



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 05:54 pm BST

PDB ID : 1LVC
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin and 2' deoxy, 3' anthraniloyl ATP
Authors : Shen, Y.; Lee, Y.-S.; Soelaiman, S.; Bergson, P.; Lu, D.; Chen, A.; Beckingham, K.; Grabarek, Z.; Mrksich, M.; Tang, W.-J.
Deposited on : 2002-05-28
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

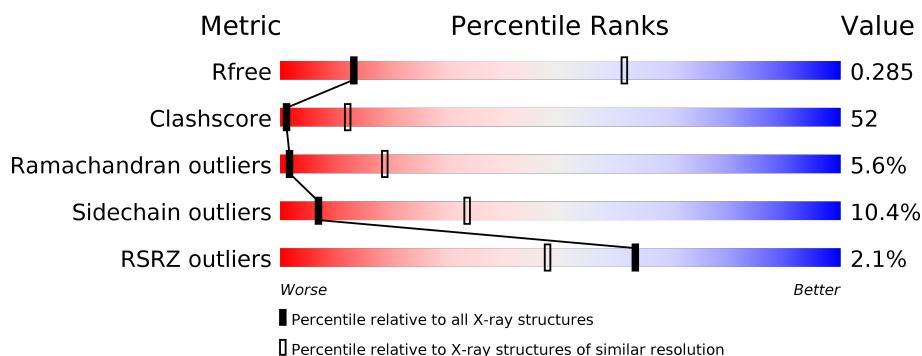
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 on 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	A	510	<div> <div></div> <div>38% 48% 9% 5%</div> </div>
1	B	510	<div> <div>3%</div> <div>22% 55% 14% 9%</div> </div>
1	C	510	<div> <div></div> <div>38% 51% 9% ..</div> </div>
2	D	149	<div> <div>3%</div> <div>34% 53% 9% .</div> </div>
2	E	149	<div> <div>7%</div> <div>38% 48% 9% .</div> </div>
2	F	149	<div> <div>5%</div> <div>36% 48% 11% .</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15302 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 calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	65	0	0
			3952	2528	673	748	3			
1	B	465	Total	C	N	O	S	113	0	0
			3794	2431	642	718	3			
1	C	503	Total	C	N	O	S	166	0	0
			4094	2616	696	779	3			

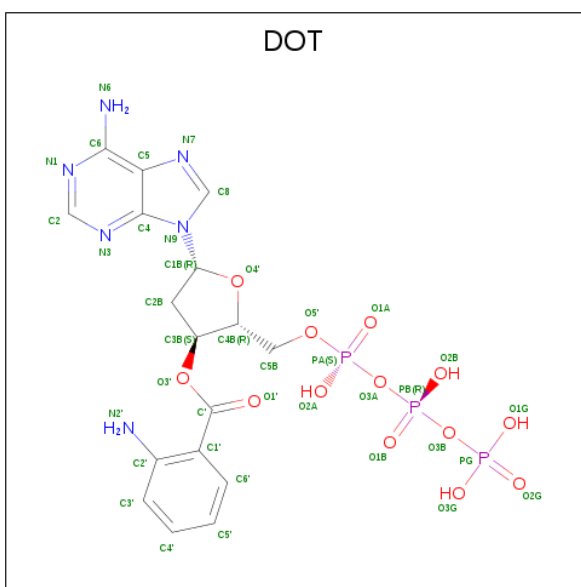
- Molecule 2 is a protein called calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	E	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	F	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			

- Molecule 3 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Yb	0	0
			1	1		
3	A	1	Total	Yb	0	0
			1	1		
3	C	1	Total	Yb	0	0
			1	1		

