



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:39 am BST

PDB ID : 6U1V
Title : Crystal structure of acyl-ACP/acyl-CoA dehydrogenase from allylmalonyl-CoA and FK506 biosynthesis, TcsD
Authors : Blake-Hedges, J.M.; Pereira, J.H.; Barajas, J.F.; Adams, P.D.; Keasling, J.D.
Deposited on : 2019-08-16
Resolution : 1.75 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 : 1.8.5 (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

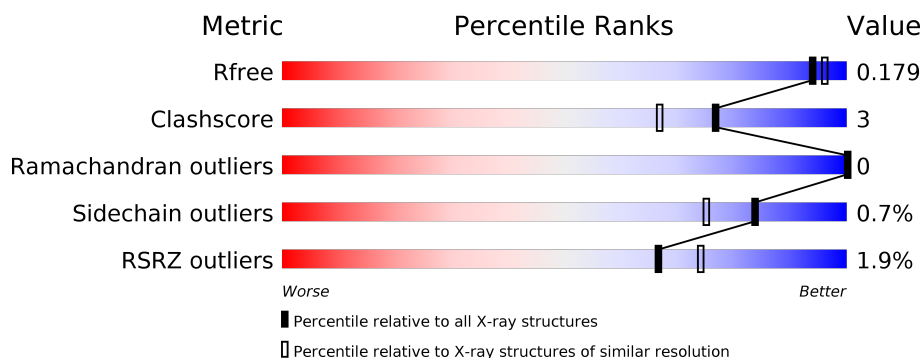
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	389	<div> <div>%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div></div> </div>
1	B	389	<div> <div>%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div></div> </div>
1	C	389	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div></div> </div>
1	D	389	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> <div></div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25470 atoms, of which 12018 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.

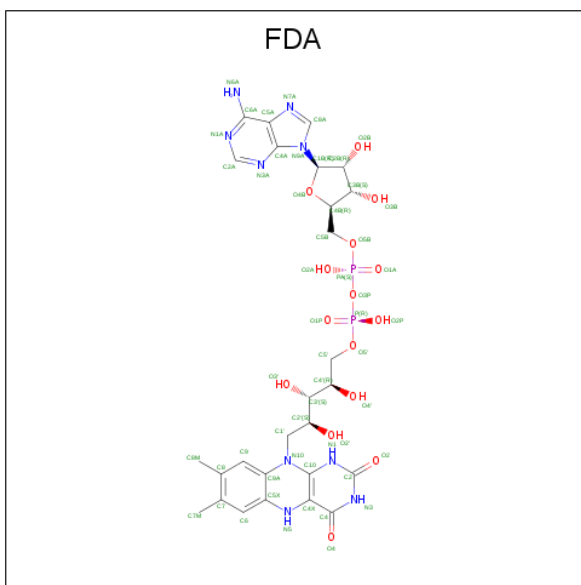
- Molecule 1 is a protein called Acyl-CoA dehydrogenase domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	3	0
			5977	1869	3004	536	553	15			
1	B	389	Total	C	H	N	O	S	0	2	0
			5975	1870	3000	536	554	15			
1	C	383	Total	C	H	N	O	S	0	2	0
			5873	1840	2950	524	544	15			
1	D	382	Total	C	H	N	O	S	0	0	0
			5842	1830	2932	523	542	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	LEU	-	expression tag	UNP I2MTW3
A	388	GLU	-	expression tag	UNP I2MTW3
A	389	HIS	-	expression tag	UNP I2MTW3
B	387	LEU	-	expression tag	UNP I2MTW3
B	388	GLU	-	expression tag	UNP I2MTW3
B	389	HIS	-	expression tag	UNP I2MTW3
C	387	LEU	-	expression tag	UNP I2MTW3
C	388	GLU	-	expression tag	UNP I2MTW3
C	389	HIS	-	expression tag	UNP I2MTW3
D	387	LEU	-	expression tag	UNP I2MTW3
D	388	GLU	-	expression tag	UNP I2MTW3
D	389	HIS	-	expression tag	UNP I2MTW3

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 86	C 27	H 33	N 9	O 15	P 2	0	0
2	B	1	Total 86	C 27	H 33	N 9	O 15	P 2	0	0
2	C	1	Total 86	C 27	H 33	N 9	O 15	P 2	0	0
2	D	1	Total 86	C 27	H 33	N 9	O 15	P 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	383	Total O 383 383	0	0
3	B	390	Total O 390 390	0	0
3	C	335	Total O 335 335	0	0
3	D	351	Total O 351 351	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Acyl-CoA dehydrogenase domain-containing protein



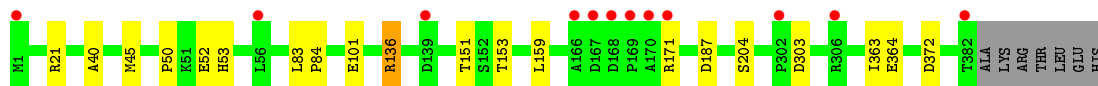
- Molecule 1: Acyl-CoA dehydrogenase domain-containing protein



- Molecule 1: Acyl-CoA dehydrogenase domain-containing protein



- Molecule 1: Acyl-CoA dehydrogenase domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.52Å 100.06Å 148.51Å 90.00° 100.31° 90.00°	Depositor
Resolution (Å)	68.40 – 1.75 68.40 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (68.40-1.75) 97.6 (68.40-1.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.146 , 0.179 0.146 , 0.179	Depositor DCC
R_{free} test set	9864 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	25470	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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: FDA

