



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:50 PM UTC

PDB ID : 3MA7 / pdb_00003ma7
Title : Crystal structure of Cardiolipin bound to mouse CD1D
Authors : Zajonc, D.M.
Deposited on : 2010-03-23
Resolution : 2.29 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

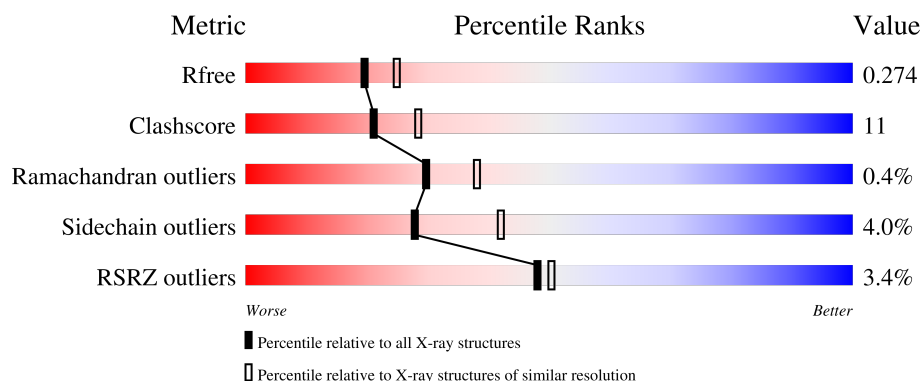
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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.



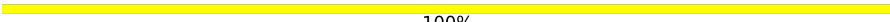
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 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	285	5% 69% 26% • •
1	C	285	4% 69% 23% • 7%
2	B	99	2% 76% 19% • •
2	D	99	83% 13% • •
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
3	G	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6280 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 T-cell surface glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	265	Total	C	N	O	S	0	0	0
			2115	1352	361	389	13			
1	A	273	Total	C	N	O	S	0	0	0
			2180	1389	376	402	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	201	HIS	ASP	engineered mutation	UNP P11609
C	280	HIS	-	expression tag	UNP P11609
C	281	HIS	-	expression tag	UNP P11609
C	282	HIS	-	expression tag	UNP P11609
C	283	HIS	-	expression tag	UNP P11609
C	284	HIS	-	expression tag	UNP P11609
C	285	HIS	-	expression tag	UNP P11609
A	201	HIS	ASP	engineered mutation	UNP P11609
A	280	HIS	-	expression tag	UNP P11609
A	281	HIS	-	expression tag	UNP P11609
A	282	HIS	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	HIS	-	expression tag	UNP P11609

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	98	Total	C	N	O	S	0	0	0
			809	517	137	148	7			
2	B	98	Total	C	N	O	S	0	0	0
			793	506	134	146	7			

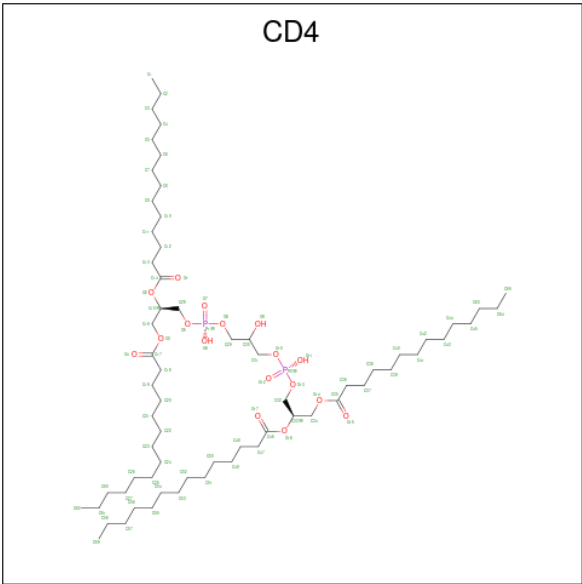
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



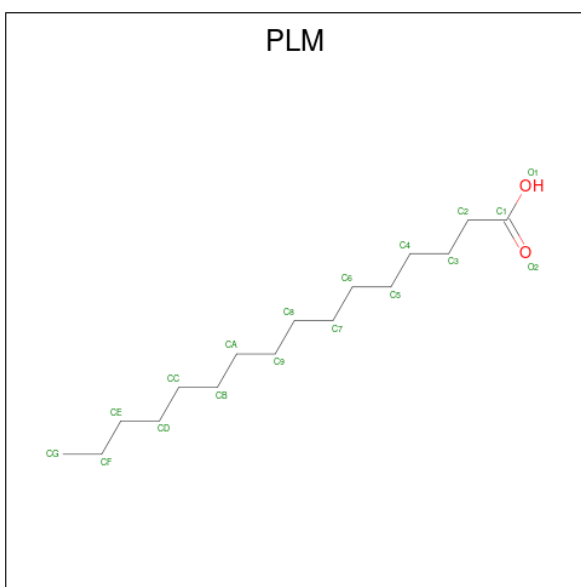
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecano yloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (CCD ID: CD4) (formula: C₆₅H₁₂₆O₁₇P₂).



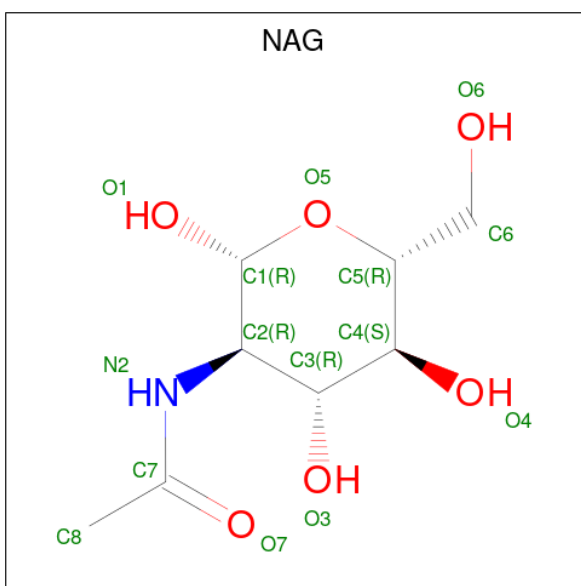
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O	P	0	0
			46	31	13	2		
4	A	1	Total	C	O	P	0	0
			46	31	13	2		

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			18	16	2		
5	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

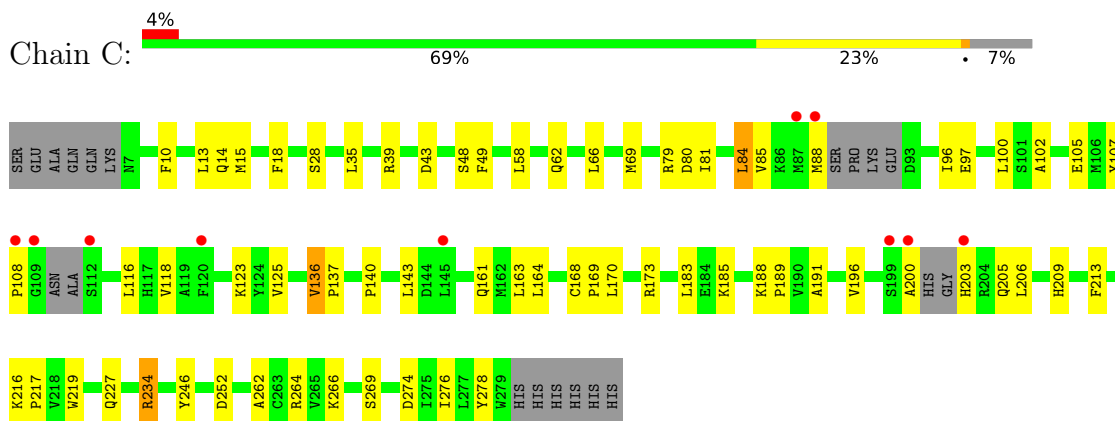
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	62	Total 62	O 62	0	0
7	D	36	Total 36	O 36	0	0
7	A	43	Total 43	O 43	0	0
7	B	16	Total 16	O 16	0	0

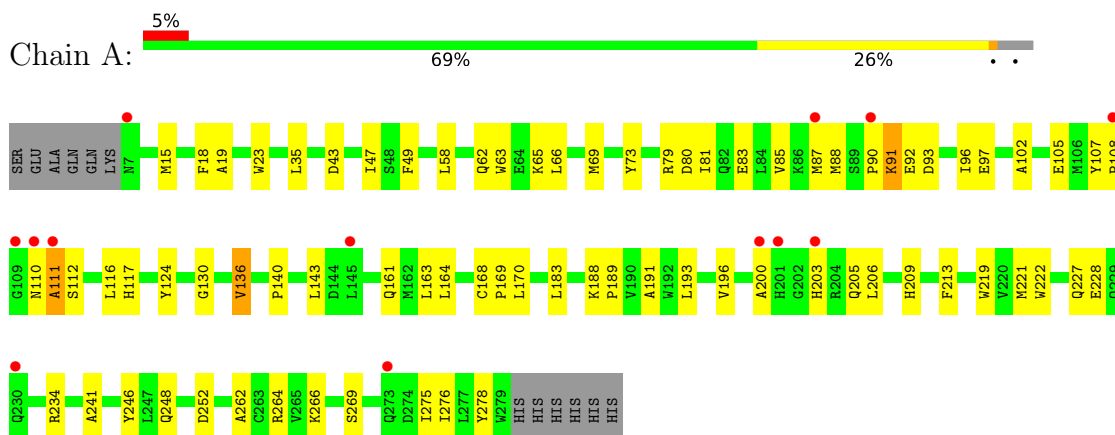
3 Residue-property plots [i](#)

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.