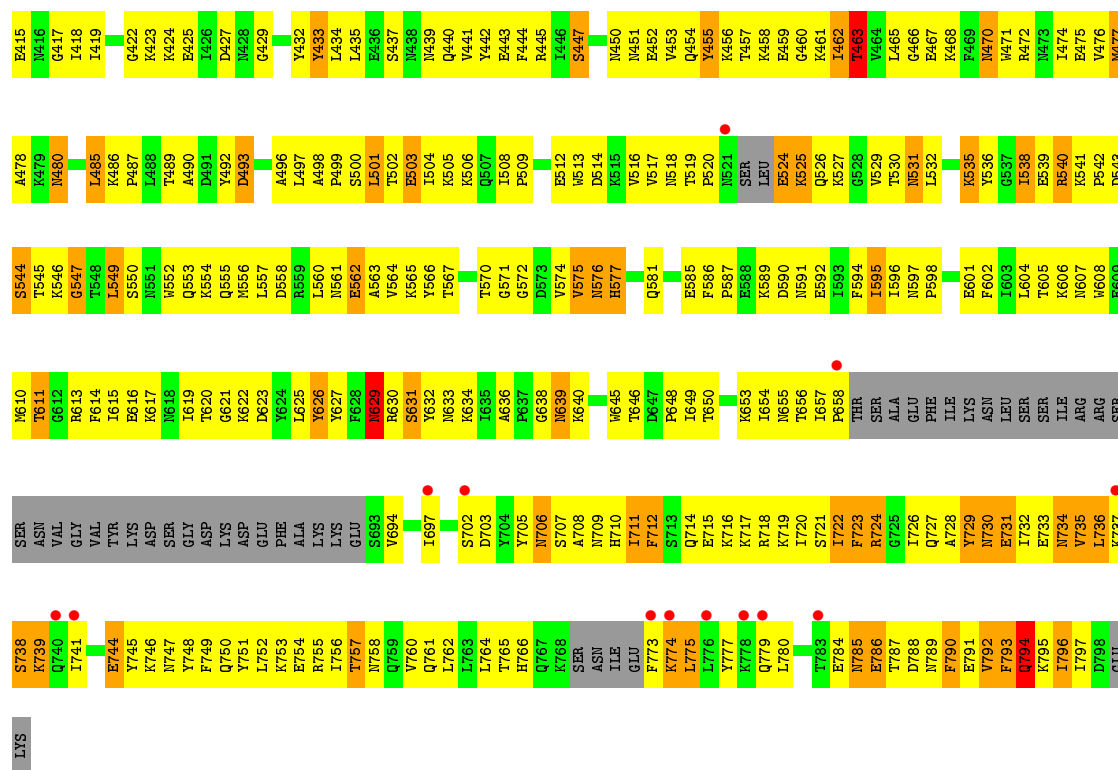
- Molecule 4 is 3'ANTHRANILOYL-2'-DEOXY-ADENOSINE-5'-TRIPHOSPHATE (three-letter code: DOT) (formula: C₁₇H₂₁N₆O₁₃P₃).



