

wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2023 – 06:21 pm GMT

PDB ID : 7ZBC

Title : Dark state crystal structure of bovine rhodopsin in Lipidic Cubic Phase

(SACLA)

Authors: Gruhl, T.; Weinert, T.; Rodrigues, M.J.; Milne, C.; Ortolani, G.; Nass, K.;

Nango, E.; Sen, S.; Johnson, P.; Cirelli, C.; Furrer, A.; Mous, S.; Skopintsev, P.; James, D.; Dworkowski, F.; Baath, P.; Kekilli, D.; Oserov, D.; Tanaka, R.; Glover, H.; Bacellar, C.; Bruenle, S.; Casadei, C.; Diethelm, A.; Gashi, D.; Gotthard, G.; Guixa-Gonzalez, R.; Joti, Y.; Kabanova, V.; Knopp, G.; Lesca, E.; Ma, P.; Martiel, I.; Muehle, J.; Owada, S.; Pamula, F.; Sarabi, S.; Tejero, O.; Tsai, C.J.; Varma, N.; Wach, A.; Boutet, S.; Tono, K.; Nogly, P.; Deupi,

X.; Iwata, S.; Neutze, R.; Standfuss, J.; Schertler, G.F.X.; Panneels, V.

Deposited on : 2022-03-23

Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

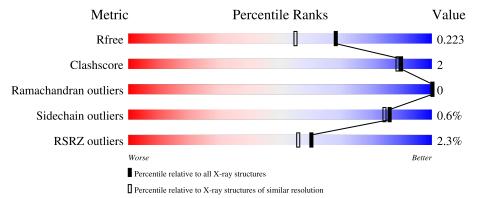
Xtriage (Phenix) : 1.13 EDS : 2.32.1

Overall quality at a glance (i) 1

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

The reported resolution of this entry is 1.80 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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					
			2%					
1	A	348	85%	• 13%				

Continued on next page...

1.1.7 (2018) buster-report

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> 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) 2.32.1



 $Continued\ from\ previous\ page...$

Mol	Chain	Length	Quality of chain					
1	В	348	2% • 13%	_				
2	С	2	100%					
2	D	2	100%					



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5509 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 Rhodopsin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	303	Total 2485	C 1666	N 377	O 419	S 23	0	11	0
1	В	304	Total 2485	C 1668	N 376	O 417	S 24	0	10	0

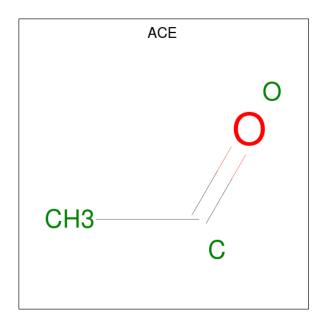
• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	С	2	Total C 28 16	N 2		0	0	0
2	D	2	Total C 28 16	N 2	O 10	0	0	0

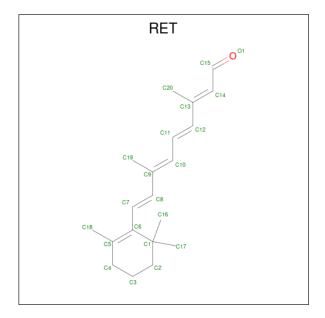
• Molecule 3 is ACETYL GROUP (three-letter code: ACE) (formula: C₂H₄O).





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

• Molecule 4 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 20 20	0	0

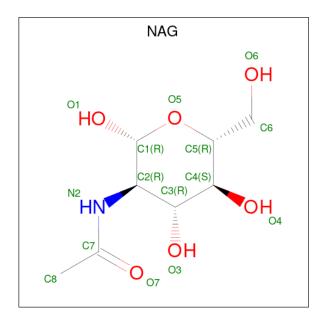
Continued on next page...



Continued from previous page...

\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total C 20 20	0	0

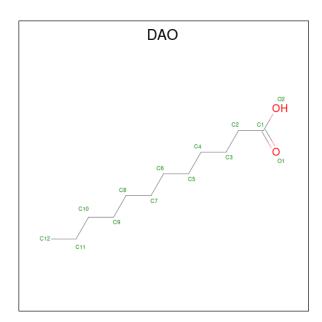
 \bullet Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 14			O 5	0	0
5	В	1	Total 14	C 8	N 1	O 5	0	0

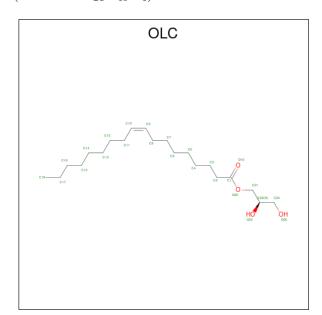
 \bullet Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: $\mathrm{C_{12}H_{24}O_2}).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 14	C 12	O 2	0	0

 \bullet Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 25 21 4	0	0
7	A	1	Total C O 22 18 4	0	0

