Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 07:28 AM EDT

PDB ID	:	3C9L
Title	:	Structure of ground-state bovine rhodospin in a hexagonal crystal form
Authors	:	Stenkamp, R.E.
Deposited on	:	2008-02-16
Resolution	:	2.65 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:

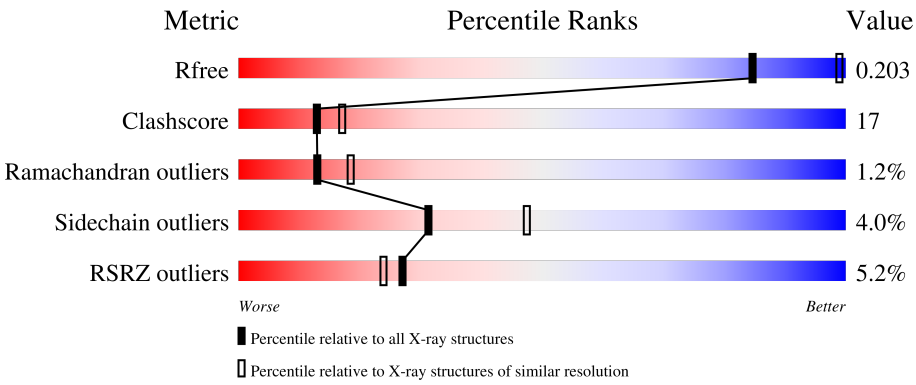
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.65 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	348	5%; 64%; 27%; • 5%
2	B	3	100%
2	C	3	33%; 67%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	C8E	A	1347	-	-	-	X
9	C8E	A	1348	-	-	-	X

2 Entry composition (i)

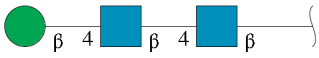
There are 10 unique types of molecules in this entry. The entry contains 2888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	329	2603	1731	403	443	26	0	0	1

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

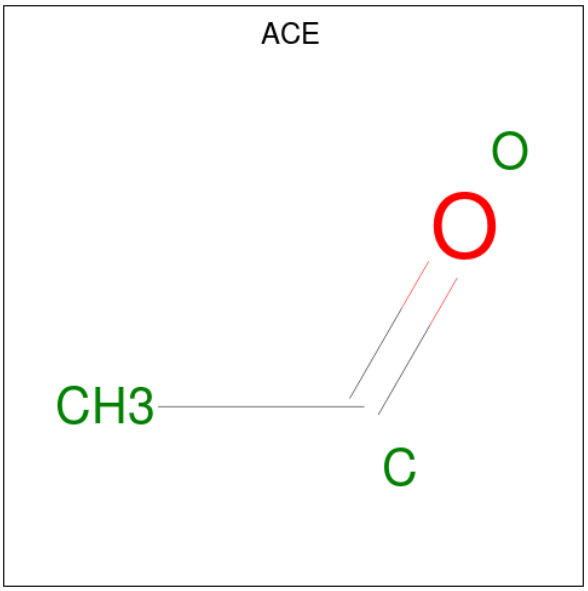


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0
2	C	3	39	22	2	15	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

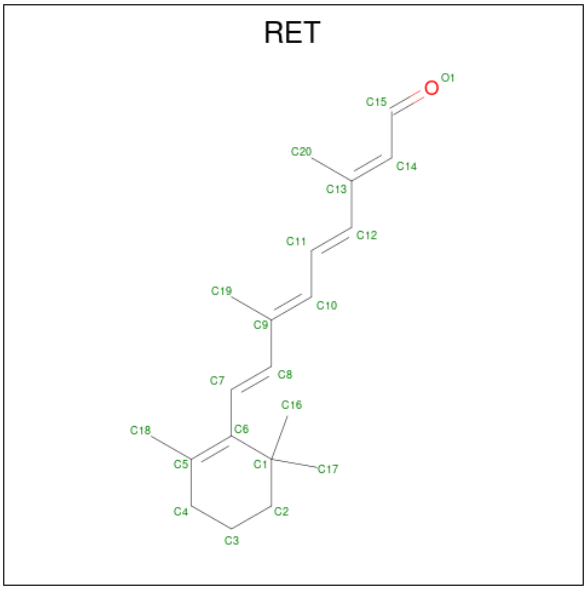
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O).



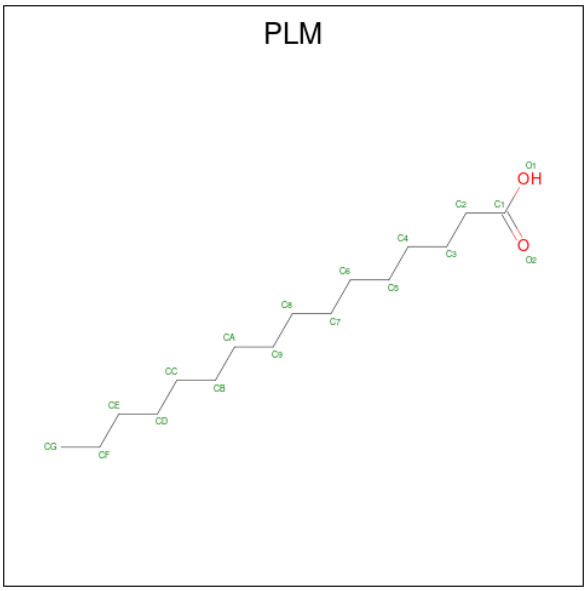
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 2 1	0	0

- Molecule 5 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



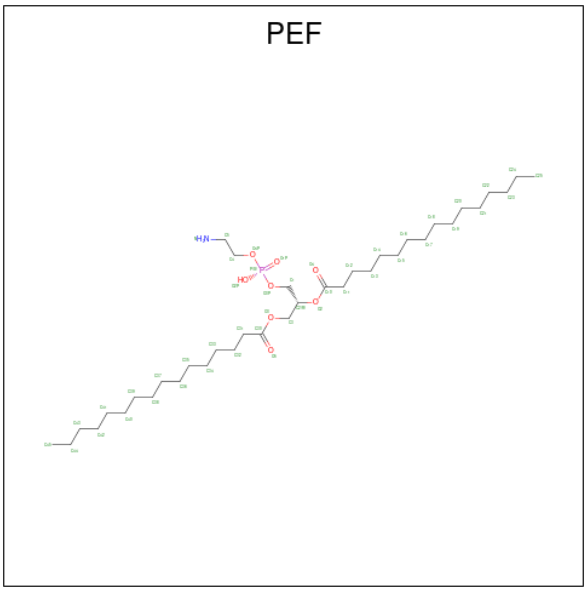
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 20 20	0	0

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



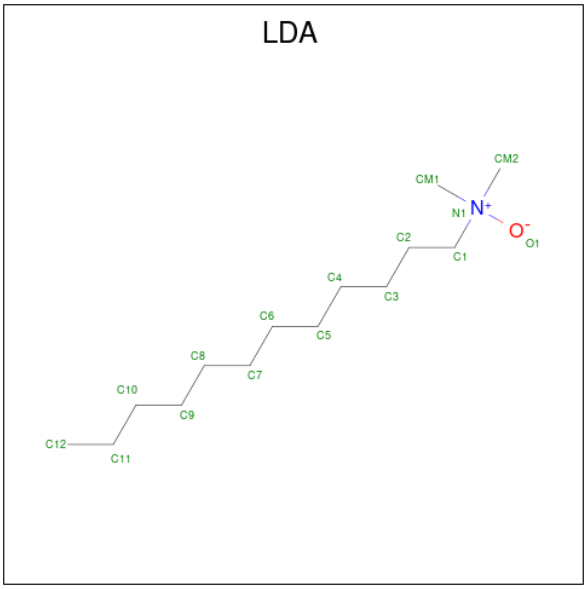
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	17	16	1	0	0
			Total	C	O		
6	A	1	17	16	1	0	0

- Molecule 7 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



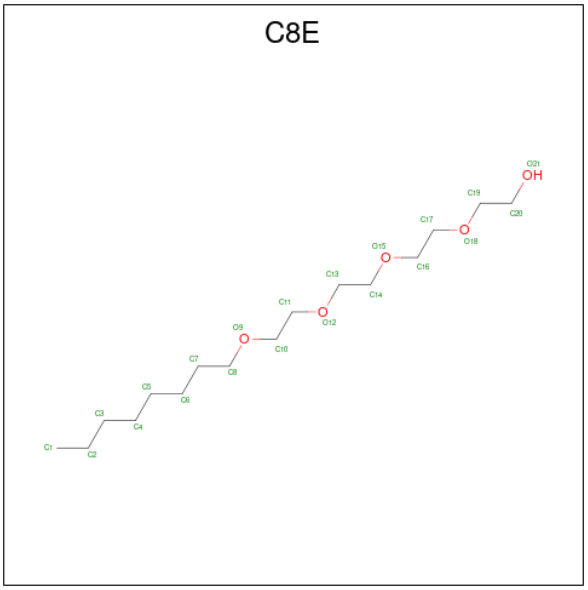
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
7	A	1	20	20	0	0

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	16	14	1	1	0	0

- Molecule 9 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	17	14	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	15	12	3	0	0
			Total	C	O		
9	A	1	10	9	1	0	0
			Total	C	O		
9	A	1	18	14	4	0	0
			Total	C	O		
9	A	1	21	16	5	0	0
			Total	C	O		
9	A	1	12	10	2	0	0

- Molecule 10 is water.