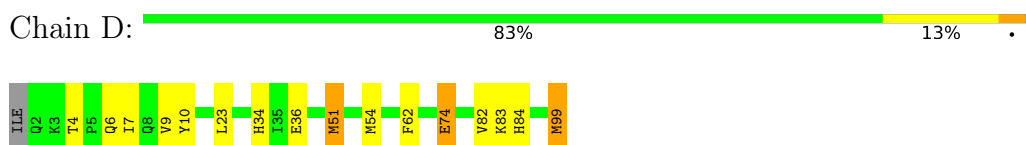
• Molecule 1: T-cell surface glycoprotein CD1d1



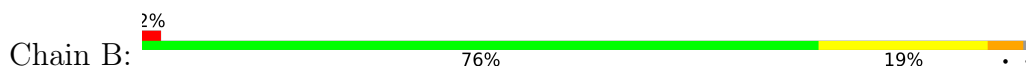
• Molecule 1: T-cell surface glycoprotein CD1d1

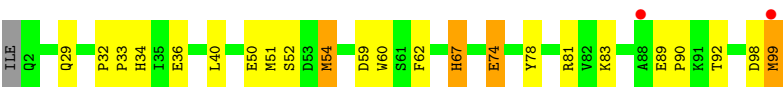


• Molecule 2: Beta-2 microglobulin



• Molecule 2: Beta-2 microglobulin

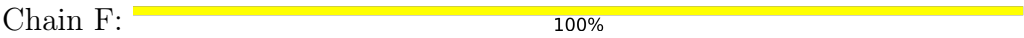




• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.77Å 50.92Å 103.17Å 102.15° 92.22° 106.21°	Depositor
Resolution (Å)	44.68 – 2.29 44.68 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.2 (44.68-2.29) 94.2 (44.68-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.232 , 0.273 0.235 , 0.274	Depositor DCC
R_{free} test set	1157 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6280	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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: CD4, NAG, PLM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	0/2245	0.90	2/3055 (0.1%)
1	C	0.81	0/2175	0.91	0/2957
2	B	0.71	0/819	0.91	1/1116 (0.1%)
2	D	0.78	0/835	0.89	2/1133 (0.2%)
All	All	0.77	0/6074	0.91	5/8261 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	SER	N-CA-C	-6.12	101.13	109.95
1	A	164	LEU	N-CA-C	5.89	117.37	111.07
2	D	4	THR	CA-C-N	5.46	125.38	119.76
2	D	4	THR	C-N-CA	5.46	125.38	119.76
2	B	29	GLN	N-CA-C	5.28	119.31	112.86

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	2180	0	2074	59	0
1	C	2115	0	2005	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	793	0	746	23	0
2	D	809	0	783	15	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	3	0
4	A	46	0	56	1	0
4	C	46	0	56	2	0
5	A	18	0	31	1	0
5	C	18	0	31	6	0
6	C	14	0	13	0	0
7	A	43	0	0	4	1
7	B	16	0	0	2	1
7	C	62	0	0	4	0
7	D	36	0	0	4	0
All	All	6280	0	5870	132	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 11.

