wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 01:04 pm GMT

PDB ID	:	6FJ3
Title	:	High resolution crystal structure of parathyroid hormone 1 receptor in complex with a peptide agonist.
Authors	:	Ehrenmann, J.; Schoppe, J.; Klenk, C.; Rappas, M.; Kummer, L.; Dore, A.S.; Pluckthun, A.
Deposited on	:	2018-01-19
Resolution	:	2.50 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 (i)) were used in the production of this report:

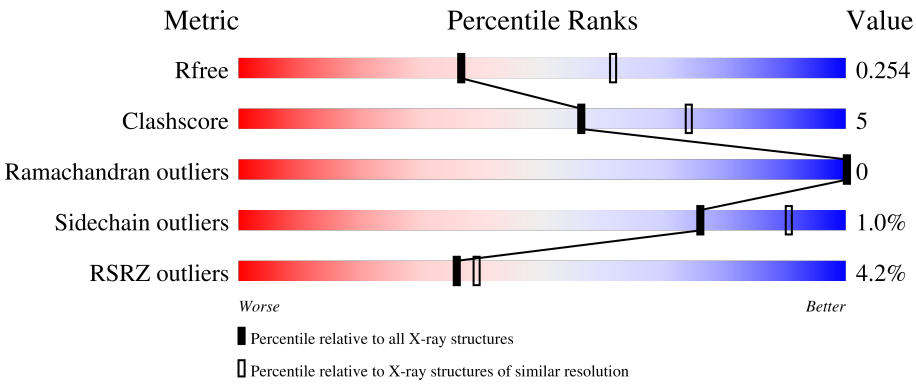
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	602	4%, 82%, 11%, 7%
2	B	35	3%, 86%, 14%
3	C	6	83%, 17%
4	D	4	100%

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Mol	Chain	Length	Quality of chain
5	E	4	25% 50% 25%

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
3	MAN	C	5	-	-	-	X
3	FUC	C	6	X	-	-	-
4	FUC	D	4	X	-	-	-
6	MAN	A	1511	-	-	-	X
6	MAN	A	1516	-	-	-	X
6	MAN	A	1517	-	-	-	X
9	PG4	A	1528	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 5352 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 Parathyroid hormone/parathyroid hormone-related peptide receptor,Parathyroid hormone/parathyroid hormone-related peptide receptor,GlgA glycogen synthase,Parathyroid hormone/parathyroid hormone-related peptide receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	562	4546	2965	767	784	30	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q03431
A	23	PRO	-	expression tag	UNP Q03431
A	191	CYS	TYR	engineered mutation	UNP Q03431
A	240	MET	LYS	engineered mutation	UNP Q03431
A	300	ALA	LEU	engineered mutation	UNP Q03431
A	312	LYS	MET	engineered mutation	UNP Q03431
A	334	ILE	VAL	engineered mutation	UNP Q03431
A	359	ASN	LYS	engineered mutation	UNP Q03431
A	407	ALA	LEU	engineered mutation	UNP Q03431
A	426	LEU	ALA	engineered mutation	UNP Q03431
A	440	ARG	GLN	engineered mutation	UNP Q03431
A	458	ALA	ILE	engineered mutation	UNP Q03431

- Molecule 2 is a protein called Parathyroid hormone.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	35	302	194	58	49	1	0	0	1

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	AC5	SER	conflict	UNP Q27IM2
B	3	AIB	SER	conflict	UNP Q27IM2

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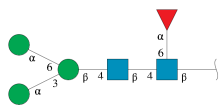
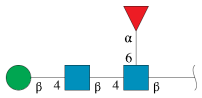
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	ASN	engineered mutation	UNP Q27IM2
B	11	HRG	LEU	conflict	UNP Q27IM2
B	12	ALA	GLY	engineered mutation	UNP Q27IM2
B	14	TRP	HIS	engineered mutation	UNP Q27IM2
B	18	NLE	VAL	conflict	UNP Q27IM2
B	34	TYR	PHE	engineered mutation	UNP Q27IM2
B	35	NH2	-	amidation	UNP Q27IM2

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	6	71	40	2	29	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

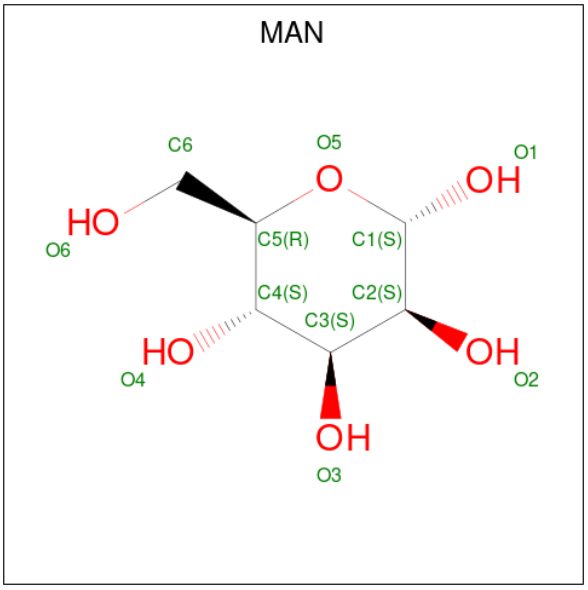


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	4	49	28	2	19	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

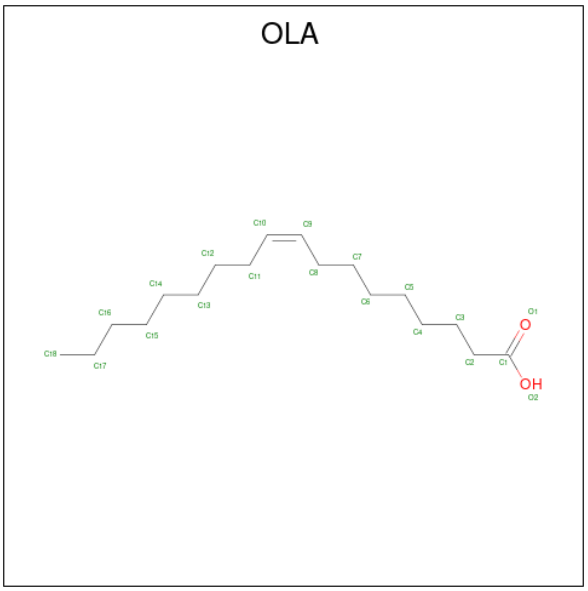
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	4	50	28	2	20	0	0	0

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



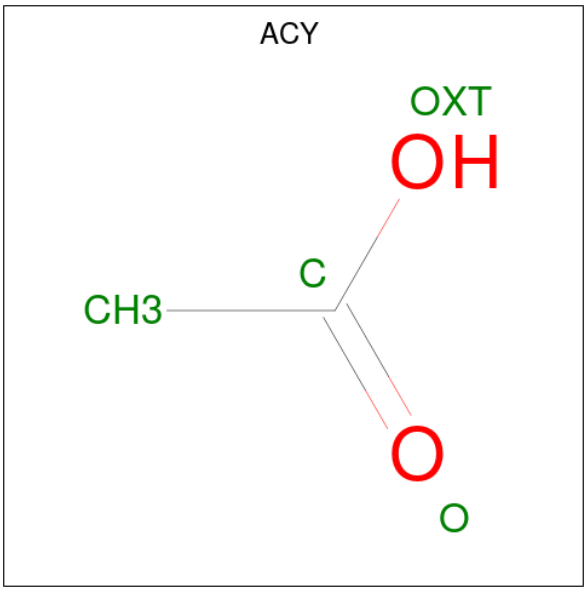
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	11	6	5		0	0
			Total	C	O			
6	A	1	11	6	5		0	0
			Total	C	O			
6	A	1	11	6	5		0	0