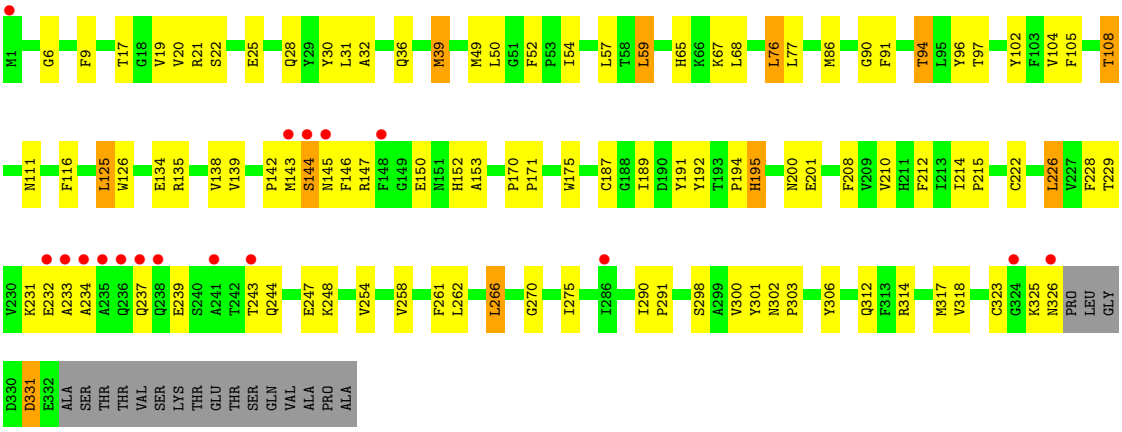
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	20	20	20	0	0

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: 5% 64% 27% • 5%



• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 33% 67%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	103.82Å 103.82Å 76.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.95 – 2.65 44.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.95-2.65) 99.8 (44.96-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.65Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, R_{free}	0.188 , 0.216 0.178 , 0.203	Depositor DCC
R_{free} test set	688 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	63.1	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.058 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2888	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: PEF, BMA, RET, ACE, NAG, C8E, LDA, ZN, PLM

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	0.44	0/2684	0.56	0/3656

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	2603	0	2565	95	0
2	B	39	0	34	0	0
2	C	39	0	34	0	0
3	A	1	0	0	0	0
4	A	3	0	3	0	0
5	A	20	0	27	2	0
6	A	34	0	62	2	0
7	A	20	0	32	0	0
8	A	16	0	31	2	0
9	A	93	0	153	3	0
10	A	20	0	0	3	0
All	All	2888	0	2941	96	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 17.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:HA	1:A:94:THR:CG2	2.10	0.80
1:A:28:GLN:HB3	1:A:31:LEU:HD12	1.67	0.76
1:A:239:GLU:HB2	1:A:244:GLN:HE21	1.53	0.74
1:A:232:GLU:HG2	1:A:232:GLU:O	1.93	0.67
1:A:76:LEU:HD22	1:A:306:TYR:CG	2.30	0.67
1:A:201:GLU:HB2	10:A:1350:HOH:O	1.95	0.66
1:A:67:LYS:HG2	1:A:331:ASP:CB	2.26	0.65
1:A:318:VAL:HG12	1:A:326:ASN:HB2	1.80	0.64
1:A:234:ALA:HB1	1:A:239:GLU:OE1	1.99	0.63
1:A:143:MET:HE3	1:A:143:MET:HA	1.79	0.62
1:A:318:VAL:CG1	1:A:326:ASN:HB2	2.29	0.62
1:A:65:HIS:HB2	1:A:68:LEU:HD22	1.82	0.62
1:A:32:ALA:HB1	1:A:36:GLN:OE1	2.00	0.62
1:A:50:LEU:HD23	6:A:1333:PLM:HG1	1.80	0.62
1:A:229:THR:HA	1:A:233:ALA:HB3	1.81	0.61
1:A:143:MET:HE2	1:A:144:SER:H	1.64	0.61
1:A:102:TYR:CZ	1:A:104:VAL:HG12	2.36	0.60
1:A:111:ASN:HB3	9:A:1344:C8E:H61	1.83	0.59
1:A:57:LEU:HD11	1:A:317:MET:HG3	1.83	0.59
1:A:187:CYS:O	5:A:1332:RET:H12	2.02	0.58
1:A:298:SER:HA	1:A:301:TYR:CE2	2.39	0.58
1:A:76:LEU:HD22	1:A:306:TYR:CD2	2.39	0.57
1:A:54:ILE:CD1	1:A:300:VAL:HG13	2.35	0.57
1:A:146:PHE:HZ	1:A:152:HIS:NE2	2.02	0.57
1:A:228:PHE:O	1:A:231:LYS:HB3	2.05	0.57
1:A:170:PRO:N	1:A:171:PRO:HD2	2.20	0.56
1:A:244:GLN:O	1:A:248:LYS:HB2	2.04	0.56
1:A:143:MET:CE	1:A:144:SER:H	2.18	0.56
1:A:229:THR:HG23	1:A:234:ALA:HB2	1.88	0.56
1:A:262:LEU:O	1:A:266:LEU:HB2	2.06	0.56
1:A:290:ILE:HB	1:A:291:PRO:HD3	1.89	0.55
1:A:91:PHE:HA	1:A:94:THR:HG23	1.86	0.55
1:A:229:THR:CG2	1:A:234:ALA:HB2	2.36	0.55
1:A:302:ASN:HB2	10:A:1368:HOH:O	2.06	0.55
1:A:68:LEU:HD12	1:A:312:GLN:NE2	2.22	0.53
1:A:192:TYR:CE1	1:A:275:ILE:HD13	2.44	0.53
1:A:96:TYR:HE1	1:A:104:VAL:HG21	1.73	0.53
1:A:20:VAL:HA	1:A:30:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:C	1:A:59:LEU:HD12	2.30	0.52
1:A:59:LEU:HD12	1:A:59:LEU:O	2.10	0.52
1:A:59:LEU:HD13	1:A:77:LEU:HD11	1.91	0.52
1:A:90:GLY:O	1:A:94:THR:HG22	2.10	0.51
1:A:146:PHE:CZ	1:A:152:HIS:NE2	2.78	0.51
1:A:111:ASN:CB	9:A:1344:C8E:H61	2.41	0.51
1:A:254:VAL:O	1:A:258:VAL:HG23	2.11	0.51
1:A:91:PHE:HA	1:A:94:THR:HG22	1.93	0.50
1:A:262:LEU:HB3	1:A:266:LEU:HD22	1.94	0.50
1:A:142:PRO:HG2	1:A:143:MET:H	1.76	0.50
1:A:171:PRO:HA	1:A:175:TRP:O	2.11	0.49
1:A:325:LYS:N	1:A:325:LYS:HD2	2.28	0.49
1:A:270:GLY:HA3	8:A:1342:LDA:H42	1.95	0.48
1:A:105:PHE:O	1:A:108:THR:HG23	2.13	0.48
1:A:222:CYS:O	1:A:226:LEU:HD12	2.14	0.48
1:A:303:PRO:O	1:A:306:TYR:HB3	2.14	0.47
1:A:65:HIS:HB3	1:A:331:ASP:CB	2.43	0.47
1:A:68:LEU:HD12	1:A:312:GLN:HE21	1.79	0.47
1:A:229:THR:C	1:A:231:LYS:H	2.17	0.47
5:A:1332:RET:C8	5:A:1332:RET:H181	2.44	0.47
1:A:229:THR:C	1:A:231:LYS:N	2.67	0.47
1:A:68:LEU:CD1	1:A:312:GLN:HE21	2.28	0.47
1:A:143:MET:HG3	1:A:144:SER:N	2.30	0.47
1:A:270:GLY:HA2	8:A:1342:LDA:H71	1.97	0.47
1:A:126:TRP:CZ2	1:A:215:PRO:HG3	2.51	0.46
1:A:22:SER:HB3	1:A:25:GLU:HG2	1.97	0.46
1:A:125:LEU:HG	1:A:261:PHE:CZ	2.50	0.46
1:A:54:ILE:HD11	1:A:300:VAL:HG13	1.98	0.46
1:A:52:PHE:CZ	6:A:1334:PLM:HF2	2.51	0.46
1:A:194:PRO:O	1:A:195:HIS:C	2.54	0.45
1:A:325:LYS:HD2	1:A:325:LYS:H	1.82	0.45
1:A:17:THR:OG1	1:A:19:VAL:HG12	2.17	0.45
1:A:96:TYR:CE1	1:A:104:VAL:HG21	2.52	0.44
1:A:243:THR:HG22	1:A:247:GLU:HG3	1.98	0.44
1:A:194:PRO:O	1:A:200:ASN:HB2	2.18	0.44
1:A:147:ARG:O	1:A:147:ARG:HG3	2.18	0.44
1:A:54:ILE:HD13	1:A:300:VAL:HG13	2.00	0.43
1:A:97:THR:HG23	1:A:102:TYR:C	2.39	0.43
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.83	0.43
1:A:233:ALA:O	1:A:237:GLN:HG2	2.19	0.43
1:A:146:PHE:HZ	1:A:152:HIS:CD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLU:OE2	1:A:138:VAL:HG21	2.18	0.42
1:A:96:TYR:HE1	1:A:104:VAL:CG2	2.33	0.42
1:A:189:ILE:HD13	1:A:189:ILE:HA	1.89	0.42
1:A:126:TRP:CH2	1:A:215:PRO:HG3	2.55	0.42
1:A:134:GLU:OE1	1:A:135:ARG:HD2	2.20	0.42
1:A:208:PHE:O	1:A:212:PHE:HB3	2.19	0.41
1:A:298:SER:HB2	10:A:1369:HOH:O	2.20	0.41
1:A:170:PRO:N	1:A:171:PRO:CD	2.83	0.41
1:A:239:GLU:CB	1:A:244:GLN:HE21	2.29	0.41
1:A:314:ARG:HD2	9:A:1346:C8E:H82	2.02	0.41
1:A:49:MET:HA	1:A:49:MET:CE	2.51	0.41
1:A:150:GLU:O	1:A:153:ALA:HB3	2.20	0.41
1:A:210:VAL:HA	1:A:214:ILE:HD12	2.03	0.41
1:A:6:GLY:HA3	1:A:9:PHE:CZ	2.56	0.40
1:A:39:MET:HA	1:A:39:MET:CE	2.52	0.40
1:A:86:MET:HG2	1:A:116:PHE:O	2.22	0.40
1:A:139:VAL:O	1:A:139:VAL:HG12	2.20	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	325/348 (93%)	302 (93%)	19 (6%)	4 (1%)	13 18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	331	ASP
1	A	195	HIS
1	A	323	CYS

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	278/296 (94%)	267 (96%)	11 (4%)	31 47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	39	MET
1	A	59	LEU
1	A	76	LEU
1	A	94	THR
1	A	108	THR
1	A	125	LEU
1	A	145	ASN
1	A	191	TYR
1	A	226	LEU
1	A	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	244	GLN
1	A	312	GLN
1	A	315	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)

6 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	0.57	0	17,19,21	0.75	0
2	NAG	B	2	2	14,14,15	0.66	0	17,19,21	0.70	0
2	BMA	B	3	2	11,11,12	0.34	0	15,15,17	0.59	0
2	NAG	C	1	1,2	14,14,15	0.59	0	17,19,21	1.20	2 (11%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	1.14	2 (11%)
2	BMA	C	3	2	11,11,12	0.34	0	15,15,17	0.60	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	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	NAG	C	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C1-O5-C5	2.93	116.16	112.19
2	C	1	NAG	C4-C3-C2	2.09	114.08	111.02
2	C	2	NAG	C4-C3-C2	-2.02	108.05	111.02
2	C	1	NAG	O7-C7-C8	-2.02	118.30	122.06

There are no chirality outliers.