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	0.56	3/3030 (0.1%)	0.72	2/4094 (0.0%)
1	B	1.07	5/3030 (0.2%)	0.82	6/4095 (0.1%)
1	C	0.47	0/2977	0.60	0/4025
1	D	0.48	0/2958	0.62	0/3999
All	All	0.69	8/11995 (0.1%)	0.70	8/16213 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	310	ARG	CZ-NH2	-46.80	0.72	1.33
1	B	310	ARG	CZ-NH1	15.65	1.53	1.33
1	A	137	ASP	CB-CG	-8.33	1.34	1.51
1	B	385	ARG	CZ-NH2	-8.13	1.22	1.33
1	B	310	ARG	NE-CZ	7.75	1.43	1.33
1	A	384	LYS	CE-NZ	7.64	1.68	1.49
1	A	137	ASP	CG-OD2	5.71	1.38	1.25
1	B	35	LEU	CG-CD1	5.41	1.71	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	385	ARG	NE-CZ-NH2	-20.79	109.90	120.30
1	A	137	ASP	CB-CG-OD1	16.08	132.78	118.30
1	B	35	LEU	CB-CG-CD2	15.15	136.75	111.00
1	B	310	ARG	NE-CZ-NH1	-14.29	113.16	120.30
1	A	137	ASP	CB-CG-OD2	-11.38	108.06	118.30
1	B	385	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	B	310	ARG	NH1-CZ-NH2	8.69	128.95	119.40
1	B	310	ARG	NE-CZ-NH2	-5.71	117.44	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	384	LYS	Peptide
1	B	384	LYS	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	A	2973	3004	3010	22	2
1	B	2975	3000	3004	24	2
1	C	2923	2950	2953	10	0
1	D	2910	2932	2932	17	0
2	A	53	33	33	0	0
2	B	53	33	33	0	0
2	C	53	33	33	0	0
2	D	53	33	33	0	0
3	A	383	0	0	8	0
3	B	390	0	0	7	0
3	C	335	0	0	3	0
3	D	351	0	0	6	0
All	All	13452	12018	12031	73	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (73) 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:A:384:LYS:NZ	1:A:384:LYS:CE	1.68	1.49
1:B:310:ARG:NE	1:B:310:ARG:NH2	1.87	1.21
1:B:310:ARG:NH2	3:B:501:HOH:O	1.74	1.17
1:B:310:ARG:NH1	1:B:310:ARG:NH2	2.06	1.03
1:B:310:ARG:NE	3:B:502:HOH:O	1.85	0.99
1:B:310:ARG:NH1	3:B:502:HOH:O	1.90	0.98
1:A:260:LYS:NZ	3:A:502:HOH:O	2.00	0.90
1:D:101:GLU:OE2	3:D:501:HOH:O	1.88	0.90
1:D:101:GLU:OE1	3:D:502:HOH:O	1.91	0.89
1:B:310:ARG:CZ	1:B:310:ARG:NH2	0.72	0.87
1:C:11:ARG:NH2	3:C:501:HOH:O	2.13	0.82
1:B:388:GLU:OE1	3:B:503:HOH:O	2.00	0.80
1:A:384:LYS:NZ	3:A:501:HOH:O	1.82	0.79
1:A:184:LEU:HD13	1:A:205:PHE:CE1	2.19	0.76
1:A:388:GLU:OE2	3:A:503:HOH:O	2.03	0.76
1:B:260:LYS:NZ	3:B:504:HOH:O	2.15	0.74
1:A:384:LYS:CE	3:A:501:HOH:O	2.37	0.73
1:A:384:LYS:HE3	3:A:534:HOH:O	1.89	0.73
1:B:310:ARG:HH21	1:B:310:ARG:CZ	1.37	0.72
1:B:310:ARG:HH22	1:B:310:ARG:CZ	1.37	0.70
1:A:384:LYS:CE	3:A:534:HOH:O	2.40	0.69
1:D:153:THR:HG23	1:D:159:LEU:HD21	1.74	0.68
1:B:310:ARG:CZ	3:B:501:HOH:O	2.42	0.67
1:D:372:ASP:OD1	3:D:503:HOH:O	2.14	0.65
1:A:153:THR:HG23	1:A:159:LEU:HD21	1.82	0.61
1:B:310:ARG:HH21	1:B:310:ARG:HG3	1.66	0.60
1:B:310:ARG:HH21	1:B:310:ARG:CD	2.14	0.59
1:B:310:ARG:CD	1:B:310:ARG:NH2	2.64	0.59
1:D:21:ARG:NH2	3:D:509:HOH:O	2.37	0.57
1:C:363:ILE:HG22	1:C:364:GLU:HG3	1.87	0.56
1:C:153:THR:HG23	1:C:159:LEU:HD21	1.88	0.56
1:B:309:LEU:HB2	3:B:501:HOH:O	2.08	0.54
1:A:153:THR:HG23	1:A:159:LEU:CD2	2.38	0.53
1:C:306:ARG:NH1	3:C:509:HOH:O	2.43	0.52
1:B:310:ARG:HH21	1:B:310:ARG:CG	2.22	0.51
1:D:53:HIS:ND1	3:D:501:HOH:O	2.34	0.51
1:A:24:ILE:H	1:A:24:ILE:HD12	1.76	0.50
1:A:384:LYS:NZ	1:A:384:LYS:CD	2.61	0.50
1:D:153:THR:HG23	1:D:159:LEU:CD2	2.43	0.49
1:C:96:SER:OG	1:C:98:GLU:HG2	2.13	0.48
1:A:303:ASP:OD2	1:A:306:ARG:NH2	2.47	0.47
1:A:378:PHE:O	1:A:382:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:LEU:HD23	1:D:151:THR:HB	1.96	0.47
1:C:136:ARG:HD2	1:C:167:ASP:OD2	2.15	0.47
1:C:372:ASP:OD1	3:C:502:HOH:O	2.20	0.46
1:D:136:ARG:NH1	1:D:136:ARG:HG3	2.29	0.46
1:A:384:LYS:C	1:A:385:ARG:HG2	2.35	0.46
1:C:306:ARG:HH12	1:C:310:ARG:HE	1.64	0.46
1:A:267:ASP:HA	3:A:502:HOH:O	2.17	0.45
1:A:306:ARG:HE	1:A:310:ARG:NH1	2.16	0.44
1:B:310:ARG:HG3	1:B:310:ARG:NH2	2.27	0.44
1:A:98:GLU:OE1	1:A:213:ASP:OD2	2.36	0.44
1:A:382:THR:C	1:A:384:LYS:H	2.21	0.43
1:A:363:ILE:HG22	1:A:364:GLU:HG3	2.00	0.43
1:B:40:ALA:HB1	1:B:111:ARG:HD3	2.01	0.43
1:D:40:ALA:HA	1:D:45:MET:HG3	2.01	0.43
1:B:50:PRO:HB2	1:B:52:GLU:HG3	2.01	0.43
1:A:384:LYS:CD	3:A:501:HOH:O	2.66	0.43
1:D:50:PRO:HB2	1:D:52:GLU:HG2	2.01	0.43
1:D:136:ARG:HH11	1:D:136:ARG:CG	2.32	0.42
1:B:328:ALA:HB1	1:B:357:VAL:HG21	2.02	0.42
1:D:83:LEU:N	1:D:84:PRO:CD	2.83	0.41
1:B:136:ARG:HB3	1:B:136:ARG:CZ	2.50	0.41
1:B:99:LEU:HD13	1:B:214:ASN:HA	2.01	0.41
1:D:303:ASP:OD1	1:D:303:ASP:N	2.47	0.41
1:C:153:THR:HG23	1:C:159:LEU:CD2	2.48	0.41
1:D:45:MET:HB2	3:D:638:HOH:O	2.19	0.41
1:C:165:SER:HB3	1:C:168:ASP:O	2.20	0.41
1:A:306:ARG:HE	1:A:310:ARG:HH12	1.69	0.41
1:B:184:LEU:HD23	1:B:184:LEU:C	2.42	0.41
1:D:187:ASP:OD2	1:D:204:SER:OG	2.34	0.40
1:D:363:ILE:HG22	1:D:364:GLU:HG3	2.03	0.40
1:B:384:LYS:C	1:B:385:ARG:HG2	2.42	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASP:OD2	1:B:385:ARG:HH22[1_455]	0.99	0.61
1:A:137:ASP:OD2	1:B:385:ARG:NH2[1_455]	1.67	0.53