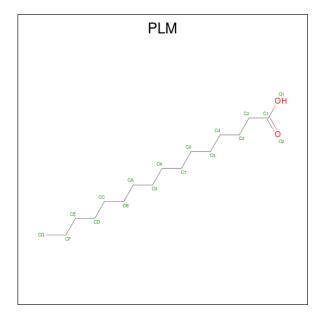
Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 7 7	0	0
7	A	1	Total C 10 10	0	0
7	A	1	Total C 12 12	0	0
7	A	1	Total C O 10 8 2	0	0
7	A	1	Total C O 25 21 4	0	0
7	A	1	Total C O 10 8 2	0	0
7	A	1	Total C O 25 21 4	0	0
7	A	1	Total C 13 13	0	0
7	В	1	Total C O 19 17 2	0	0
7	В	1	Total C O 18 14 4	0	0
7	В	1	Total C 7 7	0	0

 \bullet Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $\mathrm{C_{16}H_{32}O_2}).$





\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 17 16 1	0	0
8	В	1	Total C O 7 6 1	0	0

$\bullet\,$ Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	91	Total O 91 91	0	0
9	В	77	Total O 77 77	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: Rhodopsin Chain A: LYS GLU GLU THR SER GLN VAL ALA PRO ALA • Molecule 1: Rhodopsin Chain B: 84% 13% ASP GLU ALA SER THR LYS SER LYS SER CLU THR GLU WAL ALA ALA • Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose Chain C: 100% • Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido opyranose Chain D: 100%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	61.29Å 90.81Å 150.51Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.47 - 1.80	Depositor
Resolution (A)	10.47 - 1.80	EDS
% Data completeness	99.7 (10.47-1.80)	Depositor
(in resolution range)	99.7 (10.47-1.80)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.53 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.198 , 0.223	Depositor
R, R_{free}	0.198 , 0.223	DCC
R_{free} test set	1127 reflections (1.45%)	wwPDB-VP
Wilson B-factor $(Å^2)$	27.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.50 , 108.1	EDS
L-test for twinning ²	$ < L >=0.52, < L^2>=0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5509	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	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 56.83 % 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 2.5852e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: OLC, NAG, RET, ACE, PLM, DAO

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		
Moi Chair		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.46	0/2563	0.59	0/3501	
1	В	0.47	0/2566	0.59	0/3501	
All	All	0.47	0/5129	0.59	0/7002	

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	2485	0	2445	5	0
1	В	2485	0	2450	11	0
2	С	28	0	25	0	0
2	D	28	0	25	0	0
3	A	3	0	3	0	0
3	В	3	0	3	0	0
4	A	20	0	27	1	0
4	В	20	0	27	2	0
5	A	14	0	13	0	0
5	В	14	0	13	1	0
6	A	14	0	23	1	0

Continued on next page...



I 'omtamalod	trom	mmonia	maaa
Continued	11 0116	DICUIUUS	Daue
	.,	10	1

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	159	0	235	2	0
7	В	44	0	57	3	0
8	A	17	0	31	0	0
8	В	7	0	8	0	0
9	A	91	0	0	0	0
9	В	77	0	0	1	0
All	All	5509	0	5385	19	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.

The worst 5 of 19 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:74:TYR:CE2	1:B:150:GLU:HG2	2.42	0.55
1:B:74:TYR:HE2	1:B:150:GLU:HG2	1.76	0.50
4:A:402:RET:H10	4:A:402:RET:H202	1.93	0.50
7:A:414:OLC:H4A	1:B:36:GLN:HE21	1.77	0.50
1:B:290[B]:ILE:HG22	7:B:405:OLC:H2A	1.95	0.47

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	Perce	ntiles
1	A	308/348 (88%)	299 (97%)	9 (3%)	0	100	100
1	В	308/348 (88%)	301 (98%)	7 (2%)	0	100	100
All	All	616/696 (88%)	600 (97%)	16 (3%)	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	265/296 (90%)	264 (100%)	1 (0%)	91 89
1	В	264/296 (89%)	262 (99%)	2 (1%)	81 78
All	All	529/592 (89%)	526 (99%)	3 (1%)	86 84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	TYR
1	В	223	TYR
1	В	321	LEU

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

Mol	Chain	Res	Type
1	A	302	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 monosaccharides 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	ain Res Link		Bo	Bond lengths			Bond angles		
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	NAG	С	1	2,1	14,14,15	0.31	0	17,19,21	0.49	0	
2	NAG	С	2	2	14,14,15	0.25	0	17,19,21	0.49	0	
2	NAG	D	1	2,1	14,14,15	0.50	0	17,19,21	0.51	0	
2	NAG	D	2	2	14,14,15	0.38	0	17,19,21	0.48	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	NAG	С	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

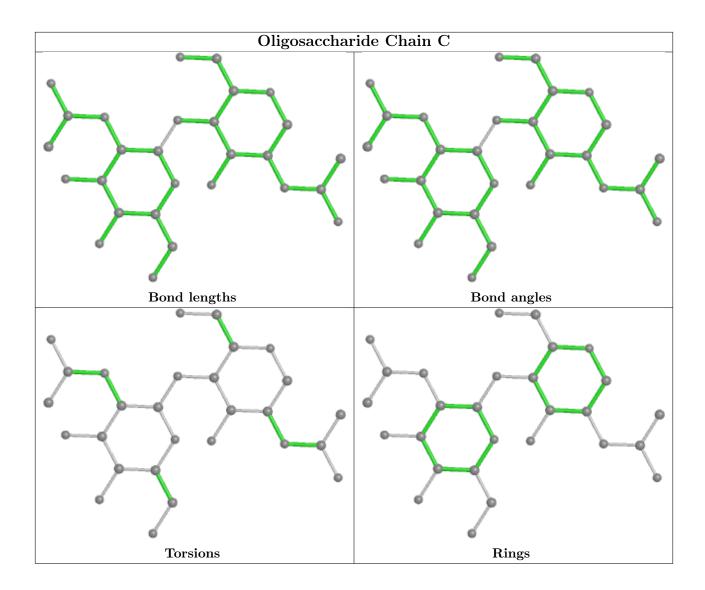
There are no torsion outliers.