All (15) torsion outliers are listed below:

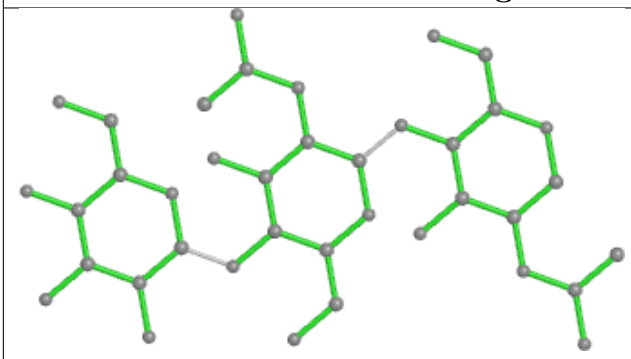
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	3	BMA	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

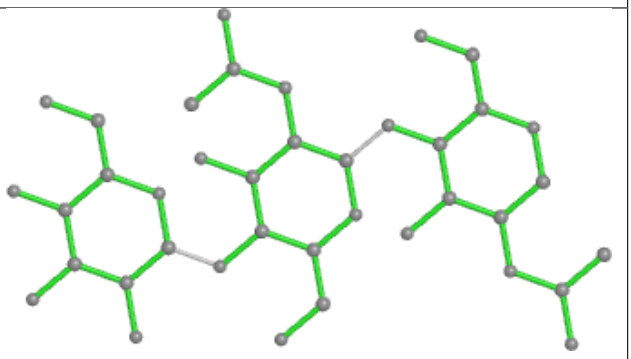
No monomer is involved in short contacts.

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

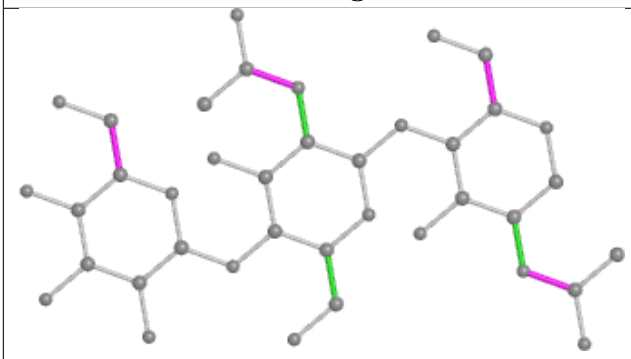
Oligosaccharide Chain B



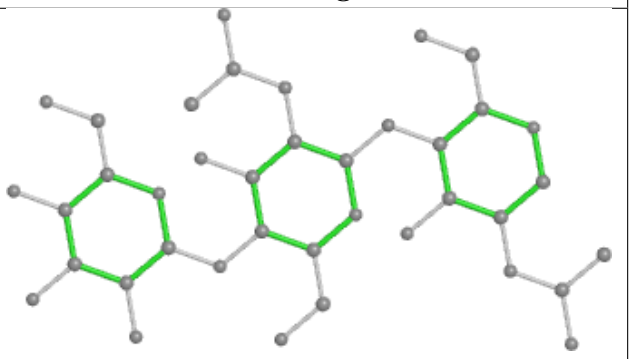
Bond lengths



Bond angles

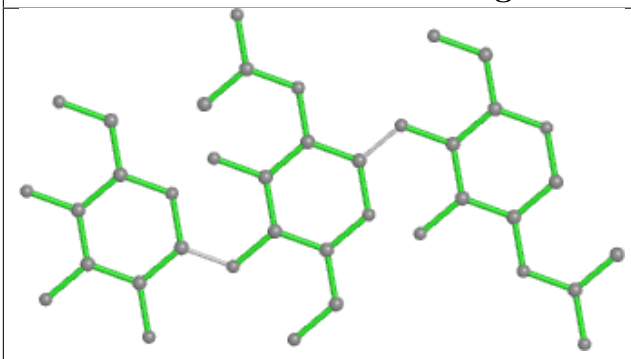


Torsions

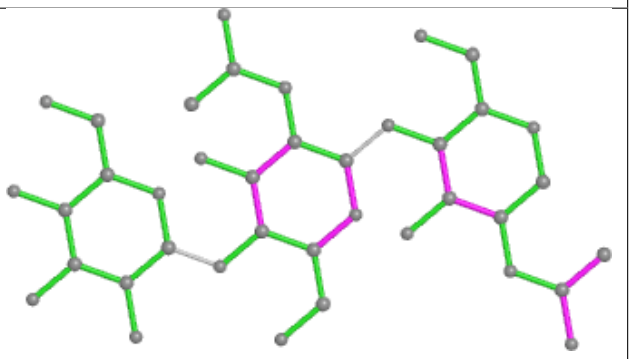


Rings

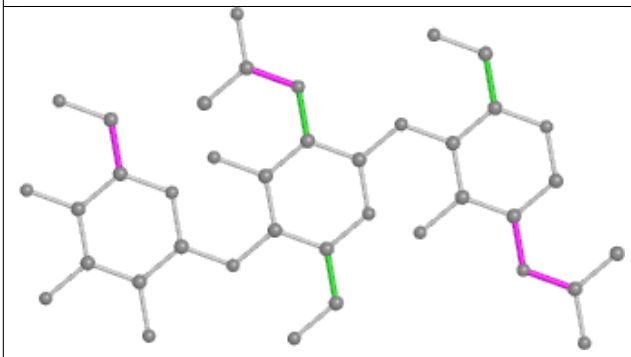
Oligosaccharide Chain C



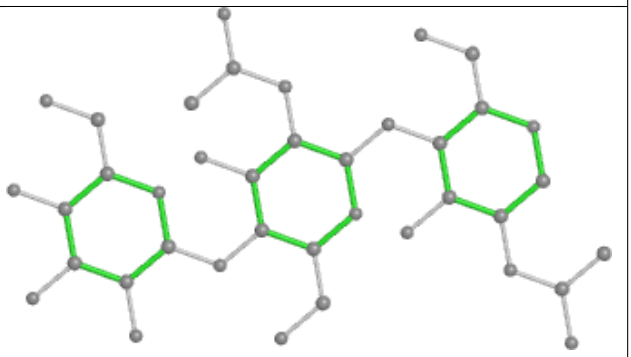
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	LDA	A	1342	-	12,15,15	2.11	1 (8%)	14,17,17	0.64	0
9	C8E	A	1345	-	9,9,20	0.34	0	8,8,19	0.51	0
4	ACE	A	0	1	1,2,2	0.85	0	1,1,1	0.32	0
9	C8E	A	1346	-	17,17,20	0.51	0	16,16,19	0.33	0
7	PEF	A	1341	-	18,18,46	0.31	0	16,16,51	0.40	0
6	PLM	A	1333	1	16,16,17	0.83	1 (6%)	15,15,17	0.64	0
9	C8E	A	1343	-	16,16,20	0.52	0	15,15,19	0.43	0
5	RET	A	1332	1	20,20,21	1.04	1 (5%)	27,27,28	1.36	5 (18%)
9	C8E	A	1348	-	11,11,20	0.39	0	10,10,19	0.46	0
9	C8E	A	1344	-	14,14,20	0.42	0	13,13,19	0.52	0
9	C8E	A	1347	-	20,20,20	0.56	0	19,19,19	0.39	0
6	PLM	A	1334	1	16,16,17	0.81	1 (6%)	15,15,17	0.69	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
8	LDA	A	1342	-	-	7/13/13/13	-
9	C8E	A	1345	-	-	5/7/7/18	-
9	C8E	A	1346	-	-	10/15/15/18	-
7	PEF	A	1341	-	-	10/14/14/50	-
6	PLM	A	1333	1	-	8/14/14/15	-
9	C8E	A	1343	-	-	12/14/14/18	-
5	RET	A	1332	1	-	1/13/30/31	0/1/1/1
9	C8E	A	1348	-	-	7/9/9/18	-
9	C8E	A	1344	-	-	9/12/12/18	-
9	C8E	A	1347	-	-	14/18/18/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLM	A	1334	1	-	11/14/14/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1342	LDA	O1-N1	-7.20	1.25	1.42
5	A	1332	RET	C14-C13	3.26	1.36	1.33
6	A	1333	PLM	O1-C1	-3.14	1.25	1.42
6	A	1334	PLM	O1-C1	-3.03	1.26	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1332	RET	C2-C1-C6	2.85	114.87	110.48
5	A	1332	RET	C20-C13-C12	2.54	122.08	118.08
5	A	1332	RET	C8-C9-C10	-2.44	115.19	118.94
5	A	1332	RET	C11-C12-C13	2.26	132.75	126.42
5	A	1332	RET	C18-C5-C6	-2.01	122.27	124.53