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	A	389/389 (100%)	385 (99%)	4 (1%)	0	100	100
1	B	389/389 (100%)	386 (99%)	3 (1%)	0	100	100
1	C	383/389 (98%)	382 (100%)	1 (0%)	0	100	100
1	D	380/389 (98%)	377 (99%)	3 (1%)	0	100	100
All	All	1541/1556 (99%)	1530 (99%)	11 (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	A	306/304 (101%)	305 (100%)	1 (0%)	92	89
1	B	306/304 (101%)	303 (99%)	3 (1%)	76	63
1	C	300/304 (99%)	297 (99%)	3 (1%)	76	63
1	D	298/304 (98%)	296 (99%)	2 (1%)	84	75
All	All	1210/1216 (100%)	1201 (99%)	9 (1%)	84	75

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

Mol	Chain	Res	Type
1	A	388	GLU
1	B	139	ASP

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Mol	Chain	Res	Type
1	B	384	LYS
1	B	385	ARG
1	C	130[A]	ILE
1	C	130[B]	ILE
1	C	136	ARG
1	D	136	ARG
1	D	171	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	46	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](#)

4 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	FDA	A	401	-	51,58,58	3.71	16 (31%)	60,89,89	2.42	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FDA	B	401	-	51,58,58	3.53	19 (37%)	60,89,89	2.13	12 (20%)
2	FDA	C	401	-	51,58,58	3.78	19 (37%)	60,89,89	2.18	15 (25%)
2	FDA	D	401	-	51,58,58	3.64	18 (35%)	60,89,89	2.33	16 (26%)

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	FDA	A	401	-	-	1/30/50/50	0/6/6/6
2	FDA	B	401	-	-	1/30/50/50	0/6/6/6
2	FDA	C	401	-	-	1/30/50/50	0/6/6/6
2	FDA	D	401	-	-	1/30/50/50	0/6/6/6

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FDA	C2B-C1B	-13.23	1.33	1.53
2	A	401	FDA	C2B-C1B	-13.22	1.33	1.53
2	C	401	FDA	C2B-C1B	-12.73	1.34	1.53
2	B	401	FDA	C2B-C1B	-12.51	1.34	1.53
2	A	401	FDA	O4B-C1B	12.41	1.58	1.41
2	D	401	FDA	O4B-C1B	11.65	1.57	1.41
2	C	401	FDA	O4B-C1B	11.64	1.57	1.41
2	B	401	FDA	O4B-C1B	11.47	1.57	1.41
2	C	401	FDA	C4X-N5	9.72	1.47	1.33
2	B	401	FDA	C10-N1	9.23	1.45	1.33
2	A	401	FDA	C10-N1	9.01	1.44	1.33
2	C	401	FDA	C10-N1	8.78	1.44	1.33
2	A	401	FDA	C4X-N5	8.04	1.44	1.33
2	D	401	FDA	C4X-N5	7.79	1.44	1.33
2	D	401	FDA	C10-N1	7.44	1.42	1.33
2	C	401	FDA	C5X-N5	7.18	1.47	1.35
2	B	401	FDA	C4X-N5	7.15	1.43	1.33
2	B	401	FDA	C5X-N5	6.60	1.46	1.35
2	D	401	FDA	C5X-N5	6.00	1.45	1.35
2	A	401	FDA	C5X-N5	5.91	1.45	1.35
2	A	401	FDA	C9A-N10	5.60	1.46	1.38
2	D	401	FDA	C9A-N10	5.58	1.46	1.38
2	B	401	FDA	C4-C4X	5.36	1.50	1.41
2	C	401	FDA	C9A-N10	5.34	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FDA	C4-C4X	5.25	1.50	1.41
2	A	401	FDA	C4-C4X	5.10	1.50	1.41
2	D	401	FDA	C4-C4X	4.82	1.49	1.41
2	A	401	FDA	O4B-C4B	-4.80	1.34	1.45
2	C	401	FDA	C4-N3	4.74	1.41	1.33
2	B	401	FDA	C9A-N10	4.70	1.44	1.38
2	D	401	FDA	C4-N3	4.61	1.41	1.33
2	D	401	FDA	O4B-C4B	-4.36	1.35	1.45
2	D	401	FDA	C1'-N10	-4.08	1.44	1.48
2	D	401	FDA	O2B-C2B	3.98	1.52	1.43
2	A	401	FDA	O2B-C2B	3.98	1.52	1.43
2	B	401	FDA	O4B-C4B	-3.80	1.36	1.45
2	A	401	FDA	C2A-N3A	3.45	1.37	1.32
2	C	401	FDA	O2B-C2B	3.37	1.50	1.43
2	C	401	FDA	O4B-C4B	-3.35	1.37	1.45
2	B	401	FDA	O2B-C2B	3.32	1.50	1.43
2	B	401	FDA	C4-N3	3.28	1.38	1.33
2	A	401	FDA	C4-N3	3.25	1.38	1.33
2	C	401	FDA	C5'-C4'	3.14	1.56	1.51
2	D	401	FDA	C6A-N6A	3.03	1.45	1.34
2	C	401	FDA	C9A-C5X	-2.99	1.36	1.42
2	C	401	FDA	C1'-N10	-2.89	1.45	1.48
2	C	401	FDA	C6A-N6A	2.87	1.44	1.34
2	C	401	FDA	C2-N1	2.83	1.43	1.38
2	B	401	FDA	C6A-N6A	2.82	1.44	1.34
2	C	401	FDA	C4X-C10	-2.74	1.36	1.38
2	A	401	FDA	C5A-C4A	-2.72	1.33	1.40
2	C	401	FDA	C2A-N3A	2.71	1.36	1.32
2	C	401	FDA	O2'-C2'	-2.65	1.37	1.43
2	A	401	FDA	C6A-N6A	2.61	1.43	1.34
2	D	401	FDA	C4X-C10	-2.47	1.36	1.38
2	D	401	FDA	C5A-C4A	-2.46	1.34	1.40
2	B	401	FDA	C2-N1	2.45	1.43	1.38
2	B	401	FDA	C6-C5X	-2.44	1.38	1.41
2	A	401	FDA	O3B-C3B	-2.43	1.37	1.43
2	C	401	FDA	C5A-C4A	-2.41	1.34	1.40
2	B	401	FDA	C5A-C4A	-2.39	1.34	1.40
2	B	401	FDA	O2'-C2'	-2.38	1.38	1.43
2	A	401	FDA	C2-N1	2.34	1.42	1.38
2	D	401	FDA	O3B-C3B	-2.33	1.37	1.43
2	B	401	FDA	C5'-C4'	2.28	1.55	1.51
2	A	401	FDA	C4A-N3A	-2.24	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FDA	C2-N3	2.19	1.42	1.38
2	D	401	FDA	C2A-N3A	2.17	1.35	1.32
2	B	401	FDA	PA-O2A	-2.16	1.45	1.55
2	D	401	FDA	C6-C5X	-2.13	1.38	1.41
2	B	401	FDA	C2A-N3A	2.12	1.35	1.32
2	D	401	FDA	PA-O5B	2.00	1.67	1.59

