



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:28 PM UTC

PDB ID : 7PE6 / pdb_00007pe6
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

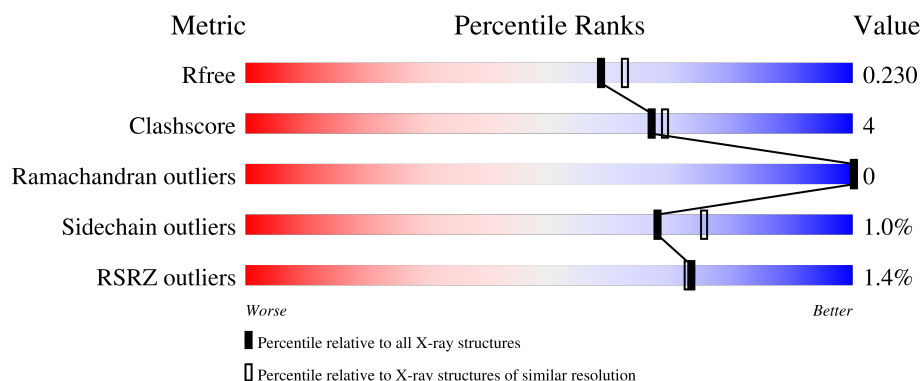
1 Overall quality at a glance

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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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% 86% 10% 5%
1	BaB	210	 % 85% 10% 5%
1	CaC	210	 3% 85% 9% 6%
1	DaD	210	 87% 8% 5%
1	EaE	210	 84% 11% 5%

2 Entry composition

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:

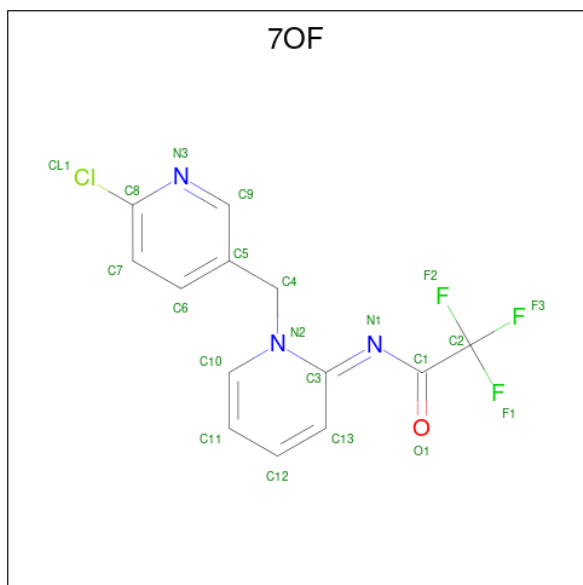
Chain	Residue	Modelled	Actual	Comment	Reference
AaA	1	ALA	-	expression tag	UNP P58154
AaA	55	ARG	GLN	engineered mutation	UNP P58154
AaA	66	ASP	ASN	engineered mutation	UNP P58154
AaA	114	VAL	MET	engineered mutation	UNP P58154
BaB	1	ALA	-	expression tag	UNP P58154
BaB	55	ARG	GLN	engineered mutation	UNP 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 (CCD ID: 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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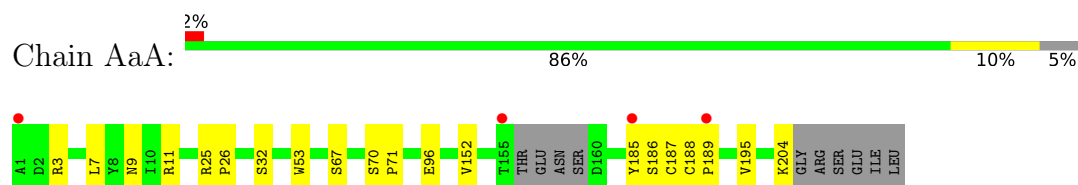
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	DaD	21	Total	O	0	0
			21	21		
3	EaE	36	Total	O	0	0
			36	36		

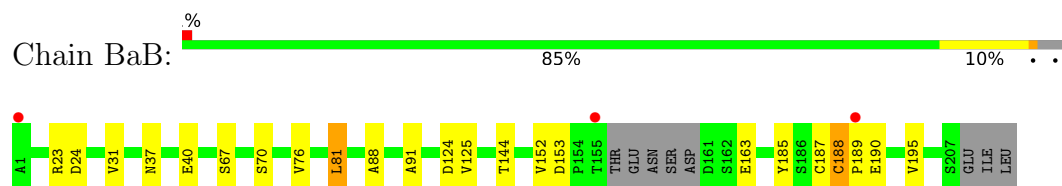
3 Residue-property plots [i](#)

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 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.

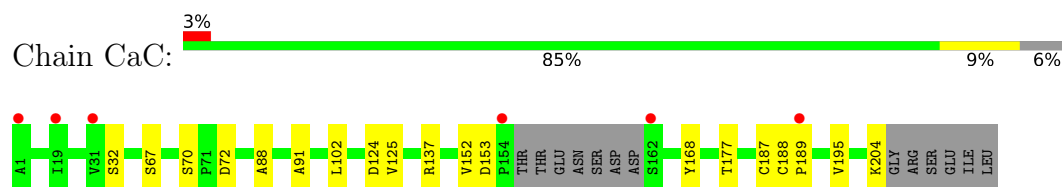
- Molecule 1: Acetylcholine-binding protein



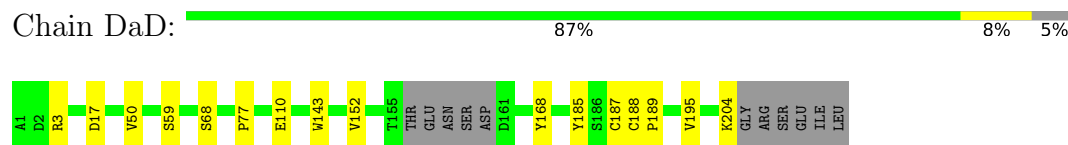
- Molecule 1: Acetylcholine-binding protein



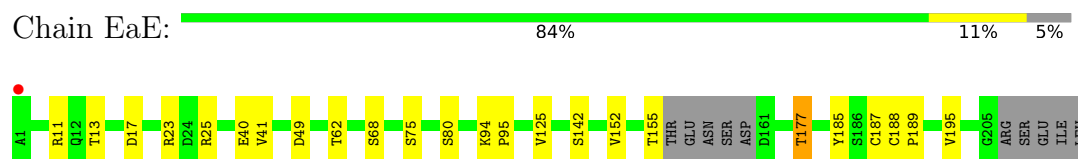
- Molecule 1: Acetylcholine-binding protein



- 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 350.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.12 – 2.01 64.12 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.12-2.01) 99.9 (64.12-2.01)	Depositor EDS
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 0.197 , 0.230	Depositor DCC
R_{free} test set	3542 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.1	EDS
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
F_o, F_c correlation	0.96	EDS
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 [i](#)