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1342	LDA	N1-C1-C2-C3
9	A	1346	C8E	O9-C10-C11-O12
9	A	1343	C8E	O9-C10-C11-O12
9	A	1347	C8E	O9-C10-C11-O12
9	A	1343	C8E	C6-C7-C8-O9
9	A	1346	C8E	O15-C16-C17-O18
9	A	1343	C8E	O12-C13-C14-O15
9	A	1345	C8E	C6-C7-C8-O9
9	A	1344	C8E	C6-C7-C8-O9
9	A	1344	C8E	O12-C13-C14-O15
9	A	1347	C8E	O18-C19-C20-O21
9	A	1348	C8E	O9-C10-C11-O12
6	A	1334	PLM	C3-C4-C5-C6
7	A	1341	PEF	C11-C12-C13-C14
9	A	1343	C8E	C3-C4-C5-C6
9	A	1345	C8E	C2-C3-C4-C5
8	A	1342	LDA	C4-C5-C6-C7
6	A	1334	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
9	A	1348	C8E	C4-C5-C6-C7
7	A	1341	PEF	C33-C34-C35-C36
6	A	1334	PLM	C5-C6-C7-C8
6	A	1334	PLM	C6-C7-C8-C9
9	A	1347	C8E	C2-C3-C4-C5
9	A	1348	C8E	C2-C3-C4-C5
9	A	1346	C8E	O12-C13-C14-O15
9	A	1345	C8E	C7-C8-O9-C10
9	A	1347	C8E	O12-C13-C14-O15
9	A	1343	C8E	C2-C3-C4-C5
9	A	1347	C8E	O15-C16-C17-O18
7	A	1341	PEF	C32-C33-C34-C35
9	A	1344	C8E	O9-C10-C11-O12
6	A	1333	PLM	C2-C3-C4-C5
6	A	1334	PLM	CB-CC-CD-CE
7	A	1341	PEF	C36-C37-C38-C39
9	A	1343	C8E	C4-C5-C6-C7
9	A	1345	C8E	C1-C2-C3-C4
6	A	1334	PLM	CD-CE-CF-CG
9	A	1348	C8E	C1-C2-C3-C4
6	A	1334	PLM	C1-C2-C3-C4
9	A	1346	C8E	C2-C3-C4-C5
7	A	1341	PEF	C35-C36-C37-C38
7	A	1341	PEF	C37-C38-C39-C40
7	A	1341	PEF	C10-C11-C12-C13
9	A	1343	C8E	C17-C16-O15-C14
9	A	1348	C8E	C7-C8-O9-C10
6	A	1334	PLM	CA-CB-CC-CD
8	A	1342	LDA	C1-C2-C3-C4
9	A	1343	C8E	C11-C10-O9-C8
6	A	1334	PLM	C8-C9-CA-CB
9	A	1344	C8E	C5-C6-C7-C8
8	A	1342	LDA	C2-C1-N1-CM1
8	A	1342	LDA	C2-C1-N1-CM2
9	A	1348	C8E	C11-C10-O9-C8
9	A	1347	C8E	C20-C19-O18-C17
9	A	1346	C8E	C17-C16-O15-C14
9	A	1347	C8E	C7-C8-O9-C10
6	A	1333	PLM	C9-CA-CB-CC
7	A	1341	PEF	C12-C13-C14-C15
6	A	1333	PLM	CC-CD-CE-CF
9	A	1344	C8E	C7-C8-O9-C10

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Mol	Chain	Res	Type	Atoms
9	A	1344	C8E	C11-C10-O9-C8
9	A	1343	C8E	C14-C13-O12-C11
9	A	1346	C8E	C14-C13-O12-C11
9	A	1347	C8E	C13-C14-O15-C16
9	A	1345	C8E	C3-C4-C5-C6
9	A	1344	C8E	C10-C11-O12-C13
9	A	1347	C8E	C17-C16-O15-C14
9	A	1343	C8E	C7-C8-O9-C10
9	A	1343	C8E	C10-C11-O12-C13
6	A	1333	PLM	O1-C1-C2-C3
9	A	1343	C8E	C13-C14-O15-C16
5	A	1332	RET	C10-C11-C12-C13
9	A	1347	C8E	C16-C17-O18-C19
7	A	1341	PEF	C31-C32-C33-C34
7	A	1341	PEF	C13-C14-C15-C16
6	A	1333	PLM	C5-C6-C7-C8
6	A	1333	PLM	C3-C4-C5-C6
9	A	1346	C8E	C4-C5-C6-C7
9	A	1344	C8E	C2-C3-C4-C5
6	A	1333	PLM	CD-CE-CF-CG
6	A	1334	PLM	C9-CA-CB-CC
9	A	1348	C8E	C3-C4-C5-C6
9	A	1346	C8E	C13-C14-O15-C16
9	A	1347	C8E	C11-C10-O9-C8
9	A	1346	C8E	C5-C6-C7-C8
9	A	1344	C8E	C3-C4-C5-C6
9	A	1347	C8E	C10-C11-O12-C13
6	A	1333	PLM	C7-C8-C9-CA
9	A	1347	C8E	C14-C13-O12-C11
6	A	1334	PLM	C4-C5-C6-C7
8	A	1342	LDA	C2-C1-N1-O1
8	A	1342	LDA	C3-C4-C5-C6
9	A	1347	C8E	C1-C2-C3-C4
9	A	1346	C8E	C7-C8-O9-C10

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1342	LDA	2	0
9	A	1346	C8E	1	0
6	A	1333	PLM	1	0

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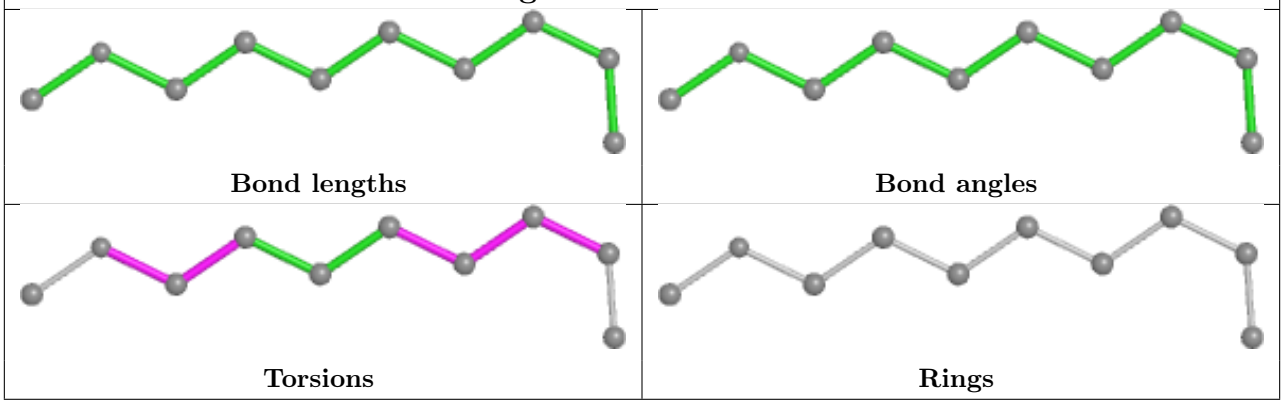
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1332	RET	2	0
9	A	1344	C8E	2	0
6	A	1334	PLM	1	0

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 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 C8E A 1345



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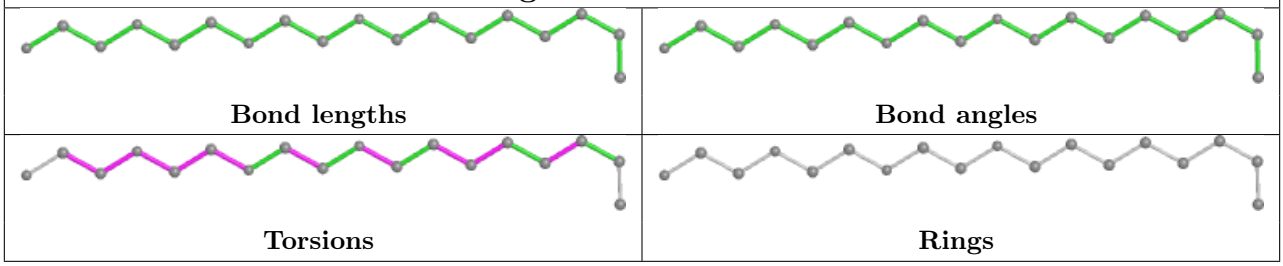
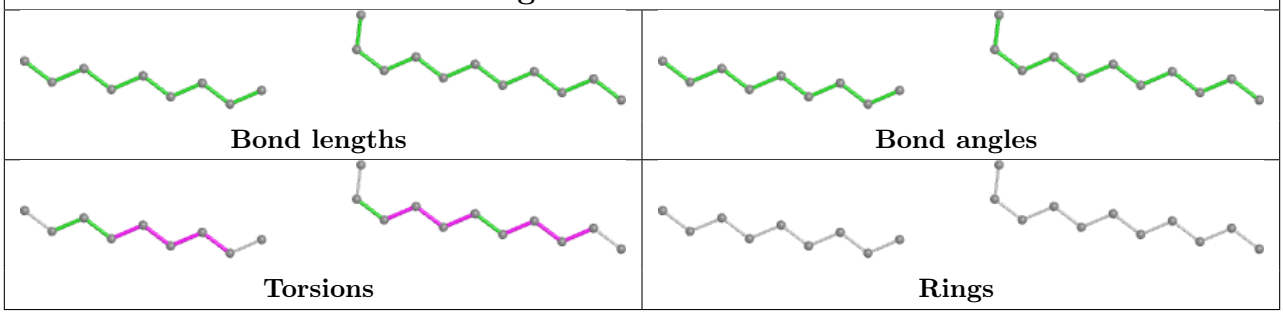
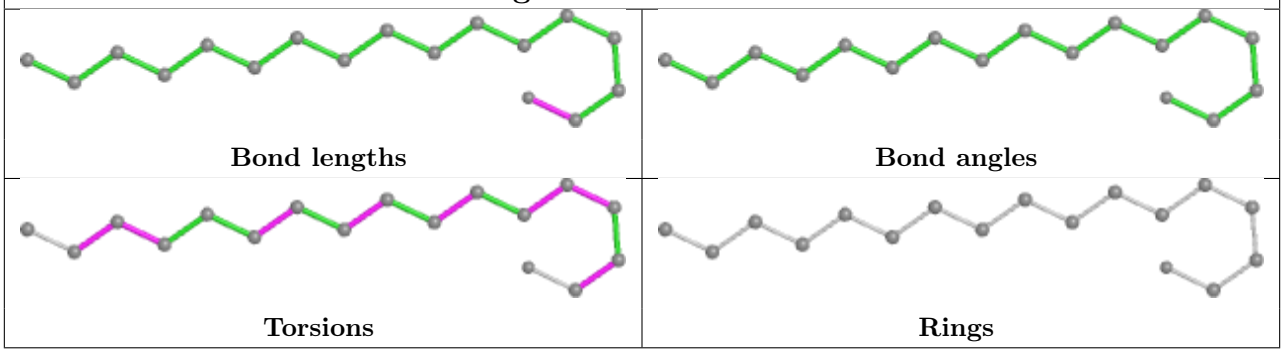


