



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2022 – 06:16 PM JST

PDB ID : 7EI4
Title : Crystal structure of MasL in complex with a novel covalent inhibitor, colimonin C
Authors : Lin, C.C.; Huang, K.F.; Yang, Y.L.
Deposited on : 2021-03-30
Resolution : 1.66 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 : 2.27
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) : 2.27

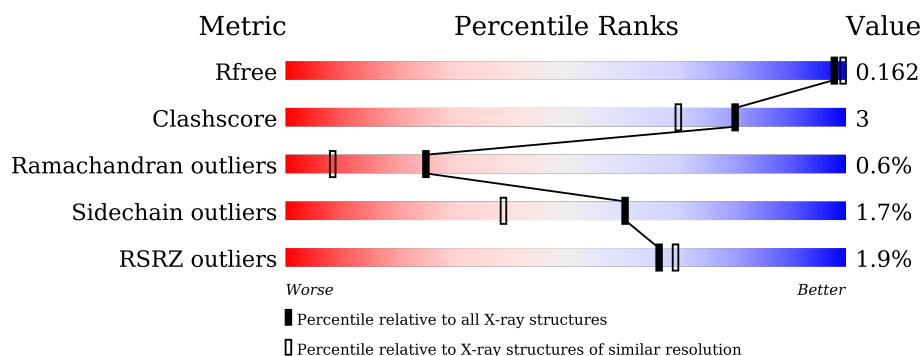
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 $\leq 5\%$. 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	407	<div> <div>2%</div> <div>90%</div> <div>5%</div> <div>.</div> <div>.</div> </div>
1	B	407	<div> <div>%</div> <div>92%</div> <div>.</div> <div>.</div> </div>
1	C	407	<div> <div>2%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	D	407	<div> <div>2%</div> <div>92%</div> <div>.</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13216 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 Acetyl-CoA C-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			2869	1793	528	540	8			
1	B	389	Total	C	N	O	S	0	0	0
			2845	1777	524	536	8			
1	C	391	Total	C	N	O	S	0	0	0
			2861	1788	526	539	8			
1	D	390	Total	C	N	O	S	0	0	0
			2853	1783	525	537	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5C7BKK5
A	2	VAL	-	expression tag	UNP A0A5C7BKK5
A	183	THR	VAL	engineered mutation	UNP A0A5C7BKK5
A	395	LYS	-	expression tag	UNP A0A5C7BKK5
A	396	LEU	-	expression tag	UNP A0A5C7BKK5
A	397	ALA	-	expression tag	UNP A0A5C7BKK5
A	398	ALA	-	expression tag	UNP A0A5C7BKK5
A	399	ALA	-	expression tag	UNP A0A5C7BKK5
A	400	LEU	-	expression tag	UNP A0A5C7BKK5
A	401	GLU	-	expression tag	UNP A0A5C7BKK5
A	402	HIS	-	expression tag	UNP A0A5C7BKK5
A	403	HIS	-	expression tag	UNP A0A5C7BKK5
A	404	HIS	-	expression tag	UNP A0A5C7BKK5
A	405	HIS	-	expression tag	UNP A0A5C7BKK5
A	406	HIS	-	expression tag	UNP A0A5C7BKK5
A	407	HIS	-	expression tag	UNP A0A5C7BKK5
B	1	MET	-	initiating methionine	UNP A0A5C7BKK5
B	2	VAL	-	expression tag	UNP A0A5C7BKK5
B	183	THR	VAL	engineered mutation	UNP A0A5C7BKK5
B	395	LYS	-	expression tag	UNP A0A5C7BKK5
B	396	LEU	-	expression tag	UNP A0A5C7BKK5