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FDA	C4-N3-C2	11.41	124.77	115.14
2	D	401	FDA	C4-N3-C2	10.70	124.18	115.14
2	C	401	FDA	C4-N3-C2	9.77	123.39	115.14
2	B	401	FDA	C4-N3-C2	9.45	123.12	115.14
2	A	401	FDA	N3A-C2A-N1A	-5.04	120.80	128.68
2	B	401	FDA	C5A-C6A-N6A	4.97	127.91	120.35
2	D	401	FDA	N3A-C2A-N1A	-4.96	120.92	128.68
2	C	401	FDA	C5A-C6A-N6A	4.74	127.55	120.35
2	B	401	FDA	N3A-C2A-N1A	-4.73	121.29	128.68
2	A	401	FDA	C3B-C2B-C1B	4.67	108.01	100.98
2	D	401	FDA	C4X-C4-N3	-4.61	117.13	123.43
2	D	401	FDA	C5A-C6A-N6A	4.58	127.32	120.35
2	A	401	FDA	C4X-C4-N3	-4.58	117.17	123.43
2	C	401	FDA	N3A-C2A-N1A	-4.56	121.55	128.68
2	B	401	FDA	C3B-C2B-C1B	4.41	107.61	100.98
2	D	401	FDA	C3B-C2B-C1B	4.18	107.26	100.98
2	C	401	FDA	C4X-C4-N3	-4.15	117.76	123.43
2	C	401	FDA	C10-C4X-N5	-3.98	118.50	121.26
2	A	401	FDA	C2B-C3B-C4B	-3.77	95.31	102.64
2	A	401	FDA	C5A-C6A-N6A	3.67	125.92	120.35
2	A	401	FDA	C9A-N10-C10	-3.62	117.17	121.91
2	B	401	FDA	C4X-C4-N3	-3.61	118.49	123.43
2	D	401	FDA	C9A-N10-C10	-3.60	117.20	121.91
2	C	401	FDA	C9A-N10-C10	-3.56	117.25	121.91
2	C	401	FDA	C3B-C2B-C1B	3.55	106.33	100.98
2	C	401	FDA	C4-C4X-N5	3.35	122.42	118.60
2	B	401	FDA	C9A-N10-C10	-3.31	117.57	121.91
2	A	401	FDA	O3'-C3'-C2'	-3.19	101.10	108.81
2	B	401	FDA	N6A-C6A-N1A	-3.15	112.03	118.57
2	B	401	FDA	C1'-N10-C10	3.06	121.15	118.41
2	D	401	FDA	C4-C4X-N5	2.99	122.02	118.60
2	A	401	FDA	N6A-C6A-N1A	-2.83	112.71	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FDA	N6A-C6A-N1A	-2.79	112.78	118.57
2	D	401	FDA	C2B-C3B-C4B	-2.79	97.23	102.64
2	B	401	FDA	O3'-C3'-C2'	-2.77	102.11	108.81
2	D	401	FDA	C1'-N10-C9A	2.75	120.46	118.29
2	D	401	FDA	C4-C4X-C10	-2.63	118.21	119.95
2	B	401	FDA	C2B-C3B-C4B	-2.63	97.52	102.64
2	C	401	FDA	N6A-C6A-N1A	-2.63	113.12	118.57
2	A	401	FDA	C10-C4X-N5	-2.62	119.45	121.26
2	A	401	FDA	C1'-N10-C9A	2.57	120.31	118.29
2	C	401	FDA	C2B-C3B-C4B	-2.50	97.79	102.64
2	A	401	FDA	C4-C4X-N5	2.44	121.39	118.60
2	D	401	FDA	C8M-C8-C9	-2.44	114.51	120.34
2	D	401	FDA	C10-C4X-N5	-2.38	119.61	121.26
2	C	401	FDA	C1B-N9A-C4A	-2.34	122.54	126.64
2	D	401	FDA	C7M-C7-C6	-2.29	114.86	120.34
2	C	401	FDA	O4'-C4'-C5'	-2.26	104.84	109.92
2	A	401	FDA	C5'-C4'-C3'	-2.23	107.90	112.20
2	C	401	FDA	C9A-C5X-N5	-2.22	118.89	122.36
2	B	401	FDA	C10-C4X-N5	-2.21	119.73	121.26
2	A	401	FDA	C8M-C8-C9	-2.20	115.09	120.34
2	D	401	FDA	C1B-N9A-C4A	-2.19	122.79	126.64
2	B	401	FDA	C8M-C8-C9	-2.17	115.15	120.34
2	D	401	FDA	C7M-C7-C8	2.14	125.11	120.74
2	C	401	FDA	P-O3P-PA	-2.10	125.63	132.83
2	A	401	FDA	C7M-C7-C6	-2.06	115.42	120.34
2	C	401	FDA	C5X-C9A-N10	2.02	119.18	117.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

