Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 04:41 PM EDT

PDB ID	:	6KXF
Title	:	The ishigamide ketosynthase/chain length factor
Authors	:	Du, D.; Katsuyama, Y.; Horiuchi, M.; Fushinobu, S.; Chen, A.; Davis, T.; Burkart, M.; Ohnishi, Y.
Deposited on	:	2019-09-10
Resolution	:	1.98 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

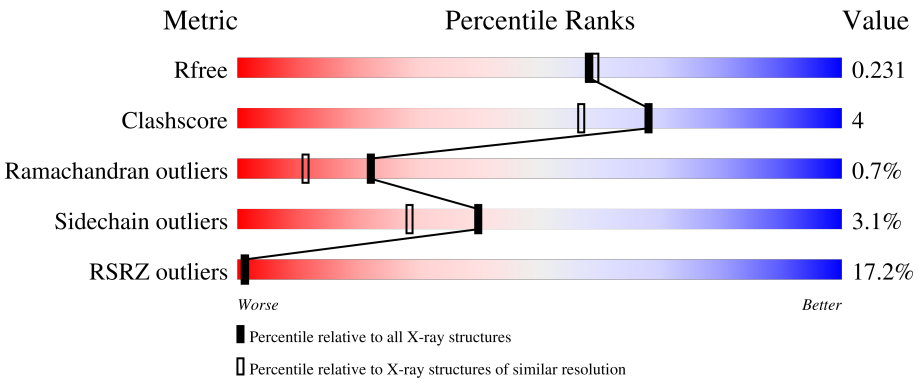
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	409	8%, 93%, 5% •
2	B	378	16%, 89%, 5% • 5%
3	C	83	60%, 51%, 27%, 8% • 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6432 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 Ketosynthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	2953	1821	537	582	13	0	0	0

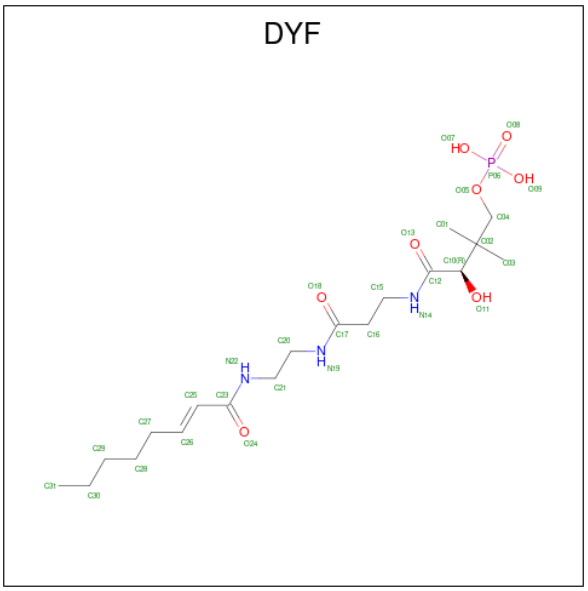
- Molecule 2 is a protein called Ketosynthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	360	2572	1602	465	496	9	0	0	0

- Molecule 3 is a protein called ACP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	73	553	347	88	115	3	0	0	0

- Molecule 4 is [(3 {R})-2,2-dimethyl-4-[[3-[2-[[({E})-oct-2-enoyl]amino]ethylamino]-3-oxidanylidene-propyl]amino]-3-oxidanyl-4-oxidanylidene-butyl] dihydrogen phosphate (three-letter code: DYF) (formula: $C_{19}H_{36}N_3O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	C	1	31	19	3	8	1	0	0

- Molecule 5 is water.

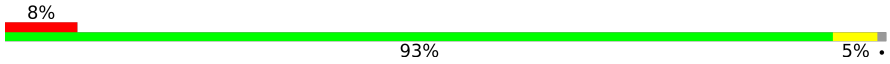
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	216	216	216	0	0
			Total	O		
5	B	101	101	101	0	0
			Total	O		
5	C	6	6	6	0	0

