



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:30 PM UTC

PDB ID : 5EN0 / pdb_00005en0
Title : Crystal Structure of T94I rhodopsin mutant
Authors : Singhal, A.; Guo, Y.; Matkovic, M.; Schertler, G.; Deupi, X.; Yan, E.; Standfuss, J.
Deposited on : 2015-11-08
Resolution : 2.81 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

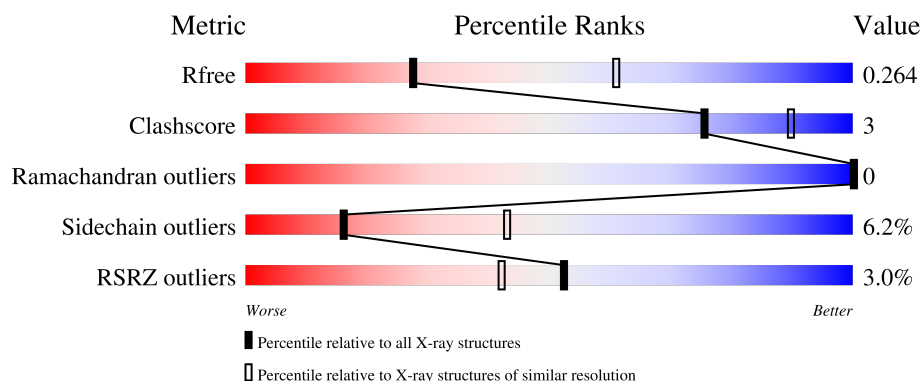
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 $\leq 5\%$. 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	349	3% 81% 11% 6%
2	B	11	9% 73% 18% 9%
3	C	4	100%

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
1	ACE	A	0	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 2863 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	327	Total	C	N	O	S	0	0	0
			2592	1727	399	438	28			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P02699
A	2	CYS	ASN	engineered mutation	UNP P02699
A	94	ILE	THR	engineered mutation	UNP P02699
A	282	CYS	ASP	engineered mutation	UNP P02699

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(t) subunit alpha-3.

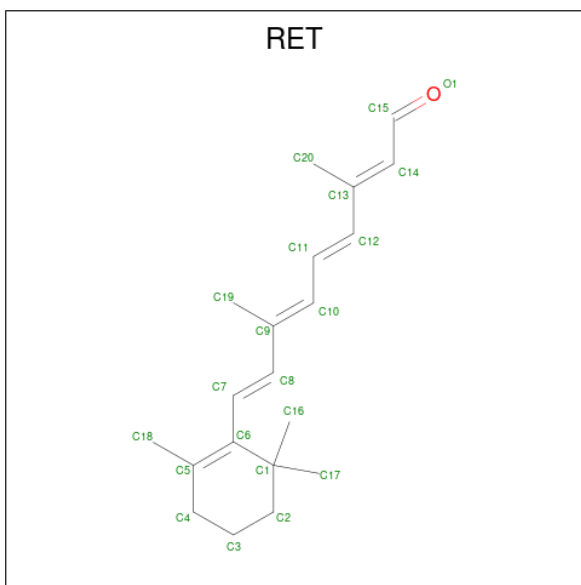
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			89	59	13	17			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



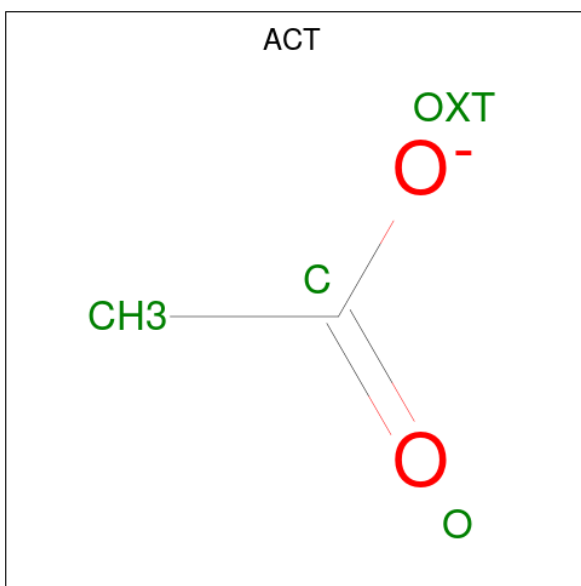
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is RETINAL (CCD ID: RET) (formula: C₂₀H₂₈O).



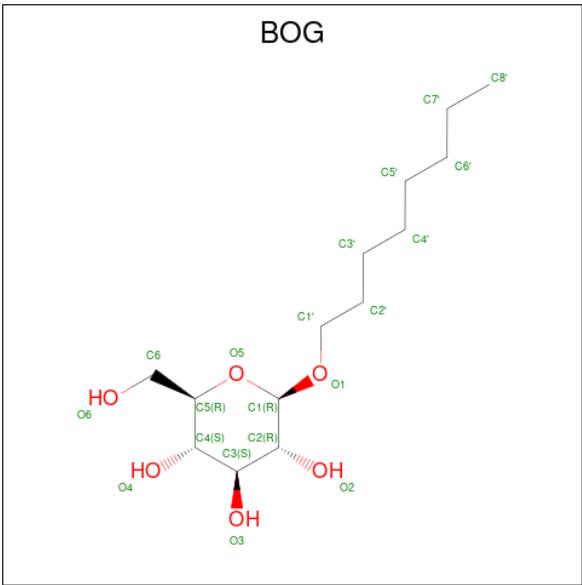
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			20	20		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