5.1 Standard geometry [i](#)

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	1.14	2/1635 (0.1%)	1.24	3/2231 (0.1%)
1	BaB	1.15	3/1648 (0.2%)	1.27	1/2247 (0.0%)
1	CaC	1.09	0/1612	1.24	2/2199 (0.1%)
1	DaD	1.16	1/1627 (0.1%)	1.26	5/2220 (0.2%)
1	EaE	1.19	4/1644 (0.2%)	1.25	2/2243 (0.1%)
All	All	1.15	10/8166 (0.1%)	1.25	13/11140 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EaE	95	PRO	C-O	-6.24	1.16	1.23
1	EaE	40	GLU	C-O	5.82	1.30	1.23
1	BaB	188	CYS	N-CA	5.64	1.50	1.45
1	AaA	26	PRO	C-O	-5.54	1.17	1.23
1	DaD	50	VAL	C-O	5.31	1.29	1.24
1	AaA	71	PRO	C-O	-5.10	1.17	1.23
1	BaB	37	ASN	C-O	5.09	1.30	1.23
1	EaE	75	SER	C-O	-5.09	1.17	1.24
1	BaB	31	VAL	C-O	5.06	1.29	1.24
1	EaE	142	SER	C-O	-5.02	1.17	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AaA	204	LYS	CA-C-O	-7.64	107.81	120.80
1	DaD	110	GLU	CB-CA-C	7.26	121.80	109.53
1	CaC	204	LYS	CA-C-O	-7.11	108.71	120.80
1	BaB	153	ASP	CB-CA-C	6.16	118.11	108.88
1	CaC	72	ASP	CA-CB-CG	6.08	118.68	112.60
1	AaA	3	ARG	CG-CD-NE	-6.07	98.65	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DaD	204	LYS	CA-C-O	-6.07	110.48	120.80
1	DaD	77	PRO	N-CA-CB	5.88	108.55	103.31
1	EaE	177	THR	CA-CB-OG1	-5.51	101.33	109.60
1	DaD	59	SER	CB-CA-C	5.48	119.24	109.38
1	EaE	49	ASP	CA-CB-CG	5.38	117.98	112.60
1	AaA	9	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	DaD	3	ARG	NE-CZ-NH2	5.01	123.71	119.20

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	13	0
1	BaB	1613	0	1567	15	0
1	CaC	1577	0	1535	11	0
1	DaD	1592	0	1546	11	0
1	EaE	1605	0	1558	16	0
2	AaA	21	0	0	1	0
2	BaB	21	0	0	2	0
2	CaC	21	0	0	0	0
2	DaD	42	0	0	4	0
2	EaE	42	0	0	2	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	57	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 (57) 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:DaD:17:ASP:OD2	1:EaE:11:ARG:NH1	2.20	0.72
1:AaA:152:VAL:HG12	1:AaA:195:VAL:HG23	1.78	0.65
1:BaB:152:VAL:HG12	1:BaB:195:VAL:HG23	1.80	0.63
1:AaA:188:CYS:HB3	1:AaA:189:PRO:HD2	1.81	0.62
1:EaE:152:VAL:HG12	1:EaE:195:VAL:HG23	1.82	0.61
1:DaD:152:VAL:HG12	1:DaD:195:VAL:HG23	1.81	0.61
1:CaC:152:VAL:HG12	1:CaC:195:VAL:HG23	1.84	0.59
1:EaE:155:THR:O	1:EaE:155:THR:HG22	2.06	0.56
1:CaC:67:SER:HA	1:CaC:70:SER:OG	2.06	0.55
1:BaB:185:TYR:OH	2:BaB:301:7OF:C11	2.55	0.54
1:DaD:188:CYS:HB3	1:DaD:189:PRO:HD2	1.90	0.54
1:CaC:187:CYS:SG	1:CaC:188:CYS:N	2.82	0.53
1:AaA:67:SER:HA	1:AaA:70:SER:OG	2.08	0.53
1:BaB:67:SER:HA	1:BaB:70:SER:OG	2.08	0.52
1:BaB:187:CYS:SG	1:BaB:188:CYS:N	2.82	0.52
1:AaA:186:SER:HB2	1:BaB:163:GLU:OE2	2.09	0.51
1:EaE:13:THR:HG21	1:EaE:62:THR:O	2.10	0.51
1:CaC:188:CYS:HB3	1:CaC:189:PRO:HD2	1.92	0.51
1:BaB:23:ARG:HG2	1:BaB:24:ASP:H	1.75	0.51
1:DaD:187:CYS:SG	1:DaD:188:CYS:N	2.84	0.51
1:EaE:23:ARG:HB2	1:EaE:25:ARG:HG3	1.93	0.50
1:AaA:187:CYS:SG	1:AaA:188:CYS:N	2.84	0.49
1:DaD:185:TYR:OH	2:DaD:301[B]:7OF:C10	2.61	0.49
1:AaA:11:ARG:NH2	1:EaE:17:ASP:OD2	2.47	0.47
1:AaA:188:CYS:HB3	1:AaA:189:PRO:CD	2.45	0.47
1:EaE:187:CYS:SG	1:EaE:188:CYS:N	2.88	0.47
1:BaB:189:PRO:HG2	1:BaB:190:GLU:OE2	2.14	0.47
1:DaD:143:TRP:CH2	2:DaD:301[B]:7OF:C11	2.99	0.46
1:DaD:185:TYR:OH	2:DaD:301[B]:7OF:C11	2.64	0.45
1:AaA:185:TYR:CZ	2:AaA:301:7OF:C10	3.00	0.45
1:BaB:185:TYR:OH	2:BaB:301:7OF:C10	2.65	0.45
1:BaB:76:VAL:HG11	1:BaB:81:LEU:HD21	1.98	0.45
1:AaA:25:ARG:NE	1:AaA:25:ARG:HA	2.31	0.45
1:BaB:152:VAL:CG1	1:BaB:195:VAL:HG23	2.44	0.45
1:EaE:152:VAL:CG1	1:EaE:195:VAL:HG23	2.47	0.44
1:DaD:152:VAL:CG1	1:DaD:195:VAL:HG23	2.46	0.44
1:AaA:7:LEU:CD2	1:EaE:17:ASP:HB2	2.48	0.44
1:CaC:124:ASP:HB2	1:DaD:168:TYR:CE1	2.53	0.43
1:DaD:143:TRP:CZ3	2:DaD:301[B]:7OF:C11	3.01	0.43
1:EaE:11:ARG:NE	1:EaE:80:SER:OG	2.50	0.43
1:EaE:185:TYR:OH	2:EaE:301[B]:7OF:C11	2.66	0.43
1:BaB:88:ALA:HB3	1:BaB:91:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AaA:152:VAL:CG1	1:AaA:195:VAL:HG23	2.46	0.43
1:CaC:88:ALA:HB3	1:CaC:91:ALA:HB2	2.01	0.42
1:EaE:188:CYS:HB3	1:EaE:189:PRO:HD2	2.00	0.42
1:EaE:41:VAL:HG13	1:EaE:125:VAL:HG11	2.01	0.42
1:BaB:125:VAL:HG12	1:BaB:125:VAL:O	2.19	0.42
1:CaC:152:VAL:CG1	1:CaC:195:VAL:HG23	2.47	0.42
1:BaB:188:CYS:HB3	1:BaB:189:PRO:HD2	2.01	0.42
1:CaC:125:VAL:HG12	1:CaC:125:VAL:O	2.19	0.42
1:AaA:53:TRP:CE3	2:EaE:301[A]:7OF:C12	3.03	0.41
1:EaE:41:VAL:HG13	1:EaE:125:VAL:CG1	2.50	0.41
1:BaB:144:THR:HG21	1:CaC:102:LEU:HB2	2.02	0.41
1:AaA:96:GLU:HG3	1:EaE:94:LYS:HE3	2.02	0.40
1:BaB:124:ASP:HB2	1:CaC:168:TYR:CE1	2.57	0.40
1:CaC:137:ARG:NH2	1:DaD:168:TYR:OH	2.55	0.40
1:EaE:125:VAL:HG12	1:EaE:125:VAL:O	2.21	0.40

