



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:29 AM BST

PDB ID : 4KU5  
Title : Crystal Structures of C143S Xanthomonas campestris OleA with Bound Lauric Acid and Lauroyl-CoA  
Authors : Goblirsch, B.R.  
Deposited on : 2013-05-21  
Resolution : 2.17 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	:	2.13.1
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)	:	2.13.1

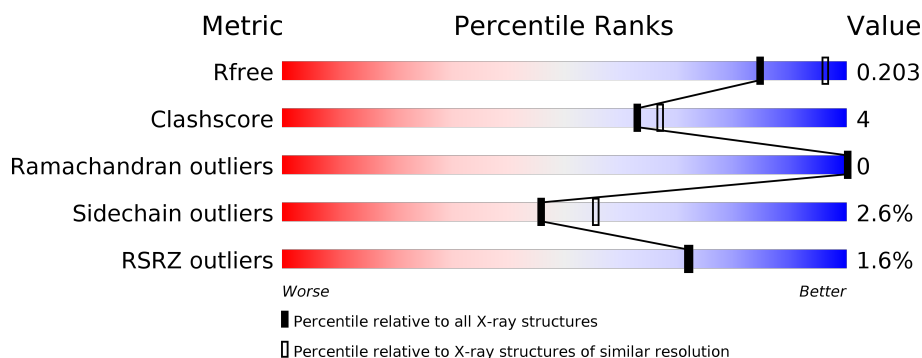
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	358	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	358	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	A	403	-	-	X	-
2	PEG	B	402	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5727 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 3-oxoacyl-[ACP] synthase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	7	0
			2620	1647	461	498	14			
1	B	337	Total	C	N	O	S	0	8	0
			2617	1642	458	503	14			

There are 42 discrepancies between the modelled and reference sequences:

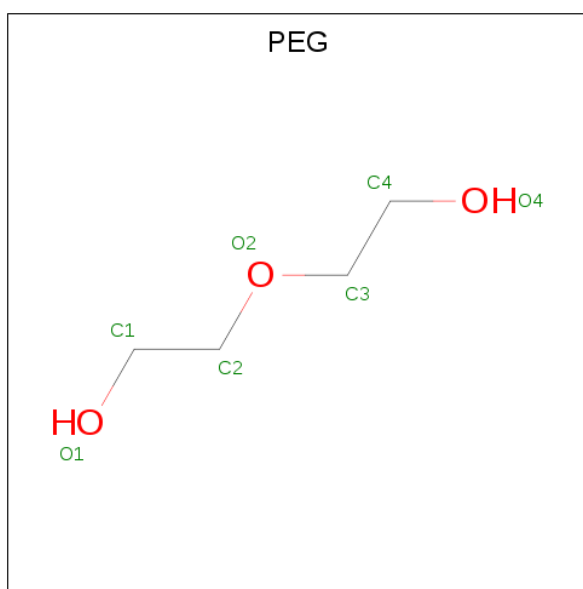
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q8PDX2
A	2	GLY	-	EXPRESSION TAG	UNP Q8PDX2
A	3	SER	-	EXPRESSION TAG	UNP Q8PDX2
A	4	SER	-	EXPRESSION TAG	UNP Q8PDX2
A	5	HIS	-	EXPRESSION TAG	UNP Q8PDX2
A	6	HIS	-	EXPRESSION TAG	UNP Q8PDX2
A	7	HIS	-	EXPRESSION TAG	UNP Q8PDX2
A	8	HIS	-	EXPRESSION TAG	UNP Q8PDX2
A	9	HIS	-	EXPRESSION TAG	UNP Q8PDX2
A	10	HIS	-	EXPRESSION TAG	UNP Q8PDX2
A	11	SER	-	EXPRESSION TAG	UNP Q8PDX2
A	12	SER	-	EXPRESSION TAG	UNP Q8PDX2
A	13	GLY	-	EXPRESSION TAG	UNP Q8PDX2
A	14	LEU	-	EXPRESSION TAG	UNP Q8PDX2
A	15	VAL	-	EXPRESSION TAG	UNP Q8PDX2
A	16	PRO	-	EXPRESSION TAG	UNP Q8PDX2
A	17	ARG	-	EXPRESSION TAG	UNP Q8PDX2
A	18	GLY	-	EXPRESSION TAG	UNP Q8PDX2
A	19	SER	-	EXPRESSION TAG	UNP Q8PDX2
A	20	HIS	-	EXPRESSION TAG	UNP Q8PDX2
A	143	SER	CYS	ENGINEERED MUTATION	UNP Q8PDX2
B	1	MET	-	INITIATING METHIONINE	UNP Q8PDX2
B	2	GLY	-	EXPRESSION TAG	UNP Q8PDX2
B	3	SER	-	EXPRESSION TAG	UNP Q8PDX2
B	4	SER	-	EXPRESSION TAG	UNP Q8PDX2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	EXPRESSION TAG	UNP Q8PDX2
B	6	HIS	-	EXPRESSION TAG	UNP Q8PDX2
B	7	HIS	-	EXPRESSION TAG	UNP Q8PDX2
B	8	HIS	-	EXPRESSION TAG	UNP Q8PDX2
B	9	HIS	-	EXPRESSION TAG	UNP Q8PDX2
B	10	HIS	-	EXPRESSION TAG	UNP Q8PDX2
B	11	SER	-	EXPRESSION TAG	UNP Q8PDX2
B	12	SER	-	EXPRESSION TAG	UNP Q8PDX2
B	13	GLY	-	EXPRESSION TAG	UNP Q8PDX2
B	14	LEU	-	EXPRESSION TAG	UNP Q8PDX2
B	15	VAL	-	EXPRESSION TAG	UNP Q8PDX2
B	16	PRO	-	EXPRESSION TAG	UNP Q8PDX2
B	17	ARG	-	EXPRESSION TAG	UNP Q8PDX2
B	18	GLY	-	EXPRESSION TAG	UNP Q8PDX2
B	19	SER	-	EXPRESSION TAG	UNP Q8PDX2
B	20	HIS	-	EXPRESSION TAG	UNP Q8PDX2
B	143	SER	CYS	ENGINEERED MUTATION	UNP Q8PDX2

