



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 08:52 am BST

PDB ID : 4YMK  
Title : Crystal Structure of Stearoyl-Coenzyme A Desaturase 1  
Authors : Bai, Y.; McCoy, J.G.; Rajashankar, K.R.; Zhou, M.  
Deposited on : 2015-03-06  
Resolution : 2.60 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](mailto: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.

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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

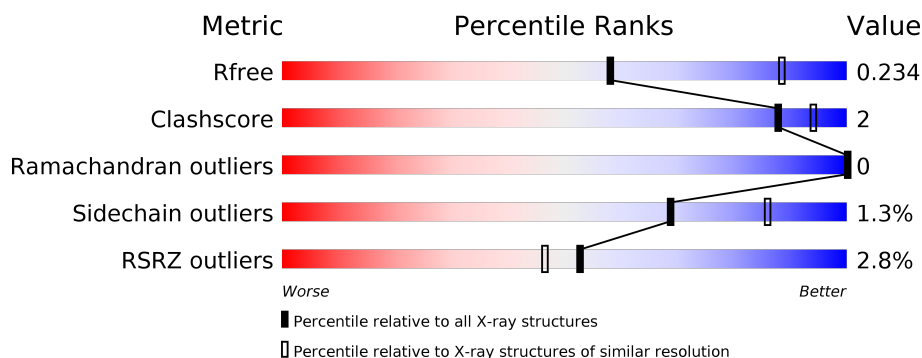
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	339	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	D	339	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5505 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 Acyl-CoA desaturase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2659	1735	459	452	13			
1	D	312	Total	C	N	O	S	0	0	0
			2572	1680	446	433	13			

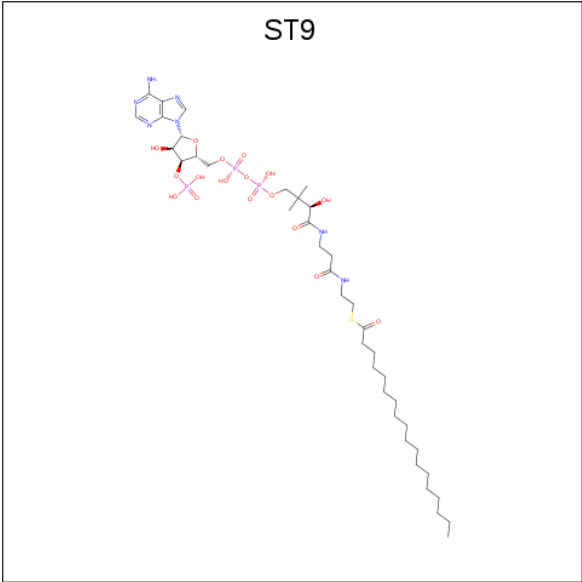
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P13516
A	356	GLU	-	expression tag	UNP P13516
A	357	ASN	-	expression tag	UNP P13516
A	358	LEU	-	expression tag	UNP P13516
A	359	TYR	-	expression tag	UNP P13516
A	360	PHE	-	expression tag	UNP P13516
A	361	GLN	-	expression tag	UNP P13516
D	23	MET	-	initiating methionine	UNP P13516
D	356	GLU	-	expression tag	UNP P13516
D	357	ASN	-	expression tag	UNP P13516
D	358	LEU	-	expression tag	UNP P13516
D	359	TYR	-	expression tag	UNP P13516
D	360	PHE	-	expression tag	UNP P13516
D	361	GLN	-	expression tag	UNP P13516

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

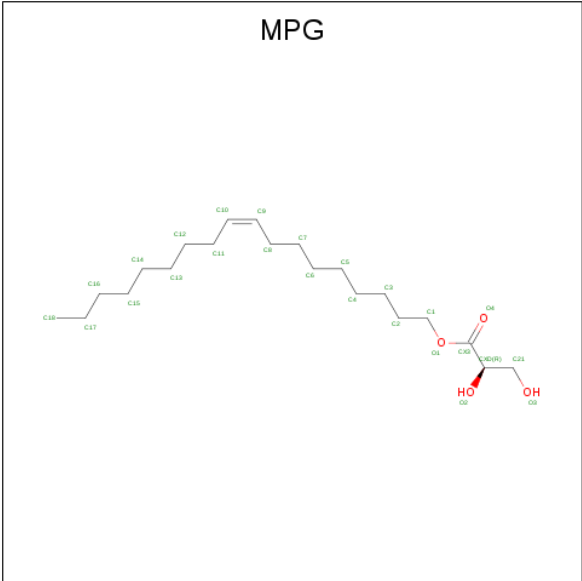
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is STEAROYL-COENZYME A (three-letter code: ST9) (formula: C<sub>39</sub>H<sub>70</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			67	39	7	17	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			67	39	7	17	3	1		