There are no ring outliers.

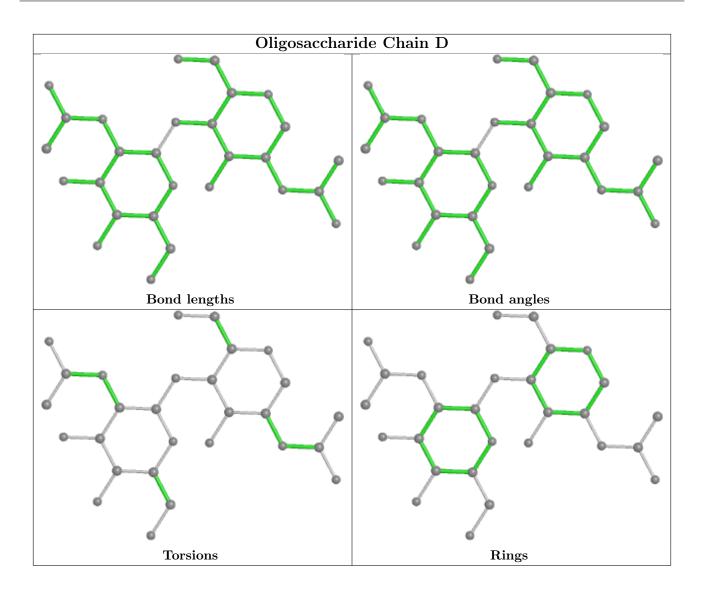
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry (i)

22 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	Tuno	Chain	Res	Link	Во	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	ACE	A	401	1	1,2,2	0.73	0	1,1,1	0.52	0	
4	RET	A	402	1	20,20,21	0.92	1 (5%)	27,27,28	0.87	1 (3%)	
7	OLC	A	414	-	24,24,24	0.23	0	25,25,25	0.26	0	



Mol	Type	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
WIOI	Type	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	403	1	14,14,15	0.27	0	17,19,21	0.42	0
3	ACE	В	401	1	1,2,2	0.97	0	1,1,1	0.30	0
7	OLC	A	415	-	12,12,24	0.26	0	11,11,25	0.13	0
7	OLC	В	405	-	17,17,24	0.28	0	18,18,25	0.37	0
7	OLC	A	405	-	24,24,24	0.31	0	25,25,25	0.34	0
7	OLC	A	409	-	11,11,24	0.23	0	10,10,25	0.31	0
6	DAO	A	404	-	13,13,13	0.72	0	13,13,13	0.62	0
5	NAG	В	403	1	14,14,15	0.26	0	17,19,21	0.52	0
7	OLC	A	406	-	21,21,24	0.28	0	22,22,25	0.29	0
8	PLM	A	410	1	16,16,17	0.48	0	15,15,17	0.50	0
4	RET	В	402	1	20,20,21	0.92	2 (10%)	27,27,28	0.80	1 (3%)
7	OLC	A	408	-	9,9,24	0.31	0	8,8,25	0.16	0
7	OLC	A	412	-	24,24,24	0.25	0	25,25,25	0.30	0
7	OLC	A	411	-	9,9,24	1.52	2 (22%)	9,9,25	1.70	2 (22%)
7	OLC	В	404	-	18,18,24	0.33	0	18,18,25	0.31	0
7	OLC	A	413	-	9,9,24	1.51	2 (22%)	9,9,25	1.69	2 (22%)
8	PLM	В	406	1	6,6,17	0.82	0	5,5,17	0.76	0
7	OLC	A	407	-	6,6,24	0.20	0	4,5,25	0.37	0
7	OLC	В	407	-	6,6,24	0.20	0	4,5,25	0.21	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	RET	A	402	1	-	1/13/30/31	0/1/1/1
7	OLC	A	414	-	-	1/24/24/24	-
5	NAG	A	403	1	-	0/6/23/26	0/1/1/1
7	OLC	A	415	-	-	2/10/10/24	-
7	OLC	В	405	-	-	5/17/17/24	-
7	OLC	A	405	ı	-	6/24/24/24	-
7	OLC	A	409	ı	-	2/9/9/24	-
6	DAO	A	404	-	-	5/11/11/11	-
5	NAG	В	403	1	-	0/6/23/26	0/1/1/1
7	OLC	A	406	-	-	4/21/21/24	-
8	PLM	A	410	1	-	3/13/14/15	-
4	RET	В	402	1	-	1/13/30/31	0/1/1/1
7	OLC	A	408	-	-	0/7/7/24	-
7	OLC	A	412	-	-	5/24/24/24	-

Continued on next page...