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

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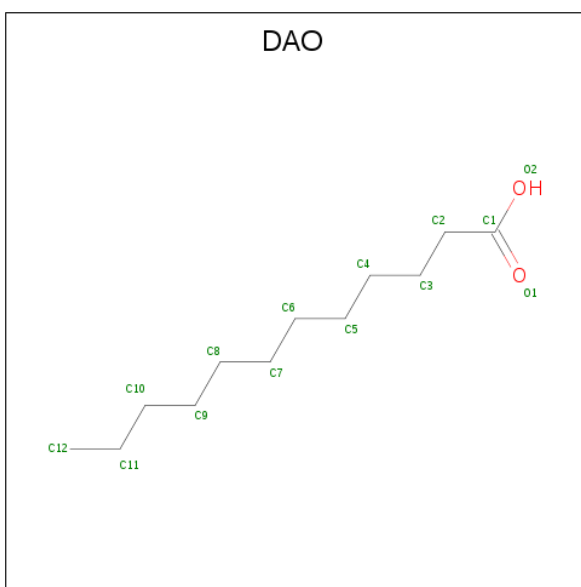
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



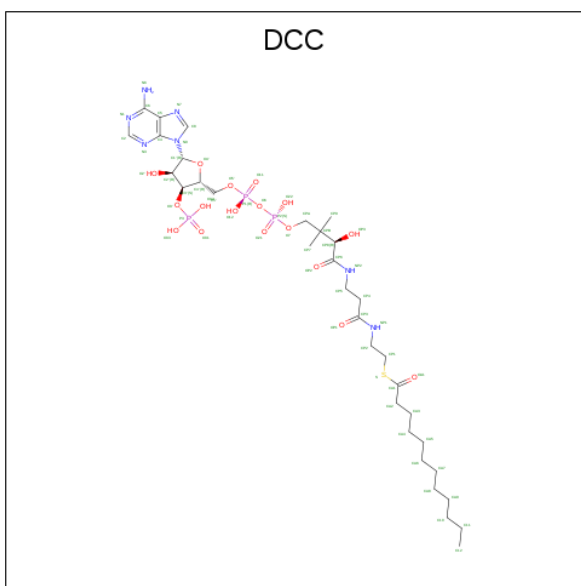
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is LAURIC ACID (three-letter code: DAO) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			14	12	2		

- Molecule 5 is DODECYL-COA (three-letter code: DCC) (formula:  $C_{33}H_{58}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			61	33	7	17	3	1		

- Molecule 6 is water.