- Molecule 7 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



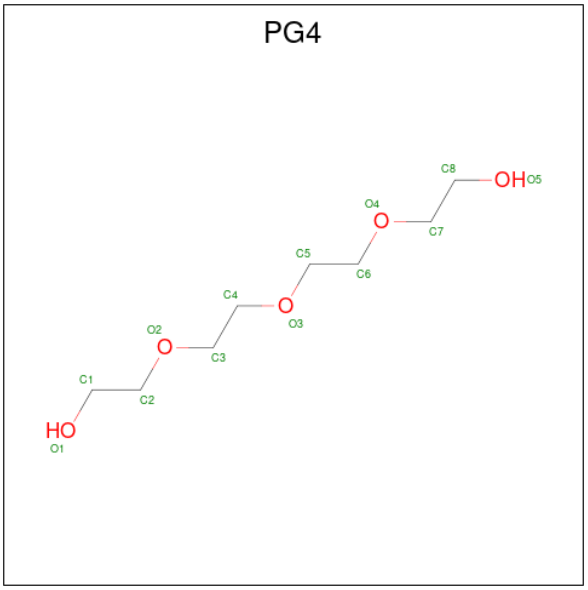
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 9 7 2	0	0
7	A	1	Total C O 11 9 2	0	0
7	A	1	Total C 7 7	0	0
7	A	1	Total C O 20 18 2	0	0
7	A	1	Total C O 20 18 2	0	0
7	A	1	Total C 7 7	0	0
7	A	1	Total C O 13 11 2	0	0
7	A	1	Total C O 20 18 2	0	0
7	A	1	Total C O 20 18 2	0	0

- Molecule 8 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	13	8	5	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
10	A	1	1	1	0	0

- Molecule 11 is water.

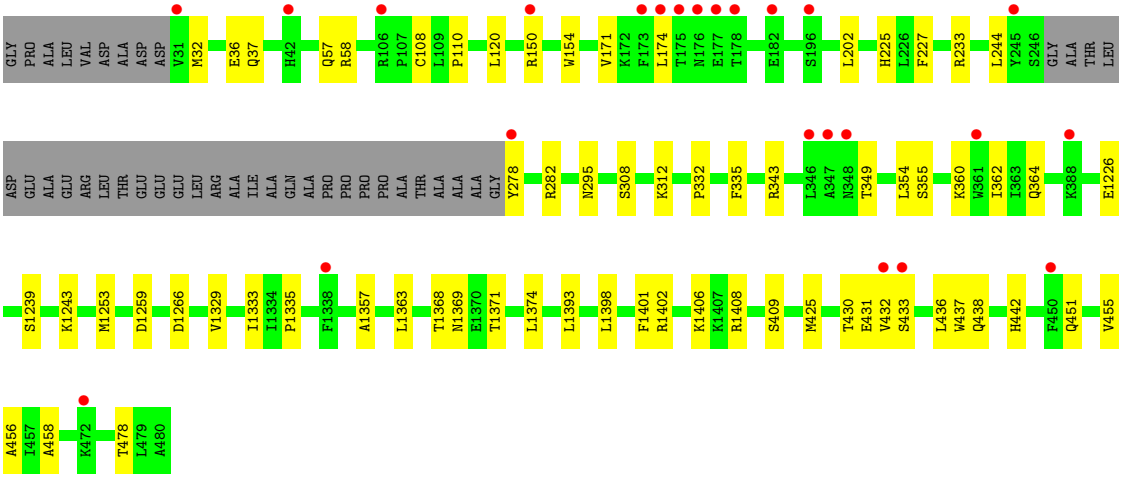
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	148	148	148	0	0
			Total	O		
11	B	8	8	8	0	0

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.

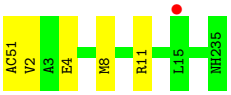
• Molecule 1: Parathyroid hormone/parathyroid hormone-related peptide receptor,Parathyroid hormone/parathyroid hormone-related peptide receptor,GlgA glycogen synthase,Parathyroid hormone/parathyroid hormone-related peptide receptor

Chain A:



• Molecule 2: Parathyroid hormone

Chain B:



• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1
NAG2
BMA3
FUC4

• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 25% 50% 25%

NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	44.12Å 52.86Å 111.87Å 80.63° 83.76° 79.16°	Depositor
Resolution (Å)	49.39 – 2.50 49.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.39-2.50) 99.8 (49.39-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.209 , 0.248 0.209 , 0.254	Depositor DCC
R_{free} test set	1662 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5352	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.46% 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: MAN, NH2, NAG, OLA, PG4, ACY, BMA, AC5, FUC, CL, NLE, AIB, YCM, HRG

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	0.24	0/4656	0.39	0/6298
2	B	0.21	0/271	0.29	0/361
All	All	0.24	0/4927	0.38	0/6659

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	4546	0	4555	40	0
2	B	302	0	307	3	0
3	C	71	0	61	2	0
4	D	49	0	43	0	0
5	E	50	0	43	4	0
6	A	33	0	30	6	0
7	A	127	0	190	5	0
8	A	4	0	3	0	0
9	A	13	0	18	4	0
10	A	1	0	0	0	0
11	A	148	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	8	0	0	0	0
All	All	5352	0	5250	52	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 5.

The worst 5 of 52 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)
6:A:1516:MAN:H2	6:A:1517:MAN:C1	1.88	1.04
6:A:1511:MAN:C1	3:C:4:MAN:O2	2.14	0.95
6:A:1516:MAN:C1	5:E:3:BMA:O3	2.25	0.84
1:A:1369:ASN:H	9:A:1528:PG4:H31	1.43	0.83
1:A:478:THR:HA	7:A:1526:OLA:H151	1.61	0.82

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	558/602 (93%)	537 (96%)	21 (4%)	0	100	100
2	B	30/35 (86%)	30 (100%)	0	0	100	100
All	All	588/637 (92%)	567 (96%)	21 (4%)	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	484/509 (95%)	479 (99%)	5 (1%)	76	90
2	B	29/29 (100%)	29 (100%)	0	100	100
All	All	513/538 (95%)	508 (99%)	5 (1%)	76	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	354	LEU
1	A	362	ILE
1	A	1259	ASP
1	A	1401	PHE

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	364	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	NLE	B	18	2	6,7,8	0.69	0	2,7,9	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HRG	B	11	2	10,11,12	0.73	0	6,12,14	0.56	0
2	AIB	B	3	2	1,5,6	1.65	0	2,7,9	0.19	0
1	YCM	A	1221	1	7,9,10	1.08	0	4,10,12	1.08	0
2	AC5	B	1	2	6,8,9	1.16	0	5,11,13	1.09	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	NLE	B	18	2	-	2/5/6/8	-
2	HRG	B	11	2	-	4/9/10/12	-
2	AIB	B	3	2	-	1/2/3/6	-
1	YCM	A	1221	1	-	3/6/8/10	-
2	AC5	B	1	2	-	2/2/12/15	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1221	YCM	CE-CD-SG-CB
2	B	1	AC5	O-C-CA-CB1
2	B	1	AC5	O-C-CA-CB2
2	B	11	HRG	N-CA-CB-CG'
2	B	11	HRG	C-CA-CB-CG'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	11	HRG	1	0
2	B	1	AC5	1	0