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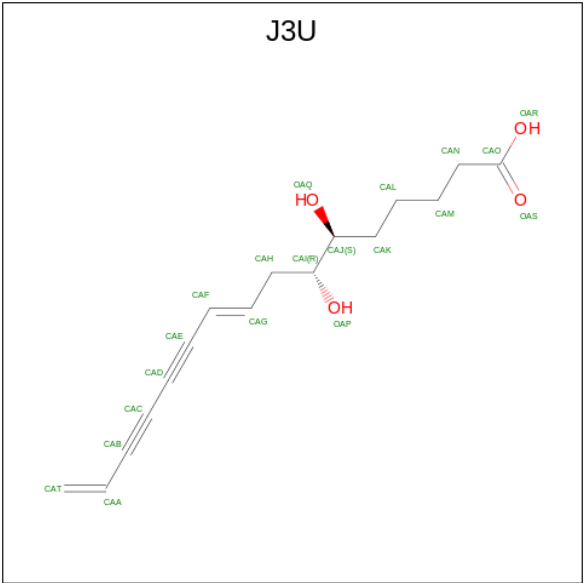
Chain	Residue	Modelled	Actual	Comment	Reference
B	397	ALA	-	expression tag	UNP A0A5C7BKK5
B	398	ALA	-	expression tag	UNP A0A5C7BKK5
B	399	ALA	-	expression tag	UNP A0A5C7BKK5
B	400	LEU	-	expression tag	UNP A0A5C7BKK5
B	401	GLU	-	expression tag	UNP A0A5C7BKK5
B	402	HIS	-	expression tag	UNP A0A5C7BKK5
B	403	HIS	-	expression tag	UNP A0A5C7BKK5
B	404	HIS	-	expression tag	UNP A0A5C7BKK5
B	405	HIS	-	expression tag	UNP A0A5C7BKK5
B	406	HIS	-	expression tag	UNP A0A5C7BKK5
B	407	HIS	-	expression tag	UNP A0A5C7BKK5
C	1	MET	-	initiating methionine	UNP A0A5C7BKK5
C	2	VAL	-	expression tag	UNP A0A5C7BKK5
C	183	THR	VAL	engineered mutation	UNP A0A5C7BKK5
C	395	LYS	-	expression tag	UNP A0A5C7BKK5
C	396	LEU	-	expression tag	UNP A0A5C7BKK5
C	397	ALA	-	expression tag	UNP A0A5C7BKK5
C	398	ALA	-	expression tag	UNP A0A5C7BKK5
C	399	ALA	-	expression tag	UNP A0A5C7BKK5
C	400	LEU	-	expression tag	UNP A0A5C7BKK5
C	401	GLU	-	expression tag	UNP A0A5C7BKK5
C	402	HIS	-	expression tag	UNP A0A5C7BKK5
C	403	HIS	-	expression tag	UNP A0A5C7BKK5
C	404	HIS	-	expression tag	UNP A0A5C7BKK5
C	405	HIS	-	expression tag	UNP A0A5C7BKK5
C	406	HIS	-	expression tag	UNP A0A5C7BKK5
C	407	HIS	-	expression tag	UNP A0A5C7BKK5
D	1	MET	-	initiating methionine	UNP A0A5C7BKK5
D	2	VAL	-	expression tag	UNP A0A5C7BKK5
D	183	THR	VAL	engineered mutation	UNP A0A5C7BKK5
D	395	LYS	-	expression tag	UNP A0A5C7BKK5
D	396	LEU	-	expression tag	UNP A0A5C7BKK5
D	397	ALA	-	expression tag	UNP A0A5C7BKK5
D	398	ALA	-	expression tag	UNP A0A5C7BKK5
D	399	ALA	-	expression tag	UNP A0A5C7BKK5
D	400	LEU	-	expression tag	UNP A0A5C7BKK5
D	401	GLU	-	expression tag	UNP A0A5C7BKK5
D	402	HIS	-	expression tag	UNP A0A5C7BKK5
D	403	HIS	-	expression tag	UNP A0A5C7BKK5
D	404	HIS	-	expression tag	UNP A0A5C7BKK5
D	405	HIS	-	expression tag	UNP A0A5C7BKK5
D	406	HIS	-	expression tag	UNP A0A5C7BKK5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	407	HIS	-	expression tag	UNP A0A5C7BKK5

- Molecule 2 is (6S,7R,9E)-6,7-bis(oxidanyl)hexadeca-9,15-dien-11,13-dynoic acid (three-letter code: J3U) (formula: C₁₆H₂₀O₄) (labeled as "Ligand of Interest" by depositor).



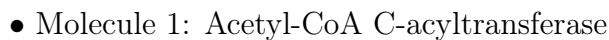
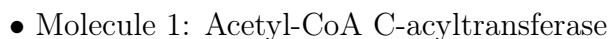
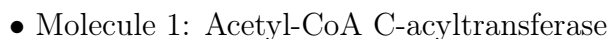
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 20 16 4	0	0
2	B	1	Total C O 20 16 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	D	1	Total C O 20 16 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	462	Total O 462 462	0	0
3	B	430	Total O 430 430	0	0
3	C	403	Total O 403 403	0	0
3	D	413	Total O 413 413	0	0

i

- Molecule 1: Acetyl-CoA C-acyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.14Å 115.08Å 125.79Å 90.00° 91.08° 90.00°	Depositor
Resolution (Å)	29.22 – 1.66 29.21 – 1.66	Depositor EDS
% Data completeness (in resolution range)	91.0 (29.22-1.66) 91.0 (29.21-1.66)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.114 , 0.162 0.116 , 0.162	Depositor DCC
R_{free} test set	9113 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13216	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1101e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: J3U

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	0.67	0/2915	0.75	0/3962
1	B	0.66	0/2891	0.75	0/3930
1	C	0.65	0/2907	0.75	0/3953
1	D	0.64	0/2899	0.73	0/3941
All	All	0.65	0/11612	0.75	0/15786

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 [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	2869	0	2887	25	0
1	B	2845	0	2856	14	0
1	C	2861	0	2876	17	0
1	D	2853	0	2867	11	0
2	A	20	0	0	1	0
2	B	20	0	0	1	0
2	C	20	0	0	0	0
2	D	20	0	0	1	0
3	A	462	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	430	0	0	7	0
3	C	403	0	0	7	0
3	D	413	0	0	7	0
All	All	13216	0	11486	61	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 3.