- Molecule 4 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (three-letter code: MPG) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	21	4		

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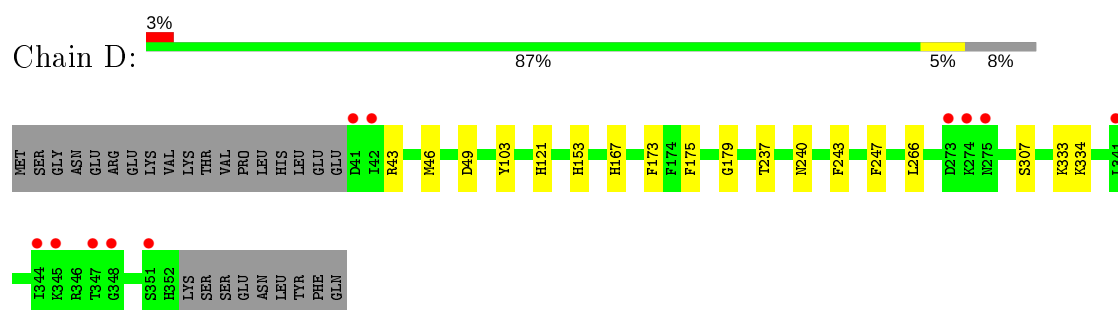
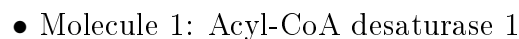
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			25	21	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	D	39	Total	O	0	0
			39	39		



- Molecule 1: Acyl-CoA desaturase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.06Å 113.77Å 141.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.41 – 2.60 47.41 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.41-2.60) 95.4 (47.41-2.61)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.203 , 0.235 0.204 , 0.234	Depositor DCC
$R_{free}$ test set	2000 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPG, ZN, ST9

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	0.21	0/2745	0.34	0/3722
1	D	0.21	0/2656	0.34	0/3603
All	All	0.21	0/5401	0.34	0/7325

There are no bond length outliers.

There are no bond angle outliers.

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	A	2659	0	2615	13	0
1	D	2572	0	2537	9	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
3	A	67	0	66	2	0
3	D	67	0	66	1	0
4	A	25	0	40	1	0
4	D	25	0	40	0	0
5	A	47	0	0	1	0
5	D	39	0	0	0	0
All	All	5505	0	5364	22	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 2.

All (22) 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:103:TYR:HB3	1:A:249:ARG:HD2	1.81	0.61
1:D:43:ARG:NH1	1:D:121:HIS:O	2.35	0.59
1:A:212:ARG:NH1	1:A:213:TYR:OH	2.36	0.59
1:D:243:PHE:HA	1:D:247:PHE:HB2	1.86	0.56
1:A:143:GLN:HB3	3:A:403:ST9:H2A	1.88	0.56
1:A:43:ARG:NH1	1:A:46:MET:O	2.40	0.54
1:A:153:HIS:CE1	3:A:403:ST9:H10A	2.45	0.51
1:D:43:ARG:NH2	1:D:49:ASP:OD2	2.44	0.50
1:A:43:ARG:HD3	1:A:46:MET:HB3	1.95	0.49
1:A:171:ARG:NH2	5:A:544:HOH:O	2.46	0.48
1:D:175:PHE:HA	1:D:179:GLY:HA3	1.95	0.48
1:D:43:ARG:HG3	1:D:333:LYS:HE3	1.95	0.48
1:D:173:PHE:HD2	1:D:266:LEU:HD12	1.78	0.48
1:D:307:SER:O	1:D:334:LYS:NZ	2.47	0.48
1:D:153:HIS:CE1	3:D:403:ST9:H10A	2.49	0.47
1:A:43:ARG:NH2	1:A:49:ASP:OD2	2.48	0.46
1:A:289:VAL:HA	4:A:404:MPG:H212	1.98	0.45
1:A:136:ILE:HG22	1:A:140:MET:HE2	1.99	0.45
1:A:117:ARG:NH2	1:A:291:GLU:OE2	2.41	0.45
1:A:117:ARG:HD3	1:A:304:TYR:O	2.17	0.44
1:D:237:THR:OG1	1:D:240:ASN:OD1	2.36	0.42
1:A:50:ILE:O	1:A:158:LYS:HG2	2.21	0.41