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	A	411	-	-	3/7/7/24	-
7	OLC	В	404	-	-	3/17/17/24	-
7	OLC	A	413	-	-	2/7/7/24	-
8	PLM	В	406	1	-	0/3/4/15	-
7	OLC	A	407	-	-	1/4/4/24	-
7	OLC	В	407	-	-	1/4/4/24	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
7	A	411	OLC	O19-C1	3.38	1.33	1.22
7	A	413	OLC	O19-C1	3.36	1.33	1.22
7	A	411	OLC	O20-C1	-3.00	1.20	1.30
4	A	402	RET	C15-C14	-2.98	1.38	1.49
7	A	413	OLC	O20-C1	-2.96	1.20	1.30

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
7	A	413	OLC	O19-C1-C2	-3.64	111.38	123.08
7	A	411	OLC	O19-C1-C2	-3.63	111.41	123.08
7	A	411	OLC	O20-C1-C2	3.55	125.44	114.03
7	A	413	OLC	O20-C1-C2	3.49	125.26	114.03
4	В	402	RET	C10-C11-C12	2.41	130.74	123.22

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	406	OLC	C2-C1-O20-C21
7	A	406	OLC	O19-C1-O20-C21
7	В	404	OLC	C2-C1-O20-C21
7	В	404	OLC	O19-C1-O20-C21
7	A	412	OLC	O19-C1-O20-C21

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	RET	1	0

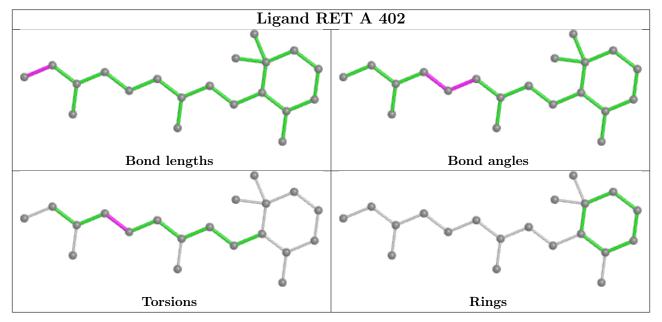
Continued on next page...



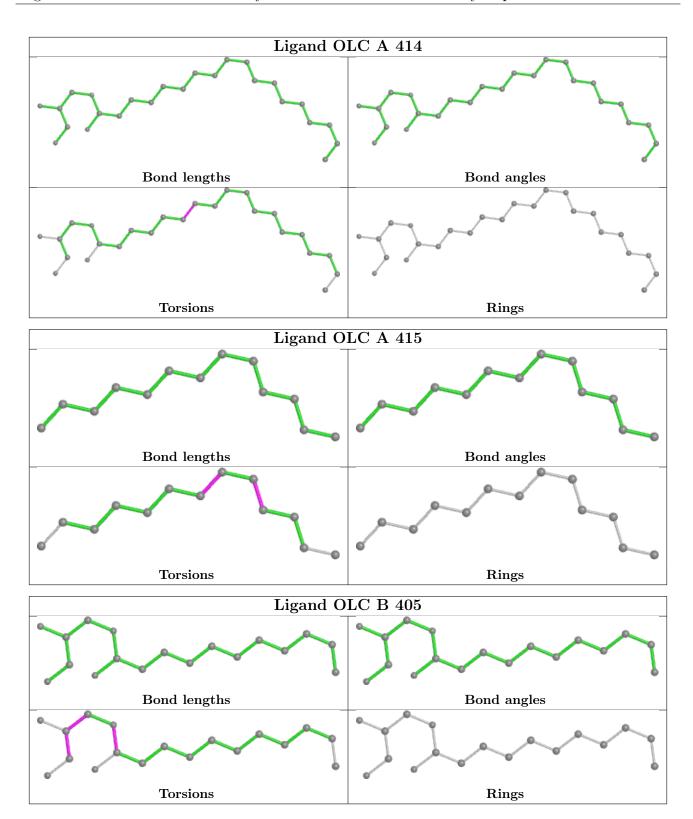
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	414	OLC	1	0
7	В	405	OLC	3	0
6	A	404	DAO	1	0
5	В	403	NAG	1	0
7	A	406	OLC	1	0
4	В	402	RET	2	0

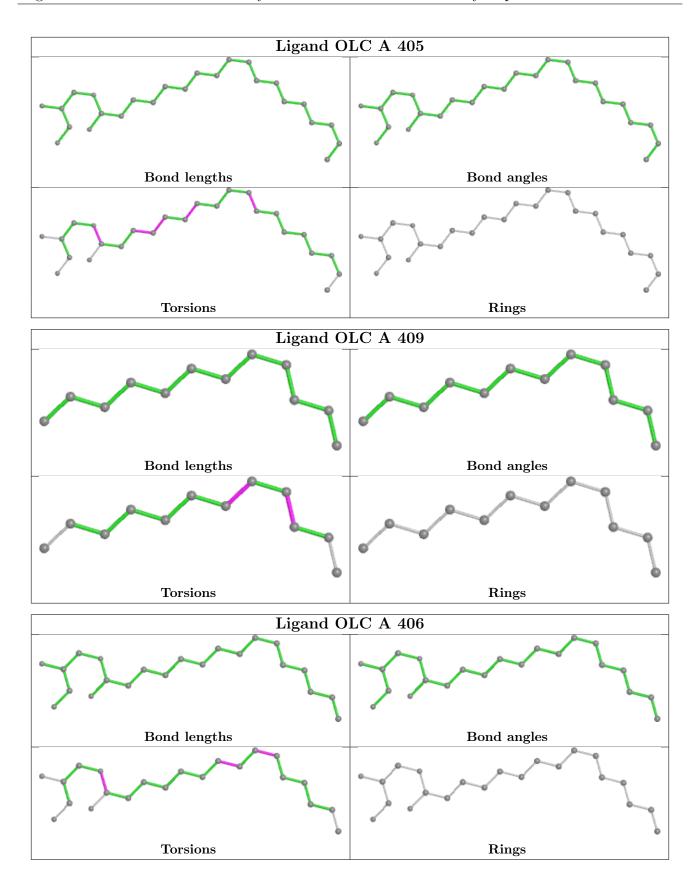
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