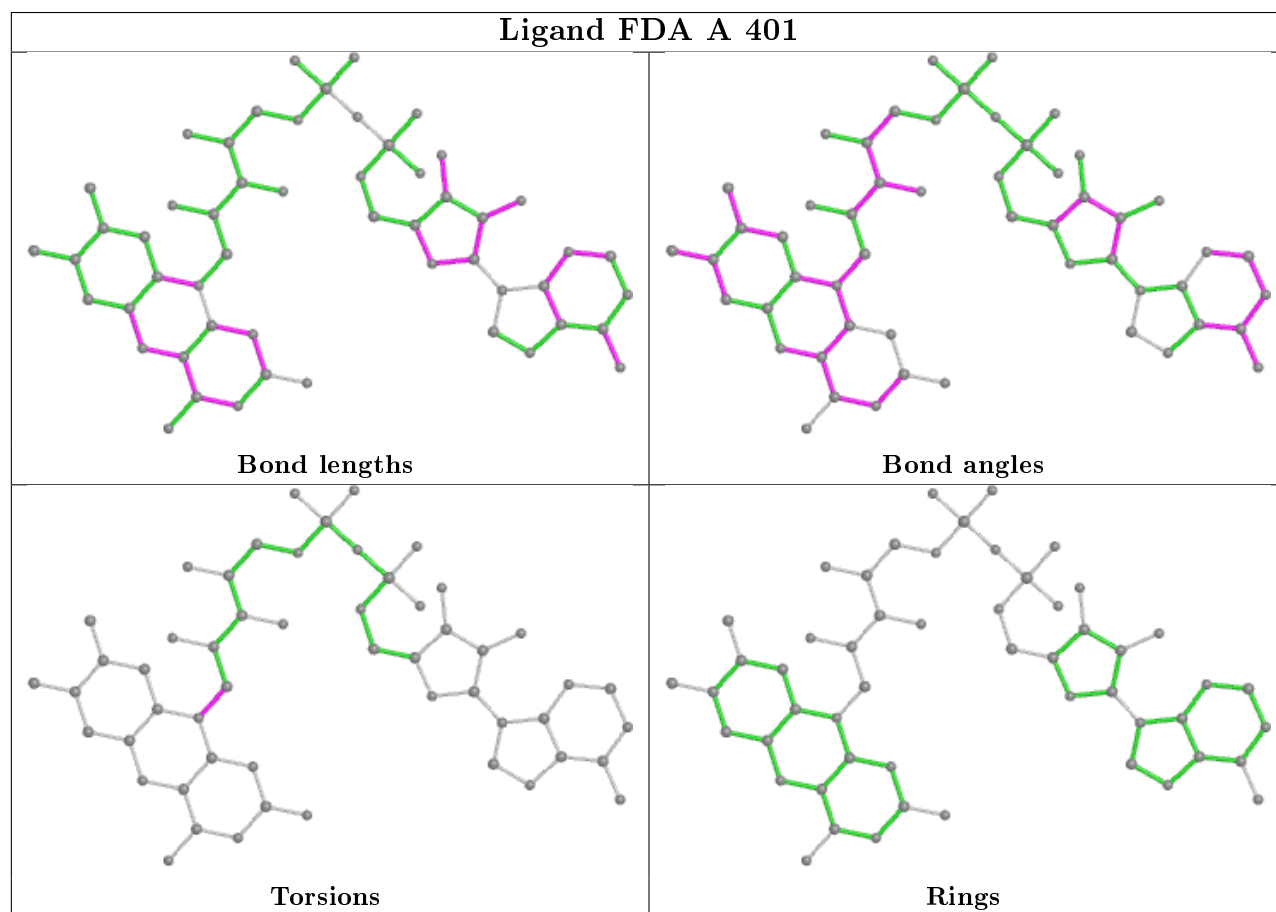
Mol	Chain	Res	Type	Atoms
2	A	401	FDA	C2'-C1'-N10-C10
2	B	401	FDA	C2'-C1'-N10-C10
2	C	401	FDA	C2'-C1'-N10-C10
2	D	401	FDA	C2'-C1'-N10-C10