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	A	320/339 (94%)	301 (94%)	19 (6%)	0	100	100
1	D	310/339 (91%)	290 (94%)	20 (6%)	0	100	100
All	All	630/678 (93%)	591 (94%)	39 (6%)	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	281/297 (95%)	277 (99%)	4 (1%)	67	85
1	D	271/297 (91%)	268 (99%)	3 (1%)	73	88
All	All	552/594 (93%)	545 (99%)	7 (1%)	69	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	87	ILE
1	A	103	TYR
1	A	167	HIS
1	D	46	MET
1	D	103	TYR
1	D	167	HIS

Some 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	MPG	D	404	-	24,24,24	0.59	0	24,25,25	0.45	0
3	ST9	D	403	-	61,69,69	0.87	2 (3%)	72,95,95	1.38	6 (8%)
3	ST9	A	403	-	61,69,69	0.88	2 (3%)	72,95,95	1.30	7 (9%)
4	MPG	A	404	-	24,24,24	0.59	0	24,25,25	0.44	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
4	MPG	D	404	-	-	4/25/25/25	-
3	ST9	D	403	-	-	17/64/84/84	0/3/3/3
3	ST9	A	403	-	-	19/64/84/84	0/3/3/3
4	MPG	A	404	-	-	6/25/25/25	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	ST9	O4B-C1B	2.98	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	ST9	O4B-C1B	2.81	1.45	1.41
3	D	403	ST9	C8A-N7A	-2.20	1.30	1.34
3	A	403	ST9	C8A-N7A	-2.14	1.30	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	403	ST9	C2-C1-S1P	6.43	120.95	113.46
3	A	403	ST9	C2-C1-S1P	5.08	119.37	113.46
3	D	403	ST9	O2-C1-C2	-3.94	119.34	123.99
3	D	403	ST9	N3A-C2A-N1A	-3.91	122.57	128.68
3	A	403	ST9	N3A-C2A-N1A	-3.84	122.68	128.68
3	A	403	ST9	O2-C1-C2	-3.14	120.28	123.99
3	A	403	ST9	C6P-C5P-N4P	2.62	120.84	116.42
3	A	403	ST9	C7P-C6P-C5P	-2.56	108.09	112.36
3	A	403	ST9	C4A-C5A-N7A	-2.30	107.00	109.40
3	A	403	ST9	CAP-C9P-N8P	2.26	121.08	116.58
3	D	403	ST9	O2-C1-S1P	-2.23	119.72	122.61
3	D	403	ST9	C4A-C5A-N7A	-2.18	107.13	109.40
3	D	403	ST9	C7P-C6P-C5P	-2.06	108.92	112.36

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	404	MPG	O1-CX3-CXD-O2
3	A	403	ST9	C1-C2-C3-C4
3	A	403	ST9	C3B-O3B-P3B-O9A
3	A	403	ST9	C5P-C6P-C7P-N8P
3	D	403	ST9	C1-C2-C3-C4
3	D	403	ST9	C5B-O5B-P1A-O1A
3	D	403	ST9	C5B-O5B-P1A-O2A
3	D	403	ST9	C3P-C2P-S1P-C1
3	D	403	ST9	C3B-O3B-P3B-O9A
3	D	403	ST9	O4B-C4B-C5B-O5B
3	D	403	ST9	C5P-C6P-C7P-N8P
4	A	404	MPG	O3-C21-CXD-O2
4	A	404	MPG	O1-CX3-CXD-O2
3	D	403	ST9	C3B-C4B-C5B-O5B
3	A	403	ST9	C4-C5-C6-C7
3	A	403	ST9	C7-C8-C9-C10
3	A	403	ST9	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	D	403	ST9	C7-C8-C9-C10
3	A	403	ST9	S1P-C2P-C3P-N4P
3	A	403	ST9	C5-C6-C7-C8
3	A	403	ST9	C2-C3-C4-C5
4	D	404	MPG	O4-CX3-CXD-O2
4	A	404	MPG	O4-CX3-CXD-O2
4	A	404	MPG	O3-C21-CXD-CX3
3	A	403	ST9	C6-C7-C8-C9
3	A	403	ST9	O2-C1-S1P-C2P
3	D	403	ST9	O2-C1-S1P-C2P
3	D	403	ST9	O2-C1-C2-C3
3	D	403	ST9	S1P-C1-C2-C3
3	A	403	ST9	C2-C1-S1P-C2P
3	D	403	ST9	C2-C1-S1P-C2P
4	A	404	MPG	C1-C2-C3-C4
3	D	403	ST9	C4-C5-C6-C7
3	A	403	ST9	C5B-O5B-P1A-O3A
3	A	403	ST9	C5B-O5B-P1A-O1A
4	A	404	MPG	O1-C1-C2-C3
3	A	403	ST9	CEP-CBP-CCP-O6A
3	D	403	ST9	C3-C4-C5-C6
3	A	403	ST9	CDP-CBP-CCP-O6A
3	A	403	ST9	C3P-C2P-S1P-C1
3	A	403	ST9	O4B-C4B-C5B-O5B
3	D	403	ST9	P1A-O3A-P2A-O6A
4	D	404	MPG	C1-C2-C3-C4
4	D	404	MPG	O1-C1-C2-C3
3	A	403	ST9	C3B-O3B-P3B-O7A
3	D	403	ST9	C5B-O5B-P1A-O3A