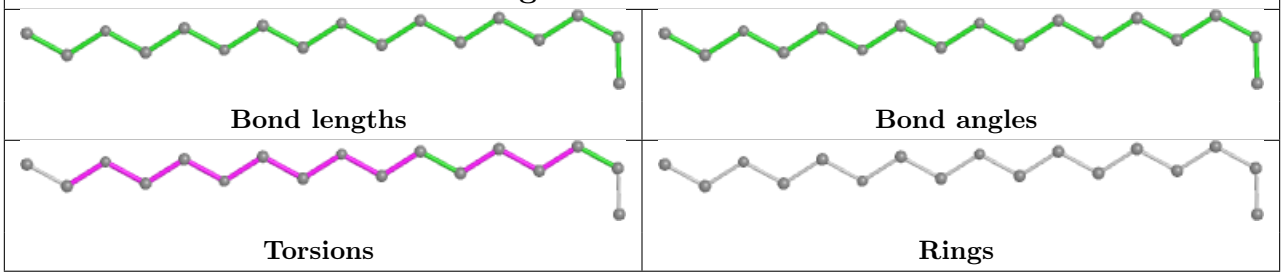
Ligand PEF A 1341



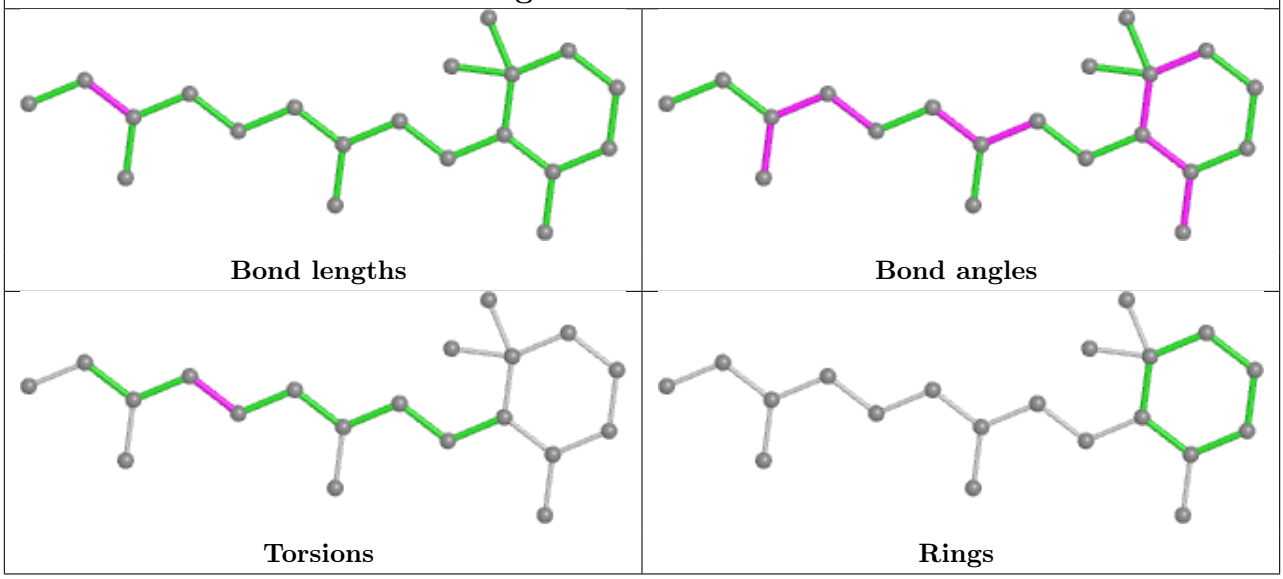
Ligand PLM A 1333



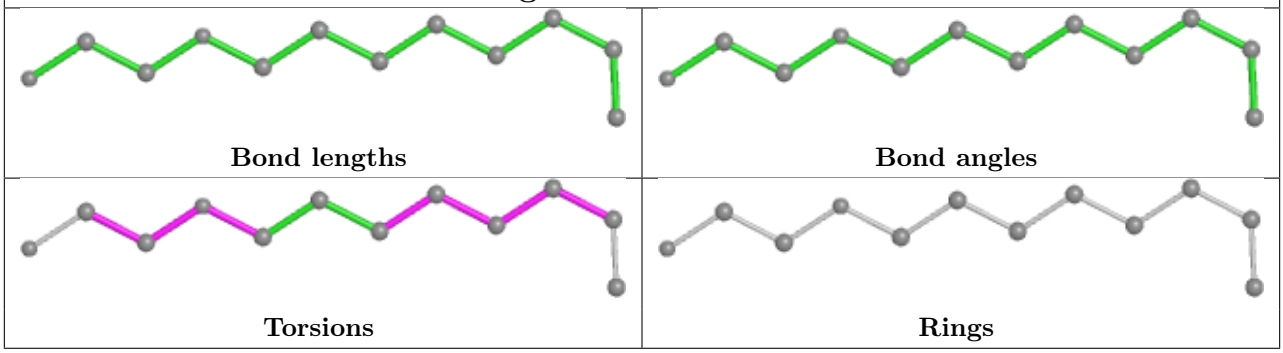
Ligand C8E A 1343



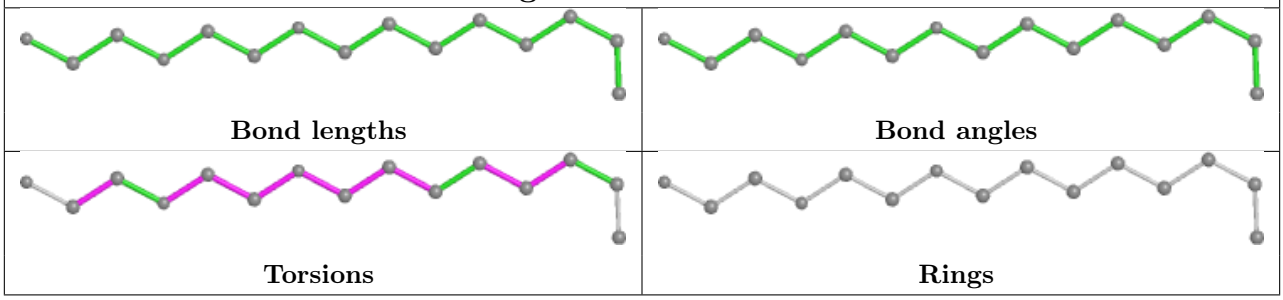
Ligand RET A 1332



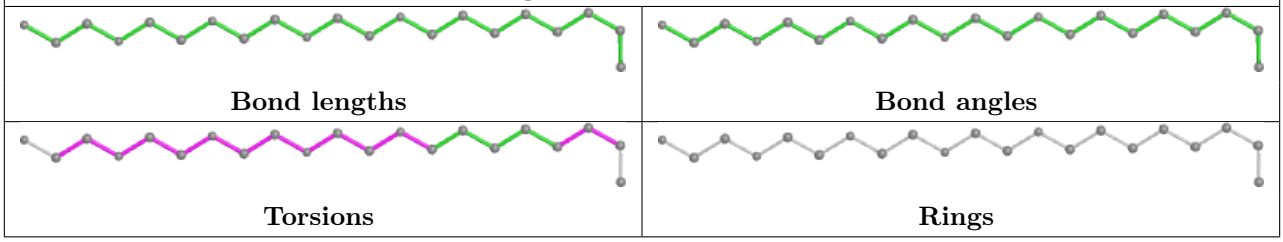
Ligand C8E A 1348



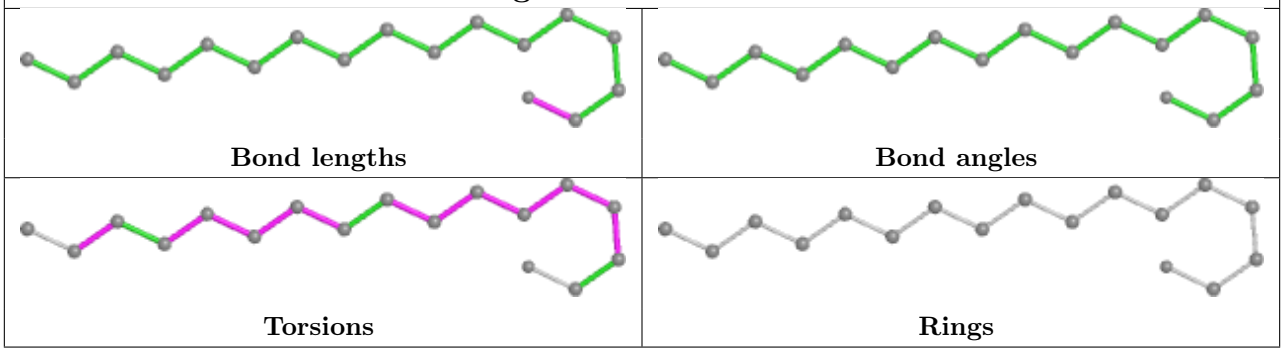
Ligand C8E A 1344



Ligand C8E A 1347



Ligand PLM A 1334



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	329/348 (94%)	0.09	17 (5%) 27 24	44, 57, 124, 183	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	ALA	6.3
1	A	236	GLN	6.1
1	A	235	ALA	6.1
1	A	233	ALA	5.8
1	A	238	GLN	5.8
1	A	241	ALA	4.8
1	A	145	ASN	4.5
1	A	144	SER	4.5
1	A	143	MET	4.0
1	A	237	GLN	3.8
1	A	1	MET	3.5
1	A	232	GLU	3.4
1	A	243	THR	3.0
1	A	324	GLY	2.9
1	A	148	PHE	2.5
1	A	326	ASN	2.4
1	A	286	ILE	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)