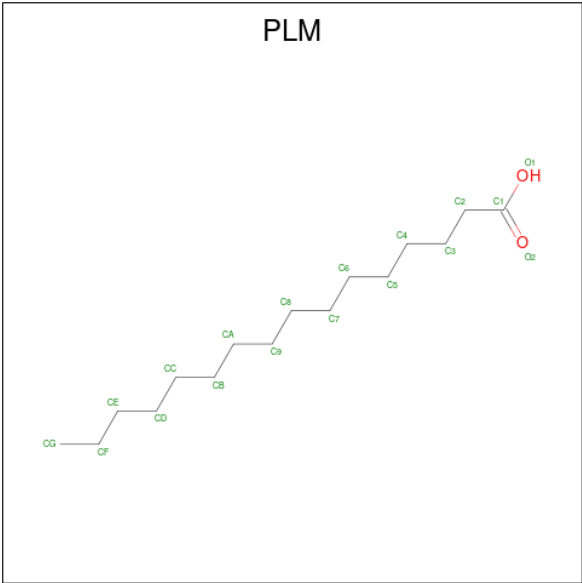
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



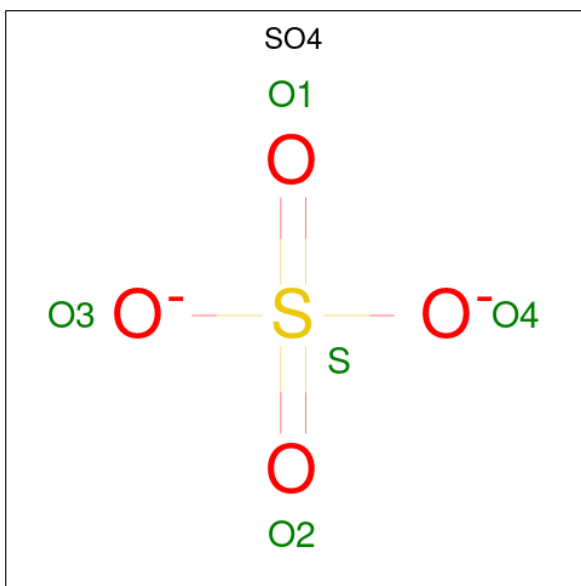
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	14	6		
6	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 7 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

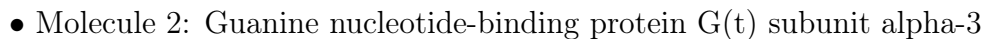


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	25	Total	O	0	0
			25	25		

- Molecule 1: Rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	242.27Å 242.27Å 111.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.81 30.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.81) 99.5 (30.00-2.81)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.207 , 0.253 0.220 , 0.264	Depositor DCC
R_{free} test set	1569 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2863	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, RET, ACE, BMA, BOG, ACT, NAG, PLM, MAN

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	1.09	3/2672 (0.1%)	1.19	6/3640 (0.2%)
2	B	1.04	0/89	1.33	0/117
All	All	1.09	3/2761 (0.1%)	1.19	6/3757 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	N-CA	6.80	1.59	1.46
1	A	282	CYS	CA-C	-6.22	1.45	1.52
1	A	302	ASN	C-O	-6.07	1.18	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	CYS	CA-CB-SG	-8.05	95.88	114.40
1	A	322	CYS	CA-CB-SG	-7.76	96.56	114.40
1	A	2	CYS	CA-CB-SG	-7.62	96.89	114.40
1	A	106	GLY	CA-C-N	6.46	126.23	119.05
1	A	106	GLY	C-N-CA	6.46	126.23	119.05
1	A	257	MET	CG-SD-CE	-5.17	89.52	100.90

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	2592	0	2569	15	0
2	B	89	0	93	1	0
3	C	50	0	43	0	0
4	A	20	0	27	1	0
5	A	8	0	6	0	0
6	A	40	0	56	0	0
7	A	34	0	62	0	0
8	A	5	0	0	0	0
9	A	25	0	0	1	0
All	All	2863	0	2856	17	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 (17) 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:135:ARG:HH12	1:A:257:MET:HE1	1.45	0.82
1:A:176:SER:O	9:A:501:HOH:O	2.04	0.74
4:A:401:RET:C8	4:A:401:RET:H181	2.33	0.57
1:A:135:ARG:NH1	1:A:257:MET:HE1	2.16	0.56
1:A:6:GLY:HA3	1:A:9:PHE:CZ	2.43	0.54
1:A:277:THR:O	1:A:278:HIS:ND1	2.44	0.50
1:A:193:THR:HG22	1:A:195:HIS:HB2	1.93	0.50
1:A:231:LYS:NZ	1:A:247:GLU:OE2	2.43	0.49
2:B:343:ASN:O	2:B:347:VAL:HB	2.13	0.48
1:A:94:ILE:HG12	1:A:186:SER:HB3	1.97	0.47
1:A:96:TYR:O	1:A:100:HIS:HD2	1.99	0.46
1:A:93:THR:HG21	1:A:113:GLU:HG3	1.99	0.44
1:A:143:MET:HE3	1:A:146:PHE:CG	2.54	0.42
1:A:61:VAL:HG13	1:A:68:LEU:CD1	2.50	0.42
1:A:41:ALA:HB1	1:A:95:LEU:HD12	2.02	0.41
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.90	0.41
1:A:322:CYS:C	1:A:323:CYS:SG	3.04	0.41