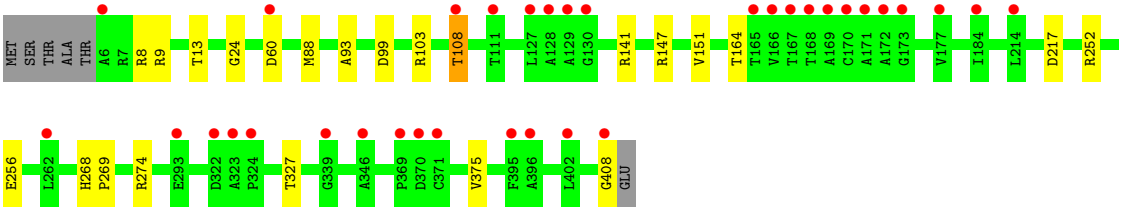
3 Residue-property plots (i)

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: Ketosynthase

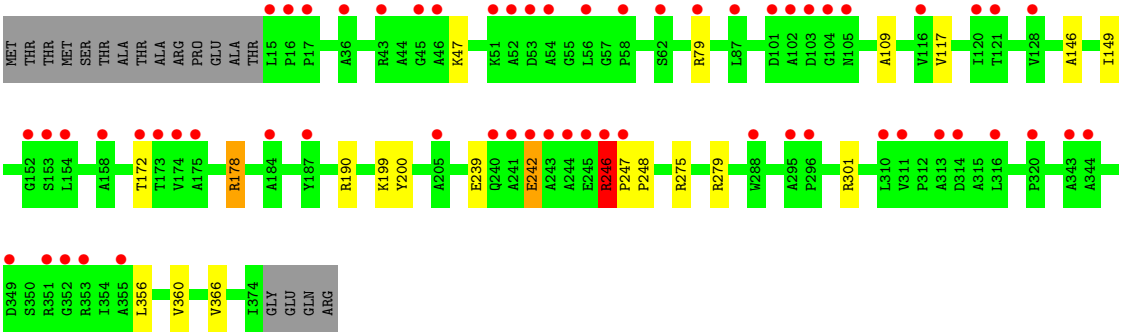
Chain A:





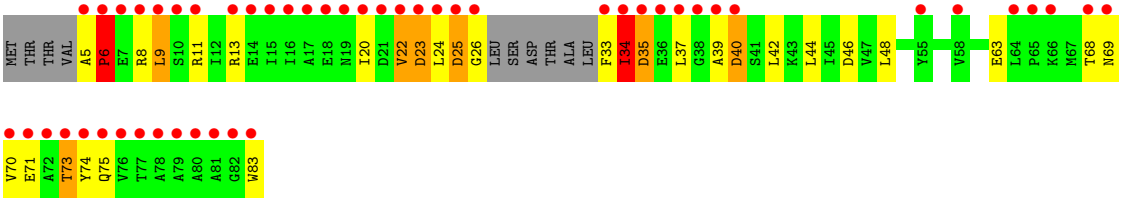
- Molecule 2: Ketosynthase

Chain B:



- Molecule 3: ACP

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.87Å 104.41Å 114.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 1.98 47.52 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.56-1.98) 99.7 (47.52-1.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0230, PHENIX	Depositor
R, R_{free}	0.179 , 0.229 0.189 , 0.231	Depositor DCC
R_{free} test set	3452 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6432	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: DYF

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	0.68	0/2999	0.79	1/4075 (0.0%)
2	B	0.58	0/2616	0.73	0/3570
3	C	0.55	0/557	0.76	1/757 (0.1%)
All	All	0.63	0/6172	0.76	2/8402 (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	2
2	B	0	5
3	C	0	3
All	All	0	10

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	6	PRO	N-CA-CB	-5.50	96.55	102.60
1	A	252	ARG	NE-CZ-NH2	-5.16	117.72	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
1	A	8	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	178	ARG	Sidechain
2	B	190	ARG	Sidechain
2	B	246	ARG	Sidechain
2	B	301	ARG	Sidechain
2	B	79	ARG	Sidechain
3	C	11	ARG	Sidechain
3	C	13	ARG	Sidechain
3	C	34	ILE	Peptide