All (132) 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)
2:D:99:MET:HE1	7:D:144:HOH:O	1.40	1.19
2:B:98:ASP:OD2	7:B:147:HOH:O	1.62	1.16
1:A:43:ASP:HB2	7:A:318:HOH:O	1.56	1.03
1:A:88:MET:HB3	1:A:91:LYS:CB	1.97	0.94
1:A:241:ALA:CB	2:B:67:HIS:CD2	2.51	0.92
1:A:241:ALA:HB2	2:B:67:HIS:HD2	1.38	0.87
1:A:91:LYS:CB	1:A:92:GLU:HA	2.05	0.86
1:A:241:ALA:CB	2:B:67:HIS:HD2	1.89	0.83
1:C:43:ASP:HB2	7:C:338:HOH:O	1.82	0.80
1:A:107:TYR:HB2	1:A:110:ASN:HB2	1.65	0.79
1:A:85:VAL:O	1:A:88:MET:HB2	1.83	0.78
1:A:241:ALA:HB2	2:B:67:HIS:CD2	2.17	0.74
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.71	0.72
1:A:241:ALA:HB1	2:B:67:HIS:CD2	2.26	0.69
1:A:91:LYS:CB	1:A:92:GLU:CA	2.73	0.67
1:A:200:ALA:HB1	1:A:203:HIS:ND1	2.10	0.66
7:A:295:HOH:O	3:G:2:NAG:O4	2.15	0.65
1:A:18:PHE:HB2	1:A:96:ILE:HB	1.79	0.64
1:A:73:TYR:HB2	4:A:2089:CD4:H33	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HD12	1:C:88:MET:HG3	1.84	0.60
1:C:69:MET:HE1	1:C:163:LEU:HD11	1.81	0.60
1:C:164:LEU:HD23	5:C:286:PLM:HF2	1.81	0.60
1:A:205:GLN:HG3	1:A:252:ASP:OD2	2.01	0.59
1:A:161:GLN:HB3	3:G:1:NAG:H82	1.84	0.59
1:C:205:GLN:HG3	1:C:252:ASP:OD2	2.02	0.59
1:A:246:TYR:OH	2:B:99:MET:HE3	2.03	0.59
1:A:97:GLU:OE2	2:B:34:HIS:HE1	1.86	0.59
1:A:88:MET:CB	1:A:91:LYS:CB	2.78	0.58
1:C:168:CYS:HB3	1:C:169:PRO:HD3	1.84	0.58
1:C:84:LEU:CD1	1:C:88:MET:HG3	2.34	0.58
1:A:191:ALA:HA	1:A:209:HIS:O	2.04	0.58
1:A:130:GLY:HA2	3:G:1:NAG:H5	1.88	0.56
1:C:18:PHE:HB2	1:C:96:ILE:HB	1.88	0.56
1:C:191:ALA:HA	1:C:209:HIS:O	2.05	0.56
2:D:99:MET:HE2	7:D:100:HOH:O	2.04	0.56
1:C:58:LEU:HD22	1:C:62:GLN:HB3	1.88	0.55
1:C:84:LEU:HD12	1:C:84:LEU:O	2.07	0.54
1:C:164:LEU:CD2	5:C:286:PLM:HF2	2.38	0.53
1:A:69:MET:HE1	1:A:163:LEU:HD11	1.91	0.53
1:C:35:LEU:HD12	1:C:183:LEU:HD23	1.91	0.53
1:C:81:ILE:O	1:C:85:VAL:HG23	2.09	0.53
2:B:52:SER:HA	7:B:107:HOH:O	2.09	0.53
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.91	0.52
1:A:107:TYR:CB	1:A:110:ASN:HB2	2.38	0.52
1:C:163:LEU:HD13	5:C:286:PLM:HG2	1.92	0.52
1:A:124:TYR:HB2	2:B:60:TRP:HE1	1.74	0.52
1:C:107:TYR:HB3	1:C:108:PRO:HD2	1.90	0.52
1:C:185:LYS:HE2	7:C:322:HOH:O	2.11	0.51
1:A:262:ALA:HB2	1:A:278:TYR:CD2	2.45	0.51
1:A:221:MET:HG2	1:A:228:GLU:HG2	1.94	0.49
1:A:19:ALA:HB3	1:A:23:TRP:HB3	1.94	0.49
1:A:81:ILE:O	1:A:85:VAL:HG23	2.13	0.48
1:A:248:GLN:OE1	2:B:99:MET:HG2	2.13	0.48
2:B:36:GLU:HB3	2:B:83:LYS:HB3	1.96	0.48
1:A:85:VAL:HG12	1:A:92:GLU:HG2	1.95	0.48
1:A:97:GLU:OE2	2:B:34:HIS:CE1	2.67	0.48
1:A:58:LEU:HD22	1:A:62:GLN:HB3	1.95	0.48
1:C:15:MET:HG2	2:D:62:PHE:HE2	1.78	0.47
1:C:188:LYS:HA	1:C:269:SER:OG	2.14	0.47
2:D:74:GLU:HA	7:D:116:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:C	1:A:116:LEU:HD23	2.39	0.47
1:A:66:LEU:HD12	1:A:69:MET:HE3	1.97	0.47
1:A:117:HIS:HB3	1:A:124:TYR:CE1	2.50	0.47
2:B:54:MET:HE2	2:B:54:MET:HB2	1.82	0.47
1:A:49:PHE:HE1	1:A:63:TRP:CZ2	2.33	0.47
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.96	0.47
2:B:67:HIS:ND1	2:B:67:HIS:C	2.73	0.47
1:A:140:PRO:HD2	1:A:143:LEU:HD12	1.96	0.47
1:A:102:ALA:HB2	1:A:116:LEU:HG	1.97	0.46
2:D:54:MET:HE2	2:D:54:MET:HB2	1.89	0.46
1:A:15:MET:HG2	2:B:62:PHE:HE2	1.80	0.46
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.97	0.46
2:B:81:ARG:HG3	2:B:92:THR:OG1	2.15	0.46
1:C:161:GLN:HB3	3:E:1:NAG:H82	1.97	0.46
1:C:102:ALA:HB2	1:C:116:LEU:HG	1.98	0.45
1:C:143:LEU:HD21	4:C:2089:CD4:H6	1.98	0.45
1:C:97:GLU:OE2	2:D:34:HIS:HE1	2.00	0.45
1:C:108:PRO:HD3	7:C:331:HOH:O	2.16	0.45
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.98	0.45
2:B:50:GLU:HB2	2:B:67:HIS:CE1	2.51	0.45
1:A:140:PRO:O	1:A:143:LEU:HB2	2.17	0.45
1:C:234:ARG:HD3	7:C:336:HOH:O	2.15	0.45
1:C:262:ALA:HB2	1:C:278:TYR:CD2	2.51	0.45
1:C:14:GLN:HB3	1:C:100:LEU:HB2	1.99	0.45
1:C:49:PHE:CD1	1:C:49:PHE:N	2.82	0.45
1:A:111:ALA:HB3	7:A:317:HOH:O	2.17	0.45
1:C:123:LYS:O	1:C:125:VAL:HG13	2.18	0.44
5:C:286:PLM:H81	5:C:286:PLM:HB2	1.48	0.44
1:A:193:LEU:HD22	1:A:222:TRP:CH2	2.52	0.44
1:C:39:ARG:HG2	1:C:48:SER:HB2	1.98	0.44
1:C:246:TYR:OH	2:D:99:MET:HE3	2.18	0.44
1:C:266:LYS:HG2	1:C:274:ASP:CG	2.43	0.44
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.47	0.44
1:C:13:LEU:O	1:C:28:SER:HA	2.18	0.44
1:A:200:ALA:CB	1:A:203:HIS:ND1	2.80	0.44
1:A:188:LYS:HA	1:A:269:SER:OG	2.18	0.44
1:C:200:ALA:HB1	1:C:203:HIS:ND1	2.33	0.43
1:C:219:TRP:HB3	1:C:266:LYS:HB2	1.99	0.43
4:C:2089:CD4:H45	5:C:286:PLM:HG1	2.00	0.43
1:C:136:VAL:O	1:C:137:PRO:C	2.61	0.43
1:C:107:TYR:HB3	1:C:108:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:MET:HE2	2:D:51:MET:HB3	1.66	0.43
2:D:10:TYR:CD1	2:D:10:TYR:N	2.86	0.43
1:C:140:PRO:HD2	1:C:143:LEU:HD12	2.01	0.42
2:B:40:LEU:O	2:B:78:TYR:HA	2.20	0.42
1:C:140:PRO:O	1:C:143:LEU:HB2	2.19	0.42
2:D:36:GLU:HB3	2:D:83:LYS:HB3	2.02	0.42
1:A:168:CYS:HB3	1:A:169:PRO:CD	2.47	0.42
1:A:264:ARG:HG3	1:A:276:ILE:HG12	2.01	0.42
2:B:74:GLU:CD	2:B:74:GLU:H	2.27	0.42
2:B:89:GLU:HA	2:B:90:PRO:HD2	1.86	0.42
1:C:79:ARG:NH2	1:C:80:ASP:OD1	2.52	0.42
1:C:264:ARG:HG3	1:C:276:ILE:HG12	2.02	0.42
2:B:59:ASP:O	2:B:60:TRP:HB2	2.19	0.42
2:D:34:HIS:O	2:D:84:HIS:HD2	2.03	0.42
1:A:79:ARG:O	1:A:83:GLU:HG2	2.20	0.42
1:A:264:ARG:HA	1:A:275:ILE:O	2.19	0.42
2:D:74:GLU:H	2:D:74:GLU:CD	2.28	0.42
1:A:65:LYS:HB3	7:A:303:HOH:O	2.20	0.42
1:A:124:TYR:CZ	1:A:136:VAL:HG21	2.55	0.42
1:C:189:PRO:HB3	1:C:213:PHE:HB3	2.01	0.41
1:A:35:LEU:HD12	1:A:183:LEU:HD23	2.03	0.41
1:C:66:LEU:HD12	1:C:69:MET:HE3	2.02	0.41
1:A:79:ARG:NH2	1:A:80:ASP:OD1	2.54	0.41
1:C:10:PHE:HZ	5:C:286:PLM:H82	1.85	0.41
1:C:100:LEU:HG	1:C:118:VAL:HG22	2.03	0.41
1:A:88:MET:HE2	1:A:91:LYS:CB	2.50	0.41
2:D:7:ILE:HG12	2:D:82:VAL:HG21	2.02	0.41
2:D:6:GLN:HB3	7:D:105:HOH:O	2.21	0.41
1:C:216:LYS:O	1:C:217:PRO:C	2.64	0.40
2:D:9:VAL:HG12	2:D:23:LEU:HD11	2.02	0.40
1:A:47:ILE:HD13	5:A:286:PLM:H51	2.02	0.40

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)
7:A:320:HOH:O	7:B:147:HOH:O[1_445]	2.18	0.02

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	271/285 (95%)	257 (95%)	11 (4%)	3 (1%)	11	13
1	C	257/285 (90%)	249 (97%)	8 (3%)	0	100	100
2	B	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
2	D	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
All	All	720/768 (94%)	688 (96%)	29 (4%)	3 (0%)	30	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
1	A	111	ALA
1	A	90	PRO

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	235/249 (94%)	226 (96%)	9 (4%)	29	44
1	C	227/249 (91%)	218 (96%)	9 (4%)	28	42
2	B	88/93 (95%)	83 (94%)	5 (6%)	18	27
2	D	92/93 (99%)	89 (97%)	3 (3%)	33	50
All	All	642/684 (94%)	616 (96%)	26 (4%)	28	42

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	84	LEU
1	C	105	GLU
1	C	136	VAL
1	C	170	LEU
1	C	173	ARG
1	C	196	VAL
1	C	206	LEU
1	C	227	GLN
1	C	234	ARG
2	D	51	MET
2	D	74	GLU
2	D	99	MET
1	A	87	MET
1	A	93	ASP
1	A	105	GLU
1	A	136	VAL
1	A	170	LEU
1	A	196	VAL
1	A	206	LEU
1	A	227	GLN
1	A	234	ARG
2	B	51	MET
2	B	54	MET
2	B	67	HIS
2	B	74	GLU
2	B	99	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	7	ASN
1	C	117	HIS
1	C	233	HIS
1	C	248	GLN
1	C	273	GLN
2	D	31	HIS
2	D	34	HIS
1	A	117	HIS
1	A	227	GLN
1	A	248	GLN
1	A	273	GLN
2	B	31	HIS
2	B	34	HIS

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Mol	Chain	Res	Type
2	B	67	HIS

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 ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.76	0	17,19,21	1.30	2 (11%)
3	NAG	E	2	3	14,14,15	0.64	0	17,19,21	1.61	3 (17%)
3	NAG	F	1	1,3	14,14,15	0.50	0	17,19,21	2.28	4 (23%)
3	NAG	F	2	3	14,14,15	0.65	0	17,19,21	1.61	2 (11%)
3	NAG	G	1	1,3	14,14,15	0.76	0	17,19,21	1.69	2 (11%)
3	NAG	G	2	3	14,14,15	0.65	0	17,19,21	1.39	4 (23%)

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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-O5-C5	7.84	122.69	112.19
3	F	2	NAG	C4-C3-C2	4.55	117.68	111.02
3	G	1	NAG	C2-N2-C7	4.20	128.53	122.90
3	G	1	NAG	C1-O5-C5	3.93	117.45	112.19
3	E	2	NAG	C1-C2-N2	-3.34	105.16	110.43
3	G	2	NAG	O4-C4-C5	2.89	116.44	109.32
3	E	2	NAG	O4-C4-C5	2.68	115.93	109.32
3	F	2	NAG	C3-C4-C5	2.63	115.01	110.23
3	E	1	NAG	O5-C1-C2	-2.60	107.27	111.29
3	F	1	NAG	C2-N2-C7	-2.47	119.59	122.90
3	F	1	NAG	C6-C5-C4	-2.36	107.21	113.02
3	G	2	NAG	O6-C6-C5	-2.29	103.55	111.33
3	G	2	NAG	O3-C3-C2	-2.13	104.98	109.40
3	F	1	NAG	C3-C4-C5	2.09	114.02	110.23
3	G	2	NAG	C3-C4-C5	-2.08	106.45	110.23
3	E	1	NAG	O6-C6-C5	-2.05	104.34	111.33
3	E	2	NAG	C6-C5-C4	2.01	117.96	113.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