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	325/349 (93%)	301 (93%)	24 (7%)	0	100	100
2	B	9/11 (82%)	9 (100%)	0	0	100	100
All	All	334/360 (93%)	310 (93%)	24 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	278/296 (94%)	262 (94%)	16 (6%)	18	47
2	B	10/10 (100%)	8 (80%)	2 (20%)	1	4
All	All	288/306 (94%)	270 (94%)	18 (6%)	16	43

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	CYS
1	A	7	PRO
1	A	19	VAL
1	A	61	VAL
1	A	64	GLN
1	A	66	LYS
1	A	108	THR
1	A	154	ILE

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Mol	Chain	Res	Type
1	A	215	PRO
1	A	226	LEU
1	A	242	THR
1	A	245	LYS
1	A	249	GLU
1	A	293	PHE
1	A	323	CYS
1	A	326	ASN
2	B	340	ILE
2	B	347	VAL

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	111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	ACE	A	0	1	1,2,2	0.92	0	0,1,1	-	-

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.

5.5 Carbohydrates

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1	3,1	14,14,15	0.61	0	17,19,21	1.41	2 (11%)
3	NAG	C	2	3	14,14,15	1.22	1 (7%)	17,19,21	1.83	5 (29%)
3	BMA	C	3	3	11,11,12	1.22	0	15,15,17	2.57	9 (60%)
3	MAN	C	4	3	11,11,12	0.70	0	15,15,17	1.99	2 (13%)

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
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O5-C1	2.77	1.48	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	6.58	121.00	112.19
3	C	3	BMA	C3-C4-C5	5.63	120.43	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	O6-C6-C5	4.46	126.52	111.33
3	C	3	BMA	O5-C5-C6	4.17	115.77	107.66
3	C	3	BMA	C1-C2-C3	3.86	115.27	109.64
3	C	1	NAG	O7-C7-N2	2.94	127.17	121.98
3	C	4	MAN	O5-C1-C2	-2.79	104.14	110.79
3	C	2	NAG	O3-C3-C2	-2.78	103.64	109.40
3	C	2	NAG	O3-C3-C4	2.59	116.47	110.38
3	C	3	BMA	O5-C1-C2	-2.56	104.68	110.79
3	C	2	NAG	O5-C5-C4	-2.49	104.77	110.83
3	C	1	NAG	C2-N2-C7	2.36	126.06	122.90
3	C	3	BMA	O3-C3-C2	-2.24	105.48	110.05
3	C	3	BMA	C2-C3-C4	2.11	114.57	110.86
3	C	2	NAG	O5-C5-C6	2.09	111.73	107.66
3	C	3	BMA	O2-C2-C1	-2.03	104.57	109.22
3	C	3	BMA	C1-O5-C5	2.03	114.90	112.19
3	C	3	BMA	O2-C2-C3	-2.01	106.00	110.15

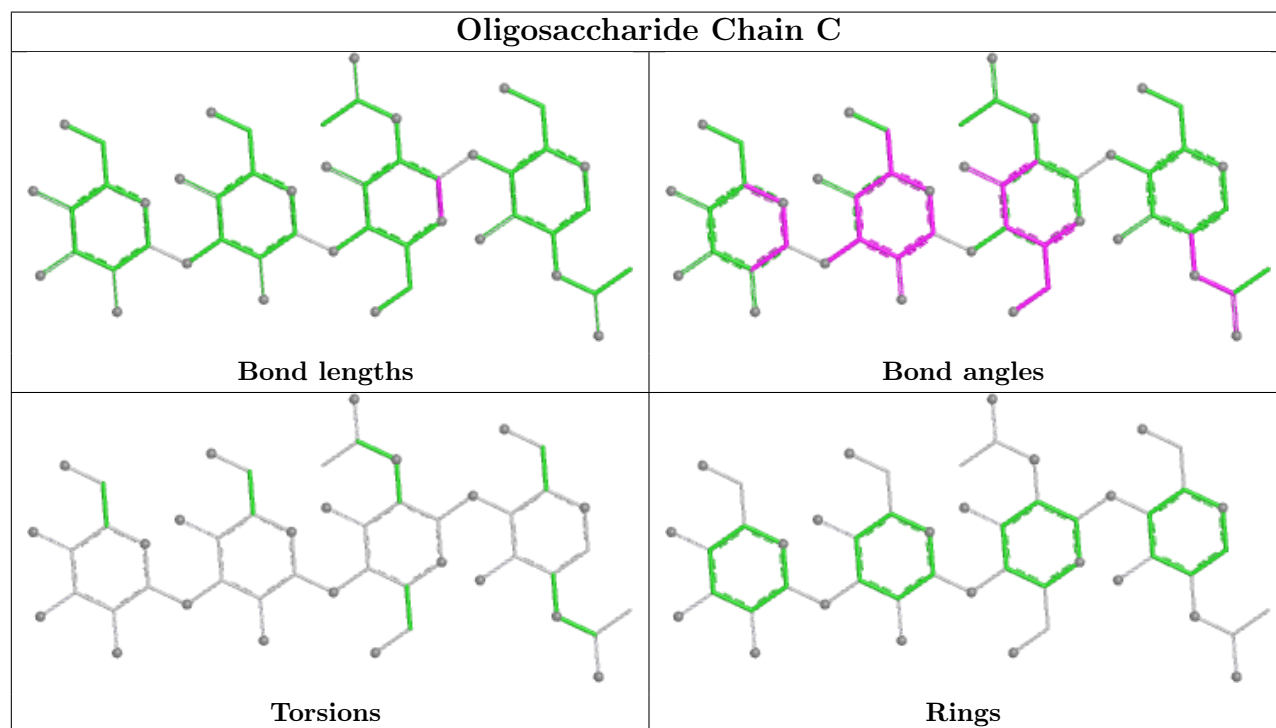
There are no chirality outliers.