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	2953	0	2898	12	0
2	B	2572	0	2566	9	0
3	C	553	0	538	25	0
4	C	31	0	0	0	0
5	A	216	0	0	3	0
5	B	101	0	0	0	0
5	C	6	0	0	1	0
All	All	6432	0	6002	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)
3:C:34:ILE:HG12	3:C:68:THR:HA	1.53	0.88
3:C:34:ILE:HB	3:C:35:ASP:HB2	1.70	0.72
3:C:34:ILE:CB	3:C:35:ASP:HB2	2.23	0.69
2:B:360:VAL:HG12	2:B:366:VAL:HG22	1.77	0.66
1:A:408:GLY:HA3	5:A:697:HOH:O	1.98	0.63
3:C:34:ILE:HD12	3:C:35:ASP:HB2	1.80	0.63
3:C:26:GLY:C	3:C:69:ASN:OD1	2.37	0.62
3:C:34:ILE:CG1	3:C:68:THR:HA	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:GLY:CA	5:A:697:HOH:O	2.48	0.61
2:B:146:ALA:HA	2:B:149:ILE:HD12	1.80	0.61
2:B:242:GLU:CD	2:B:242:GLU:H	2.01	0.61
3:C:6:PRO:HG2	5:C:206:HOH:O	2.04	0.57
1:A:9:ARG:HD2	1:A:256:GLU:OE2	2.06	0.56
3:C:22:VAL:HG12	3:C:23:ASP:H	1.71	0.55
3:C:69:ASN:C	3:C:71:GLU:H	2.08	0.55
3:C:34:ILE:HD12	3:C:35:ASP:CB	2.36	0.55
3:C:69:ASN:O	3:C:73:THR:HG23	2.08	0.53
3:C:34:ILE:CD1	3:C:35:ASP:HB2	2.39	0.52
1:A:268:HIS:ND1	1:A:269:PRO:HD2	2.25	0.52
1:A:108:THR:HA	1:A:164:THR:O	2.10	0.52
3:C:48:LEU:HD23	3:C:48:LEU:C	2.30	0.52
1:A:147:ARG:O	1:A:151:VAL:HG22	2.11	0.51
3:C:35:ASP:HA	3:C:39:ALA:CB	2.41	0.51
3:C:33:PHE:CB	3:C:69:ASN:ND2	2.73	0.51
2:B:239:GLU:OE1	2:B:246:ARG:NH2	2.44	0.50
1:A:13:THR:O	1:A:93:ALA:HA	2.12	0.50
3:C:35:ASP:N	3:C:39:ALA:HB2	2.26	0.49
3:C:40:ASP:OD2	3:C:42:LEU:HB2	2.12	0.48
3:C:34:ILE:CA	3:C:35:ASP:HB2	2.43	0.48
2:B:275:ARG:NH2	2:B:279:ARG:HD3	2.29	0.47
3:C:33:PHE:CB	3:C:69:ASN:HD21	2.28	0.46
3:C:8:ARG:HG2	3:C:83:TRP:CH2	2.51	0.46
1:A:24:GLY:HA2	1:A:88:MET:CE	2.47	0.45
3:C:9:LEU:HD22	3:C:74:TYR:CD1	2.52	0.44
3:C:34:ILE:HG22	3:C:44:LEU:HD11	2.00	0.44
1:A:327:THR:O	1:A:375:VAL:HA	2.18	0.43
1:A:99:ASP:O	1:A:103:ARG:HD2	2.19	0.43
3:C:70:VAL:HG12	3:C:70:VAL:O	2.20	0.42
2:B:109:ALA:O	2:B:199:LYS:HE3	2.20	0.42
1:A:268:HIS:CE1	1:A:269:PRO:HD2	2.55	0.42
2:B:247:PRO:HA	2:B:248:PRO:HD2	1.81	0.41
3:C:5:ALA:HB3	3:C:6:PRO:HD3	2.03	0.41
2:B:117:VAL:HA	2:B:172:THR:O	2.21	0.41
2:B:356:LEU:C	2:B:356:LEU:HD23	2.41	0.41
3:C:69:ASN:C	3:C:71:GLU:N	2.74	0.40
1:A:408:GLY:HA2	5:A:697:HOH:O	2.18	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	401/409 (98%)	385 (96%)	16 (4%)	0	100	100
2	B	358/378 (95%)	343 (96%)	15 (4%)	0	100	100
3	C	69/83 (83%)	51 (74%)	12 (17%)	6 (9%)	1	0
All	All	828/870 (95%)	779 (94%)	43 (5%)	6 (1%)	22	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	6	PRO
3	C	35	ASP
3	C	37	LEU
3	C	40	ASP
3	C	22	VAL
3	C	25	ASP

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	299/304 (98%)	295 (99%)	4 (1%)	69	64
2	B	250/264 (95%)	245 (98%)	5 (2%)	55	48
3	C	58/70 (83%)	48 (83%)	10 (17%)	2	0
All	All	607/638 (95%)	588 (97%)	19 (3%)	40	28