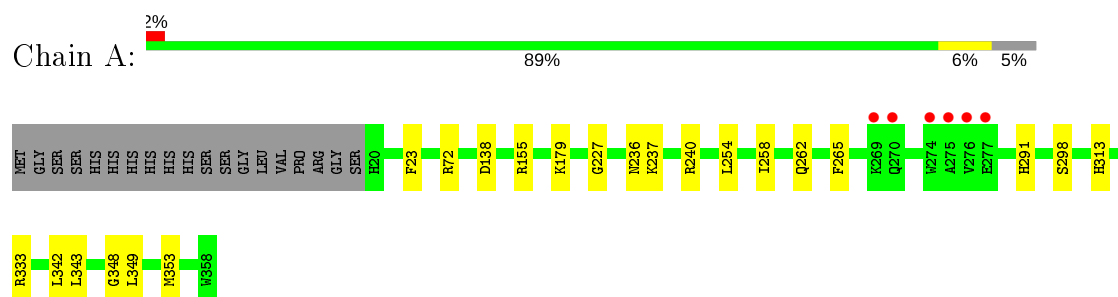
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total 210	O 210	0	7
6	B	165	Total 165	O 165	0	0



### 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: 3-oxoacyl-[ACP] synthase III



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.20Å 85.38Å 102.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.01 – 2.17 44.01 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.01-2.17) 94.6 (44.01-2.17)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.02 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.159 , 0.203 0.159 , 0.203	Depositor DCC
$R_{free}$ test set	1945 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5727	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: PO4, PEG, DAO, DCC

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	0.34	0/2672	0.47	0/3618
1	B	0.33	0/2661	0.47	0/3603
All	All	0.33	0/5333	0.47	0/7221