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
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%)	81	87
1	BaB	187/195 (96%)	185 (99%)	2 (1%)	65	73
1	CaC	183/195 (94%)	180 (98%)	3 (2%)	55	62
1	DaD	185/195 (95%)	184 (100%)	1 (0%)	81	87
1	EaE	186/195 (95%)	184 (99%)	2 (1%)	65	73
All	All	927/975 (95%)	918 (99%)	9 (1%)	68	75

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	EaE	301[A]	-	19,22,22	0.53	0	25,31,31	1.01	1 (4%)
2	7OF	CaC	301	-	19,22,22	0.60	0	25,31,31	1.02	1 (4%)
2	7OF	EaE	301[B]	-	19,22,22	0.63	0	25,31,31	0.93	1 (4%)
2	7OF	DaD	301[B]	-	19,22,22	0.68	0	25,31,31	0.97	2 (8%)
2	7OF	AaA	301	-	19,22,22	0.61	0	25,31,31	0.92	0
2	7OF	DaD	301[A]	-	19,22,22	0.64	0	25,31,31	1.02	1 (4%)
2	7OF	BaB	301	-	19,22,22	0.79	0	25,31,31	0.96	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	EaE	301[A]	-	-	1/14/14/14	0/2/2/2
2	7OF	CaC	301	-	-	1/14/14/14	0/2/2/2
2	7OF	EaE	301[B]	-	-	2/14/14/14	0/2/2/2
2	7OF	DaD	301[B]	-	-	1/14/14/14	0/2/2/2
2	7OF	AaA	301	-	-	0/14/14/14	0/2/2/2
2	7OF	DaD	301[A]	-	-	0/14/14/14	0/2/2/2
2	7OF	BaB	301	-	-	0/14/14/14	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DaD	301[A]	7OF	C13-C3-N1	2.58	131.20	128.32
2	EaE	301[A]	7OF	C13-C3-N1	2.47	131.08	128.32
2	CaC	301	7OF	C13-C3-N1	2.36	130.96	128.32
2	EaE	301[B]	7OF	C12-C13-C3	2.04	122.23	119.60
2	DaD	301[B]	7OF	C12-C13-C3	2.01	122.20	119.60
2	DaD	301[B]	7OF	C13-C3-N1	2.01	130.56	128.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DaD	301[B]	7OF	C2-C1-N1-C3
2	EaE	301[A]	7OF	C2-C1-N1-C3
2	EaE	301[B]	7OF	C2-C1-N1-C3
2	CaC	301	7OF	O1-C1-C2-F2
2	EaE	301[B]	7OF	N1-C1-C2-F3

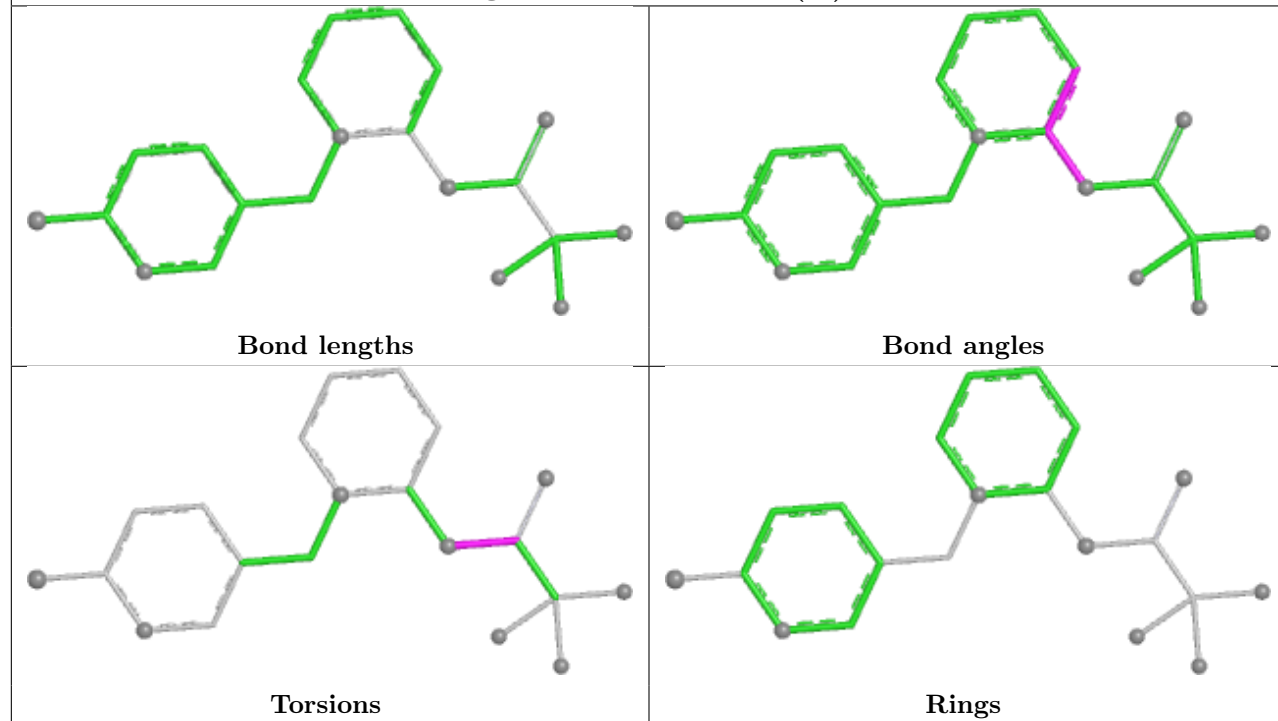
There are no ring outliers.

5 monomers are involved in 9 short contacts:

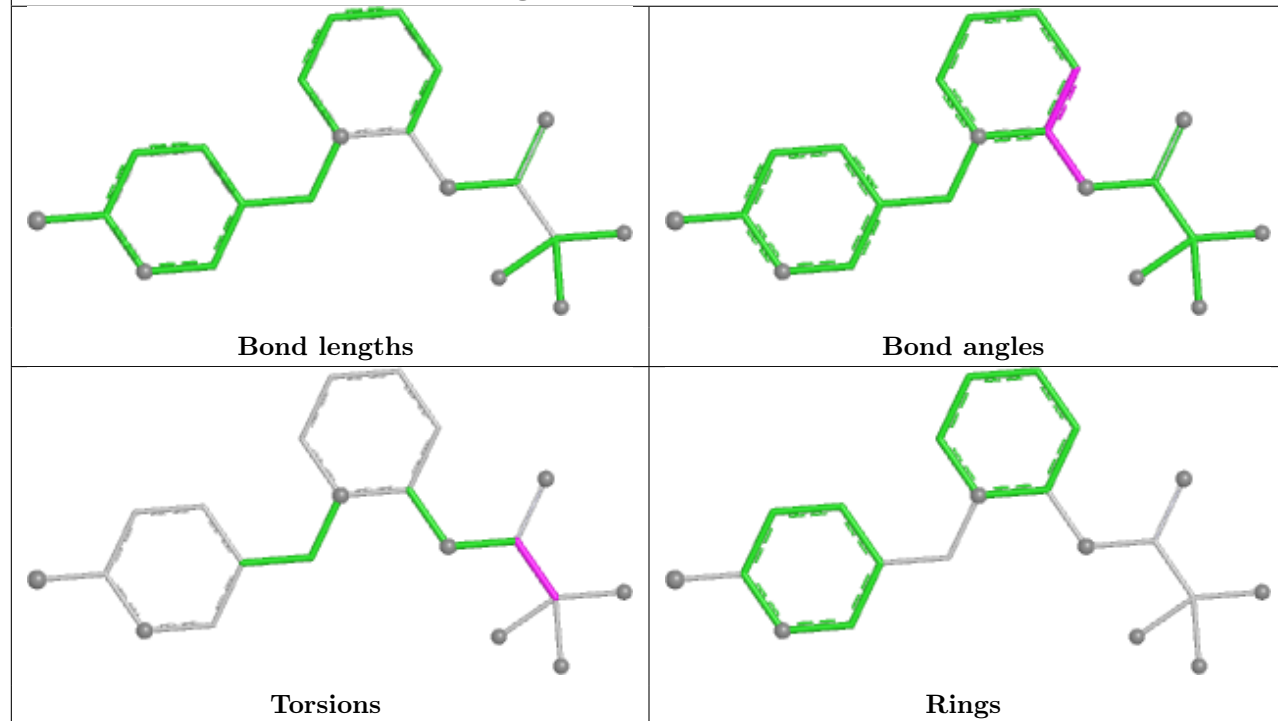
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EaE	301[A]	7OF	1	0
2	EaE	301[B]	7OF	1	0
2	DaD	301[B]	7OF	4	0
2	AaA	301	7OF	1	0
2	BaB	301	7OF	2	0