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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PLM	A	405	1	15,16,17	0.55	0	14,15,17	0.36	0
6	BOG	A	404	-	20,20,20	0.76	1 (5%)	25,25,25	1.63	7 (28%)
5	ACT	A	403	-	3,3,3	0.87	0	3,3,3	0.84	0
6	BOG	A	411	-	20,20,20	0.87	1 (5%)	25,25,25	1.86	7 (28%)
5	ACT	A	402	-	3,3,3	0.99	0	3,3,3	2.00	1 (33%)
4	RET	A	401	1	20,20,21	0.95	1 (5%)	27,27,28	1.68	8 (29%)
7	PLM	A	406	1	15,16,17	0.49	0	14,15,17	0.81	0
8	SO4	A	412	-	4,4,4	0.49	0	6,6,6	0.35	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
7	PLM	A	405	1	-	6/14/14/15	-
6	BOG	A	404	-	-	7/11/31/31	0/1/1/1
6	BOG	A	411	-	-	4/11/31/31	0/1/1/1
4	RET	A	401	1	-	0/13/30/31	0/1/1/1
7	PLM	A	406	1	-	4/14/14/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	411	BOG	O1-C1	2.45	1.44	1.40
4	A	401	RET	C14-C13	2.41	1.35	1.33
6	A	404	BOG	O1-C1	2.32	1.44	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	411	BOG	C4-C3-C2	4.73	119.14	110.83
6	A	411	BOG	O5-C5-C4	-4.23	102.08	109.70
6	A	411	BOG	O3-C3-C4	-3.50	102.14	110.38
4	A	401	RET	C8-C9-C10	-3.27	113.87	119.01
6	A	404	BOG	C4-C3-C2	-3.26	105.10	110.83
4	A	401	RET	C18-C5-C6	-3.26	120.93	124.48
5	A	402	ACT	OXT-C-CH3	2.80	126.79	115.05
4	A	401	RET	C19-C9-C8	2.76	122.30	118.09
4	A	401	RET	C11-C10-C9	-2.75	123.43	127.28
6	A	404	BOG	O5-C5-C6	2.68	113.09	106.44
6	A	404	BOG	C1-C2-C3	-2.68	104.37	110.01
6	A	404	BOG	C1-O5-C5	2.63	118.85	113.72
4	A	401	RET	C10-C11-C12	-2.54	115.85	123.20
4	A	401	RET	C11-C12-C13	-2.49	119.55	126.36
6	A	404	BOG	C3-C4-C5	-2.43	105.83	110.23
4	A	401	RET	C8-C7-C6	-2.41	120.56	127.00
4	A	401	RET	C7-C8-C9	-2.33	122.79	126.23
6	A	411	BOG	O4-C4-C5	2.25	114.86	109.32
6	A	411	BOG	O4-C4-C3	-2.22	105.13	110.38
6	A	411	BOG	O5-C1-C2	2.11	114.70	110.37
6	A	404	BOG	O5-C5-C4	-2.06	105.98	109.70
6	A	404	BOG	O3-C3-C4	2.06	115.24	110.38
6	A	411	BOG	C1-C2-C3	2.04	114.30	110.01

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	404	BOG	C4-C5-C6-O6
6	A	404	BOG	C2'-C1'-O1-C1
6	A	411	BOG	O5-C5-C6-O6
7	A	406	PLM	C4-C5-C6-C7
7	A	406	PLM	C6-C7-C8-C9
6	A	404	BOG	C4'-C5'-C6'-C7'
7	A	405	PLM	CB-CC-CD-CE
6	A	404	BOG	O5-C5-C6-O6
6	A	411	BOG	C4-C5-C6-O6
7	A	406	PLM	C3-C4-C5-C6
6	A	404	BOG	C3'-C4'-C5'-C6'
7	A	405	PLM	CA-CB-CC-CD
6	A	411	BOG	C3'-C4'-C5'-C6'
7	A	405	PLM	C6-C7-C8-C9
6	A	404	BOG	C1'-C2'-C3'-C4'