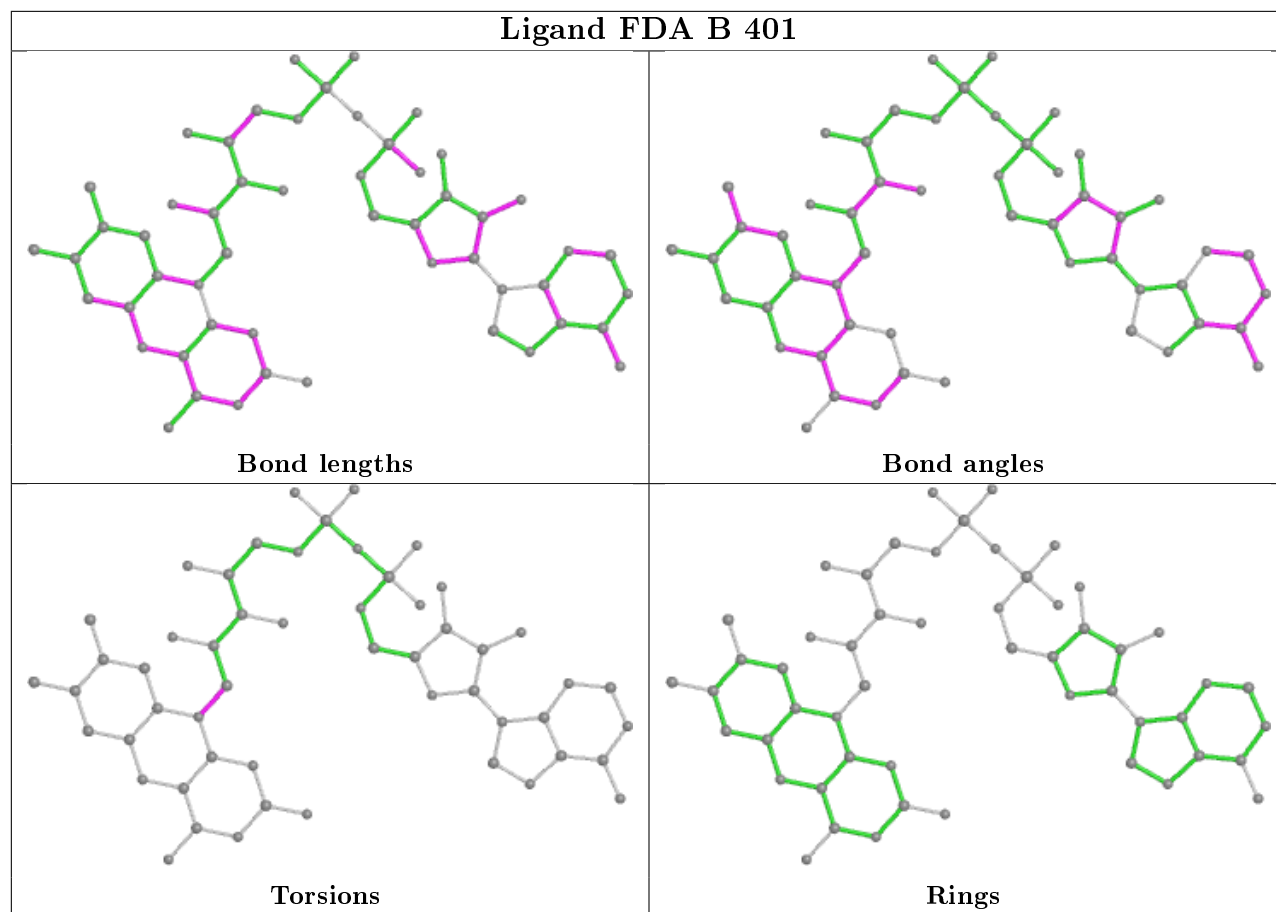
There are no ring outliers.

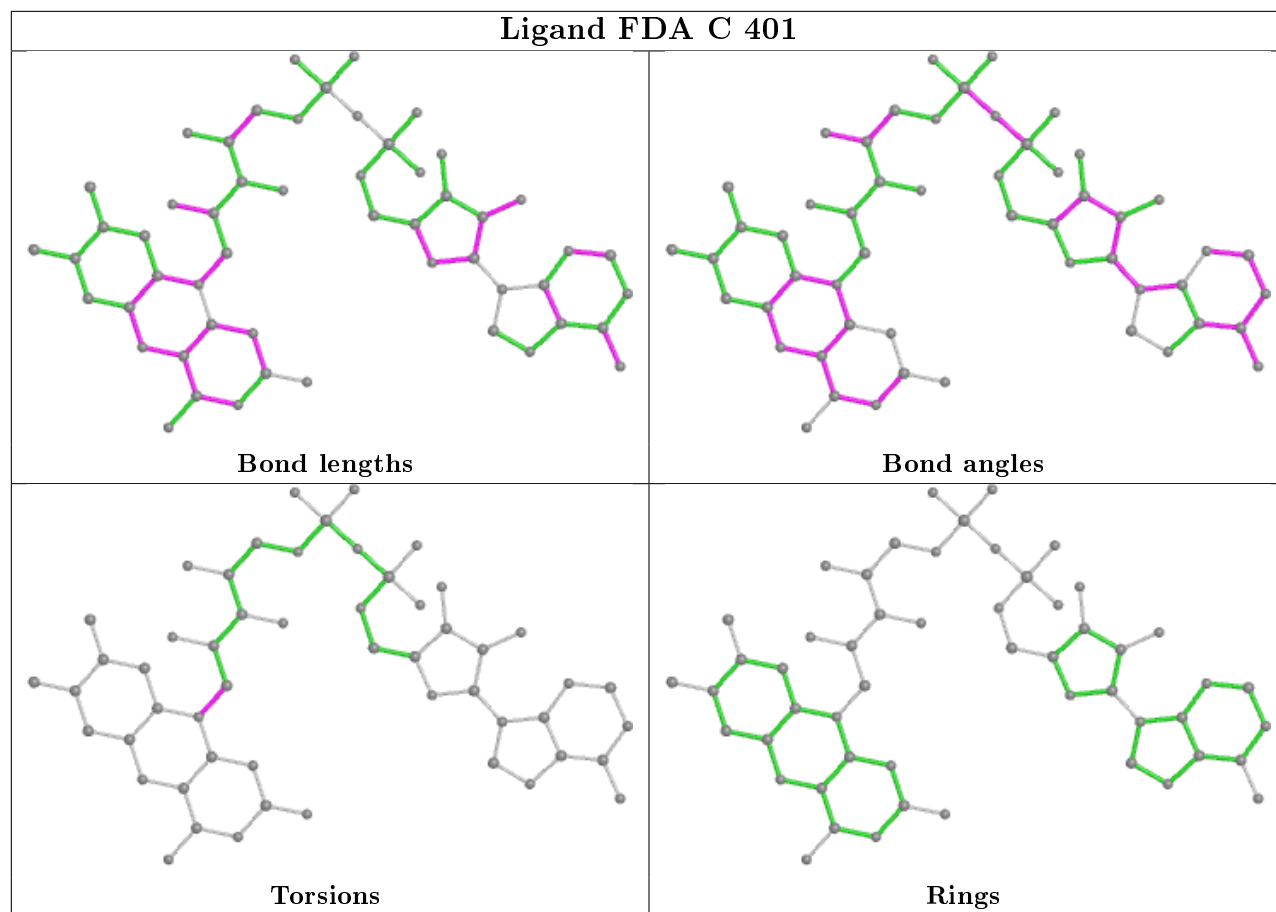
No monomer is involved in short contacts.