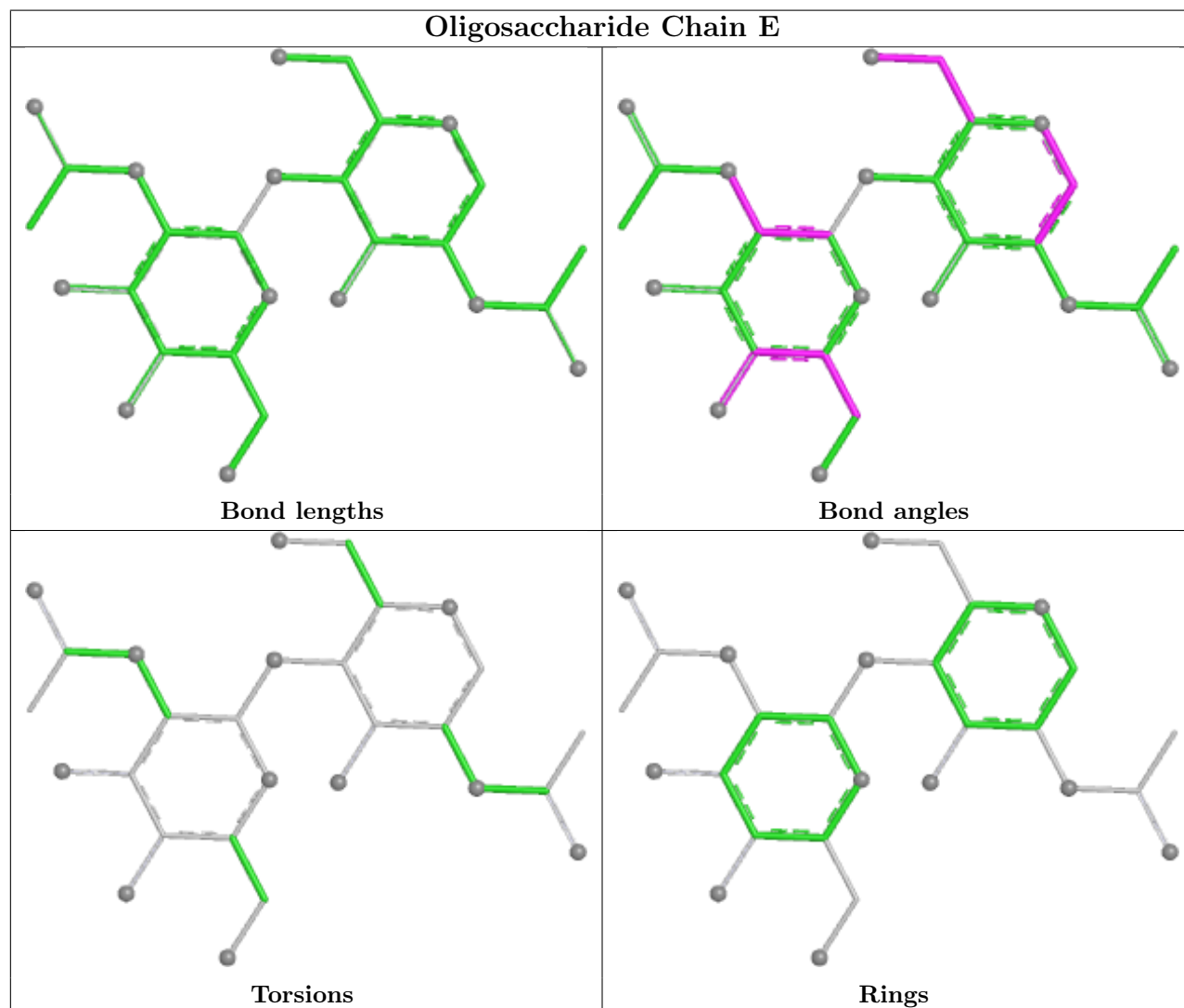
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

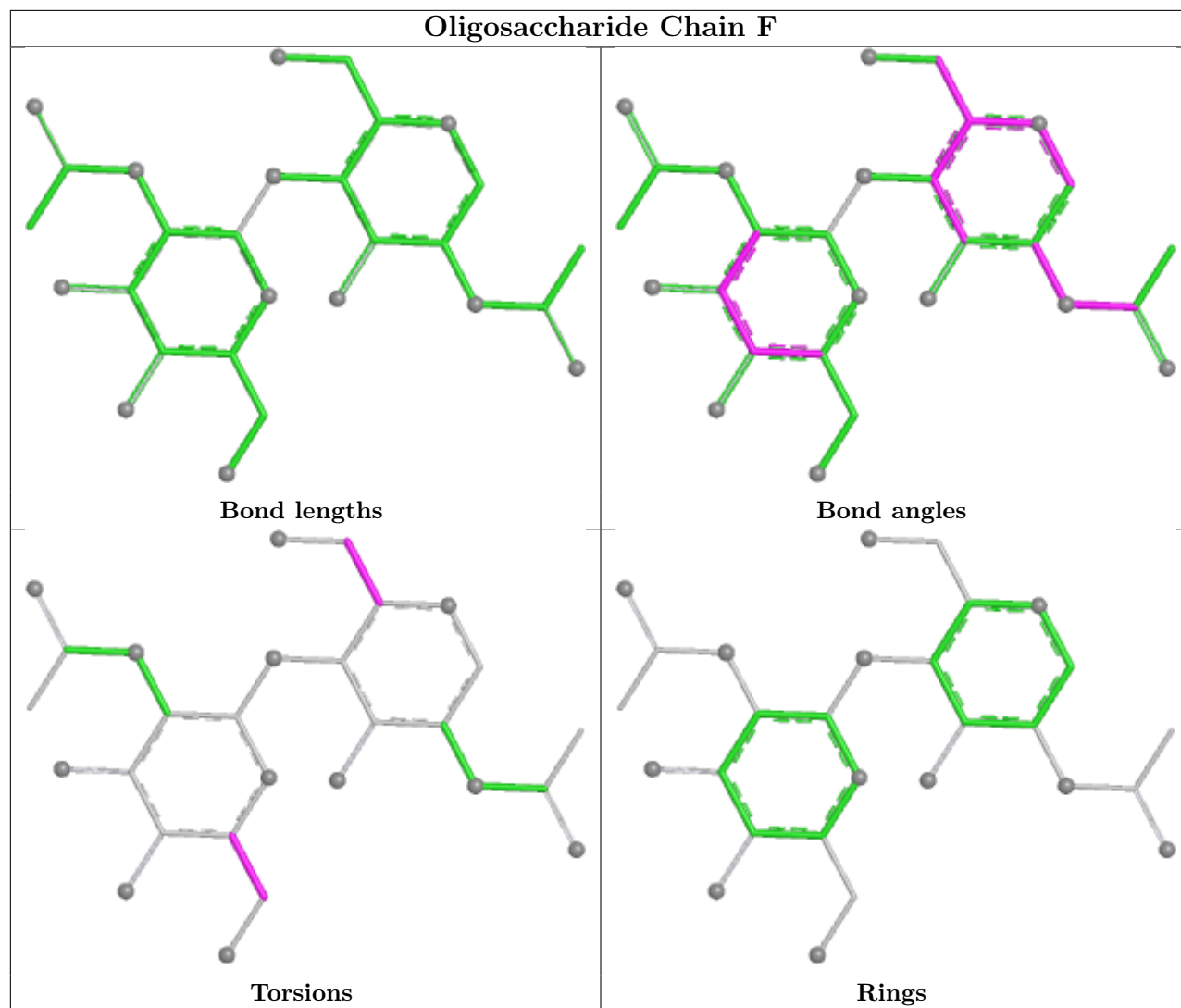
There are no ring outliers.