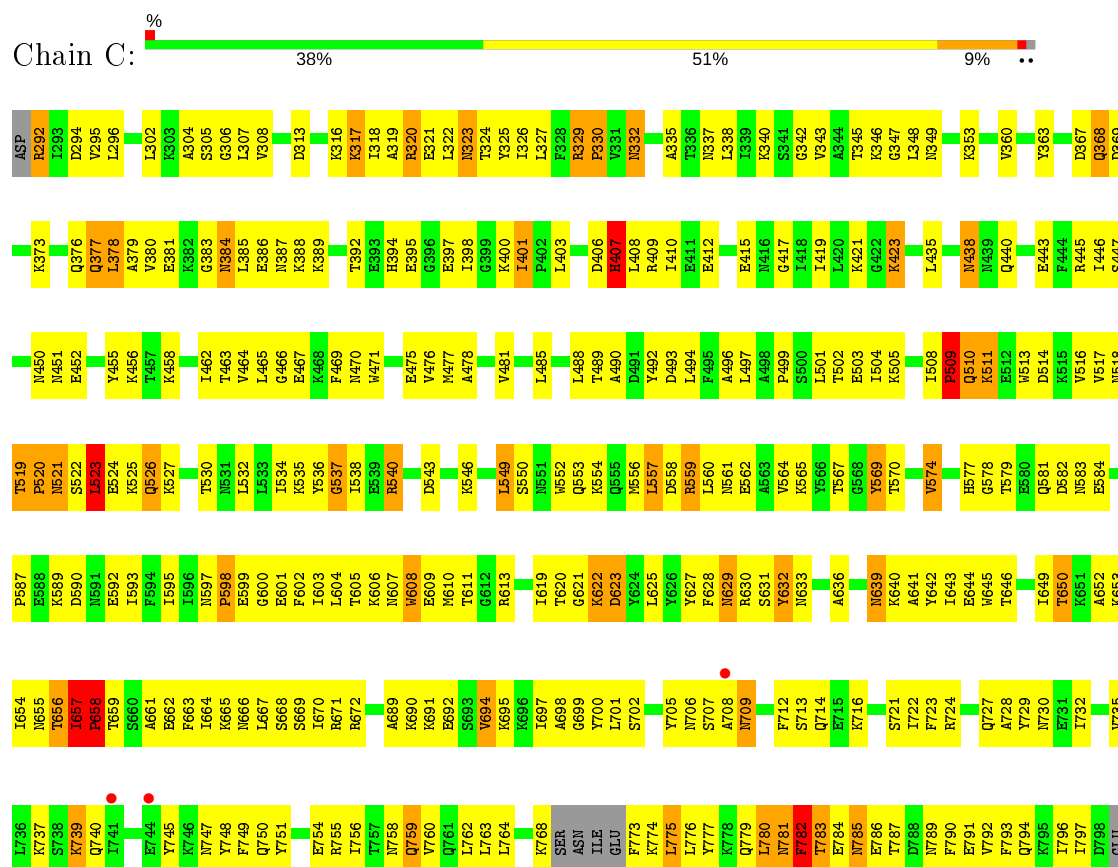
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 39	C 17	N 6	O 13	P 3	0	0
4	C	1	Total 39	C 17	N 6	O 13	P 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total Ca 2 2	0	0
5	F	2	Total Ca 2 2	0	0
5	E	2	Total Ca 2 2	0	0



• Molecule 1: calmodulin-sensitive adenylate cyclase



E140	A73	ME1
F141	R74	ALA
V142	K75	ASP
Q143	M76	GLN
M144		LEU
M145	T79	T5
T146	D80	E6
A147	S81	E7
LVS	E82	Q8
	E83	Q9
	E84	K10
	R85	E11
	R86	F12
	E87	K13
	A88	E14
	R89	A15
	R90	F16
	V91	S17
	F92	L18
	D93	F19
	R94	D20
		K21
	Y99	D22
	I100	
	A101	G25
	A102	T26
	A103	I27
	E104	T28
	L105	
	R106	K36
	H107	R37
	V108	S38
	M109	L39
	T110	G40
		Q41
	K115	
	L116	T44
	T117	E45
	D118	A46
	E119	E47
	F120	L48
	V121	Q49
	D122	D50
	E123	M51
	M124	I52
	I125	M53
	R126	E54
	E127	
	A128	G61
	D129	T62
	I130	I63
	D131	D64
	G132	F65
	D133	P66
	G134	E67
	Q135	F68
	V136	L69
	N137	T70
	F138	M71
	F139	M72