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	108	THR
1	A	217	ASP
1	A	274	ARG
2	B	47	LYS
2	B	178	ARG
2	B	200	TYR
2	B	242	GLU
2	B	246	ARG
3	C	9	LEU
3	C	20	ILE
3	C	23	ASP
3	C	24	LEU
3	C	25	ASP
3	C	34	ILE
3	C	46	ASP
3	C	63	GLU
3	C	73	THR
3	C	75	GLN

Sometimes 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)

1 ligand is 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	$\#\|Z\| > 2$
4	DYF	C	101	3,1	27,30,30	1.90	4 (14%)	36,39,39	4.40	11 (30%)

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	DYF	C	101	3,1	-	14/37/37/37	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	101	DYF	C12-N14	4.87	1.44	1.33
4	C	101	DYF	C21-N22	-4.65	1.35	1.46
4	C	101	DYF	C17-N19	4.46	1.43	1.33
4	C	101	DYF	C25-C23	3.34	1.55	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	101	DYF	O24-C23-N22	-15.99	95.78	122.23
4	C	101	DYF	C21-N22-C23	13.52	142.37	122.54
4	C	101	DYF	C25-C23-N22	12.22	138.00	114.97
4	C	101	DYF	C20-C21-N22	-5.43	93.40	111.44
4	C	101	DYF	C16-C17-N19	-4.54	108.78	116.42
4	C	101	DYF	O09-P06-O05	2.80	114.19	106.73
4	C	101	DYF	O11-C10-C02	-2.58	104.17	110.25
4	C	101	DYF	C20-N19-C17	2.53	127.53	122.84
4	C	101	DYF	C03-C02-C10	2.35	112.89	108.82
4	C	101	DYF	O18-C17-N19	2.24	127.23	123.01
4	C	101	DYF	O09-P06-O08	2.10	118.89	110.68

There are no chirality outliers.

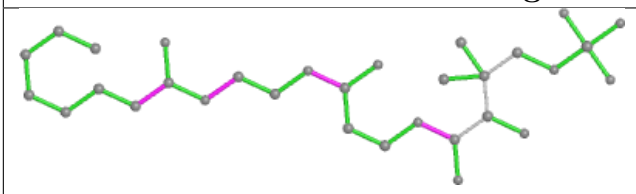
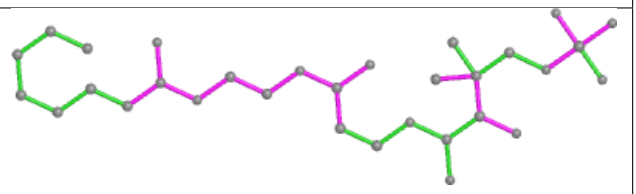
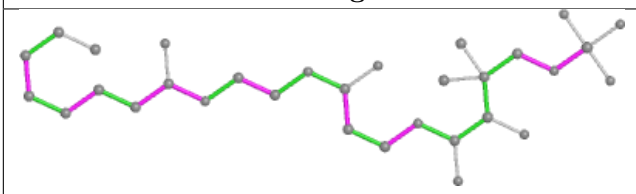
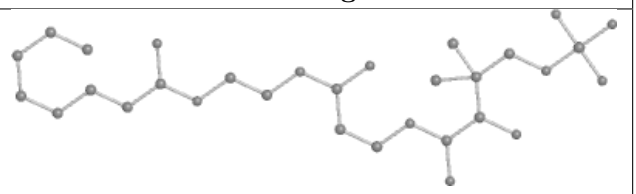
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	101	DYF	C25-C23-N22-C21
4	C	101	DYF	O24-C23-N22-C21
4	C	101	DYF	C04-O05-P06-O07
4	C	101	DYF	C04-O05-P06-O09
4	C	101	DYF	N22-C23-C25-C26
4	C	101	DYF	N19-C20-C21-N22
4	C	101	DYF	O24-C23-C25-C26
4	C	101	DYF	C16-C15-N14-C12
4	C	101	DYF	C27-C28-C29-C30
4	C	101	DYF	C04-O05-P06-O08
4	C	101	DYF	C15-C16-C17-O18
4	C	101	DYF	C15-C16-C17-N19
4	C	101	DYF	C25-C26-C27-C28
4	C	101	DYF	C02-C04-O05-P06