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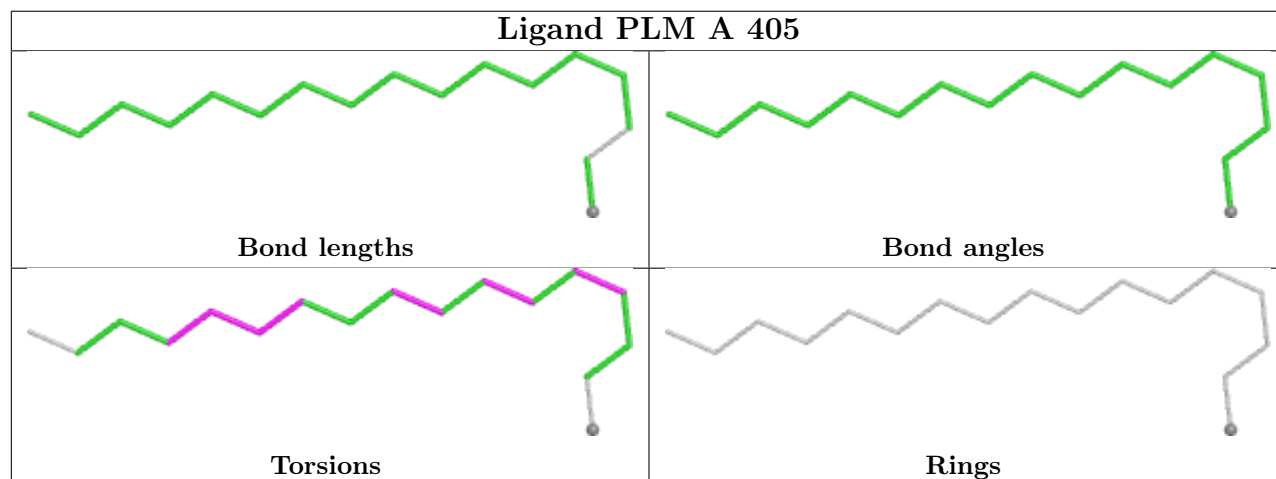
Mol	Chain	Res	Type	Atoms
7	A	406	PLM	C9-CA-CB-CC
7	A	405	PLM	C9-CA-CB-CC
6	A	411	BOG	C5'-C6'-C7'-C8'
6	A	404	BOG	O1-C1'-C2'-C3'
7	A	405	PLM	C4-C5-C6-C7
7	A	405	PLM	C2-C3-C4-C5

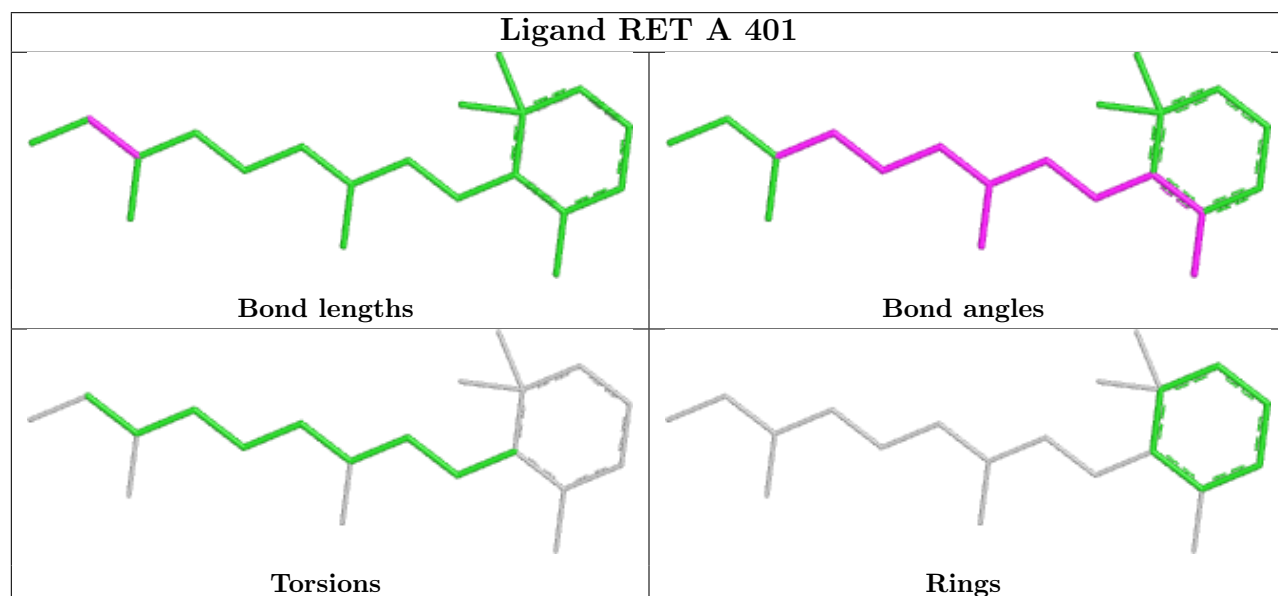
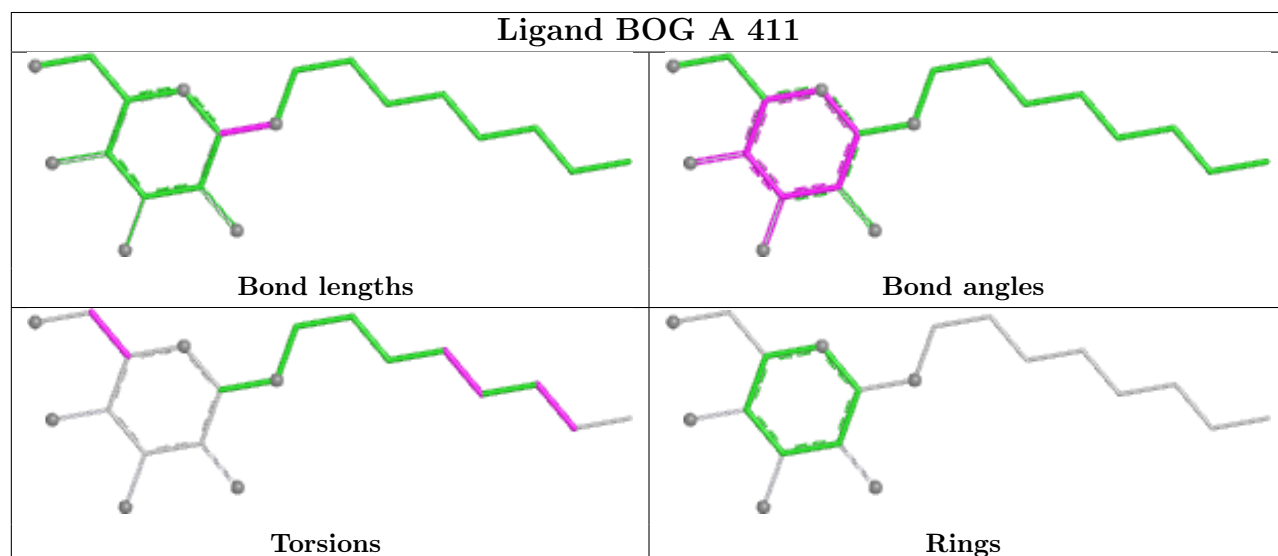
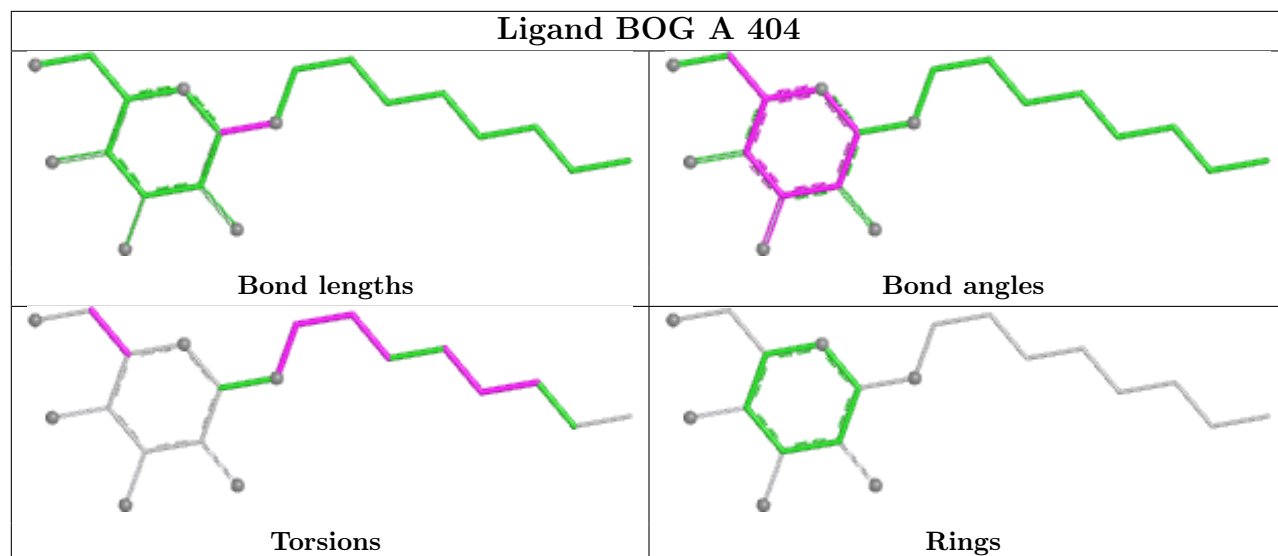
There are no ring outliers.