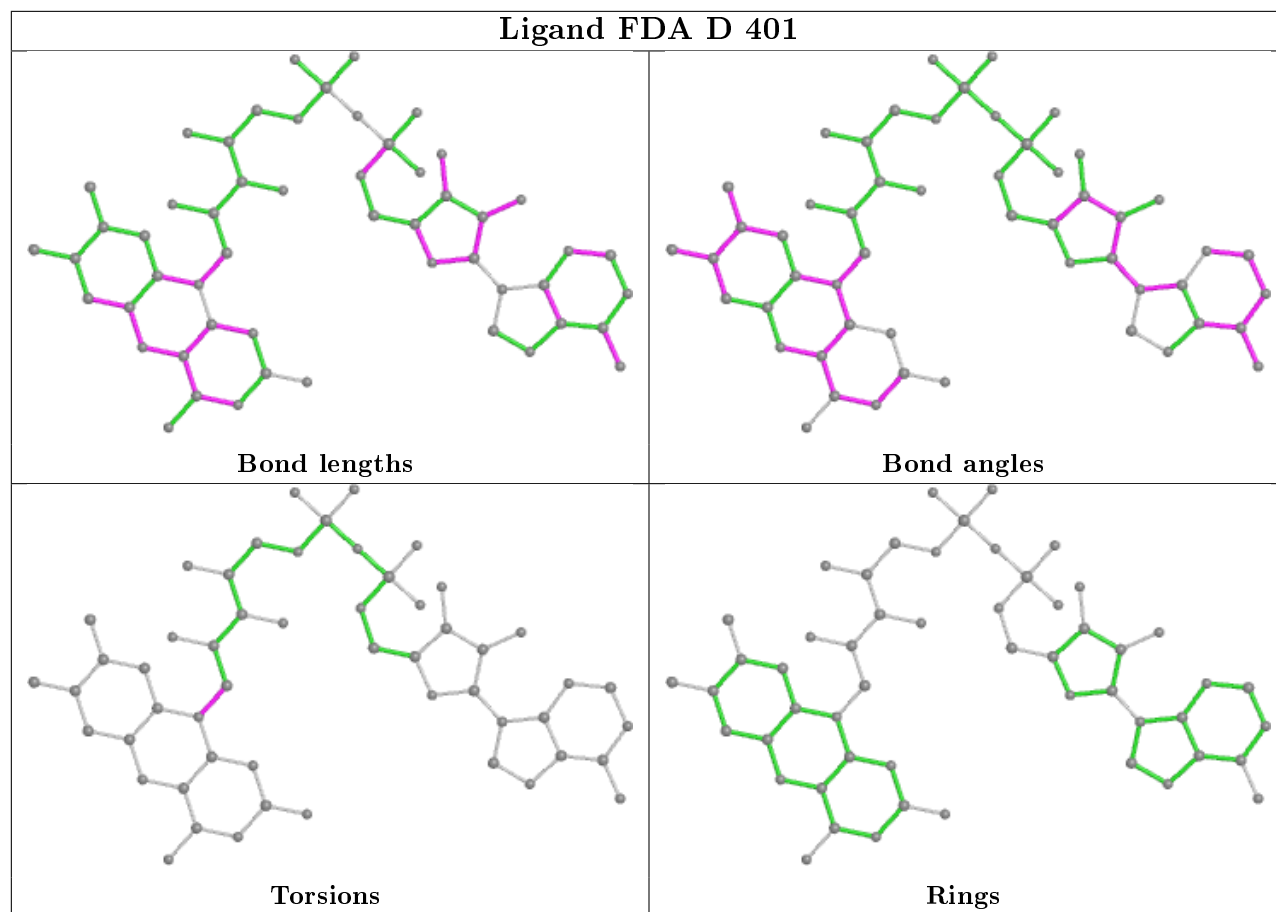
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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 ⓘ

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	A	388/389 (99%)	-0.18	5 (1%) 77 83	13, 20, 47, 88	0
1	B	389/389 (100%)	-0.20	5 (1%) 77 83	12, 20, 46, 100	0
1	C	383/389 (98%)	-0.09	7 (1%) 68 76	15, 25, 52, 93	0
1	D	382/389 (98%)	-0.13	12 (3%) 49 55	13, 22, 50, 80	0
All	All	1542/1556 (99%)	-0.15	29 (1%) 66 74	12, 21, 50, 100	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.9
1	C	383	ALA	5.5
1	D	167	ASP	5.0
1	D	139	ASP	4.5
1	B	387	LEU	4.5
1	A	386	THR	4.2
1	A	387	LEU	4.1
1	C	302	PRO	3.8
1	B	389	HIS	3.6
1	D	168	ASP	3.6
1	D	1	MET	3.5
1	D	302	PRO	3.4
1	B	385	ARG	3.4
1	A	385	ARG	3.0
1	D	382	THR	3.0
1	A	384	LYS	2.8
1	D	166	ALA	2.8
1	D	170	ALA	2.7
1	B	1	MET	2.6
1	C	168	ASP	2.6
1	A	1	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	167	ASP	2.5
1	D	171	ARG	2.5
1	D	169	PRO	2.5
1	B	386	THR	2.4
1	D	306	ARG	2.1
1	C	171	ARG	2.1
1	D	56	LEU	2.1
1	C	136	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