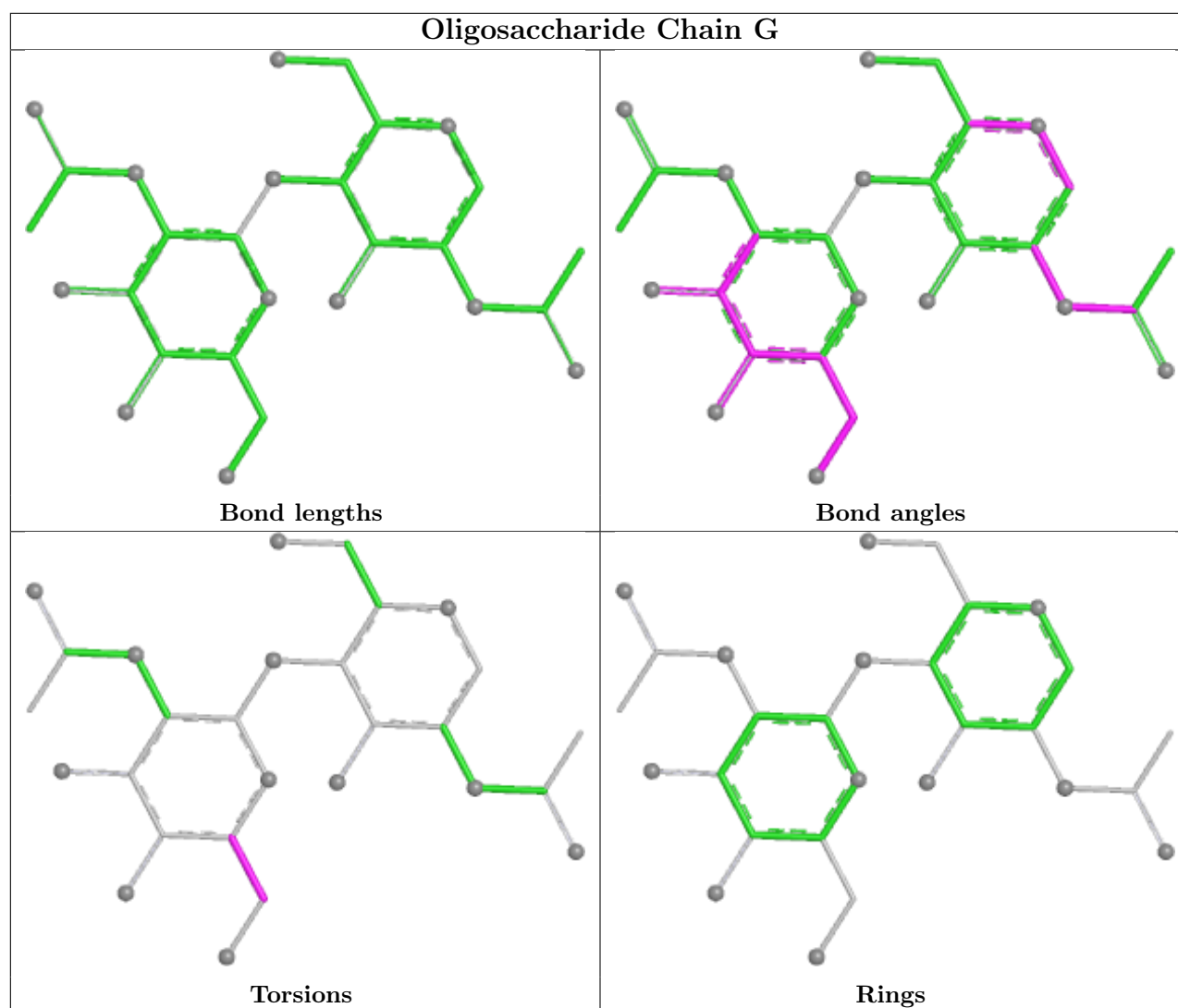
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	2	0
3	E	1	NAG	1	0
3	G	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.







5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
4	CD4	A	2089	-	45,45,83	0.97	1 (2%)	49,54,95	1.01	3 (6%)
6	NAG	C	501	1	14,14,15	0.44	0	17,19,21	2.10	3 (17%)
5	PLM	C	286	-	17,17,17	0.65	0	17,17,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CD4	C	2089	-	45,45,83	1.04	2 (4%)	49,54,95	1.39	4 (8%)
5	PLM	A	286	-	17,17,17	0.81	0	17,17,17	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CD4	A	2089	-	-	32/50/50/94	-
6	NAG	C	501	1	-	2/6/23/26	0/1/1/1
5	PLM	C	286	-	-	9/15/15/15	-
4	CD4	C	2089	-	-	24/50/50/94	-
5	PLM	A	286	-	-	9/15/15/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2089	CD4	P2-O12	4.06	1.63	1.50
4	A	2089	CD4	P2-O12	3.56	1.61	1.50
4	C	2089	CD4	P2-O11	2.07	1.62	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	501	NAG	C1-O5-C5	6.64	121.08	112.19
4	C	2089	CD4	O2-C14-C13	5.26	122.86	111.48
4	C	2089	CD4	C28-C15-C16	-4.01	102.44	111.78
6	C	501	NAG	C2-N2-C7	-3.69	117.96	122.90
4	A	2089	CD4	O2-C14-C13	3.54	119.14	111.48
4	C	2089	CD4	O13-P2-O10	3.11	114.77	106.67
4	C	2089	CD4	O2-C15-C28	2.97	119.01	108.34
6	C	501	NAG	C4-C3-C2	-2.78	106.95	111.02
4	A	2089	CD4	O13-P2-O10	2.22	112.47	106.67
4	A	2089	CD4	O2-C14-O1	-2.21	118.54	123.70

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2089	CD4	C28-O5-P1-O8
4	C	2089	CD4	C29-O8-P1-O5
4	C	2089	CD4	C31-O10-P2-O12
4	A	2089	CD4	C13-C14-O2-C15
4	A	2089	CD4	C28-O5-P1-O7
4	A	2089	CD4	C29-O8-P1-O5
4	A	2089	CD4	C29-O8-P1-O7
4	A	2089	CD4	C31-O10-P2-O12
4	A	2089	CD4	O1-C14-O2-C15
4	A	2089	CD4	C18-C17-O3-C16
4	C	2089	CD4	O8-C29-C30-O9
4	C	2089	CD4	O9-C30-C31-O10
4	A	2089	CD4	O4-C17-O3-C16
4	C	2089	CD4	O8-C29-C30-C31
4	A	2089	CD4	C29-C30-C31-O10
5	C	286	PLM	C8-C9-CA-CB
6	C	501	NAG	C4-C5-C6-O6
4	A	2089	CD4	O9-C30-C31-O10
6	C	501	NAG	O5-C5-C6-O6
4	C	2089	CD4	C18-C17-O3-C16
4	A	2089	CD4	C17-C18-C19-C20
4	A	2089	CD4	C11-C12-C13-C14
5	C	286	PLM	C1-C2-C3-C4
4	C	2089	CD4	O4-C17-O3-C16
4	A	2089	CD4	C23-C24-C25-C26
4	A	2089	CD4	C28-C15-C16-O3
5	A	286	PLM	C4-C5-C6-C7
4	A	2089	CD4	C21-C22-C23-C24
5	C	286	PLM	CD-CE-CF-CG
4	A	2089	CD4	C4-C5-C6-C7
5	A	286	PLM	CB-CC-CD-CE
5	A	286	PLM	C7-C8-C9-CA
4	A	2089	CD4	C2-C3-C4-C5
4	C	2089	CD4	C16-C15-C28-O5
4	C	2089	CD4	C10-C11-C12-C13
5	A	286	PLM	CA-CB-CC-CD
5	A	286	PLM	C1-C2-C3-C4
4	A	2089	CD4	C11-C10-C9-C8
4	A	2089	CD4	C20-C21-C22-C23
4	A	2089	CD4	C6-C7-C8-C9
4	A	2089	CD4	O2-C15-C16-O3
4	A	2089	CD4	C19-C20-C21-C22
5	C	286	PLM	C2-C3-C4-C5