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DYF C 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	403/409 (98%)	0.70	34 (8%)	11	12	32, 41, 60, 79	0
2	B	360/378 (95%)	1.06	60 (16%)	1	1	37, 53, 83, 107	0
3	C	73/83 (87%)	3.45	50 (68%)	0	0	56, 89, 114, 120	0
All	All	836/870 (96%)	1.09	144 (17%)	1	1	32, 48, 89, 120	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	37	LEU	11.0
3	C	22	VAL	10.4
3	C	21	ASP	9.7
3	C	15	ILE	9.4
3	C	34	ILE	9.3
3	C	5	ALA	8.7
3	C	78	ALA	8.0
3	C	83	TRP	6.6
3	C	10	SER	6.3
3	C	24	LEU	6.2
3	C	23	ASP	5.9
3	C	6	PRO	5.6
2	B	102	ALA	5.5
3	C	75	GLN	5.5
3	C	74	TYR	5.4
3	C	70	VAL	5.3
3	C	80	ALA	5.2
3	C	73	THR	5.2
3	C	33	PHE	5.0
2	B	247	PRO	4.8
1	A	129	ALA	4.8
2	B	243	ALA	4.8
1	A	323	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	103	ASP	4.7
2	B	104	GLY	4.6
2	B	105	ASN	4.4
2	B	15	LEU	4.4
2	B	154	LEU	4.4
3	C	38	GLY	4.4
3	C	20	ILE	4.4
2	B	52	ALA	4.4
3	C	13	ARG	4.4
2	B	79	ARG	4.2
1	A	60	ASP	4.1
3	C	18	GLU	4.1
2	B	314	ASP	4.1
3	C	19	ASN	4.0
3	C	68	THR	4.0
1	A	128	ALA	4.0
2	B	43	ARG	3.9
3	C	11	ARG	3.8
3	C	39	ALA	3.7
3	C	69	ASN	3.7
3	C	25	ASP	3.7
3	C	9	LEU	3.7
3	C	79	ALA	3.6
1	A	322	ASP	3.6
2	B	51	LYS	3.6
1	A	166	VAL	3.6
3	C	71	GLU	3.4
1	A	171	ALA	3.4
3	C	17	ALA	3.4
2	B	120	ILE	3.4
3	C	58	VAL	3.3
3	C	14	GLU	3.3
1	A	167	THR	3.3
3	C	72	ALA	3.3
2	B	311	VAL	3.2
2	B	296	PRO	3.2
2	B	101	ASP	3.1
1	A	6	ALA	3.1
2	B	175	ALA	3.1
3	C	82	GLY	3.1
2	B	174	VAL	3.1
1	A	127	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	53	ASP	3.0
2	B	62	SER	3.0
2	B	288	TRP	3.0
1	A	371	CYS	3.0
2	B	36	ALA	3.0
1	A	169	ALA	3.0
2	B	316	LEU	3.0
3	C	76	VAL	3.0
1	A	170	CYS	3.0
2	B	172	THR	2.9
3	C	77	THR	2.9
1	A	396	ALA	2.9
1	A	346	ALA	2.9
3	C	16	ILE	2.8
2	B	351	ARG	2.8
3	C	81	ALA	2.8
3	C	35	ASP	2.8
2	B	87	LEU	2.8
2	B	313	ALA	2.7
1	A	111	THR	2.7
3	C	7	GLU	2.6
3	C	8	ARG	2.6
2	B	242	GLU	2.6
2	B	355	ALA	2.6
1	A	172	ALA	2.6
2	B	241	ALA	2.6
2	B	244	ALA	2.6
1	A	130	GLY	2.6
2	B	320	PRO	2.5
1	A	324	PRO	2.5
2	B	17	PRO	2.5
2	B	310	LEU	2.5
2	B	153	SER	2.5
2	B	344	ALA	2.5
3	C	65	PRO	2.5
2	B	46	ALA	2.5
1	A	339	GLY	2.4
2	B	245	GLU	2.4
1	A	370	ASP	2.4
1	A	408	GLY	2.4
2	B	349	ASP	2.4
2	B	246	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	108	THR	2.4
1	A	395	PHE	2.4
1	A	165	THR	2.4
2	B	58	PRO	2.4
2	B	54	ALA	2.3
2	B	343	ALA	2.3
3	C	36	GLU	2.3
1	A	402	LEU	2.3
2	B	128	VAL	2.3
1	A	293	GLU	2.2
1	A	173	GLY	2.2
3	C	55	TYR	2.2
1	A	168	THR	2.2
2	B	240	GLN	2.2
1	A	177	VAL	2.2
2	B	16	PRO	2.2
2	B	187	TYR	2.2
1	A	184	ILE	2.2
1	A	262	LEU	2.2
3	C	64	LEU	2.1
3	C	40	ASP	2.1
3	C	66	LYS	2.1
2	B	205	ALA	2.1
2	B	353	ARG	2.1
2	B	352	GLY	2.1
2	B	184	ALA	2.1
2	B	116	VAL	2.1
1	A	214	LEU	2.1
1	A	369	PRO	2.1
2	B	45	GLY	2.1
3	C	26	GLY	2.1
2	B	295	ALA	2.1
2	B	152	GLY	2.1
2	B	121	THR	2.0
2	B	158	ALA	2.0
2	B	56	LEU	2.0
2	B	173	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