5.5 Carbohydrates (i)

14 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	0.27	0	17,19,21	0.62	0
3	NAG	C	2	3	14,14,15	0.26	0	17,19,21	0.59	0
3	BMA	C	3	3	11,11,12	0.21	0	15,15,17	0.72	0
3	MAN	C	4	3	11,11,12	0.24	0	15,15,17	0.67	0
3	MAN	C	5	3	11,11,12	0.25	0	15,15,17	0.66	0
3	FUC	C	6	3	10,10,11	0.24	0	14,14,16	0.54	0
4	NAG	D	1	1,4	14,14,15	0.26	0	17,19,21	0.70	0
4	NAG	D	2	4	14,14,15	0.29	0	17,19,21	0.66	0
4	BMA	D	3	4	11,11,12	0.22	0	15,15,17	0.71	0
4	FUC	D	4	4	10,10,11	0.26	0	14,14,16	0.67	0
5	NAG	E	1	1,5	14,14,15	0.29	0	17,19,21	0.84	0
5	NAG	E	2	5	14,14,15	0.29	0	17,19,21	1.89	3 (17%)
5	BMA	E	3	5	11,11,12	0.24	0	15,15,17	0.73	0
5	MAN	E	4	5	11,11,12	0.23	0	15,15,17	0.61	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
3	NAG	C	1	3,1	-	4/6/23/26	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
3	MAN	C	5	3	-	1/2/19/22	0/1/1/1
3	FUC	C	6	3	1/1/4/5	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	FUC	D	4	4	1/1/4/5	-	0/1/1/1
5	NAG	E	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C2-N2-C7	5.70	131.01	122.90
5	E	2	NAG	C1-C2-N2	2.79	115.25	110.49
5	E	2	NAG	C8-C7-N2	2.30	119.99	116.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	6	FUC	C1
4	D	4	FUC	C1

5 of 13 torsion outliers are listed below:

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

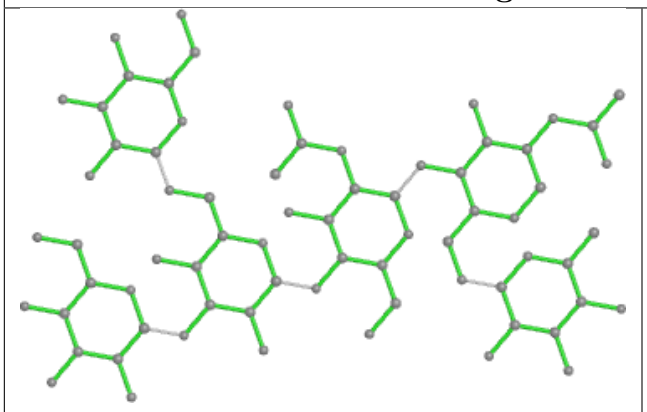
There are no ring outliers.

4 monomers are involved in 6 short contacts:

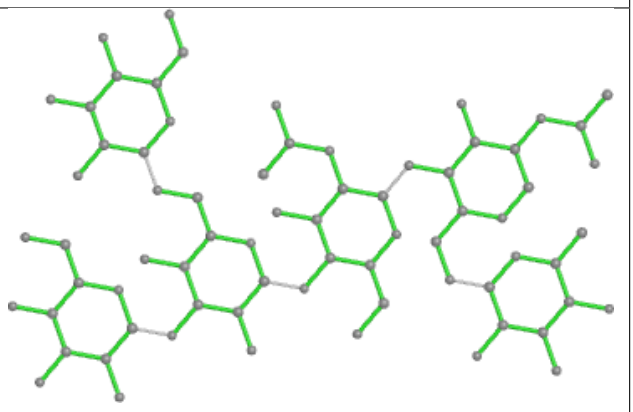
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	3	BMA	3	0
5	E	1	NAG	1	0
3	C	4	MAN	2	0
5	E	2	NAG	1	0