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 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.

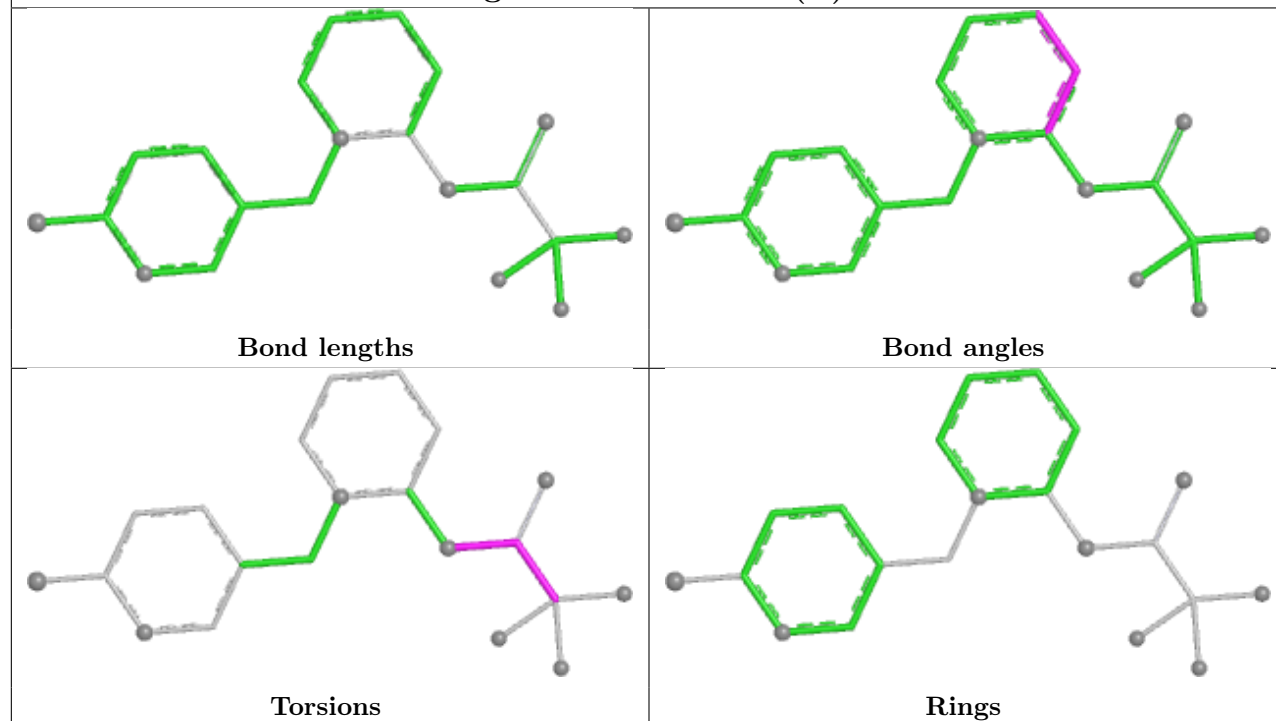
Ligand 7OF EaE 301 (A)