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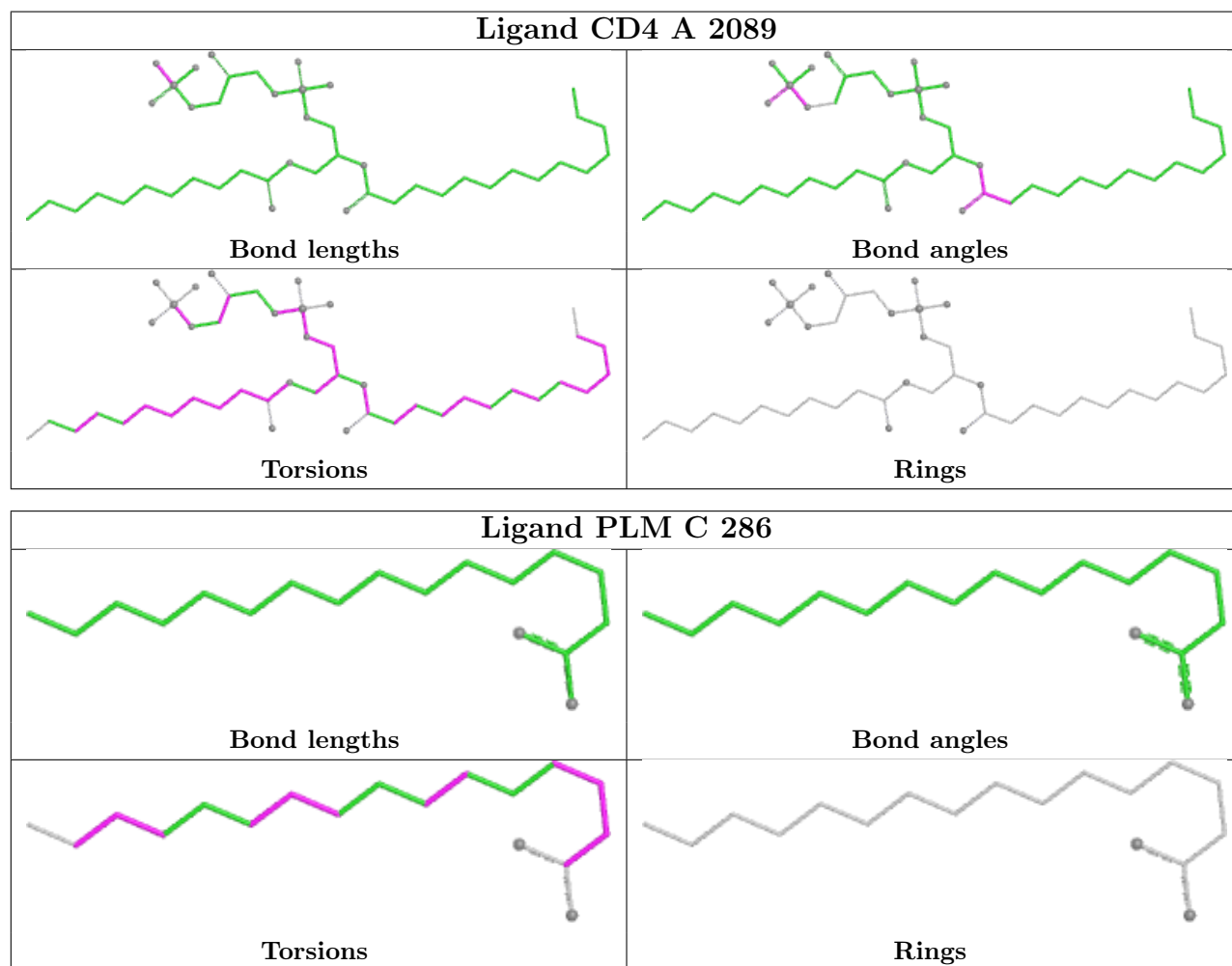
Mol	Chain	Res	Type	Atoms
4	C	2089	CD4	C30-C29-O8-P1
4	A	2089	CD4	O2-C15-C28-O5
4	C	2089	CD4	C30-C31-O10-P2
4	A	2089	CD4	C1-C2-C3-C4
5	A	286	PLM	C5-C6-C7-C8
5	A	286	PLM	C3-C4-C5-C6
4	A	2089	CD4	C16-C15-C28-O5
4	C	2089	CD4	O2-C15-C28-O5
5	C	286	PLM	C9-CA-CB-CC
4	C	2089	CD4	C2-C3-C4-C5
4	C	2089	CD4	C18-C19-C20-C21
4	C	2089	CD4	C19-C20-C21-C22
5	C	286	PLM	CC-CD-CE-CF
4	C	2089	CD4	C29-C30-C31-O10
4	A	2089	CD4	C3-C4-C5-C6
5	C	286	PLM	C5-C6-C7-C8
4	C	2089	CD4	C28-O5-P1-O7
4	C	2089	CD4	C29-O8-P1-O7
4	A	2089	CD4	C29-O8-P1-O6
4	A	2089	CD4	C18-C19-C20-C21
4	A	2089	CD4	C9-C10-C11-C12
4	C	2089	CD4	C5-C6-C7-C8
4	A	2089	CD4	C15-C28-O5-P1
4	C	2089	CD4	C22-C23-C24-C25
5	A	286	PLM	O2-C1-C2-C3
4	C	2089	CD4	C24-C25-C26-C27
4	C	2089	CD4	C6-C7-C8-C9
5	A	286	PLM	O1-C1-C2-C3
4	C	2089	CD4	C9-C10-C11-C12
4	A	2089	CD4	O3-C17-C18-C19
5	C	286	PLM	O2-C1-C2-C3
5	C	286	PLM	O1-C1-C2-C3
4	A	2089	CD4	O4-C17-C18-C19

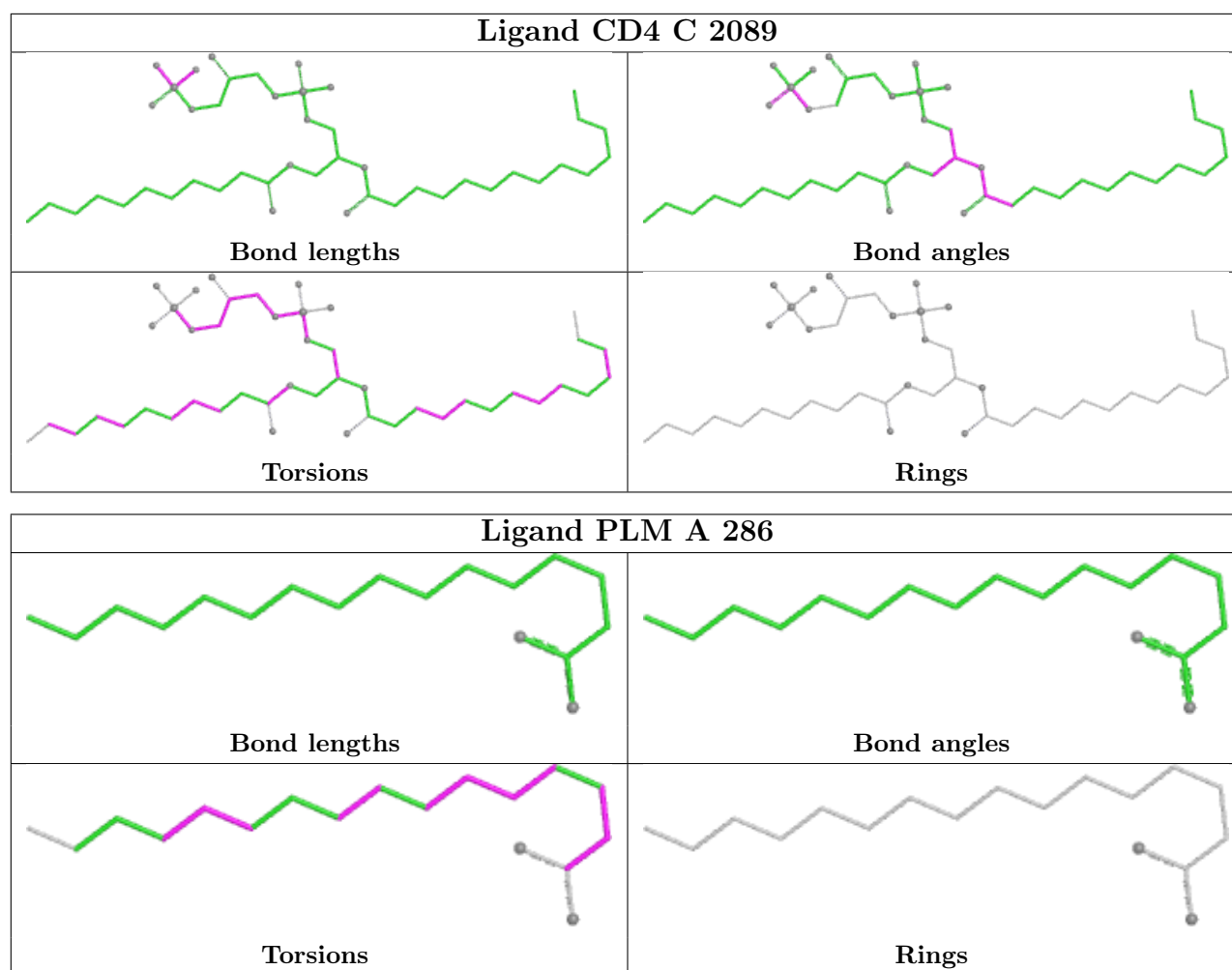
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2089	CD4	1	0
5	C	286	PLM	6	0
4	C	2089	CD4	2	0
5	A	286	PLM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	273/285 (95%)	0.54	13 (4%) 35 37	35, 47, 71, 90	0
1	C	265/285 (92%)	0.35	10 (3%) 44 46	29, 41, 70, 94	0
2	B	98/99 (98%)	0.30	2 (2%) 65 66	36, 47, 63, 69	0
2	D	98/99 (98%)	0.20	0 100 100	30, 44, 56, 63	0
All	All	734/768 (95%)	0.39	25 (3%) 48 50	29, 45, 68, 94	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	87	MET	4.1
1	A	145	LEU	3.4
1	C	120	PHE	3.4
1	C	88	MET	3.3
1	C	145	LEU	3.0
1	C	203	HIS	2.9
1	C	199	SER	2.8
1	A	201	HIS	2.8
1	A	90	PRO	2.8
1	A	273	GLN	2.7
1	C	200	ALA	2.6
1	A	111	ALA	2.6
1	C	108	PRO	2.6
1	A	230	GLN	2.5
1	A	87	MET	2.5
2	B	99	MET	2.5
1	A	7	ASN	2.4
1	C	109	GLY	2.4
1	A	200	ALA	2.3
1	A	203	HIS	2.2
1	A	108	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	109	GLY	2.2
1	A	110	ASN	2.1
2	B	88	ALA	2.1
1	C	112	SER	2.0