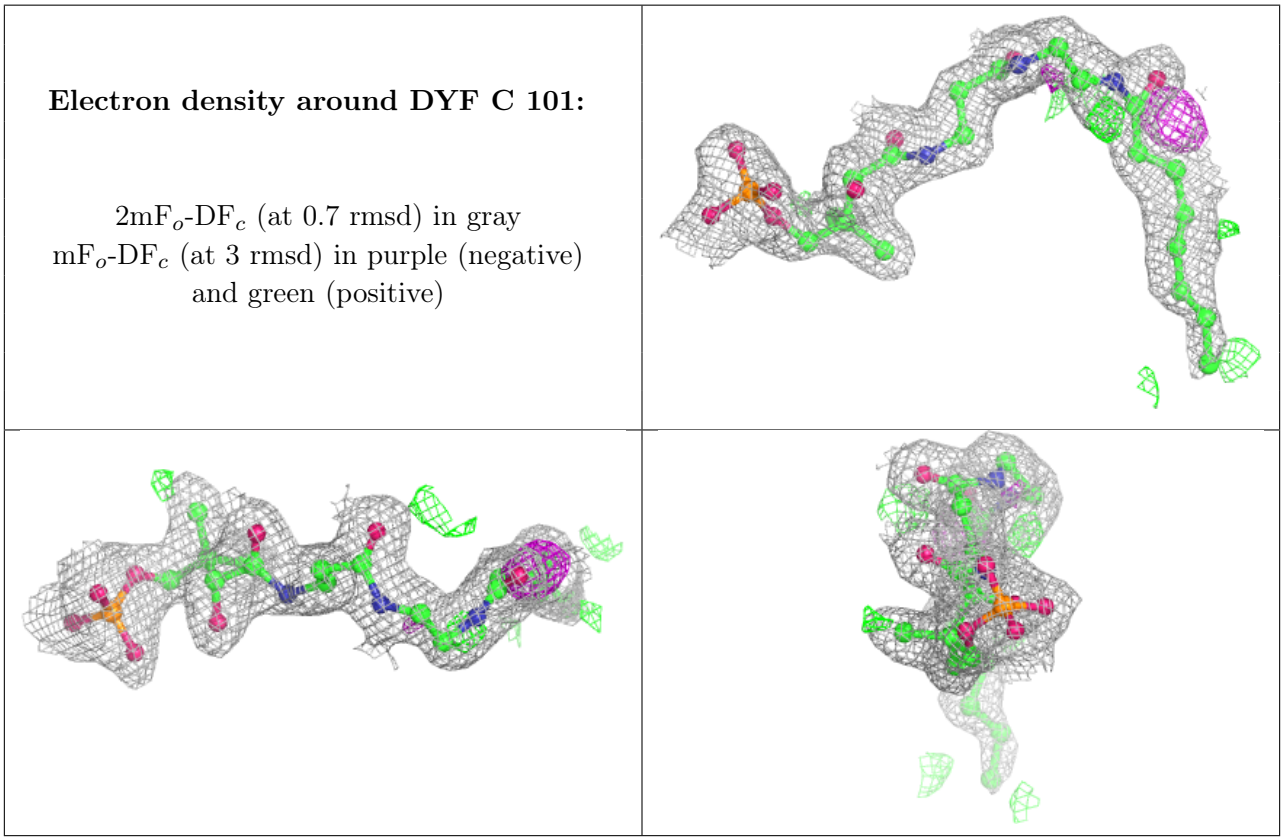
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DYF	C	101	31/31	0.86	0.19	41,52,71,82	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 DYF C 101:

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.