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,

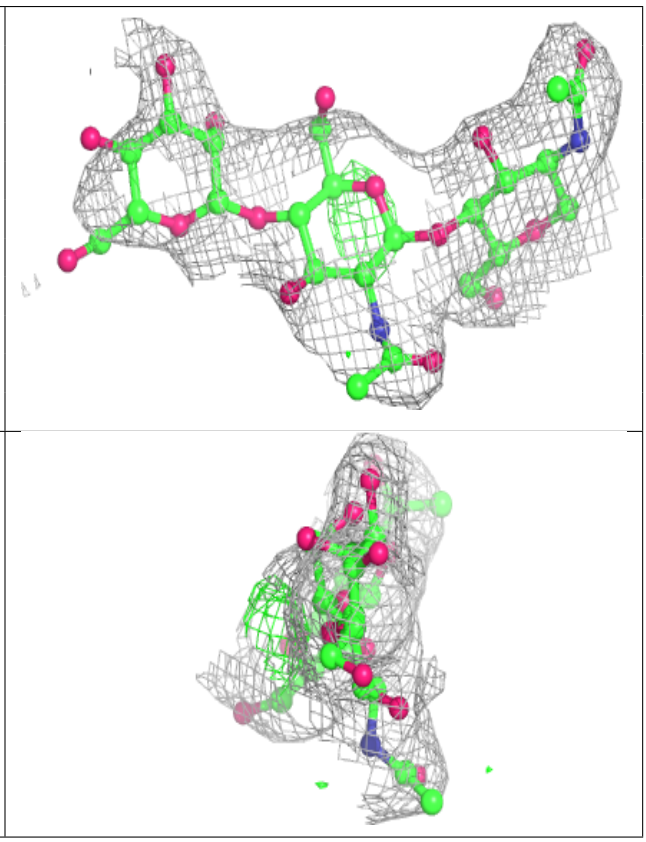
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	2	14/15	0.83	0.26	117,126,136,142	0
2	BMA	B	3	11/12	0.85	0.43	141,147,150,151	0
2	BMA	C	3	11/12	0.85	0.14	130,136,140,141	0
2	NAG	C	1	14/15	0.91	0.21	82,96,104,114	0
2	NAG	C	2	14/15	0.93	0.24	118,126,132,135	0
2	NAG	B	1	14/15	0.97	0.19	81,90,101,107	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.

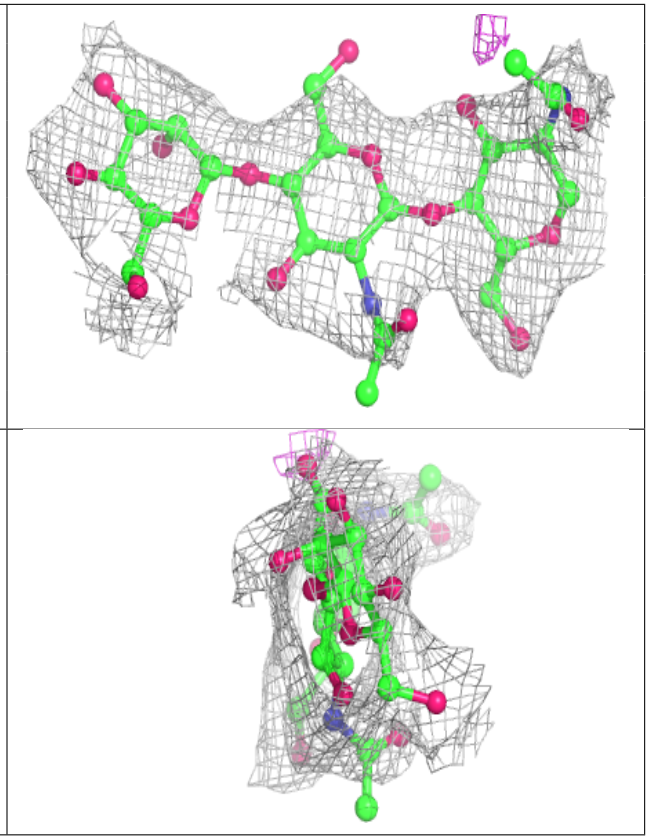
Electron density around Chain B:

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 Chain C:

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



6.4 Ligands (i)

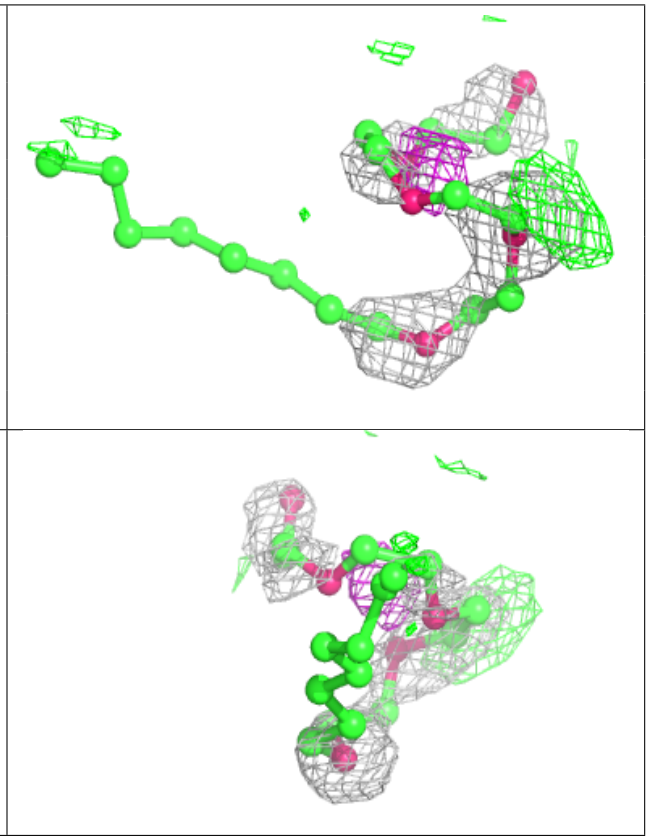
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	C8E	A	1347	21/21	0.57	0.54	80,100,122,133	0
9	C8E	A	1348	12/21	0.74	0.42	76,81,89,100	0
9	C8E	A	1343	17/21	0.86	0.36	65,72,80,86	0
9	C8E	A	1346	18/21	0.86	0.32	62,73,95,103	0
4	ACE	A	0	3/3	0.86	0.76	100,100,102,105	0
6	PLM	A	1334	17/18	0.86	0.38	76,84,93,94	0
8	LDA	A	1342	16/16	0.88	0.21	54,61,78,79	0
7	PEF	A	1341	20/47	0.89	0.26	45,65,94,95	0
9	C8E	A	1345	10/21	0.92	0.25	54,69,78,88	0
9	C8E	A	1344	15/21	0.92	0.20	54,67,83,86	0
3	ZN	A	1349	1/1	0.93	0.08	95,95,95,95	1
6	PLM	A	1333	17/18	0.94	0.28	58,66,87,89	0
5	RET	A	1332	20/21	0.97	0.21	45,51,56,57	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.

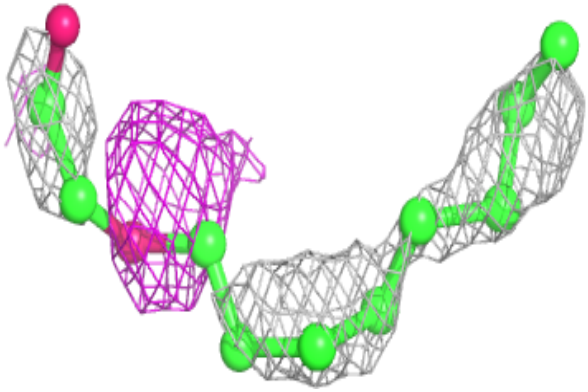
Electron density around C8E A 1347:

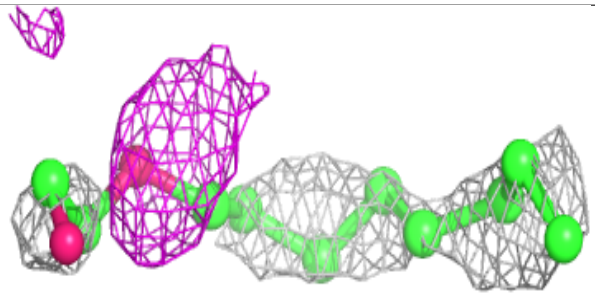
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

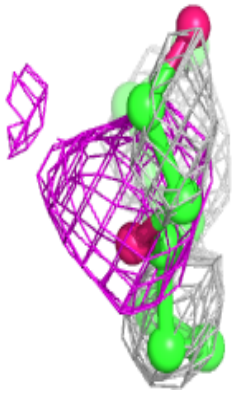


Electron density around C8E A 1348:

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

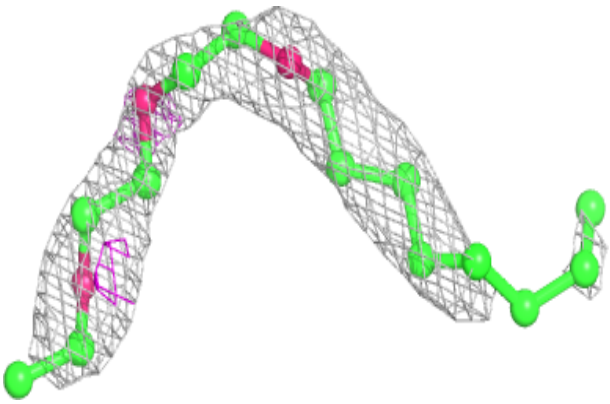


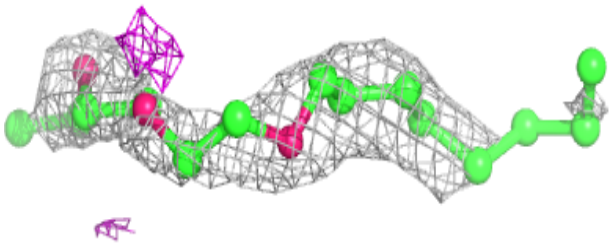


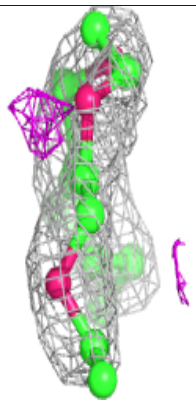


Electron density around C8E A 1343:

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

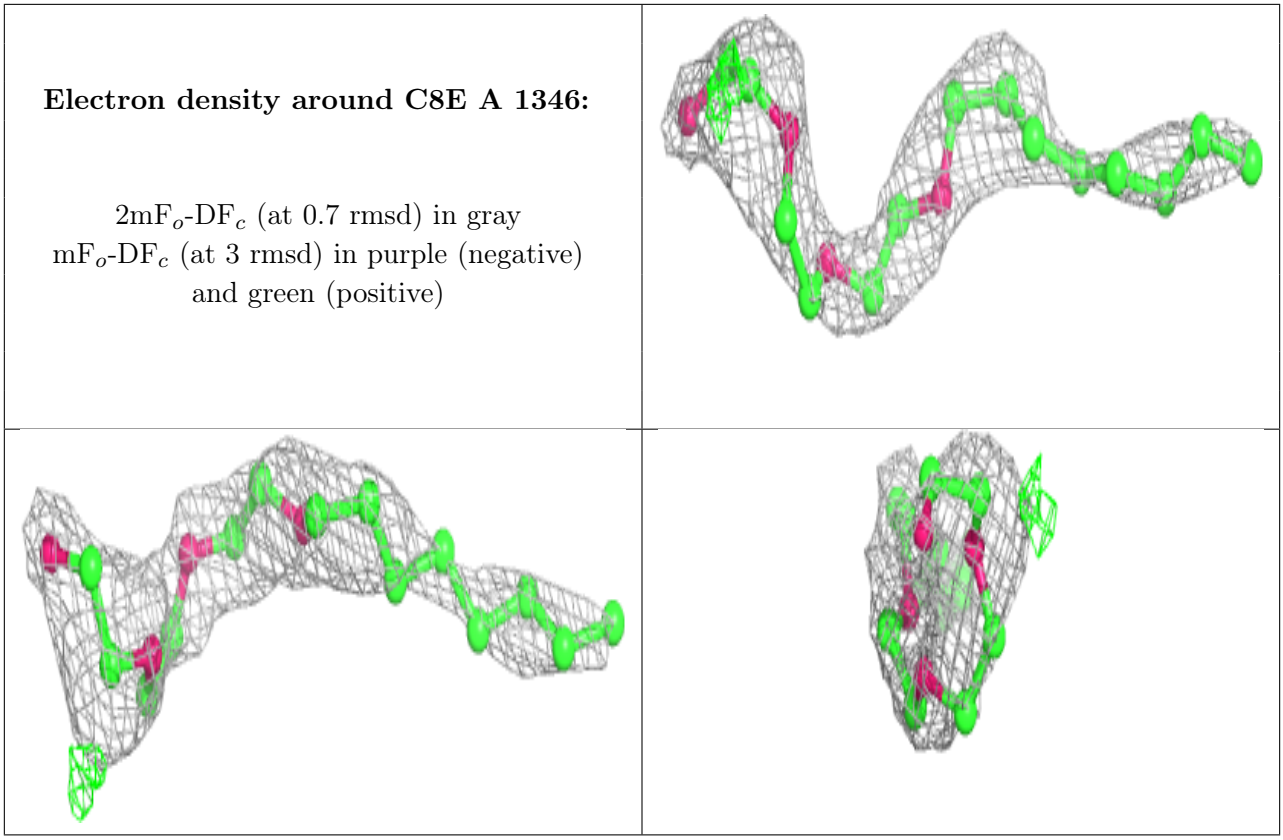






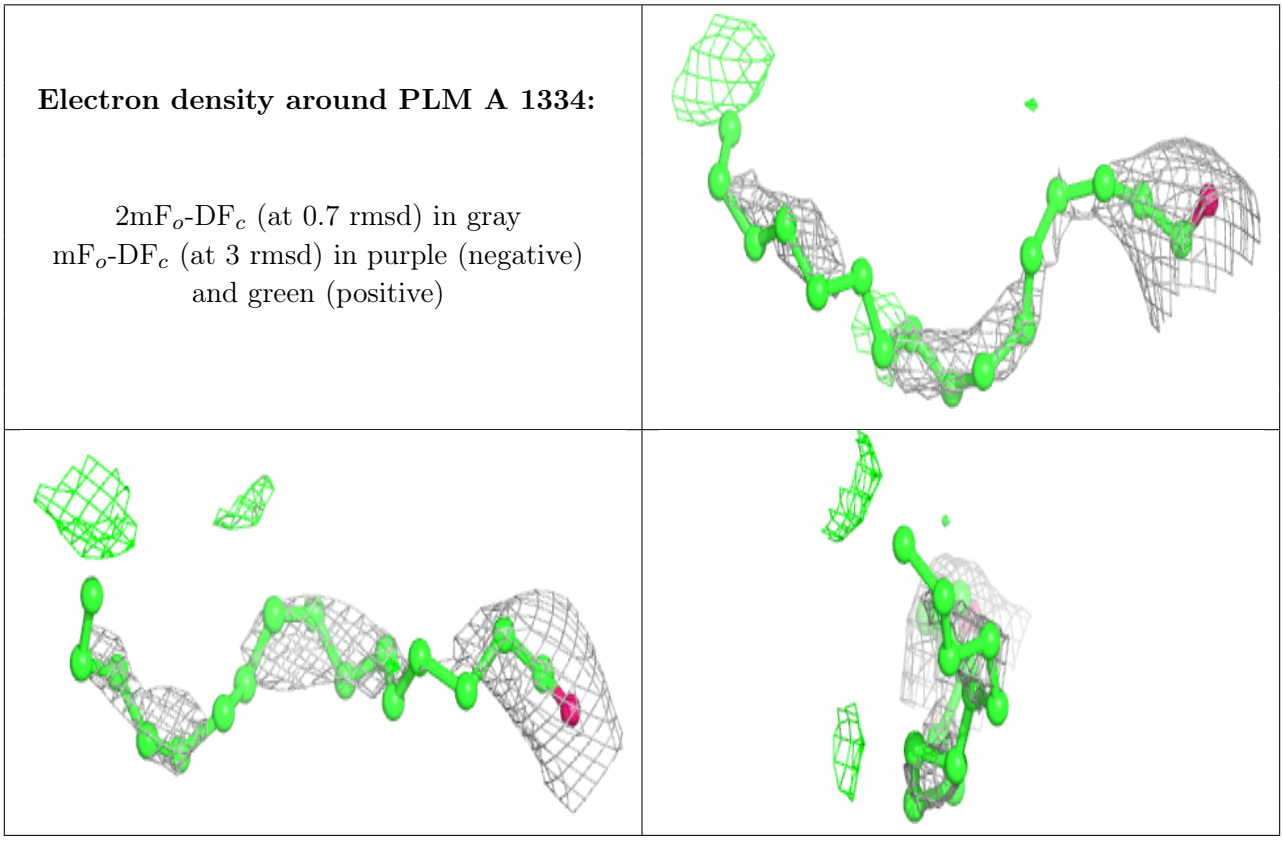
Electron density around C8E A 1346:

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



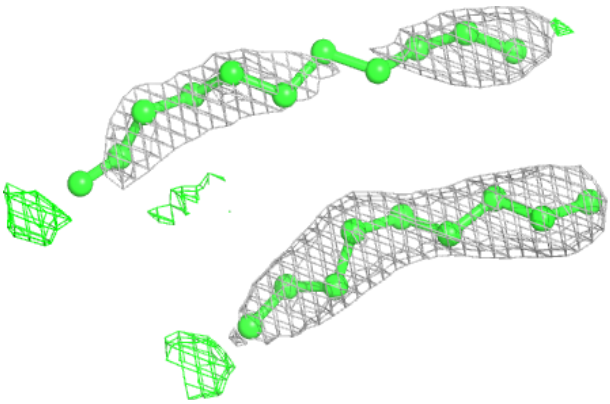
Electron density around PLM A 1334:

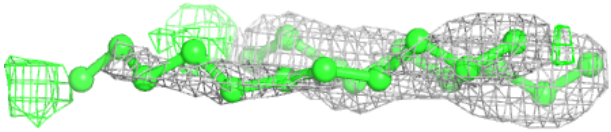
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

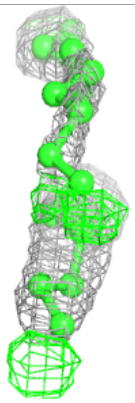


Electron density around PEF A 1341:

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

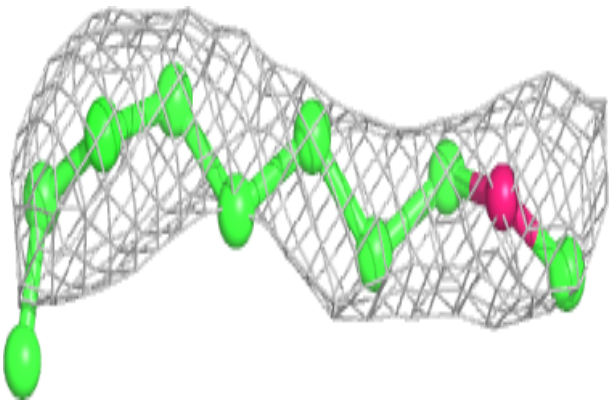


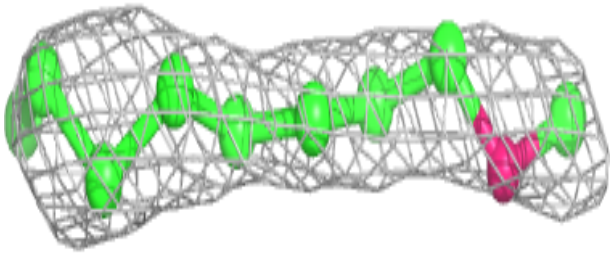


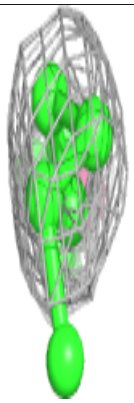


Electron density around C8E A 1345:

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

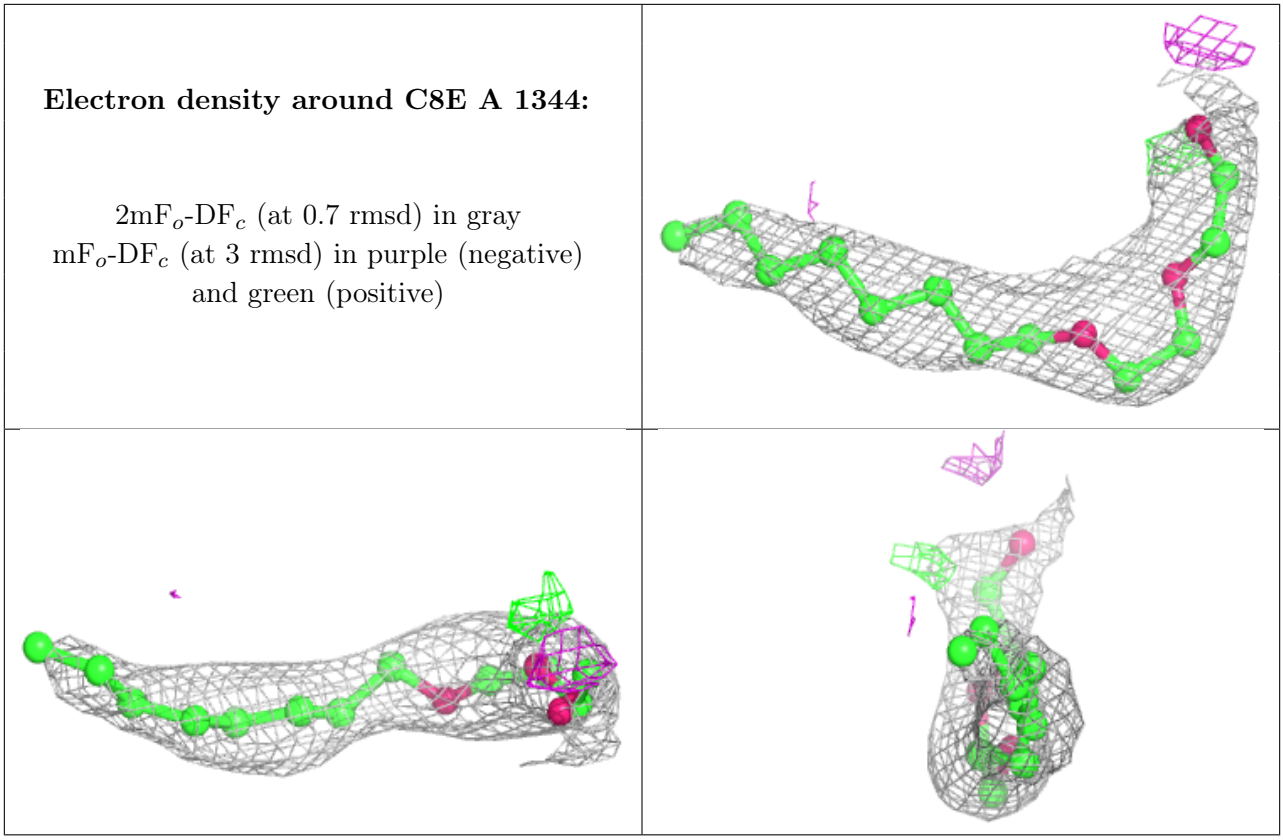






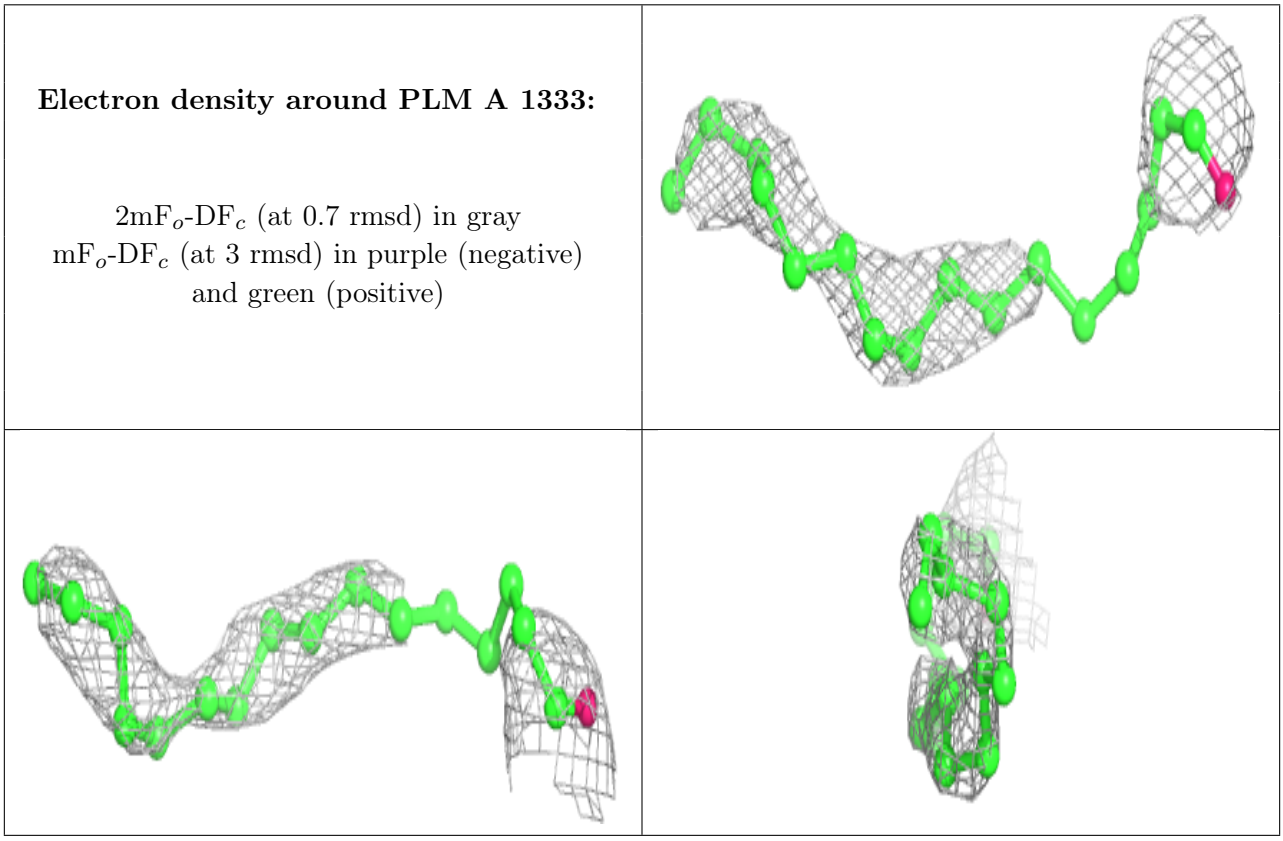
Electron density around C8E A 1344:

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



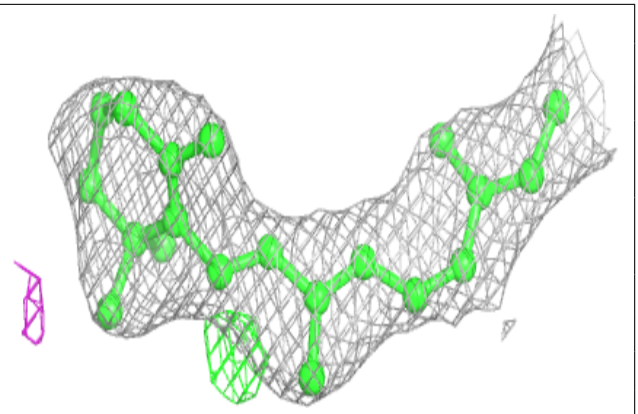
Electron density around PLM A 1333:

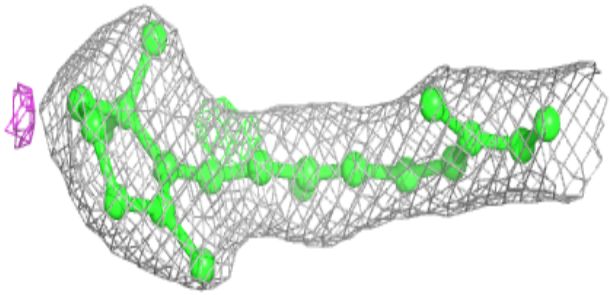
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

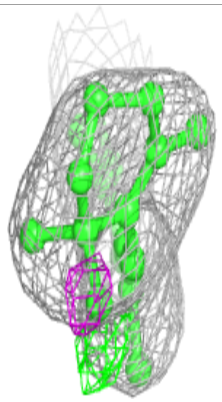


Electron density around RET A 1332:

$2mF_o$-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.