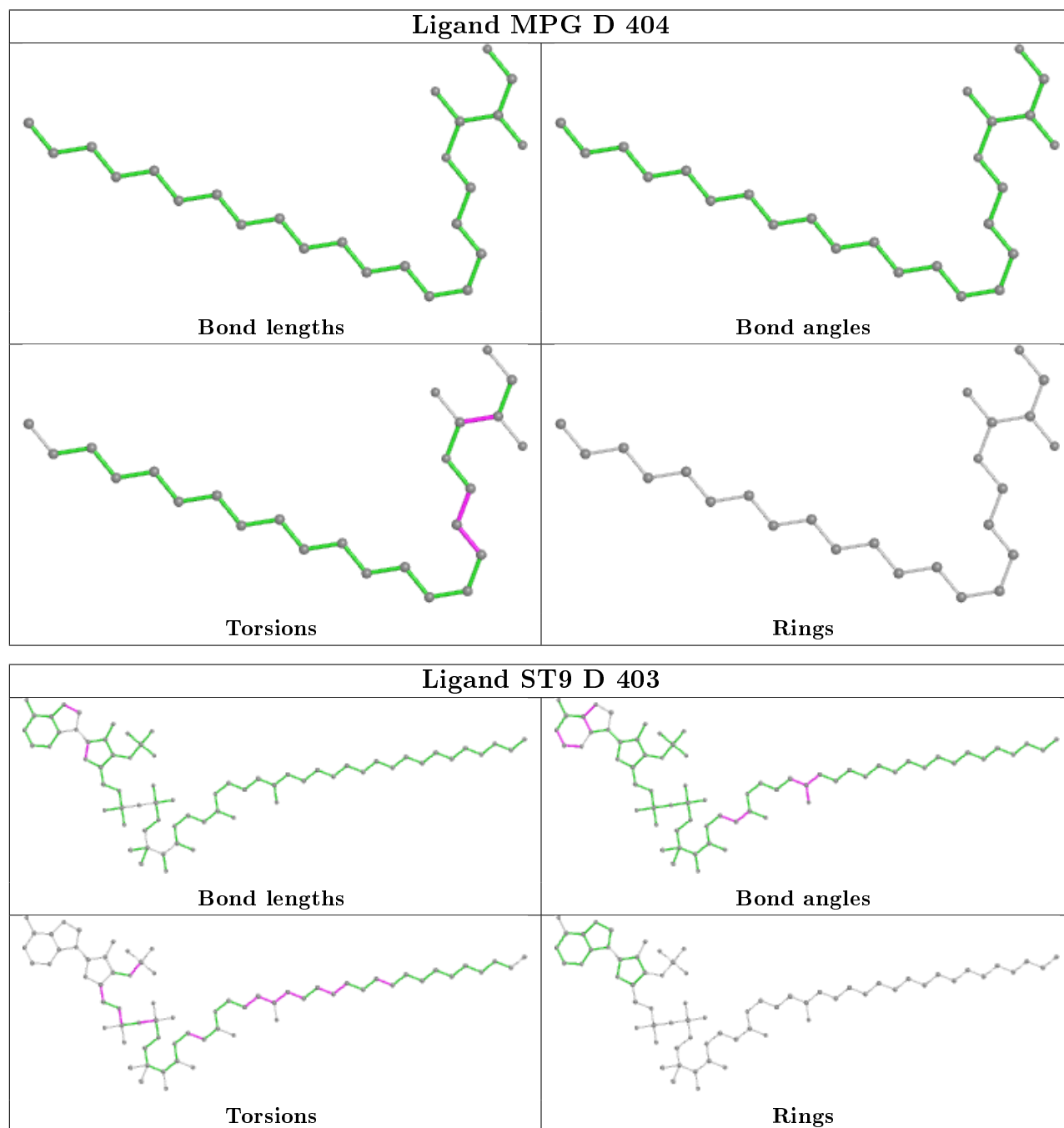
There are no ring outliers.