All (61) 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:D:179:ARG:HD3	1:D:227:GLU:OE2	1.76	0.84
1:B:136:MET:HE1	3:C:672:HOH:O	1.79	0.82
1:B:186:GLN:HG3	3:B:607:HOH:O	1.80	0.78
3:B:742:HOH:O	1:C:136:MET:HE1	1.90	0.71
1:B:368:ARG:NH1	3:B:601:HOH:O	2.23	0.71
1:A:136:MET:CE	3:D:671:HOH:O	2.39	0.71
1:A:175:GLU:O	1:A:179:ARG:HD3	1.93	0.68
1:A:49:ARG:HD3	3:A:719:HOH:O	1.97	0.65
1:A:135:ARG:NH2	2:D:500:J3U:OAR	2.29	0.63
1:A:105:ARG:HD2	3:B:722:HOH:O	1.98	0.62
1:B:136:MET:CG	3:C:846:HOH:O	2.48	0.62
1:B:145:LEU:HD11	1:C:136:MET:HE2	1.82	0.62
1:A:136:MET:HE1	3:D:671:HOH:O	1.99	0.61
1:B:136:MET:CB	3:C:846:HOH:O	2.49	0.61
2:B:500:J3U:OAR	1:C:135:ARG:NH2	2.32	0.61
1:C:41:GLU:HB2	3:C:862:HOH:O	2.01	0.61
3:A:655:HOH:O	1:D:136:MET:HE1	2.00	0.60
1:A:41:GLU:HG3	3:A:639:HOH:O	2.02	0.59
1:A:145:LEU:HD11	1:D:136:MET:HE2	1.83	0.59
1:C:179:ARG:HD3	1:C:227:GLU:OE1	2.03	0.58
1:B:136:MET:HE2	1:C:145:LEU:HD11	1.87	0.57
1:A:145:LEU:HD11	1:D:136:MET:CE	2.34	0.56
3:C:820:HOH:O	1:D:105:ARG:HD2	2.07	0.55
1:B:145:LEU:HD11	1:C:136:MET:CE	2.39	0.53
1:B:280:ILE:H	1:B:304:GLN:NE2	2.07	0.52
1:C:280:ILE:H	1:C:304:GLN:NE2	2.07	0.52
1:B:136:MET:HB3	3:C:846:HOH:O	2.10	0.52
1:B:204:VAL:HG13	3:B:910:HOH:O	2.11	0.50
1:A:221:ASN:H	1:A:221:ASN:HD22	1.59	0.50
1:A:382:GLY:H	2:A:500:J3U:CAT	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:MET:CE	1:C:145:LEU:HD11	2.44	0.47
1:A:34:HIS:CE1	3:A:601:HOH:O	2.67	0.47
1:D:136:MET:CB	3:D:908:HOH:O	2.63	0.47
1:B:52:GLU:HG3	1:B:53:VAL:N	2.31	0.46
1:A:217:LYS:HE3	1:A:217:LYS:HB3	1.70	0.46
1:C:52:GLU:HG3	1:C:53:VAL:N	2.31	0.45
1:A:136:MET:CG	3:D:901:HOH:O	2.64	0.45
3:B:936:HOH:O	1:C:136:MET:CG	2.65	0.45
1:D:381:ILE:HB	1:D:385:GLN:HB2	1.99	0.45
1:A:396:LEU:HD23	1:A:396:LEU:N	2.32	0.44
1:C:58:VAL:HG21	1:C:352:ILE:HG22	1.99	0.44
1:A:208:THR:HG23	1:A:211:GLY:O	2.18	0.44
1:A:368:ARG:NH1	3:A:610:HOH:O	2.50	0.44
1:D:52:GLU:HG3	1:D:53:VAL:N	2.33	0.44
1:A:58:VAL:HG21	1:A:352:ILE:HG22	1.99	0.43
1:A:34:HIS:CD2	1:A:204:VAL:HG12	2.52	0.43
1:A:136:MET:CB	3:D:901:HOH:O	2.65	0.43
1:C:276:VAL:CG1	1:C:392:GLU:HB3	2.49	0.43
1:A:52:GLU:HG3	1:A:53:VAL:N	2.33	0.43
1:C:4:ASP:N	3:C:609:HOH:O	2.52	0.43
3:B:936:HOH:O	1:C:136:MET:CB	2.65	0.42
1:D:4:ASP:HA	3:D:887:HOH:O	2.18	0.42
1:B:58:VAL:HG21	1:B:352:ILE:HG22	2.00	0.42
1:D:58:VAL:HG21	1:D:352:ILE:HG22	2.00	0.42
1:A:381:ILE:HB	1:A:385:GLN:HB2	2.02	0.42
1:A:204:VAL:HG22	1:A:215:PHE:HB3	2.02	0.41
1:C:381:ILE:HB	1:C:385:GLN:HB2	2.02	0.41
1:C:239:LYS:HE2	1:C:239:LYS:HB3	1.81	0.41
1:A:136:MET:HE3	3:D:671:HOH:O	2.10	0.41
1:A:208:THR:CG2	1:A:211:GLY:O	2.69	0.40
1:D:53:VAL:O	1:D:83:ALA:HA	2.21	0.40

