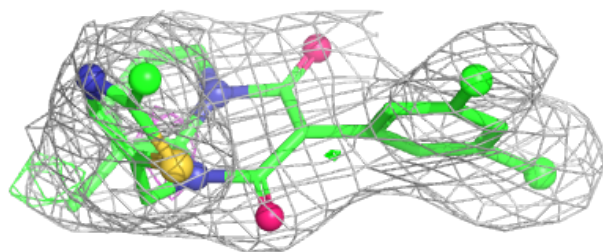
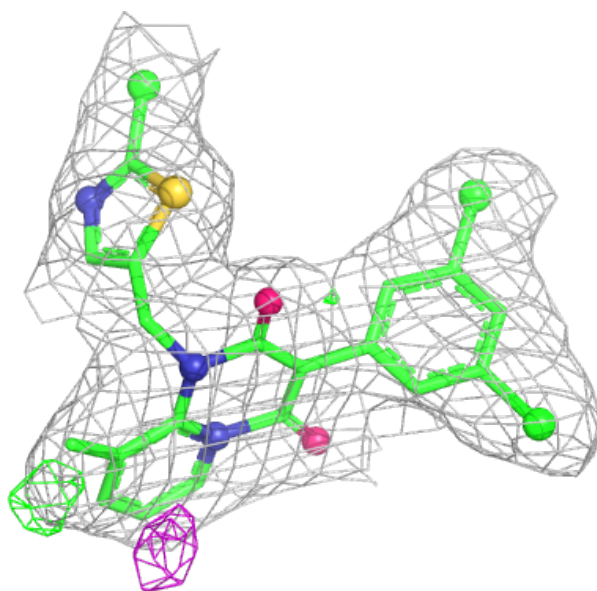
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	7JI	CaC	301	28/28	0.87	0.14	38,44,52,59	0
2	7JI	BaB	301	28/28	0.89	0.17	38,50,65,73	0
2	7JI	DaD	301	28/28	0.94	0.14	32,38,58,64	0
2	7JI	EaE	301	28/28	0.94	0.17	33,39,50,57	0
2	7JI	EaE	302	28/28	0.95	0.12	29,35,59,67	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.

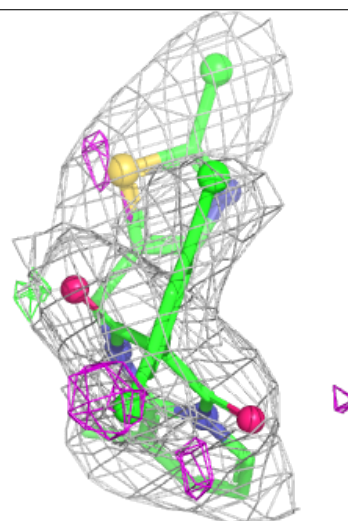
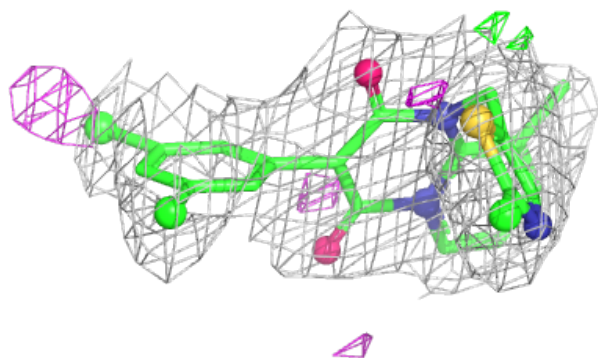
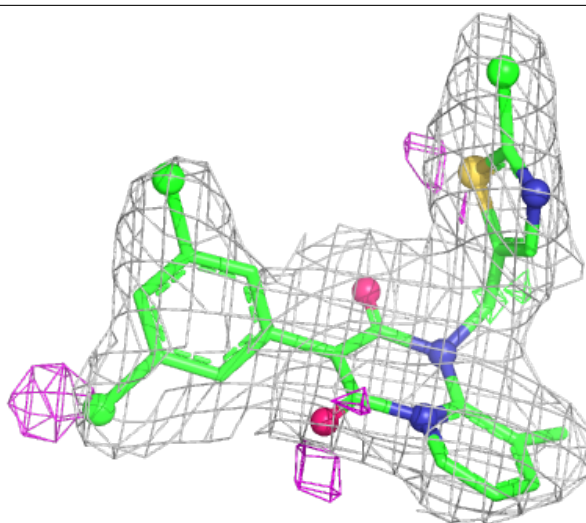
Electron density around 7JI CaC 301:

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



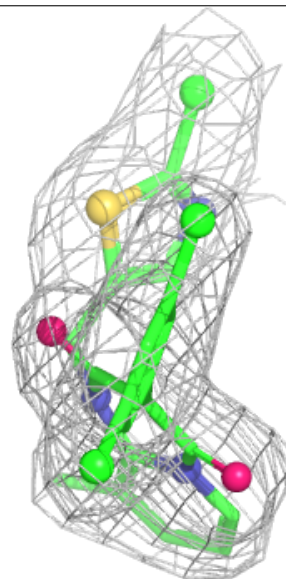
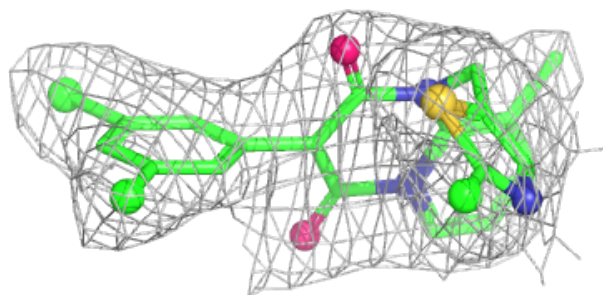
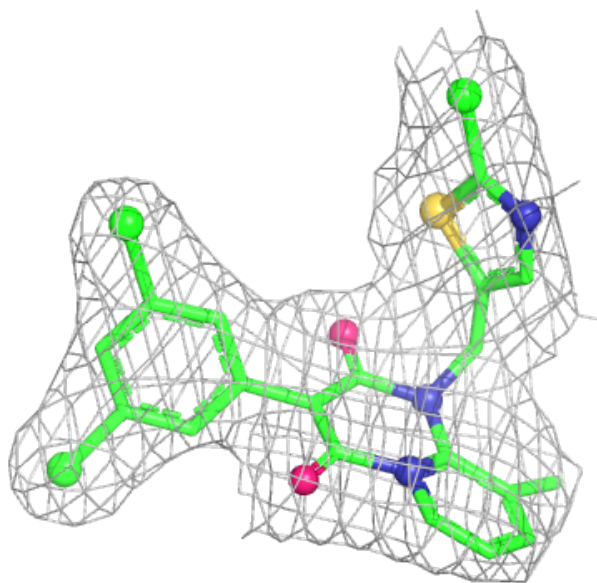
Electron density around 7JI BaB 301:

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



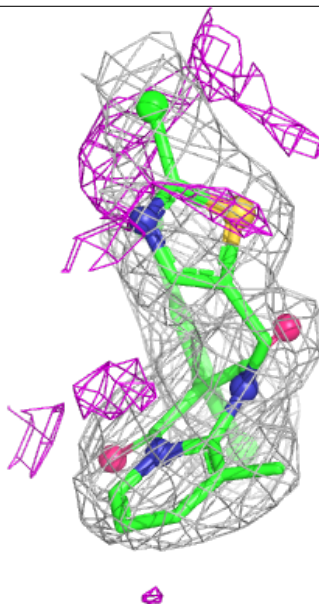
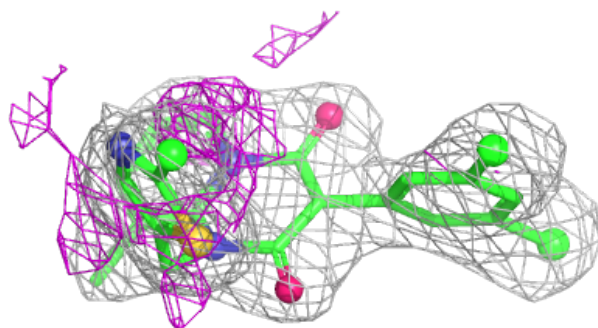
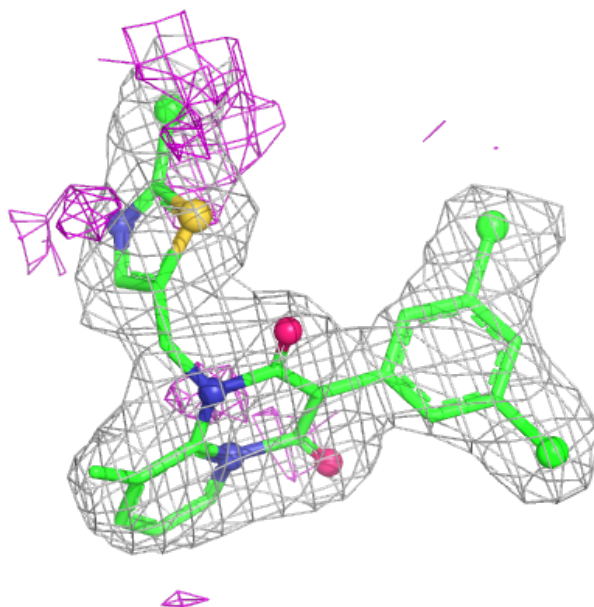
Electron density around 7JI DaD 301:

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



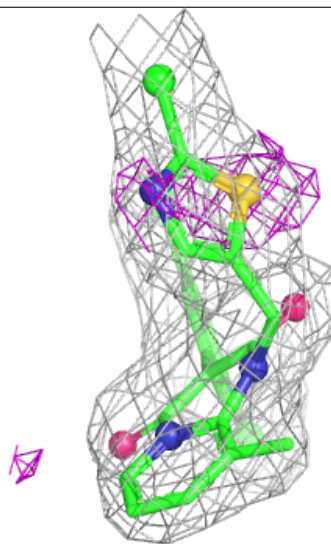
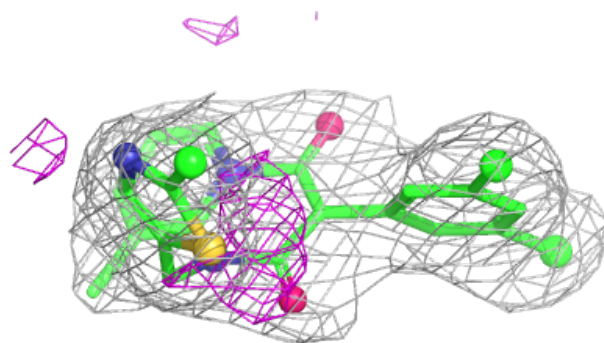
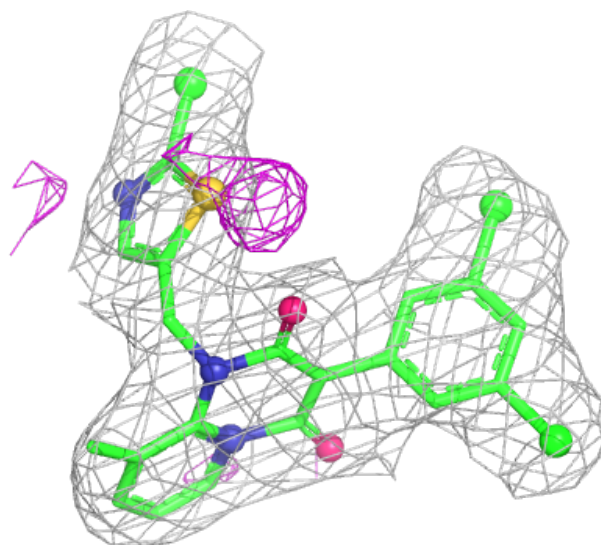
Electron density around 7JI EaE 301:

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



Electron density around 7JI EaE 302:

$2mF_o-DF_c$ (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.