



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 07:46 PM BST

PDB ID : 3L9R
Title : Crystal structure of bovine CD1b3 with endogenously bound ligands
Authors : Zajonc, D.M.; Girardi, E.
Deposited on : 2010-01-05
Resolution : 2.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

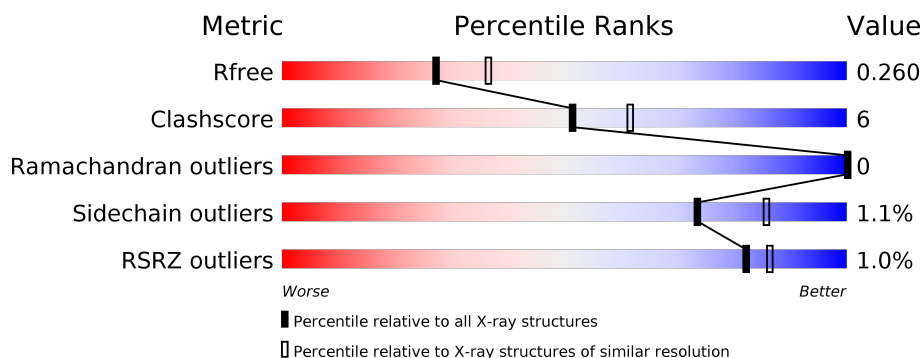
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	283	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 90% 7% • </div> </div>
1	C	283	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 85% 11% • </div> </div>
1	E	283	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 83% 14% • </div> </div>
1	G	283	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 86% 11% • </div> </div>
2	B	98	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 78% 21% • </div> </div>
2	D	98	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 92% 8% • </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	98	<div><div></div><div>%</div><div>94%6%</div></div>
2	H	98	<div><div></div><div>2%</div><div>89%11%</div></div>
3	I	6	<div><div></div><div>100%</div></div>
4	J	5	<div><div></div><div>80%20%</div></div>
4	K	5	<div><div></div><div>40%20%40%</div></div>
4	L	5	<div><div></div><div>40%60%</div></div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 12721 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 CD1b3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2124	1355	364	395	10			
1	C	274	Total	C	N	O	S	0	0	0
			2114	1350	364	390	10			
1	E	275	Total	C	N	O	S	0	2	0
			2143	1364	367	401	11			
1	G	275	Total	C	N	O	S	0	0	0
			2125	1355	367	393	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	HIS	-	expression tag	UNP Q1L1H6
A	279	HIS	-	expression tag	UNP Q1L1H6
A	280	HIS	-	expression tag	UNP Q1L1H6
A	281	HIS	-	expression tag	UNP Q1L1H6
A	282	HIS	-	expression tag	UNP Q1L1H6
A	283	HIS	-	expression tag	UNP Q1L1H6
C	278	HIS	-	expression tag	UNP Q1L1H6
C	279	HIS	-	expression tag	UNP Q1L1H6
C	280	HIS	-	expression tag	UNP Q1L1H6
C	281	HIS	-	expression tag	UNP Q1L1H6
C	282	HIS	-	expression tag	UNP Q1L1H6
C	283	HIS	-	expression tag	UNP Q1L1H6
E	278	HIS	-	expression tag	UNP Q1L1H6
E	279	HIS	-	expression tag	UNP Q1L1H6
E	280	HIS	-	expression tag	UNP Q1L1H6
E	281	HIS	-	expression tag	UNP Q1L1H6
E	282	HIS	-	expression tag	UNP Q1L1H6
E	283	HIS	-	expression tag	UNP Q1L1H6
G	278	HIS	-	expression tag	UNP Q1L1H6
G	279	HIS	-	expression tag	UNP Q1L1H6
G	280	HIS	-	expression tag	UNP Q1L1H6

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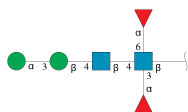
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Chain	Residue	Modelled	Actual	Comment	Reference
G	281	HIS	-	expression tag	UNP Q1L1H6
G	282	HIS	-	expression tag	UNP Q1L1H6
G	283	HIS	-	expression tag	UNP Q1L1H6

- Molecule 2 is a protein called Beta-2-microglobulin.

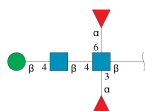
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			782	501	134	145	2			
2	D	98	Total	C	N	O	S	0	0	0
			780	500	134	144	2			
2	F	98	Total	C	N	O	S	0	0	0
			778	501	132	143	2			
2	H	98	Total	C	N	O	S	0	0	0
			786	504	134	146	2			

- 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)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	6	Total	C	N	O	0	0	0
			70	40	2	28			

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



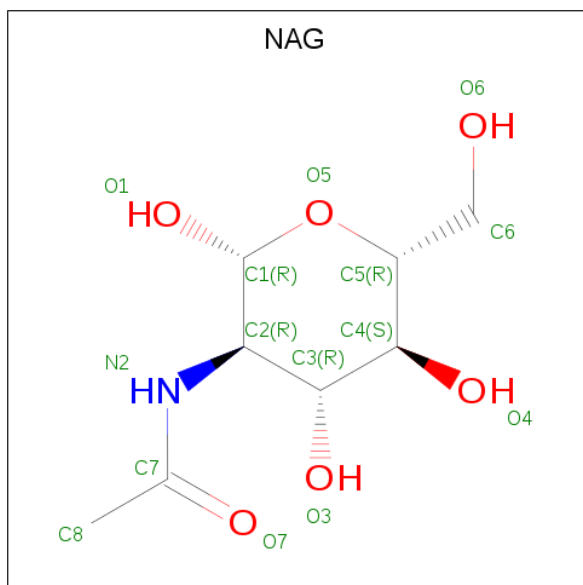
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			59	34	2	23			
4	K	5	Total	C	N	O	0	0	0
			59	34	2	23			

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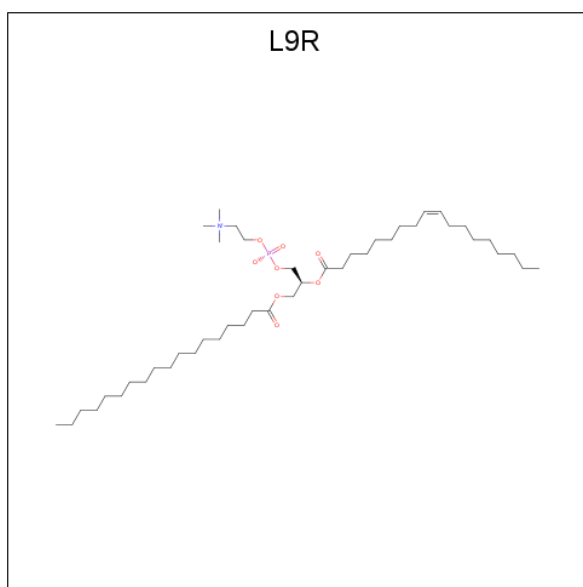
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	5	Total	C	N	O	0	0	0
			59	34	2	23			

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



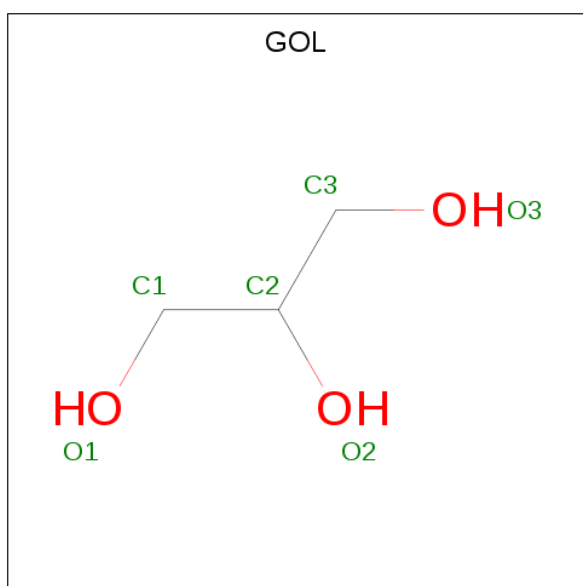
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is (2S)-3-(octadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: L9R) (formula: $C_{44}H_{86}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
6	E	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



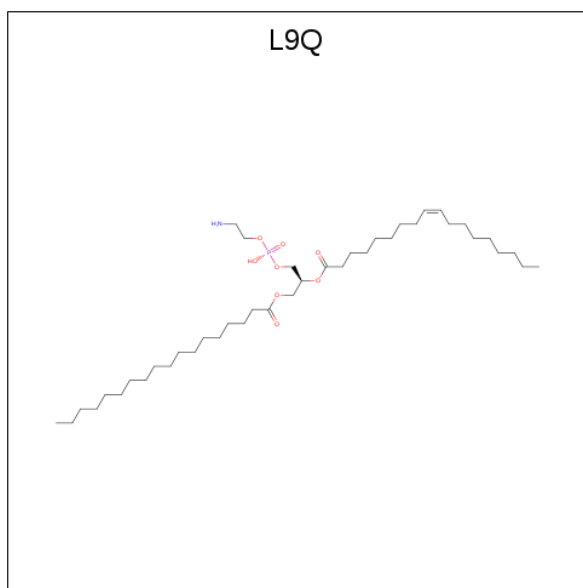
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is (1S)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(octadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: L9Q) (formula: C₄₁H₈₀NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
8	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	1	Total Cl 1 1	0	0
9	C	1	Total Cl 1 1	0	0

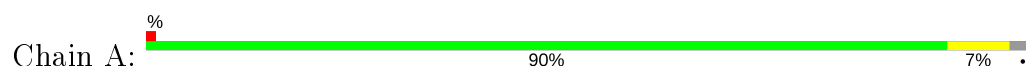
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	93	Total O 93 93	0	0
10	B	21	Total O 21 21	0	0
10	C	90	Total O 90 90	0	0
10	D	19	Total O 19 19	0	0
10	E	114	Total O 114 114	0	0
10	F	27	Total O 27 27	0	0
10	G	111	Total O 111 111	0	0
10	H	31	Total O 31 31	0	0

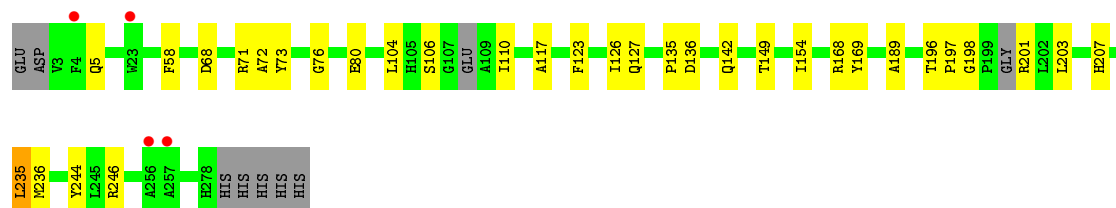
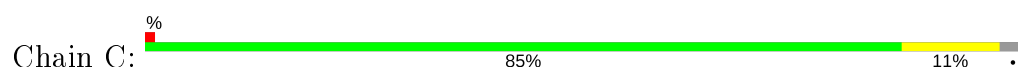
3 Residue-property plots [i](#)

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.