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

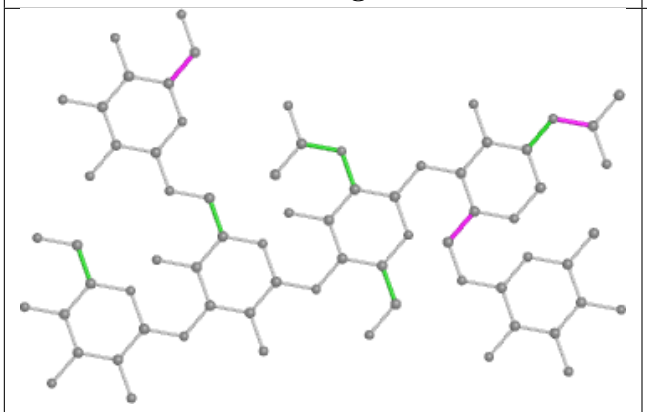
Oligosaccharide Chain C



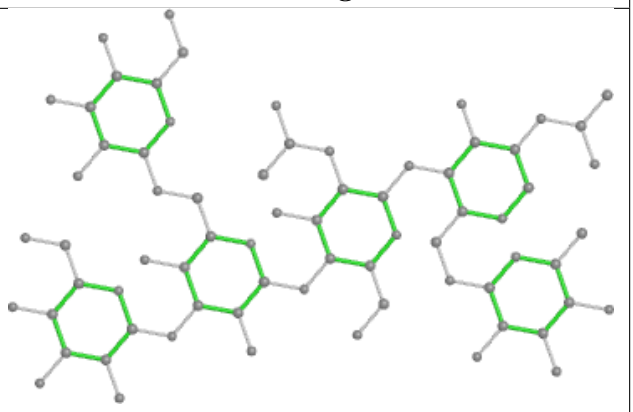
Bond lengths



Bond angles

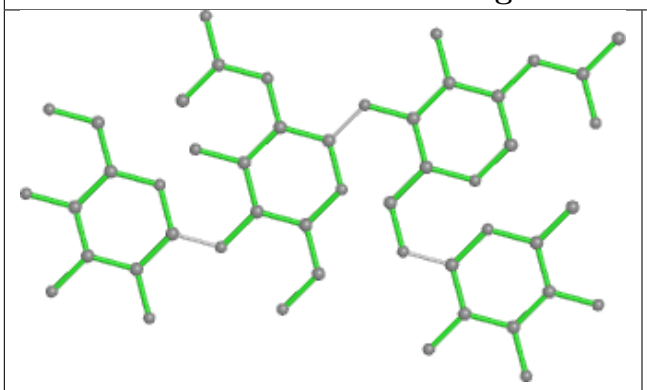


Torsions

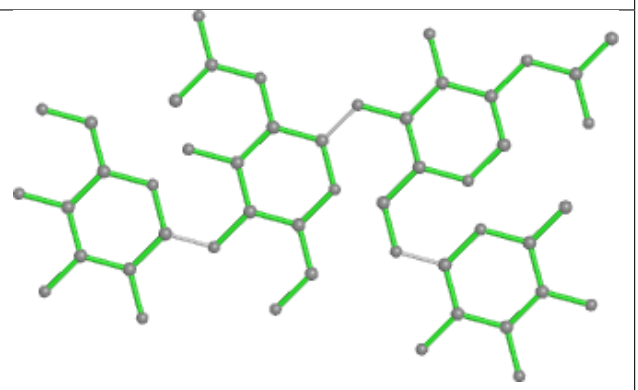


Rings

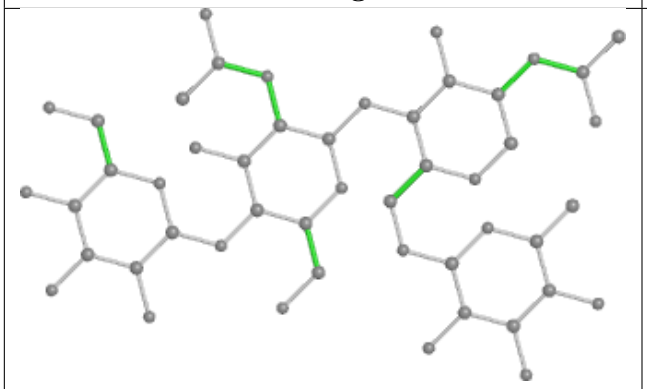
Oligosaccharide Chain D



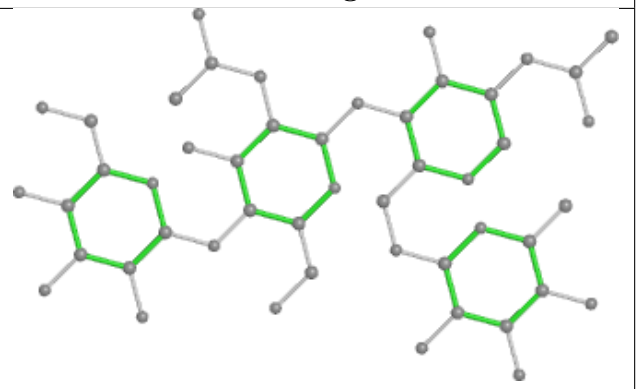
Bond lengths



Bond angles

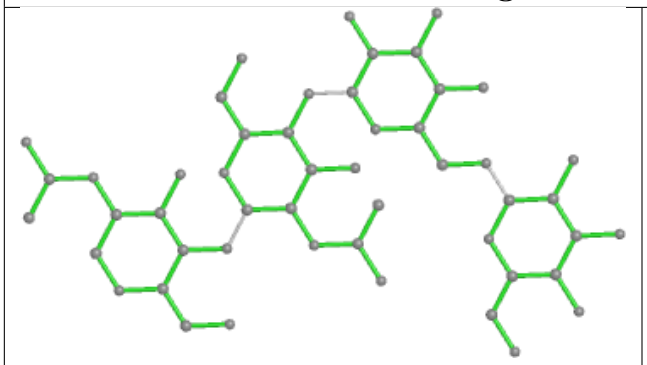


Torsions

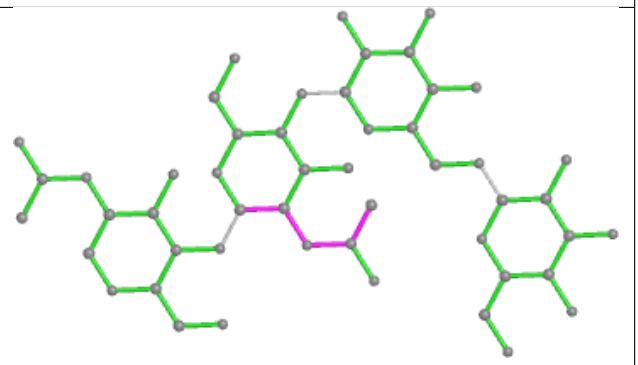


Rings

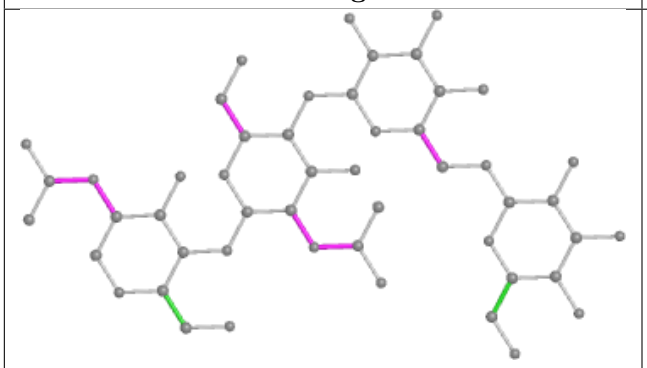
Oligosaccharide Chain E



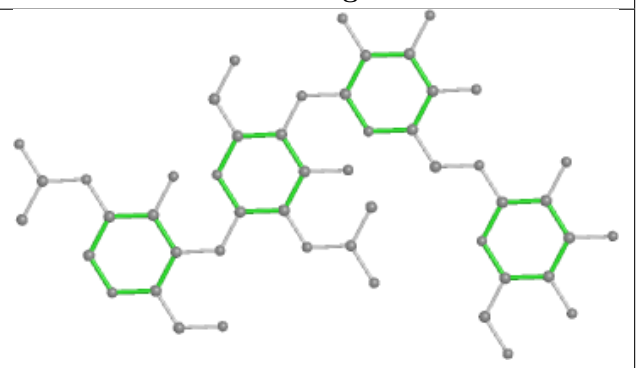
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\#\|Z\| > 2$
7	OLA	A	1518	-	8,8,19	0.70	0	8,8,19	1.01	0
7	OLA	A	1521	-	19,19,19	0.49	0	19,19,19	0.80	0
7	OLA	A	1519	-	10,10,19	0.62	0	10,10,19	0.99	0
8	ACY	A	1527	-	3,3,3	0.77	0	3,3,3	0.72	0
7	OLA	A	1524	-	12,12,19	0.61	0	12,12,19	0.96	0
6	MAN	A	1517	-	11,11,12	0.22	0	15,15,17	0.57	0
7	OLA	A	1523	-	6,6,19	0.33	0	4,5,19	0.51	0
7	OLA	A	1520	-	6,6,19	0.23	0	5,5,19	0.52	0
9	PG4	A	1528	-	12,12,12	0.42	0	11,11,11	0.54	0
7	OLA	A	1526	-	19,19,19	0.47	0	19,19,19	0.90	1 (5%)
6	MAN	A	1511	-	11,11,12	0.32	0	15,15,17	0.63	0
7	OLA	A	1525	-	19,19,19	0.48	0	19,19,19	0.84	0
7	OLA	A	1522	-	19,19,19	0.49	0	19,19,19	0.82	0
6	MAN	A	1516	-	11,11,12	0.24	0	15,15,17	0.65	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	OLA	A	1518	-	-	3/6/6/17	-
7	OLA	A	1521	-	-	0/17/17/17	-
7	OLA	A	1519	-	-	0/8/8/17	-
7	OLA	A	1524	-	-	3/10/10/17	-
6	MAN	A	1517	-	-	0/2/19/22	0/1/1/1
7	OLA	A	1523	-	-	0/4/4/17	-
7	OLA	A	1520	-	-	0/4/4/17	-
9	PG4	A	1528	-	-	5/10/10/10	-
7	OLA	A	1526	-	-	4/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	1511	-	-	0/2/19/22	0/1/1/1
7	OLA	A	1525	-	-	7/17/17/17	-
7	OLA	A	1522	-	-	2/17/17/17	-
6	MAN	A	1516	-	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1526	OLA	C3-C2-C1	-2.44	108.33	114.47

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1528	PG4	O2-C3-C4-O3
6	A	1516	MAN	O5-C5-C6-O6
7	A	1526	OLA	C14-C15-C16-C17
7	A	1526	OLA	C13-C14-C15-C16
7	A	1526	OLA	C11-C12-C13-C14

There are no ring outliers.