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	2620	0	2660	16	0
1	B	2617	0	2643	28	0
2	A	21	0	30	9	0
2	B	14	0	20	8	0
3	A	5	0	0	0	0
4	B	14	0	23	0	0
5	B	61	0	54	1	0
6	A	210	0	0	4	0
6	B	165	0	0	8	0
All	All	5727	0	5430	46	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 (46) 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:102:LYS:HE2	2:B:404:PEG:H22	1.62	0.80
1:A:313:HIS:NE2	2:A:401:PEG:H32	2.06	0.70
1:B:114[A]:ASP:OD1	6:B:617:HOH:O	2.12	0.67
1:B:102:LYS:HA	2:B:402:PEG:H11	1.76	0.66
1:B:240:ARG:NH1	6:B:640:HOH:O	2.29	0.66
1:B:158:GLU:OE1	6:B:619:HOH:O	2.13	0.65
2:A:402:PEG:H11	6:A:686:HOH:O	1.97	0.64
1:B:251:ARG:NH2	5:B:403:DCC:O12	2.31	0.62
1:B:333:ARG:NH2	6:B:612:HOH:O	2.20	0.61
1:B:193:GLU:OE1	6:B:615:HOH:O	2.16	0.61
1:B:102:LYS:HD3	2:B:402:PEG:H11	1.86	0.56
1:B:102:LYS:HE3	2:B:402:PEG:H41	1.87	0.55
1:B:114[B]:ASP:OD2	1:B:114[B]:ASP:N	2.39	0.55
1:A:227:GLY:O	2:A:403:PEG:H42	2.07	0.55
2:A:401:PEG:H31	6:A:545:HOH:O	2.09	0.51
1:A:227:GLY:H	2:A:403:PEG:C4	2.24	0.51
1:B:180:THR:O	1:B:184[B]:MET:HG2	2.12	0.50
1:B:113:ARG:NH2	1:B:138:ASP:OD2	2.46	0.49
1:B:289:ARG:HB3	1:B:290:PRO:HD3	1.95	0.49
1:B:102:LYS:HE2	2:B:404:PEG:H41	1.95	0.49
1:A:155:ARG:HB3	6:A:684:HOH:O	2.14	0.48
1:B:91:LYS:NZ	6:B:589:HOH:O	2.39	0.48
1:A:236:ASN:O	1:A:240:ARG:NH1	2.47	0.47
1:B:255:ILE:O	6:B:584:HOH:O	2.20	0.47
1:B:330[B]:GLU:OE2	6:B:514:HOH:O	2.20	0.47
1:B:69:ILE:HD13	1:B:202:THR:HA	1.97	0.47
1:B:252:LEU:HD22	1:B:256:GLU:HG2	1.97	0.47
2:A:402:PEG:H41	2:A:402:PEG:H21	1.77	0.46
1:A:23:PHE:CZ	2:A:403:PEG:H31	2.51	0.46
1:A:254:LEU:HB2	1:A:291[B]:HIS:CE1	2.51	0.45
1:B:295:PHE:O	1:B:298[A]:SER:OG	2.33	0.45
1:A:343:LEU:HD22	1:A:353:MET:HG2	1.98	0.45
1:A:227:GLY:O	2:A:403:PEG:H22	2.17	0.45
1:A:23:PHE:CE2	2:A:403:PEG:H31	2.52	0.44
1:A:138:ASP:HB2	1:B:140:ALA:HB3	2.00	0.44
1:B:108:ASN:HB3	1:B:138:ASP:OD1	2.17	0.44
1:A:333:ARG:NH1	6:A:657:HOH:O	2.50	0.43
1:B:51:PRO:O	1:B:55:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:HE3	2:B:402:PEG:C4	2.48	0.43
1:B:102:LYS:HE3	2:B:402:PEG:H22	2.00	0.43
1:A:237:LYS:HA	1:A:240:ARG:NH1	2.34	0.42
1:A:348:GLY:N	1:A:349:LEU:HA	2.35	0.41
1:A:254:LEU:O	1:A:258:ILE:HG12	2.21	0.41
1:A:179:LYS:HD3	1:A:179:LYS:HA	1.86	0.41
1:B:36:ALA:HB3	1:B:73:ARG:HB3	2.04	0.40
1:B:102:LYS:CE	2:B:402:PEG:H22	2.51	0.40

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	344/358 (96%)	337 (98%)	7 (2%)	0	100	100
1	B	343/358 (96%)	334 (97%)	9 (3%)	0	100	100
All	All	687/716 (96%)	671 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	281/290 (97%)	276 (98%)	5 (2%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	280/290 (97%)	271 (97%)	9 (3%)	39	47
All	All	561/580 (97%)	547 (98%)	14 (2%)	46	57