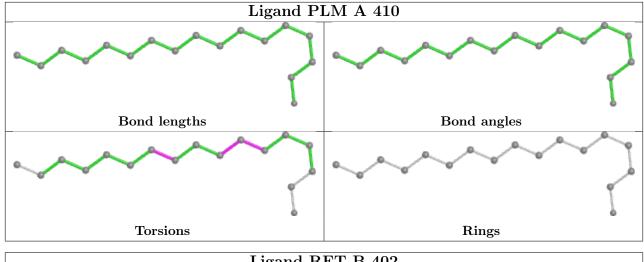


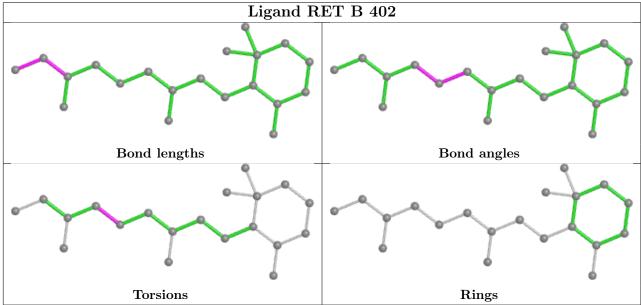


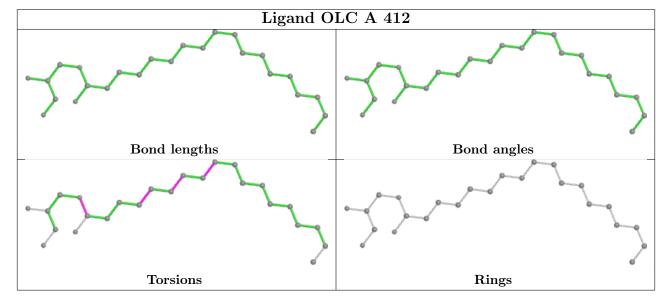




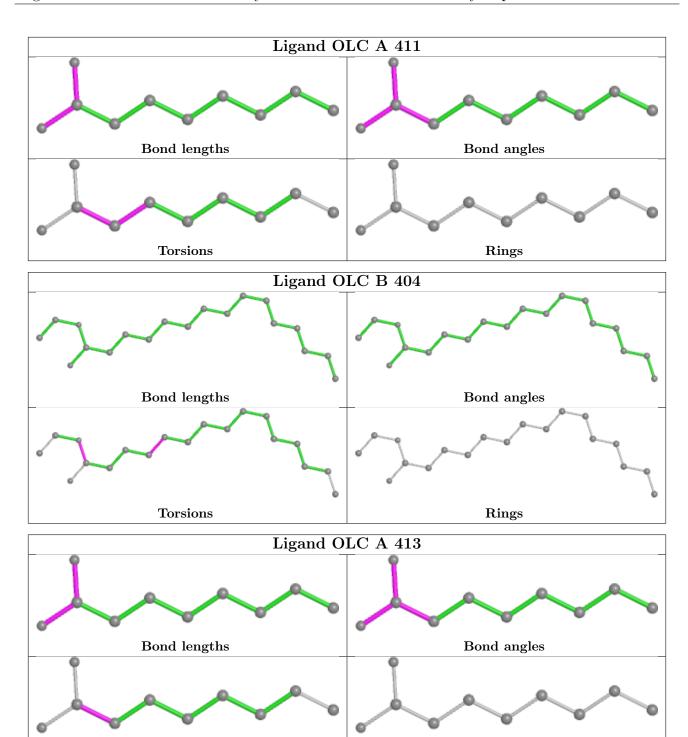








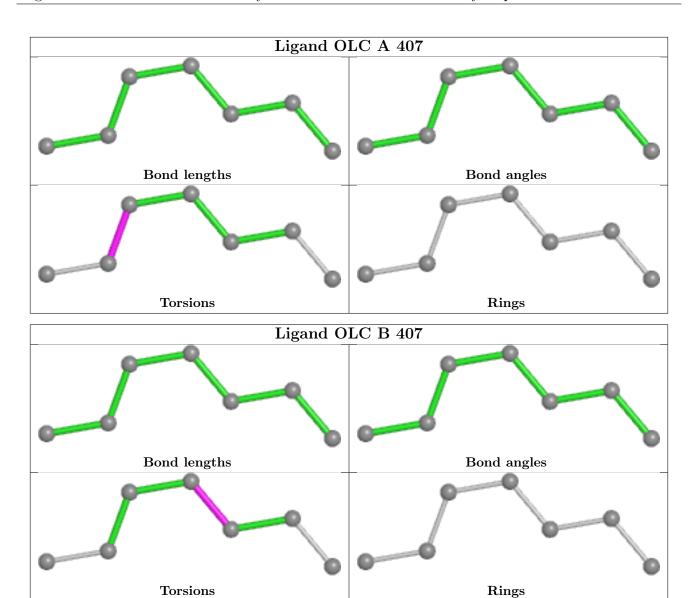






Torsions

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, 95^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	303/348 (87%)	-0.38	6 (1%) 65 61	19, 28, 51, 79	0
1	В	304/348 (87%)	-0.38	8 (2%) 56 51	19, 27, 51, 79	0
All	All	607/696 (87%)	-0.38	14 (2%) 60 56	19, 28, 51, 79	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	244	GLN	4.5
1	A	223	TYR	4.1
1	A	1	MET	3.8
1	A	229	THR	3.8
1	В	223	TYR	3.6

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

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

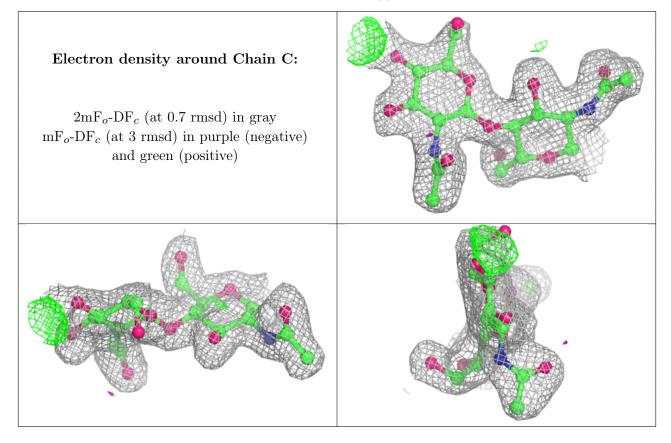
6.3 Carbohydrates (i)

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^{th} 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.