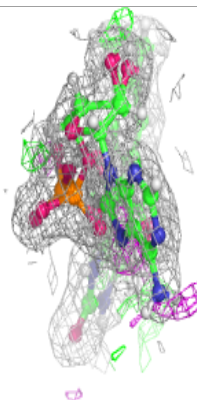
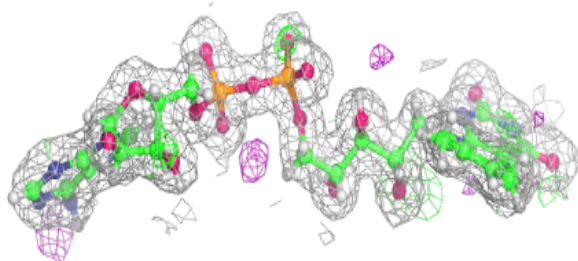
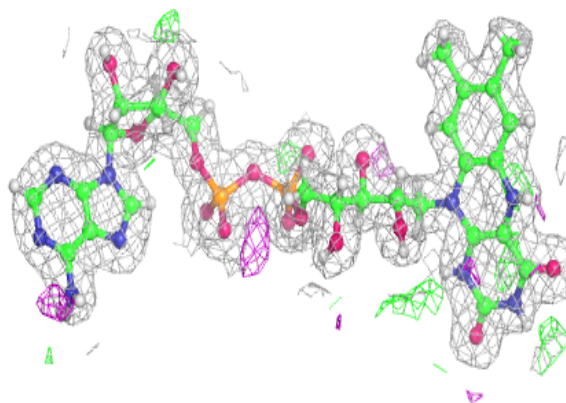
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FDA	A	401	53/53	0.98	0.10	11,17,22,25	0
2	FDA	B	401	53/53	0.98	0.11	11,17,24,26	0
2	FDA	C	401	53/53	0.98	0.08	12,19,27,28	0
2	FDA	D	401	53/53	0.98	0.08	11,18,27,33	0

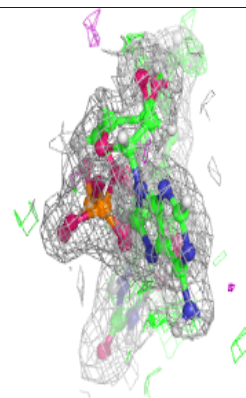
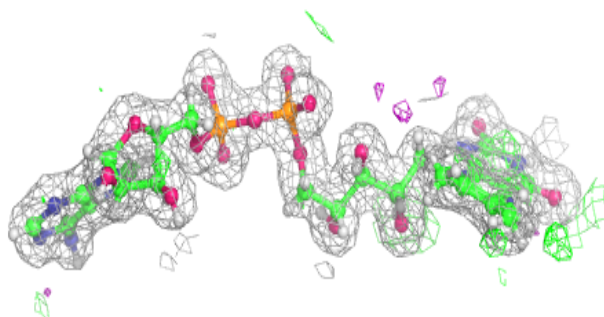
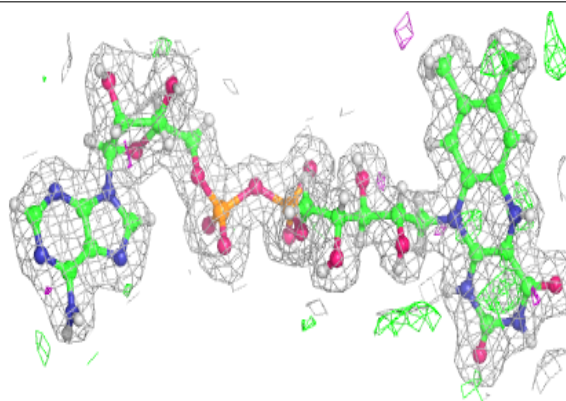
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FDA A 401:

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

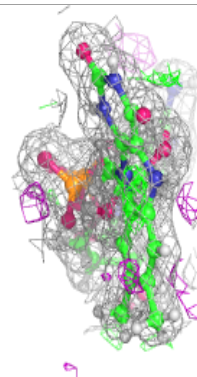
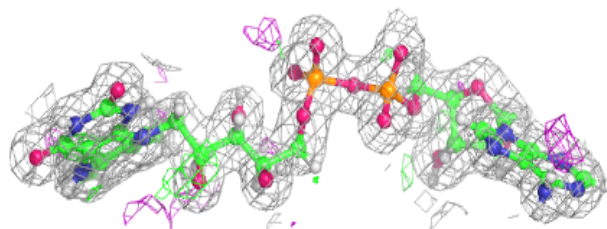
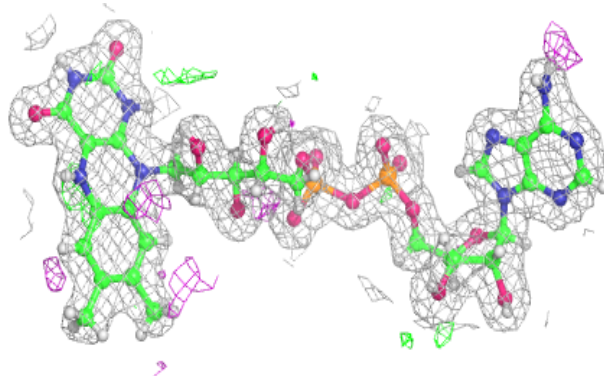
**Electron density around FDA B 401:**

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

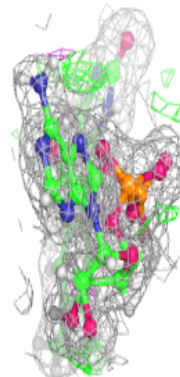
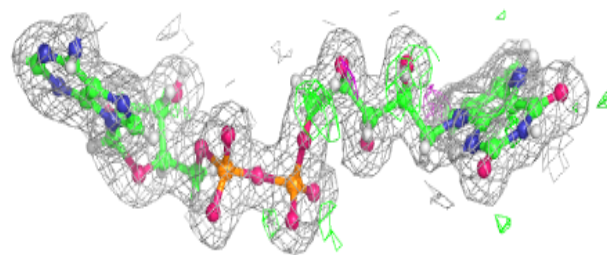
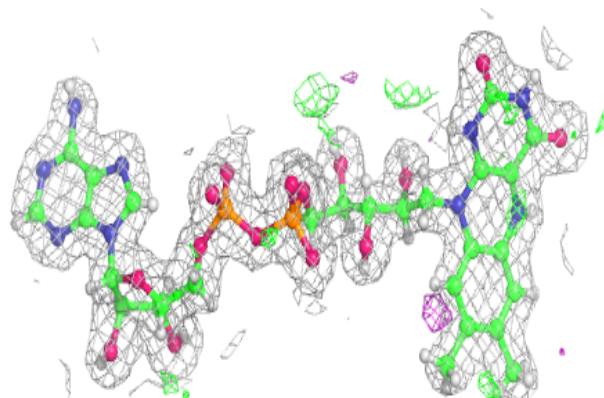


Electron density around FDA C 401:

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

**Electron density around FDA D 401:**

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



6.5 Other polymers

There are no such residues in this entry.