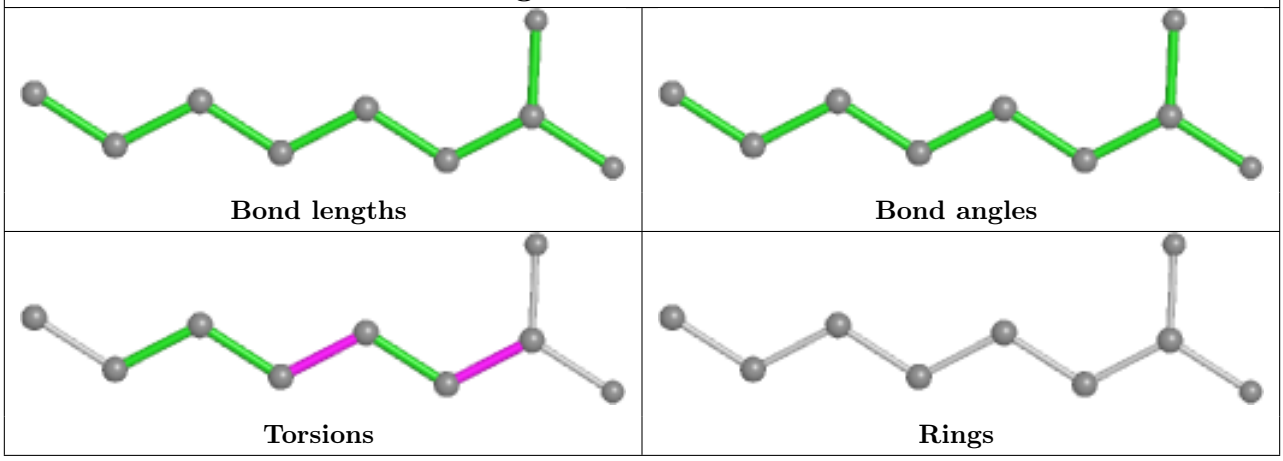
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1519	OLA	1	0
6	A	1517	MAN	2	0
7	A	1523	OLA	1	0
9	A	1528	PG4	4	0
7	A	1526	OLA	2	0
6	A	1511	MAN	2	0
7	A	1525	OLA	1	0
6	A	1516	MAN	4	0

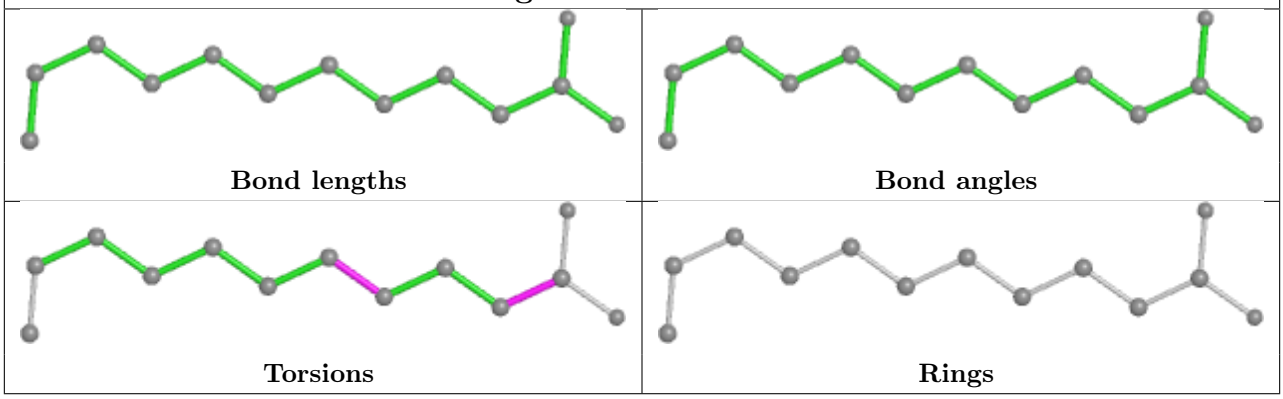
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