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

Mol	Chain	Res	Type
1	A	72	ARG
1	A	262	GLN
1	A	265	PHE
1	A	298	SER
1	A	342	LEU
1	B	48	ARG
1	B	72	ARG
1	B	252	LEU
1	B	253	LEU
1	B	271	VAL
1	B	287	VAL
1	B	288	SER
1	B	316	ILE
1	B	333	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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
3	PO4	A	404	-	4,4,4	0.86	0	6,6,6	1.26	1 (16%)
2	PEG	B	404	-	6,6,6	0.53	0	5,5,5	0.65	0
2	PEG	A	403	-	6,6,6	0.53	0	5,5,5	0.63	0
5	DCC	B	403	-	55,63,63	1.67	9 (16%)	66,89,89	1.92	17 (25%)
2	PEG	B	402	-	6,6,6	0.53	0	5,5,5	0.74	0
2	PEG	A	402	-	6,6,6	0.52	0	5,5,5	0.62	0
2	PEG	A	401	-	6,6,6	0.53	0	5,5,5	0.63	0
4	DAO	B	401	-	10,13,13	0.29	0	9,13,13	0.82	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	PEG	B	404	-	-	2/4/4/4	-
2	PEG	A	403	-	-	1/4/4/4	-
5	DCC	B	403	-	-	26/58/78/78	0/3/3/3
2	PEG	B	402	-	-	2/4/4/4	-
2	PEG	A	402	-	-	2/4/4/4	-
2	PEG	A	401	-	-	2/4/4/4	-
4	DAO	B	401	-	-	5/9/11/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	DCC	CP6-NP2	5.92	1.46	1.33
5	B	403	DCC	CP3-NP1	5.62	1.46	1.33
5	B	403	DCC	C2'-C1'	-3.70	1.48	1.53
5	B	403	DCC	OP3-CP8	3.52	1.48	1.42
5	B	403	DCC	C2-N3	3.02	1.37	1.32
5	B	403	DCC	C6-N6	2.83	1.44	1.34
5	B	403	DCC	C2'-C3'	-2.26	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	DCC	O2'-C2'	-2.23	1.37	1.43
5	B	403	DCC	CP9-CPB	-2.12	1.49	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	DCC	O12-P1-O5'	-5.49	82.27	107.75
5	B	403	DCC	O5'-P1-O11	-5.47	87.68	109.07
5	B	403	DCC	N3-C2-N1	-5.42	120.20	128.68
5	B	403	DCC	CA2-CA1-S	4.47	118.66	113.46
5	B	403	DCC	OA1-CA1-CA2	-3.93	119.35	123.99
5	B	403	DCC	P2-O6-P1	-3.68	120.19	132.83
5	B	403	DCC	OA1-CA1-S	-3.32	118.31	122.61
5	B	403	DCC	CP8-CP6-NP2	3.12	122.79	116.58
5	B	403	DCC	CP1-S-CA1	2.62	110.02	101.87
3	A	404	PO4	O2-P-O1	-2.58	101.44	110.89
5	B	403	DCC	O7-P2-O21	2.57	119.13	109.07
5	B	403	DCC	O22-P2-O7	2.52	119.45	107.75
5	B	403	DCC	CP4-CP5-NP2	-2.33	107.19	111.90
5	B	403	DCC	C4-C5-N7	-2.18	107.13	109.40
5	B	403	DCC	CP9-CPB-CPA	2.15	111.74	108.23
5	B	403	DCC	OP1-CP3-NP1	-2.13	118.99	123.01
5	B	403	DCC	CP4-CP3-NP1	2.06	119.88	116.42
5	B	403	DCC	OP3-CP8-CPB	2.05	115.08	110.25

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	403	DCC	C3'-C4'-C5'-O5'
5	B	403	DCC	O4'-C4'-C5'-O5'
5	B	403	DCC	C5'-O5'-P1-O11
5	B	403	DCC	C5'-O5'-P1-O12
5	B	403	DCC	C5'-O5'-P1-O6
5	B	403	DCC	CPA-O7-P2-O22
5	B	403	DCC	CP6-CP8-CPB-CPA
5	B	403	DCC	CP6-CP8-CPB-CP7
5	B	403	DCC	OP2-CP6-CP8-OP3
5	B	403	DCC	NP2-CP6-CP8-OP3
5	B	403	DCC	CP8-CP6-NP2-CP5
5	B	403	DCC	CP3-CP4-CP5-NP2
5	B	403	DCC	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
2	A	402	PEG	C4-C3-O2-C2
2	A	401	PEG	C4-C3-O2-C2
5	B	403	DCC	OP2-CP6-NP2-CP5
2	B	402	PEG	O2-C3-C4-O4
5	B	403	DCC	C11-C10-CA9-CA8
4	B	401	DAO	C2-C3-C4-C5
4	B	401	DAO	C7-C8-C9-C10
5	B	403	DCC	CA6-CA7-CA8-CA9
2	B	404	PEG	O1-C1-C2-O2
4	B	401	DAO	C5-C6-C7-C8
5	B	403	DCC	CA2-CA3-CA4-CA5
4	B	401	DAO	C3-C4-C5-C6
5	B	403	DCC	CA5-CA6-CA7-CA8
5	B	403	DCC	CA3-CA4-CA5-CA6
5	B	403	DCC	CP6-CP8-CPB-CP9
5	B	403	DCC	CPA-O7-P2-O21
2	A	402	PEG	C1-C2-O2-C3
5	B	403	DCC	CA4-CA5-CA6-CA7
2	B	402	PEG	O1-C1-C2-O2
2	B	404	PEG	O2-C3-C4-O4
4	B	401	DAO	C9-C10-C11-C12
2	A	403	PEG	C1-C2-O2-C3
5	B	403	DCC	CP2-CP1-S-CA1
5	B	403	DCC	CA7-CA8-CA9-C10
2	A	401	PEG	O1-C1-C2-O2
5	B	403	DCC	C3'-O3'-P3-O31
5	B	403	DCC	C3'-O3'-P3-O32