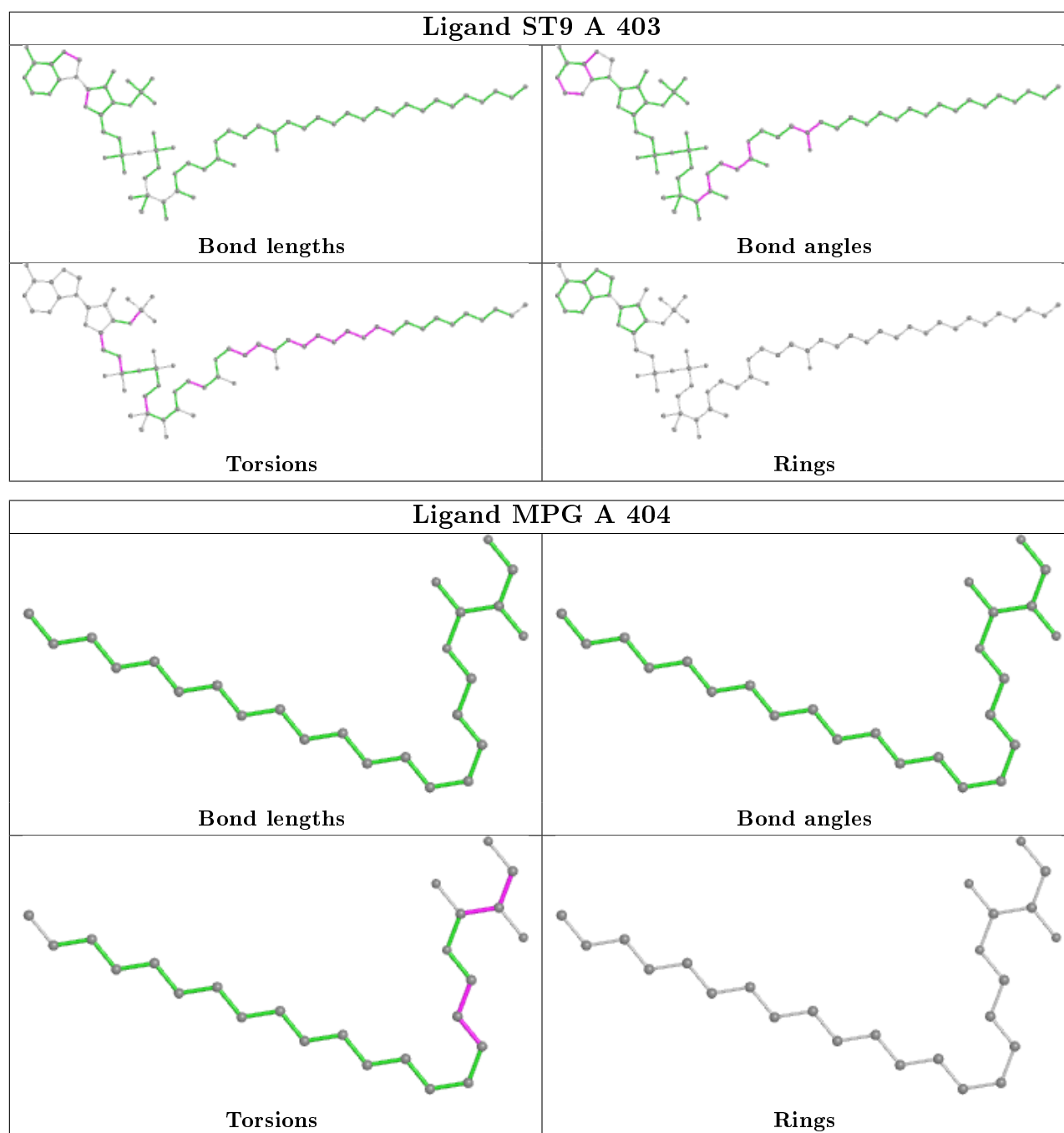
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	ST9	1	0
3	A	403	ST9	2	0
4	A	404	MPG	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	322/339 (94%)	-0.14	7 (2%) 62 56	25, 40, 61, 104	0
1	D	312/339 (92%)	-0.04	11 (3%) 44 36	33, 48, 73, 110	0
All	All	634/678 (93%)	-0.09	18 (2%) 53 46	25, 44, 69, 110	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	42	ILE	6.0
1	A	40	GLU	4.6
1	A	345	LYS	4.5
1	A	341	LEU	3.8
1	D	41	ASP	3.8
1	D	274	LYS	3.7
1	D	345	LYS	3.5
1	D	344	ILE	2.9
1	D	275	ASN	2.8
1	A	45	GLU	2.7
1	A	42	ILE	2.7
1	D	347	THR	2.6
1	A	346	ARG	2.4
1	D	351	SER	2.4
1	D	348	GLY	2.4
1	A	41	ASP	2.3
1	D	273	ASP	2.2
1	D	341	LEU	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 carbohydrates in this entry.