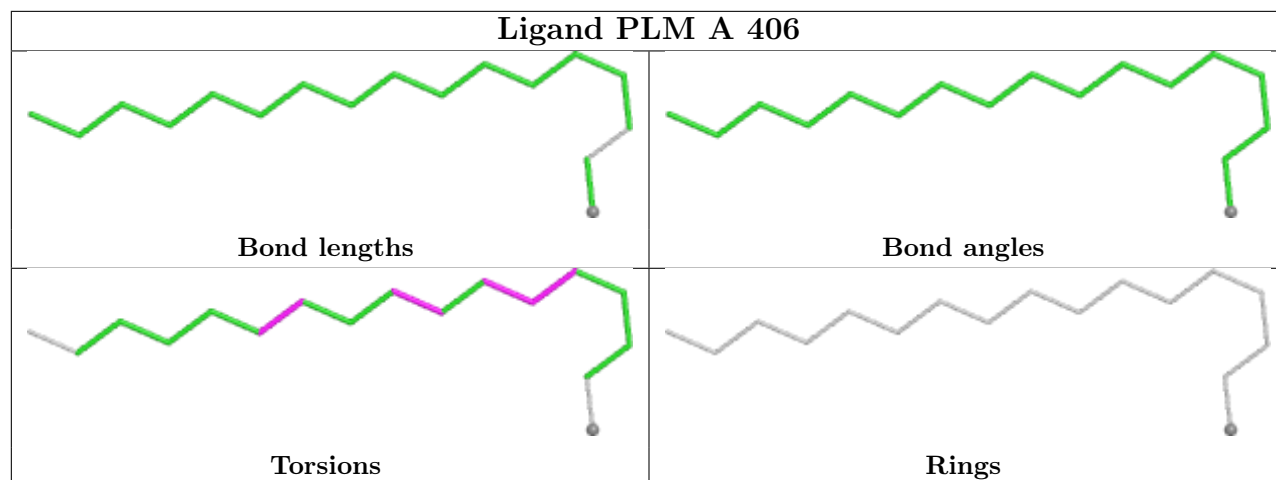
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	RET	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 [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	326/349 (93%)	-0.19	9 (2%) 55 44	36, 55, 81, 120	0
2	B	11/11 (100%)	0.48	1 (9%) 15 11	55, 66, 87, 92	0
All	All	337/360 (93%)	-0.17	10 (2%) 52 42	36, 55, 84, 120	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	340	ILE	5.1
1	A	311	LYS	4.6
1	A	312	GLN	4.2
1	A	283	PHE	3.1
1	A	2	CYS	2.9
1	A	66	LYS	2.8
1	A	325	LYS	2.5
1	A	282	CYS	2.5
1	A	145	ASN	2.2
1	A	8	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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.