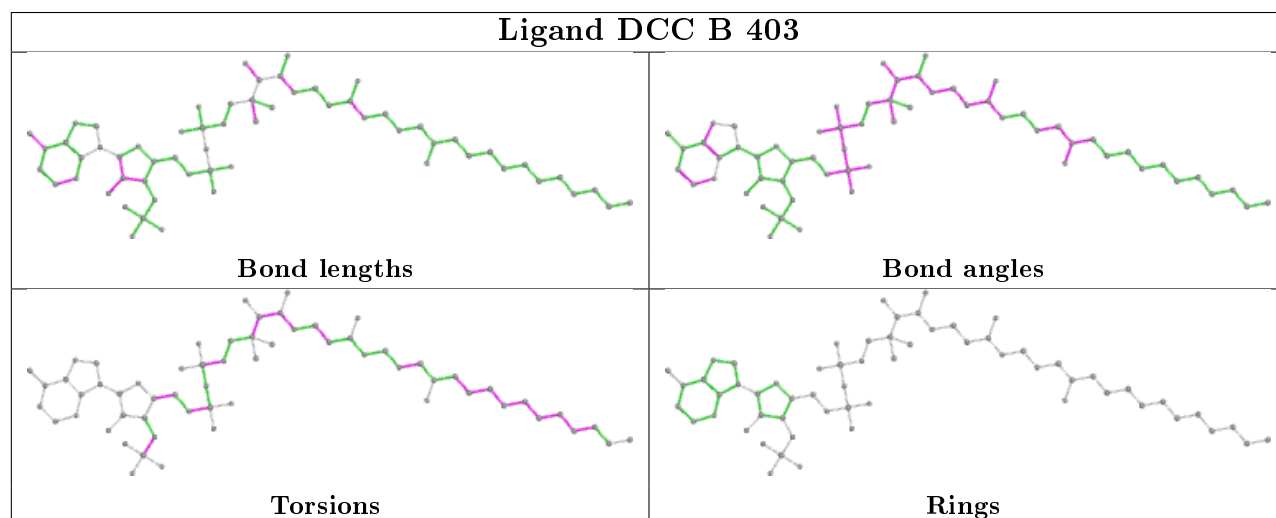
There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	404	PEG	2	0
2	A	403	PEG	5	0
5	B	403	DCC	1	0
2	B	402	PEG	6	0
2	A	402	PEG	2	0
2	A	401	PEG	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.



## 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	339/358 (94%)	-0.37	6 (1%) 68 69	16, 29, 48, 79	0
1	B	337/358 (94%)	-0.11	5 (1%) 73 74	18, 33, 59, 84	0
All	All	676/716 (94%)	-0.24	11 (1%) 72 72	16, 31, 57, 84	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	59	LYS	3.8
1	B	78	ASP	3.7
1	A	276	VAL	3.5
1	A	270	GLN	3.2
1	B	300	GLY	2.9
1	A	275	ALA	2.8
1	B	270	GLN	2.7
1	A	277	GLU	2.6
1	B	277	GLU	2.2
1	A	269	LYS	2.2
1	A	274	TRP	2.1