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

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

6.3 Carbohydrates [i](#)

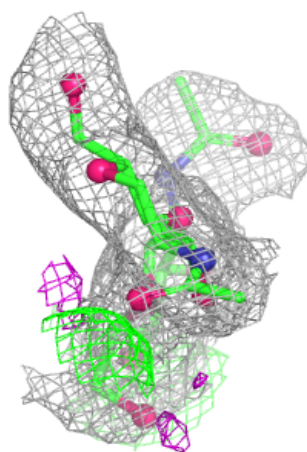
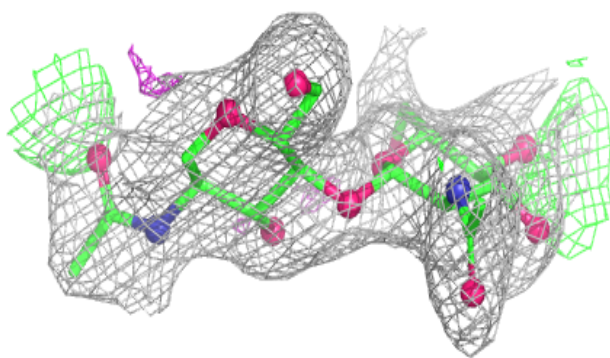
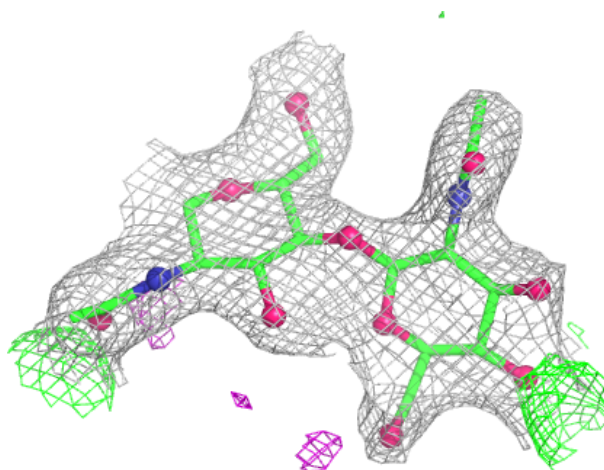
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.72	0.13	72,80,87,90	0
3	NAG	E	2	14/15	0.78	0.13	50,54,60,61	0
3	NAG	F	1	14/15	0.85	0.11	60,66,73,74	0
3	NAG	G	2	14/15	0.89	0.12	42,47,54,55	0
3	NAG	E	1	14/15	0.91	0.08	38,43,47,49	0
3	NAG	G	1	14/15	0.94	0.08	34,38,42,45	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.

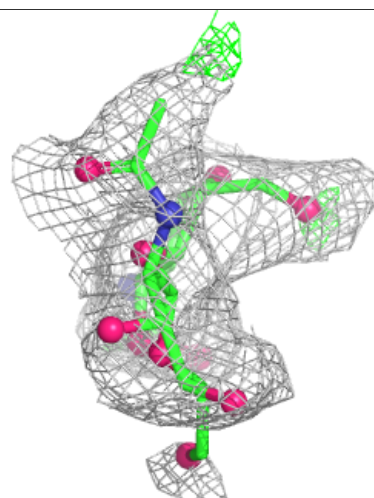
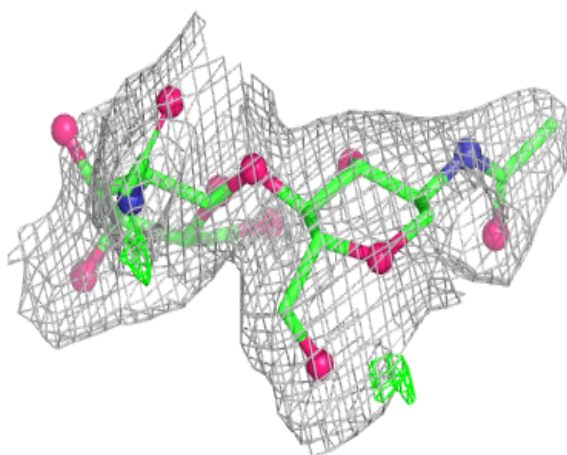
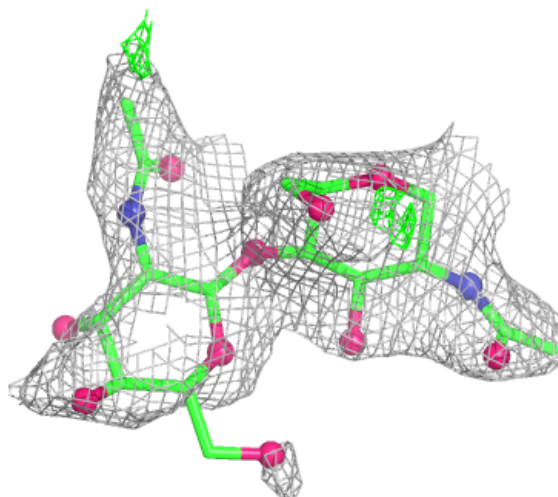
Electron density around Chain E:

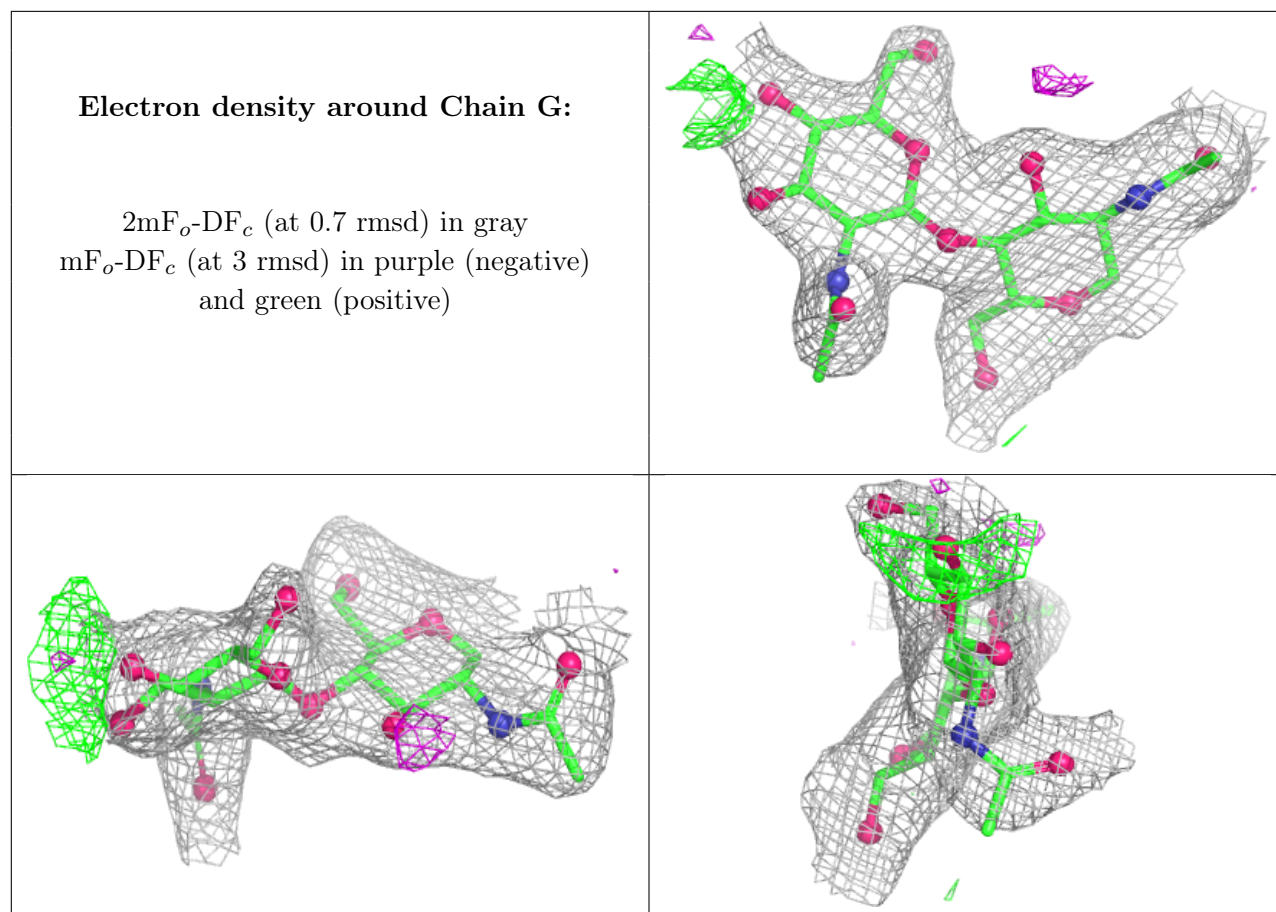
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