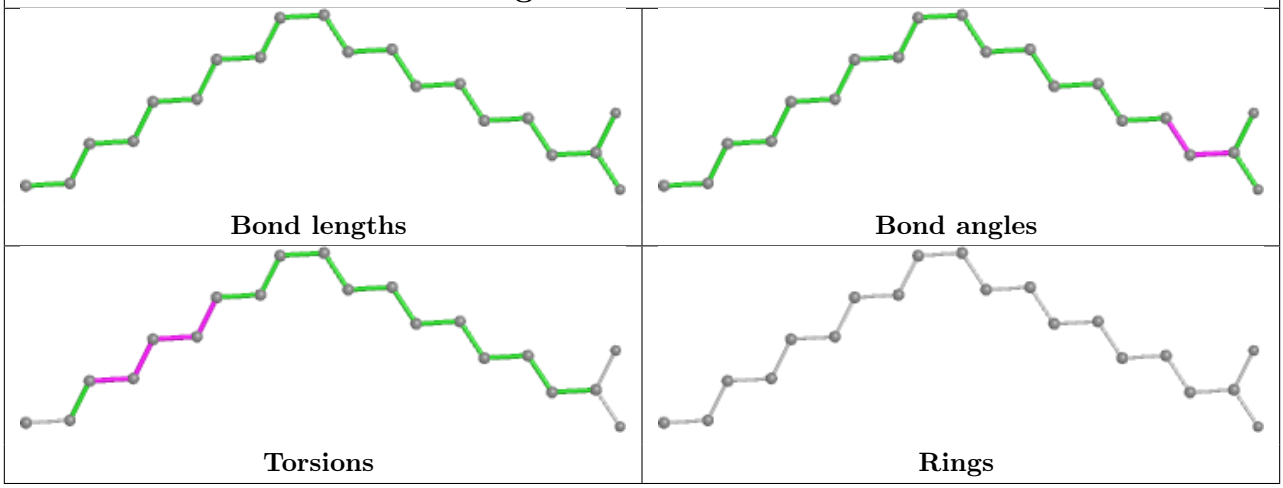
Ligand OLA A 1518

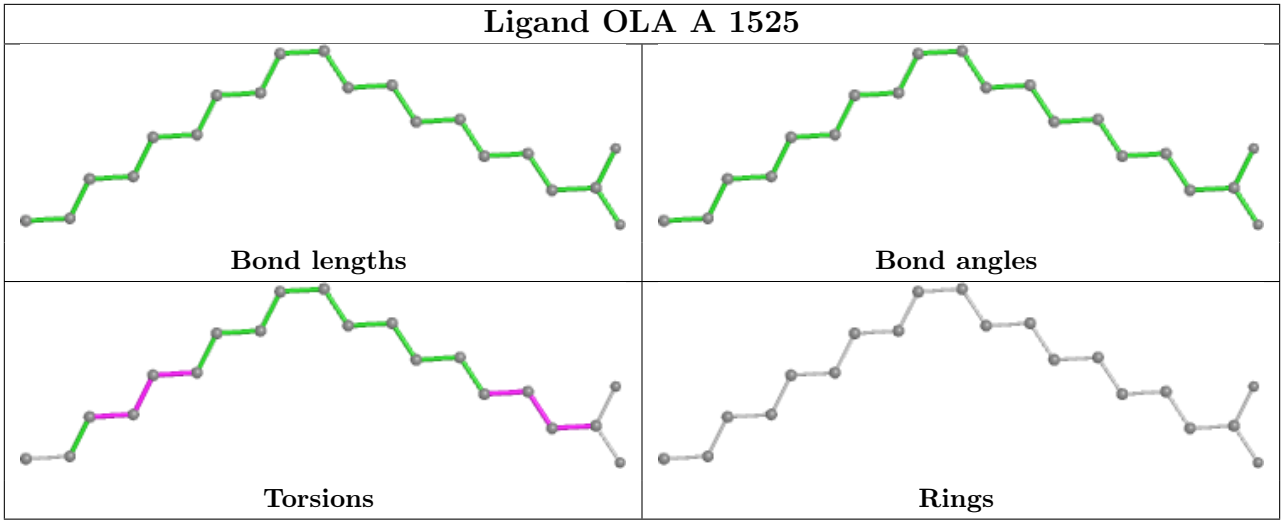


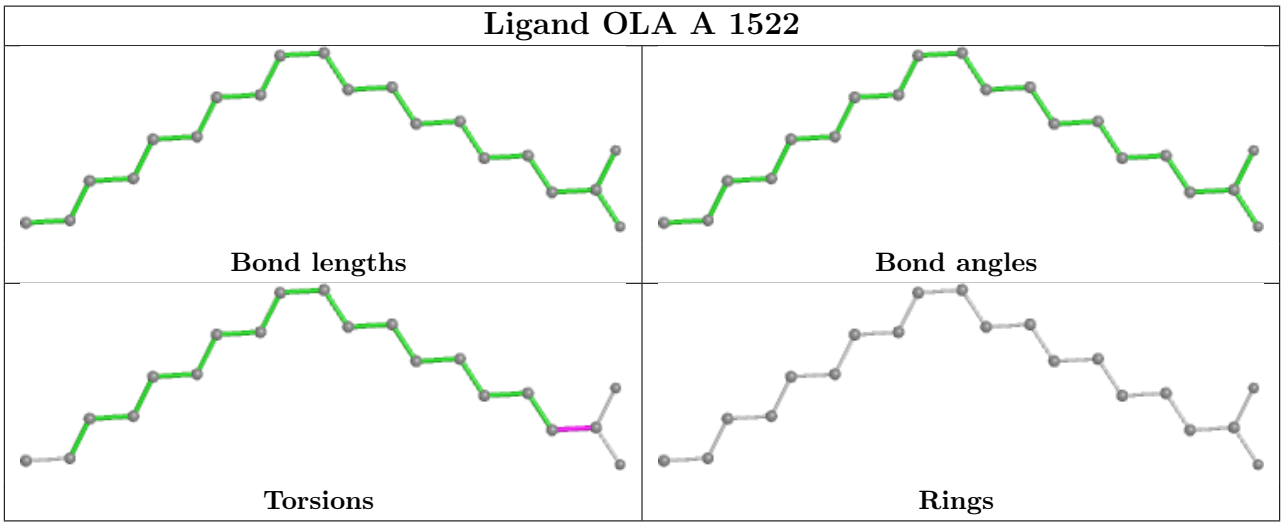
Ligand OLA A 1524



Ligand OLA A 1526







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	34:TYR	C	35:NH2	N	1.06

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	561/602 (93%)	0.27	24 (4%)	35	38	31, 68, 143, 212	0
2	B	30/35 (85%)	0.21	1 (3%)	46	50	49, 87, 115, 137	0
All	All	591/637 (92%)	0.26	25 (4%)	36	39	31, 69, 141, 212	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	THR	9.3
1	A	176	ASN	6.4
1	A	245	TYR	4.6
1	A	173	PHE	4.5
1	A	432	VAL	4.5

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
2	AC5	B	1	8/9	0.85	0.23	110,118,120,120	0
2	HRG	B	11	12/13	0.91	0.18	93,108,137,137	0
1	YCM	A	1221	10/11	0.94	0.17	57,67,79,84	0
2	AIB	B	3	6/7	0.96	0.22	101,104,108,123	0
2	NLE	B	18	8/9	0.96	0.23	75,85,100,102	0

6.3 Carbohydrates (i)

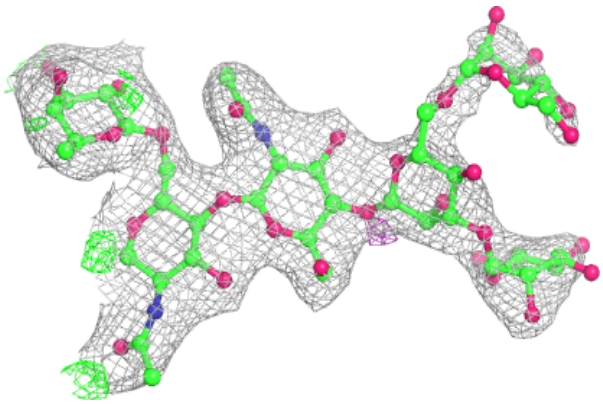
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

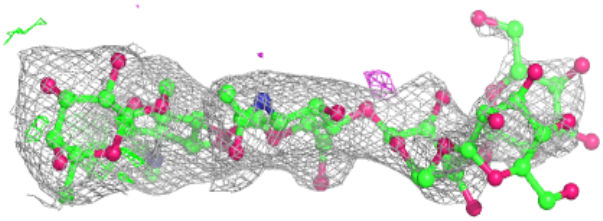
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	E	3	11/12	0.52	0.21	145,149,156,159	0
5	NAG	E	2	14/15	0.54	0.38	155,158,162,162	0
5	MAN	E	4	11/12	0.58	0.32	140,143,145,146	0
4	BMA	D	3	11/12	0.61	0.24	124,130,134,135	0
3	MAN	C	5	11/12	0.70	0.52	89,94,97,98	11
5	NAG	E	1	14/15	0.78	0.26	114,136,142,149	0
3	MAN	C	4	11/12	0.83	0.38	97,101,105,109	11
4	FUC	D	4	10/11	0.84	0.27	105,113,116,117	10
3	BMA	C	3	11/12	0.87	0.24	96,102,106,108	11
4	NAG	D	2	14/15	0.87	0.14	91,101,107,115	0
4	NAG	D	1	14/15	0.91	0.10	53,67,85,96	0
3	FUC	C	6	10/11	0.94	0.16	51,55,61,64	0
3	NAG	C	1	14/15	0.96	0.16	37,45,56,59	0
3	NAG	C	2	14/15	0.96	0.16	44,56,73,85	0

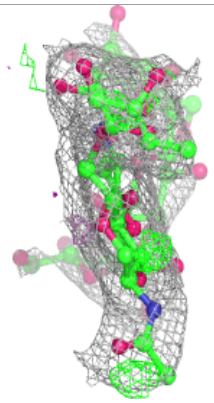
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