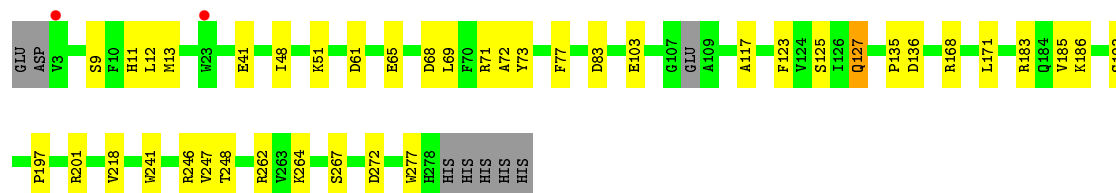
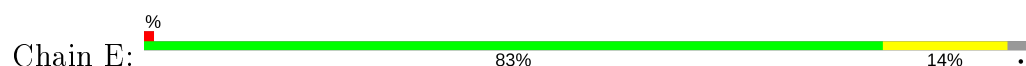
• Molecule 1: CD1b3



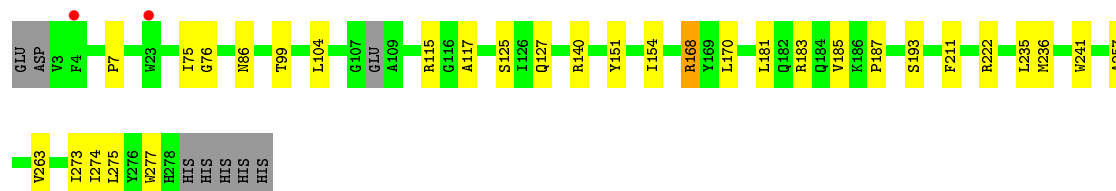
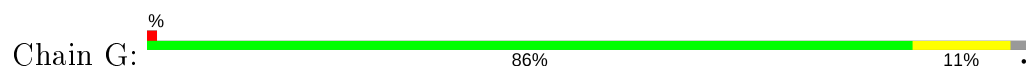
• Molecule 1: CD1b3



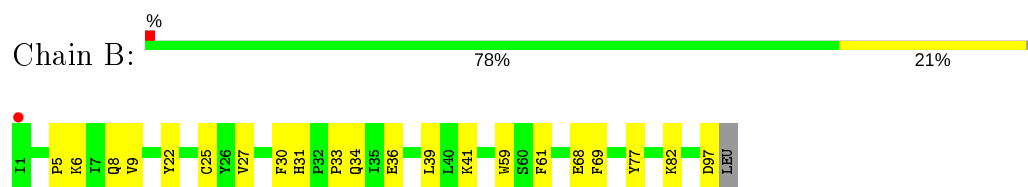
• Molecule 1: CD1b3



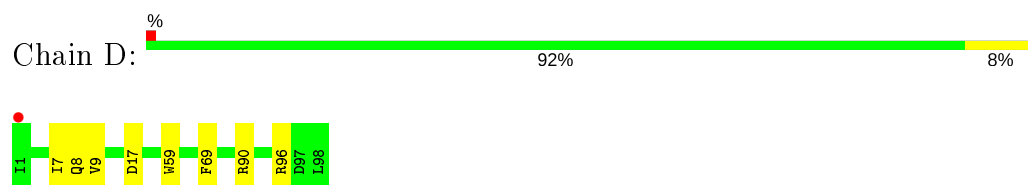
• Molecule 1: CD1b3



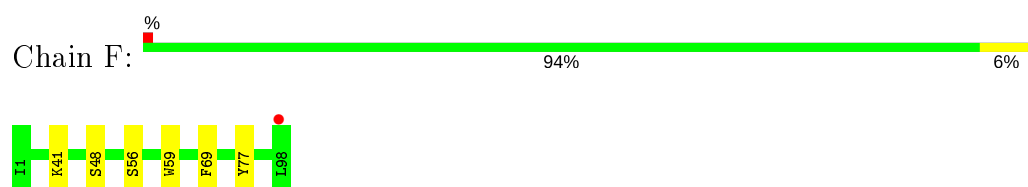
- Molecule 2: Beta-2-microglobulin



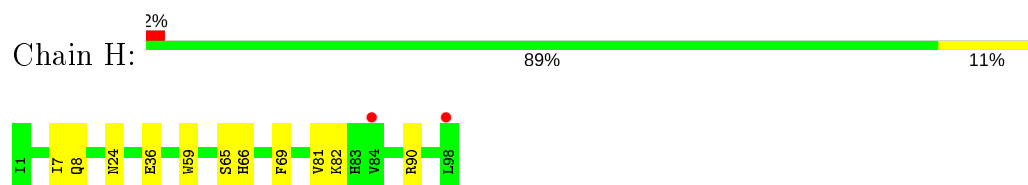
- Molecule 2: Beta-2-microglobulin



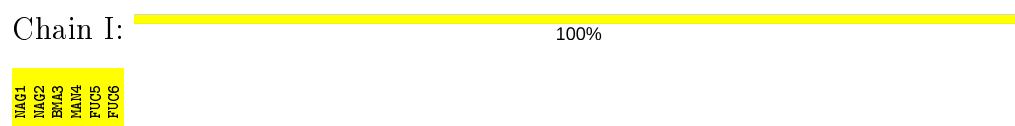
- Molecule 2: Beta-2-microglobulin



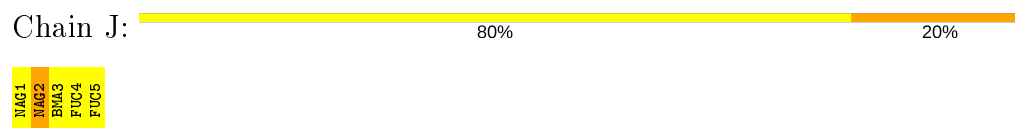
- Molecule 2: Beta-2-microglobulin



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



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



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

Chain K:  40% 20% 40%



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

Chain L:  40% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.53Å 139.97Å 111.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.30 45.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.00-2.30) 99.4 (45.84-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.201 , 0.248 0.213 , 0.260	Depositor DCC
R_{free} test set	4805 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 17.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.127 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12721	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, L9R, CL, L9Q, FUC, 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	0.61	0/2181	0.66	0/2969
1	C	0.61	0/2170	0.65	1/2953 (0.0%)
1	E	0.61	0/2199	0.67	2/2991 (0.1%)
1	G	0.64	0/2182	0.69	1/2970 (0.0%)
2	B	0.55	0/808	0.61	0/1104
2	D	0.50	0/806	0.58	0/1102
2	F	0.56	0/804	0.64	0/1100
2	H	0.54	0/812	0.61	0/1110
All	All	0.60	0/11962	0.65	4/16299 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	262	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	E	71	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	G	168	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	235	LEU	CA-CB-CG	-5.12	103.52	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2124	0	2015	22	0
1	C	2114	0	2003	30	0
1	E	2143	0	2032	38	0
1	G	2125	0	2020	29	0
2	B	782	0	716	13	0
2	D	780	0	702	6	0
2	F	778	0	704	2	0
2	H	786	0	713	6	0
3	I	70	0	61	0	0
4	J	59	0	52	2	0
4	K	59	0	52	2	0
4	L	59	0	52	1	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	E	28	0	26	1	0
5	G	14	0	13	3	0
6	A	54	0	86	6	0
6	E	54	0	86	11	1
7	A	6	0	8	0	0
7	C	18	0	24	0	0
7	E	6	0	8	3	0
7	G	24	0	32	1	0
8	C	51	0	79	10	0
8	G	51	0	79	3	1
9	C	1	0	0	0	0
9	G	1	0	0	0	0
10	A	93	0	0	2	0
10	B	21	0	0	0	0
10	C	90	0	0	1	0
10	D	19	0	0	0	0
10	E	114	0	0	5	0
10	F	27	0	0	0	0
10	G	111	0	0	0	0
10	H	31	0	0	0	0
All	All	12721	0	11589	134	1

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 6.