## 6.4 Ligands

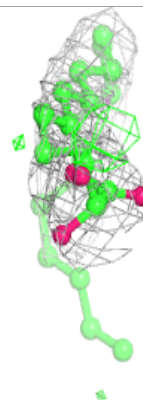
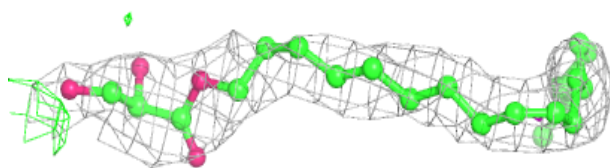
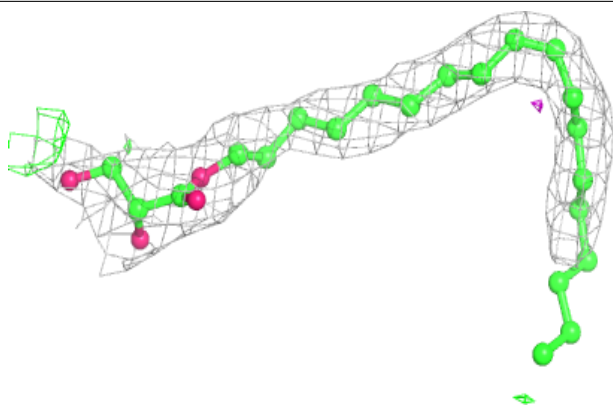
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MPG	D	404	25/25	0.74	0.32	49,63,86,89	0
4	MPG	A	404	25/25	0.83	0.26	46,62,79,82	0
3	ST9	D	403	67/67	0.93	0.17	32,46,87,107	0
3	ST9	A	403	67/67	0.95	0.16	23,39,63,80	0
2	ZN	D	402	1/1	0.99	0.12	38,38,38,38	0
2	ZN	D	401	1/1	0.99	0.17	38,38,38,38	0
2	ZN	A	402	1/1	1.00	0.14	31,31,31,31	0
2	ZN	A	401	1/1	1.00	0.18	34,34,34,34	0

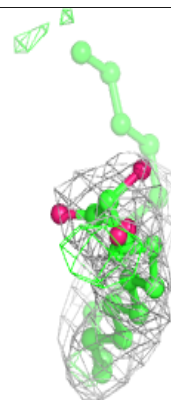
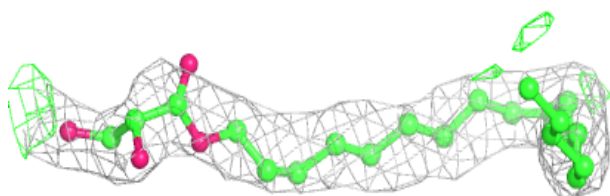
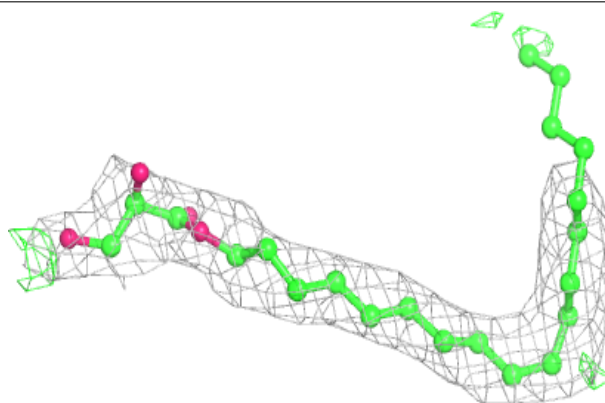
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around MPG D 404:**