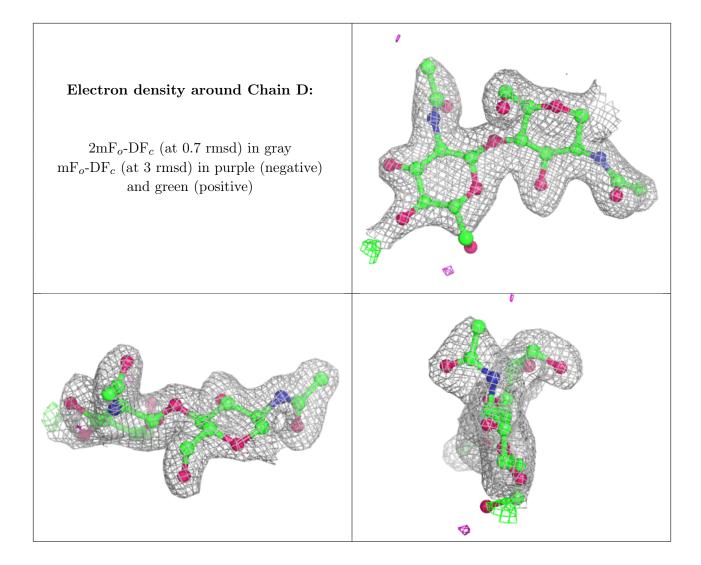
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	NAG	С	2	14/15	0.89	0.14	36,43,53,68	0
2	NAG	D	2	14/15	0.90	0.25	47,58,74,80	0
2	NAG	D	1	14/15	0.93	0.11	30,36,40,40	0
2	NAG	С	1	14/15	0.95	0.08	27,32,36,37	0



The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.







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^{th} 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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
8	PLM	В	406	7/18	0.71	0.12	64,67,69,75	0
7	OLC	В	404	19/25	0.72	0.14	47,61,80,81	0
8	PLM	A	410	17/18	0.74	0.17	54,64,76,80	0
7	OLC	A	409	12/25	0.74	0.14	40,52,66,68	0
7	OLC	A	414	25/25	0.77	0.17	40,59,83,88	0
7	OLC	A	406	22/25	0.77	0.18	48,65,88,91	0
7	OLC	A	412	25/25	0.80	0.14	48,59,68,72	0
7	OLC	A	415	13/25	0.81	0.13	42,51,61,64	0
3	ACE	A	401	3/3	0.82	0.48	71,71,74,81	0