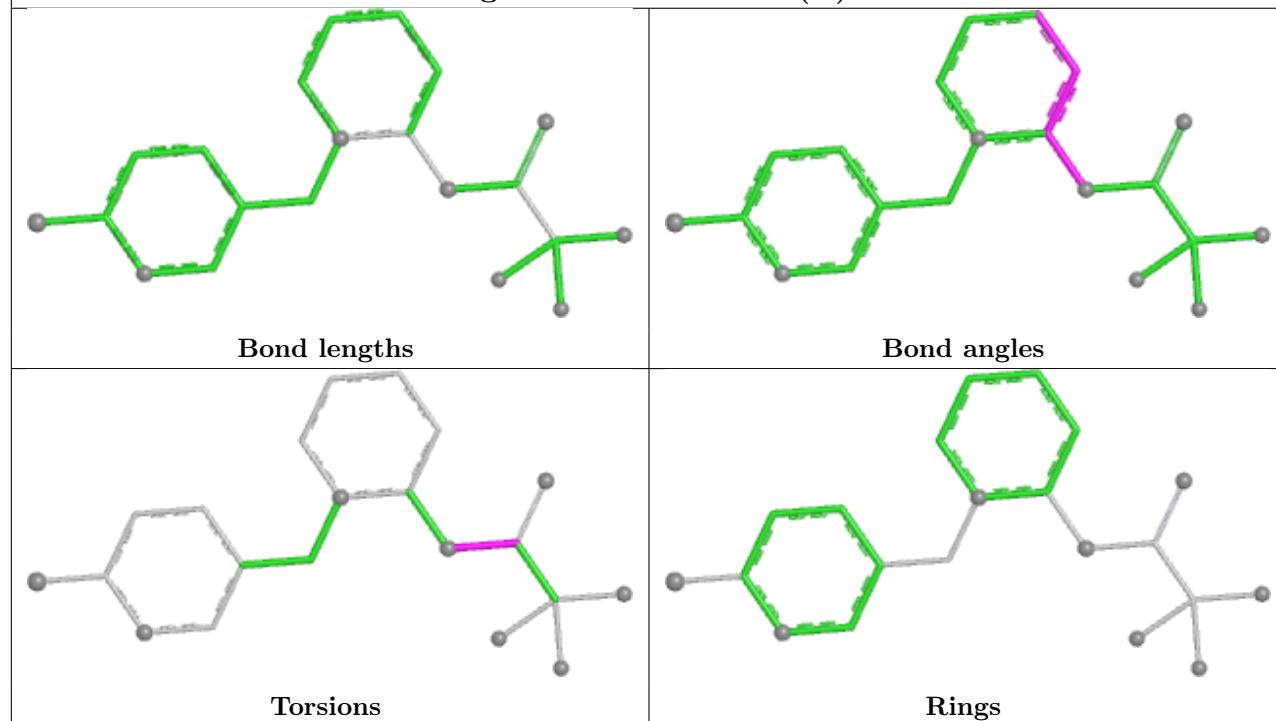
Ligand 7OF CaC 301



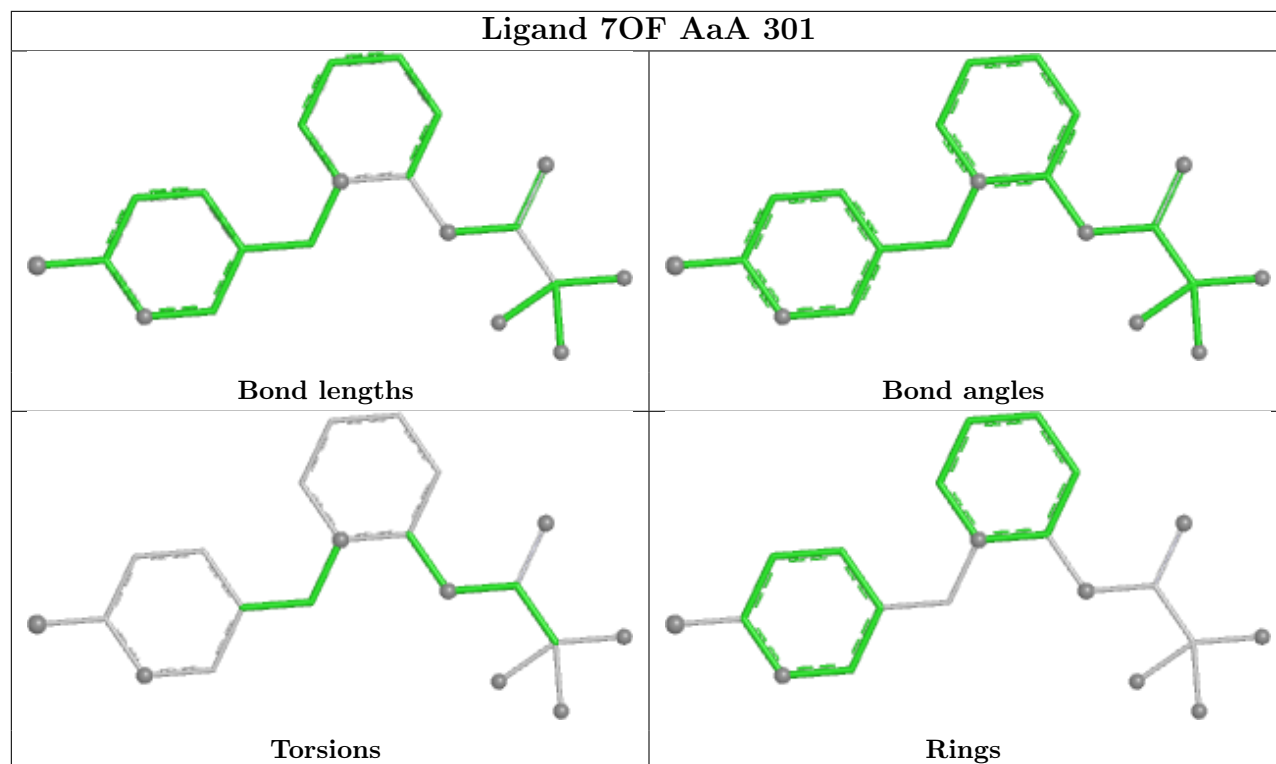
Ligand 7OF EaE 301 (B)



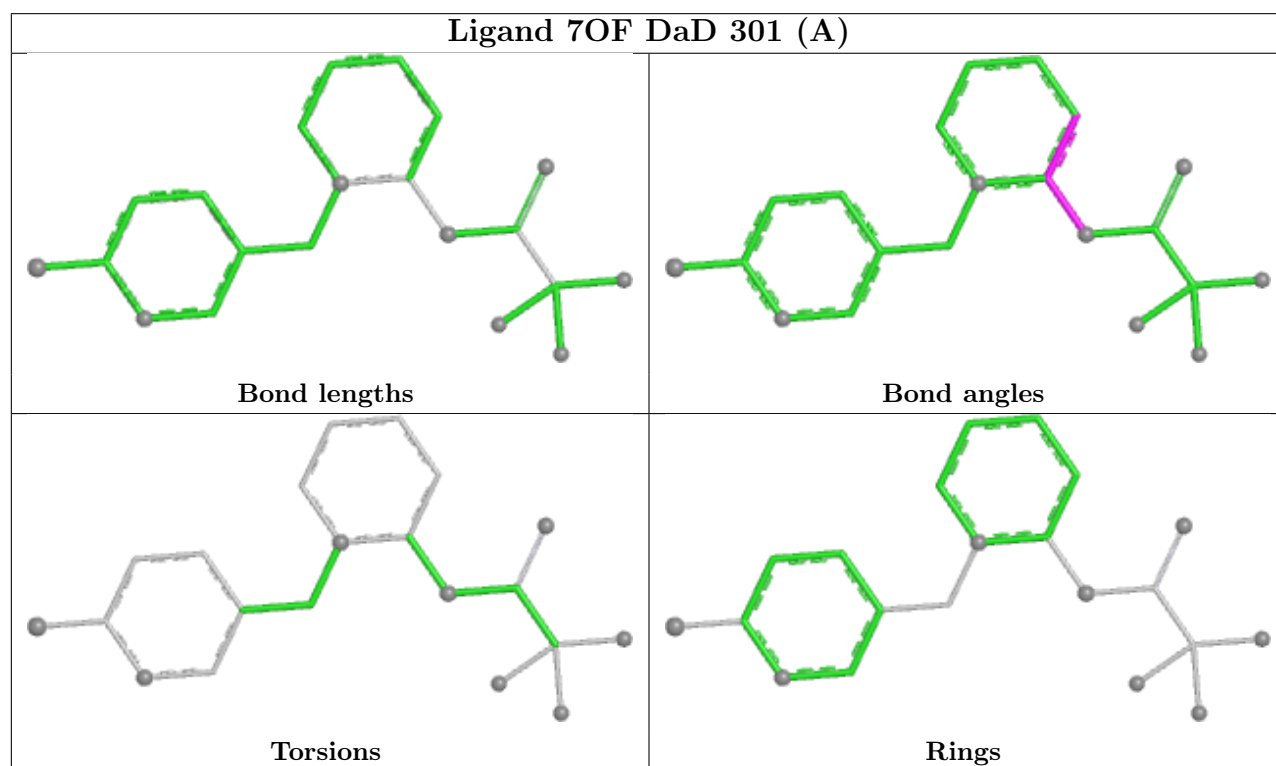
Ligand 7OF DaD 301 (B)