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 167.92Å 341.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.60 29.95 – 3.60	Depositor EDS
% Data completeness (in resolution range)	90.6 (29.96-3.60) 95.9 (29.95-3.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.00 (at 3.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.281 , 0.307 0.253 , 0.285	Depositor DCC
R_{free} test set	1945 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	98.5	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15302	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: CA, YB, DOT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.49	0/4027	0.82	13/5419 (0.2%)
1	B	0.51	0/3867	0.78	9/5204 (0.2%)
1	C	0.51	1/4172 (0.0%)	0.82	16/5613 (0.3%)
2	D	0.38	0/1137	0.59	2/1527 (0.1%)
2	E	0.40	0/1137	0.61	2/1527 (0.1%)
2	F	0.37	0/1137	0.74	3/1527 (0.2%)
All	All	0.48	1/15477 (0.0%)	0.78	45/20817 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	658	PRO	CA-C	-5.34	1.42	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	106	ARG	NE-CZ-NH1	-14.10	113.25	120.30
2	F	106	ARG	NE-CZ-NH2	13.51	127.06	120.30
1	A	613	ARG	NE-CZ-NH1	-11.05	114.77	120.30
1	C	613	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	C	613	ARG	NE-CZ-NH1	10.64	125.62	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	3952	0	3999	403	0
1	B	3794	0	3828	500	0
1	C	4094	0	4134	394	0
2	D	1125	0	1049	113	0
2	E	1125	0	1049	103	0
2	F	1125	0	1049	109	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	39	0	17	8	0
4	C	39	0	17	5	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
All	All	15302	0	15142	1552	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 52.

The worst 5 of 1552 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:ASN:ND2	1:B:631:SER:H	1.14	1.44
1:C:456:LYS:HB2	1:C:470:ASN:O	1.22	1.34
1:C:456:LYS:CB	1:C:470:ASN:O	1.84	1.24
1:C:659:THR:HG22	1:C:661:ALA:H	1.08	1.14
1:A:456:LYS:HB2	1:A:470:ASN:O	1.46	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/510 (94%)	386 (81%)	71 (15%)	22 (5%)	2	23
1	B	457/510 (90%)	335 (73%)	89 (20%)	33 (7%)	1	13
1	C	499/510 (98%)	384 (77%)	93 (19%)	22 (4%)	2	23
2	D	141/149 (95%)	105 (74%)	28 (20%)	8 (6%)	1	18
2	E	141/149 (95%)	108 (77%)	24 (17%)	9 (6%)	1	17
2	F	141/149 (95%)	108 (77%)	23 (16%)	10 (7%)	1	14
All	All	1858/1977 (94%)	1426 (77%)	328 (18%)	104 (6%)	2	19

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	521	ASN
1	B	566	TYR
1	B	571	GLY
1	B	757	THR

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	A	433/455 (95%)	394 (91%)	39 (9%)	9	39
1	B	414/455 (91%)	351 (85%)	63 (15%)	3	19
1	C	448/455 (98%)	405 (90%)	43 (10%)	8	37
2	D	121/127 (95%)	113 (93%)	8 (7%)	16	51
2	E	121/127 (95%)	112 (93%)	9 (7%)	13	46
2	F	121/127 (95%)	111 (92%)	10 (8%)	11	42
All	All	1658/1746 (95%)	1486 (90%)	172 (10%)	7	33

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	552	TRP
1	B	741	ILE
2	E	74	ARG
1	B	577	HIS
1	B	639	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	551	ASN
1	B	706	ASN
1	C	759	GLN
1	B	629	ASN
1	B	730	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DOT	A	999	3	36,42,42	5.12	20 (55%)	44,64,64	7.86	22 (50%)
4	DOT	C	1999	3	36,42,42	5.11	20 (55%)	44,64,64	7.86	24 (54%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DOT	A	999	3	-	6/26/42/42	0/4/4/4
4	DOT	C	1999	3	-	3/26/42/42	0/4/4/4

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	DOT	C1'-C2'	20.34	1.70	1.41
4	C	1999	DOT	C1'-C2'	20.22	1.70	1.41
4	A	999	DOT	C3'-C2'	15.16	1.74	1.40
4	C	1999	DOT	C3'-C2'	15.15	1.74	1.40
4	C	1999	DOT	C8-N7	6.62	1.46	1.34

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	DOT	C3'-C2'-N2'	26.73	171.91	120.13
4	C	1999	DOT	C3'-C2'-N2'	26.72	171.90	120.13
4	A	999	DOT	C3'-C2'-C1'	-24.77	94.08	118.10
4	C	1999	DOT	C3'-C2'-C1'	-24.72	94.13	118.10
4	A	999	DOT	C1'-C2'-N2'	-24.51	90.26	122.67