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	388/407 (95%)	378 (97%)	8 (2%)	2 (0%)	29	11
1	B	385/407 (95%)	374 (97%)	9 (2%)	2 (0%)	29	11
1	C	387/407 (95%)	377 (97%)	7 (2%)	3 (1%)	19	5
1	D	386/407 (95%)	376 (97%)	8 (2%)	2 (0%)	29	11
All	All	1546/1628 (95%)	1505 (97%)	32 (2%)	9 (1%)	25	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	ILE
1	B	352	ILE
1	C	352	ILE
1	D	352	ILE
1	A	89	VAL
1	B	89	VAL
1	C	89	VAL
1	D	89	VAL
1	C	66	ASN

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	286/298 (96%)	280 (98%)	6 (2%)	53	29
1	B	283/298 (95%)	280 (99%)	3 (1%)	73	57
1	C	285/298 (96%)	278 (98%)	7 (2%)	47	22
1	D	284/298 (95%)	281 (99%)	3 (1%)	73	57
All	All	1138/1192 (96%)	1119 (98%)	19 (2%)	60	39

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

Mol	Chain	Res	Type
1	A	59	LEU
1	A	136	MET
1	A	208	THR
1	A	221	ASN
1	A	239	LYS
1	A	396	LEU
1	B	37	LYS
1	B	127	MET
1	B	239	LYS
1	C	37	LYS
1	C	59	LEU
1	C	105	ARG
1	C	127	MET
1	C	234	ARG
1	C	239	LYS
1	C	272	GLN
1	D	179	ARG
1	D	239	LYS
1	D	395	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	B	304	GLN
1	C	304	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

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	J3U	C	500	-	16,19,19	3.78	7 (43%)	14,21,21	1.47	2 (14%)
2	J3U	D	500	-	16,19,19	3.52	5 (31%)	14,21,21	2.12	6 (42%)
2	J3U	B	500	-	16,19,19	4.92	7 (43%)	14,21,21	1.84	2 (14%)
2	J3U	A	500	-	16,19,19	9.60	6 (37%)	14,21,21	1.90	5 (35%)

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	J3U	C	500	-	-	5/17/20/20	-
2	J3U	D	500	-	-	7/17/20/20	-
2	J3U	B	500	-	-	4/17/20/20	-
2	J3U	A	500	-	-	9/17/20/20	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	J3U	CAB-CAC	25.25	1.42	1.21
2	A	500	J3U	CAE-CAD	23.90	1.41	1.21
2	A	500	J3U	CAF-CAE	-12.34	1.22	1.42
2	B	500	J3U	CAF-CAE	-11.68	1.23	1.42
2	D	500	J3U	CAF-CAE	-11.27	1.24	1.42
2	B	500	J3U	CAA-CAB	-9.98	1.29	1.42
2	A	500	J3U	CAA-CAB	9.79	1.55	1.42
2	C	500	J3U	CAE-CAD	-9.22	1.13	1.21
2	B	500	J3U	CAB-CAC	-8.76	1.13	1.21
2	C	500	J3U	CAF-CAE	-7.45	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	J3U	CAA-CAB	-7.37	1.32	1.42
2	B	500	J3U	CAE-CAD	-6.01	1.15	1.21
2	D	500	J3U	CAB-CAC	5.57	1.25	1.21
2	B	500	J3U	CAC-CAD	-4.06	1.29	1.37
2	D	500	J3U	CAE-CAD	3.97	1.24	1.21
2	C	500	J3U	CAC-CAD	-2.90	1.31	1.37
2	D	500	J3U	CAF-CAG	2.65	1.53	1.29
2	A	500	J3U	CAT-CAA	2.63	1.59	1.26
2	C	500	J3U	CAF-CAG	2.61	1.53	1.29
2	B	500	J3U	CAF-CAG	2.56	1.52	1.29
2	A	500	J3U	CAF-CAG	2.38	1.51	1.29
2	D	500	J3U	CAT-CAA	2.38	1.56	1.26
2	C	500	J3U	CAB-CAC	2.37	1.23	1.21
2	C	500	J3U	CAT-CAA	2.34	1.55	1.26
2	B	500	J3U	CAT-CAA	2.28	1.54	1.26