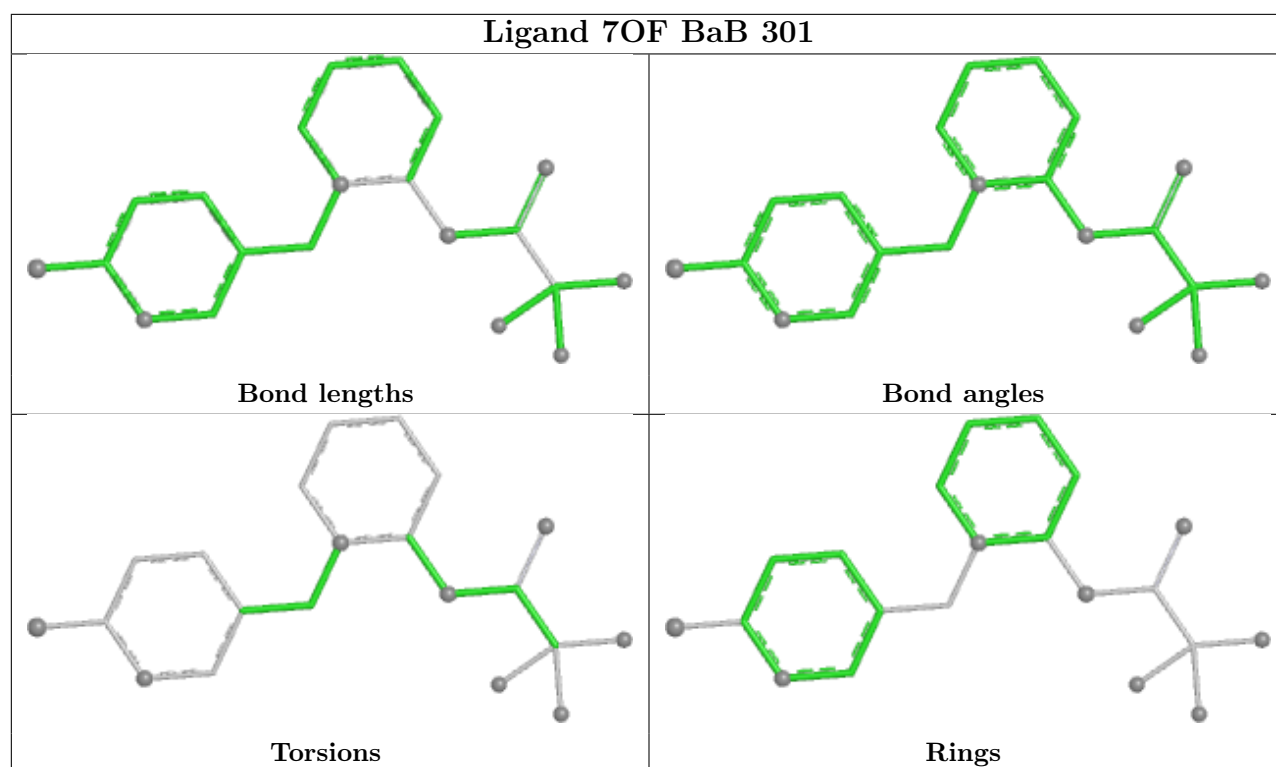


Ligand 7OF AaA 301



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	200/210 (95%)	0.02	4 (2%) 65 64	37, 53, 96, 113	0
1	BaB	202/210 (96%)	0.31	3 (1%) 72 71	42, 62, 98, 124	0
1	CaC	197/210 (93%)	0.23	6 (3%) 52 51	44, 66, 97, 117	0
1	DaD	199/210 (94%)	0.04	0 100 100	38, 55, 89, 104	0
1	EaE	200/210 (95%)	-0.07	1 (0%) 87 87	30, 50, 85, 116	1 (0%)
All	All	998/1050 (95%)	0.10	14 (1%) 73 73	30, 58, 95, 124	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BaB	1	ALA	3.4
1	EaE	1	ALA	3.4
1	CaC	162	SER	2.8
1	AaA	155	THR	2.6
1	BaB	155	THR	2.6
1	CaC	1	ALA	2.6
1	CaC	154	PRO	2.5
1	AaA	185	TYR	2.5
1	AaA	1	ALA	2.5
1	CaC	31	VAL	2.4
1	CaC	189	PRO	2.2
1	CaC	19	ILE	2.2
1	BaB	189	PRO	2.1
1	AaA	189	PRO	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

There are no oligosaccharides in this entry.

6.4 Ligands

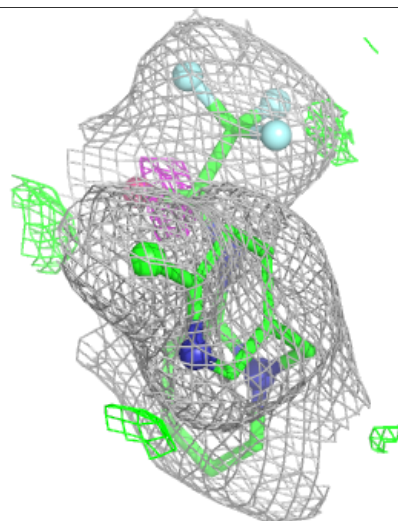
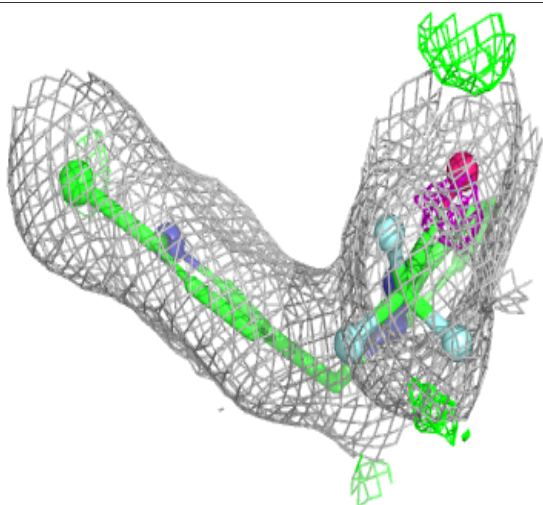
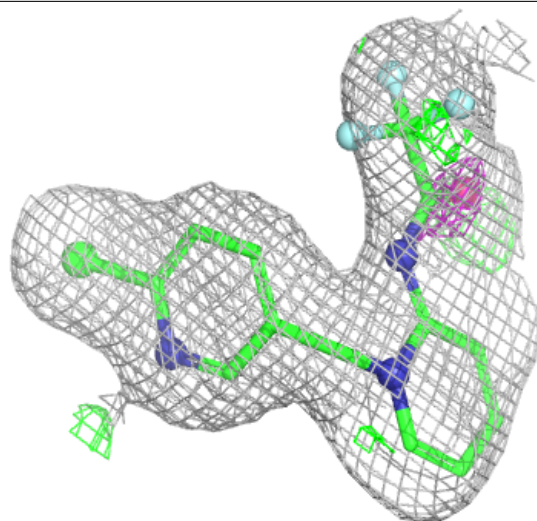
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	7OF	DaD	301[A]	21/21	0.90	0.11	42,52,60,65	21
2	7OF	DaD	301[B]	21/21	0.90	0.11	44,53,67,73	21
2	7OF	CaC	301	21/21	0.91	0.10	52,66,91,98	0
2	7OF	BaB	301	21/21	0.92	0.09	54,73,89,107	0
2	7OF	AaA	301	21/21	0.92	0.10	57,68,88,92	0
2	7OF	EaE	301[A]	21/21	0.93	0.10	48,59,70,73	21
2	7OF	EaE	301[B]	21/21	0.93	0.10	48,54,73,78	21

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.