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

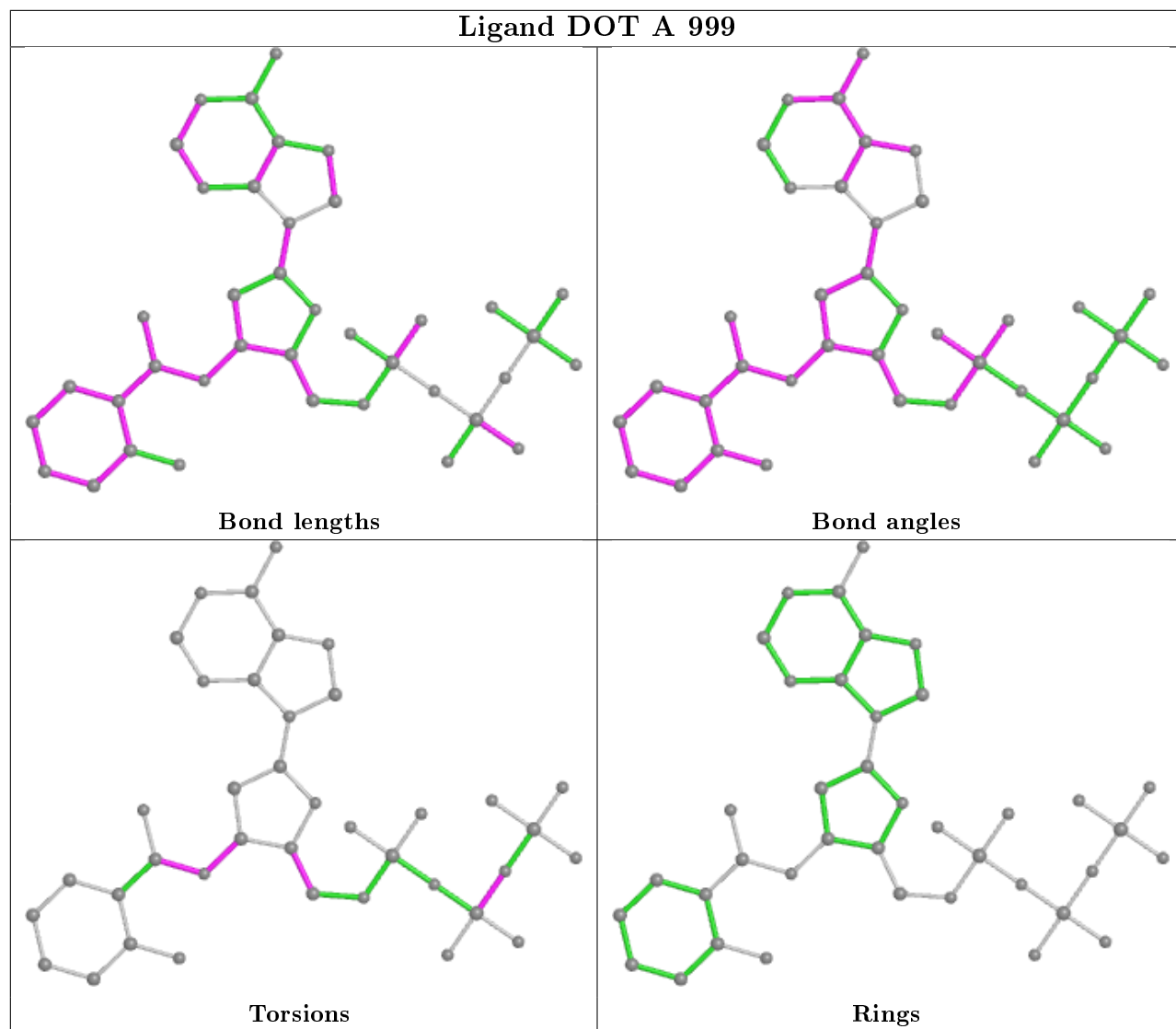
Mol	Chain	Res	Type	Atoms
4	C	1999	DOT	O4'-C4B-C5B-O5'
4	C	1999	DOT	C2B-C3B-O3'-C'
4	A	999	DOT	O4'-C4B-C5B-O5'
4	A	999	DOT	O1'-C'-O3'-C3B
4	A	999	DOT	C1'-C'-O3'-C3B