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	J3U	CAL-CAK-CAJ	-4.54	106.72	114.18
2	A	500	J3U	CAL-CAK-CAJ	-4.44	106.89	114.18
2	D	500	J3U	CAL-CAK-CAJ	-4.40	106.95	114.18
2	D	500	J3U	CAM-CAL-CAK	-3.51	101.22	113.62
2	B	500	J3U	CAL-CAM-CAN	-3.22	101.22	113.76
2	C	500	J3U	CAM-CAL-CAK	-3.09	102.70	113.62
2	C	500	J3U	OAP-CAI-CAJ	-2.64	104.31	109.72
2	A	500	J3U	CAM-CAL-CAK	-2.57	104.52	113.62
2	D	500	J3U	CAK-CAJ-CAI	-2.57	107.25	113.35
2	A	500	J3U	CAF-CAE-CAD	-2.49	173.02	177.30
2	D	500	J3U	CAF-CAE-CAD	-2.38	173.21	177.30
2	D	500	J3U	CAL-CAM-CAN	-2.17	105.30	113.76
2	D	500	J3U	OAP-CAI-CAJ	-2.14	105.32	109.72
2	A	500	J3U	CAL-CAM-CAN	-2.14	105.43	113.76
2	A	500	J3U	CAE-CAD-CAC	-2.09	174.70	177.49

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	J3U	OAP-CAI-CAJ-CAK
2	A	500	J3U	CAH-CAI-CAJ-CAK
2	A	500	J3U	OAP-CAI-CAJ-OAQ

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Mol	Chain	Res	Type	Atoms
2	A	500	J3U	CAH-CAI-CAJ-OAQ
2	A	500	J3U	CAG-CAH-CAI-OAP
2	A	500	J3U	CAD-CAE-CAF-CAG
2	B	500	J3U	CAA-CAB-CAC-CAD
2	C	500	J3U	CAL-CAM-CAN-CAO
2	C	500	J3U	CAA-CAB-CAC-CAD
2	D	500	J3U	OAP-CAI-CAJ-CAK
2	D	500	J3U	CAH-CAI-CAJ-CAK
2	D	500	J3U	OAP-CAI-CAJ-OAQ
2	D	500	J3U	CAH-CAI-CAJ-OAQ
2	D	500	J3U	CAA-CAB-CAC-CAD
2	C	500	J3U	OAP-CAI-CAJ-OAQ
2	D	500	J3U	CAK-CAL-CAM-CAN
2	B	500	J3U	CAD-CAE-CAF-CAG
2	C	500	J3U	CAD-CAE-CAF-CAG
2	D	500	J3U	CAD-CAE-CAF-CAG
2	B	500	J3U	CAJ-CAK-CAL-CAM
2	A	500	J3U	CAL-CAM-CAN-CAO
2	A	500	J3U	CAG-CAH-CAI-CAJ
2	C	500	J3U	CAJ-CAK-CAL-CAM
2	A	500	J3U	CAA-CAB-CAC-CAD
2	B	500	J3U	OAQ-CAJ-CAK-CAL