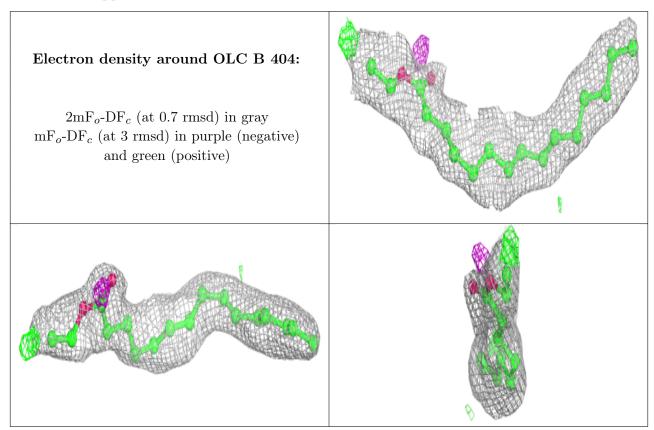
Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
7	OLC	A	405	25/25	0.83	0.13	51,61,73,87	0
7	OLC	A	408	10/25	0.84	0.11	40,50,56,61	0
5	NAG	A	403	14/15	0.84	0.19	42,56,64,68	0
7	OLC	В	405	18/25	0.85	0.16	37,50,63,65	0
7	OLC	В	407	7/25	0.86	0.12	39,44,53,60	0
7	OLC	A	413	10/25	0.88	0.09	46,61,74,77	0
7	OLC	A	411	10/25	0.89	0.10	55,66,70,74	0
6	DAO	A	404	14/14	0.89	0.15	39,52,62,69	0
7	OLC	A	407	7/25	0.90	0.08	41,44,49,49	0
5	NAG	В	403	14/15	0.91	0.12	33,40,44,45	0
4	RET	A	402	20/21	0.96	0.06	18,22,29,30	0
4	RET	В	402	20/21	0.97	0.06	18,21,30,37	0
3	ACE	В	401	3/3	0.99	0.10	34,34,35,37	0

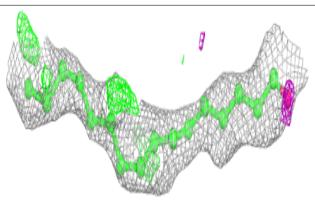
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

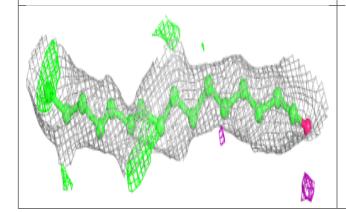


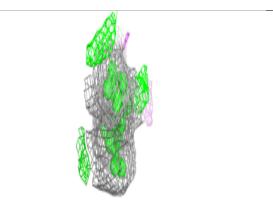


Electron density around PLM A 410:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

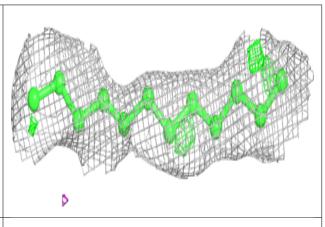


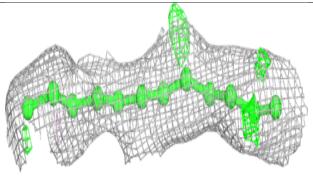


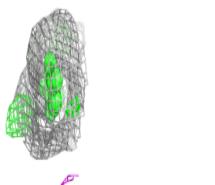


Electron density around OLC A 409:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



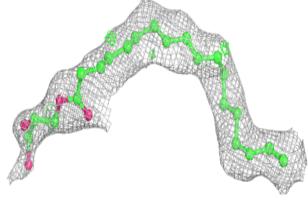


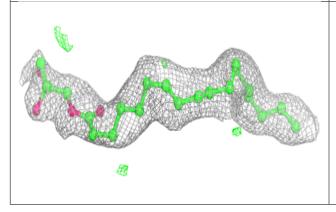


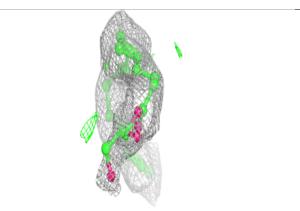


Electron density around OLC A 414:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

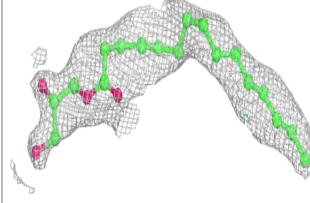


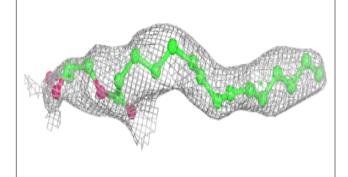


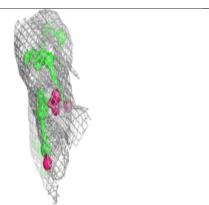


Electron density around OLC A 406:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



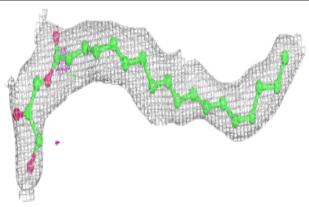


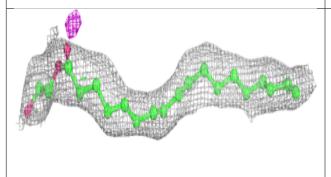


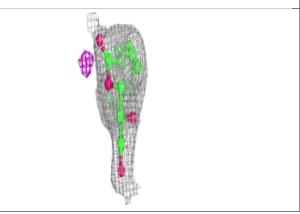


Electron density around OLC A 412:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

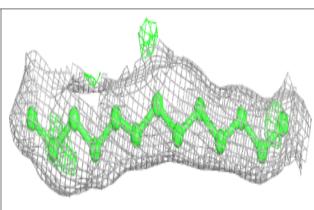


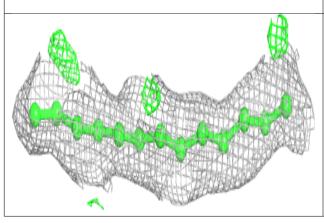


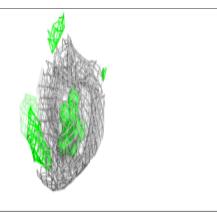


Electron density around OLC A 415:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