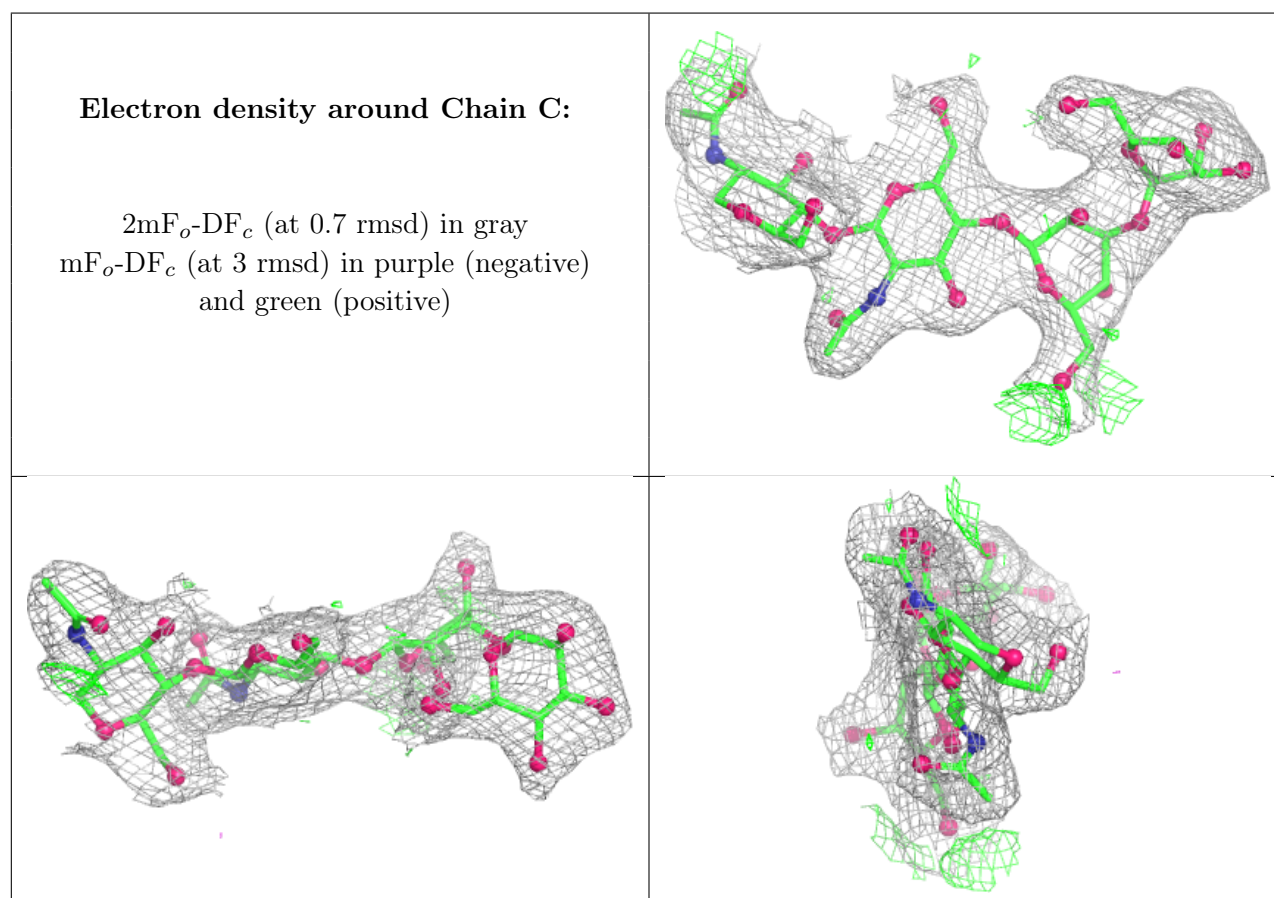
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	ACE	A	0	3/3	-0.05	0.66	83,83,106,109	0

6.3 Carbohydrates ⓘ

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
3	BMA	C	3	11/12	0.86	0.11	61,74,81,82	0
3	MAN	C	4	11/12	0.94	0.10	60,74,85,90	0
3	NAG	C	2	14/15	0.97	0.07	30,32,43,58	0
3	NAG	C	1	14/15	0.99	0.05	39,41,50,56	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 ⓘ

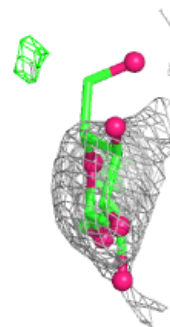
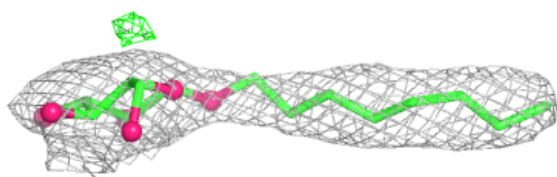
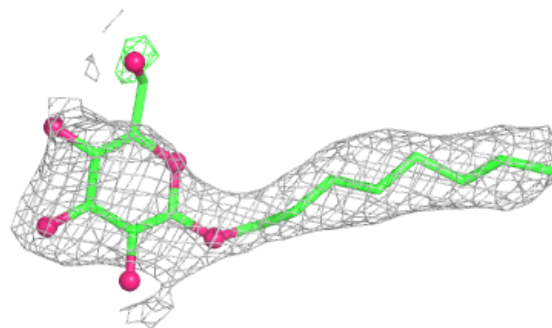
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	A	402	4/4	0.78	0.32	76,80,92,94	0
6	BOG	A	404	20/20	0.86	0.19	66,107,139,149	0
7	PLM	A	405	17/18	0.88	0.26	71,93,113,123	0
5	ACT	A	403	4/4	0.90	0.20	80,86,89,93	0
8	SO4	A	412	5/5	0.90	0.27	101,102,123,126	0
6	BOG	A	411	20/20	0.91	0.15	63,82,98,101	0
7	PLM	A	406	17/18	0.92	0.15	55,65,99,104	0
4	RET	A	401	20/21	0.95	0.16	85,95,117,118	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.