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

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

### 6.3 Carbohydrates [i](#)

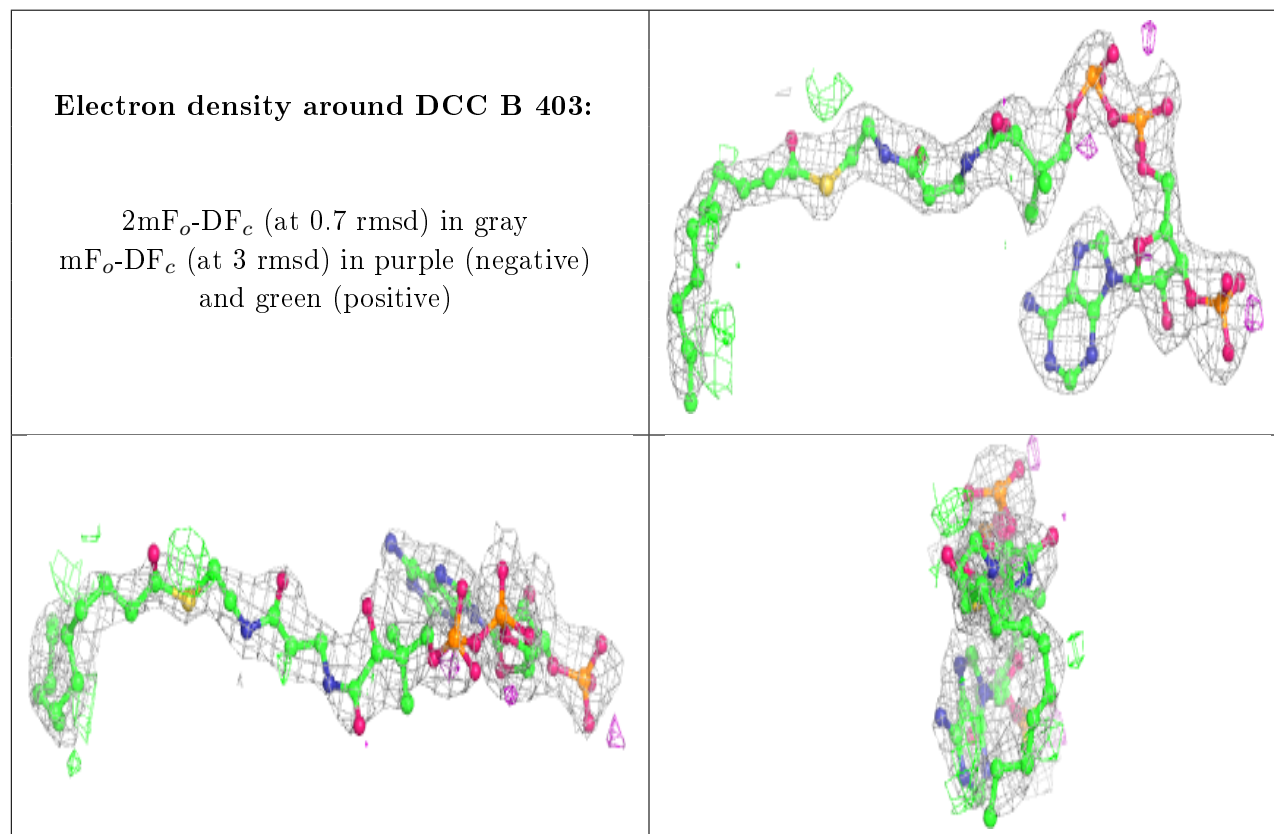
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	PO4	A	404	5/5	0.84	0.16	55,61,104,107	0
5	DCC	B	403	61/61	0.84	0.18	31,48,83,232	61
2	PEG	B	402	7/7	0.85	0.18	51,61,64,64	0
2	PEG	A	402	7/7	0.85	0.19	52,54,60,62	0
2	PEG	A	401	7/7	0.85	0.13	48,55,59,61	0
2	PEG	A	403	7/7	0.86	0.18	63,68,73,74	0
4	DAO	B	401	14/14	0.90	0.19	26,42,49,50	0
2	PEG	B	404	7/7	0.92	0.18	52,53,54,59	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.