The worst 5 of 134 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:E:103:GLU:HB2	7:E:284:GOL:H32	1.54	0.86
1:E:73:TYR:HB2	6:E:285:L9R:H32	1.59	0.82
1:A:73:TYR:HA	6:A:284:L9R:H3	1.62	0.81
1:E:72:ALA:CB	6:E:285:L9R:H5A	2.12	0.80
1:E:72:ALA:HB2	6:E:285:L9R:H5A	1.64	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:285:L9R:O1P	8:G:289:L9Q:O31[3_554]	2.04	0.16

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	271/283 (96%)	261 (96%)	10 (4%)	0	100	100
1	C	268/283 (95%)	258 (96%)	10 (4%)	0	100	100
1	E	273/283 (96%)	269 (98%)	4 (2%)	0	100	100
1	G	271/283 (96%)	266 (98%)	5 (2%)	0	100	100
2	B	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
2	D	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
2	F	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
2	H	96/98 (98%)	96 (100%)	0	0	100	100
All	All	1466/1524 (96%)	1429 (98%)	37 (2%)	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	223/240 (93%)	223 (100%)	0	100	100
1	C	221/240 (92%)	219 (99%)	2 (1%)	78	89
1	E	226/240 (94%)	224 (99%)	2 (1%)	78	89
1	G	223/240 (93%)	221 (99%)	2 (1%)	78	89
2	B	84/94 (89%)	83 (99%)	1 (1%)	71	84
2	D	81/94 (86%)	80 (99%)	1 (1%)	71	84
2	F	81/94 (86%)	78 (96%)	3 (4%)	34	48
2	H	83/94 (88%)	81 (98%)	2 (2%)	49	66
All	All	1222/1336 (92%)	1209 (99%)	13 (1%)	73	86

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	127	GLN
2	F	48	SER
1	G	235	LEU
1	E	83	ASP
1	G	86	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	127	GLN
1	C	152	GLN
1	G	127	GLN
1	C	89	GLN
2	D	34	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

21 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	I	1	1,3	14,14,15	0.61	0	17,19,21	1.75	5 (29%)
3	NAG	I	2	3	14,14,15	0.78	1 (7%)	17,19,21	0.95	0
3	BMA	I	3	3	11,11,12	0.79	0	15,15,17	1.35	2 (13%)
3	MAN	I	4	3	11,11,12	0.57	0	15,15,17	1.32	1 (6%)
3	FUC	I	5	3	10,10,11	0.56	0	14,14,16	0.93	1 (7%)
3	FUC	I	6	3	10,10,11	0.70	0	14,14,16	0.93	1 (7%)
4	NAG	J	1	1,4	14,14,15	0.85	1 (7%)	17,19,21	0.88	1 (5%)
4	NAG	J	2	4	14,14,15	0.76	0	17,19,21	1.02	1 (5%)
4	BMA	J	3	4	11,11,12	0.63	0	15,15,17	1.09	1 (6%)
4	FUC	J	4	4	10,10,11	0.62	0	14,14,16	0.63	0
4	FUC	J	5	4	10,10,11	0.62	0	14,14,16	0.94	1 (7%)
4	NAG	K	1	1,4	14,14,15	0.77	0	17,19,21	1.48	2 (11%)
4	NAG	K	2	4	14,14,15	0.77	0	17,19,21	1.27	2 (11%)
4	BMA	K	3	4	11,11,12	0.63	0	15,15,17	1.18	1 (6%)
4	FUC	K	4	4	10,10,11	0.55	0	14,14,16	0.83	0
4	FUC	K	5	4	10,10,11	0.78	0	14,14,16	0.91	0
4	NAG	L	1	1,4	14,14,15	0.84	0	17,19,21	0.79	0
4	NAG	L	2	4	14,14,15	0.69	0	17,19,21	0.89	0
4	BMA	L	3	4	11,11,12	0.52	0	15,15,17	1.01	1 (6%)
4	FUC	L	4	4	10,10,11	0.70	0	14,14,16	1.11	1 (7%)
4	FUC	L	5	4	10,10,11	0.81	0	14,14,16	0.76	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	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
3	FUC	I	5	3	-	-	0/1/1/1
3	FUC	I	6	3	-	-	0/1/1/1
4	NAG	J	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
4	FUC	J	4	4	-	-	0/1/1/1
4	FUC	J	5	4	-	-	0/1/1/1
4	NAG	K	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	FUC	K	4	4	-	-	0/1/1/1
4	FUC	K	5	4	-	-	0/1/1/1
4	NAG	L	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	BMA	L	3	4	-	1/2/19/22	0/1/1/1
4	FUC	L	4	4	-	-	0/1/1/1
4	FUC	L	5	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	O5-C1	-2.06	1.40	1.43
3	I	2	NAG	O5-C1	-2.04	1.40	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1	NAG	C2-N2-C7	3.90	128.46	122.90
3	I	4	MAN	C1-O5-C5	3.65	117.14	112.19
3	I	3	BMA	C1-C2-C3	3.45	113.90	109.67
4	J	3	BMA	C1-O5-C5	3.43	116.84	112.19
3	I	1	NAG	C2-N2-C7	-3.41	118.05	122.90

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

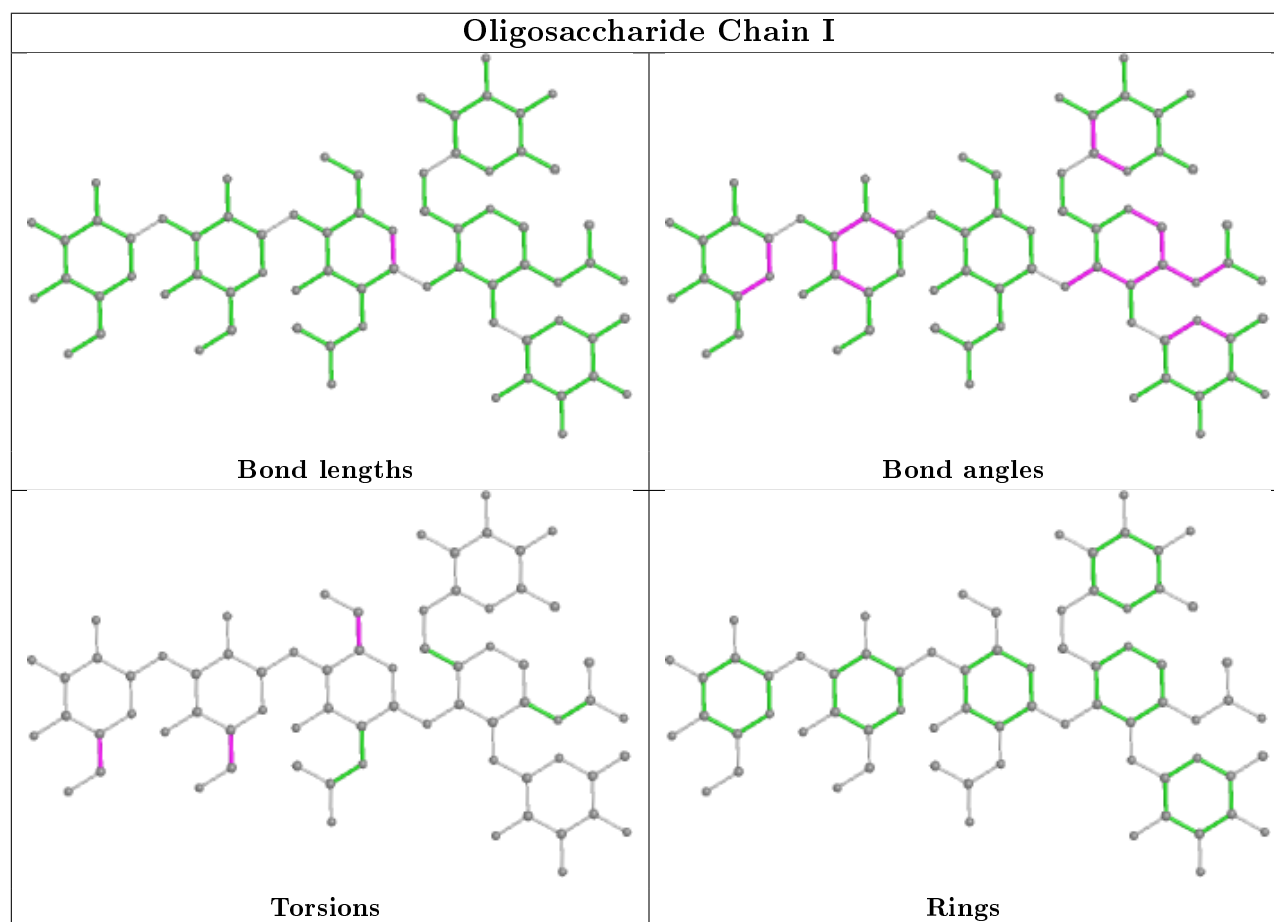
Mol	Chain	Res	Type	Atoms
3	I	3	BMA	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6