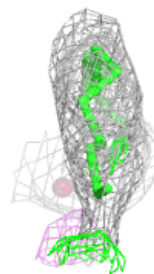
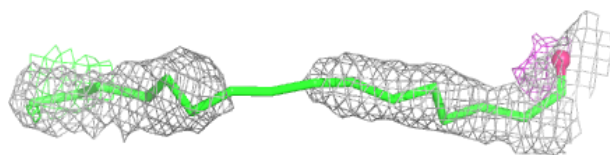
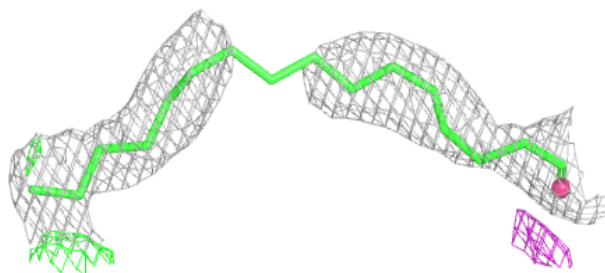
Electron density around BOG A 404:

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

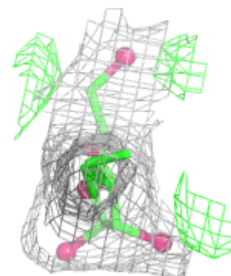
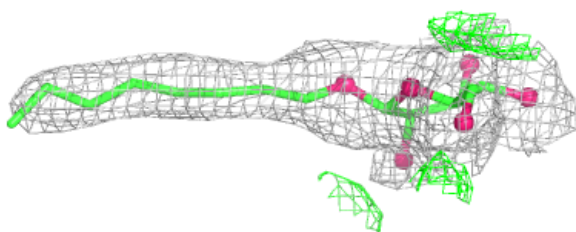
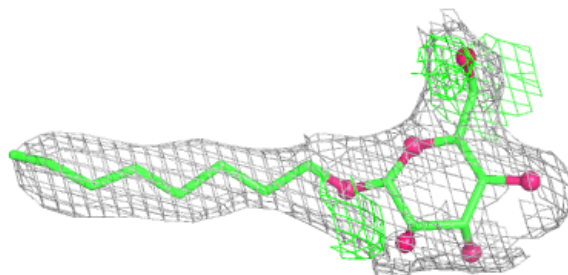


Electron density around PLM A 405:

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

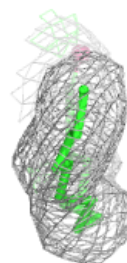
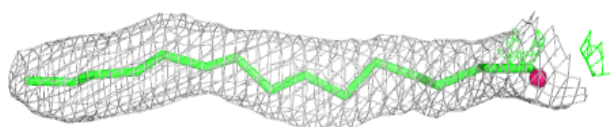
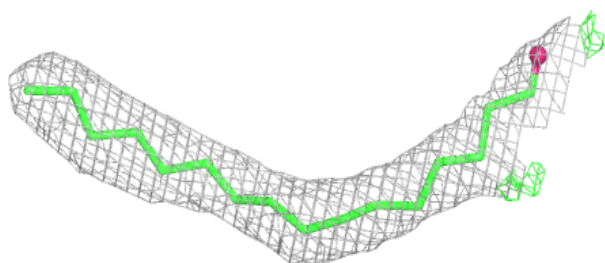
**Electron density around BOG A 411:**

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

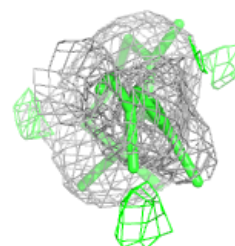
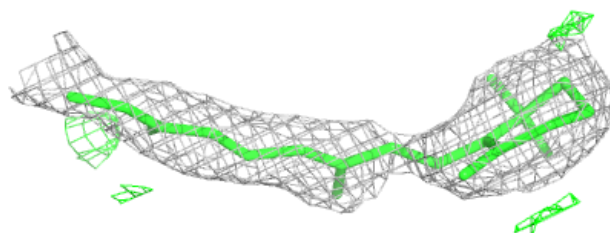
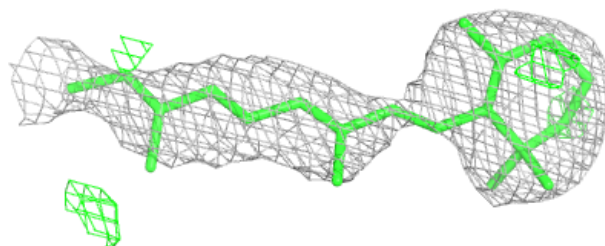


Electron density around PLM A 406:

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

**Electron density around RET A 401:**

$2mF_o-DF_c$ (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.