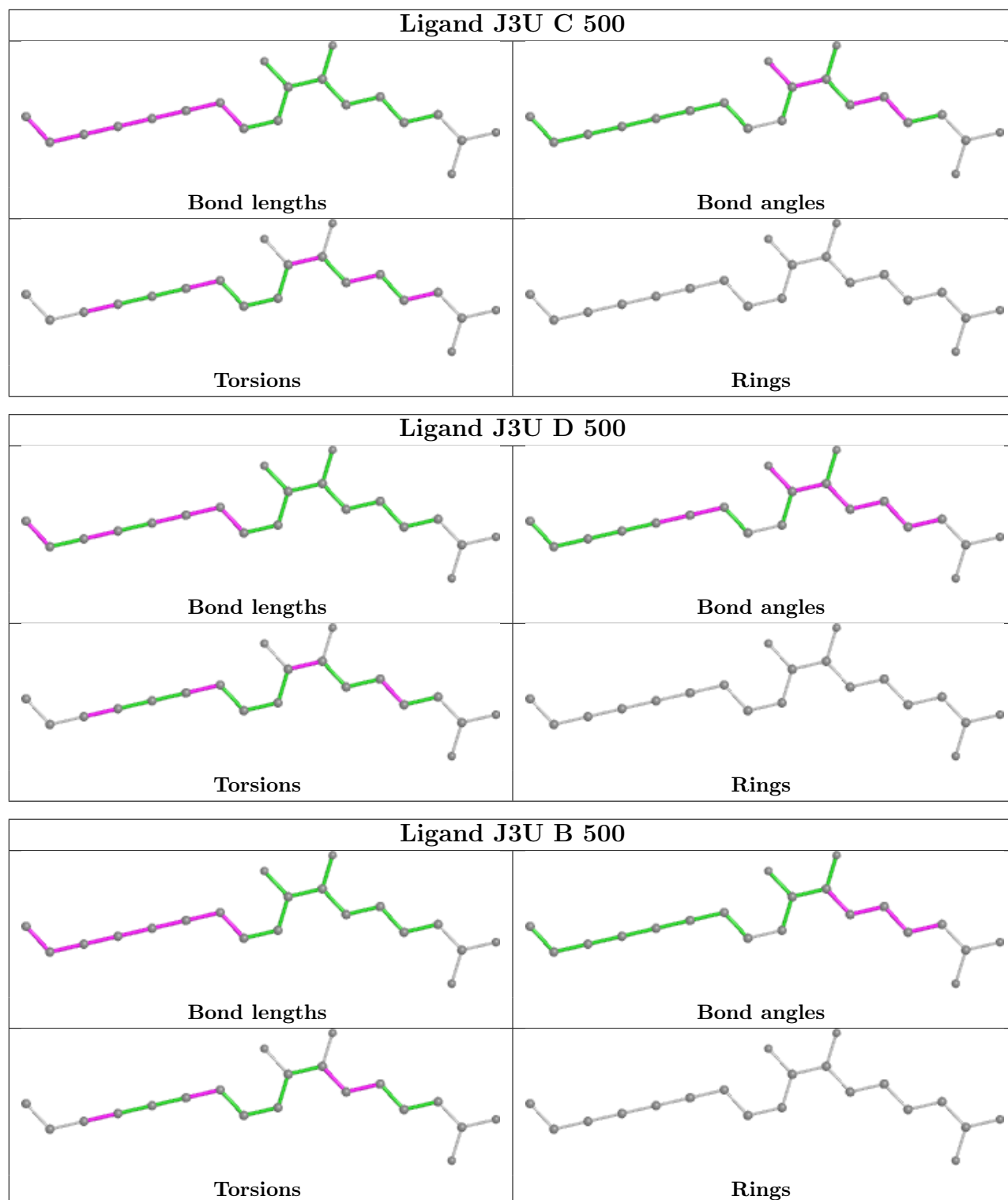
There are no ring outliers.

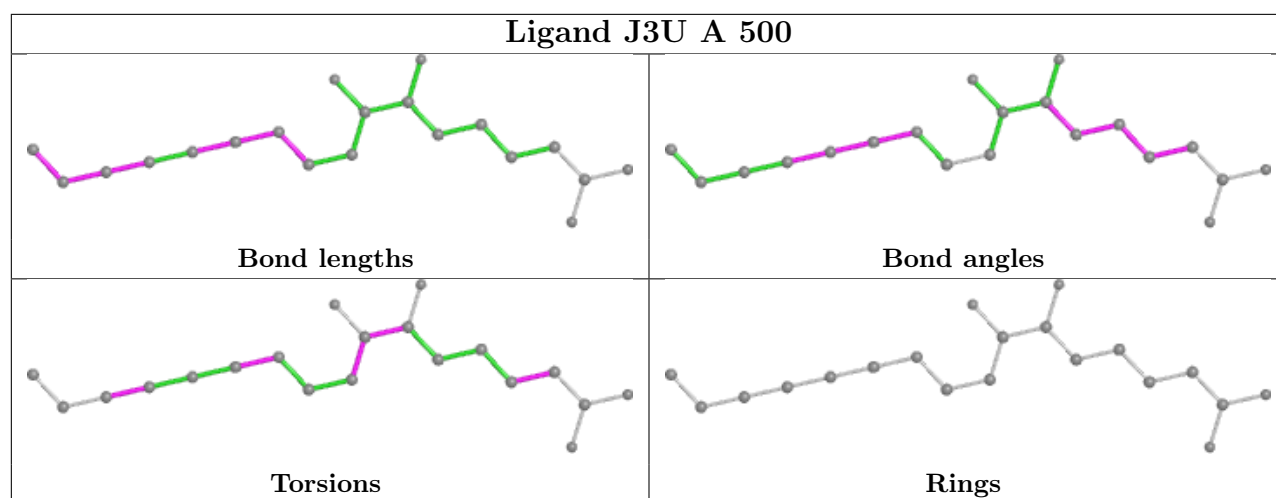
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	J3U	1	0
2	B	500	J3U	1	0
2	A	500	J3U	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 ⓘ