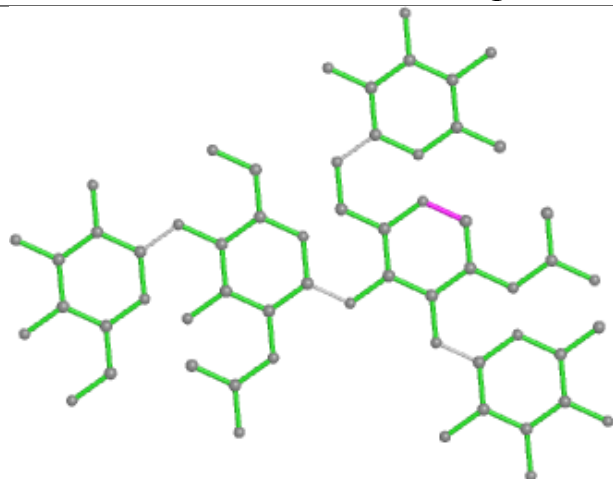
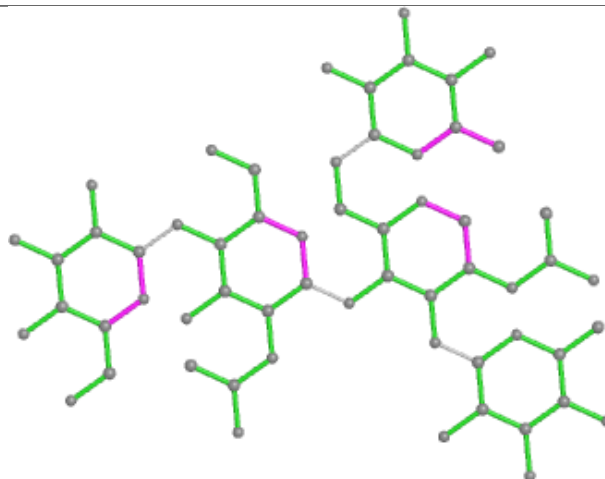
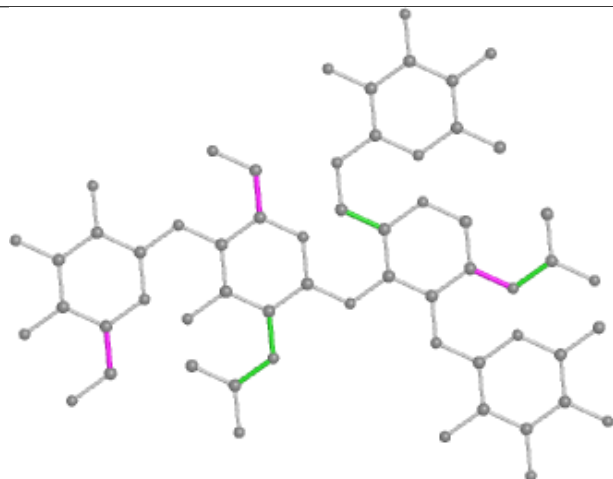
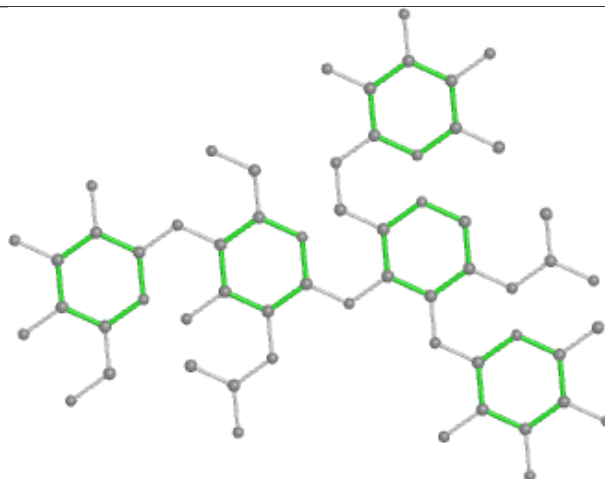
There are no ring outliers.

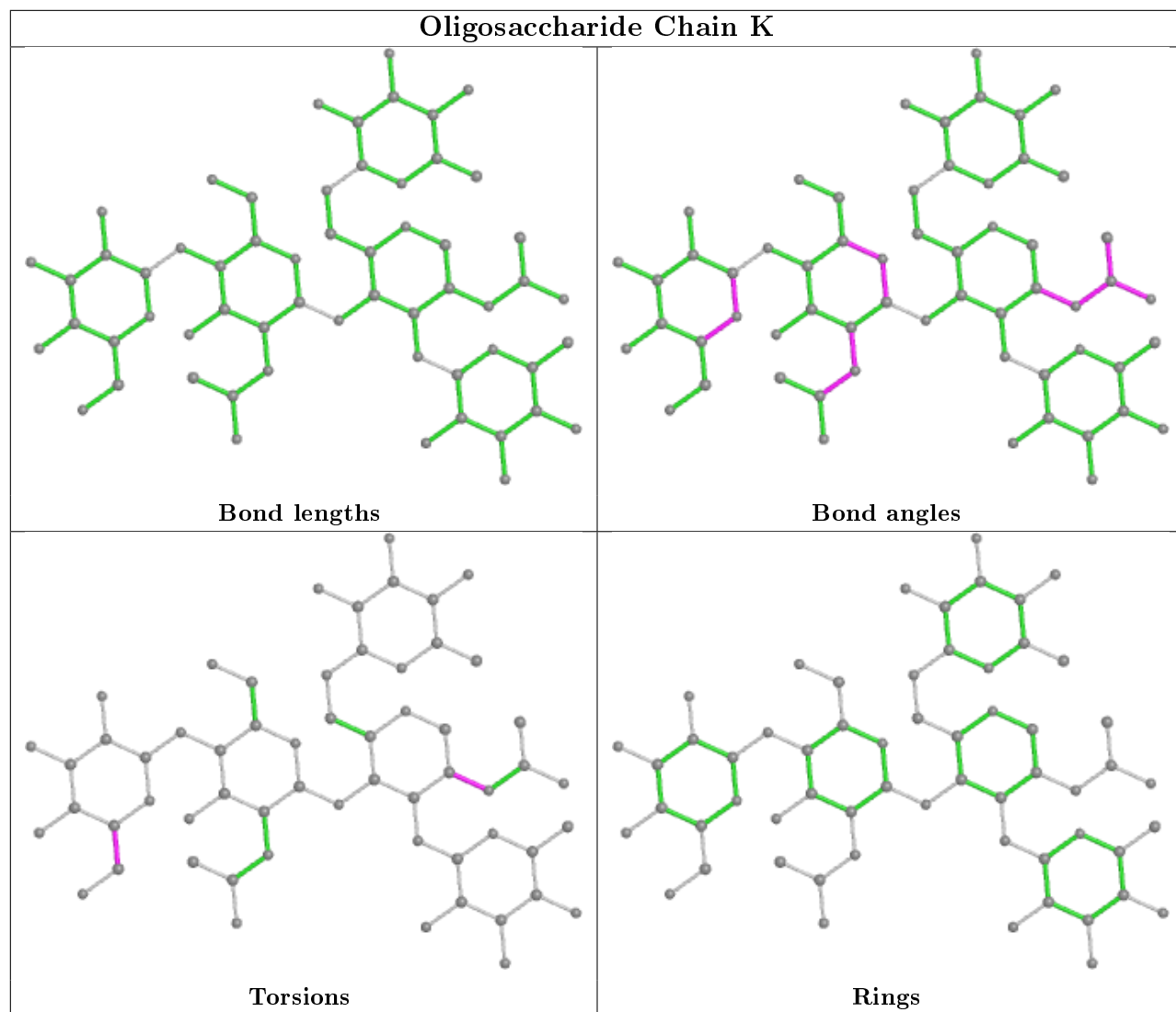
5 monomers are involved in 5 short contacts:

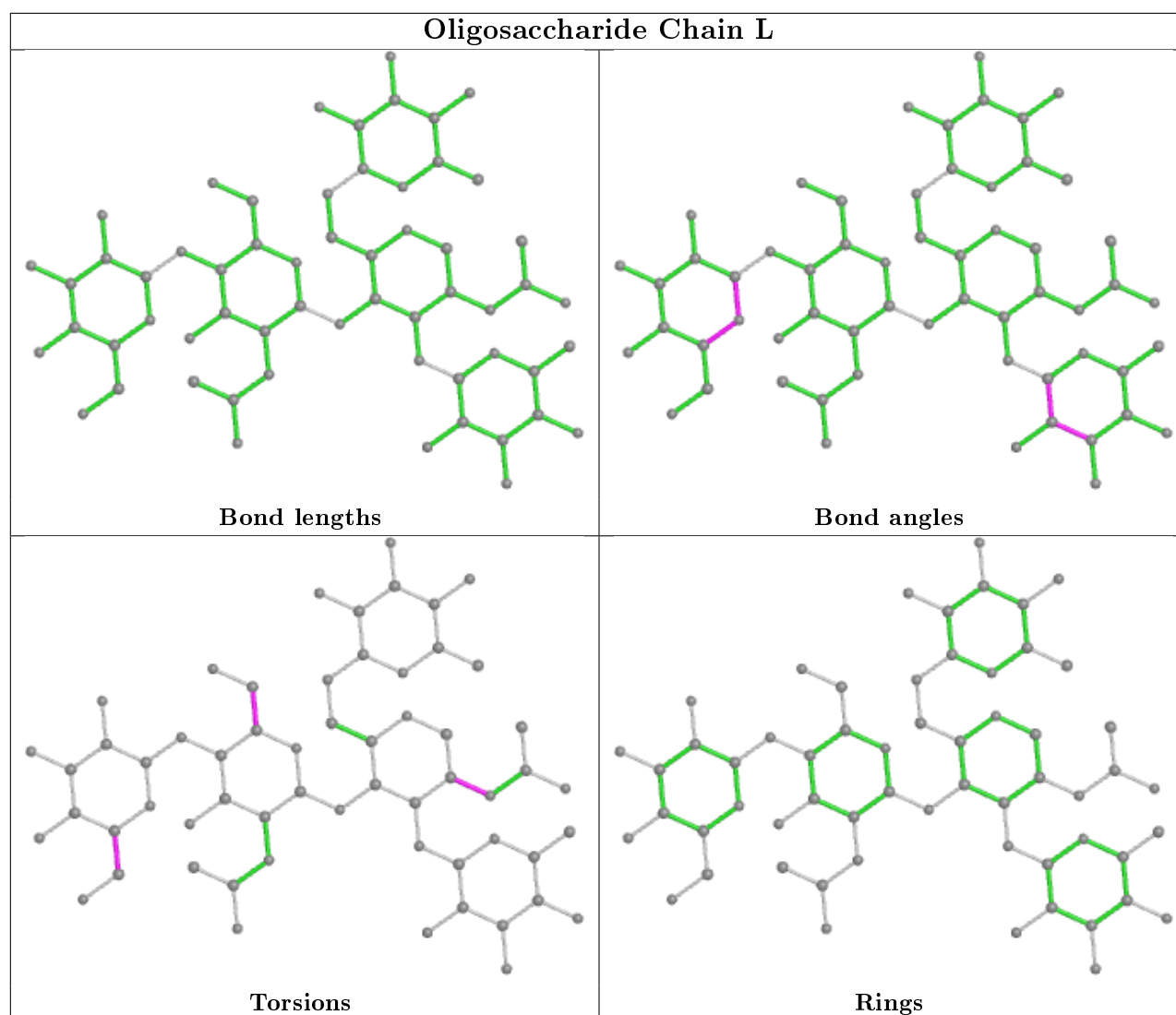
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0
4	J	2	NAG	1	0
4	L	1	NAG	1	0
4	J	4	FUC	2	0
4	K	2	NAG	1	0