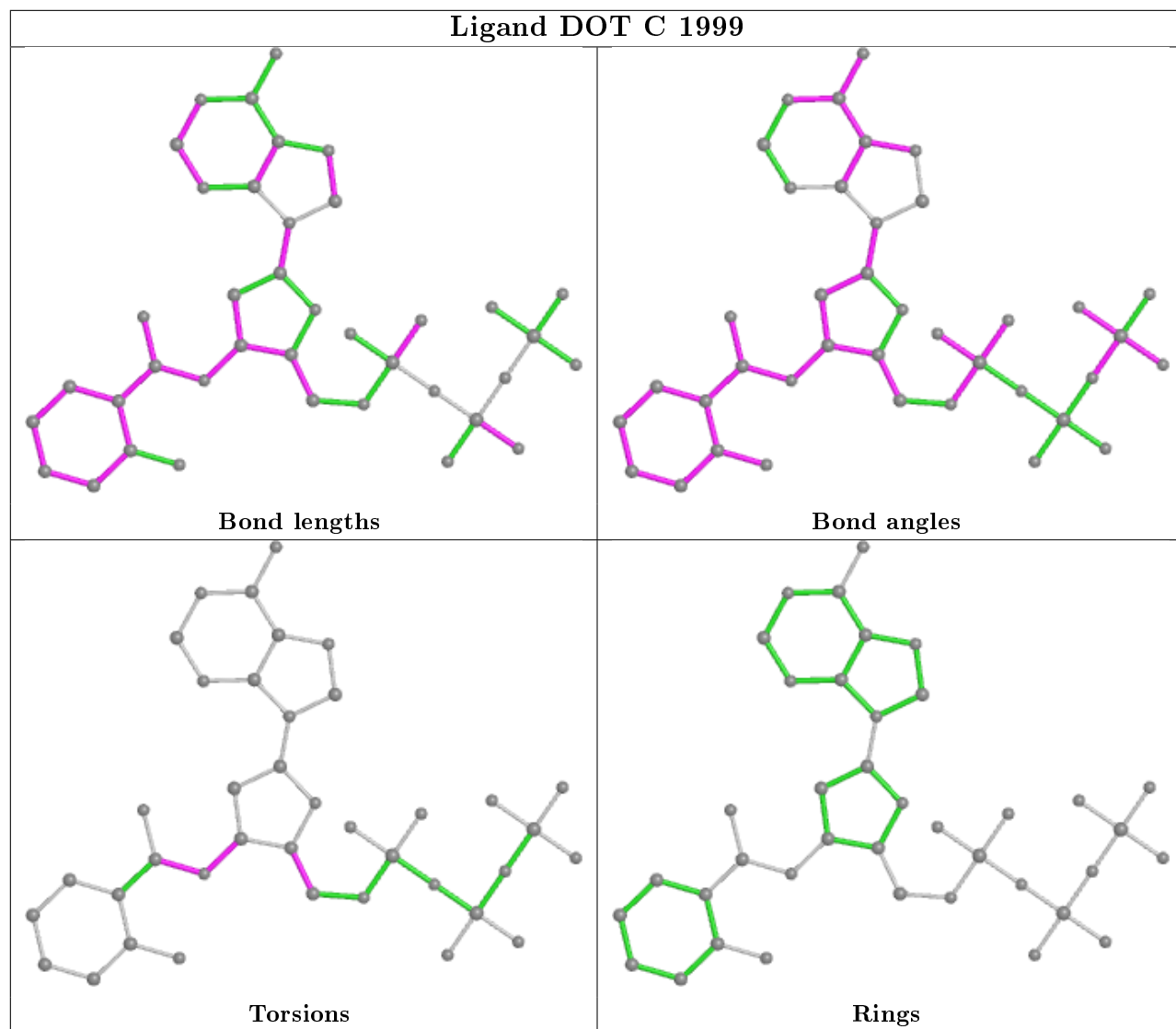
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	DOT	8	0
4	C	1999	DOT	5	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.