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	392/407 (96%)	-0.47	9 (2%) 60 61	5, 12, 30, 77	0
1	B	389/407 (95%)	-0.45	6 (1%) 73 77	7, 15, 31, 63	0
1	C	391/407 (96%)	-0.41	7 (1%) 68 71	8, 16, 36, 66	0
1	D	390/407 (95%)	-0.40	8 (2%) 63 65	8, 16, 33, 63	0
All	All	1562/1628 (95%)	-0.43	30 (1%) 66 69	5, 15, 32, 77	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	208	THR	4.6
1	A	208	THR	4.4
1	D	239	LYS	4.1
1	D	211	GLY	4.0
1	D	310	GLN	3.8
1	A	239	LYS	3.8
1	B	239	LYS	3.7
1	C	239	LYS	3.7
1	C	397	ALA	3.6
1	C	207	THR	3.4
1	A	207	THR	3.1
1	C	4	ASP	3.1
1	B	211	GLY	3.1
1	D	234	ARG	3.0
1	A	234	ARG	2.9
1	B	234	ARG	2.9
1	A	4	ASP	2.7
1	A	211	GLY	2.6
1	D	4	ASP	2.5
1	A	3	LYS	2.5
1	D	240	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	213	THR	2.4
1	B	4	ASP	2.3
1	D	207	THR	2.3
1	B	310	GLN	2.3
1	C	234	ARG	2.3
1	A	396	LEU	2.2
1	C	240	ASP	2.2
1	B	240	ASP	2.0
1	A	213	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](#)

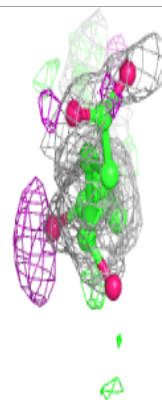
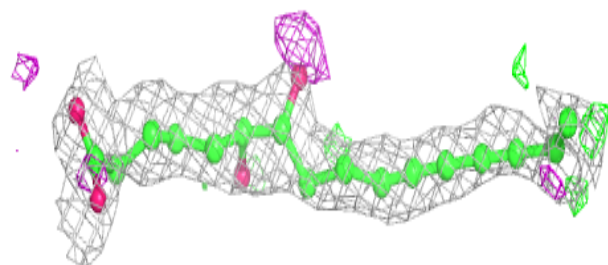
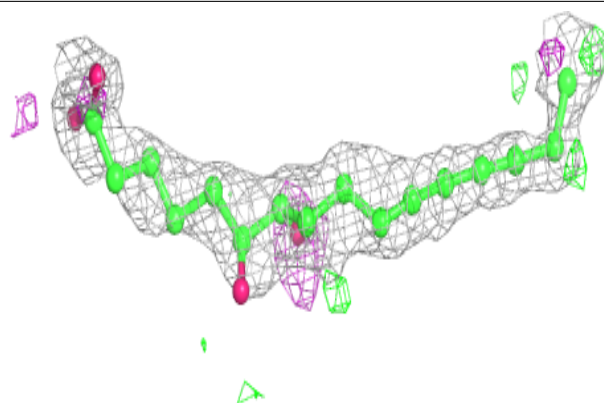
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	J3U	D	500	20/20	0.74	0.18	32,43,55,55	0
2	J3U	C	500	20/20	0.80	0.17	32,42,53,61	0
2	J3U	B	500	20/20	0.80	0.18	33,44,58,70	0
2	J3U	A	500	20/20	0.84	0.17	20,40,60,62	0

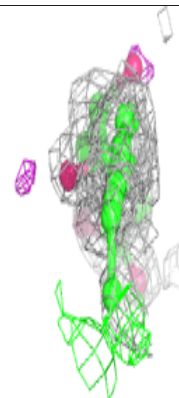
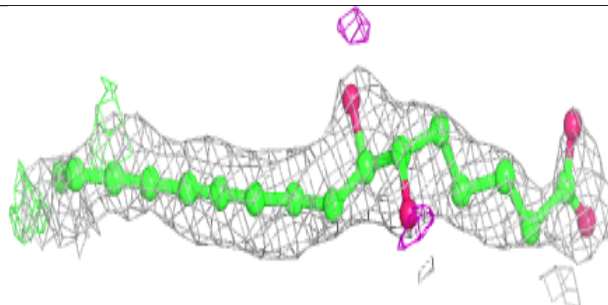
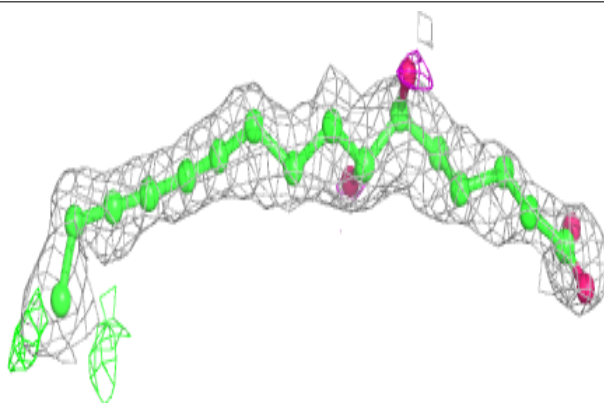
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around J3U D 500:

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

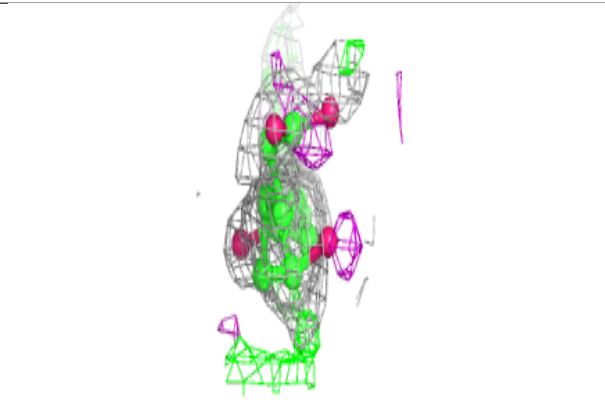
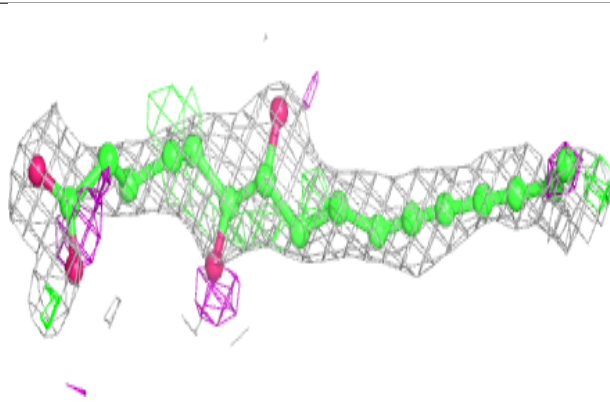
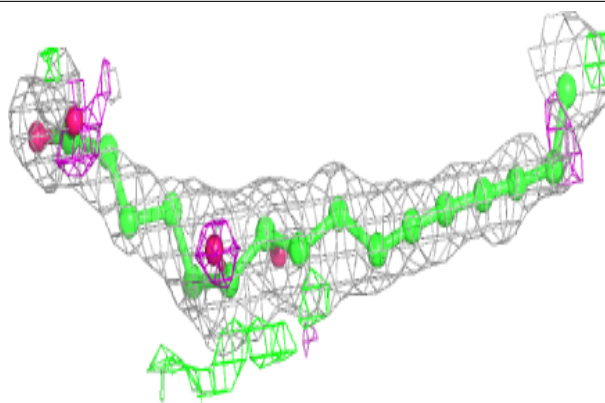
**Electron density around J3U C 500:**

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

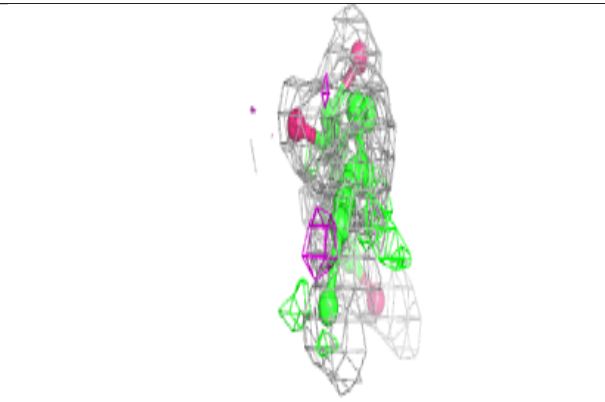
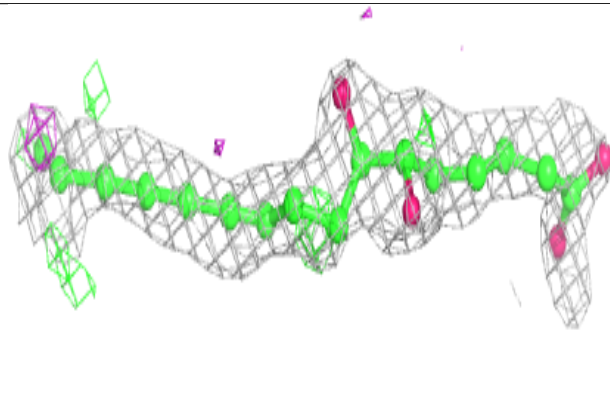
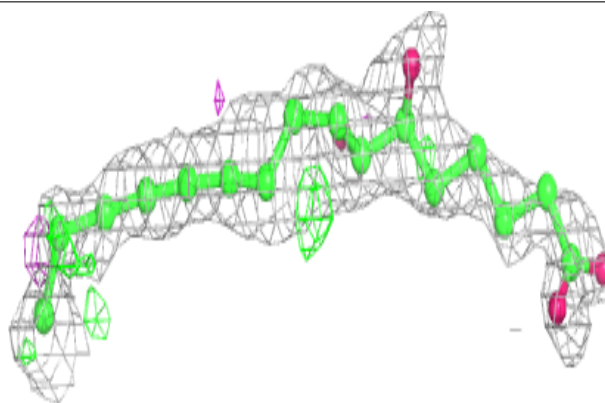


Electron density around J3U B 500:

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

**Electron density around J3U A 500:**

$2mF_o-DF_c$ (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.