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 J**Bond lengths****Bond angles****Torsions****Rings**





5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	GOL	G	284	-	5,5,5	0.26	0	5,5,5	0.35	0
7	GOL	G	286	-	5,5,5	0.39	0	5,5,5	0.35	0
7	GOL	C	285	-	5,5,5	0.20	0	5,5,5	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	500	1	14,14,15	0.52	0	17,19,21	1.06	2 (11%)
5	NAG	A	500	1	14,14,15	0.52	0	17,19,21	1.58	4 (23%)
8	L9Q	G	289	-	50,50,50	0.90	1 (2%)	53,55,55	1.02	1 (1%)
5	NAG	G	500	1	14,14,15	0.64	0	17,19,21	1.35	2 (11%)
7	GOL	G	287	-	5,5,5	0.37	0	5,5,5	0.48	0
6	L9R	A	284	-	53,53,53	1.07	5 (9%)	59,61,61	1.28	5 (8%)
7	GOL	E	284	-	5,5,5	0.37	0	5,5,5	0.26	0
5	NAG	E	500	1	14,14,15	0.43	0	17,19,21	2.23	5 (29%)
8	L9Q	C	284	-	50,50,50	0.87	2 (4%)	53,55,55	0.79	2 (3%)
7	GOL	C	286	-	5,5,5	0.44	0	5,5,5	0.33	0
7	GOL	A	285	-	5,5,5	0.27	0	5,5,5	0.35	0
5	NAG	E	508	1	14,14,15	0.61	0	17,19,21	1.60	2 (11%)
7	GOL	C	288	-	5,5,5	0.49	0	5,5,5	0.74	0
6	L9R	E	285	-	53,53,53	1.25	7 (13%)	59,61,61	1.54	6 (10%)
7	GOL	G	285	-	5,5,5	0.28	0	5,5,5	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	GOL	G	284	-	-	4/4/4/4	-
7	GOL	G	286	-	-	0/4/4/4	-
7	GOL	C	285	-	-	2/4/4/4	-
5	NAG	C	500	1	-	0/6/23/26	0/1/1/1
5	NAG	A	500	1	-	2/6/23/26	0/1/1/1
8	L9Q	G	289	-	-	20/54/54/54	-
5	NAG	G	500	1	-	2/6/23/26	0/1/1/1
7	GOL	G	287	-	-	0/4/4/4	-
6	L9R	A	284	-	-	34/57/57/57	-
7	GOL	E	284	-	-	0/4/4/4	-
5	NAG	E	500	1	-	4/6/23/26	0/1/1/1
8	L9Q	C	284	-	-	21/54/54/54	-
7	GOL	C	286	-	-	2/4/4/4	-
7	GOL	A	285	-	-	4/4/4/4	-
5	NAG	E	508	1	-	2/6/23/26	0/1/1/1
7	GOL	C	288	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	L9R	E	285	-	-	32/57/57/57	-
7	GOL	G	285	-	-	0/4/4/4	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	285	L9R	C3-C2	3.43	1.61	1.50
6	E	285	L9R	O3-C3	2.71	1.51	1.45
6	E	285	L9R	O3-C11	2.39	1.40	1.33
6	A	284	L9R	C1-C2	2.33	1.57	1.50
8	G	289	L9Q	P-O4P	2.29	1.68	1.59

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	500	NAG	C1-O5-C5	7.09	121.80	112.19
6	E	285	L9R	O3-C3-C2	5.92	125.68	108.43
6	A	284	L9R	O2-C31-C32	5.41	123.16	111.50
6	E	285	L9R	C3-C2-C1	5.41	124.57	111.79
8	G	289	L9Q	O2-C31-C32	4.71	121.65	111.50

There are no chirality outliers.

5 of 130 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	284	L9Q	O4P-C4-C5-N
8	G	289	L9Q	O4P-C4-C5-N
6	A	284	L9R	O11-C11-O3-C3
6	A	284	L9R	C12-C11-O3-C3
6	A	284	L9R	O4P-C4-C5-N

There are no ring outliers.

8 monomers are involved in 39 short contacts:

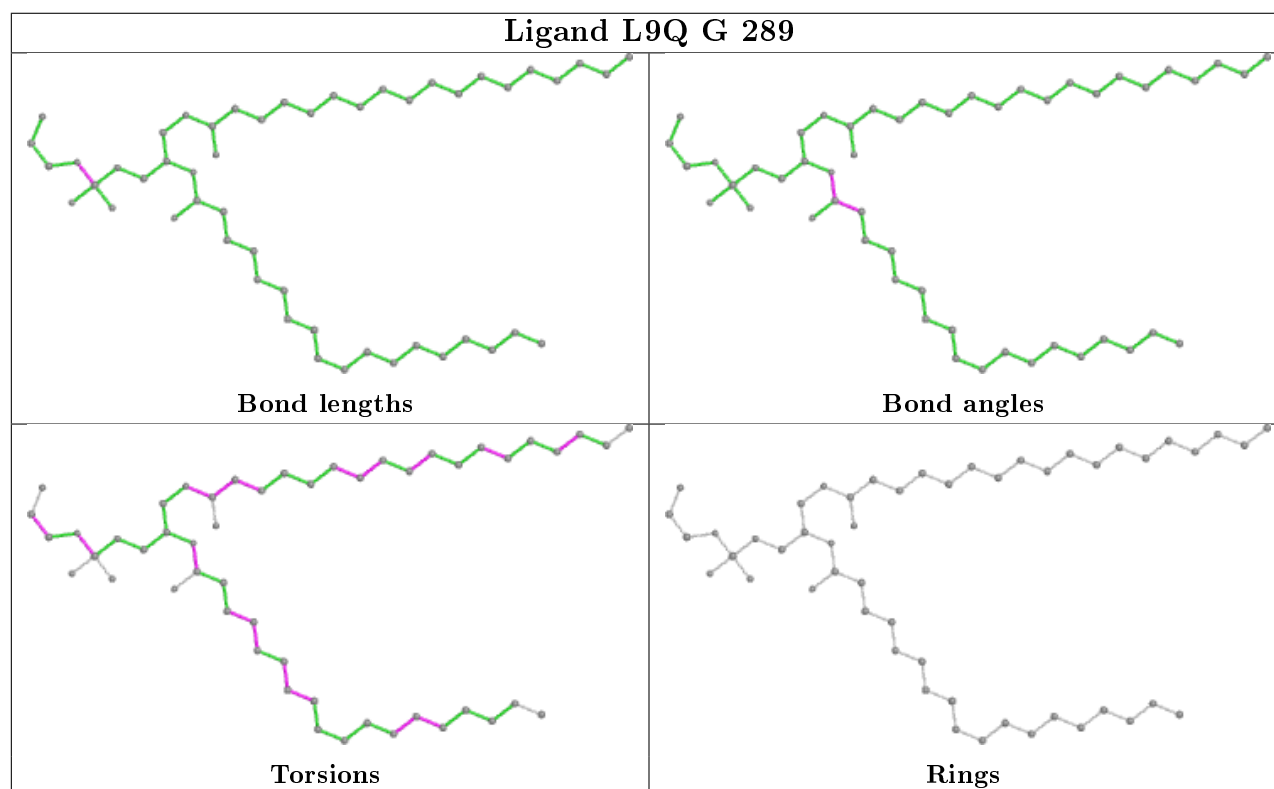
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	286	GOL	1	0
8	G	289	L9Q	3	1
5	G	500	NAG	3	0
6	A	284	L9R	6	0
7	E	284	GOL	3	0
8	C	284	L9Q	10	0