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	A	485/510 (95%)	-0.44	1 (0%) 95 91	14, 58, 137, 162	16 (3%)
1	B	457/510 (89%)	-0.28	13 (2%) 53 37	13, 58, 158, 165	12 (2%)
1	C	491/510 (96%)	-0.38	3 (0%) 89 81	13, 61, 137, 162	19 (3%)
2	D	143/149 (95%)	0.13	5 (3%) 44 29	49, 143, 180, 183	0
2	E	143/149 (95%)	0.17	10 (6%) 16 9	48, 144, 180, 182	0
2	F	143/149 (95%)	0.16	8 (5%) 24 14	49, 143, 180, 183	0
All	All	1862/1977 (94%)	-0.25	40 (2%) 63 48	13, 66, 166, 183	47 (2%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	697	ILE	5.4
2	F	62	THR	4.1
2	E	79	THR	3.5
2	E	21	LYS	3.3
2	E	19	PHE	3.3

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 carbohydrates in this entry.

6.4 Ligands

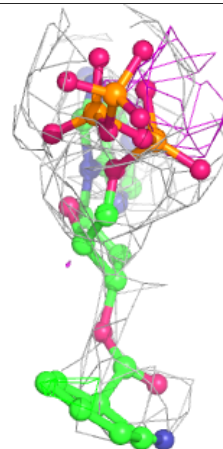
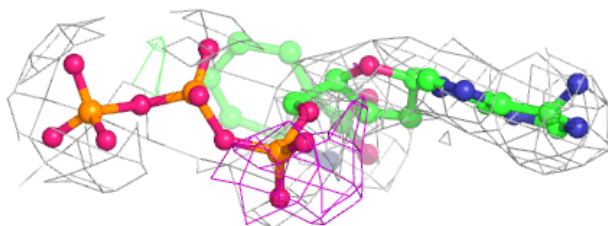
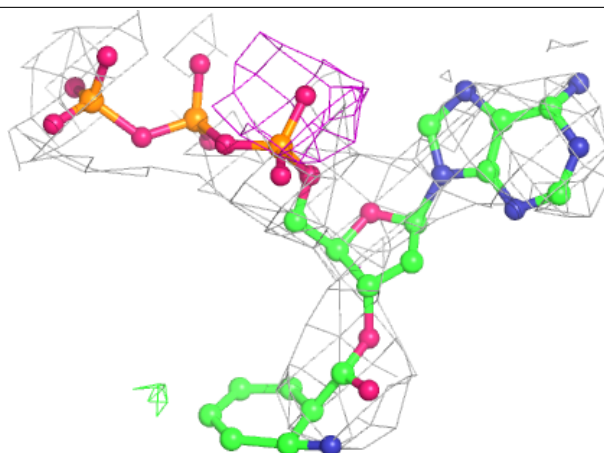
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