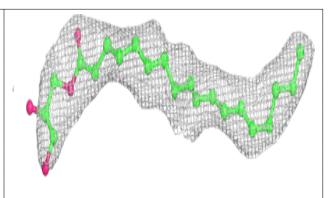


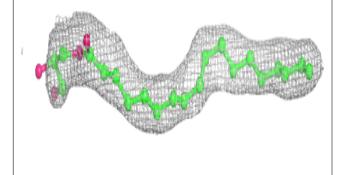




Electron density around OLC A 405:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

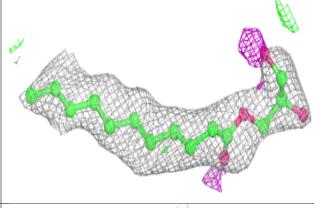


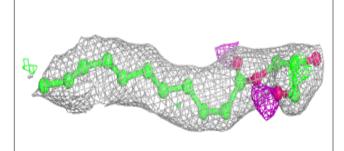


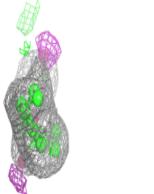


Electron density around OLC B 405:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



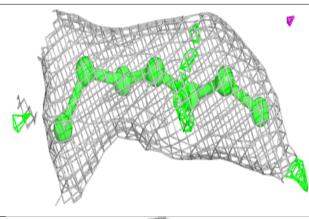


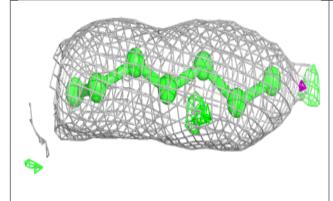


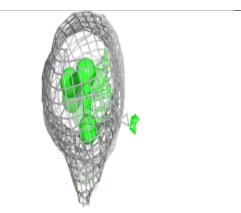


Electron density around OLC B 407:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

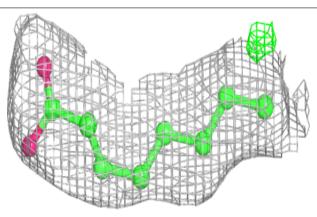


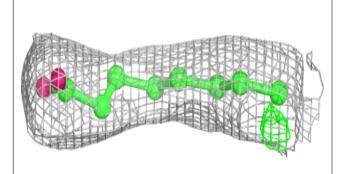


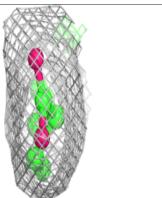


Electron density around OLC A 413:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



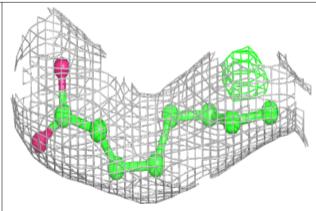


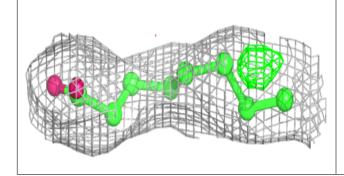


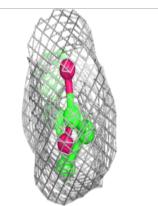


Electron density around OLC A 411:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

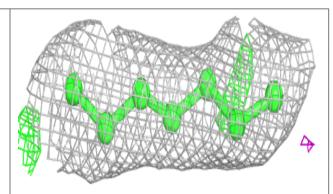


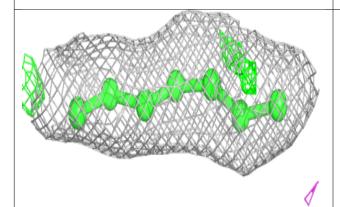


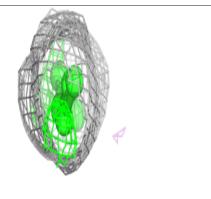


Electron density around OLC A 407:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



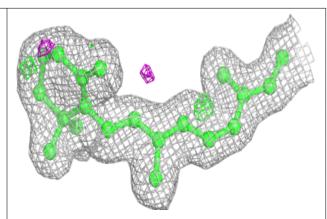


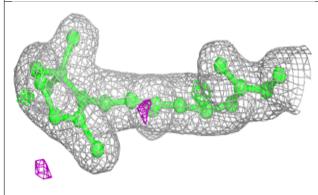


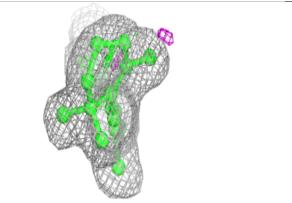


Electron density around RET A 402:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

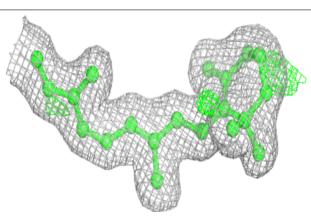


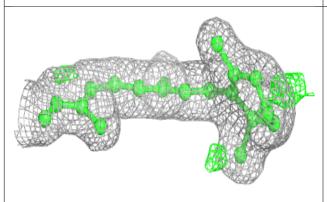


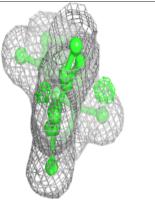


Electron density around RET B 402:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