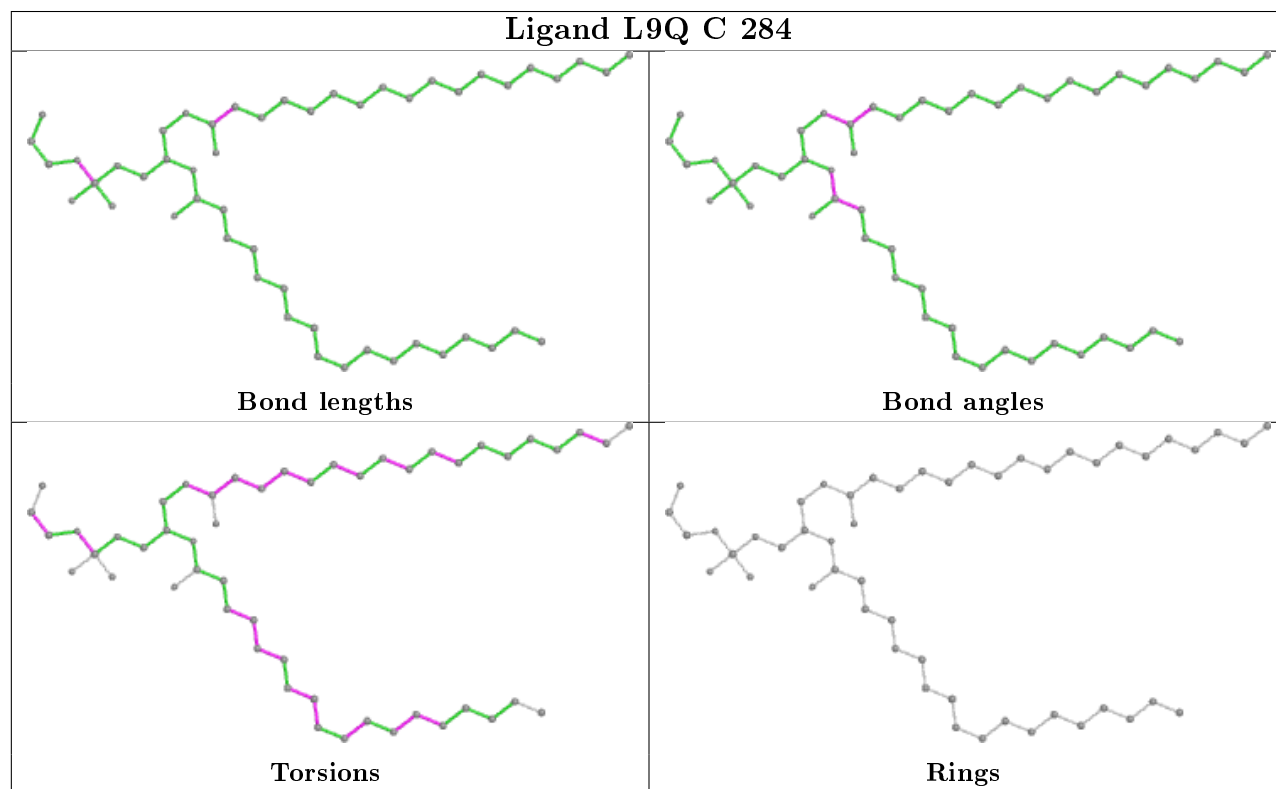
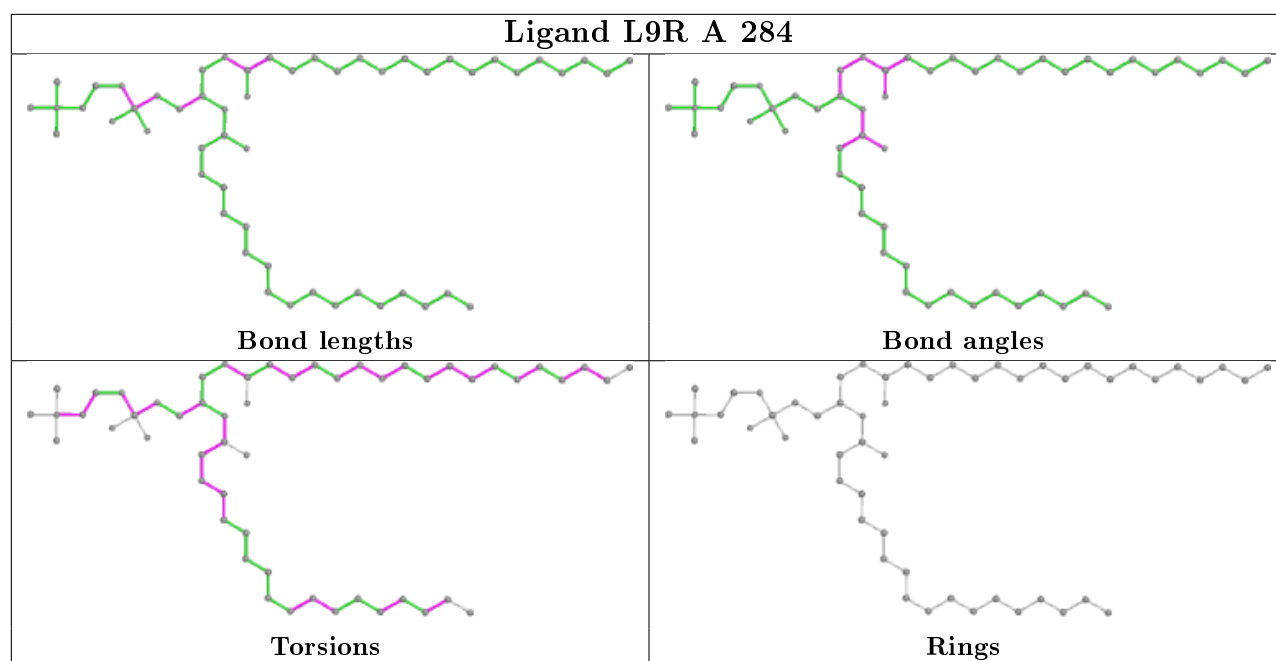
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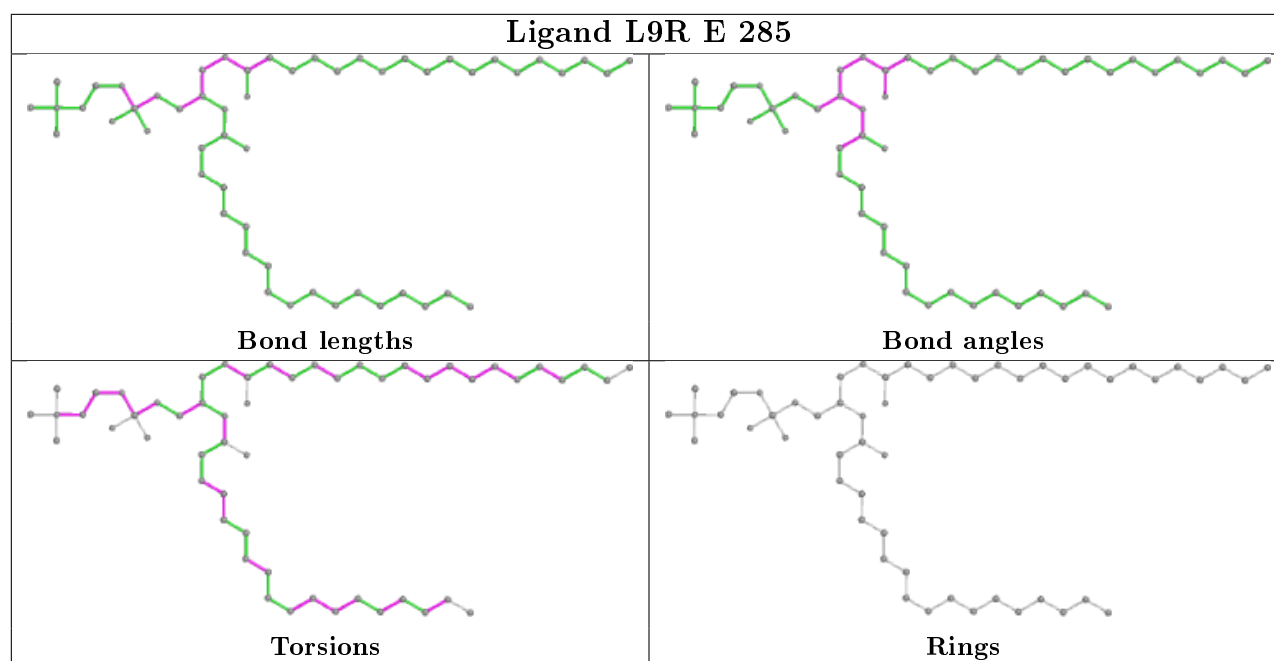
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	508	NAG	1	0
6	E	285	L9R	11	1

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/283 (97%)	-0.01	2 (0%) 87 91	23, 39, 63, 73	0
1	C	274/283 (96%)	0.06	4 (1%) 73 79	21, 40, 65, 77	0
1	E	275/283 (97%)	-0.02	2 (0%) 87 91	21, 36, 58, 69	0
1	G	275/283 (97%)	-0.00	2 (0%) 87 91	21, 36, 60, 69	0
2	B	97/98 (98%)	0.03	1 (1%) 82 86	29, 54, 88, 124	0
2	D	98/98 (100%)	0.17	1 (1%) 82 86	31, 59, 91, 111	0
2	F	98/98 (100%)	-0.09	1 (1%) 82 86	27, 43, 66, 73	0
2	H	98/98 (100%)	0.00	2 (2%) 65 71	28, 51, 76, 95	0
All	All	1490/1524 (97%)	0.01	15 (1%) 82 86	21, 40, 71, 124	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	PHE	4.8
2	B	1	ILE	4.5
1	G	4	PHE	4.0
1	G	23	TRP	3.8
2	D	1	ILE	3.6

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

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

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,

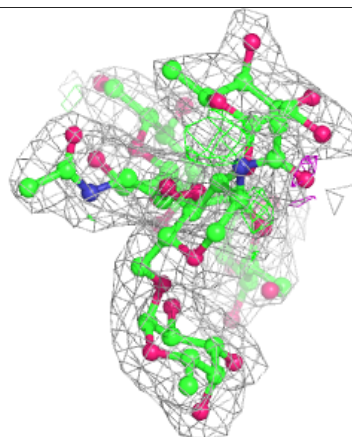
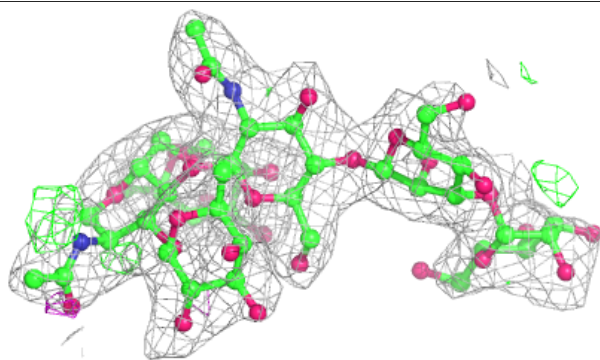
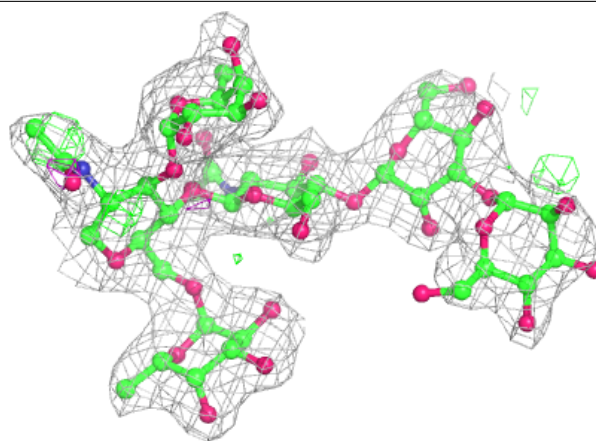
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	J	3	11/12	0.75	0.16	62,69,76,77	0
4	BMA	K	3	11/12	0.85	0.15	59,66,71,73	0
3	BMA	I	3	11/12	0.86	0.12	67,74,82,83	0
3	MAN	I	4	11/12	0.89	0.16	80,88,98,99	0
4	BMA	L	3	11/12	0.90	0.13	63,69,75,75	0
4	FUC	L	4	10/11	0.92	0.16	47,52,58,59	0
3	FUC	I	5	10/11	0.92	0.12	50,55,61,61	0
3	NAG	I	1	14/15	0.93	0.16	38,43,48,51	0
4	NAG	J	2	14/15	0.94	0.11	43,48,52,58	0
4	FUC	K	4	10/11	0.94	0.10	45,50,54,54	0
4	FUC	J	5	10/11	0.96	0.17	41,46,49,51	0
4	FUC	L	5	10/11	0.96	0.15	40,44,47,50	0
4	NAG	L	2	14/15	0.96	0.10	37,46,51,57	0
4	NAG	J	1	14/15	0.97	0.12	32,36,44,44	0
3	NAG	I	2	14/15	0.97	0.12	42,49,56,60	0
4	FUC	K	5	10/11	0.97	0.14	32,38,41,44	0
4	FUC	J	4	10/11	0.97	0.10	48,53,60,60	0
4	NAG	L	1	14/15	0.98	0.11	29,34,40,43	0
3	FUC	I	6	10/11	0.98	0.09	35,40,45,49	0
4	NAG	K	1	14/15	0.98	0.13	31,35,40,42	0
4	NAG	K	2	14/15	0.98	0.13	36,44,49,53	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.