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

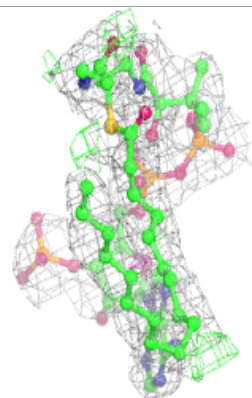
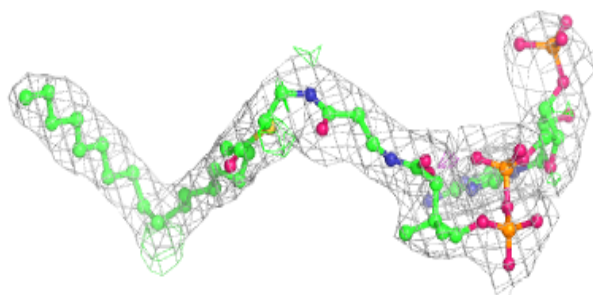
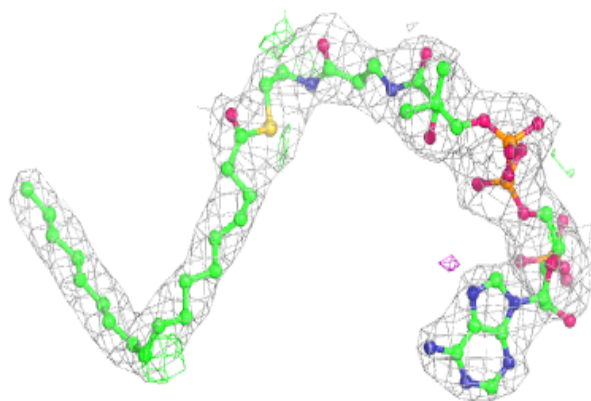
**Electron density around MPG A 404:**

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

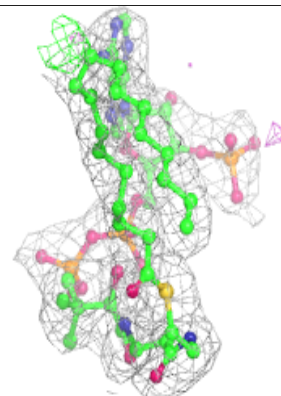
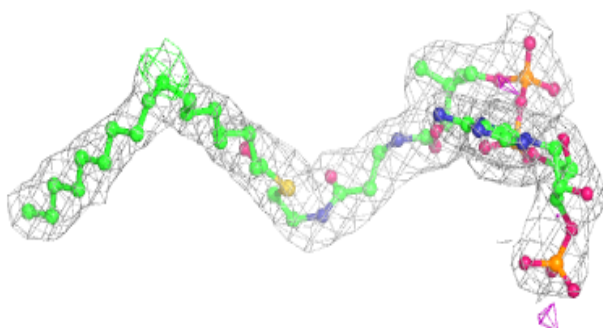
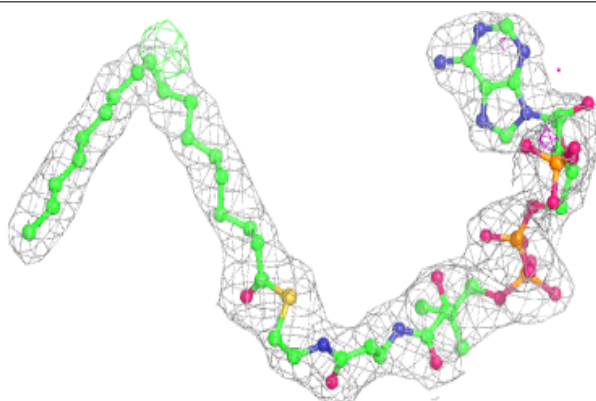


**Electron density around ST9 D 403:**

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

**Electron density around ST9 A 403:**

$2mF_o-DF_c$  (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.