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





6.4 Ligands [i](#)

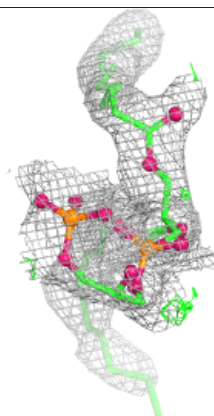
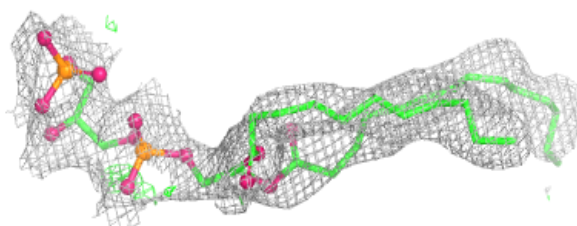
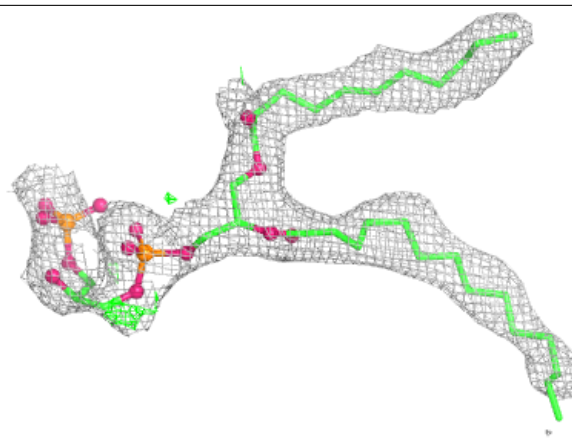
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CD4	C	2089	46/84	0.84	0.14	35,57,94,96	0
4	CD4	A	2089	46/84	0.87	0.14	41,64,97,100	0
6	NAG	C	501	14/15	0.89	0.10	58,63,66,72	0
5	PLM	A	286	18/18	0.90	0.14	41,46,62,62	0
5	PLM	C	286	18/18	0.92	0.12	43,44,56,58	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.

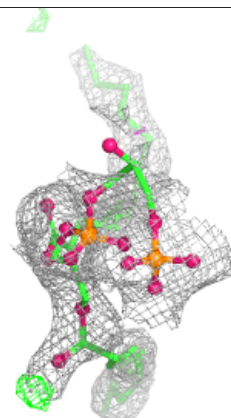
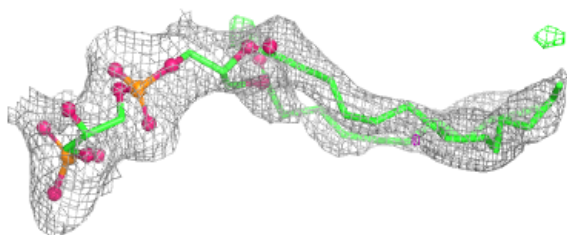
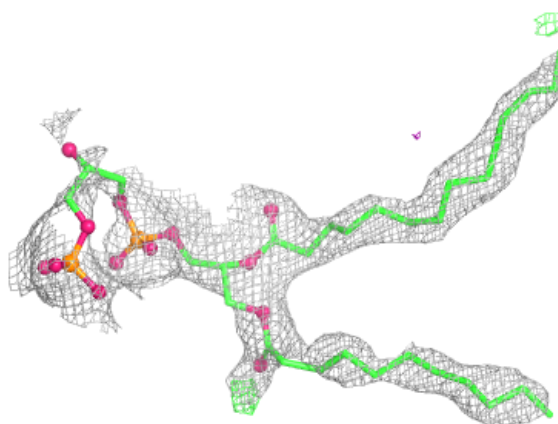
Electron density around CD4 C 2089:

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



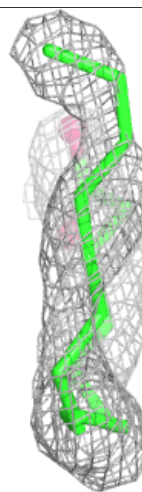
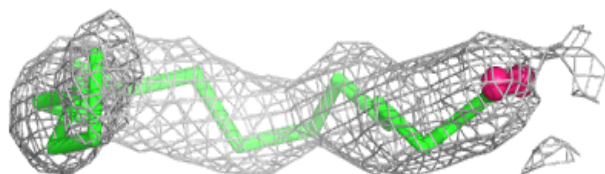
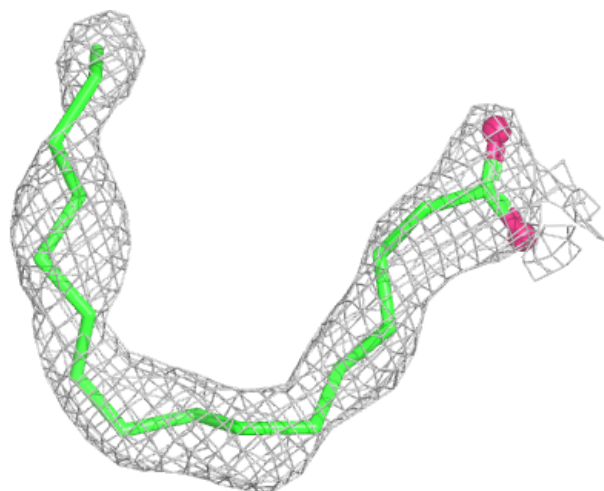
Electron density around CD4 A 2089:

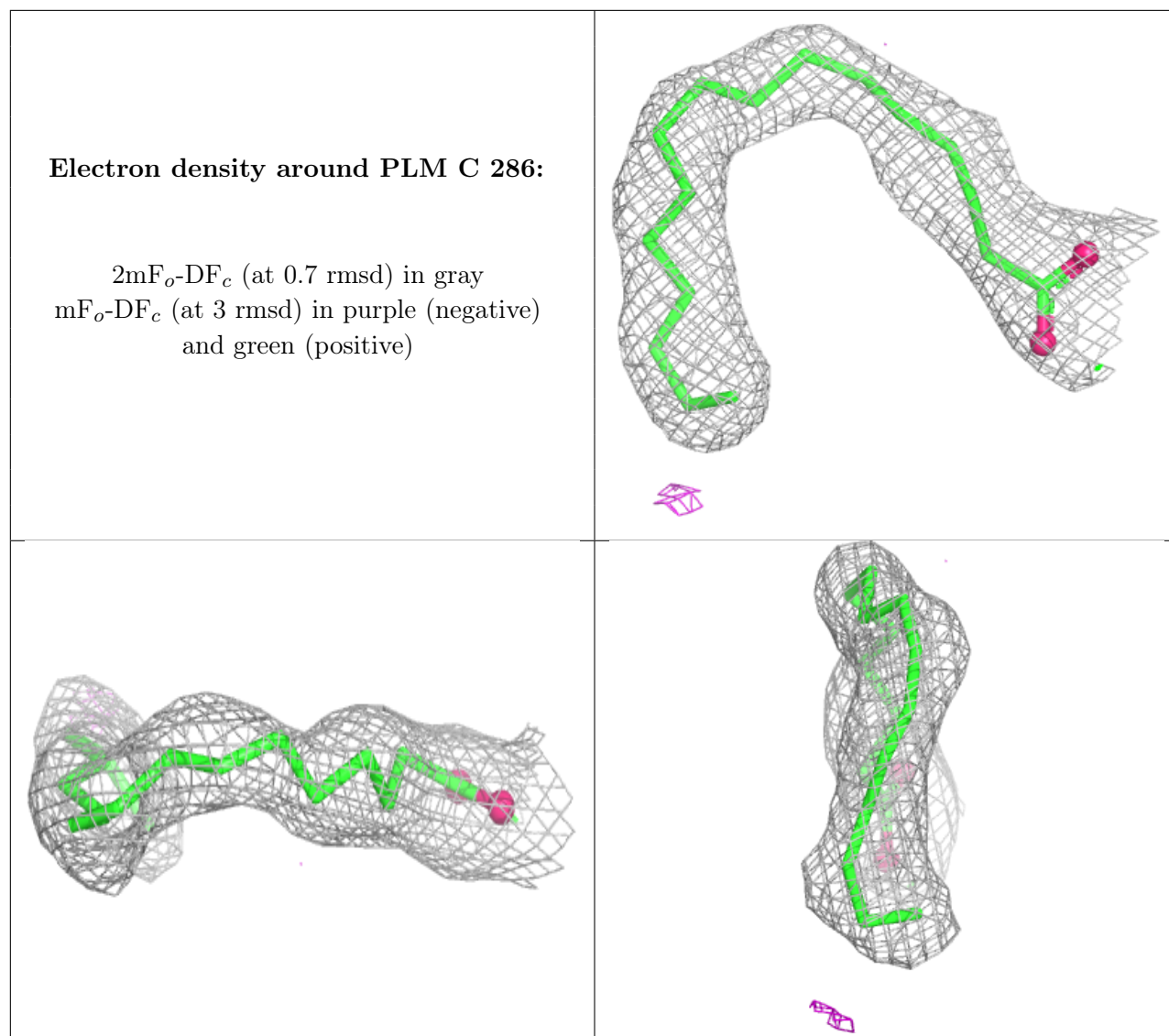
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLM A 286:

$2mF_o-DF_c$ (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.