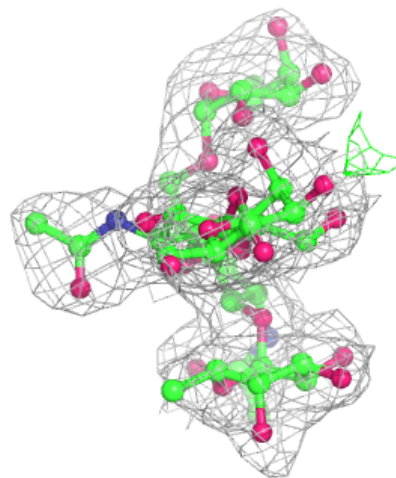
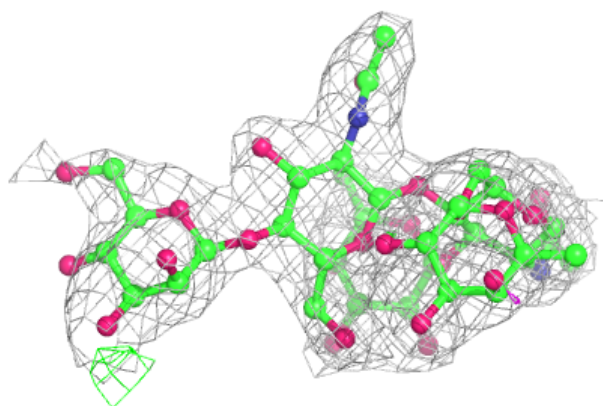
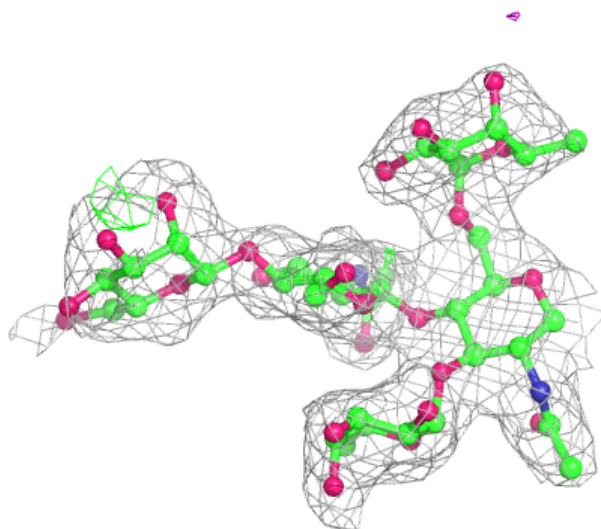
Electron density around Chain I:

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



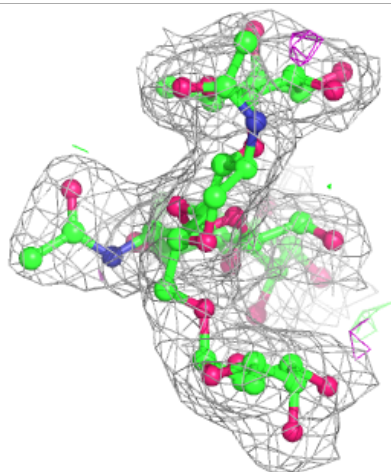
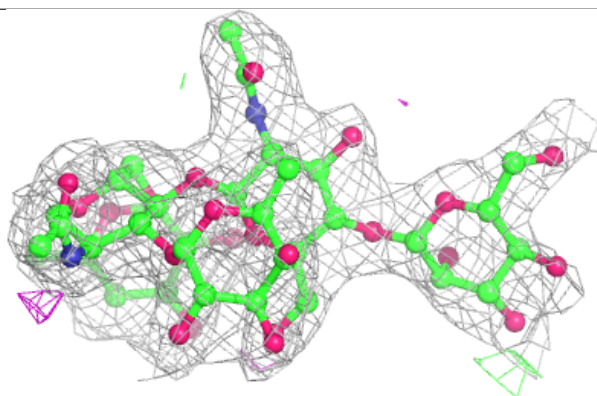
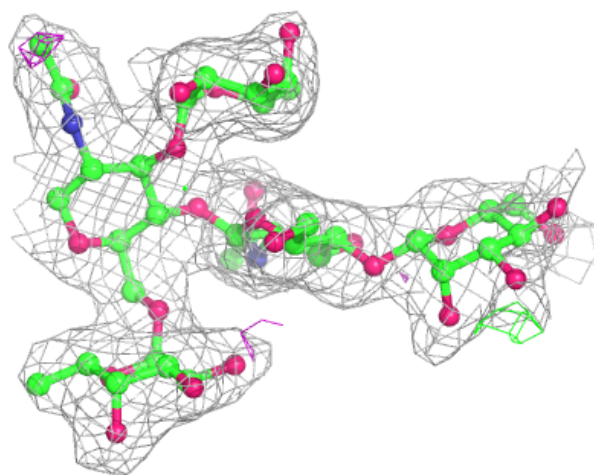
Electron density around Chain J:

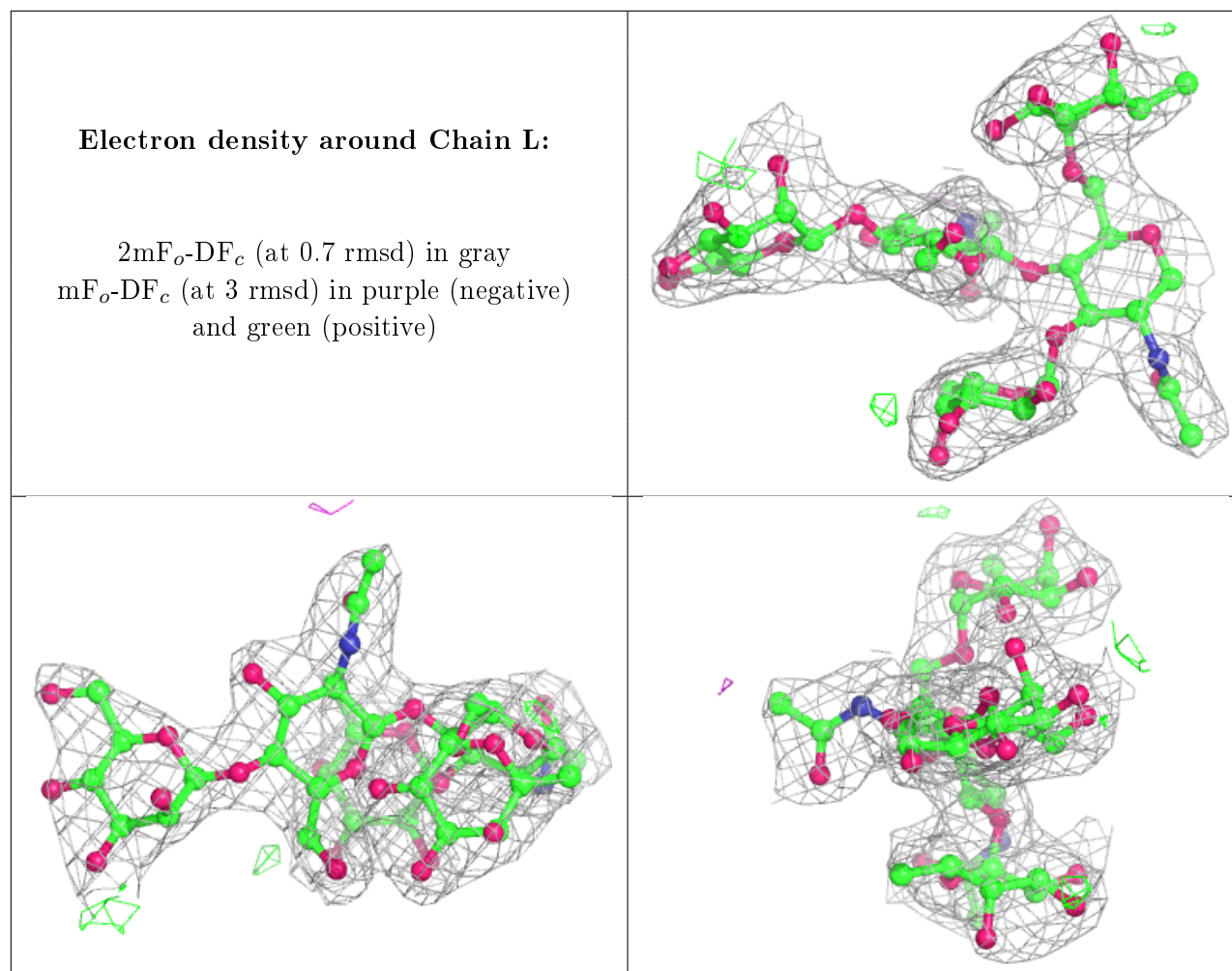
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (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
5	NAG	G	500	14/15	0.66	0.21	60,70,78,80	0
8	L9Q	G	289	51/51	0.69	0.30	34,51,81,83	0
7	GOL	G	286	6/6	0.73	0.17	66,67,69,69	0
8	L9Q	C	284	51/51	0.74	0.31	31,58,86,88	0
5	NAG	A	500	14/15	0.74	0.17	86,94,98,100	0
5	NAG	C	500	14/15	0.74	0.15	78,87,91,93	0
6	L9R	E	285	54/54	0.76	0.26	31,56,82,85	0
6	L9R	A	284	54/54	0.77	0.22	38,59,86,87	0
5	NAG	E	500	14/15	0.79	0.14	79,87,95,96	0
5	NAG	E	508	14/15	0.86	0.13	63,72,77,81	0