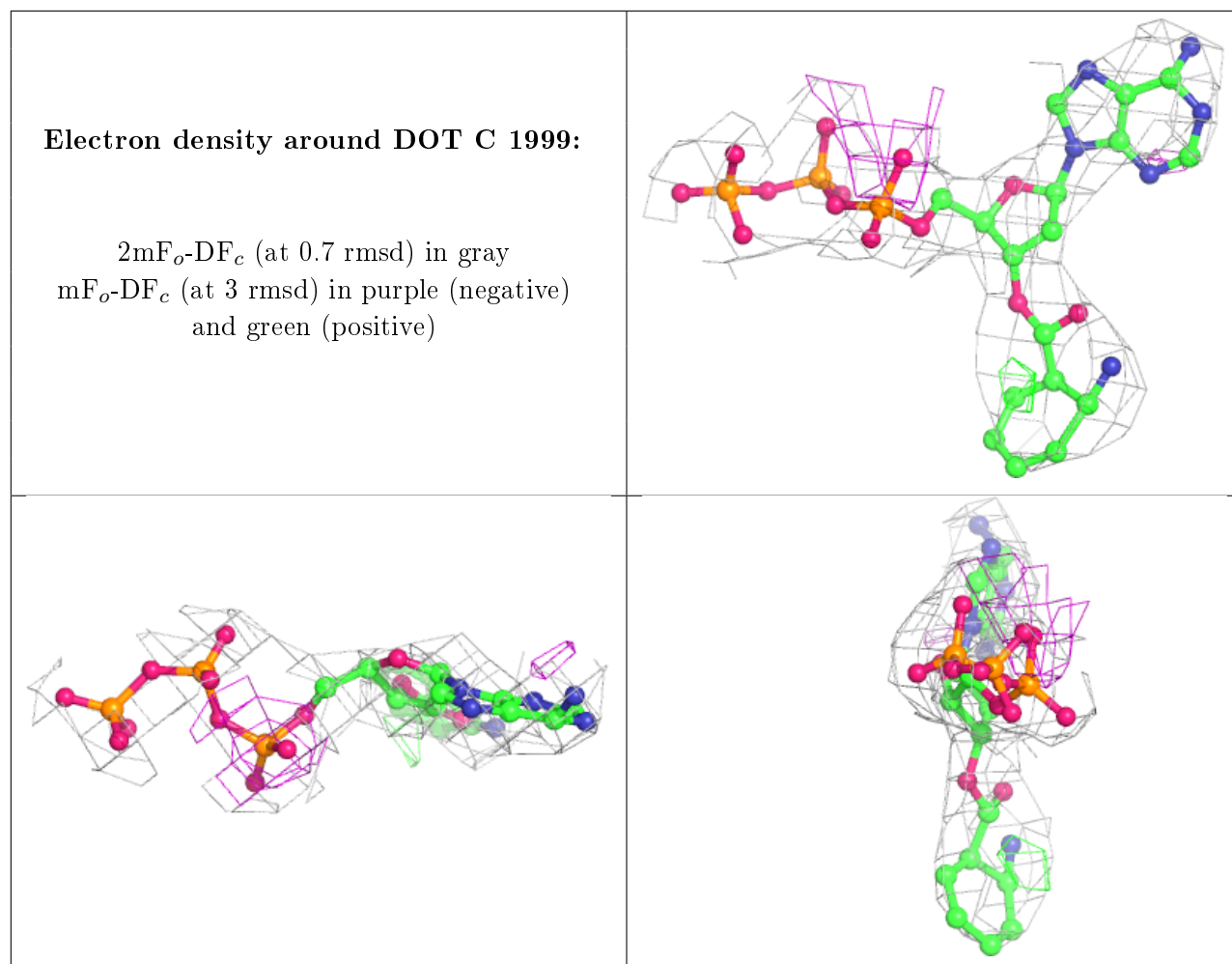
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	F	805	1/1	0.86	0.12	82,82,82,82	0
5	CA	E	802	1/1	0.86	0.04	75,75,75,75	0
4	DOT	A	999	39/39	0.87	0.29	52,80,92,92	0
3	YB	A	901	1/1	0.87	0.08	135,135,135,135	0
5	CA	F	804	1/1	0.88	0.14	70,70,70,70	0
4	DOT	C	1999	39/39	0.88	0.26	45,80,83,84	0
5	CA	D	800	1/1	0.94	0.11	65,65,65,65	0
3	YB	C	903	1/1	0.96	0.04	124,124,124,124	0
5	CA	D	801	1/1	0.98	0.04	51,51,51,51	0
3	YB	B	902	1/1	0.98	0.09	142,142,142,142	0
5	CA	E	803	1/1	0.99	0.06	70,70,70,70	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 DOT A 999:

$2mF_o-DF_c$ (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.