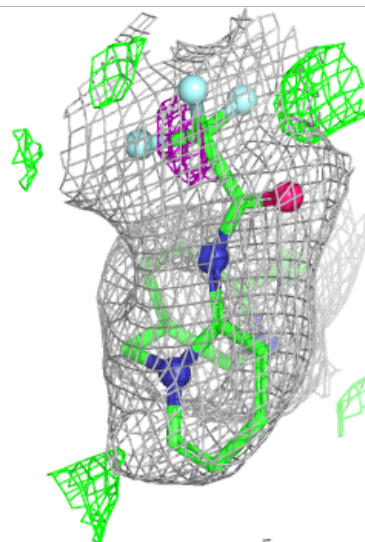
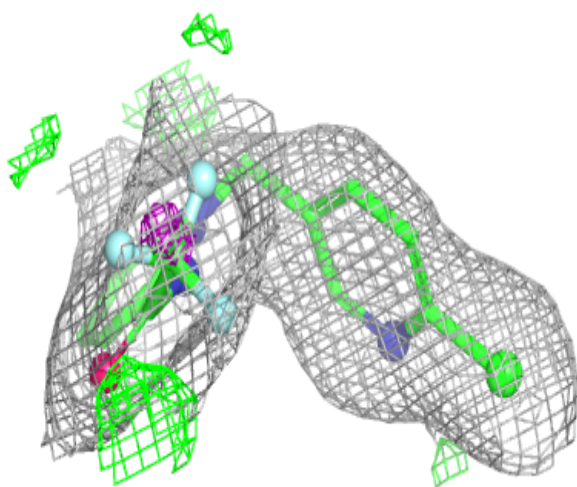
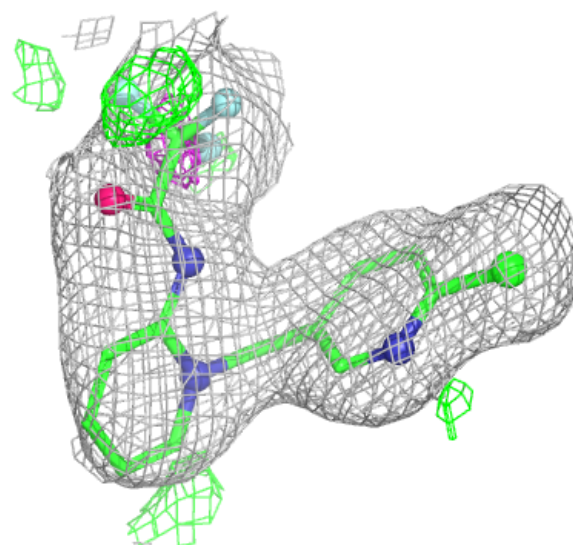
Electron density around 7OF DaD 301 (A):

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



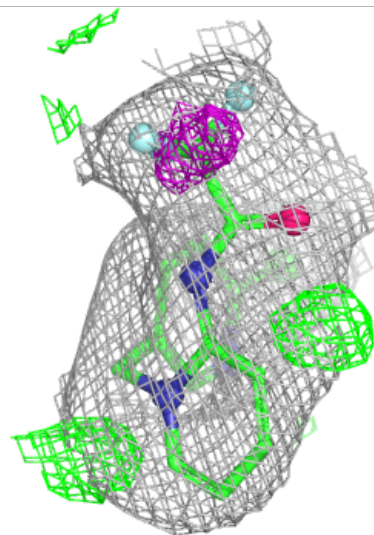
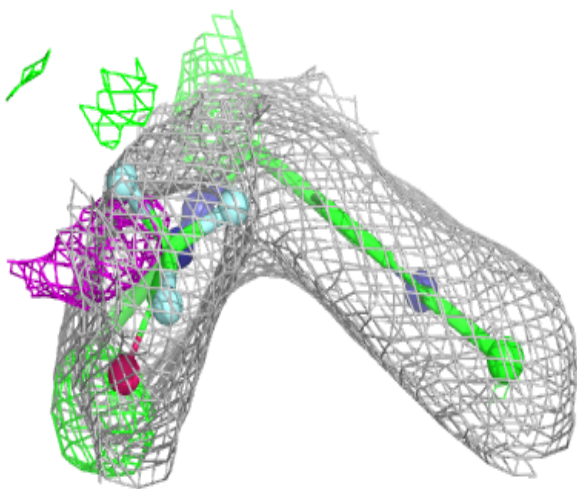
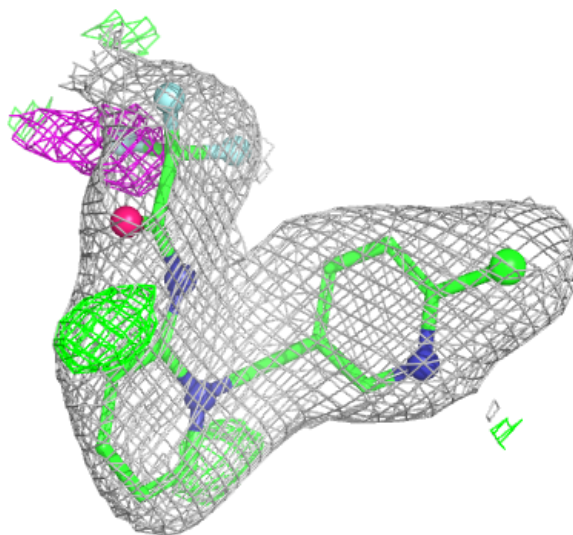
Electron density around 7OF DaD 301 (B):

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



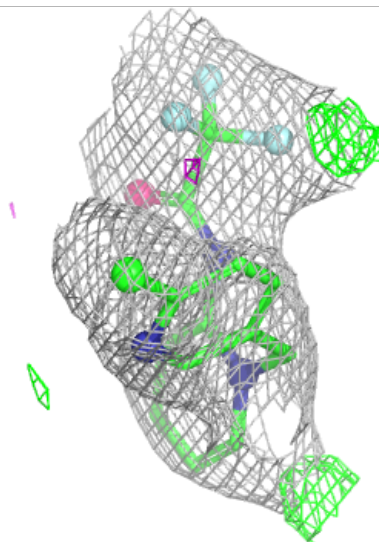
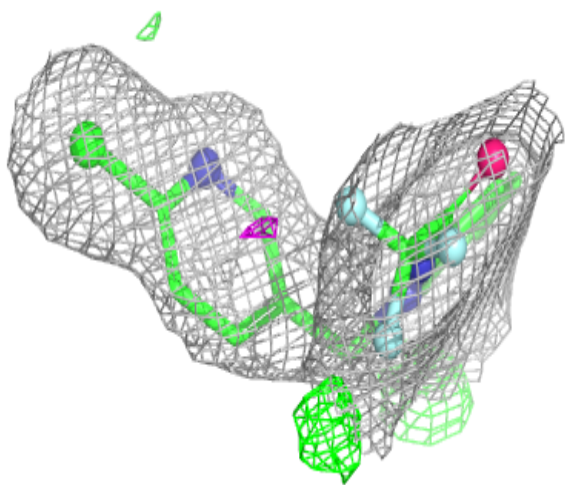
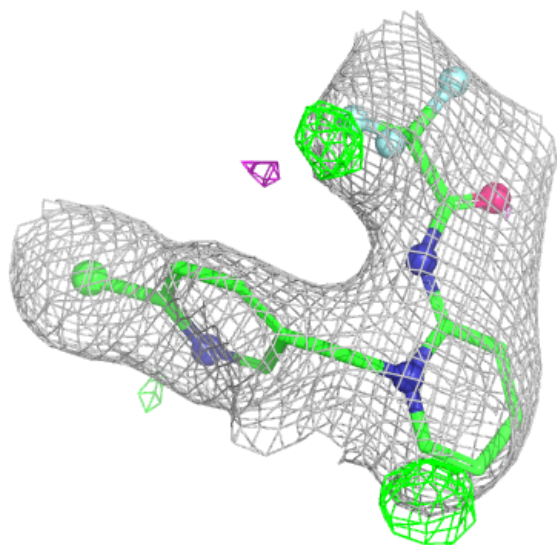
Electron density around 7OF CaC 301:

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



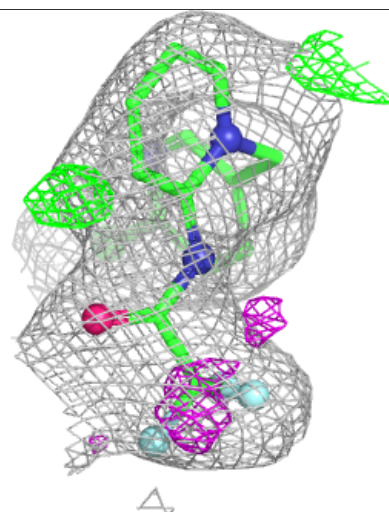
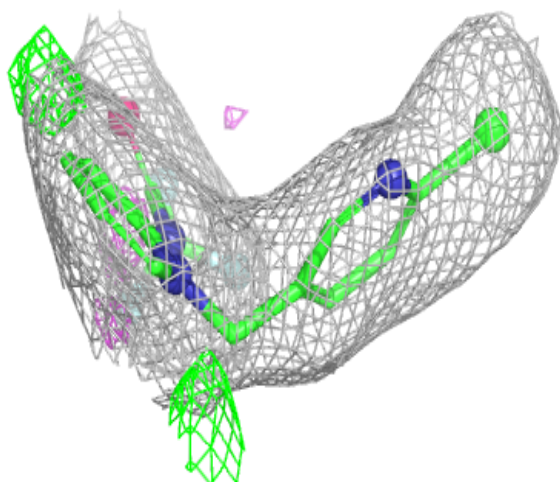
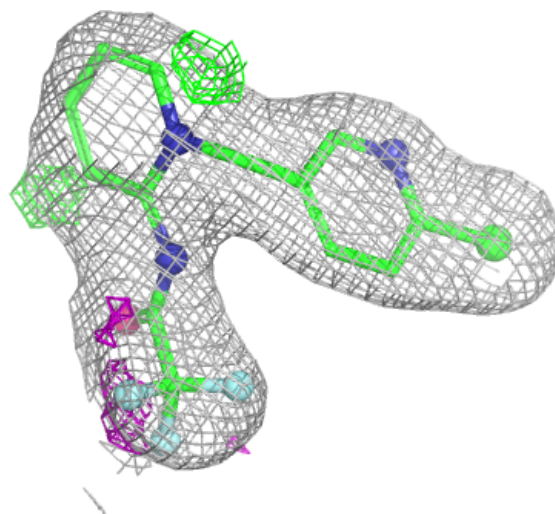
Electron density around 7OF BaB 301:

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



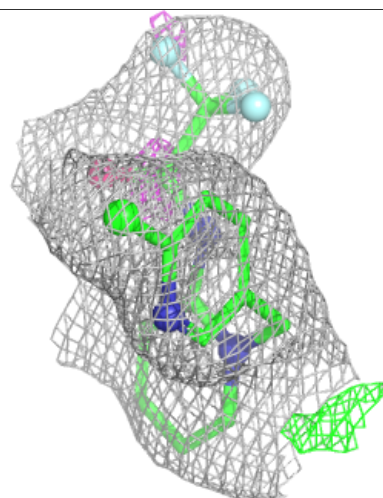
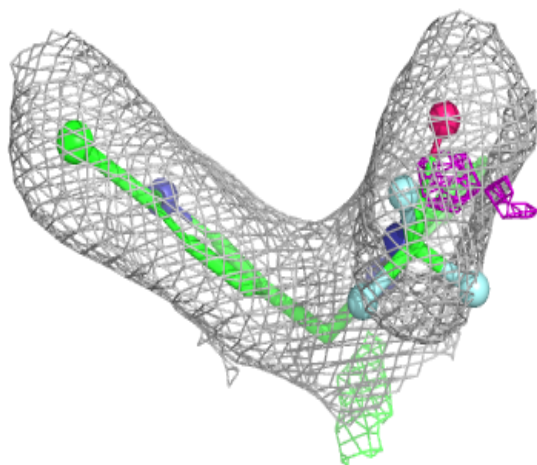
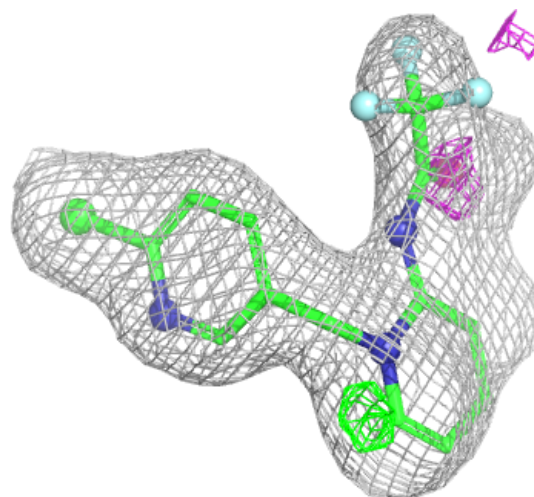
Electron density around 7OF AaA 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



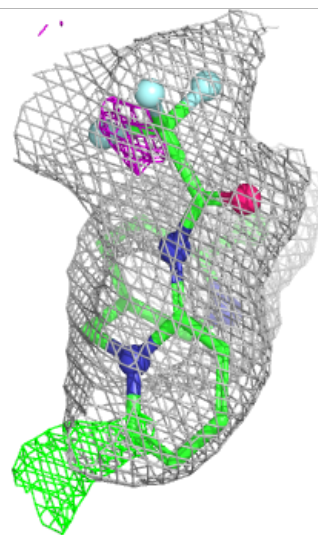
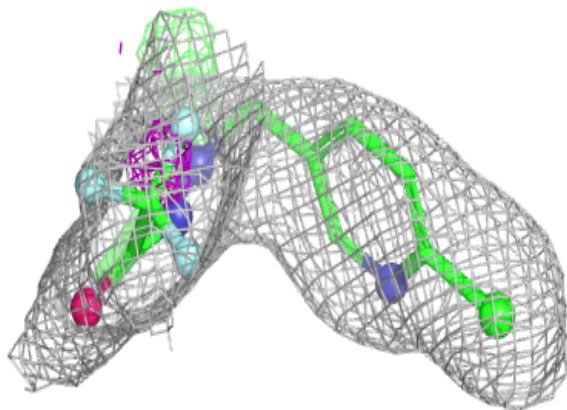
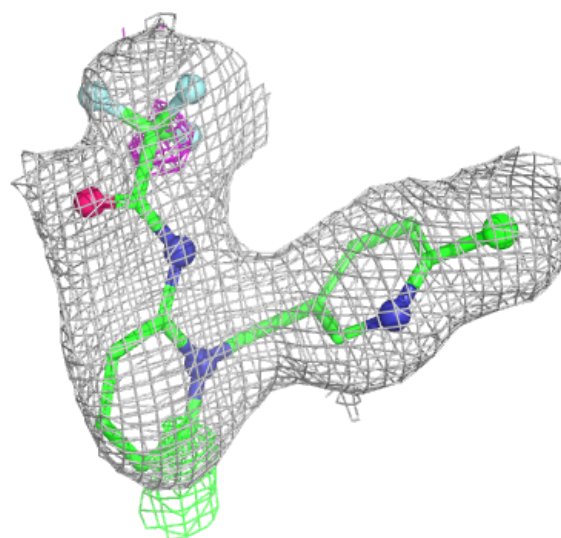
Electron density around 7OF EaE 301 (A):

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



Electron density around 7OF EaE 301 (B):

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.