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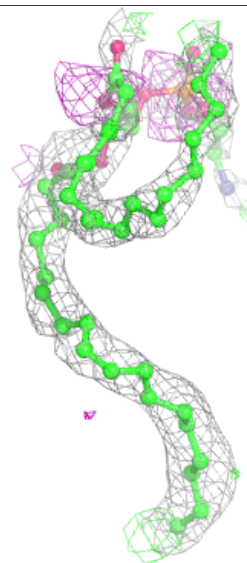
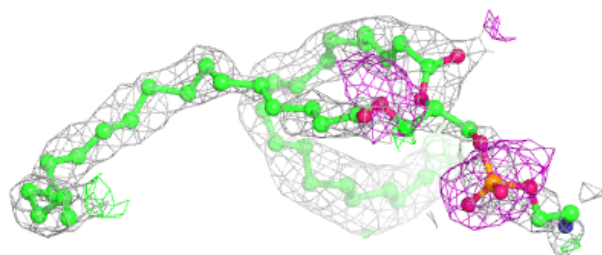
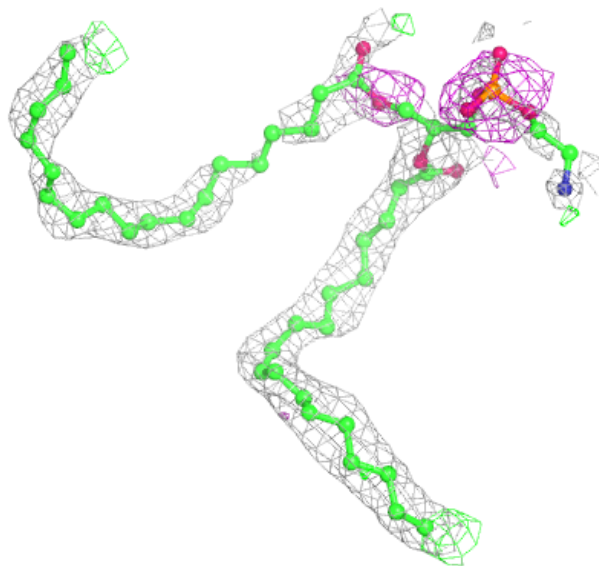
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	E	284	6/6	0.89	0.19	53,54,55,56	0
7	GOL	C	285	6/6	0.90	0.19	41,45,46,48	0
7	GOL	C	288	6/6	0.91	0.17	51,52,55,56	0
7	GOL	G	285	6/6	0.91	0.12	44,45,46,46	0
7	GOL	C	286	6/6	0.92	0.18	53,56,57,59	0
7	GOL	G	287	6/6	0.95	0.14	47,48,50,51	0
7	GOL	A	285	6/6	0.95	0.14	56,56,57,58	0
7	GOL	G	284	6/6	0.95	0.18	55,55,55,55	0
9	CL	C	287	1/1	0.98	0.12	35,35,35,35	0
9	CL	G	288	1/1	0.99	0.14	30,30,30,30	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.

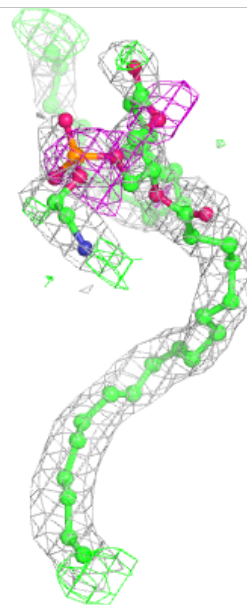
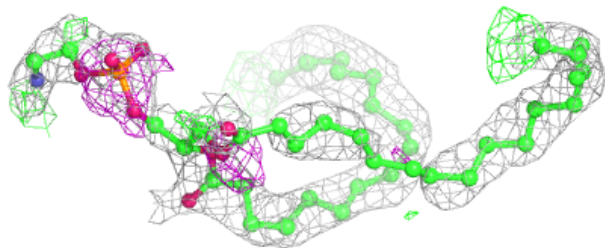
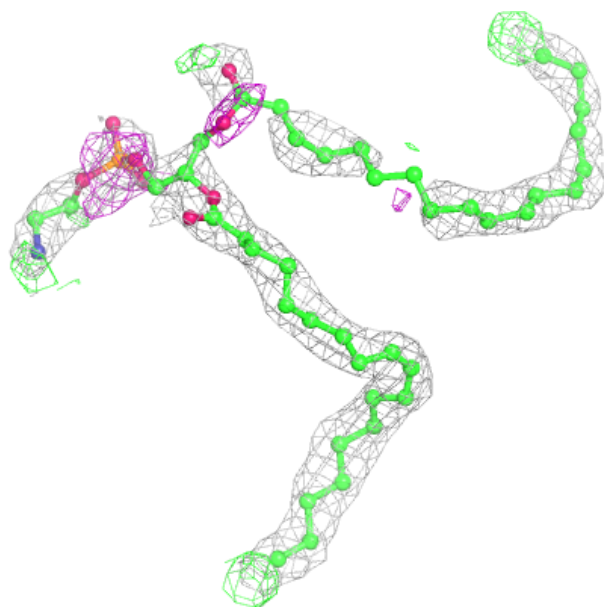
Electron density around L9Q G 289:

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



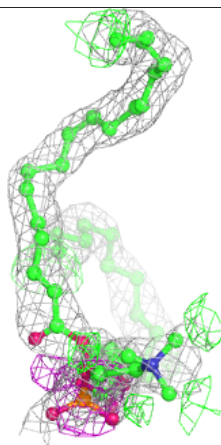
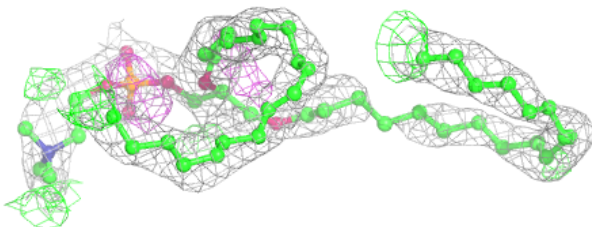
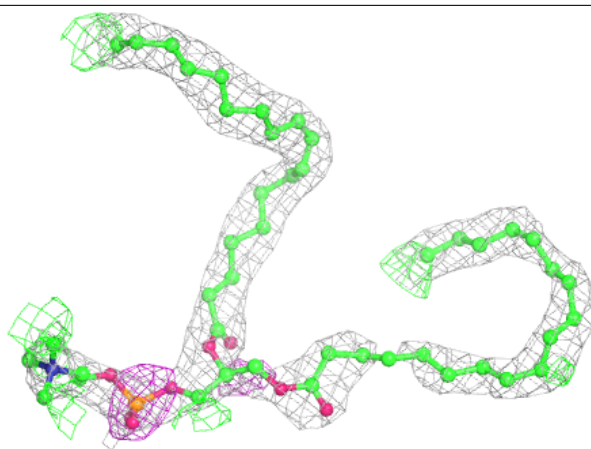
Electron density around L9Q C 284:

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



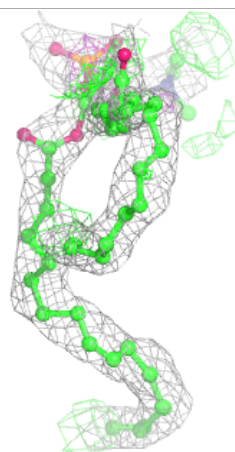
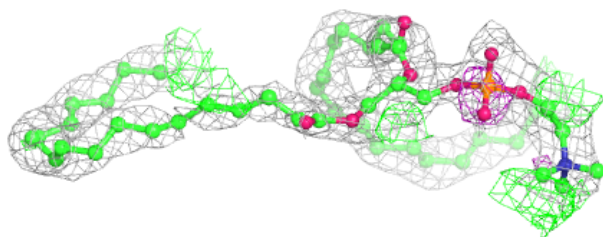
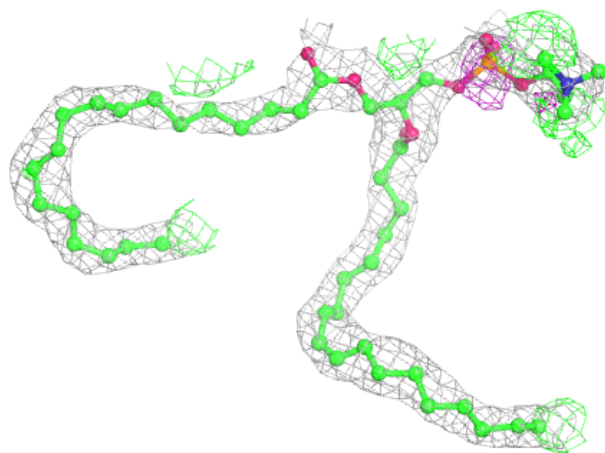
Electron density around L9R E 285:

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



Electron density around L9R A 284:

$2mF_o-DF_c$ (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.