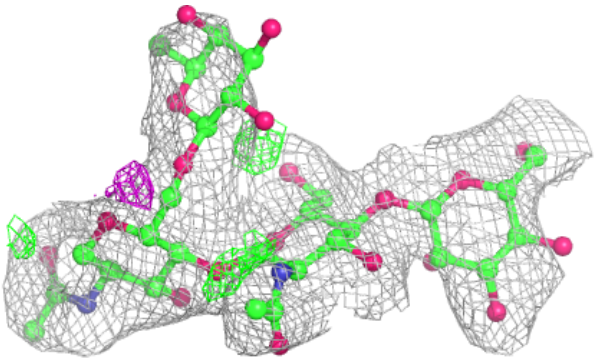


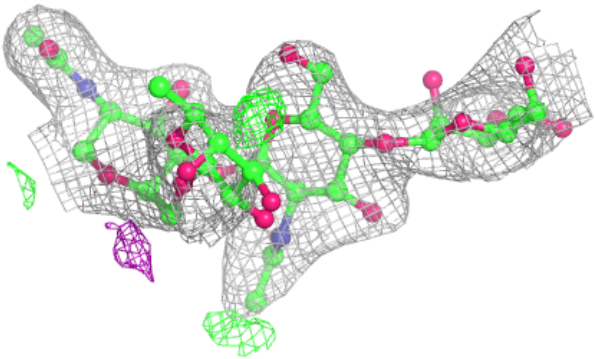


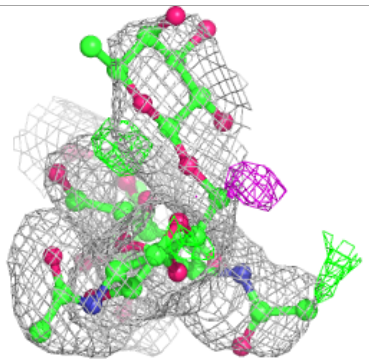


Electron density around Chain D:

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

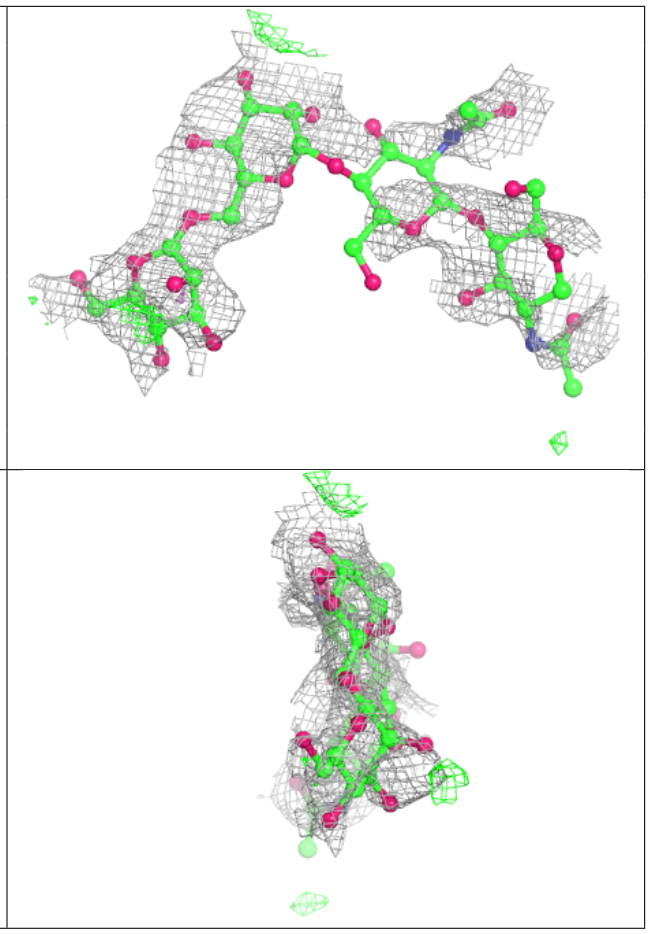






Electron density around Chain E:

$2mF_o$-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
7	OLA	A	1524	13/20	0.45	0.31	103,129,149,149	0
6	MAN	A	1517	11/12	0.46	0.41	110,116,118,119	11
10	CL	A	1529	1/1	0.48	0.34	211,211,211,211	0
7	OLA	A	1526	20/20	0.63	0.21	89,99,112,113	0
7	OLA	A	1525	20/20	0.64	0.28	88,95,104,104	0
8	ACY	A	1527	4/4	0.67	0.27	101,105,105,107	0
6	MAN	A	1516	11/12	0.68	0.50	130,134,137,138	11
9	PG4	A	1528	13/13	0.69	0.41	158,167,169,169	0
7	OLA	A	1522	20/20	0.72	0.28	91,105,116,116	4
7	OLA	A	1519	11/20	0.75	0.18	106,108,110,110	0
6	MAN	A	1511	11/12	0.76	0.72	105,106,106,107	11
7	OLA	A	1523	7/20	0.79	0.34	104,108,108,109	0

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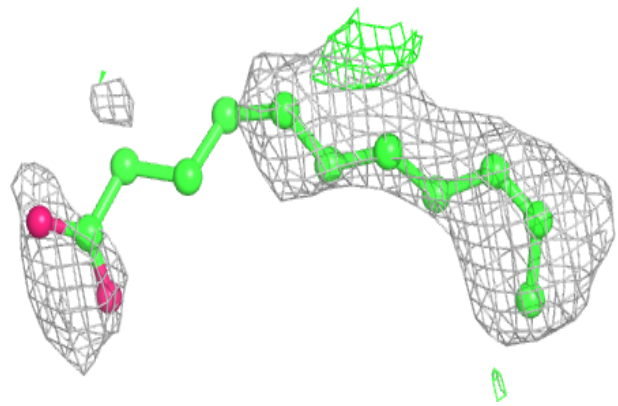
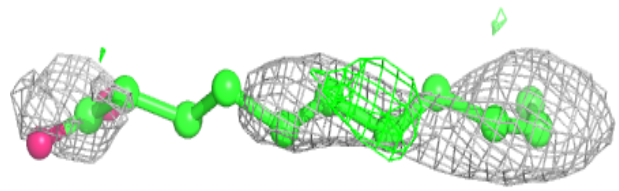
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	OLA	A	1521	20/20	0.82	0.31	84,88,101,102	5
7	OLA	A	1520	7/20	0.88	0.19	90,91,93,94	0
7	OLA	A	1518	9/20	0.88	0.10	92,95,105,106	0

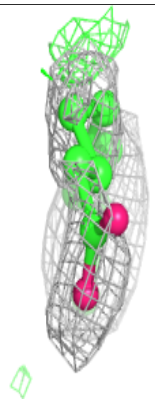
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1524:

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

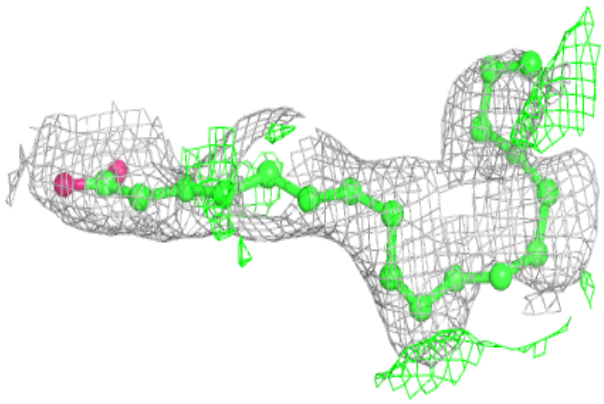


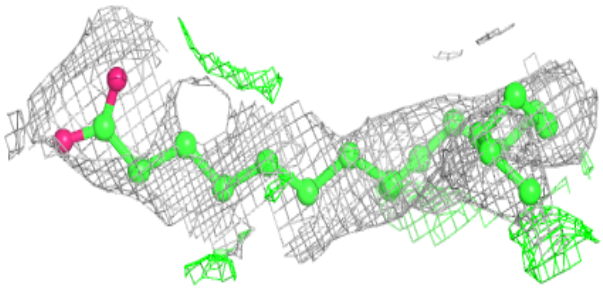


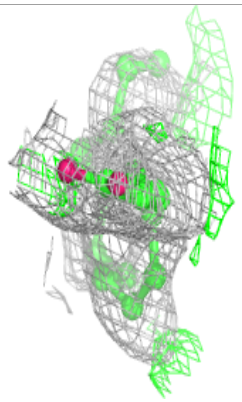


Electron density around OLA A 1526:

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

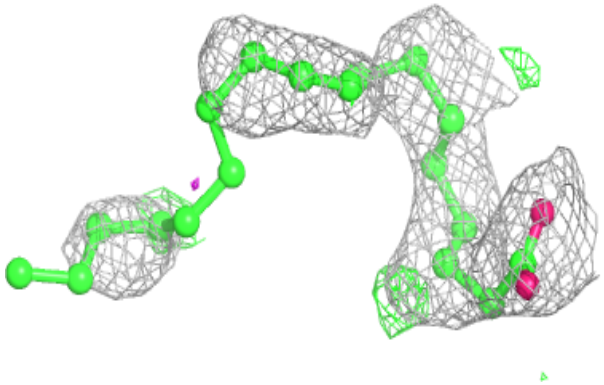


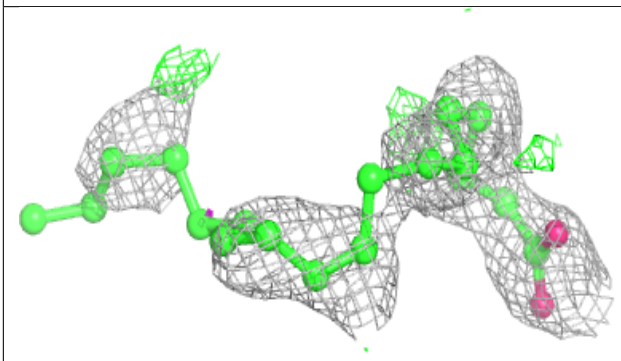


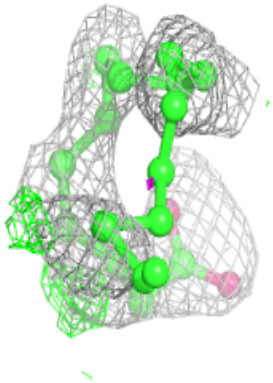


Electron density around OLA A 1525:

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

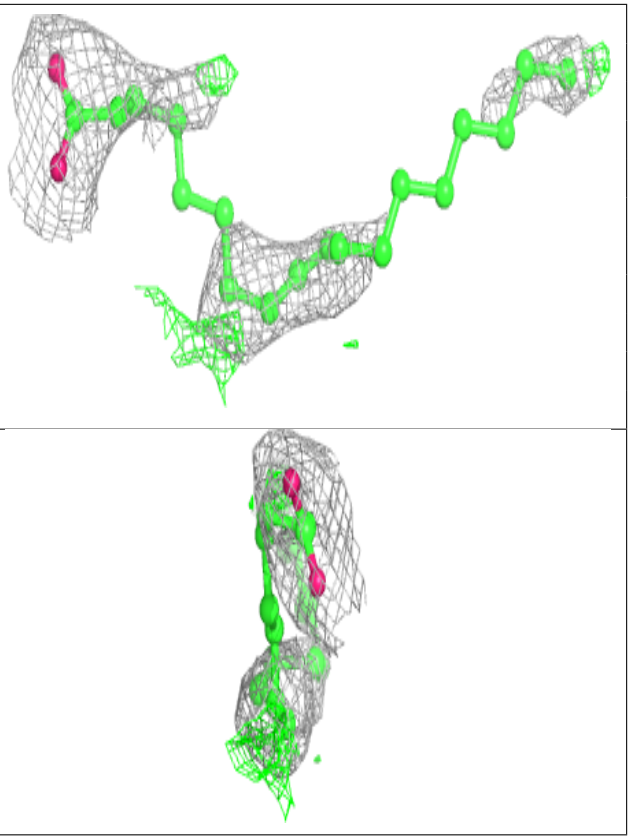


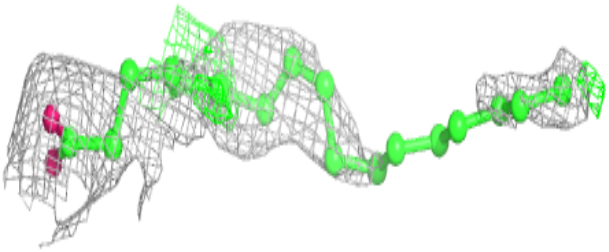




Electron density around OLA A 1522:

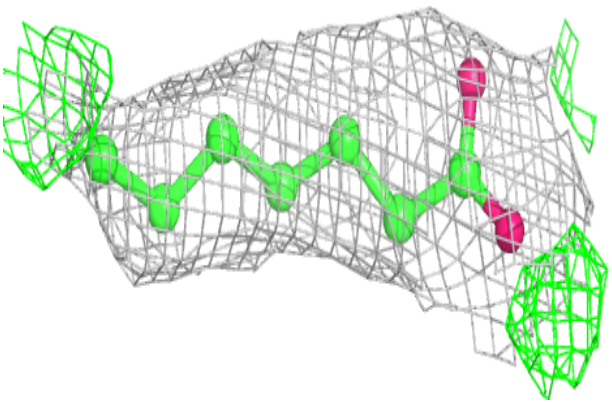
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

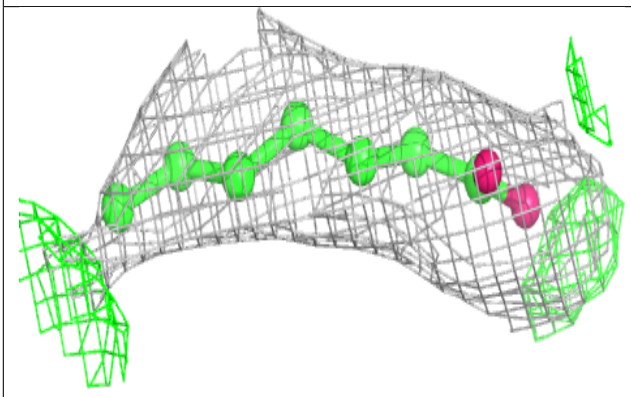


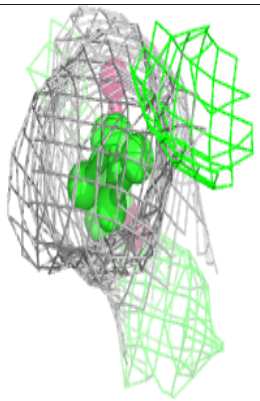


Electron density around OLA A 1518:

$2mF_o$-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.